



## Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 08:51 AM UTC

PDB ID : 9JZR / pdb\_00009jzr  
EMDB ID : EMD-61940  
Title : Structure of PSI-LHCI-LHCII supercomplex from Bryopsis corticulans  
Authors : Liu, X.Y.; Wang, W.D.  
Deposited on : 2024-10-14  
Resolution : 2.73 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

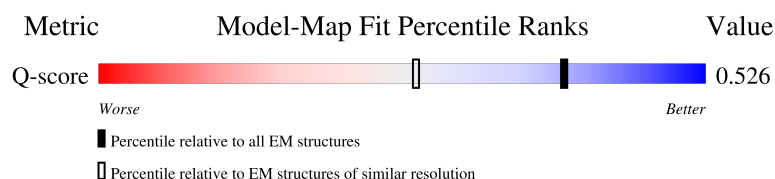
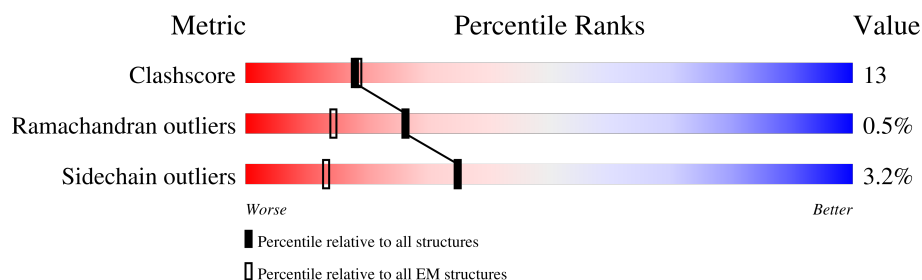


# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.73 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|--|
| Clashscore            | 229148                      | 23984                       | -  |
| Ramachandran outliers | 224038                      | 23583                       | -  |
| Sidechain outliers    | 223484                      | 23102                       | -  |
| Q-score               | -                           | 25397                       | 10432 ( 2.23 - 3.23 )                                    |









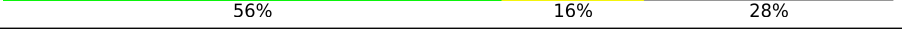

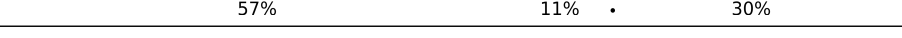
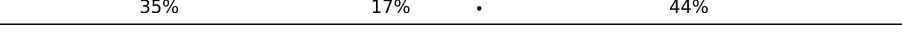

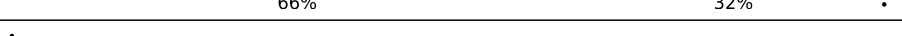


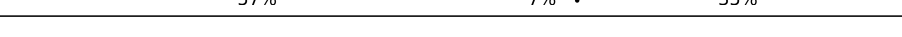








The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | 0     | 245    |                  |
| 2   | 1     | 226    |                  |
| 2   | 5     | 226    |                  |
| 3   | 2     | 256    |                  |

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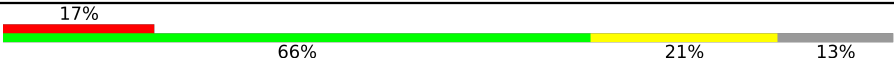



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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 4   | 3     | 281    |    |
| 5   | 6     | 267    |    |
| 6   | 7     | 264    |    |
| 7   | 4     | 248    |    |
| 7   | 8     | 248    |    |
| 8   | 9     | 222    |    |
| 9   | A     | 751    |    |
| 10  | B     | 734    |    |
| 11  | D     | 198    |    |
| 12  | E     | 91     |    |
| 13  | F     | 236    |    |
| 14  | G     | 167    |   |
| 15  | I     | 36     |  |
| 16  | J     | 41     |  |
| 17  | L     | 204    |  |
| 18  | C     | 81     |  |
| 19  | K     | 123    |  |
| 20  | M     | 32     |  |
| 21  | O     | 137    |  |
| 22  | a     | 250    |  |
| 22  | h     | 250    |  |
| 23  | c     | 254    |  |
| 24  | b     | 251    |  |
| 25  | d     | 280    |  |
| 25  | g     | 280    |  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 26  | f     | 259    |  |
| 27  | H     | 133    |  |
| 28  | i     | 282    |  |
| 29  | e     | 250    |  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 30  | CHL  | 0     | 301 | X         | -        | -       | -                |
| 30  | CHL  | 0     | 302 | X         | -        | -       | -                |
| 30  | CHL  | 0     | 305 | X         | -        | -       | -                |
| 30  | CHL  | 0     | 306 | X         | -        | -       | -                |
| 30  | CHL  | 1     | 302 | X         | -        | -       | -                |
| 30  | CHL  | 1     | 305 | X         | -        | -       | -                |
| 30  | CHL  | 1     | 306 | X         | -        | -       | -                |
| 30  | CHL  | 1     | 307 | X         | -        | -       | -                |
| 30  | CHL  | 1     | 313 | X         | -        | -       | -                |
| 30  | CHL  | 2     | 301 | X         | -        | -       | -                |
| 30  | CHL  | 2     | 302 | X         | -        | -       | -                |
| 30  | CHL  | 2     | 305 | X         | -        | -       | -                |
| 30  | CHL  | 2     | 306 | X         | -        | -       | -                |
| 30  | CHL  | 2     | 307 | X         | -        | -       | -                |
| 30  | CHL  | 2     | 308 | X         | -        | -       | -                |
| 30  | CHL  | 2     | 313 | X         | -        | -       | -                |
| 30  | CHL  | 2     | 319 | X         | -        | -       | -                |
| 30  | CHL  | 3     | 302 | X         | -        | -       | -                |
| 30  | CHL  | 3     | 305 | X         | -        | -       | -                |
| 30  | CHL  | 3     | 307 | X         | -        | -       | -                |
| 30  | CHL  | 4     | 302 | X         | -        | -       | -                |
| 30  | CHL  | 4     | 305 | X         | -        | -       | -                |
| 30  | CHL  | 4     | 306 | X         | -        | -       | -                |
| 30  | CHL  | 4     | 307 | X         | -        | -       | -                |
| 30  | CHL  | 4     | 308 | X         | -        | -       | -                |
| 30  | CHL  | 4     | 313 | X         | -        | -       | -                |
| 30  | CHL  | 4     | 319 | X         | -        | -       | -                |
| 30  | CHL  | 5     | 301 | X         | -        | -       | -                |
| 30  | CHL  | 5     | 302 | X         | -        | -       | -                |
| 30  | CHL  | 5     | 305 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 30  | CHL  | 5     | 306 | X         | -        | -       | -                |
| 30  | CHL  | 5     | 307 | X         | -        | -       | -                |
| 30  | CHL  | 5     | 313 | X         | -        | -       | -                |
| 30  | CHL  | 6     | 301 | X         | -        | -       | -                |
| 30  | CHL  | 6     | 302 | X         | -        | -       | -                |
| 30  | CHL  | 6     | 305 | X         | -        | -       | -                |
| 30  | CHL  | 6     | 306 | X         | -        | -       | -                |
| 30  | CHL  | 6     | 307 | X         | -        | -       | -                |
| 30  | CHL  | 6     | 308 | X         | -        | -       | -                |
| 30  | CHL  | 6     | 313 | X         | -        | -       | -                |
| 30  | CHL  | 6     | 315 | X         | -        | -       | -                |
| 30  | CHL  | 7     | 301 | X         | -        | -       | -                |
| 30  | CHL  | 7     | 302 | X         | -        | -       | -                |
| 30  | CHL  | 7     | 305 | X         | -        | -       | -                |
| 30  | CHL  | 7     | 306 | X         | -        | -       | -                |
| 30  | CHL  | 7     | 307 | X         | -        | -       | -                |
| 30  | CHL  | 7     | 313 | X         | -        | -       | -                |
| 30  | CHL  | 8     | 301 | X         | -        | -       | -                |
| 30  | CHL  | 8     | 302 | X         | -        | -       | -                |
| 30  | CHL  | 8     | 305 | X         | -        | -       | -                |
| 30  | CHL  | 8     | 306 | X         | -        | -       | -                |
| 30  | CHL  | 8     | 307 | X         | -        | -       | -                |
| 30  | CHL  | 8     | 308 | X         | -        | -       | -                |
| 30  | CHL  | 8     | 313 | X         | -        | -       | -                |
| 30  | CHL  | 8     | 315 | X         | -        | -       | -                |
| 30  | CHL  | 9     | 301 | X         | -        | -       | -                |
| 30  | CHL  | 9     | 305 | X         | -        | -       | -                |
| 30  | CHL  | 9     | 306 | X         | -        | -       | -                |
| 30  | CHL  | 9     | 313 | X         | -        | -       | -                |
| 30  | CHL  | a     | 601 | X         | -        | -       | -                |
| 30  | CHL  | a     | 602 | X         | -        | -       | -                |
| 30  | CHL  | a     | 605 | X         | -        | -       | -                |
| 30  | CHL  | a     | 606 | X         | -        | -       | -                |
| 30  | CHL  | a     | 607 | X         | -        | -       | -                |
| 30  | CHL  | a     | 608 | X         | -        | -       | -                |
| 30  | CHL  | a     | 609 | X         | -        | -       | -                |
| 30  | CHL  | a     | 614 | X         | -        | -       | -                |
| 30  | CHL  | b     | 601 | X         | -        | -       | -                |
| 30  | CHL  | b     | 602 | X         | -        | -       | -                |
| 30  | CHL  | b     | 606 | X         | -        | -       | -                |
| 30  | CHL  | b     | 607 | X         | -        | -       | -                |
| 30  | CHL  | b     | 608 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 30  | CHL  | b     | 609 | X         | -        | -       | -                |
| 30  | CHL  | b     | 614 | X         | -        | -       | -                |
| 30  | CHL  | c     | 601 | X         | -        | -       | -                |
| 30  | CHL  | c     | 602 | X         | -        | -       | -                |
| 30  | CHL  | c     | 605 | X         | -        | -       | -                |
| 30  | CHL  | c     | 606 | X         | -        | -       | -                |
| 30  | CHL  | c     | 607 | X         | -        | -       | -                |
| 30  | CHL  | c     | 608 | X         | -        | -       | -                |
| 30  | CHL  | c     | 609 | X         | -        | -       | -                |
| 30  | CHL  | c     | 614 | X         | -        | -       | -                |
| 30  | CHL  | d     | 601 | X         | -        | -       | -                |
| 30  | CHL  | d     | 602 | X         | -        | -       | -                |
| 30  | CHL  | d     | 605 | X         | -        | -       | -                |
| 30  | CHL  | d     | 606 | X         | -        | -       | -                |
| 30  | CHL  | d     | 607 | X         | -        | -       | -                |
| 30  | CHL  | d     | 608 | X         | -        | -       | -                |
| 30  | CHL  | d     | 609 | X         | -        | -       | -                |
| 30  | CHL  | d     | 614 | X         | -        | -       | -                |
| 30  | CHL  | e     | 601 | X         | -        | -       | -                |
| 30  | CHL  | e     | 602 | X         | -        | -       | -                |
| 30  | CHL  | e     | 605 | X         | -        | -       | -                |
| 30  | CHL  | e     | 606 | X         | -        | -       | -                |
| 30  | CHL  | e     | 607 | X         | -        | -       | -                |
| 30  | CHL  | e     | 608 | X         | -        | -       | -                |
| 30  | CHL  | e     | 609 | X         | -        | -       | -                |
| 30  | CHL  | e     | 614 | X         | -        | -       | -                |
| 30  | CHL  | f     | 601 | X         | -        | -       | -                |
| 30  | CHL  | f     | 602 | X         | -        | -       | -                |
| 30  | CHL  | f     | 605 | X         | -        | -       | -                |
| 30  | CHL  | f     | 606 | X         | -        | -       | -                |
| 30  | CHL  | f     | 607 | X         | -        | -       | -                |
| 30  | CHL  | f     | 608 | X         | -        | -       | -                |
| 30  | CHL  | f     | 609 | X         | -        | -       | -                |
| 30  | CHL  | f     | 614 | X         | -        | -       | -                |
| 30  | CHL  | g     | 601 | X         | -        | -       | -                |
| 30  | CHL  | g     | 602 | X         | -        | -       | -                |
| 30  | CHL  | g     | 605 | X         | -        | -       | -                |
| 30  | CHL  | g     | 606 | X         | -        | -       | -                |
| 30  | CHL  | g     | 607 | X         | -        | -       | -                |
| 30  | CHL  | g     | 608 | X         | -        | -       | -                |
| 30  | CHL  | g     | 609 | X         | -        | -       | -                |
| 30  | CHL  | g     | 614 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 30  | CHL  | h     | 601 | X         | -        | -       | -                |
| 30  | CHL  | h     | 602 | X         | -        | -       | -                |
| 30  | CHL  | h     | 605 | X         | -        | -       | -                |
| 30  | CHL  | h     | 606 | X         | -        | -       | -                |
| 30  | CHL  | h     | 607 | X         | -        | -       | -                |
| 30  | CHL  | h     | 608 | X         | -        | -       | -                |
| 30  | CHL  | h     | 609 | X         | -        | -       | -                |
| 30  | CHL  | h     | 614 | X         | -        | -       | -                |
| 30  | CHL  | i     | 601 | X         | -        | -       | -                |
| 30  | CHL  | i     | 602 | X         | -        | -       | -                |
| 30  | CHL  | i     | 605 | X         | -        | -       | -                |
| 30  | CHL  | i     | 606 | X         | -        | X       | -                |
| 30  | CHL  | i     | 607 | X         | -        | -       | -                |
| 30  | CHL  | i     | 608 | X         | -        | -       | -                |
| 30  | CHL  | i     | 609 | X         | -        | -       | -                |
| 30  | CHL  | i     | 614 | X         | -        | -       | -                |
| 31  | CLA  | 0     | 303 | X         | -        | -       | -                |
| 31  | CLA  | 0     | 304 | X         | -        | -       | -                |
| 31  | CLA  | 0     | 308 | X         | -        | -       | -                |
| 31  | CLA  | 0     | 309 | X         | -        | -       | -                |
| 31  | CLA  | 0     | 310 | X         | -        | -       | -                |
| 31  | CLA  | 0     | 311 | X         | -        | -       | -                |
| 31  | CLA  | 0     | 312 | X         | -        | -       | -                |
| 31  | CLA  | 0     | 313 | X         | -        | -       | -                |
| 31  | CLA  | 0     | 321 | X         | -        | -       | -                |
| 31  | CLA  | 1     | 303 | X         | -        | -       | -                |
| 31  | CLA  | 1     | 304 | X         | -        | -       | -                |
| 31  | CLA  | 1     | 308 | X         | -        | -       | -                |
| 31  | CLA  | 1     | 309 | X         | -        | -       | -                |
| 31  | CLA  | 1     | 310 | X         | -        | -       | -                |
| 31  | CLA  | 1     | 311 | X         | -        | -       | -                |
| 31  | CLA  | 1     | 312 | X         | -        | -       | -                |
| 31  | CLA  | 1     | 314 | X         | -        | -       | -                |
| 31  | CLA  | 2     | 303 | X         | -        | -       | -                |
| 31  | CLA  | 2     | 304 | X         | -        | -       | -                |
| 31  | CLA  | 2     | 309 | X         | -        | -       | -                |
| 31  | CLA  | 2     | 310 | X         | -        | -       | -                |
| 31  | CLA  | 2     | 311 | X         | -        | -       | -                |
| 31  | CLA  | 2     | 312 | X         | -        | -       | -                |
| 31  | CLA  | 2     | 314 | X         | -        | -       | -                |
| 31  | CLA  | 3     | 303 | X         | -        | -       | -                |
| 31  | CLA  | 3     | 304 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 31  | CLA  | 3     | 306 | X         | -        | -       | -                |
| 31  | CLA  | 3     | 308 | X         | -        | -       | -                |
| 31  | CLA  | 3     | 309 | X         | -        | -       | -                |
| 31  | CLA  | 3     | 310 | X         | -        | -       | -                |
| 31  | CLA  | 3     | 311 | X         | -        | -       | -                |
| 31  | CLA  | 3     | 312 | X         | -        | -       | -                |
| 31  | CLA  | 3     | 313 | X         | -        | -       | -                |
| 31  | CLA  | 3     | 318 | X         | -        | -       | -                |
| 31  | CLA  | 3     | 320 | X         | -        | -       | -                |
| 31  | CLA  | 4     | 303 | X         | -        | -       | -                |
| 31  | CLA  | 4     | 304 | X         | -        | -       | -                |
| 31  | CLA  | 4     | 309 | X         | -        | -       | -                |
| 31  | CLA  | 4     | 310 | X         | -        | -       | -                |
| 31  | CLA  | 4     | 311 | X         | -        | -       | -                |
| 31  | CLA  | 4     | 312 | X         | -        | -       | -                |
| 31  | CLA  | 4     | 314 | X         | -        | -       | -                |
| 31  | CLA  | 5     | 303 | X         | -        | -       | -                |
| 31  | CLA  | 5     | 304 | X         | -        | -       | -                |
| 31  | CLA  | 5     | 308 | X         | -        | -       | -                |
| 31  | CLA  | 5     | 309 | X         | -        | -       | -                |
| 31  | CLA  | 5     | 310 | X         | -        | -       | -                |
| 31  | CLA  | 5     | 311 | X         | -        | -       | -                |
| 31  | CLA  | 5     | 312 | X         | -        | -       | -                |
| 31  | CLA  | 5     | 314 | X         | -        | -       | -                |
| 31  | CLA  | 6     | 303 | X         | -        | -       | -                |
| 31  | CLA  | 6     | 304 | X         | -        | -       | -                |
| 31  | CLA  | 6     | 309 | X         | -        | -       | -                |
| 31  | CLA  | 6     | 310 | X         | -        | -       | -                |
| 31  | CLA  | 6     | 311 | X         | -        | -       | -                |
| 31  | CLA  | 6     | 312 | X         | -        | -       | -                |
| 31  | CLA  | 6     | 314 | X         | -        | -       | -                |
| 31  | CLA  | 6     | 317 | X         | -        | -       | -                |
| 31  | CLA  | 6     | 318 | X         | -        | -       | -                |
| 31  | CLA  | 6     | 320 | X         | -        | -       | -                |
| 31  | CLA  | 7     | 303 | X         | -        | -       | -                |
| 31  | CLA  | 7     | 304 | X         | -        | -       | -                |
| 31  | CLA  | 7     | 308 | X         | -        | -       | -                |
| 31  | CLA  | 7     | 309 | X         | -        | -       | -                |
| 31  | CLA  | 7     | 310 | X         | -        | -       | -                |
| 31  | CLA  | 7     | 311 | X         | -        | -       | -                |
| 31  | CLA  | 7     | 312 | X         | -        | -       | -                |
| 31  | CLA  | 7     | 315 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 31  | CLA  | 7     | 316 | X         | -        | -       | -                |
| 31  | CLA  | 7     | 317 | X         | -        | -       | -                |
| 31  | CLA  | 7     | 318 | X         | -        | -       | -                |
| 31  | CLA  | 8     | 303 | X         | -        | -       | -                |
| 31  | CLA  | 8     | 304 | X         | -        | -       | -                |
| 31  | CLA  | 8     | 309 | X         | -        | -       | -                |
| 31  | CLA  | 8     | 310 | X         | -        | -       | -                |
| 31  | CLA  | 8     | 311 | X         | -        | -       | -                |
| 31  | CLA  | 8     | 312 | X         | -        | -       | -                |
| 31  | CLA  | 8     | 314 | X         | -        | -       | -                |
| 31  | CLA  | 9     | 300 | X         | -        | -       | -                |
| 31  | CLA  | 9     | 302 | X         | -        | -       | -                |
| 31  | CLA  | 9     | 303 | X         | -        | -       | -                |
| 31  | CLA  | 9     | 304 | X         | -        | -       | -                |
| 31  | CLA  | 9     | 308 | X         | -        | -       | -                |
| 31  | CLA  | 9     | 309 | X         | -        | -       | -                |
| 31  | CLA  | 9     | 310 | X         | -        | -       | -                |
| 31  | CLA  | 9     | 311 | X         | -        | -       | -                |
| 31  | CLA  | 9     | 312 | X         | -        | -       | -                |
| 31  | CLA  | A     | 802 | X         | -        | -       | -                |
| 31  | CLA  | A     | 803 | X         | -        | -       | -                |
| 31  | CLA  | A     | 804 | X         | -        | -       | -                |
| 31  | CLA  | A     | 805 | X         | -        | -       | -                |
| 31  | CLA  | A     | 806 | X         | -        | -       | -                |
| 31  | CLA  | A     | 807 | X         | -        | -       | -                |
| 31  | CLA  | A     | 808 | X         | -        | -       | -                |
| 31  | CLA  | A     | 809 | X         | -        | -       | -                |
| 31  | CLA  | A     | 810 | X         | -        | -       | -                |
| 31  | CLA  | A     | 811 | X         | -        | -       | -                |
| 31  | CLA  | A     | 812 | X         | -        | -       | -                |
| 31  | CLA  | A     | 813 | X         | -        | -       | -                |
| 31  | CLA  | A     | 814 | X         | -        | -       | -                |
| 31  | CLA  | A     | 815 | X         | -        | -       | -                |
| 31  | CLA  | A     | 816 | X         | -        | -       | -                |
| 31  | CLA  | A     | 817 | X         | -        | -       | -                |
| 31  | CLA  | A     | 818 | X         | -        | -       | -                |
| 31  | CLA  | A     | 819 | X         | -        | -       | -                |
| 31  | CLA  | A     | 820 | X         | -        | -       | -                |
| 31  | CLA  | A     | 821 | X         | -        | -       | -                |
| 31  | CLA  | A     | 822 | X         | -        | -       | -                |
| 31  | CLA  | A     | 823 | X         | -        | -       | -                |
| 31  | CLA  | A     | 824 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 31  | CLA  | A     | 825 | X         | -        | -       | -                |
| 31  | CLA  | A     | 826 | X         | -        | -       | -                |
| 31  | CLA  | A     | 827 | X         | -        | -       | -                |
| 31  | CLA  | A     | 828 | X         | -        | -       | -                |
| 31  | CLA  | A     | 829 | X         | -        | -       | -                |
| 31  | CLA  | A     | 830 | X         | -        | -       | -                |
| 31  | CLA  | A     | 831 | X         | -        | -       | -                |
| 31  | CLA  | A     | 832 | X         | -        | -       | -                |
| 31  | CLA  | A     | 833 | X         | -        | -       | -                |
| 31  | CLA  | A     | 834 | X         | -        | -       | -                |
| 31  | CLA  | A     | 835 | X         | -        | -       | -                |
| 31  | CLA  | A     | 836 | X         | -        | -       | -                |
| 31  | CLA  | A     | 837 | X         | -        | -       | -                |
| 31  | CLA  | A     | 838 | X         | -        | -       | -                |
| 31  | CLA  | A     | 839 | X         | -        | -       | -                |
| 31  | CLA  | A     | 840 | X         | -        | -       | -                |
| 31  | CLA  | A     | 841 | X         | -        | -       | -                |
| 31  | CLA  | A     | 843 | X         | -        | -       | -                |
| 31  | CLA  | A     | 852 | X         | -        | -       | -                |
| 31  | CLA  | A     | 853 | X         | -        | -       | -                |
| 31  | CLA  | B     | 801 | X         | -        | -       | -                |
| 31  | CLA  | B     | 803 | X         | -        | -       | -                |
| 31  | CLA  | B     | 805 | X         | -        | -       | -                |
| 31  | CLA  | B     | 806 | X         | -        | -       | -                |
| 31  | CLA  | B     | 807 | X         | -        | -       | -                |
| 31  | CLA  | B     | 808 | X         | -        | -       | -                |
| 31  | CLA  | B     | 809 | X         | -        | -       | -                |
| 31  | CLA  | B     | 810 | X         | -        | -       | -                |
| 31  | CLA  | B     | 811 | X         | -        | -       | -                |
| 31  | CLA  | B     | 812 | X         | -        | -       | -                |
| 31  | CLA  | B     | 813 | X         | -        | -       | -                |
| 31  | CLA  | B     | 814 | X         | -        | -       | -                |
| 31  | CLA  | B     | 815 | X         | -        | -       | -                |
| 31  | CLA  | B     | 816 | X         | -        | -       | -                |
| 31  | CLA  | B     | 817 | X         | -        | -       | -                |
| 31  | CLA  | B     | 818 | X         | -        | -       | -                |
| 31  | CLA  | B     | 819 | X         | -        | -       | -                |
| 31  | CLA  | B     | 820 | X         | -        | -       | -                |
| 31  | CLA  | B     | 821 | X         | -        | -       | -                |
| 31  | CLA  | B     | 822 | X         | -        | -       | -                |
| 31  | CLA  | B     | 823 | X         | -        | -       | -                |
| 31  | CLA  | B     | 824 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 31  | CLA  | B     | 825 | X         | -        | -       | -                |
| 31  | CLA  | B     | 826 | X         | -        | -       | -                |
| 31  | CLA  | B     | 827 | X         | -        | -       | -                |
| 31  | CLA  | B     | 828 | X         | -        | -       | -                |
| 31  | CLA  | B     | 829 | X         | -        | -       | -                |
| 31  | CLA  | B     | 830 | X         | -        | -       | -                |
| 31  | CLA  | B     | 831 | X         | -        | -       | -                |
| 31  | CLA  | B     | 832 | X         | -        | -       | -                |
| 31  | CLA  | B     | 833 | X         | -        | -       | -                |
| 31  | CLA  | B     | 834 | X         | -        | -       | -                |
| 31  | CLA  | B     | 835 | X         | -        | -       | -                |
| 31  | CLA  | B     | 836 | X         | -        | -       | -                |
| 31  | CLA  | B     | 837 | X         | -        | -       | -                |
| 31  | CLA  | B     | 838 | X         | -        | -       | -                |
| 31  | CLA  | B     | 839 | X         | -        | -       | -                |
| 31  | CLA  | B     | 840 | X         | -        | -       | -                |
| 31  | CLA  | B     | 841 | X         | -        | -       | -                |
| 31  | CLA  | B     | 850 | X         | -        | -       | -                |
| 31  | CLA  | F     | 301 | X         | -        | -       | -                |
| 31  | CLA  | G     | 101 | X         | -        | -       | -                |
| 31  | CLA  | G     | 102 | X         | -        | -       | -                |
| 31  | CLA  | G     | 103 | X         | -        | -       | -                |
| 31  | CLA  | H     | 201 | X         | -        | -       | -                |
| 31  | CLA  | H     | 202 | X         | -        | -       | -                |
| 31  | CLA  | H     | 204 | X         | -        | -       | -                |
| 31  | CLA  | H     | 205 | X         | -        | -       | -                |
| 31  | CLA  | J     | 103 | X         | -        | -       | -                |
| 31  | CLA  | K     | 101 | X         | -        | -       | -                |
| 31  | CLA  | K     | 102 | X         | -        | -       | -                |
| 31  | CLA  | K     | 104 | X         | -        | -       | -                |
| 31  | CLA  | K     | 105 | X         | -        | -       | -                |
| 31  | CLA  | L     | 201 | X         | -        | -       | -                |
| 31  | CLA  | L     | 202 | X         | -        | -       | -                |
| 31  | CLA  | L     | 203 | X         | -        | -       | -                |
| 31  | CLA  | L     | 204 | X         | -        | -       | -                |
| 31  | CLA  | L     | 207 | X         | -        | -       | -                |
| 31  | CLA  | M     | 101 | X         | -        | -       | -                |
| 31  | CLA  | O     | 201 | X         | -        | -       | -                |
| 31  | CLA  | O     | 202 | X         | -        | -       | -                |
| 31  | CLA  | O     | 203 | X         | -        | -       | -                |
| 31  | CLA  | O     | 206 | X         | -        | -       | -                |
| 31  | CLA  | a     | 603 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 31  | CLA  | a     | 604 | X         | -        | -       | -                |
| 31  | CLA  | a     | 610 | X         | -        | -       | -                |
| 31  | CLA  | a     | 611 | X         | -        | -       | -                |
| 31  | CLA  | a     | 612 | X         | -        | -       | -                |
| 31  | CLA  | a     | 613 | X         | -        | -       | -                |
| 31  | CLA  | b     | 603 | X         | -        | -       | -                |
| 31  | CLA  | b     | 604 | X         | -        | -       | -                |
| 31  | CLA  | b     | 610 | X         | -        | -       | -                |
| 31  | CLA  | b     | 611 | X         | -        | -       | -                |
| 31  | CLA  | b     | 612 | X         | -        | -       | -                |
| 31  | CLA  | b     | 613 | X         | -        | -       | -                |
| 31  | CLA  | c     | 603 | X         | -        | -       | -                |
| 31  | CLA  | c     | 604 | X         | -        | -       | -                |
| 31  | CLA  | c     | 610 | X         | -        | -       | -                |
| 31  | CLA  | c     | 611 | X         | -        | -       | -                |
| 31  | CLA  | c     | 612 | X         | -        | -       | -                |
| 31  | CLA  | c     | 613 | X         | -        | -       | -                |
| 31  | CLA  | d     | 603 | X         | -        | -       | -                |
| 31  | CLA  | d     | 604 | X         | -        | -       | -                |
| 31  | CLA  | d     | 610 | X         | -        | -       | -                |
| 31  | CLA  | d     | 611 | X         | -        | -       | -                |
| 31  | CLA  | d     | 612 | X         | -        | -       | -                |
| 31  | CLA  | d     | 613 | X         | -        | -       | -                |
| 31  | CLA  | e     | 603 | X         | -        | -       | -                |
| 31  | CLA  | e     | 604 | X         | -        | -       | -                |
| 31  | CLA  | e     | 610 | X         | -        | -       | -                |
| 31  | CLA  | e     | 611 | X         | -        | -       | -                |
| 31  | CLA  | e     | 612 | X         | -        | -       | -                |
| 31  | CLA  | e     | 613 | X         | -        | -       | -                |
| 31  | CLA  | f     | 603 | X         | -        | -       | -                |
| 31  | CLA  | f     | 604 | X         | -        | -       | -                |
| 31  | CLA  | f     | 610 | X         | -        | -       | -                |
| 31  | CLA  | f     | 611 | X         | -        | -       | -                |
| 31  | CLA  | f     | 612 | X         | -        | -       | -                |
| 31  | CLA  | f     | 613 | X         | -        | -       | -                |
| 31  | CLA  | g     | 603 | X         | -        | -       | -                |
| 31  | CLA  | g     | 604 | X         | -        | -       | -                |
| 31  | CLA  | g     | 610 | X         | -        | -       | -                |
| 31  | CLA  | g     | 611 | X         | -        | -       | -                |
| 31  | CLA  | g     | 612 | X         | -        | -       | -                |
| 31  | CLA  | g     | 613 | X         | -        | -       | -                |
| 31  | CLA  | h     | 603 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 31  | CLA  | h     | 604 | X         | -        | -       | -                |
| 31  | CLA  | h     | 610 | X         | -        | -       | -                |
| 31  | CLA  | h     | 611 | X         | -        | -       | -                |
| 31  | CLA  | h     | 612 | X         | -        | -       | -                |
| 31  | CLA  | h     | 613 | X         | -        | -       | -                |
| 31  | CLA  | i     | 603 | X         | -        | -       | -                |
| 31  | CLA  | i     | 604 | X         | -        | X       | -                |
| 31  | CLA  | i     | 610 | X         | -        | -       | -                |
| 31  | CLA  | i     | 611 | X         | -        | -       | -                |
| 31  | CLA  | i     | 612 | X         | -        | -       | -                |
| 31  | CLA  | i     | 613 | X         | -        | -       | -                |
| 39  | CL0  | A     | 857 | X         | -        | -       | -                |
| 42  | NEX  | f     | 523 | -         | -        | X       | -                |
| 42  | NEX  | i     | 523 | -         | -        | X       | -                |



## 2 Entry composition [i](#)

There are 42 unique types of molecules in this entry. The entry contains 77090 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Chlorophyll a-b binding protein, chloroplastic.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | 0     | 213      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1640  | 1063 | 270 | 296 | 11 |         |       |

- Molecule 2 is a protein called Chlorophyll a-b binding protein, chloroplastic.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 2   | 1     | 195      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1478  | 950 | 243 | 273 | 12 |         |       |
| 2   | 5     | 195      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1484  | 956 | 243 | 273 | 12 |         |       |

- Molecule 3 is a protein called Chlorophyll a-b binding protein, chloroplastic.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | 2     | 216      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1667  | 1082 | 269 | 304 | 12 |         |       |

- Molecule 4 is a protein called Chlorophyll a-b binding protein, chloroplastic.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4   | 3     | 228      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1768  | 1141 | 288 | 329 | 10 |         |       |

- Molecule 5 is a protein called Chlorophyll a-b binding protein, chloroplastic.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 5   | 6     | 229      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1797  | 1182 | 292 | 313 | 10 |         |       |

- Molecule 6 is a protein called Chlorophyll a-b binding protein, chloroplastic.



| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 6   | 7     | 228      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1758  | 1137 | 291 | 319 | 11 |         |       |

- Molecule 7 is a protein called Chlorophyll a-b binding protein, chloroplastic.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 7   | 8     | 205      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1574  | 1035 | 256 | 274 | 9 |         |       |
| 7   | 4     | 207      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1569  | 1030 | 257 | 273 | 9 |         |       |

- Molecule 8 is a protein called Chlorophyll a-b binding protein, chloroplastic.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | 9     | 189      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1453  | 932 | 245 | 267 | 9 |         |       |

- Molecule 9 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

| Mol | Chain | Residues | Atoms |      |     |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|-------|
| 9   | A     | 746      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5872  | 3836 | 998 | 1016 | 22 |         |       |

- Molecule 10 is a protein called photosystem I.

| Mol | Chain | Residues | Atoms |      |     |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|-------|
| 10  | B     | 733      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5824  | 3824 | 979 | 1002 | 19 |         |       |

- Molecule 11 is a protein called Photosystem I reaction center subunit II, chloroplastic.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | D     | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1109  | 709 | 193 | 202 | 5 |         |       |

- Molecule 12 is a protein called PsaE.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 12  | E     | 64       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 509   | 323 | 90 | 95 | 1 |         |       |

- Molecule 13 is a protein called Photosystem I reaction center subunit III.



| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | F     | 165      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1273  | 810 | 224 | 235 | 4 |         |       |

- Molecule 14 is a protein called PsaG.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | G     | 93       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 726   | 471 | 119 | 136 |   |         |       |

- Molecule 15 is a protein called Photosystem I reaction center subunit VIII.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 15  | I     | 35       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 262   | 180 | 37 | 43 | 2 |         |       |

- Molecule 16 is a protein called Photosystem I reaction center subunit IX.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 16  | J     | 41       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 336   | 232 | 49 | 54 | 1 |         |       |

- Molecule 17 is a protein called PSI subunit V.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | L     | 162      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1195  | 773 | 192 | 226 | 4 |         |       |

- Molecule 18 is a protein called Photosystem I iron-sulfur center.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 18  | C     | 80       | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 602   | 370 | 105 | 116 | 11 |         |       |

- Molecule 19 is a protein called PsaK.

| Mol | Chain | Residues | Atoms |     |    |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|-------|
| 19  | K     | 80       | Total | C   | N  | O   | S | 0       | 0     |
|     |       |          | 558   | 363 | 92 | 100 | 3 |         |       |

- Molecule 20 is a protein called Photosystem I reaction center subunit XII.



| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 20  | M     | 31       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 238   | 158 | 37 | 43 |         |       |

- Molecule 21 is a protein called PsaO.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | O     | 92       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 728   | 488 | 116 | 120 | 4 |         |       |

- Molecule 22 is a protein called Lhcb-a.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 22  | a     | 198      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1511  | 978 | 243 | 279 | 11 |         |       |
| 22  | h     | 201      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1520  | 985 | 245 | 280 | 10 |         |       |

- Molecule 23 is a protein called Lhcb-c.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 23  | c     | 219      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1680  | 1083 | 271 | 317 | 9 |         |       |

- Molecule 24 is a protein called Lhcb-b.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 24  | b     | 209      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1609  | 1038 | 265 | 295 | 11 |         |       |

- Molecule 25 is a protein called Lhcb-d.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 25  | d     | 217      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1634  | 1059 | 260 | 305 | 10 |         |       |
| 25  | g     | 199      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1502  | 971  | 238 | 283 | 10 |         |       |

- Molecule 26 is a protein called Lhcb-f.

| Mol | Chain | Residues | Atoms |      |     |     |   |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---|---------|-------|
| 26  | f     | 225      | Total | C    | N   | O   | P | S | 0       | 0     |
|     |       |          | 1727  | 1107 | 282 | 330 | 1 | 7 |         |       |



- Molecule 27 is a protein called PsaH.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27  | H     | 94       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 717   | 451 | 126 | 139 | 1 |         |       |

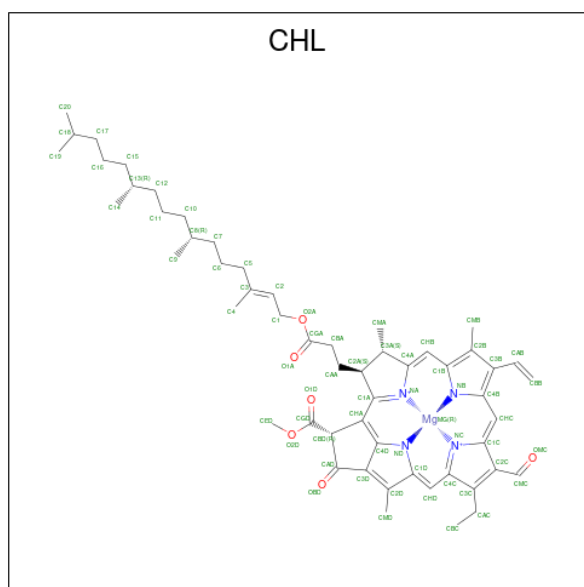
- Molecule 28 is a protein called Lhcb-i.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 28  | i     | 237      | Total | C    | N   | O   | P S | 0       | 0     |
|     |       |          | 1834  | 1179 | 305 | 342 | 1 7 |         |       |

- Molecule 29 is a protein called Lhcb-e.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 29  | e     | 216      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1647  | 1066 | 261 | 310 | 10 |         |       |

- Molecule 30 is CHLOROPHYLL B (CCD ID: CHL) (formula:  $C_{55}H_{70}MgN_4O_6$ ) (labeled as "Ligand of Interest" by depositor).





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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 30  | 0     | 1        | Total<br>48 | C<br>37 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 30  | 1     | 1        | Total<br>64 | C<br>53 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 30  | 1     | 1        | Total<br>51 | C<br>40 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 30  | 1     | 1        | Total<br>48 | C<br>37 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 30  | 1     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 30  | 1     | 1        | Total<br>62 | C<br>51 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 30  | 2     | 1        | Total<br>61 | C<br>50 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 30  | 2     | 1        | Total<br>64 | C<br>53 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 30  | 2     | 1        | Total<br>43 | C<br>34 | Mg<br>1 | N<br>4 | O<br>4 | 0       |
| 30  | 2     | 1        | Total<br>48 | C<br>37 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 30  | 2     | 1        | Total<br>51 | C<br>40 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 30  | 2     | 1        | Total<br>47 | C<br>36 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 30  | 2     | 1        | Total<br>51 | C<br>40 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 30  | 2     | 1        | Total<br>61 | C<br>50 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 30  | 3     | 1        | Total<br>62 | C<br>51 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 30  | 3     | 1        | Total<br>51 | C<br>40 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 30  | 3     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 30  | 5     | 1        | Total<br>52 | C<br>41 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 30  | 5     | 1        | Total<br>64 | C<br>53 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 30  | 5     | 1        | Total<br>46 | C<br>35 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 30  | 5     | 1        | Total<br>48 | C<br>37 | Mg<br>1 | N<br>4 | O<br>6 | 0       |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 30  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 36 | 1  | 4 | 6 |         |
| 30  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 36 | 1  | 4 | 6 |         |
| 30  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 61    | 50 | 1  | 4 | 6 |         |
| 30  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 64    | 53 | 1  | 4 | 6 |         |
| 30  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |
| 30  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 40 | 1  | 4 | 6 |         |
| 30  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 40 | 1  | 4 | 6 |         |
| 30  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 49 | 1  | 4 | 6 |         |
| 30  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 52    | 41 | 1  | 4 | 6 |         |
| 30  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |
| 30  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 63    | 52 | 1  | 4 | 6 |         |
| 30  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 64    | 53 | 1  | 4 | 6 |         |
| 30  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 48    | 37 | 1  | 4 | 6 |         |
| 30  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 61    | 50 | 1  | 4 | 6 |         |
| 30  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 40 | 1  | 4 | 6 |         |
| 30  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 36 | 1  | 4 | 6 |         |
| 30  | 8     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 61    | 50 | 1  | 4 | 6 |         |
| 30  | 8     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 64    | 53 | 1  | 4 | 6 |         |
| 30  | 8     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 36 | 1  | 4 | 6 |         |
| 30  | 8     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 40 | 1  | 4 | 6 |         |
| 30  | 8     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 40 | 1  | 4 | 6 |         |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 30  | 8     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 36 | 1  | 4 | 6 |         |
| 30  | 8     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 56    | 45 | 1  | 4 | 6 |         |
| 30  | 8     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |
| 30  | 9     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 36 | 1  | 4 | 6 |         |
| 30  | 9     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 40 | 1  | 4 | 6 |         |
| 30  | 9     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 48    | 37 | 1  | 4 | 6 |         |
| 30  | 9     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 36 | 1  | 4 | 6 |         |
| 30  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 36 | 1  | 4 | 6 |         |
| 30  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 64    | 53 | 1  | 4 | 6 |         |
| 30  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |
| 30  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 40 | 1  | 4 | 6 |         |
| 30  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 39 | 1  | 4 | 6 |         |
| 30  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 49    | 38 | 1  | 4 | 6 |         |
| 30  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 59    | 48 | 1  | 4 | 6 |         |
| 30  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 42    | 33 | 1  | 4 | 4 |         |
| 30  | c     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 56    | 45 | 1  | 4 | 6 |         |
| 30  | c     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 61    | 50 | 1  | 4 | 6 |         |
| 30  | c     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |
| 30  | c     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 44    | 35 | 1  | 4 | 4 |         |
| 30  | c     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 36 | 1  | 4 | 6 |         |
| 30  | c     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 30  | c     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 30  | c     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 42    | 33 | 1  | 4 | 4 |         |
| 30  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 30  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 64    | 53 | 1  | 4 | 6 |         |
| 30  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 40 | 1  | 4 | 6 |         |
| 30  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 36 | 1  | 4 | 6 |         |
| 30  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 30  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 43 | 1  | 4 | 6 |         |
| 30  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 42    | 33 | 1  | 4 | 4 |         |
| 30  | d     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 40 | 1  | 4 | 6 |         |
| 30  | d     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 64    | 53 | 1  | 4 | 6 |         |
| 30  | d     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |
| 30  | d     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 40 | 1  | 4 | 6 |         |
| 30  | d     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 36 | 1  | 4 | 6 |         |
| 30  | d     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 40 | 1  | 4 | 6 |         |
| 30  | d     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 30  | d     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 42    | 33 | 1  | 4 | 4 |         |
| 30  | f     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 30  | f     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 64    | 53 | 1  | 4 | 6 |         |
| 30  | f     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |
| 30  | f     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 40 | 1  | 4 | 6 |         |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 30  | f     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 36 | 1  | 4 | 6 |         |
| 30  | f     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 40 | 1  | 4 | 6 |         |
| 30  | f     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 30  | f     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 42    | 33 | 1  | 4 | 4 |         |
| 30  | g     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 52    | 41 | 1  | 4 | 6 |         |
| 30  | g     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 52    | 41 | 1  | 4 | 6 |         |
| 30  | g     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |
| 30  | g     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 40 | 1  | 4 | 6 |         |
| 30  | g     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 40 | 1  | 4 | 6 |         |
| 30  | g     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |
| 30  | g     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 36 | 1  | 4 | 6 |         |
| 30  | g     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 42    | 33 | 1  | 4 | 4 |         |
| 30  | h     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 36 | 1  | 4 | 6 |         |
| 30  | h     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 64    | 53 | 1  | 4 | 6 |         |
| 30  | h     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |
| 30  | h     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 40 | 1  | 4 | 6 |         |
| 30  | h     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 35 | 1  | 4 | 6 |         |
| 30  | h     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 35 | 1  | 4 | 6 |         |
| 30  | h     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 36 | 1  | 4 | 6 |         |
| 30  | h     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 42    | 33 | 1  | 4 | 4 |         |
| 30  | i     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 36 | 1  | 4 | 6 |         |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 30  | i     | 1        | Total<br>61 | C<br>50 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 30  | i     | 1        | Total<br>43 | C<br>34 | Mg<br>1 | N<br>4 | O<br>4 | 0       |
| 30  | i     | 1        | Total<br>51 | C<br>40 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 30  | i     | 1        | Total<br>47 | C<br>36 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 30  | i     | 1        | Total<br>50 | C<br>39 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 30  | i     | 1        | Total<br>48 | C<br>37 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 30  | i     | 1        | Total<br>42 | C<br>33 | Mg<br>1 | N<br>4 | O<br>4 | 0       |
| 30  | e     | 1        | Total<br>51 | C<br>40 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 30  | e     | 1        | Total<br>61 | C<br>50 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 30  | e     | 1        | Total<br>43 | C<br>34 | Mg<br>1 | N<br>4 | O<br>4 | 0       |
| 30  | e     | 1        | Total<br>51 | C<br>40 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 30  | e     | 1        | Total<br>47 | C<br>36 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 30  | e     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 30  | e     | 1        | Total<br>61 | C<br>50 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 30  | e     | 1        | Total<br>42 | C<br>33 | Mg<br>1 | N<br>4 | O<br>4 | 0       |
| 30  | 4     | 1        | Total<br>53 | C<br>42 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 30  | 4     | 1        | Total<br>43 | C<br>34 | Mg<br>1 | N<br>4 | O<br>4 | 0       |
| 30  | 4     | 1        | Total<br>48 | C<br>37 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 30  | 4     | 1        | Total<br>51 | C<br>40 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 30  | 4     | 1        | Total<br>47 | C<br>36 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 30  | 4     | 1        | Total<br>51 | C<br>40 | Mg<br>1 | N<br>4 | O<br>6 | 0       |

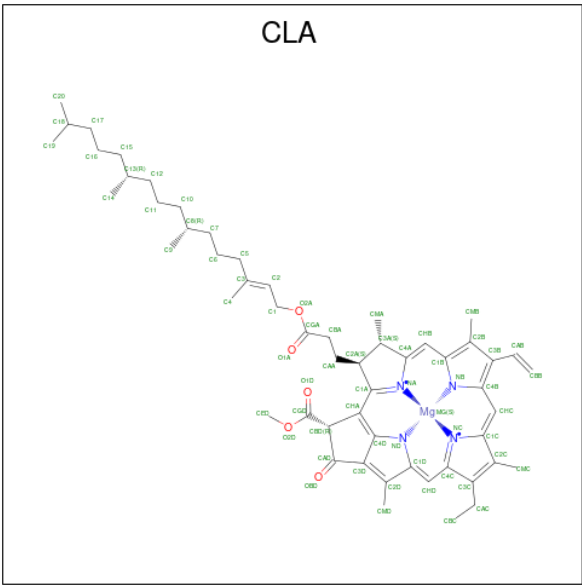
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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 30  | 4     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 43 | 1  | 4 | 6 |         |

- Molecule 31 is CHLOROPHYLL A (CCD ID: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 31  | 0     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 62    | 52 | 1  | 4 | 5 |         |
| 31  | 0     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 52    | 42 | 1  | 4 | 5 |         |
| 31  | 0     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 31  | 0     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 31  | 0     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 41    | 33 | 1  | 4 | 3 |         |
| 31  | 0     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 37 | 1  | 4 | 5 |         |
| 31  | 0     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 31  | 0     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |
| 31  | 0     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 31  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 56    | 46 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 31  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 52    | 42 | 1  | 4 | 5 |         |
| 31  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 31  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 31  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 63    | 53 | 1  | 4 | 5 |         |
| 31  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 52    | 42 | 1  | 4 | 5 |         |
| 31  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 31  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |
| 31  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 56    | 46 | 1  | 4 | 5 |         |
| 31  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 31  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 31  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 31  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 48    | 38 | 1  | 4 | 5 |         |
| 31  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 31  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 31  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 31  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 31  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 37 | 1  | 4 | 5 |         |
| 31  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 31  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 31  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 62    | 52 | 1  | 4 | 5 |         |
| 31  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 31  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 31  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 31  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |
| 31  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 52    | 42 | 1  | 4 | 5 |         |
| 31  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 59    | 49 | 1  | 4 | 5 |         |
| 31  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 52    | 42 | 1  | 4 | 5 |         |
| 31  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |
| 31  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 31  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 31  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 31  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 56    | 46 | 1  | 4 | 5 |         |
| 31  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |
| 31  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 52    | 42 | 1  | 4 | 5 |         |
| 31  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |
| 31  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 58    | 48 | 1  | 4 | 5 |         |
| 31  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 31  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 48    | 38 | 1  | 4 | 5 |         |
| 31  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 56    | 46 | 1  | 4 | 5 |         |
| 31  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 31  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 31  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 31  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |
| 31  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 31  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 31  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 31  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 59    | 49 | 1  | 4 | 5 |         |
| 31  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 37    | 31 | 1  | 4 | 1 |         |
| 31  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 52    | 42 | 1  | 4 | 5 |         |
| 31  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 31  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 37 | 1  | 4 | 5 |         |
| 31  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 49    | 39 | 1  | 4 | 5 |         |
| 31  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 31  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 31  | 8     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |
| 31  | 8     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 31  | 8     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 31  | 8     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |
| 31  | 8     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |
| 31  | 8     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 56    | 46 | 1  | 4 | 5 |         |
| 31  | 8     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 31  | 9     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 58    | 48 | 1  | 4 | 5 |         |
| 31  | 9     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 31  | 9     | 1        | Total<br>48 | C<br>38 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | 9     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | 9     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | 9     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | 9     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 31  | 9     | 1        | Total<br>52 | C<br>42 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | 9     | 1        | Total<br>56 | C<br>46 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | A     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | A     | 1        | Total<br>54 | C<br>44 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | A     | 1        | Total<br>54 | C<br>44 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | A     | 1        | Total<br>57 | C<br>47 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 31  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 31  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 61    | 51 | 1  | 4 | 5 |         |
| 31  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 31  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 31  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 31  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 31  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 49    | 39 | 1  | 4 | 5 |         |
| 31  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |
| 31  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 31  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 31  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 31  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 31  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 31  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 31  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 31  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 31  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 31  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |
| 31  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 57    | 47 | 1  | 4 | 5 |         |
| 31  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 31  | A     | 1        | Total<br>61 | C<br>51 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | A     | 1        | Total<br>56 | C<br>46 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | A     | 1        | Total<br>52 | C<br>42 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | B     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | B     | 1        | Total<br>62 | C<br>52 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | B     | 1        | Total<br>52 | C<br>42 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | B     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | B     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 31  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 31  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 31  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 59    | 49 | 1  | 4 | 5 |         |
| 31  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 31  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 56    | 46 | 1  | 4 | 5 |         |
| 31  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 31  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 31  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 52    | 42 | 1  | 4 | 5 |         |
| 31  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 31  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 31  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 31  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 31  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 31  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 31  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 56    | 46 | 1  | 4 | 5 |         |
| 31  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 31  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 31  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 31  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 61    | 51 | 1  | 4 | 5 |         |
| 31  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 31  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 31  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | B     | 1        | Total<br>47 | C<br>37 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | B     | 1        | Total<br>47 | C<br>37 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | F     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | G     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | G     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | G     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | J     | 1        | Total<br>42 | C<br>34 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 31  | L     | 1        | Total<br>58 | C<br>48 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | L     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | L     | 1        | Total<br>63 | C<br>53 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | L     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | L     | 1        | Total<br>47 | C<br>37 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | K     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | K     | 1        | Total<br>53 | C<br>43 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | K     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | K     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | M     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 31  | O     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 31  | O     | 1        | Total<br>38 | C<br>30 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 31  | O     | 1        | Total<br>38 | C<br>30 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 31  | O     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | a     | 1        | Total<br>53 | C<br>43 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | a     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | a     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | a     | 1        | Total<br>57 | C<br>47 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | a     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | a     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | c     | 1        | Total<br>52 | C<br>42 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | c     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | c     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | c     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | c     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | c     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | b     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | b     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | b     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | b     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | b     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 31  | b     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | d     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | d     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | d     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | d     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | d     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | d     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | f     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | f     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | f     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | f     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | f     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | f     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | g     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | g     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | g     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | g     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | g     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | g     | 1        | Total<br>47 | C<br>37 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | h     | 1        | Total<br>49 | C<br>39 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | h     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 31  | h     | 1        | Total<br>47 | C<br>37 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | h     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 31  | h     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | h     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | H     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | H     | 1        | Total<br>47 | C<br>37 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | H     | 1        | Total<br>47 | C<br>37 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | H     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | i     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | i     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | i     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | i     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | i     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | i     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | e     | 1        | Total<br>57 | C<br>47 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | e     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | e     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | e     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | e     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | e     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | 4     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

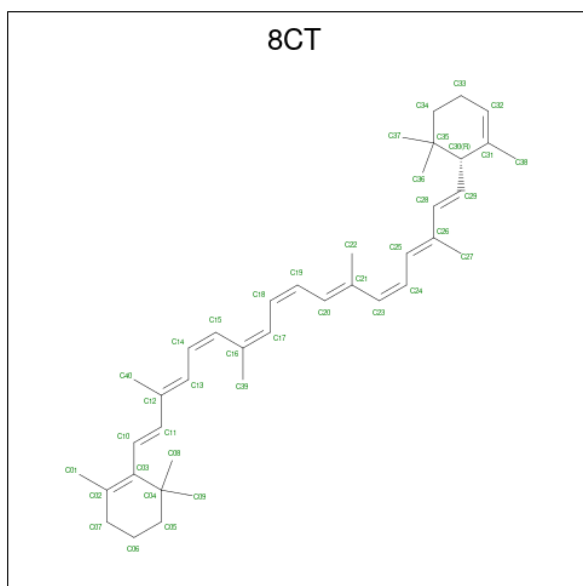
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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 31  | 4     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 31  | 4     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 31  | 4     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 31  | 4     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 48    | 38 | 1  | 4 | 5 |         |
| 31  | 4     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 53    | 43 | 1  | 4 | 5 |         |
| 31  | 4     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |

- Molecule 32 is (6'R,11cis,11'cis,13cis,15cis)-4',5'-didehydro-5',6'-dihydro-beta,beta-carotene (CCD ID: 8CT) (formula: C<sub>40</sub>H<sub>56</sub>) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 32  | 0     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 32  | 1     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 32  | 2     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 32  | 3     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 32  | 3     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |

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| Mol | Chain | Residues | Atoms            | AltConf |
|-----|-------|----------|------------------|---------|
| 32  | 6     | 1        | Total C<br>40 40 | 0       |
| 32  | 7     | 1        | Total C<br>40 40 | 0       |
| 32  | 7     | 1        | Total C<br>40 40 | 0       |
| 32  | 7     | 1        | Total C<br>40 40 | 0       |
| 32  | 8     | 1        | Total C<br>40 40 | 0       |
| 32  | 8     | 1        | Total C<br>40 40 | 0       |
| 32  | 9     | 1        | Total C<br>40 40 | 0       |
| 32  | A     | 1        | Total C<br>40 40 | 0       |
| 32  | A     | 1        | Total C<br>40 40 | 0       |
| 32  | A     | 1        | Total C<br>40 40 | 0       |
| 32  | A     | 1        | Total C<br>40 40 | 0       |
| 32  | A     | 1        | Total C<br>40 40 | 0       |
| 32  | A     | 1        | Total C<br>40 40 | 0       |
| 32  | A     | 1        | Total C<br>40 40 | 0       |
| 32  | B     | 1        | Total C<br>40 40 | 0       |
| 32  | B     | 1        | Total C<br>40 40 | 0       |
| 32  | B     | 1        | Total C<br>40 40 | 0       |
| 32  | B     | 1        | Total C<br>40 40 | 0       |
| 32  | B     | 1        | Total C<br>40 40 | 0       |
| 32  | B     | 1        | Total C<br>40 40 | 0       |
| 32  | B     | 1        | Total C<br>40 40 | 0       |
| 32  | B     | 1        | Total C<br>40 40 | 0       |

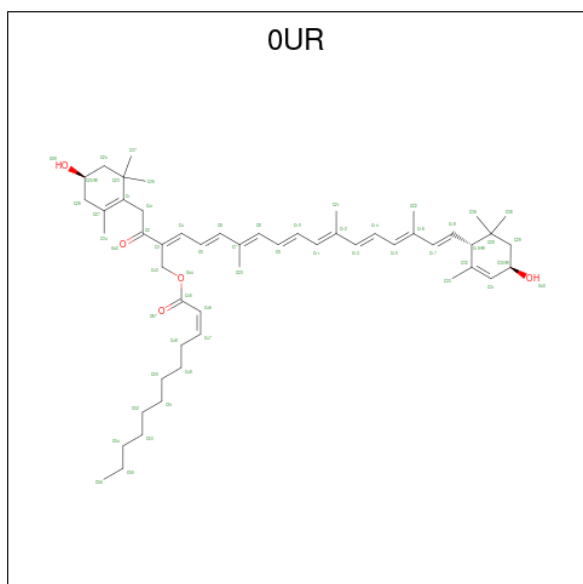
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| Mol | Chain | Residues | Atoms            | AltConf |
|-----|-------|----------|------------------|---------|
| 32  | F     | 1        | Total C<br>40 40 | 0       |
| 32  | G     | 1        | Total C<br>40 40 | 0       |
| 32  | I     | 1        | Total C<br>40 40 | 0       |
| 32  | J     | 1        | Total C<br>40 40 | 0       |
| 32  | J     | 1        | Total C<br>40 40 | 0       |
| 32  | L     | 1        | Total C<br>40 40 | 0       |
| 32  | L     | 1        | Total C<br>40 40 | 0       |
| 32  | L     | 1        | Total C<br>40 40 | 0       |
| 32  | K     | 1        | Total C<br>40 40 | 0       |
| 32  | M     | 1        | Total C<br>40 40 | 0       |
| 32  | O     | 1        | Total C<br>40 40 | 0       |
| 32  | 4     | 1        | Total C<br>40 40 | 0       |

- Molecule 33 is Siphonein (CCD ID: 0UR) (formula:  $C_{52}H_{76}O_5$ ) (labeled as "Ligand of Interest" by depositor).





| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 33  | 0     | 1        | Total | C  | O | 0       |
|     |       |          | 52    | 47 | 5 |         |
| 33  | 0     | 1        | Total | C  | O | 0       |
|     |       |          | 52    | 47 | 5 |         |
| 33  | 1     | 1        | Total | C  | O | 0       |
|     |       |          | 52    | 47 | 5 |         |
| 33  | 1     | 1        | Total | C  | O | 0       |
|     |       |          | 52    | 47 | 5 |         |
| 33  | 2     | 1        | Total | C  | O | 0       |
|     |       |          | 51    | 46 | 5 |         |
| 33  | 2     | 1        | Total | C  | O | 0       |
|     |       |          | 50    | 45 | 5 |         |
| 33  | 3     | 1        | Total | C  | O | 0       |
|     |       |          | 51    | 46 | 5 |         |
| 33  | 5     | 1        | Total | C  | O | 0       |
|     |       |          | 51    | 46 | 5 |         |
| 33  | 5     | 1        | Total | C  | O | 0       |
|     |       |          | 52    | 47 | 5 |         |
| 33  | 6     | 1        | Total | C  | O | 0       |
|     |       |          | 51    | 46 | 5 |         |
| 33  | 6     | 1        | Total | C  | O | 0       |
|     |       |          | 52    | 47 | 5 |         |
| 33  | 7     | 1        | Total | C  | O | 0       |
|     |       |          | 51    | 46 | 5 |         |
| 33  | 8     | 1        | Total | C  | O | 0       |
|     |       |          | 51    | 46 | 5 |         |
| 33  | 8     | 1        | Total | C  | O | 0       |
|     |       |          | 52    | 47 | 5 |         |
| 33  | 9     | 1        | Total | C  | O | 0       |
|     |       |          | 52    | 47 | 5 |         |
| 33  | 9     | 1        | Total | C  | O | 0       |
|     |       |          | 52    | 47 | 5 |         |
| 33  | O     | 1        | Total | C  | O | 0       |
|     |       |          | 52    | 47 | 5 |         |
| 33  | a     | 1        | Total | C  | O | 0       |
|     |       |          | 47    | 42 | 5 |         |
| 33  | c     | 1        | Total | C  | O | 0       |
|     |       |          | 52    | 47 | 5 |         |
| 33  | b     | 1        | Total | C  | O | 0       |
|     |       |          | 52    | 47 | 5 |         |
| 33  | d     | 1        | Total | C  | O | 0       |
|     |       |          | 49    | 44 | 5 |         |
| 33  | f     | 1        | Total | C  | O | 0       |
|     |       |          | 49    | 44 | 5 |         |

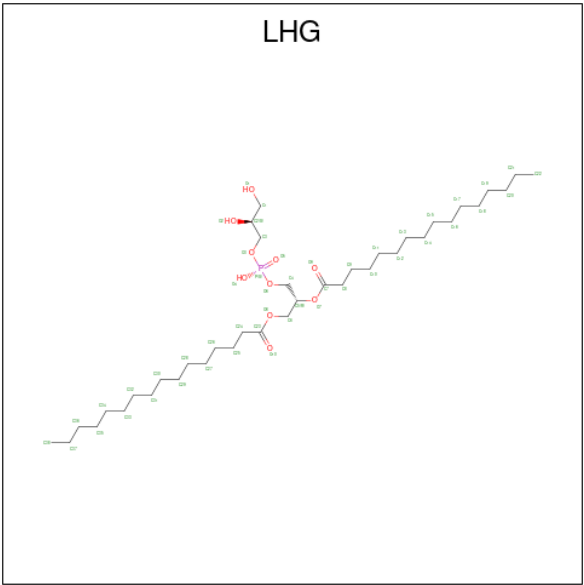
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| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 33  | g     | 1        | Total | C  | O | 0       |
|     |       |          | 52    | 47 | 5 |         |
| 33  | h     | 1        | Total | C  | O | 0       |
|     |       |          | 52    | 47 | 5 |         |
| 33  | i     | 1        | Total | C  | O | 0       |
|     |       |          | 50    | 45 | 5 |         |
| 33  | e     | 1        | Total | C  | O | 0       |
|     |       |          | 52    | 47 | 5 |         |
| 33  | 4     | 1        | Total | C  | O | 0       |
|     |       |          | 51    | 46 | 5 |         |
| 33  | 4     | 1        | Total | C  | O | 0       |
|     |       |          | 50    | 45 | 5 |         |

- Molecule 34 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 34  | 0     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 34  | 1     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 34  | 2     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 32    | 21 | 10 | 1 |         |
| 34  | 3     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 36    | 25 | 10 | 1 |         |
| 34  | 3     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 37    | 26 | 10 | 1 |         |

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| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 34  | 5     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 37    | 26 | 10 | 1 |         |
| 34  | 6     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 37    | 26 | 10 | 1 |         |
| 34  | 6     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 31    | 20 | 10 | 1 |         |
| 34  | 7     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 30    | 19 | 10 | 1 |         |
| 34  | 7     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 38    | 27 | 10 | 1 |         |
| 34  | 7     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 39    | 28 | 10 | 1 |         |
| 34  | 8     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 44    | 33 | 10 | 1 |         |
| 34  | 9     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 47    | 36 | 10 | 1 |         |
| 34  | A     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 34  | A     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 27    | 16 | 10 | 1 |         |
| 34  | A     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 42    | 31 | 10 | 1 |         |
| 34  | B     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 23    | 12 | 10 | 1 |         |
| 34  | B     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 43    | 32 | 10 | 1 |         |
| 34  | G     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 38    | 27 | 10 | 1 |         |
| 34  | K     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 43    | 34 | 8  | 1 |         |
| 34  | M     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 46    | 35 | 10 | 1 |         |
| 34  | a     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 43    | 32 | 10 | 1 |         |
| 34  | c     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 40    | 29 | 10 | 1 |         |
| 34  | b     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 41    | 30 | 10 | 1 |         |
| 34  | d     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 36    | 25 | 10 | 1 |         |
| 34  | f     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 40    | 29 | 10 | 1 |         |

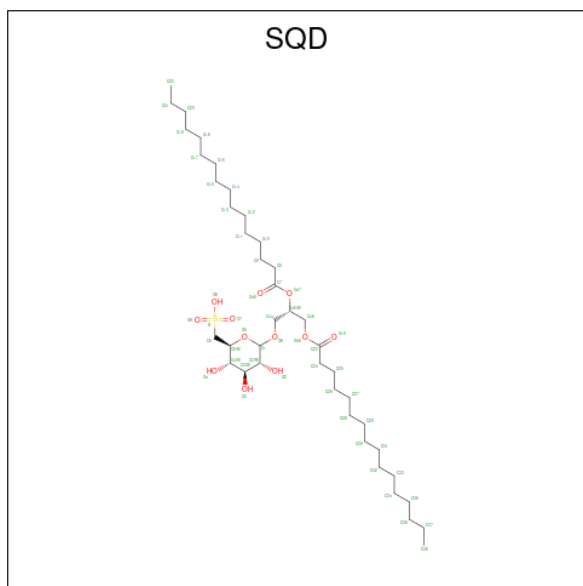
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| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 34  | g     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 30    | 19 | 10 | 1 |         |
| 34  | h     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 39    | 28 | 10 | 1 |         |
| 34  | H     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 31    | 20 | 10 | 1 |         |
| 34  | i     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 30    | 19 | 10 | 1 |         |
| 34  | e     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 43    | 32 | 10 | 1 |         |
| 34  | 4     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 32    | 21 | 10 | 1 |         |

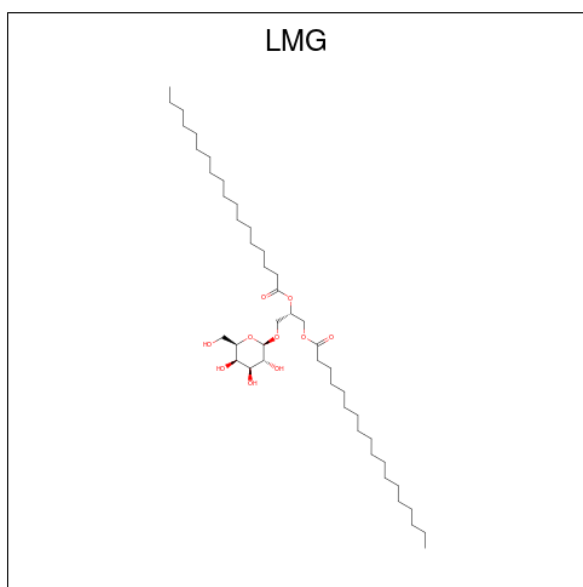
- Molecule 35 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula:  $C_{41}H_{78}O_{12}S$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
| 35  | 0     | 1        | Total | C  | O | S | 0       |
|     |       |          | 36    | 26 | 9 | 1 |         |

- Molecule 36 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula:  $C_{45}H_{86}O_{10}$ ) (labeled as "Ligand of Interest" by depositor).

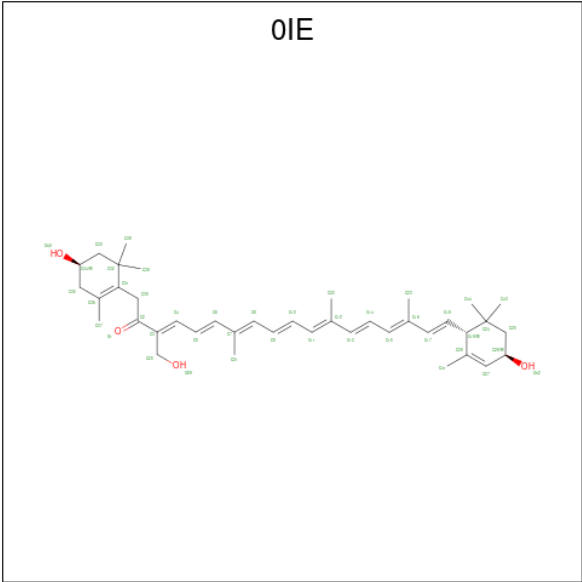




| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 36  | 2     | 1        | Total | C  | O  | 0       |
|     |       |          | 36    | 26 | 10 |         |
| 36  | 3     | 1        | Total | C  | O  | 0       |
|     |       |          | 36    | 26 | 10 |         |
| 36  | 9     | 1        | Total | C  | O  | 0       |
|     |       |          | 55    | 45 | 10 |         |
| 36  | A     | 1        | Total | C  | O  | 0       |
|     |       |          | 36    | 26 | 10 |         |
| 36  | B     | 1        | Total | C  | O  | 0       |
|     |       |          | 42    | 32 | 10 |         |
| 36  | J     | 1        | Total | C  | O  | 0       |
|     |       |          | 29    | 19 | 10 |         |
| 36  | J     | 1        | Total | C  | O  | 0       |
|     |       |          | 46    | 36 | 10 |         |
| 36  | L     | 1        | Total | C  | O  | 0       |
|     |       |          | 31    | 21 | 10 |         |
| 36  | L     | 1        | Total | C  | O  | 0       |
|     |       |          | 37    | 27 | 10 |         |
| 36  | O     | 1        | Total | C  | O  | 0       |
|     |       |          | 39    | 29 | 10 |         |

- Molecule 37 is Siphonaxanthin (CCD ID: 0IE) (formula:  $C_{40}H_{56}O_4$ ) (labeled as "Ligand of Interest" by depositor).





| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 37  | 3     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 37  | 7     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 37  | a     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 37  | a     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 37  | c     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 37  | c     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 37  | b     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 37  | b     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 37  | d     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 37  | d     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 37  | f     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 37  | f     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 37  | g     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 37  | g     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |

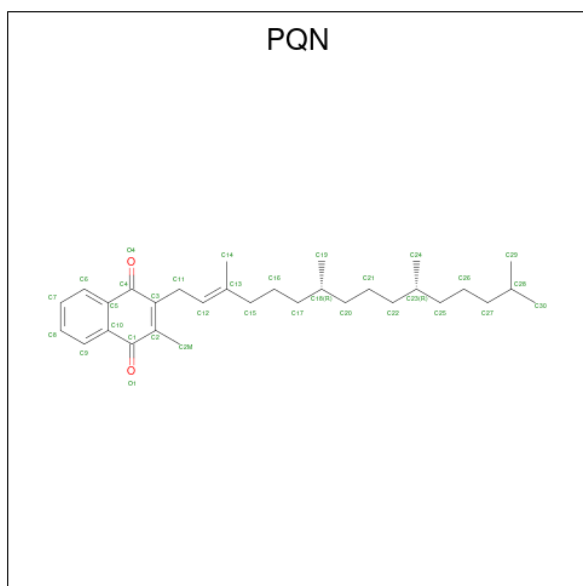
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| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 37  | h     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 37  | h     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 37  | i     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 37  | i     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 37  | e     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 37  | e     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |

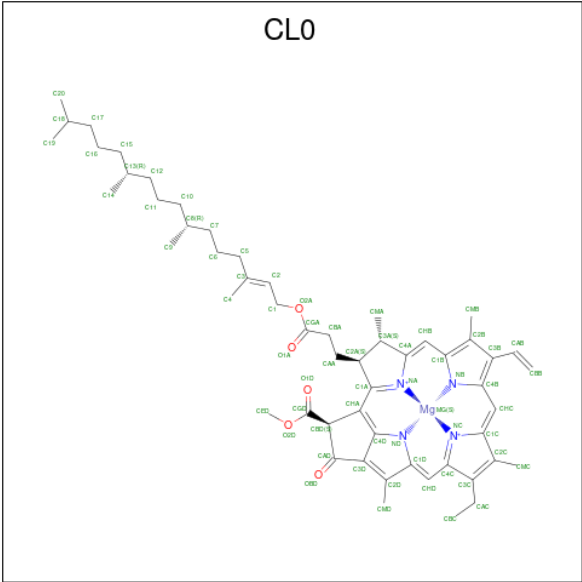
- Molecule 38 is PHYLLOQUINONE (CCD ID: PQN) (formula:  $C_{31}H_{46}O_2$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 38  | A     | 1        | Total | C  | O | 0       |
|     |       |          | 33    | 31 | 2 |         |
| 38  | B     | 1        | Total | C  | O | 0       |
|     |       |          | 33    | 31 | 2 |         |

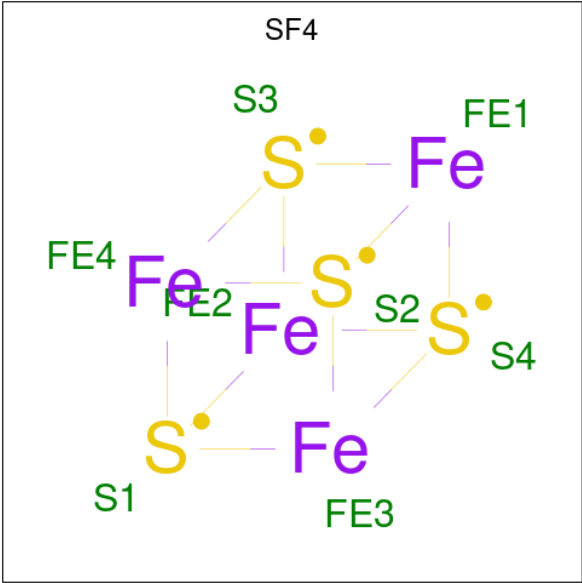
- Molecule 39 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula:  $C_{55}H_{72}MgN_4O_5$ ) (labeled as "Ligand of Interest" by depositor).





| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 39  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |

- Molecule 40 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 40  | B     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 40  | C     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |

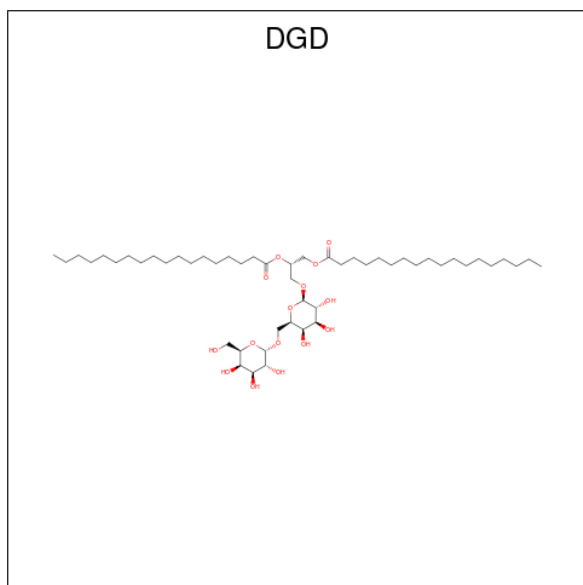
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| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 40  | C     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |

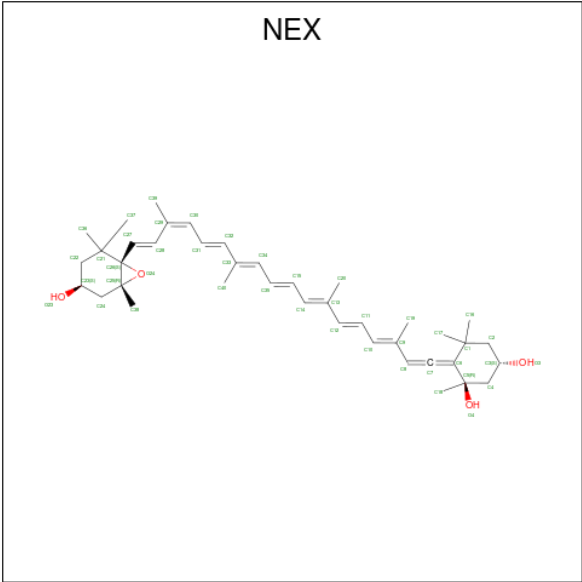
- Molecule 41 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:  $C_{51}H_{96}O_{15}$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 41  | B     | 1        | Total | C  | O  | 0       |
|     |       |          | 56    | 41 | 15 |         |

- Molecule 42 is (1R,3R)-6-{(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula:  $C_{40}H_{56}O_4$ ) (labeled as "Ligand of Interest" by depositor).





| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 42  | a     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 42  | c     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 42  | b     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 42  | d     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 42  | f     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 42  | g     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 42  | h     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 42  | i     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 42  | e     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |

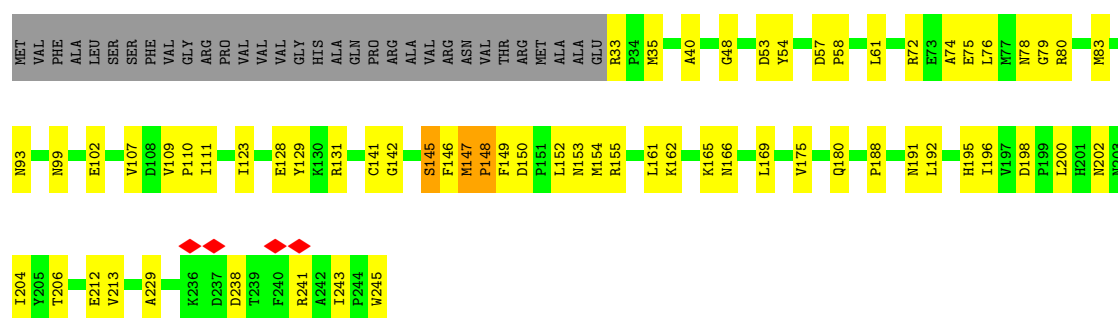


### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

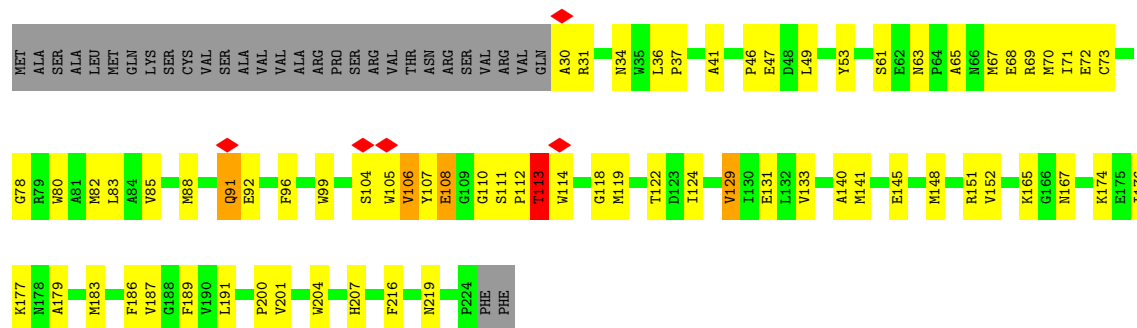
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic

Chain 0: 



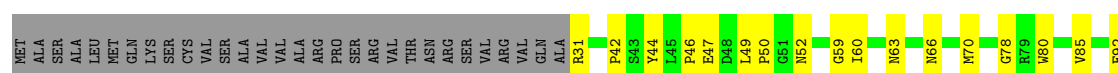
- Molecule 2: Chlorophyll a-b binding protein, chloroplastic

Chain 1: 

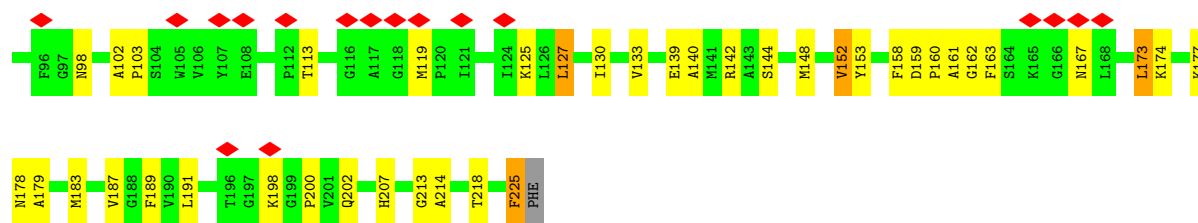


- Molecule 2: Chlorophyll a-b binding protein, chloroplastic

Chain 5: 

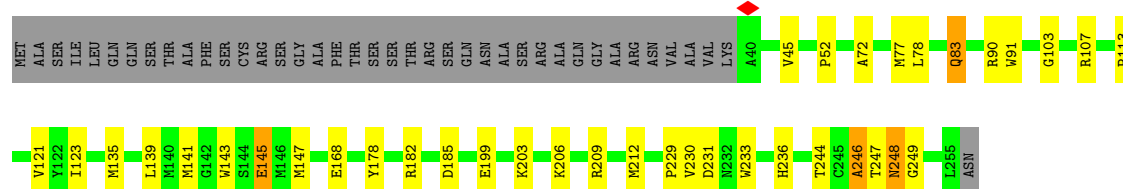






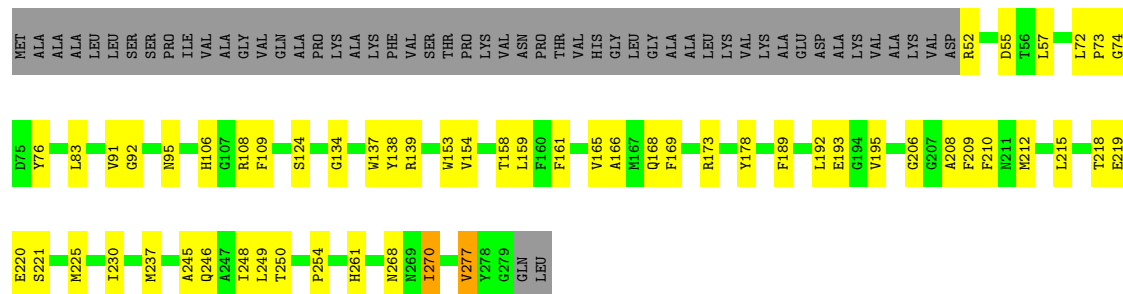
- Molecule 3: Chlorophyll a-b binding protein, chloroplastic

Chain 2: 70% 13% 16%



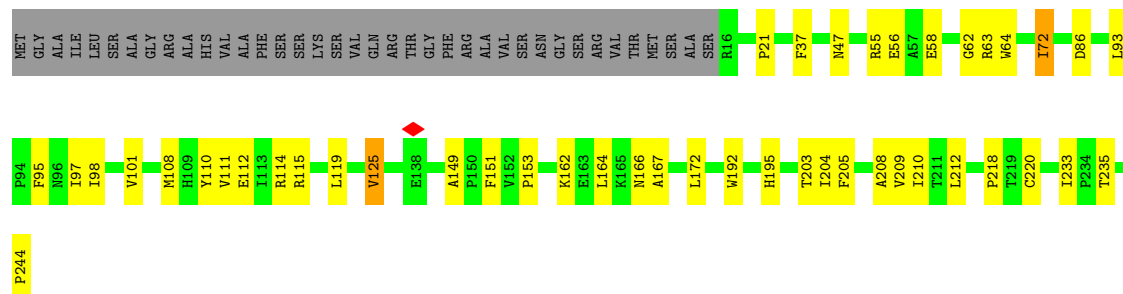
- Molecule 4: Chlorophyll a-b binding protein, chloroplastic

Chain 3: 61% 20% 19%



- Molecule 5: Chlorophyll a-b binding protein, chloroplastic

Chain 6: 69% 16% 14%



- Molecule 6: Chlorophyll a-b binding protein, chloroplastic

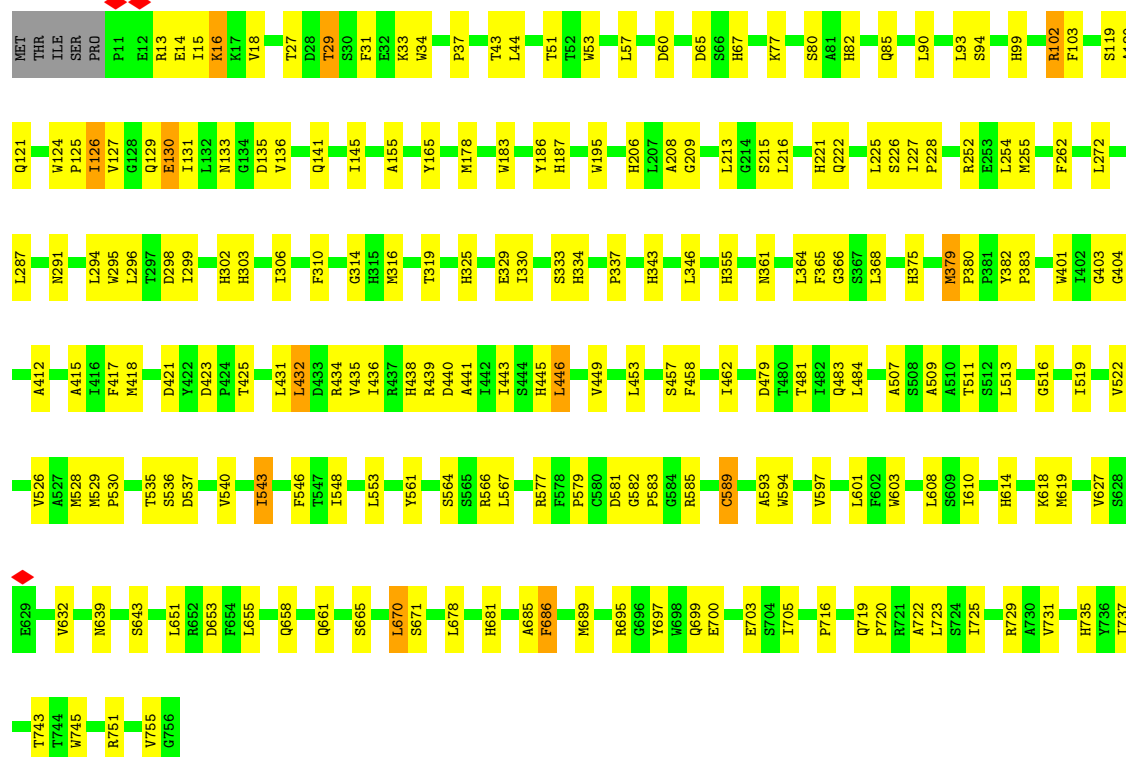
Chain 7: 66% 19% 14%






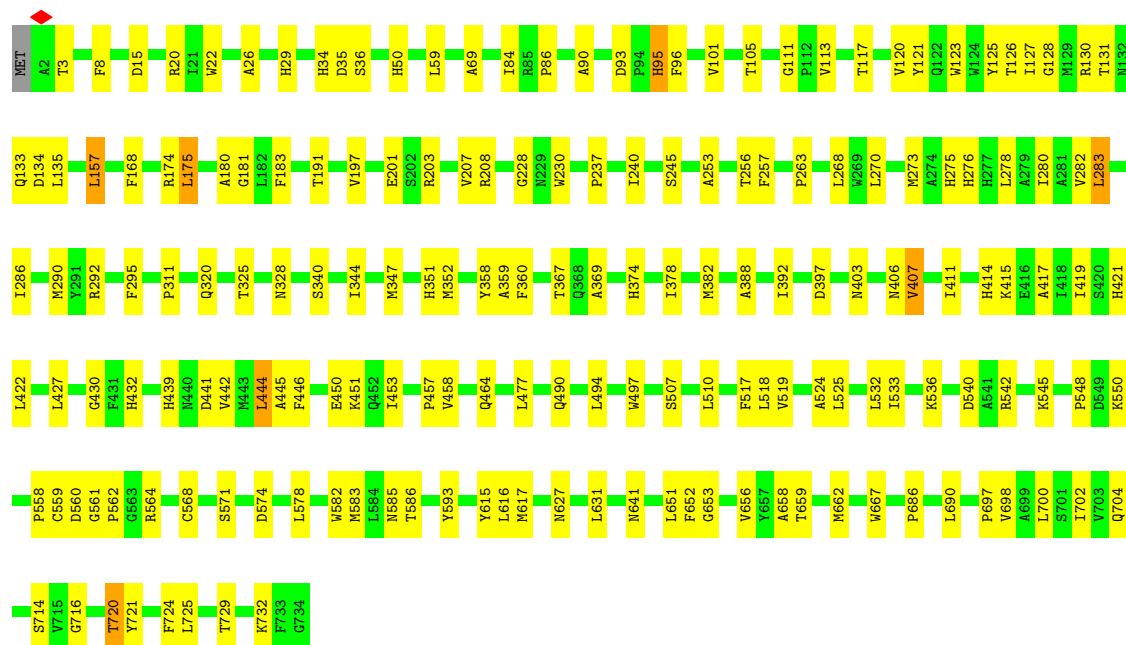


Chain A:  72% 26% ..



• Molecule 10: photosystem I

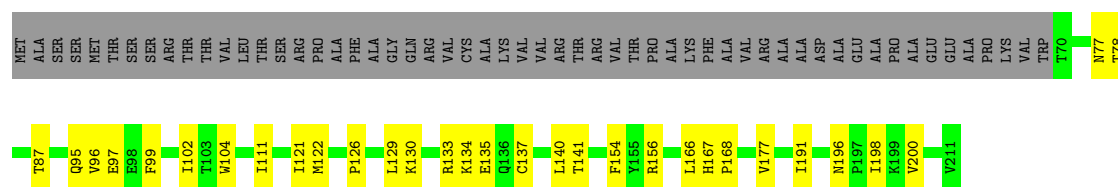
Chain B:  75% 23% .



• Molecule 11: Photosystem I reaction center subunit II, chloroplastic

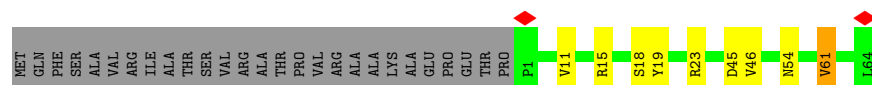


Chain D: 



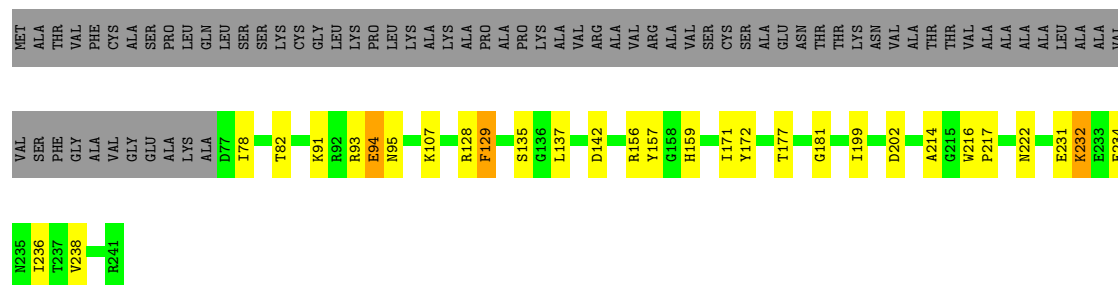
• Molecule 12: PsaE

Chain E: 




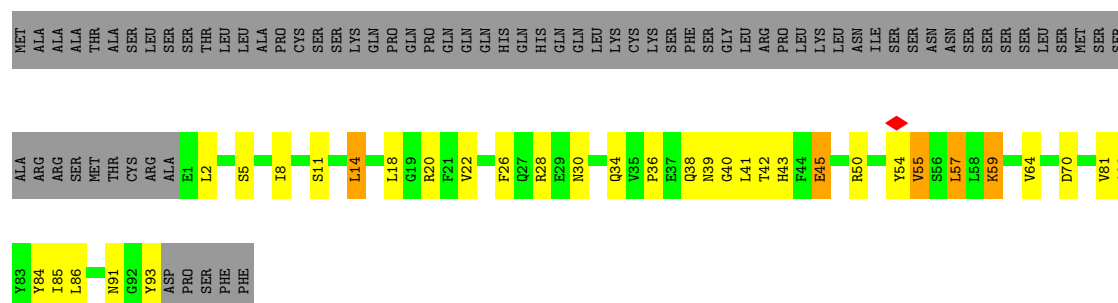
• Molecule 13: Photosystem I reaction center subunit III

Chain F: 



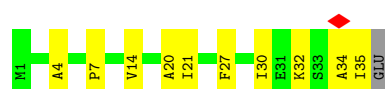
• Molecule 14: PsaG

Chain G: 



• Molecule 15: Photosystem I reaction center subunit VIII

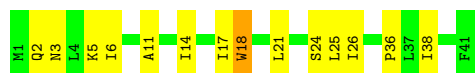
Chain I: 



• Molecule 16: Photosystem I reaction center subunit IX

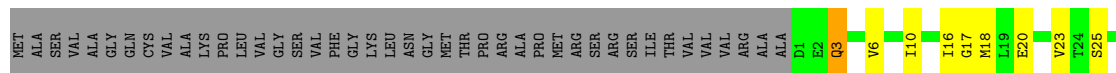


Chain J:  66% 32% .



• Molecule 17: PSI subunit V

Chain L:  64% 15% 21%



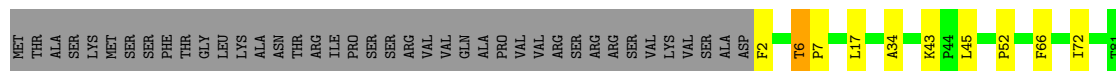
• Molecule 18: Photosystem I iron-sulfur center

Chain C:  74% 25% .




• Molecule 19: PsaK

Chain K:  57% 7% 35%



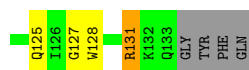
• Molecule 20: Photosystem I reaction center subunit XII

Chain M:  84% 12% .



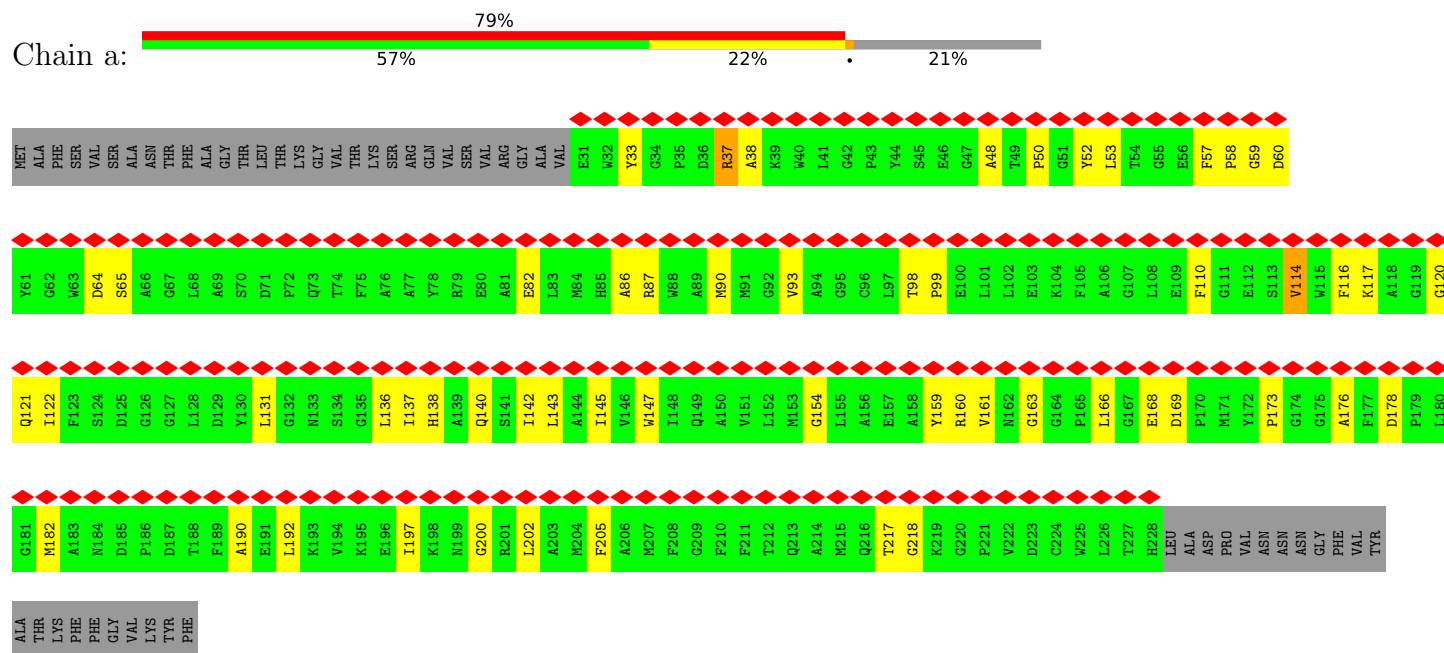
• Molecule 21: PsaO

Chain O:  57% 9% 33%

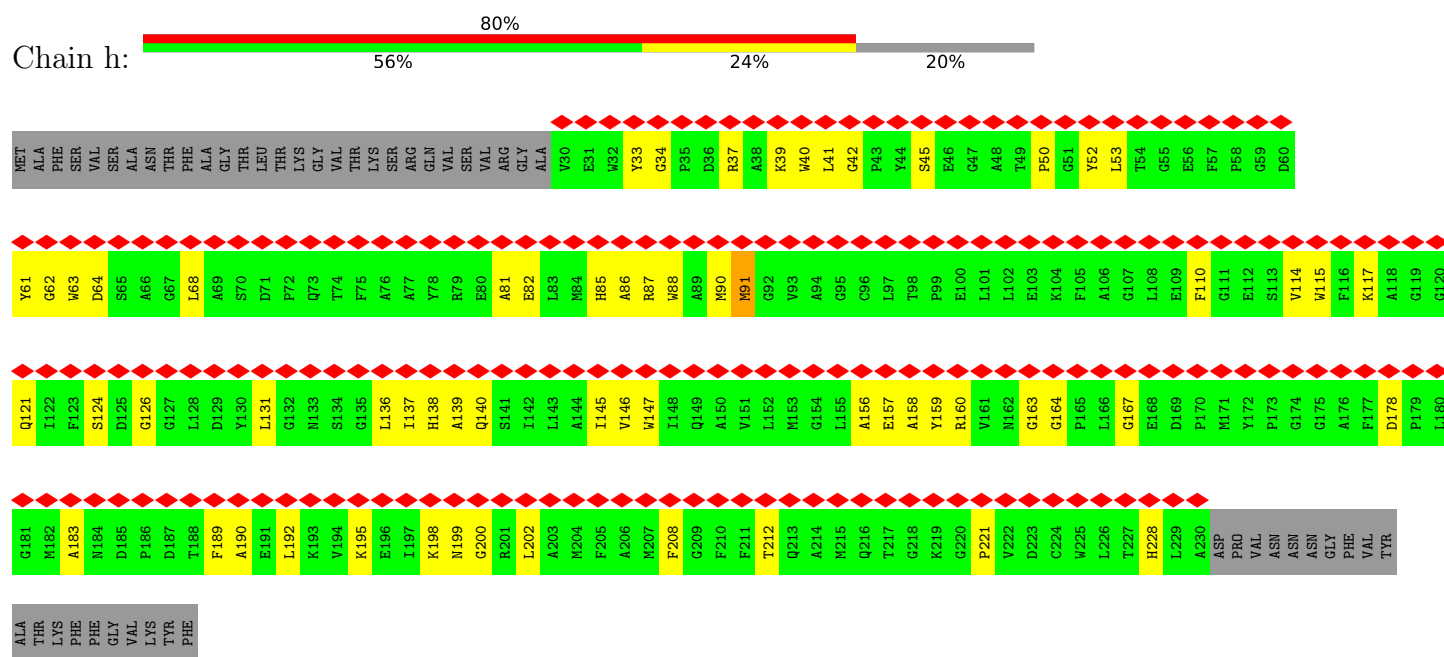




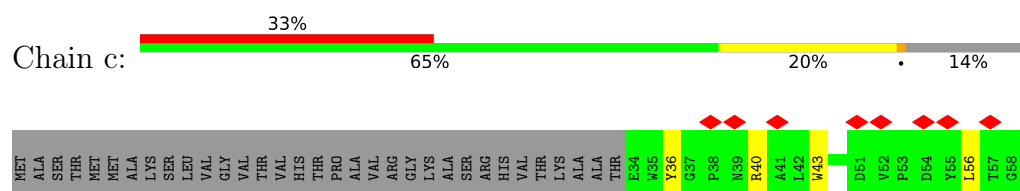
- Molecule 22: Lhcb-a



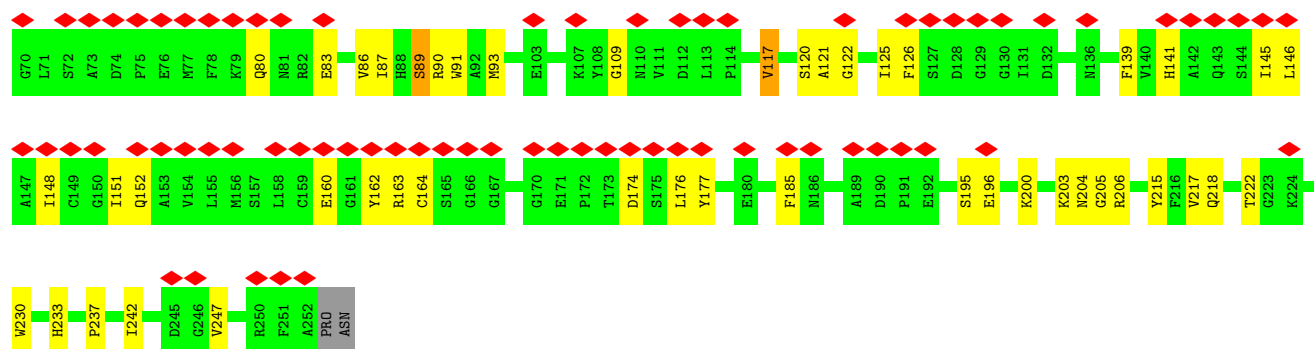
- Molecule 22: Lhcb-a



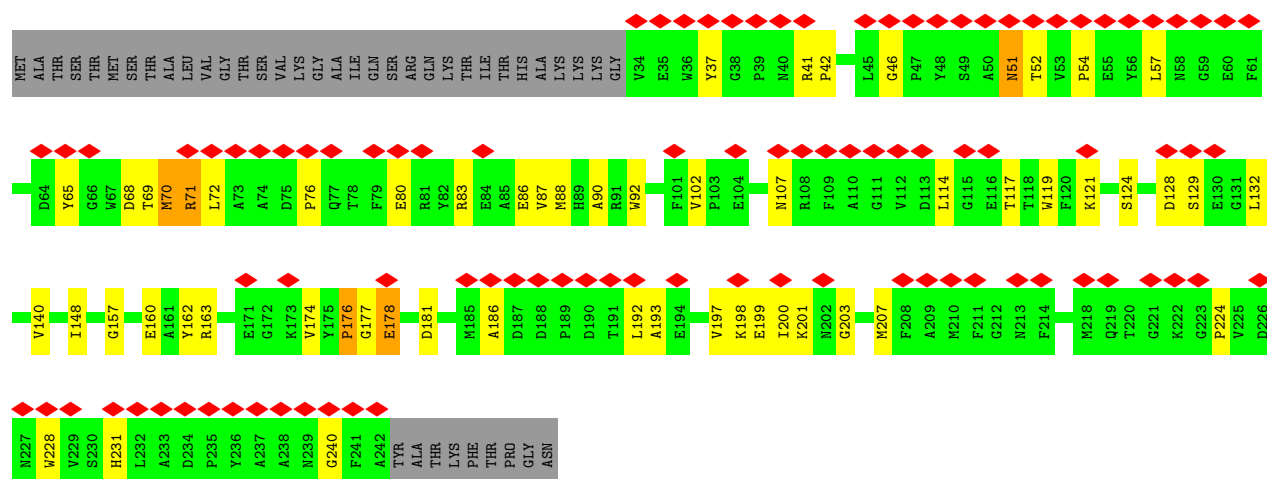
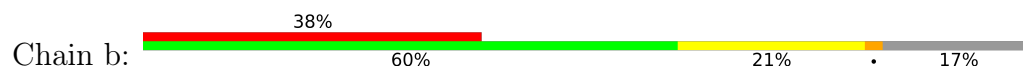
- Molecule 23: Lhcb-c



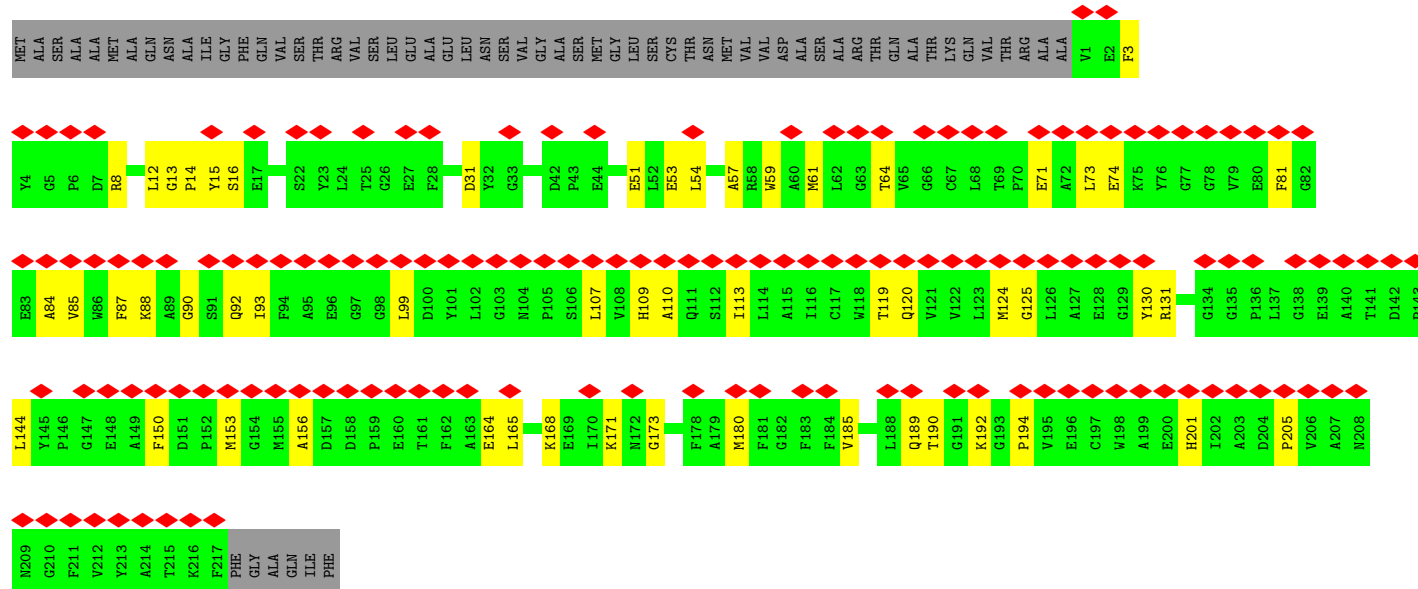




• Molecule 24: Lhcb-b

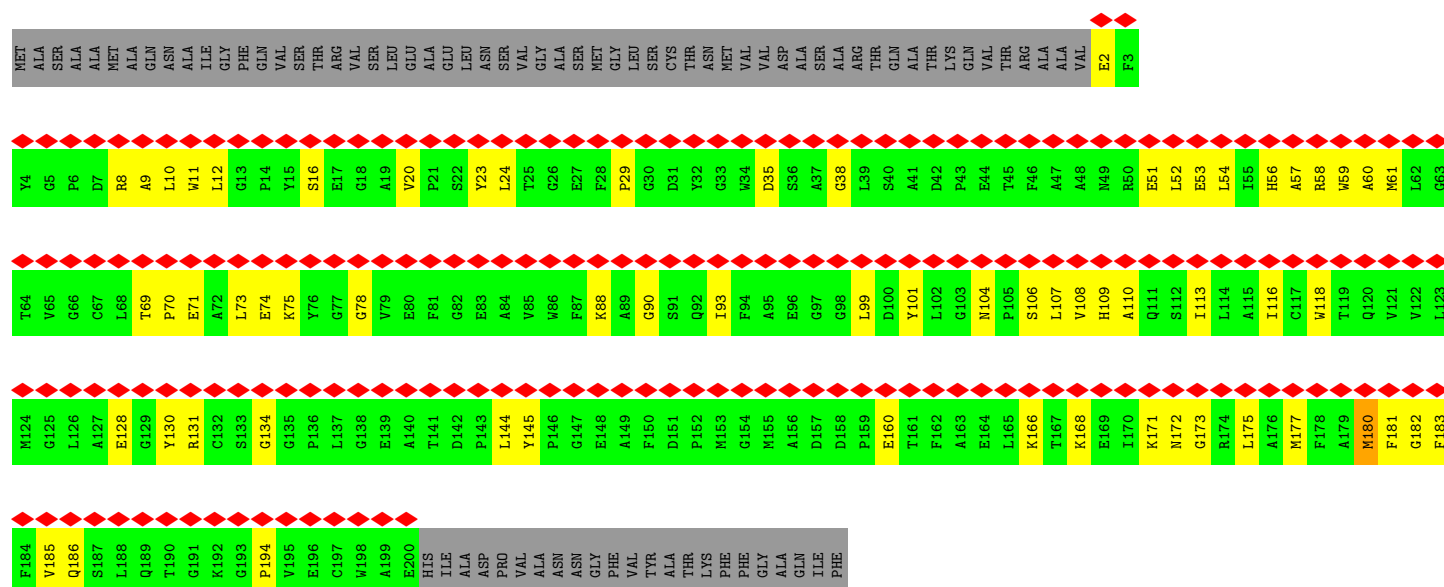


• Molecule 25: Lhcb-d

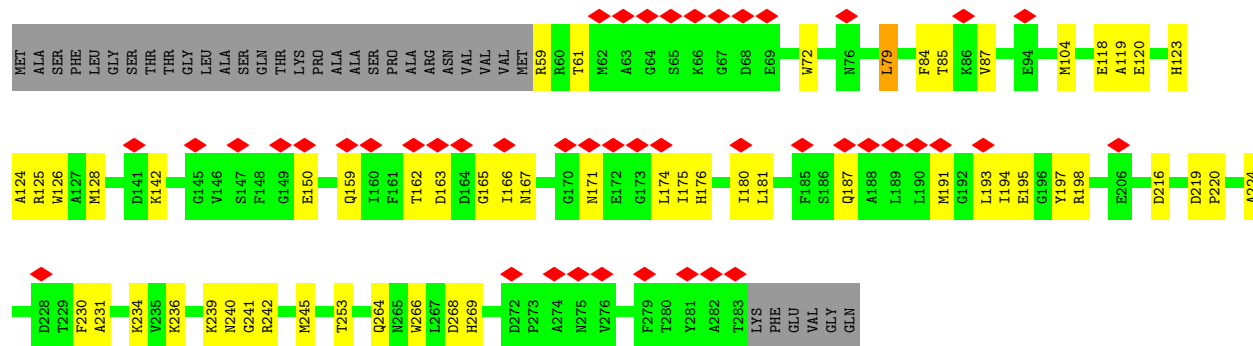




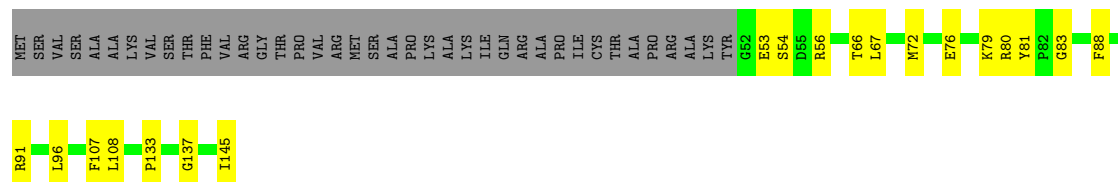
- Molecule 25: Lhcb-d



- Molecule 26: Lhcb-f



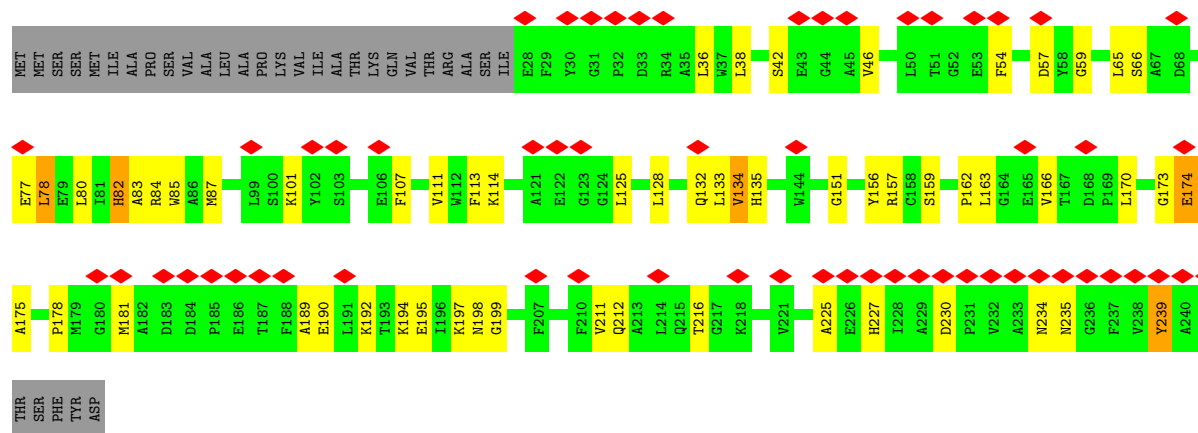
- Molecule 27: PsaH



- Molecule 28: Lhcb-i









## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|---|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 213217                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TECNAI SPHERA                       | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 60                                      | Depositor |
| Minimum defocus (nm)                 | 1000                                    | Depositor |
| Maximum defocus (nm)                 | 2000                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 BIOQUANTUM (6k x 4k)           | Depositor |
| Maximum map value                    | 1.557                                   | Depositor |
| Minimum map value                    | -0.337                                  | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 0.027                                   | Depositor |
| Recommended contour level            | 0.217                                   | Depositor |
| Map size (Å)                         | 532.48, 532.48, 532.48                  | wwPDB     |
| Map dimensions                       | 512, 512, 512                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.04, 1.04, 1.04                        | Depositor |



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: LMG, 0IE, NEX, CLA, TPO, 0UR, SQD, LHG, PQN, SF4, CL0, CHL, DGD, 8CT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |               | Bond angles |               |
|-----|-------|--------------|---------------|-------------|---------------|
|     |       | RMSZ         | # Z  >5       | RMSZ        | # Z  >5       |
| 1   | 0     | 0.27         | 0/1685        | 0.38        | 0/2285        |
| 2   | 1     | 0.41         | 1/1523 (0.1%) | 0.45        | 1/2073 (0.0%) |
| 2   | 5     | 0.21         | 0/1530        | 0.41        | 0/2082        |
| 3   | 2     | 0.47         | 2/1727 (0.1%) | 0.42        | 2/2351 (0.1%) |
| 4   | 3     | 0.25         | 0/1818        | 0.32        | 0/2466        |
| 5   | 6     | 0.22         | 0/1862        | 0.29        | 0/2542        |
| 6   | 7     | 0.22         | 0/1812        | 0.31        | 0/2468        |
| 7   | 4     | 0.34         | 0/1619        | 0.62        | 1/2206 (0.0%) |
| 7   | 8     | 0.20         | 0/1627        | 0.41        | 2/2217 (0.1%) |
| 8   | 9     | 0.53         | 0/1492        | 0.48        | 1/2036 (0.0%) |
| 9   | A     | 0.42         | 1/6069 (0.0%) | 0.35        | 1/8267 (0.0%) |
| 10  | B     | 0.37         | 0/6034        | 0.35        | 0/8239        |
| 11  | D     | 0.21         | 0/1135        | 0.34        | 0/1533        |
| 12  | E     | 0.19         | 0/521         | 0.26        | 0/706         |
| 13  | F     | 0.21         | 0/1298        | 0.31        | 0/1748        |
| 14  | G     | 0.25         | 0/743         | 0.41        | 0/1010        |
| 15  | I     | 0.60         | 0/269         | 0.45        | 0/367         |
| 16  | J     | 0.25         | 0/346         | 0.37        | 0/472         |
| 17  | L     | 0.22         | 0/1224        | 0.34        | 0/1673        |
| 18  | C     | 0.25         | 0/612         | 0.37        | 0/830         |
| 19  | K     | 0.20         | 0/567         | 0.27        | 0/769         |
| 20  | M     | 0.66         | 0/241         | 0.34        | 0/325         |
| 21  | O     | 0.22         | 0/760         | 0.32        | 0/1042        |
| 22  | a     | 0.12         | 0/1559        | 0.32        | 1/2116 (0.0%) |
| 22  | h     | 0.10         | 0/1568        | 0.28        | 0/2132        |
| 23  | c     | 0.13         | 0/1733        | 0.30        | 0/2363        |
| 24  | b     | 0.17         | 0/1658        | 0.34        | 0/2254        |
| 25  | d     | 0.12         | 0/1685        | 0.29        | 0/2296        |
| 25  | g     | 0.11         | 0/1548        | 0.26        | 0/2106        |
| 26  | f     | 0.13         | 0/1765        | 0.27        | 0/2399        |
| 27  | H     | 0.18         | 0/729         | 0.34        | 0/979         |
| 28  | i     | 0.10         | 0/1881        | 0.30        | 0/2561        |



| Mol | Chain | Bond lengths |                | Bond angles |                |
|-----|-------|--------------|----------------|-------------|----------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5        |
| 29  | e     | 0.11         | 0/1697         | 0.29        | 0/2311         |
| All | All   | 0.29         | 4/52337 (0.0%) | 0.36        | 9/71224 (0.0%) |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3   | 2     | 246 | ALA  | CA-C  | -5.28 | 1.46        | 1.52     |
| 9   | A     | 689 | MET  | CA-C  | -5.24 | 1.45        | 1.52     |
| 2   | 1     | 113 | THR  | CA-C  | -5.19 | 1.45        | 1.53     |
| 3   | 2     | 247 | THR  | N-CA  | -5.09 | 1.39        | 1.46     |

All (9) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 7   | 4     | 180 | PHE  | N-CA-C  | -13.97 | 96.79       | 112.72   |
| 8   | 9     | 163 | ARG  | N-CA-C  | -8.39  | 102.09      | 111.07   |
| 7   | 8     | 109 | GLY  | CA-C-N  | 6.66   | 129.49      | 123.10   |
| 7   | 8     | 109 | GLY  | C-N-CA  | 6.66   | 129.49      | 123.10   |
| 2   | 1     | 108 | GLU  | N-CA-C  | -6.25  | 104.35      | 112.23   |
| 3   | 2     | 248 | ASN  | N-CA-C  | -5.79  | 105.89      | 113.12   |
| 3   | 2     | 247 | THR  | N-CA-C  | -5.35  | 104.55      | 111.71   |
| 9   | A     | 686 | PHE  | N-CA-C  | -5.27  | 104.95      | 111.33   |
| 22  | a     | 37  | ARG  | CB-CA-C | -5.09  | 109.73      | 115.79   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 0     | 1640  | 0        | 1609     | 50      | 0            |
| 2   | 1     | 1478  | 0        | 1423     | 56      | 0            |
| 2   | 5     | 1484  | 0        | 1427     | 42      | 0            |
| 3   | 2     | 1667  | 0        | 1562     | 27      | 0            |
| 4   | 3     | 1768  | 0        | 1702     | 49      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 5   | 6     | 1797  | 0        | 1752     | 37      | 0            |
| 6   | 7     | 1758  | 0        | 1701     | 48      | 0            |
| 7   | 4     | 1569  | 0        | 1551     | 65      | 0            |
| 7   | 8     | 1574  | 0        | 1550     | 51      | 0            |
| 8   | 9     | 1453  | 0        | 1404     | 42      | 0            |
| 9   | A     | 5872  | 0        | 5715     | 162     | 0            |
| 10  | B     | 5824  | 0        | 5603     | 149     | 0            |
| 11  | D     | 1109  | 0        | 1124     | 26      | 0            |
| 12  | E     | 509   | 0        | 506      | 9       | 0            |
| 13  | F     | 1273  | 0        | 1290     | 23      | 0            |
| 14  | G     | 726   | 0        | 717      | 32      | 0            |
| 15  | I     | 262   | 0        | 279      | 9       | 0            |
| 16  | J     | 336   | 0        | 355      | 13      | 0            |
| 17  | L     | 1195  | 0        | 1187     | 25      | 0            |
| 18  | C     | 602   | 0        | 591      | 22      | 0            |
| 19  | K     | 558   | 0        | 591      | 7       | 0            |
| 20  | M     | 238   | 0        | 248      | 4       | 0            |
| 21  | O     | 728   | 0        | 699      | 16      | 0            |
| 22  | a     | 1511  | 0        | 1426     | 44      | 0            |
| 22  | h     | 1520  | 0        | 1429     | 56      | 0            |
| 23  | c     | 1680  | 0        | 1582     | 47      | 0            |
| 24  | b     | 1609  | 0        | 1531     | 51      | 0            |
| 25  | d     | 1634  | 0        | 1535     | 49      | 0            |
| 25  | g     | 1502  | 0        | 1412     | 51      | 0            |
| 26  | f     | 1727  | 0        | 1634     | 62      | 0            |
| 27  | H     | 717   | 0        | 684      | 22      | 0            |
| 28  | i     | 1834  | 0        | 1741     | 91      | 0            |
| 29  | e     | 1647  | 0        | 1559     | 48      | 0            |
| 30  | 0     | 215   | 0        | 172      | 13      | 0            |
| 30  | 1     | 291   | 0        | 262      | 19      | 0            |
| 30  | 2     | 426   | 0        | 344      | 21      | 0            |
| 30  | 3     | 179   | 0        | 166      | 9       | 0            |
| 30  | 4     | 347   | 0        | 251      | 22      | 0            |
| 30  | 5     | 304   | 0        | 228      | 16      | 0            |
| 30  | 6     | 425   | 0        | 344      | 22      | 0            |
| 30  | 7     | 334   | 0        | 280      | 20      | 0            |
| 30  | 8     | 420   | 0        | 332      | 20      | 0            |
| 30  | 9     | 193   | 0        | 132      | 4       | 0            |
| 30  | a     | 405   | 0        | 307      | 21      | 0            |
| 30  | b     | 390   | 0        | 341      | 25      | 0            |
| 30  | c     | 425   | 0        | 362      | 32      | 0            |
| 30  | d     | 415   | 0        | 331      | 24      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 30  | e     | 422   | 0        | 345      | 24      | 0            |
| 30  | f     | 430   | 0        | 364      | 24      | 0            |
| 30  | g     | 381   | 0        | 266      | 15      | 0            |
| 30  | h     | 386   | 0        | 280      | 19      | 0            |
| 30  | i     | 389   | 0        | 282      | 32      | 0            |
| 31  | 0     | 478   | 0        | 426      | 26      | 0            |
| 31  | 1     | 434   | 0        | 386      | 18      | 0            |
| 31  | 2     | 389   | 0        | 356      | 9       | 0            |
| 31  | 3     | 603   | 0        | 554      | 23      | 0            |
| 31  | 4     | 371   | 0        | 324      | 13      | 0            |
| 31  | 5     | 409   | 0        | 340      | 13      | 0            |
| 31  | 6     | 527   | 0        | 456      | 15      | 0            |
| 31  | 7     | 569   | 0        | 496      | 26      | 0            |
| 31  | 8     | 364   | 0        | 314      | 6       | 0            |
| 31  | 9     | 496   | 0        | 458      | 19      | 0            |
| 31  | A     | 2599  | 0        | 2656     | 135     | 0            |
| 31  | B     | 2357  | 0        | 2336     | 146     | 0            |
| 31  | F     | 45    | 0        | 33       | 3       | 0            |
| 31  | G     | 141   | 0        | 105      | 2       | 0            |
| 31  | H     | 200   | 0        | 160      | 4       | 0            |
| 31  | J     | 42    | 0        | 31       | 2       | 0            |
| 31  | K     | 209   | 0        | 176      | 9       | 0            |
| 31  | L     | 260   | 0        | 221      | 11      | 0            |
| 31  | M     | 46    | 0        | 33       | 0       | 0            |
| 31  | O     | 168   | 0        | 108      | 7       | 0            |
| 31  | a     | 315   | 0        | 266      | 10      | 0            |
| 31  | b     | 320   | 0        | 276      | 11      | 0            |
| 31  | c     | 303   | 0        | 244      | 9       | 0            |
| 31  | d     | 306   | 0        | 250      | 11      | 0            |
| 31  | e     | 317   | 0        | 270      | 13      | 0            |
| 31  | f     | 315   | 0        | 266      | 12      | 0            |
| 31  | g     | 280   | 0        | 208      | 19      | 0            |
| 31  | h     | 273   | 0        | 200      | 11      | 0            |
| 31  | i     | 292   | 0        | 228      | 38      | 0            |
| 32  | 0     | 40    | 0        | 0        | 0       | 0            |
| 32  | 1     | 40    | 0        | 0        | 0       | 0            |
| 32  | 2     | 40    | 0        | 0        | 0       | 0            |
| 32  | 3     | 80    | 0        | 0        | 1       | 0            |
| 32  | 4     | 40    | 0        | 0        | 1       | 0            |
| 32  | 6     | 40    | 0        | 0        | 0       | 0            |
| 32  | 7     | 120   | 0        | 0        | 1       | 0            |
| 32  | 8     | 80    | 0        | 0        | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 32  | 9     | 40    | 0        | 0        | 0       | 0            |
| 32  | A     | 240   | 0        | 0        | 1       | 0            |
| 32  | B     | 320   | 0        | 0        | 2       | 0            |
| 32  | F     | 40    | 0        | 0        | 0       | 0            |
| 32  | G     | 40    | 0        | 0        | 0       | 0            |
| 32  | I     | 40    | 0        | 0        | 0       | 0            |
| 32  | J     | 80    | 0        | 0        | 1       | 0            |
| 32  | K     | 40    | 0        | 0        | 0       | 0            |
| 32  | L     | 120   | 0        | 0        | 1       | 0            |
| 32  | M     | 40    | 0        | 0        | 0       | 0            |
| 32  | O     | 40    | 0        | 0        | 0       | 0            |
| 33  | 0     | 104   | 0        | 0        | 1       | 0            |
| 33  | 1     | 104   | 0        | 0        | 1       | 0            |
| 33  | 2     | 101   | 0        | 0        | 3       | 0            |
| 33  | 3     | 51    | 0        | 0        | 1       | 0            |
| 33  | 4     | 101   | 0        | 0        | 3       | 0            |
| 33  | 5     | 103   | 0        | 0        | 4       | 0            |
| 33  | 6     | 103   | 0        | 0        | 1       | 0            |
| 33  | 7     | 51    | 0        | 0        | 2       | 0            |
| 33  | 8     | 103   | 0        | 0        | 3       | 0            |
| 33  | 9     | 104   | 0        | 0        | 3       | 0            |
| 33  | O     | 52    | 0        | 0        | 1       | 0            |
| 33  | a     | 47    | 0        | 0        | 2       | 0            |
| 33  | b     | 52    | 0        | 0        | 3       | 0            |
| 33  | c     | 52    | 0        | 0        | 1       | 0            |
| 33  | d     | 49    | 0        | 0        | 1       | 0            |
| 33  | e     | 52    | 0        | 0        | 0       | 0            |
| 33  | f     | 49    | 0        | 0        | 0       | 0            |
| 33  | g     | 52    | 0        | 0        | 0       | 0            |
| 33  | h     | 52    | 0        | 0        | 1       | 0            |
| 33  | i     | 50    | 0        | 0        | 2       | 0            |
| 34  | 0     | 49    | 0        | 74       | 4       | 0            |
| 34  | 1     | 49    | 0        | 74       | 6       | 0            |
| 34  | 2     | 32    | 0        | 34       | 3       | 0            |
| 34  | 3     | 73    | 0        | 84       | 4       | 0            |
| 34  | 4     | 32    | 0        | 34       | 0       | 0            |
| 34  | 5     | 37    | 0        | 44       | 1       | 0            |
| 34  | 6     | 68    | 0        | 76       | 5       | 0            |
| 34  | 7     | 107   | 0        | 127      | 4       | 0            |
| 34  | 8     | 44    | 0        | 58       | 0       | 0            |
| 34  | 9     | 47    | 0        | 63       | 5       | 0            |
| 34  | A     | 118   | 0        | 152      | 8       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 34  | B     | 66    | 0        | 75       | 4       | 0            |
| 34  | G     | 38    | 0        | 46       | 2       | 0            |
| 34  | H     | 31    | 0        | 32       | 0       | 0            |
| 34  | K     | 43    | 0        | 60       | 4       | 0            |
| 34  | M     | 46    | 0        | 65       | 4       | 0            |
| 34  | a     | 43    | 0        | 56       | 4       | 0            |
| 34  | b     | 41    | 0        | 52       | 2       | 0            |
| 34  | c     | 40    | 0        | 50       | 5       | 0            |
| 34  | d     | 36    | 0        | 42       | 5       | 0            |
| 34  | e     | 43    | 0        | 56       | 5       | 0            |
| 34  | f     | 40    | 0        | 50       | 5       | 0            |
| 34  | g     | 30    | 0        | 30       | 3       | 0            |
| 34  | h     | 39    | 0        | 48       | 4       | 0            |
| 34  | i     | 30    | 0        | 30       | 4       | 0            |
| 35  | 0     | 36    | 0        | 41       | 2       | 0            |
| 36  | 2     | 36    | 0        | 42       | 0       | 0            |
| 36  | 3     | 36    | 0        | 42       | 1       | 0            |
| 36  | 9     | 55    | 0        | 86       | 4       | 0            |
| 36  | A     | 36    | 0        | 42       | 3       | 0            |
| 36  | B     | 42    | 0        | 54       | 1       | 0            |
| 36  | J     | 75    | 0        | 93       | 3       | 0            |
| 36  | L     | 68    | 0        | 76       | 3       | 0            |
| 36  | O     | 39    | 0        | 48       | 1       | 0            |
| 37  | 3     | 44    | 0        | 0        | 0       | 0            |
| 37  | 7     | 44    | 0        | 0        | 0       | 0            |
| 37  | a     | 88    | 0        | 0        | 0       | 0            |
| 37  | b     | 88    | 0        | 0        | 2       | 0            |
| 37  | c     | 88    | 0        | 0        | 1       | 0            |
| 37  | d     | 88    | 0        | 0        | 0       | 0            |
| 37  | e     | 88    | 0        | 0        | 0       | 0            |
| 37  | f     | 88    | 0        | 0        | 0       | 0            |
| 37  | g     | 88    | 0        | 0        | 0       | 0            |
| 37  | h     | 88    | 0        | 0        | 2       | 0            |
| 37  | i     | 88    | 0        | 0        | 4       | 0            |
| 38  | A     | 33    | 0        | 46       | 5       | 0            |
| 38  | B     | 33    | 0        | 46       | 1       | 0            |
| 39  | A     | 65    | 0        | 72       | 7       | 0            |
| 40  | B     | 8     | 0        | 0        | 1       | 0            |
| 40  | C     | 16    | 0        | 0        | 0       | 0            |
| 41  | B     | 56    | 0        | 70       | 3       | 0            |
| 42  | a     | 44    | 0        | 56       | 7       | 0            |
| 42  | b     | 44    | 0        | 56       | 3       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 42  | c     | 44    | 0        | 56       | 5       | 0            |
| 42  | d     | 44    | 0        | 56       | 10      | 0            |
| 42  | e     | 44    | 0        | 56       | 3       | 0            |
| 42  | f     | 44    | 0        | 56       | 26      | 0            |
| 42  | g     | 44    | 0        | 56       | 8       | 0            |
| 42  | h     | 44    | 0        | 56       | 15      | 0            |
| 42  | i     | 44    | 0        | 56       | 35      | 0            |
| All | All   | 77090 | 0        | 69459    | 1948    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (1948) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:i:179:VAL:HG11 | 30:i:606:CHL:HED2 | 1.28                     | 1.16              |
| 42:i:523:NEX:H362 | 31:i:604:CLA:C4B  | 1.79                     | 1.11              |
| 42:a:523:NEX:H241 | 31:a:604:CLA:H2   | 1.36                     | 1.05              |
| 1:0:147:MET:HB3   | 1:0:148:PRO:HD2   | 1.42                     | 1.00              |
| 2:5:160:PRO:HD2   | 33:5:501:0UR:C30  | 1.90                     | 1.00              |
| 42:i:523:NEX:H362 | 31:i:604:CLA:C3B  | 1.94                     | 0.97              |
| 42:i:523:NEX:H383 | 31:i:604:CLA:C1B  | 1.96                     | 0.95              |
| 42:i:523:NEX:C36  | 31:i:604:CLA:CHC  | 2.44                     | 0.95              |
| 26:f:193:LEU:CD2  | 42:h:523:NEX:H172 | 1.99                     | 0.93              |
| 31:A:805:CLA:H11  | 31:A:806:CLA:HBB1 | 1.51                     | 0.92              |
| 39:A:857:CL0:H15  | 31:B:803:CLA:HED1 | 1.52                     | 0.92              |
| 25:d:124:MET:HE1  | 42:d:523:NEX:H30  | 1.53                     | 0.90              |
| 26:f:194:ILE:HD11 | 42:f:523:NEX:C34  | 2.01                     | 0.89              |
| 42:i:523:NEX:H362 | 31:i:604:CLA:CHC  | 2.03                     | 0.89              |
| 42:d:523:NEX:H241 | 31:d:604:CLA:H2   | 1.56                     | 0.87              |
| 42:a:523:NEX:H241 | 31:a:604:CLA:C2   | 2.05                     | 0.86              |
| 9:A:29:THR:HG21   | 9:A:183:TRP:HE1   | 1.39                     | 0.85              |
| 8:9:145:MET:HB3   | 8:9:153:PRO:HD3   | 1.58                     | 0.83              |
| 26:f:193:LEU:HD21 | 42:h:523:NEX:H172 | 1.61                     | 0.82              |
| 25:d:15:TYR:CE2   | 42:h:523:NEX:O3   | 2.33                     | 0.82              |
| 2:1:78:GLY:HA3    | 2:1:179:ALA:HB1   | 1.61                     | 0.81              |
| 2:1:174:LYS:HD3   | 31:1:311:CLA:HBA1 | 1.64                     | 0.80              |
| 22:a:86:ALA:HB1   | 22:a:200:GLY:HA3  | 1.64                     | 0.79              |
| 26:f:193:LEU:HD23 | 42:h:523:NEX:H172 | 1.65                     | 0.78              |
| 42:i:523:NEX:H363 | 31:i:604:CLA:CHC  | 2.11                     | 0.78              |
| 31:B:803:CLA:HBB  | 31:B:805:CLA:H202 | 1.66                     | 0.77              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:g:128:GLU:HG2  | 25:g:131:ARG:HE   | 1.50                     | 0.76              |
| 31:B:824:CLA:H52  | 31:B:825:CLA:H142 | 1.67                     | 0.76              |
| 29:e:211:VAL:HG21 | 31:e:613:CLA:HAC2 | 1.67                     | 0.75              |
| 28:i:184:MET:HE1  | 42:i:523:NEX:H30  | 1.68                     | 0.75              |
| 7:8:146:ARG:O     | 7:8:158:ASN:ND2   | 2.20                     | 0.75              |
| 17:L:35:ASN:HB3   | 31:L:202:CLA:HAC1 | 1.69                     | 0.75              |
| 8:9:152:PHE:O     | 8:9:153:PRO:C     | 2.29                     | 0.75              |
| 28:i:159:LEU:HD13 | 30:i:606:CHL:CMD  | 2.18                     | 0.74              |
| 30:9:306:CHL:HHC  | 30:9:306:CHL:HBB1 | 1.67                     | 0.74              |
| 28:i:159:LEU:HD13 | 30:i:606:CHL:HMD2 | 1.70                     | 0.74              |
| 7:4:146:ARG:NH1   | 30:4:319:CHL:OBD  | 2.20                     | 0.74              |
| 26:f:266:TRP:HE1  | 30:f:614:CHL:HMC  | 1.52                     | 0.74              |
| 9:A:65:ASP:OD2    | 9:A:355:HIS:NE2   | 2.20                     | 0.73              |
| 31:A:809:CLA:HAB  | 31:B:833:CLA:HMD2 | 1.69                     | 0.73              |
| 31:A:832:CLA:HBB2 | 17:L:67:LEU:HD13  | 1.69                     | 0.73              |
| 30:2:319:CHL:HBB1 | 30:2:319:CHL:HHC  | 1.70                     | 0.73              |
| 1:0:147:MET:O     | 1:0:148:PRO:C     | 2.31                     | 0.73              |
| 30:e:602:CHL:HHC  | 30:e:602:CHL:HBB1 | 1.71                     | 0.73              |
| 5:6:115:ARG:NH2   | 30:6:308:CHL:O1D  | 2.21                     | 0.73              |
| 30:a:609:CHL:H2A  | 24:b:69:THR:HG21  | 1.70                     | 0.73              |
| 23:c:43:TRP:HE1   | 30:c:601:CHL:HAA1 | 1.52                     | 0.72              |
| 2:1:204:TRP:HE1   | 30:1:313:CHL:HMC  | 1.55                     | 0.72              |
| 2:5:78:GLY:HA3    | 2:5:179:ALA:HB1   | 1.71                     | 0.72              |
| 6:7:85:SER:HB2    | 6:7:198:GLY:HA3   | 1.70                     | 0.72              |
| 7:8:88:ARG:NH1    | 30:8:307:CHL:OBD  | 2.20                     | 0.72              |
| 9:A:252:ARG:NH1   | 9:A:262:PHE:O     | 2.22                     | 0.72              |
| 30:4:319:CHL:HHC  | 30:4:319:CHL:HBB1 | 1.70                     | 0.72              |
| 26:f:194:ILE:CD1  | 42:f:523:NEX:C34  | 2.67                     | 0.72              |
| 9:A:577:ARG:NH1   | 34:A:844:LHG:O10  | 2.23                     | 0.72              |
| 25:d:201:HIS:HD1  | 25:d:205:PRO:HG3  | 1.53                     | 0.72              |
| 28:i:184:MET:HE1  | 42:i:523:NEX:H32  | 1.71                     | 0.72              |
| 30:7:306:CHL:HBB1 | 30:7:306:CHL:HHC  | 1.72                     | 0.71              |
| 30:8:305:CHL:HHC  | 30:8:305:CHL:HBB1 | 1.72                     | 0.71              |
| 25:g:57:ALA:HB1   | 25:g:173:GLY:HA3  | 1.72                     | 0.71              |
| 9:A:206:HIS:HB3   | 31:A:825:CLA:HED2 | 1.71                     | 0.71              |
| 31:A:804:CLA:H61  | 31:A:809:CLA:H202 | 1.71                     | 0.71              |
| 25:d:51:GLU:HA    | 25:d:144:LEU:HD21 | 1.71                     | 0.71              |
| 5:6:114:ARG:NH1   | 30:8:301:CHL:OBD  | 2.22                     | 0.71              |
| 2:1:113:THR:HG21  | 30:1:305:CHL:HMD3 | 1.71                     | 0.71              |
| 10:B:415:LYS:HZ3  | 13:F:238:VAL:HG21 | 1.55                     | 0.71              |
| 31:d:603:CLA:H12  | 29:e:65:LEU:HD11  | 1.73                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 34:1:601:LHG:H122 | 30:4:319:CHL:H2   | 1.73                     | 0.71              |
| 31:A:825:CLA:HBA1 | 31:A:829:CLA:H203 | 1.73                     | 0.71              |
| 23:c:36:TYR:HE2   | 23:c:195:SER:HB3  | 1.54                     | 0.71              |
| 24:b:90:ALA:HB1   | 24:b:203:GLY:HA3  | 1.72                     | 0.71              |
| 22:h:163:GLY:HA3  | 30:h:608:CHL:HMC  | 1.71                     | 0.71              |
| 5:6:101:VAL:HG22  | 30:6:306:CHL:HBC1 | 1.73                     | 0.70              |
| 30:c:601:CHL:H52  | 30:b:609:CHL:HBB1 | 1.71                     | 0.70              |
| 28:i:184:MET:HE2  | 30:i:606:CHL:HMA1 | 1.73                     | 0.70              |
| 18:C:15:THR:OG1   | 18:C:19:ARG:NH1   | 2.24                     | 0.70              |
| 30:0:301:CHL:HBB2 | 30:0:302:CHL:HHD  | 1.71                     | 0.70              |
| 8:9:152:PHE:CB    | 8:9:153:PRO:HD2   | 2.21                     | 0.70              |
| 9:A:601:LEU:HD21  | 31:A:830:CLA:HBC1 | 1.71                     | 0.70              |
| 13:F:202:ASP:HA   | 36:J:102:LMG:HC61 | 1.73                     | 0.70              |
| 7:8:149:GLN:HB2   | 7:8:158:ASN:HD21  | 1.57                     | 0.70              |
| 26:f:197:TYR:OH   | 42:f:523:NEX:C19  | 2.40                     | 0.70              |
| 17:L:99:ILE:HD11  | 34:M:104:LHG:H111 | 1.74                     | 0.69              |
| 26:f:124:ALA:HB1  | 26:f:241:GLY:HA3  | 1.71                     | 0.69              |
| 8:9:170:LYS:NZ    | 34:9:601:LHG:O4   | 2.21                     | 0.69              |
| 30:6:301:CHL:O1A  | 6:7:137:HIS:ND1   | 2.25                     | 0.69              |
| 5:6:203:THR:HG22  | 5:6:205:PHE:H     | 1.56                     | 0.69              |
| 7:4:43:ILE:HG22   | 7:4:45:LEU:H      | 1.57                     | 0.69              |
| 28:i:69:ARG:H     | 28:i:69:ARG:HD3   | 1.57                     | 0.69              |
| 11:D:167:HIS:HB3  | 11:D:168:PRO:HD3  | 1.75                     | 0.69              |
| 25:d:57:ALA:HB1   | 25:d:173:GLY:HA3  | 1.72                     | 0.69              |
| 31:8:304:CLA:H192 | 30:8:307:CHL:HAA2 | 1.75                     | 0.69              |
| 29:e:125:LEU:HD21 | 31:e:604:CLA:HAA2 | 1.75                     | 0.69              |
| 42:d:523:NEX:H31  | 30:d:606:CHL:HBA2 | 1.75                     | 0.69              |
| 7:4:49:ASP:N      | 7:4:49:ASP:OD1    | 2.26                     | 0.69              |
| 28:i:131:GLU:HA   | 28:i:144:ALA:HB1  | 1.75                     | 0.68              |
| 30:4:306:CHL:HBB1 | 30:4:306:CHL:HHC  | 1.74                     | 0.68              |
| 34:0:601:LHG:HC91 | 34:0:601:LHG:H281 | 1.74                     | 0.68              |
| 7:4:226:TRP:HZ3   | 30:4:313:CHL:HMC  | 1.58                     | 0.68              |
| 30:8:301:CHL:HHC  | 30:8:301:CHL:HBB1 | 1.74                     | 0.68              |
| 9:A:511:THR:HG21  | 31:A:827:CLA:HAB  | 1.74                     | 0.68              |
| 14:G:11:SER:HB3   | 14:G:81:VAL:HG13  | 1.74                     | 0.68              |
| 9:A:13:ARG:HE     | 19:K:43:LYS:HE3   | 1.58                     | 0.68              |
| 7:4:226:TRP:CZ3   | 30:4:313:CHL:HMC  | 2.29                     | 0.68              |
| 26:f:193:LEU:HB2  | 42:f:523:NEX:C20  | 2.24                     | 0.68              |
| 2:1:30:ALA:N      | 2:1:47:GLU:O      | 2.27                     | 0.68              |
| 31:5:303:CLA:HBC1 | 31:5:308:CLA:HAC1 | 1.75                     | 0.68              |
| 10:B:120:VAL:HG21 | 31:B:811:CLA:HED1 | 1.74                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:K:104:CLA:HAC2 | 30:c:601:CHL:HMC  | 1.75                     | 0.68              |
| 9:A:543:ILE:HD13  | 39:A:857:CL0:H59  | 1.75                     | 0.67              |
| 10:B:290:MET:HB2  | 31:B:822:CLA:HBC3 | 1.75                     | 0.67              |
| 14:G:55:VAL:O     | 14:G:59:LYS:NZ    | 2.27                     | 0.67              |
| 26:f:197:TYR:OH   | 42:f:523:NEX:H192 | 1.94                     | 0.67              |
| 42:i:523:NEX:H222 | 31:i:604:CLA:C4B  | 2.24                     | 0.67              |
| 13:F:137:LEU:HD21 | 16:J:38:ILE:HG21  | 1.77                     | 0.67              |
| 28:i:259:TRP:HE1  | 30:i:614:CHL:HMC  | 1.58                     | 0.67              |
| 25:g:8:ARG:NH2    | 25:g:24:LEU:O     | 2.28                     | 0.67              |
| 28:i:159:LEU:CD1  | 30:i:606:CHL:HMD3 | 2.25                     | 0.67              |
| 42:i:523:NEX:C36  | 31:i:604:CLA:C4B  | 2.62                     | 0.67              |
| 25:d:190:THR:HG22 | 25:d:192:LYS:H    | 1.59                     | 0.67              |
| 25:d:15:TYR:HE2   | 42:h:523:NEX:O3   | 1.74                     | 0.67              |
| 7:8:161:PRO:HG2   | 7:8:166:LYS:HG3   | 1.76                     | 0.67              |
| 5:6:208:ALA:HB2   | 5:6:218:PRO:HD3   | 1.77                     | 0.67              |
| 7:4:182:PRO:HD2   | 33:4:501:0UR:C30  | 2.25                     | 0.67              |
| 2:1:88:MET:HB3    | 2:1:99:TRP:HB3    | 1.77                     | 0.66              |
| 9:A:77:LYS:NZ     | 31:A:811:CLA:OBD  | 2.28                     | 0.66              |
| 23:c:242:ILE:HG22 | 30:c:614:CHL:HED1 | 1.77                     | 0.66              |
| 26:f:193:LEU:HB2  | 42:f:523:NEX:H203 | 1.77                     | 0.66              |
| 2:5:113:THR:OG1   | 2:5:119:MET:SD    | 2.53                     | 0.66              |
| 29:e:197:LYS:NZ   | 34:e:630:LHG:O4   | 2.29                     | 0.66              |
| 3:2:168:GLU:OE2   | 3:2:182:ARG:NH2   | 2.28                     | 0.66              |
| 31:A:819:CLA:H8   | 31:A:819:CLA:HAB  | 1.76                     | 0.66              |
| 22:h:198:LYS:NZ   | 34:h:630:LHG:O4   | 2.29                     | 0.66              |
| 7:4:239:TRP:H     | 7:4:243:LEU:HD11  | 1.61                     | 0.66              |
| 5:6:55:ARG:NH1    | 5:6:58:GLU:OE1    | 2.29                     | 0.66              |
| 10:B:230:TRP:O    | 31:B:817:CLA:H3A  | 1.95                     | 0.66              |
| 30:b:608:CHL:HBA1 | 30:b:608:CHL:H122 | 1.77                     | 0.66              |
| 2:5:92:GLU:HB2    | 2:5:98:ASN:HA     | 1.77                     | 0.66              |
| 9:A:209:GLY:O     | 9:A:213:LEU:HB2   | 1.95                     | 0.65              |
| 34:i:630:LHG:HC91 | 34:i:630:LHG:H261 | 1.78                     | 0.65              |
| 7:4:84:LEU:HD12   | 7:4:176:PRO:HG2   | 1.77                     | 0.65              |
| 30:0:305:CHL:HHC  | 30:0:305:CHL:HBB1 | 1.77                     | 0.65              |
| 24:b:228:TRP:HE1  | 30:b:614:CHL:HMC  | 1.60                     | 0.65              |
| 34:d:630:LHG:H292 | 34:d:630:LHG:H101 | 1.77                     | 0.65              |
| 1:0:33:ARG:NH2    | 1:0:53:ASP:O      | 2.30                     | 0.65              |
| 6:7:86:ARG:NH1    | 30:7:307:CHL:OBD  | 2.24                     | 0.65              |
| 24:b:80:GLU:OE1   | 24:b:83:ARG:NH2   | 2.29                     | 0.65              |
| 28:i:272:PHE:O    | 28:i:274:TYR:N    | 2.30                     | 0.65              |
| 9:A:441:ALA:O     | 9:A:445:HIS:ND1   | 2.26                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:a:606:CHL:HHC  | 30:a:606:CHL:HBB1 | 1.79                     | 0.65              |
| 9:A:379:MET:HE3   | 31:A:818:CLA:HBD  | 1.79                     | 0.65              |
| 13:F:231:GLU:HG3  | 13:F:232:LYS:H    | 1.62                     | 0.65              |
| 2:1:216:PHE:HB3   | 31:1:312:CLA:H12  | 1.79                     | 0.65              |
| 31:g:603:CLA:H12  | 22:h:68:LEU:HD11  | 1.78                     | 0.65              |
| 1:0:147:MET:CB    | 1:0:148:PRO:HD2   | 2.23                     | 0.64              |
| 30:5:301:CHL:HHC  | 30:5:301:CHL:HBB1 | 1.77                     | 0.64              |
| 26:f:159:GLN:HB2  | 26:f:166:ILE:HG22 | 1.79                     | 0.64              |
| 22:h:86:ALA:HB1   | 22:h:200:GLY:HA3  | 1.78                     | 0.64              |
| 1:0:147:MET:HB3   | 1:0:148:PRO:CD    | 2.22                     | 0.64              |
| 22:h:157:GLU:OE1  | 22:h:160:ARG:NH2  | 2.26                     | 0.64              |
| 8:9:160:THR:HA    | 31:9:309:CLA:HAA2 | 1.78                     | 0.64              |
| 28:i:159:LEU:CD1  | 30:i:606:CHL:CMD  | 2.75                     | 0.64              |
| 28:i:184:MET:CE   | 42:i:523:NEX:H32  | 2.26                     | 0.64              |
| 2:1:177:LYS:NZ    | 34:1:601:LHG:O4   | 2.31                     | 0.64              |
| 30:2:306:CHL:HHC  | 30:2:306:CHL:HBB1 | 1.78                     | 0.64              |
| 5:6:62:GLY:HA3    | 5:6:167:ALA:HB1   | 1.79                     | 0.64              |
| 31:8:304:CLA:HED2 | 31:8:304:CLA:H2A  | 1.78                     | 0.64              |
| 26:f:125:ARG:NH1  | 30:f:608:CHL:OBD  | 2.29                     | 0.64              |
| 2:1:70:MET:HA     | 2:1:73:CYS:SG     | 2.38                     | 0.64              |
| 30:8:307:CHL:HHC  | 30:8:307:CHL:HBB1 | 1.80                     | 0.64              |
| 29:e:162:PRO:HG2  | 42:e:523:NEX:H192 | 1.80                     | 0.64              |
| 4:3:124:SER:HB2   | 4:3:134:GLY:HA3   | 1.80                     | 0.64              |
| 1:0:54:TYR:OH     | 1:0:165:LYS:NZ    | 2.31                     | 0.64              |
| 35:0:603:SQD:H45  | 20:M:24:ARG:HD2   | 1.79                     | 0.64              |
| 31:5:309:CLA:HAB  | 33:5:501:OUR:C13  | 2.28                     | 0.64              |
| 6:7:97:GLY:HA3    | 31:7:304:CLA:HBC3 | 1.78                     | 0.64              |
| 31:A:822:CLA:HAA2 | 19:K:34:ALA:HB3   | 1.79                     | 0.64              |
| 42:i:523:NEX:H222 | 31:i:604:CLA:NB   | 2.13                     | 0.64              |
| 24:b:160:GLU:OE1  | 24:b:163:ARG:NH1  | 2.31                     | 0.63              |
| 42:i:523:NEX:H383 | 31:i:604:CLA:CHB  | 2.28                     | 0.63              |
| 34:d:630:LHG:H271 | 34:d:630:LHG:HC62 | 1.80                     | 0.63              |
| 9:A:272:LEU:HD11  | 19:K:72:ILE:HG23  | 1.80                     | 0.63              |
| 9:A:375:HIS:ND1   | 31:A:818:CLA:OBD  | 2.27                     | 0.63              |
| 11:D:134:LYS:NZ   | 18:C:47:ASP:OD2   | 2.30                     | 0.63              |
| 28:i:117:ALA:HB1  | 28:i:234:GLY:HA3  | 1.81                     | 0.63              |
| 6:7:140:GLU:OE1   | 6:7:143:ARG:NH2   | 2.28                     | 0.63              |
| 9:A:671:SER:HB2   | 10:B:445:ALA:HB1  | 1.81                     | 0.63              |
| 7:4:198:VAL:O     | 7:4:202:ARG:HG2   | 1.98                     | 0.63              |
| 2:5:174:LYS:O     | 2:5:178:ASN:ND2   | 2.28                     | 0.63              |
| 9:A:31:PHE:O      | 16:J:3:ASN:HB3    | 1.99                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:B:130:ARG:NH2  | 10:B:245:SER:OG   | 2.31                     | 0.63              |
| 25:d:168:LYS:NZ   | 31:d:612:CLA:O1A  | 2.31                     | 0.63              |
| 25:g:99:LEU:HD11  | 31:g:604:CLA:HAA2 | 1.80                     | 0.63              |
| 29:e:163:LEU:HB2  | 30:e:608:CHL:HBB1 | 1.81                     | 0.63              |
| 16:J:14:ILE:HD12  | 16:J:17:ILE:HD11  | 1.81                     | 0.63              |
| 31:O:313:CLA:HBB2 | 8:9:120:ALA:HB1   | 1.81                     | 0.63              |
| 2:1:129:VAL:HG13  | 14:G:14:LEU:HD22  | 1.80                     | 0.63              |
| 3:2:90:ARG:NH1    | 30:2:307:CHL:OBD  | 2.28                     | 0.63              |
| 5:6:192:TRP:HE1   | 30:6:313:CHL:HMC  | 1.63                     | 0.63              |
| 7:8:147:ARG:NH2   | 30:8:308:CHL:O1D  | 2.32                     | 0.62              |
| 25:g:74:GLU:HG3   | 25:g:75:LYS:HG3   | 1.81                     | 0.62              |
| 42:g:523:NEX:O24  | 30:g:606:CHL:HAA1 | 1.98                     | 0.62              |
| 28:i:179:VAL:HG11 | 30:i:606:CHL:CED  | 2.18                     | 0.62              |
| 28:i:64:TRP:HZ2   | 31:i:611:CLA:H2A  | 1.62                     | 0.62              |
| 10:B:627:ASN:OD1  | 10:B:732:LYS:NZ   | 2.32                     | 0.62              |
| 5:6:63:ARG:NH1    | 30:6:307:CHL:OBD  | 2.27                     | 0.62              |
| 28:i:183:LEU:HD11 | 30:i:606:CHL:H43  | 1.82                     | 0.62              |
| 7:8:220:LYS:NZ    | 7:8:228:SER:OG    | 2.32                     | 0.62              |
| 10:B:690:LEU:HD11 | 17:L:38:ALA:HB1   | 1.82                     | 0.62              |
| 25:d:54:LEU:HD23  | 25:d:144:LEU:HD22 | 1.82                     | 0.62              |
| 10:B:125:TYR:O    | 10:B:130:ARG:NH1  | 2.32                     | 0.62              |
| 42:i:523:NEX:H362 | 31:i:604:CLA:CAB  | 2.30                     | 0.62              |
| 29:e:83:ALA:HB1   | 29:e:199:GLY:HA3  | 1.82                     | 0.62              |
| 1:0:93:ASN:ND2    | 1:0:99:ASN:OD1    | 2.32                     | 0.62              |
| 26:f:193:LEU:CD1  | 42:f:523:NEX:H203 | 2.30                     | 0.62              |
| 25:g:54:LEU:HD23  | 25:g:144:LEU:HD22 | 1.81                     | 0.62              |
| 37:i:521:OIE:C38  | 30:i:606:CHL:OMC  | 2.47                     | 0.62              |
| 2:1:124:ILE:HG21  | 14:G:91:ASN:HA    | 1.80                     | 0.62              |
| 6:7:148:LYS:NZ    | 31:7:317:CLA:O1D  | 2.30                     | 0.62              |
| 3:2:139:LEU:HB3   | 30:2:319:CHL:H43  | 1.81                     | 0.62              |
| 30:7:307:CHL:HBB1 | 30:7:307:CHL:HHC  | 1.81                     | 0.62              |
| 28:i:183:LEU:O    | 42:i:523:NEX:H201 | 2.00                     | 0.62              |
| 5:6:56:GLU:HG2    | 5:6:119:LEU:HD22  | 1.81                     | 0.61              |
| 6:7:57:ALA:O      | 6:7:78:ARG:NH2    | 2.33                     | 0.61              |
| 26:f:266:TRP:NE1  | 30:f:614:CHL:HMC  | 2.15                     | 0.61              |
| 2:1:165:LYS:HG3   | 2:1:167:ASN:H     | 1.66                     | 0.61              |
| 31:A:839:CLA:HAB  | 31:A:839:CLA:H122 | 1.82                     | 0.61              |
| 11:D:87:THR:HA    | 17:L:17:GLY:O     | 2.00                     | 0.61              |
| 31:6:311:CLA:HHC  | 31:6:311:CLA:HBB1 | 1.81                     | 0.61              |
| 9:A:479:ASP:O     | 9:A:483:GLN:NE2   | 2.33                     | 0.61              |
| 5:6:162:LYS:O     | 5:6:166:ASN:ND2   | 2.25                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 34:9:601:LHG:H311 | 34:9:601:LHG:H122 | 1.82                     | 0.61              |
| 26:f:193:LEU:HD21 | 42:h:523:NEX:H163 | 1.82                     | 0.61              |
| 42:h:523:NEX:C31  | 30:h:606:CHL:HBA2 | 2.30                     | 0.61              |
| 7:8:171:ASN:ND2   | 7:8:176:PRO:O     | 2.30                     | 0.61              |
| 10:B:50:HIS:HE1   | 31:B:808:CLA:H171 | 1.66                     | 0.61              |
| 42:i:523:NEX:H241 | 31:i:604:CLA:O2A  | 1.99                     | 0.61              |
| 9:A:446:LEU:HD13  | 9:A:553:LEU:HA    | 1.83                     | 0.61              |
| 17:L:55:THR:HG21  | 31:L:203:CLA:HED2 | 1.82                     | 0.61              |
| 22:h:87:ARG:NH1   | 30:h:608:CHL:OBD  | 2.34                     | 0.61              |
| 26:f:194:ILE:HD11 | 42:f:523:NEX:C35  | 2.30                     | 0.61              |
| 5:6:244:PRO:HB3   | 31:6:317:CLA:HAB  | 1.82                     | 0.61              |
| 42:h:523:NEX:H392 | 30:h:606:CHL:HBB  | 1.83                     | 0.61              |
| 8:9:200:HIS:CG    | 31:9:312:CLA:HAA2 | 2.36                     | 0.61              |
| 10:B:3:THR:HB     | 15:I:34:ALA:HA    | 1.82                     | 0.61              |
| 28:i:183:LEU:CD1  | 30:i:606:CHL:H43  | 2.31                     | 0.60              |
| 2:1:37:PRO:HB3    | 7:4:162:ILE:HG13  | 1.82                     | 0.60              |
| 4:3:83:LEU:HD12   | 30:3:302:CHL:H11  | 1.83                     | 0.60              |
| 9:A:457:SER:HB2   | 9:A:543:ILE:HG13  | 1.81                     | 0.60              |
| 31:B:809:CLA:H2   | 31:B:809:CLA:HED3 | 1.83                     | 0.60              |
| 31:B:817:CLA:HBD  | 31:B:817:CLA:HBA1 | 1.83                     | 0.60              |
| 14:G:11:SER:HA    | 14:G:14:LEU:HD23  | 1.82                     | 0.60              |
| 42:f:523:NEX:H383 | 31:f:604:CLA:C1B  | 2.31                     | 0.60              |
| 2:1:207:HIS:CG    | 31:1:312:CLA:HAA2 | 2.36                     | 0.60              |
| 22:h:195:LYS:O    | 22:h:199:ASN:ND2  | 2.28                     | 0.60              |
| 30:e:602:CHL:H41  | 31:e:603:CLA:HBA2 | 1.82                     | 0.60              |
| 7:4:53:TRP:HZ2    | 7:4:68:LYS:HG3    | 1.66                     | 0.60              |
| 42:i:523:NEX:C22  | 31:i:604:CLA:C1C  | 2.79                     | 0.60              |
| 42:i:523:NEX:H221 | 31:i:604:CLA:C1C  | 2.31                     | 0.60              |
| 9:A:287:LEU:HD21  | 9:A:380:PRO:HD2   | 1.84                     | 0.60              |
| 9:A:661:GLN:OE1   | 9:A:751:ARG:NH1   | 2.34                     | 0.60              |
| 10:B:207:VAL:O    | 10:B:208:ARG:NH1  | 2.34                     | 0.60              |
| 7:4:83:GLU:OE2    | 7:4:202:ARG:NE    | 2.34                     | 0.60              |
| 7:4:156:SER:HB3   | 7:4:158:ASN:H     | 1.67                     | 0.60              |
| 30:5:301:CHL:H42  | 7:8:138:LEU:HD12  | 1.83                     | 0.60              |
| 28:i:93:GLY:N     | 30:i:602:CHL:OBD  | 2.34                     | 0.60              |
| 6:7:156:ASP:OD1   | 6:7:159:PHE:N     | 2.30                     | 0.60              |
| 29:e:157:ARG:NH2  | 30:e:609:CHL:O1D  | 2.34                     | 0.60              |
| 31:A:828:CLA:H162 | 31:A:828:CLA:H101 | 1.84                     | 0.60              |
| 2:5:46:PRO:HG2    | 2:5:49:LEU:HB2    | 1.84                     | 0.59              |
| 14:G:20:ARG:HD3   | 31:G:103:CLA:HBB1 | 1.84                     | 0.59              |
| 25:d:168:LYS:HD2  | 31:d:612:CLA:HBD  | 1.82                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:g:107:LEU:HD23 | 30:g:605:CHL:HED2 | 1.82                     | 0.59              |
| 31:A:837:CLA:H141 | 31:L:203:CLA:H141 | 1.85                     | 0.59              |
| 31:L:204:CLA:HBA2 | 36:L:211:LMG:H131 | 1.84                     | 0.59              |
| 25:g:175:LEU:HD11 | 31:g:611:CLA:HHD  | 1.83                     | 0.59              |
| 14:G:36:PRO:HB2   | 14:G:43:HIS:CD2   | 2.36                     | 0.59              |
| 42:c:523:NEX:H392 | 30:c:606:CHL:HMB2 | 1.82                     | 0.59              |
| 30:2:313:CHL:HED3 | 4:3:158:THR:HG23  | 1.85                     | 0.59              |
| 9:A:368:LEU:HD11  | 31:A:819:CLA:H72  | 1.83                     | 0.59              |
| 9:A:404:GLY:HA3   | 9:A:608:LEU:HD11  | 1.84                     | 0.59              |
| 23:c:90:ARG:NH1   | 30:c:608:CHL:OBD  | 2.34                     | 0.59              |
| 25:g:52:LEU:O     | 25:g:56:HIS:ND1   | 2.32                     | 0.59              |
| 10:B:105:THR:HG21 | 27:H:133:PRO:HB3  | 1.83                     | 0.59              |
| 25:d:124:MET:HE1  | 42:d:523:NEX:C30  | 2.31                     | 0.59              |
| 22:h:50:PRO:HG2   | 22:h:64:ASP:HB3   | 1.85                     | 0.59              |
| 22:h:195:LYS:HD3  | 31:h:612:CLA:HAA2 | 1.85                     | 0.59              |
| 31:4:309:CLA:HAB  | 33:4:501:OUR:C13  | 2.33                     | 0.59              |
| 1:0:129:TYR:OH    | 27:H:91:ARG:NH2   | 2.36                     | 0.59              |
| 26:f:224:ALA:HB1  | 26:f:230:PHE:HD1  | 1.68                     | 0.59              |
| 31:f:613:CLA:H102 | 34:f:630:LHG:H131 | 1.85                     | 0.59              |
| 22:h:91:MET:HE1   | 31:h:610:CLA:HAC1 | 1.84                     | 0.59              |
| 31:9:308:CLA:H43  | 36:9:602:LMG:H381 | 1.84                     | 0.59              |
| 1:0:35:MET:HB3    | 1:0:40:ALA:HB3    | 1.84                     | 0.59              |
| 22:h:88:TRP:CE2   | 30:h:608:CHL:HED2 | 2.37                     | 0.59              |
| 28:i:45:LYS:O     | 28:i:50:ARG:NH1   | 2.36                     | 0.59              |
| 28:i:69:ARG:NH1   | 28:i:85:THR:O     | 2.36                     | 0.59              |
| 30:i:606:CHL:HMB1 | 30:i:609:CHL:HAC1 | 1.85                     | 0.59              |
| 4:3:52:ARG:HB3    | 4:3:57:LEU:HD21   | 1.85                     | 0.58              |
| 7:8:226:TRP:HE1   | 30:8:313:CHL:HMC  | 1.67                     | 0.58              |
| 42:f:523:NEX:H403 | 30:f:606:CHL:HBA2 | 1.85                     | 0.58              |
| 8:9:53:ALA:O      | 8:9:74:ARG:NH2    | 2.29                     | 0.58              |
| 25:g:61:MET:HE1   | 31:g:610:CLA:HAB  | 1.84                     | 0.58              |
| 2:5:139:GLU:OE1   | 2:5:142:ARG:NH2   | 2.32                     | 0.58              |
| 9:A:82:HIS:ND1    | 31:A:813:CLA:OBD  | 2.31                     | 0.58              |
| 28:i:198:GLY:HA3  | 30:i:608:CHL:HBC3 | 1.85                     | 0.58              |
| 7:4:157:VAL:HG21  | 30:4:307:CHL:HMC  | 1.85                     | 0.58              |
| 22:a:114:VAL:HG23 | 22:a:117:LYS:HB2  | 1.84                     | 0.58              |
| 24:b:163:ARG:NH2  | 30:b:609:CHL:O1D  | 2.35                     | 0.58              |
| 25:d:71:GLU:HA    | 25:d:84:ALA:HB1   | 1.85                     | 0.58              |
| 28:i:111:GLU:O    | 28:i:115:GLN:NE2  | 2.35                     | 0.58              |
| 9:A:665:SER:HB2   | 9:A:670:LEU:HB2   | 1.86                     | 0.58              |
| 23:c:203:LYS:NZ   | 34:c:630:LHG:O5   | 2.36                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:f:198:ARG:NH2  | 30:f:609:CHL:O1D  | 2.36                     | 0.58              |
| 26:f:216:ASP:OD1  | 28:i:44:ARG:NH1   | 2.36                     | 0.58              |
| 25:g:93:ILE:HG21  | 25:g:113:ILE:HB   | 1.85                     | 0.58              |
| 7:8:229:HIS:CG    | 31:8:312:CLA:HAA2 | 2.39                     | 0.58              |
| 22:a:59:GLY:H     | 22:a:197:ILE:HG21 | 1.67                     | 0.58              |
| 42:f:523:NEX:H172 | 28:i:76:LEU:HD11  | 1.84                     | 0.58              |
| 28:i:159:LEU:HD12 | 30:i:606:CHL:HMD3 | 1.86                     | 0.58              |
| 22:h:115:TRP:HD1  | 22:h:221:PRO:HD3  | 1.67                     | 0.58              |
| 6:7:226:HIS:CG    | 31:7:312:CLA:HAA2 | 2.39                     | 0.58              |
| 31:A:821:CLA:HMB2 | 31:A:825:CLA:HMA3 | 1.86                     | 0.58              |
| 21:O:65:TRP:CD1   | 21:O:120:CYS:HG   | 2.21                     | 0.58              |
| 25:g:171:LYS:NZ   | 34:g:630:LHG:O4   | 2.37                     | 0.58              |
| 22:h:50:PRO:HD2   | 22:h:53:LEU:HD12  | 1.85                     | 0.58              |
| 2:5:66:ASN:O      | 2:5:70:MET:HG2    | 2.03                     | 0.58              |
| 9:A:566:ARG:NH2   | 11:D:87:THR:O     | 2.37                     | 0.58              |
| 11:D:111:ILE:HG12 | 11:D:121:ILE:HG12 | 1.85                     | 0.58              |
| 28:i:84:LEU:HD13  | 28:i:93:GLY:HA2   | 1.85                     | 0.58              |
| 14:G:36:PRO:HB2   | 14:G:43:HIS:HD2   | 1.69                     | 0.57              |
| 31:e:603:CLA:HAC1 | 30:e:607:CHL:HBB2 | 1.85                     | 0.57              |
| 26:f:123:HIS:HB3  | 26:f:245:MET:HE3  | 1.86                     | 0.57              |
| 28:i:71:LEU:HD21  | 28:i:80:PRO:HG3   | 1.86                     | 0.57              |
| 30:2:313:CHL:HHB  | 34:7:602:LHG:H101 | 1.85                     | 0.57              |
| 36:3:602:LMG:O3   | 36:A:856:LMG:O2   | 2.21                     | 0.57              |
| 2:5:148:MET:O     | 2:5:152:VAL:HG12  | 2.04                     | 0.57              |
| 10:B:406:ASN:OD1  | 10:B:407:VAL:N    | 2.36                     | 0.57              |
| 25:g:51:GLU:HA    | 25:g:144:LEU:HD21 | 1.85                     | 0.57              |
| 42:g:523:NEX:H362 | 31:g:604:CLA:C4B  | 2.33                     | 0.57              |
| 42:i:523:NEX:H363 | 31:i:604:CLA:HHC  | 1.83                     | 0.57              |
| 29:e:84:ARG:NE    | 29:e:195:GLU:OE2  | 2.35                     | 0.57              |
| 10:B:457:PRO:HG3  | 10:B:517:PHE:HB2  | 1.86                     | 0.57              |
| 6:7:196:LYS:NZ    | 34:7:601:LHG:O5   | 2.33                     | 0.57              |
| 9:A:745:TRP:NE1   | 31:A:828:CLA:O1A  | 2.38                     | 0.57              |
| 18:C:3:HIS:CE1    | 18:C:76:SER:HB2   | 2.40                     | 0.57              |
| 9:A:627:VAL:HG22  | 9:A:632:VAL:HG22  | 1.85                     | 0.57              |
| 10:B:311:PRO:HG2  | 34:B:852:LHG:HC31 | 1.87                     | 0.57              |
| 34:M:104:LHG:O1   | 34:M:104:LHG:O9   | 2.23                     | 0.57              |
| 21:O:127:GLY:O    | 31:O:203:CLA:HMA1 | 2.04                     | 0.57              |
| 31:O:303:CLA:H42  | 27:H:108:LEU:HD21 | 1.85                     | 0.57              |
| 7:8:168:PRO:HB3   | 7:8:178:GLY:HA3   | 1.86                     | 0.57              |
| 30:c:601:CHL:HMA3 | 34:c:630:LHG:H111 | 1.87                     | 0.57              |
| 4:3:178:TYR:HE2   | 34:3:603:LHG:HC41 | 1.70                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:7:182:ALA:HB2   | 31:7:309:CLA:HAA2 | 1.86                     | 0.57              |
| 7:8:125:MET:HE2   | 30:8:305:CHL:HHD  | 1.85                     | 0.57              |
| 9:A:651:LEU:HD22  | 10:B:651:LEU:HD21 | 1.87                     | 0.57              |
| 9:A:685:ALA:HB3   | 31:B:801:CLA:HBB2 | 1.87                     | 0.57              |
| 26:f:193:LEU:HD12 | 42:f:523:NEX:H203 | 1.87                     | 0.57              |
| 29:e:38:LEU:HB2   | 29:e:42:SER:HB3   | 1.86                     | 0.57              |
| 4:3:52:ARG:NH1    | 4:3:55:ASP:OD2    | 2.33                     | 0.56              |
| 9:A:697:TYR:OH    | 31:B:801:CLA:OBD  | 2.21                     | 0.56              |
| 31:A:839:CLA:HAA2 | 31:A:852:CLA:HMB1 | 1.87                     | 0.56              |
| 27:H:83:GLY:N     | 28:i:53:TRP:O     | 2.24                     | 0.56              |
| 33:i:520:OUR:C13  | 31:i:610:CLA:HAB  | 2.35                     | 0.56              |
| 8:9:148:LEU:O     | 8:9:149:ASN:C     | 2.48                     | 0.56              |
| 9:A:120:ALA:H     | 9:A:145:ILE:HG12  | 1.70                     | 0.56              |
| 11:D:95:GLN:HA    | 27:H:67:LEU:HD13  | 1.87                     | 0.56              |
| 12:E:18:SER:OG    | 18:C:61:ASP:OD2   | 2.21                     | 0.56              |
| 12:E:54:ASN:CG    | 18:C:61:ASP:HB2   | 2.29                     | 0.56              |
| 17:L:109:GLU:OE2  | 17:L:111:GLN:NE2  | 2.36                     | 0.56              |
| 1:0:153:ASN:O     | 1:0:155:ARG:NH1   | 2.38                     | 0.56              |
| 1:0:195:HIS:CG    | 31:0:312:CLA:HAA2 | 2.40                     | 0.56              |
| 2:5:183:MET:HB2   | 30:5:302:CHL:HMC  | 1.87                     | 0.56              |
| 31:A:832:CLA:H143 | 38:B:842:PQN:H191 | 1.87                     | 0.56              |
| 30:a:606:CHL:HBC2 | 30:a:607:CHL:HHD  | 1.87                     | 0.56              |
| 26:f:150:GLU:N    | 26:f:159:GLN:OE1  | 2.38                     | 0.56              |
| 26:f:159:GLN:HE21 | 26:f:166:ILE:HG22 | 1.69                     | 0.56              |
| 1:0:198:ASP:OD1   | 1:0:202:ASN:ND2   | 2.39                     | 0.56              |
| 42:d:523:NEX:O24  | 30:d:606:CHL:HAA1 | 2.05                     | 0.56              |
| 28:i:226:LEU:HD23 | 28:i:229:LYS:HD2  | 1.88                     | 0.56              |
| 11:D:96:VAL:HG23  | 11:D:97:GLU:HG3   | 1.87                     | 0.56              |
| 11:D:133:ARG:NH2  | 11:D:135:GLU:OE1  | 2.38                     | 0.56              |
| 28:i:161:TYR:CD1  | 31:i:604:CLA:H2   | 2.41                     | 0.56              |
| 1:0:229:ALA:HB2   | 36:9:602:LMG:H292 | 1.87                     | 0.56              |
| 30:0:305:CHL:HBC2 | 30:0:306:CHL:HHD  | 1.87                     | 0.56              |
| 3:2:45:VAL:HG11   | 3:2:52:PRO:HG3    | 1.85                     | 0.56              |
| 3:2:233:TRP:HE1   | 30:2:313:CHL:HMC  | 1.71                     | 0.56              |
| 8:9:66:ASP:HB3    | 8:9:69:ARG:HB2    | 1.88                     | 0.56              |
| 24:b:46:GLY:HA3   | 30:b:601:CHL:HBB1 | 1.88                     | 0.56              |
| 22:h:37:ARG:O     | 22:h:39:LYS:NZ    | 2.38                     | 0.56              |
| 31:4:309:CLA:H102 | 31:4:311:CLA:HMB1 | 1.87                     | 0.56              |
| 31:A:840:CLA:H11  | 31:A:840:CLA:C4D  | 2.36                     | 0.56              |
| 7:4:243:LEU:HD23  | 31:4:314:CLA:C1D  | 2.36                     | 0.56              |
| 30:2:313:CHL:HBB2 | 5:6:212:LEU:HD13  | 1.87                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:6:110:TYR:CZ    | 5:6:114:ARG:HD2   | 2.40                     | 0.56              |
| 7:8:115:THR:OG1   | 7:8:116:GLU:N     | 2.39                     | 0.56              |
| 36:9:602:LMG:H332 | 36:9:602:LMG:H162 | 1.88                     | 0.56              |
| 31:B:823:CLA:H11  | 34:B:854:LHG:H242 | 1.88                     | 0.56              |
| 6:7:109:GLU:O     | 6:7:115:ASN:ND2   | 2.35                     | 0.56              |
| 9:A:516:GLY:HA2   | 9:A:530:PRO:HB3   | 1.88                     | 0.56              |
| 26:f:236:LYS:O    | 26:f:240:ASN:ND2  | 2.31                     | 0.56              |
| 31:B:810:CLA:HBC1 | 20:M:12:ILE:HA    | 1.88                     | 0.56              |
| 17:L:51:GLU:OE1   | 27:H:81:TYR:OH    | 2.24                     | 0.56              |
| 24:b:132:LEU:HD21 | 31:b:604:CLA:HAA2 | 1.88                     | 0.56              |
| 25:g:88:LYS:HG2   | 30:g:607:CHL:HED2 | 1.88                     | 0.56              |
| 1:0:188:PRO:O     | 33:0:501:OUR:O39  | 2.24                     | 0.55              |
| 4:3:248:ILE:HD12  | 31:A:815:CLA:H62  | 1.87                     | 0.55              |
| 9:A:418:MET:HE1   | 9:A:432:LEU:HD21  | 1.88                     | 0.55              |
| 9:A:585:ARG:NH2   | 11:D:135:GLU:OE2  | 2.37                     | 0.55              |
| 31:O:206:CLA:H11  | 31:f:611:CLA:H11  | 1.87                     | 0.55              |
| 22:a:178:ASP:OD1  | 33:a:520:OUR:O40  | 2.24                     | 0.55              |
| 29:e:230:ASP:O    | 29:e:234:ASN:ND2  | 2.35                     | 0.55              |
| 31:4:309:CLA:H102 | 31:4:311:CLA:CMB  | 2.36                     | 0.55              |
| 30:b:607:CHL:HBB1 | 30:b:607:CHL:HHC  | 1.88                     | 0.55              |
| 25:d:189:GLN:O    | 25:d:190:THR:OG1  | 2.23                     | 0.55              |
| 1:0:61:LEU:HD11   | 31:0:303:CLA:H72  | 1.88                     | 0.55              |
| 2:5:50:PRO:HA     | 2:5:173:LEU:HD22  | 1.88                     | 0.55              |
| 10:B:369:ALA:HB1  | 10:B:725:LEU:HD11 | 1.89                     | 0.55              |
| 23:c:185:PHE:HA   | 29:e:178:PRO:HB2  | 1.87                     | 0.55              |
| 37:i:521:OIE:C30  | 30:i:606:CHL:CBB  | 2.84                     | 0.55              |
| 24:b:51:ASN:O     | 24:b:51:ASN:ND2   | 2.37                     | 0.55              |
| 28:i:179:VAL:CG1  | 30:i:606:CHL:HED2 | 2.20                     | 0.55              |
| 1:0:146:PHE:CE1   | 28:i:209:PRO:HB2  | 2.40                     | 0.55              |
| 30:7:301:CHL:HMA3 | 34:7:601:LHG:H112 | 1.87                     | 0.55              |
| 31:B:824:CLA:HBB1 | 31:B:831:CLA:HBC2 | 1.88                     | 0.55              |
| 2:5:103:PRO:HG3   | 30:5:305:CHL:HMC  | 1.87                     | 0.55              |
| 6:7:87:TRP:CE2    | 30:7:307:CHL:HED2 | 2.42                     | 0.55              |
| 31:7:304:CLA:HMB2 | 30:7:305:CHL:HBB1 | 1.88                     | 0.55              |
| 9:A:567:LEU:O     | 11:D:133:ARG:NH1  | 2.36                     | 0.55              |
| 30:d:606:CHL:HMB1 | 30:d:609:CHL:HMC  | 1.88                     | 0.55              |
| 29:e:194:LYS:O    | 29:e:198:ASN:ND2  | 2.31                     | 0.55              |
| 4:3:91:VAL:HA     | 34:3:603:LHG:HC31 | 1.89                     | 0.55              |
| 6:7:235:ILE:HD12  | 31:7:312:CLA:H42  | 1.89                     | 0.55              |
| 17:L:20:GLU:OE1   | 17:L:25:SER:OG    | 2.20                     | 0.55              |
| 42:i:523:NEX:C36  | 31:i:604:CLA:HHC  | 2.35                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 34:1:601:LHG:H282 | 34:1:601:LHG:HC82 | 1.88                     | 0.55              |
| 2:5:31:ARG:NH2    | 2:5:47:GLU:OE1    | 2.40                     | 0.55              |
| 8:9:66:ASP:OD1    | 8:9:67:ALA:N      | 2.38                     | 0.55              |
| 16:J:24:SER:HB2   | 31:J:103:CLA:HAB  | 1.88                     | 0.55              |
| 24:b:186:ALA:HB1  | 24:b:192:LEU:HD13 | 1.89                     | 0.55              |
| 28:i:119:TRP:CE2  | 30:i:608:CHL:HED2 | 2.42                     | 0.55              |
| 31:A:802:CLA:H151 | 31:H:201:CLA:HBC3 | 1.89                     | 0.55              |
| 10:B:417:ALA:O    | 10:B:421:HIS:ND1  | 2.36                     | 0.55              |
| 26:f:219:ASP:O    | 28:i:44:ARG:NH2   | 2.32                     | 0.55              |
| 42:g:523:NEX:H383 | 31:g:604:CLA:C1B  | 2.36                     | 0.55              |
| 4:3:108:ARG:NH1   | 30:3:307:CHL:OBD  | 2.31                     | 0.54              |
| 6:7:117:PRO:HG2   | 6:7:120:VAL:HG22  | 1.89                     | 0.54              |
| 22:a:192:LEU:HD21 | 31:a:610:CLA:H12  | 1.88                     | 0.54              |
| 24:b:70:MET:O     | 24:b:71:ARG:C     | 2.49                     | 0.54              |
| 26:f:193:LEU:HD21 | 42:h:523:NEX:C17  | 2.35                     | 0.54              |
| 29:e:113:PHE:HD2  | 29:e:114:LYS:HG3  | 1.73                     | 0.54              |
| 2:1:92:GLU:OE1    | 2:1:201:VAL:N     | 2.35                     | 0.54              |
| 30:2:307:CHL:HHC  | 30:2:307:CHL:HBB1 | 1.87                     | 0.54              |
| 25:g:168:LYS:O    | 25:g:172:ASN:ND2  | 2.34                     | 0.54              |
| 29:e:235:ASN:O    | 29:e:239:TYR:N    | 2.40                     | 0.54              |
| 3:2:147:MET:HA    | 30:2:319:CHL:HED3 | 1.88                     | 0.54              |
| 9:A:228:PRO:HG3   | 9:A:255:MET:HE1   | 1.88                     | 0.54              |
| 9:A:655:LEU:HD11  | 39:A:857:CL0:H43  | 1.88                     | 0.54              |
| 31:A:841:CLA:H71  | 31:B:839:CLA:H43  | 1.90                     | 0.54              |
| 21:O:110:MET:HG2  | 21:O:114:HIS:CE1  | 2.43                     | 0.54              |
| 24:b:37:TYR:CE1   | 24:b:193:ALA:HB1  | 2.42                     | 0.54              |
| 1:0:141:CYS:SG    | 1:0:142:GLY:N     | 2.80                     | 0.54              |
| 31:1:303:CLA:H42  | 31:B:823:CLA:HMB2 | 1.88                     | 0.54              |
| 9:A:537:ASP:OD1   | 9:A:618:LYS:NZ    | 2.39                     | 0.54              |
| 10:B:191:THR:HG21 | 10:B:278:LEU:HB2  | 1.90                     | 0.54              |
| 31:B:839:CLA:H201 | 15:I:20:ALA:HB2   | 1.90                     | 0.54              |
| 42:a:523:NEX:O24  | 30:a:606:CHL:HAA1 | 2.06                     | 0.54              |
| 42:i:523:NEX:H222 | 31:i:604:CLA:CHC  | 2.37                     | 0.54              |
| 7:4:94:LEU:HD11   | 7:4:207:ALA:HB3   | 1.90                     | 0.54              |
| 9:A:102:ARG:HD3   | 9:A:103:PHE:CZ    | 2.43                     | 0.54              |
| 10:B:168:PHE:O    | 10:B:174:ARG:NH2  | 2.39                     | 0.54              |
| 22:a:142:ILE:HG23 | 22:a:143:LEU:HD12 | 1.90                     | 0.54              |
| 25:d:15:TYR:HE2   | 42:h:523:NEX:C3   | 2.20                     | 0.54              |
| 31:d:610:CLA:H62  | 31:d:612:CLA:HMA3 | 1.90                     | 0.54              |
| 22:h:110:PHE:HE1  | 22:h:131:LEU:HA   | 1.73                     | 0.54              |
| 2:5:46:PRO:O      | 2:5:52:ASN:ND2    | 2.41                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:7:177:ASP:OD1   | 33:7:501:0UR:O40  | 2.25                     | 0.54              |
| 7:8:72:ASP:OD1    | 7:8:75:THR:OG1    | 2.23                     | 0.54              |
| 31:9:302:CLA:HED2 | 31:9:302:CLA:H2A  | 1.90                     | 0.54              |
| 10:B:464:GLN:NE2  | 31:B:836:CLA:OBD  | 2.35                     | 0.54              |
| 22:a:37:ARG:NH1   | 22:a:60:ASP:O     | 2.40                     | 0.54              |
| 22:a:161:VAL:HG12 | 24:b:52:THR:HG22  | 1.89                     | 0.54              |
| 23:c:230:TRP:HE1  | 30:c:614:CHL:HMC  | 1.72                     | 0.54              |
| 22:h:39:LYS:HD3   | 22:h:45:SER:HB2   | 1.90                     | 0.54              |
| 1:0:123:ILE:HD13  | 30:0:305:CHL:H11  | 1.90                     | 0.54              |
| 9:A:302:HIS:HB2   | 31:A:818:CLA:C1B  | 2.38                     | 0.54              |
| 31:A:832:CLA:H41  | 31:A:841:CLA:HBC2 | 1.90                     | 0.54              |
| 34:B:852:LHG:O3   | 34:B:852:LHG:O1   | 2.21                     | 0.54              |
| 25:d:150:PHE:HD2  | 30:d:608:CHL:H2   | 1.72                     | 0.54              |
| 7:4:144:GLU:OE2   | 7:4:147:ARG:NH2   | 2.40                     | 0.54              |
| 30:1:307:CHL:HBA1 | 30:1:307:CHL:H13  | 1.90                     | 0.54              |
| 2:5:80:TRP:CE2    | 30:5:307:CHL:HED2 | 2.43                     | 0.54              |
| 9:A:453:LEU:HB3   | 9:A:546:PHE:HB2   | 1.90                     | 0.54              |
| 25:g:60:ALA:HB1   | 25:g:180:MET:HG3  | 1.89                     | 0.54              |
| 30:g:606:CHL:HBB1 | 30:g:606:CHL:HHC  | 1.89                     | 0.54              |
| 22:h:121:GLN:O    | 22:h:124:SER:OG   | 2.26                     | 0.54              |
| 7:4:179:ILE:C     | 7:4:181:ASP:H     | 2.15                     | 0.54              |
| 2:1:148:MET:SD    | 2:1:148:MET:N     | 2.78                     | 0.54              |
| 31:9:302:CLA:HAB  | 33:9:502:0UR:C6   | 2.38                     | 0.54              |
| 10:B:50:HIS:ND1   | 31:B:814:CLA:OBD  | 2.32                     | 0.54              |
| 10:B:542:ARG:NH2  | 11:D:196:ASN:OD1  | 2.39                     | 0.54              |
| 30:f:601:CHL:H52  | 30:e:609:CHL:HBB1 | 1.90                     | 0.54              |
| 22:h:147:TRP:HZ2  | 30:i:614:CHL:HBD  | 1.74                     | 0.54              |
| 28:i:92:TYR:OH    | 34:i:630:LHG:O5   | 2.25                     | 0.54              |
| 10:B:131:THR:HG22 | 10:B:133:GLN:H    | 1.73                     | 0.53              |
| 10:B:237:PRO:HB3  | 10:B:256:THR:HG21 | 1.90                     | 0.53              |
| 10:B:450:GLU:OE2  | 13:F:128:ARG:NH1  | 2.41                     | 0.53              |
| 7:4:53:TRP:CZ2    | 7:4:68:LYS:HG3    | 2.43                     | 0.53              |
| 31:9:302:CLA:HBC1 | 34:9:601:LHG:H271 | 1.91                     | 0.53              |
| 10:B:347:MET:HG3  | 10:B:351:HIS:CE1  | 2.43                     | 0.53              |
| 24:b:181:ASP:OD1  | 33:b:520:0UR:O40  | 2.25                     | 0.53              |
| 2:1:104:SER:HG    | 2:1:105:TRP:CD1   | 2.26                     | 0.53              |
| 5:6:37:PHE:HB2    | 30:6:302:CHL:HMD1 | 1.91                     | 0.53              |
| 31:B:818:CLA:H41  | 31:B:834:CLA:HAA2 | 1.91                     | 0.53              |
| 30:a:609:CHL:HED3 | 24:b:69:THR:HG22  | 1.90                     | 0.53              |
| 25:g:182:GLY:O    | 25:g:186:GLN:HG2  | 2.07                     | 0.53              |
| 28:i:89:PRO:HB3   | 28:i:227:LYS:HB3  | 1.91                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 34:3:603:LHG:HC32 | 34:3:603:LHG:HC62 | 1.89                     | 0.53              |
| 5:6:210:ILE:HD12  | 31:6:317:CLA:HMC2 | 1.90                     | 0.53              |
| 8:9:161:SER:HB3   | 8:9:164:VAL:HG22  | 1.89                     | 0.53              |
| 9:A:639:ASN:O     | 9:A:643:SER:HB3   | 2.09                     | 0.53              |
| 10:B:560:ASP:OD2  | 10:B:564:ARG:NH2  | 2.33                     | 0.53              |
| 18:C:3:HIS:CD2    | 18:C:69:LEU:HA    | 2.43                     | 0.53              |
| 23:c:233:HIS:CG   | 31:c:613:CLA:HAA2 | 2.44                     | 0.53              |
| 34:6:601:LHG:H292 | 34:6:601:LHG:H112 | 1.89                     | 0.53              |
| 42:g:523:NEX:H362 | 31:g:604:CLA:CHC  | 2.39                     | 0.53              |
| 1:0:154:MET:HE3   | 31:0:309:CLA:HED1 | 1.90                     | 0.53              |
| 25:g:104:ASN:ND2  | 25:g:106:SER:OG   | 2.41                     | 0.53              |
| 7:4:108:ILE:H     | 7:4:108:ILE:HD13  | 1.74                     | 0.53              |
| 9:A:543:ILE:CD1   | 39:A:857:CL0:H59  | 2.39                     | 0.53              |
| 12:E:23:ARG:NH2   | 12:E:45:ASP:OD2   | 2.42                     | 0.53              |
| 31:c:603:CLA:HAC1 | 30:c:607:CHL:HBB2 | 1.91                     | 0.53              |
| 2:1:34:ASN:HB3    | 7:4:162:ILE:HD11  | 1.91                     | 0.53              |
| 6:7:109:GLU:HG2   | 30:7:306:CHL:HED2 | 1.90                     | 0.53              |
| 8:9:160:THR:O     | 8:9:161:SER:C     | 2.52                     | 0.53              |
| 9:A:415:ALA:HB1   | 9:A:593:ALA:HB1   | 1.90                     | 0.53              |
| 11:D:102:ILE:HD13 | 11:D:140:LEU:HD23 | 1.91                     | 0.53              |
| 42:f:523:NEX:H362 | 31:f:604:CLA:CHC  | 2.39                     | 0.53              |
| 30:g:601:CHL:HMD1 | 34:g:630:LHG:H251 | 1.90                     | 0.53              |
| 27:H:88:PHE:HB2   | 31:H:204:CLA:HBC3 | 1.90                     | 0.53              |
| 31:3:309:CLA:H191 | 30:7:301:CHL:H43  | 1.91                     | 0.53              |
| 9:A:80:SER:OG     | 9:A:186:TYR:HB2   | 2.09                     | 0.53              |
| 9:A:155:ALA:HB2   | 9:A:383:PRO:HD2   | 1.90                     | 0.53              |
| 9:A:519:ILE:HG12  | 9:A:529:MET:HG3   | 1.91                     | 0.53              |
| 25:d:171:LYS:NZ   | 34:d:630:LHG:O4   | 2.42                     | 0.53              |
| 7:4:196:LYS:HD3   | 31:4:311:CLA:HAA2 | 1.91                     | 0.53              |
| 31:5:304:CLA:HBA1 | 30:5:305:CHL:C1D  | 2.38                     | 0.53              |
| 6:7:144:TRP:NE1   | 31:7:317:CLA:OBD  | 2.32                     | 0.53              |
| 9:A:382:TYR:OH    | 31:A:829:CLA:OBD  | 2.25                     | 0.53              |
| 21:O:128:TRP:HA   | 31:O:203:CLA:CMA  | 2.38                     | 0.53              |
| 37:b:522:OIE:O1   | 37:b:522:OIE:O29  | 2.25                     | 0.53              |
| 26:f:269:HIS:CG   | 31:f:613:CLA:HAA2 | 2.43                     | 0.53              |
| 2:1:80:TRP:CE2    | 30:1:307:CHL:HED2 | 2.44                     | 0.52              |
| 8:9:43:SER:OG     | 14:G:59:LYS:NZ    | 2.32                     | 0.52              |
| 10:B:616:LEU:HD12 | 31:B:803:CLA:H11  | 1.91                     | 0.52              |
| 23:c:174:ASP:OD2  | 23:c:177:TYR:N    | 2.37                     | 0.52              |
| 31:d:612:CLA:HED2 | 31:d:612:CLA:H2A  | 1.91                     | 0.52              |
| 25:g:131:ARG:NH2  | 30:g:609:CHL:O1D  | 2.40                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:h:139:ALA:HB1  | 22:h:145:ILE:HD11 | 1.91                     | 0.52              |
| 30:0:301:CHL:HBB2 | 30:0:302:CHL:CHD  | 2.39                     | 0.52              |
| 4:3:83:LEU:HB2    | 30:3:302:CHL:O1A  | 2.09                     | 0.52              |
| 10:B:117:THR:HA   | 10:B:367:THR:HG22 | 1.90                     | 0.52              |
| 10:B:276:HIS:HB2  | 31:B:818:CLA:C1B  | 2.38                     | 0.52              |
| 7:8:161:PRO:HG3   | 30:8:315:CHL:C4C  | 2.40                     | 0.52              |
| 9:A:294:LEU:HB2   | 9:A:299:ILE:HD11  | 1.90                     | 0.52              |
| 31:B:810:CLA:HBB  | 31:B:811:CLA:HBB  | 1.92                     | 0.52              |
| 21:O:51:LEU:O     | 21:O:53:ALA:N     | 2.41                     | 0.52              |
| 30:g:608:CHL:HBD  | 31:g:610:CLA:HAC2 | 1.91                     | 0.52              |
| 7:4:158:ASN:ND2   | 7:4:158:ASN:O     | 2.43                     | 0.52              |
| 4:3:168:GLN:HE22  | 31:3:318:CLA:C1A  | 2.23                     | 0.52              |
| 5:6:151:PHE:CE2   | 5:6:153:PRO:HG3   | 2.45                     | 0.52              |
| 10:B:105:THR:HG22 | 10:B:111:GLY:C    | 2.34                     | 0.52              |
| 31:B:801:CLA:CGA  | 31:B:801:CLA:H3A  | 2.39                     | 0.52              |
| 24:b:54:PRO:HD2   | 24:b:57:LEU:HD12  | 1.91                     | 0.52              |
| 25:g:71:GLU:HA    | 25:g:74:GLU:HG2   | 1.90                     | 0.52              |
| 30:4:305:CHL:HBB1 | 30:4:305:CHL:HHC  | 1.90                     | 0.52              |
| 2:1:106:VAL:HG23  | 2:1:107:TYR:CG    | 2.45                     | 0.52              |
| 9:A:102:ARG:HG3   | 9:A:165:TYR:OH    | 2.09                     | 0.52              |
| 10:B:442:VAL:HG21 | 31:B:833:CLA:HAC2 | 1.92                     | 0.52              |
| 9:A:678:LEU:HD11  | 10:B:617:MET:HB2  | 1.90                     | 0.52              |
| 10:B:320:GLN:O    | 10:B:406:ASN:ND2  | 2.41                     | 0.52              |
| 31:B:829:CLA:HBB1 | 31:B:829:CLA:HHC  | 1.92                     | 0.52              |
| 24:b:92:TRP:CE2   | 30:b:608:CHL:HED2 | 2.45                     | 0.52              |
| 25:d:8:ARG:NE     | 25:d:31:ASP:O     | 2.33                     | 0.52              |
| 26:f:126:TRP:CE2  | 30:f:608:CHL:HED2 | 2.45                     | 0.52              |
| 6:7:235:ILE:HG13  | 31:7:312:CLA:H11  | 1.92                     | 0.52              |
| 21:O:65:TRP:HH2   | 21:O:113:TRP:HA   | 1.74                     | 0.52              |
| 37:c:522:OIE:C15  | 34:c:630:LHG:H112 | 2.40                     | 0.52              |
| 22:h:158:ALA:HB2  | 28:i:73:MET:HE2   | 1.92                     | 0.52              |
| 3:2:141:MET:HE2   | 30:2:308:CHL:C2C  | 2.39                     | 0.52              |
| 2:5:173:LEU:HD12  | 2:5:177:LYS:HE3   | 1.90                     | 0.52              |
| 10:B:26:ALA:HA    | 31:B:830:CLA:H43  | 1.92                     | 0.52              |
| 22:a:145:ILE:HG22 | 30:a:605:CHL:HAC1 | 1.91                     | 0.52              |
| 23:c:200:LYS:O    | 23:c:204:ASN:ND2  | 2.32                     | 0.52              |
| 7:8:41:ARG:NH1    | 7:8:61:ASP:O      | 2.41                     | 0.52              |
| 10:B:268:LEU:HD22 | 31:B:818:CLA:HBA1 | 1.92                     | 0.52              |
| 31:B:824:CLA:H2A  | 31:B:824:CLA:HED3 | 1.92                     | 0.52              |
| 24:b:201:LYS:NZ   | 34:b:630:LHG:O5   | 2.42                     | 0.52              |
| 26:f:166:ILE:HD11 | 30:f:606:CHL:HMD3 | 1.92                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:3:261:HIS:CG    | 31:3:312:CLA:HAA2 | 2.45                     | 0.51              |
| 39:A:857:CL0:H14  | 31:B:805:CLA:NA   | 2.25                     | 0.51              |
| 23:c:83:GLU:HA    | 23:c:176:LEU:HD21 | 1.91                     | 0.51              |
| 28:i:71:LEU:HD13  | 28:i:77:THR:HG21  | 1.92                     | 0.51              |
| 4:3:209:PHE:O     | 4:3:212:MET:HG3   | 2.10                     | 0.51              |
| 8:9:100:GLN:HG2   | 8:9:106:VAL:HB    | 1.91                     | 0.51              |
| 9:A:343:HIS:CE1   | 34:A:845:LHG:HC12 | 2.45                     | 0.51              |
| 10:B:295:PHE:HA   | 14:G:57:LEU:HD22  | 1.91                     | 0.51              |
| 7:4:245:LYS:O     | 7:4:247:ILE:N     | 2.38                     | 0.51              |
| 30:0:305:CHL:NC   | 30:0:306:CHL:HBC3 | 2.25                     | 0.51              |
| 31:5:309:CLA:H121 | 31:5:311:CLA:HBC1 | 1.91                     | 0.51              |
| 7:8:196:LYS:O     | 7:8:200:ASN:ND2   | 2.26                     | 0.51              |
| 10:B:560:ASP:OD1  | 18:C:66:ARG:NH1   | 2.39                     | 0.51              |
| 24:b:121:LYS:HA   | 30:b:607:CHL:HED2 | 1.92                     | 0.51              |
| 28:i:81:PRO:HD2   | 28:i:84:LEU:HD12  | 1.92                     | 0.51              |
| 28:i:83:TYR:OH    | 28:i:95:ASP:OD2   | 2.21                     | 0.51              |
| 38:A:842:PQN:H28  | 31:F:301:CLA:HBC1 | 1.93                     | 0.51              |
| 10:B:411:ILE:HA   | 10:B:414:HIS:CE1  | 2.45                     | 0.51              |
| 36:B:853:LMG:H121 | 20:M:10:ILE:HG21  | 1.92                     | 0.51              |
| 22:a:136:LEU:HD23 | 30:a:605:CHL:HED2 | 1.92                     | 0.51              |
| 30:0:301:CHL:H52  | 8:9:127:VAL:HG21  | 1.93                     | 0.51              |
| 2:5:125:LYS:H     | 2:5:125:LYS:HD2   | 1.75                     | 0.51              |
| 31:7:309:CLA:HAB  | 33:7:501:0UR:C13  | 2.41                     | 0.51              |
| 10:B:270:LEU:HD23 | 10:B:273:MET:HE3  | 1.93                     | 0.51              |
| 31:B:809:CLA:H151 | 31:B:829:CLA:HBB2 | 1.93                     | 0.51              |
| 17:L:68:GLY:O     | 17:L:71:ARG:HG3   | 2.10                     | 0.51              |
| 23:c:91:TRP:CE2   | 30:c:608:CHL:HED2 | 2.46                     | 0.51              |
| 25:g:59:TRP:CE2   | 30:g:608:CHL:HED2 | 2.46                     | 0.51              |
| 7:8:91:MET:SD     | 31:8:309:CLA:HAB  | 2.51                     | 0.51              |
| 17:L:10:ILE:HG21  | 17:L:16:ILE:HB    | 1.91                     | 0.51              |
| 30:d:607:CHL:HED1 | 29:e:242:LYS:HD2  | 1.92                     | 0.51              |
| 26:f:193:LEU:CB   | 42:f:523:NEX:C20  | 2.89                     | 0.51              |
| 27:H:79:LYS:HB3   | 28:i:54:TRP:CZ2   | 2.45                     | 0.51              |
| 28:i:246:VAL:HG21 | 31:i:613:CLA:HAC2 | 1.92                     | 0.51              |
| 7:4:110:LEU:HD12  | 7:4:111:PRO:HD2   | 1.90                     | 0.51              |
| 1:0:238:ASP:N     | 1:0:238:ASP:OD1   | 2.44                     | 0.51              |
| 2:1:69:ARG:HH21   | 34:B:854:LHG:HC5  | 1.74                     | 0.51              |
| 3:2:209:ARG:HA    | 3:2:212:MET:HE3   | 1.93                     | 0.51              |
| 30:6:301:CHL:OBD  | 6:7:142:ARG:NH1   | 2.44                     | 0.51              |
| 9:A:643:SER:OG    | 9:A:653:ASP:OD2   | 2.22                     | 0.51              |
| 10:B:545:LYS:NZ   | 12:E:18:SER:O     | 2.44                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 42:f:523:NEX:H222 | 31:f:604:CLA:C1C  | 2.40                     | 0.51              |
| 28:i:161:TYR:HB2  | 28:i:168:ILE:HD13 | 1.93                     | 0.51              |
| 6:7:248:VAL:HG12  | 6:7:255:ILE:HB    | 1.92                     | 0.51              |
| 10:B:93:ASP:OD1   | 10:B:95:HIS:ND1   | 2.41                     | 0.51              |
| 10:B:422:LEU:HD13 | 10:B:532:LEU:HA   | 1.93                     | 0.51              |
| 31:B:808:CLA:H122 | 31:B:808:CLA:HBD  | 1.93                     | 0.51              |
| 24:b:231:HIS:CG   | 31:b:613:CLA:HAA2 | 2.46                     | 0.51              |
| 28:i:64:TRP:HB3   | 28:i:228:VAL:HG11 | 1.93                     | 0.51              |
| 3:2:244:THR:HG21  | 4:3:158:THR:OG1   | 2.10                     | 0.51              |
| 31:9:308:CLA:H43  | 36:9:602:LMG:H402 | 1.92                     | 0.51              |
| 9:A:126:ILE:HG22  | 9:A:129:GLN:OE1   | 2.10                     | 0.51              |
| 10:B:490:GLN:HA   | 10:B:494:LEU:HB3  | 1.93                     | 0.51              |
| 22:h:202:LEU:HD11 | 31:h:611:CLA:HHD  | 1.93                     | 0.51              |
| 34:6:601:LHG:O3   | 34:6:601:LHG:O1   | 2.28                     | 0.51              |
| 9:A:222:GLN:O     | 9:A:227:ILE:HG12  | 2.11                     | 0.51              |
| 9:A:507:ALA:O     | 9:A:509:ALA:N     | 2.43                     | 0.51              |
| 18:C:3:HIS:HD2    | 18:C:69:LEU:HA    | 1.76                     | 0.51              |
| 9:A:29:THR:HG23   | 36:A:856:LMG:O4   | 2.11                     | 0.50              |
| 11:D:191:ILE:HG21 | 18:C:62:PHE:HD2   | 1.75                     | 0.50              |
| 24:b:70:MET:O     | 24:b:72:LEU:N     | 2.45                     | 0.50              |
| 25:d:74:GLU:HB2   | 25:d:81:PHE:HD2   | 1.74                     | 0.50              |
| 26:f:193:LEU:CB   | 42:f:523:NEX:H203 | 2.40                     | 0.50              |
| 22:h:40:TRP:NE1   | 22:h:62:GLY:O     | 2.44                     | 0.50              |
| 28:i:82:SER:OG    | 28:i:83:TYR:N     | 2.44                     | 0.50              |
| 29:e:77:GLU:HA    | 29:e:170:LEU:HD21 | 1.92                     | 0.50              |
| 2:1:61:SER:OG     | 2:1:67:MET:SD     | 2.53                     | 0.50              |
| 31:3:320:CLA:HBC3 | 31:3:320:CLA:HHD  | 1.94                     | 0.50              |
| 2:5:49:LEU:HD22   | 30:5:302:CHL:HED2 | 1.93                     | 0.50              |
| 8:9:124:ILE:HG21  | 30:9:305:CHL:HED2 | 1.93                     | 0.50              |
| 8:9:167:ALA:O     | 8:9:171:ASN:ND2   | 2.29                     | 0.50              |
| 10:B:126:THR:HG21 | 10:B:358:TYR:HD1  | 1.76                     | 0.50              |
| 22:a:52:TYR:OH    | 22:a:64:ASP:OD2   | 2.22                     | 0.50              |
| 28:i:159:LEU:HB2  | 28:i:170:ALA:HB2  | 1.93                     | 0.50              |
| 7:4:202:ARG:HD2   | 30:4:302:CHL:C4C  | 2.41                     | 0.50              |
| 4:3:109:PHE:CE1   | 31:3:308:CLA:HBC3 | 2.46                     | 0.50              |
| 10:B:560:ASP:CG   | 18:C:66:ARG:HH12  | 2.19                     | 0.50              |
| 11:D:130:LYS:NZ   | 27:H:66:THR:O     | 2.33                     | 0.50              |
| 14:G:18:LEU:HD23  | 14:G:22:VAL:HG21  | 1.93                     | 0.50              |
| 23:c:126:PHE:HE1  | 23:c:145:ILE:HG21 | 1.76                     | 0.50              |
| 22:h:156:ALA:O    | 22:h:160:ARG:HG3  | 2.12                     | 0.50              |
| 7:4:205:MET:HB2   | 30:4:302:CHL:HMC  | 1.94                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:4:310:CLA:HED2 | 31:4:310:CLA:H2A  | 1.92                     | 0.50              |
| 3:2:72:ALA:HB1    | 3:2:78:LEU:HD13   | 1.92                     | 0.50              |
| 11:D:154:PHE:CZ   | 11:D:167:HIS:HB2  | 2.47                     | 0.50              |
| 23:c:120:SER:O    | 23:c:122:GLY:N    | 2.44                     | 0.50              |
| 42:i:523:NEX:H31  | 30:i:606:CHL:HBA2 | 1.93                     | 0.50              |
| 4:3:221:SER:O     | 4:3:225:MET:HG2   | 2.11                     | 0.50              |
| 30:6:301:CHL:H2   | 6:7:138:TYR:HB2   | 1.92                     | 0.50              |
| 9:A:37:PRO:HB2    | 9:A:53:TRP:HH2    | 1.77                     | 0.50              |
| 10:B:174:ARG:HB2  | 31:B:814:CLA:HBC2 | 1.92                     | 0.50              |
| 10:B:347:MET:HE1  | 31:B:819:CLA:H13  | 1.94                     | 0.50              |
| 25:d:107:LEU:O    | 25:d:109:HIS:N    | 2.45                     | 0.50              |
| 3:2:141:MET:O     | 3:2:145:GLU:HB2   | 2.11                     | 0.50              |
| 6:7:107:TRP:CZ3   | 6:7:212:ALA:HB2   | 2.47                     | 0.50              |
| 31:B:806:CLA:H3A  | 31:B:806:CLA:CGA  | 2.42                     | 0.50              |
| 13:F:91:LYS:HE3   | 13:F:95:ASN:HD21  | 1.75                     | 0.50              |
| 18:C:17:CYS:SG    | 18:C:18:VAL:N     | 2.85                     | 0.50              |
| 42:a:523:NEX:H31  | 30:a:606:CHL:HBA2 | 1.93                     | 0.50              |
| 28:i:229:LYS:HD3  | 31:i:612:CLA:HAA2 | 1.93                     | 0.50              |
| 2:1:191:LEU:HD12  | 31:1:312:CLA:HAC2 | 1.94                     | 0.50              |
| 5:6:114:ARG:HE    | 30:6:307:CHL:CMC  | 2.25                     | 0.50              |
| 9:A:579:PRO:HB3   | 9:A:725:ILE:HB    | 1.94                     | 0.50              |
| 10:B:292:ARG:NH1  | 14:G:34:GLN:O     | 2.45                     | 0.50              |
| 30:h:608:CHL:HHC  | 30:h:608:CHL:HBB1 | 1.92                     | 0.50              |
| 7:8:131:VAL:HG12  | 7:8:135:MET:HE2   | 1.93                     | 0.50              |
| 31:B:817:CLA:H8   | 14:G:84:TYR:CE1   | 2.47                     | 0.50              |
| 31:B:827:CLA:HMB2 | 31:B:834:CLA:HBA1 | 1.94                     | 0.50              |
| 28:i:267:ALA:O    | 28:i:269:ALA:N    | 2.45                     | 0.50              |
| 2:1:36:LEU:HD13   | 30:4:319:CHL:HMA3 | 1.93                     | 0.50              |
| 31:A:803:CLA:H93  | 31:A:808:CLA:H172 | 1.93                     | 0.50              |
| 22:a:160:ARG:HA   | 30:a:608:CHL:C3C  | 2.41                     | 0.50              |
| 30:c:608:CHL:H171 | 30:c:608:CHL:HBA1 | 1.94                     | 0.50              |
| 7:4:238:VAL:HG22  | 7:4:243:LEU:HD21  | 1.93                     | 0.50              |
| 3:2:91:TRP:CE2    | 30:2:307:CHL:HED2 | 2.47                     | 0.49              |
| 4:3:106:HIS:HB3   | 4:3:237:MET:HE3   | 1.94                     | 0.49              |
| 8:9:156:PRO:HG2   | 33:9:501:OUR:C30  | 2.42                     | 0.49              |
| 31:A:808:CLA:H2   | 31:A:828:CLA:H43  | 1.94                     | 0.49              |
| 31:A:830:CLA:H93  | 31:A:840:CLA:HED3 | 1.93                     | 0.49              |
| 11:D:99:PHE:CE1   | 27:H:67:LEU:HD21  | 2.47                     | 0.49              |
| 26:f:239:LYS:NZ   | 34:f:630:LHG:O4   | 2.35                     | 0.49              |
| 29:e:181:MET:HE3  | 31:e:610:CLA:H11  | 1.94                     | 0.49              |
| 30:1:302:CHL:H42  | 31:B:841:CLA:HBB2 | 1.94                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:5:158:PHE:O     | 2:5:160:PRO:HD3   | 2.13                     | 0.49              |
| 5:6:112:GLU:OE1   | 5:6:115:ARG:NH1   | 2.30                     | 0.49              |
| 10:B:477:LEU:HD13 | 31:B:834:CLA:HMD1 | 1.93                     | 0.49              |
| 10:B:721:TYR:HB2  | 31:B:805:CLA:HED3 | 1.93                     | 0.49              |
| 13:F:214:ALA:HB3  | 7:4:67:LEU:HD22   | 1.94                     | 0.49              |
| 25:d:201:HIS:CD2  | 31:d:613:CLA:H3A  | 2.47                     | 0.49              |
| 42:i:523:NEX:H222 | 31:i:604:CLA:C1C  | 2.42                     | 0.49              |
| 31:2:309:CLA:HAB  | 33:2:501:OUR:C13  | 2.42                     | 0.49              |
| 2:5:159:ASP:OD1   | 33:5:501:OUR:O40  | 2.30                     | 0.49              |
| 10:B:344:ILE:HG23 | 31:B:819:CLA:H61  | 1.93                     | 0.49              |
| 31:B:811:CLA:O1A  | 31:B:828:CLA:HBD  | 2.12                     | 0.49              |
| 12:E:54:ASN:OD1   | 18:C:61:ASP:N     | 2.45                     | 0.49              |
| 13:F:78:ILE:HD11  | 13:F:157:TYR:HB2  | 1.93                     | 0.49              |
| 19:K:6:THR:HG23   | 19:K:7:PRO:HD3    | 1.93                     | 0.49              |
| 42:f:523:NEX:H31  | 30:f:606:CHL:HBA2 | 1.93                     | 0.49              |
| 7:4:238:VAL:HB    | 31:4:312:CLA:H11  | 1.94                     | 0.49              |
| 31:A:840:CLA:H202 | 31:F:301:CLA:HBB1 | 1.93                     | 0.49              |
| 10:B:559:CYS:SG   | 10:B:561:GLY:N    | 2.75                     | 0.49              |
| 29:e:84:ARG:NH1   | 30:e:608:CHL:OBD  | 2.34                     | 0.49              |
| 9:A:131:ILE:HG21  | 10:B:446:PHE:HA   | 1.95                     | 0.49              |
| 11:D:191:ILE:HG21 | 18:C:62:PHE:CD2   | 2.48                     | 0.49              |
| 22:a:120:GLY:O    | 22:a:122:ILE:N    | 2.45                     | 0.49              |
| 23:c:196:GLU:HG2  | 23:c:200:LYS:HE3  | 1.94                     | 0.49              |
| 25:d:85:VAL:HG23  | 25:d:88:LYS:HB2   | 1.93                     | 0.49              |
| 26:f:163:ASP:O    | 26:f:165:GLY:N    | 2.45                     | 0.49              |
| 42:h:523:NEX:C29  | 30:h:606:CHL:HHB  | 2.42                     | 0.49              |
| 2:1:165:LYS:HE3   | 2:1:167:ASN:HB2   | 1.94                     | 0.49              |
| 31:A:803:CLA:HBB2 | 31:A:811:CLA:H121 | 1.95                     | 0.49              |
| 23:c:148:ILE:HG12 | 30:c:605:CHL:HAC1 | 1.95                     | 0.49              |
| 25:g:11:TRP:CE2   | 25:g:12:LEU:HG    | 2.48                     | 0.49              |
| 25:g:58:ARG:HD3   | 31:g:610:CLA:C3C  | 2.43                     | 0.49              |
| 22:h:81:ALA:O     | 22:h:85:HIS:ND1   | 2.34                     | 0.49              |
| 28:i:119:TRP:O    | 37:i:521:OIE:O29  | 2.31                     | 0.49              |
| 4:3:166:ALA:HB1   | 32:3:402:8CT:C18  | 2.42                     | 0.49              |
| 31:A:853:CLA:HHC  | 31:A:853:CLA:HBB1 | 1.94                     | 0.49              |
| 10:B:631:LEU:HD22 | 10:B:724:PHE:HA   | 1.94                     | 0.49              |
| 24:b:224:PRO:O    | 33:b:520:OUR:O39  | 2.31                     | 0.49              |
| 30:b:602:CHL:H41  | 31:b:603:CLA:HBA1 | 1.94                     | 0.49              |
| 31:d:603:CLA:H71  | 31:e:603:CLA:H92  | 1.95                     | 0.49              |
| 34:h:630:LHG:H291 | 34:h:630:LHG:HC91 | 1.93                     | 0.49              |
| 28:i:143:GLU:HG3  | 28:i:148:LYS:HB3  | 1.93                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:0:128:GLU:OE1   | 1:0:131:ARG:NH2   | 2.39                     | 0.49              |
| 31:0:311:CLA:H2A  | 31:0:311:CLA:O1A  | 2.13                     | 0.49              |
| 2:1:31:ARG:NH1    | 2:1:41:ALA:HB2    | 2.28                     | 0.49              |
| 9:A:583:PRO:HD3   | 10:B:561:GLY:HA2  | 1.94                     | 0.49              |
| 14:G:20:ARG:HG3   | 14:G:64:VAL:HG11  | 1.95                     | 0.49              |
| 19:K:52:PRO:HG2   | 31:K:104:CLA:HBC2 | 1.94                     | 0.49              |
| 23:c:93:MET:SD    | 31:c:610:CLA:HAB  | 2.52                     | 0.49              |
| 25:g:116:ILE:HG12 | 30:g:605:CHL:HAC1 | 1.93                     | 0.49              |
| 7:4:88:ARG:NH1    | 30:4:307:CHL:OBD  | 2.33                     | 0.49              |
| 3:2:244:THR:HG23  | 3:2:246:ALA:H     | 1.77                     | 0.49              |
| 4:3:245:ALA:HA    | 31:A:815:CLA:H61  | 1.94                     | 0.49              |
| 31:L:201:CLA:H51  | 31:L:203:CLA:H43  | 1.94                     | 0.49              |
| 24:b:162:TYR:HB3  | 30:b:608:CHL:CMC  | 2.43                     | 0.49              |
| 25:d:124:MET:HE2  | 30:d:606:CHL:HMA1 | 1.95                     | 0.49              |
| 7:4:105:ASN:O     | 7:4:105:ASN:ND2   | 2.42                     | 0.49              |
| 1:0:111:ILE:HG13  | 28:i:162:LEU:HD22 | 1.94                     | 0.49              |
| 30:2:319:CHL:H62  | 30:2:319:CHL:H41  | 1.57                     | 0.49              |
| 31:3:306:CLA:HBC2 | 34:3:601:LHG:H251 | 1.95                     | 0.49              |
| 9:A:85:GLN:HE21   | 31:A:805:CLA:HMB3 | 1.78                     | 0.49              |
| 9:A:221:HIS:CE1   | 9:A:225:LEU:HD12  | 2.48                     | 0.49              |
| 10:B:197:VAL:O    | 10:B:201:GLU:HB2  | 2.12                     | 0.49              |
| 10:B:422:LEU:HG   | 31:B:838:CLA:HBB1 | 1.94                     | 0.49              |
| 31:B:850:CLA:OBD  | 13:F:156:ARG:NH1  | 2.44                     | 0.49              |
| 11:D:77:ASN:O     | 27:H:56:ARG:NH1   | 2.46                     | 0.49              |
| 14:G:18:LEU:O     | 14:G:22:VAL:HB    | 2.12                     | 0.49              |
| 26:f:119:ALA:O    | 26:f:123:HIS:ND1  | 2.44                     | 0.49              |
| 29:e:77:GLU:HA    | 29:e:170:LEU:HD11 | 1.94                     | 0.49              |
| 2:1:200:PRO:O     | 33:1:501:OUR:O39  | 2.32                     | 0.48              |
| 7:8:119:ASN:HA    | 30:8:306:CHL:HED2 | 1.94                     | 0.48              |
| 9:A:581:ASP:OD2   | 9:A:585:ARG:NH1   | 2.44                     | 0.48              |
| 13:F:94:GLU:HG2   | 13:F:129:PHE:HB3  | 1.95                     | 0.48              |
| 22:a:50:PRO:HG2   | 22:a:64:ASP:HB3   | 1.95                     | 0.48              |
| 22:a:143:LEU:HG   | 30:b:614:CHL:HED3 | 1.95                     | 0.48              |
| 23:c:162:TYR:HB3  | 30:c:608:CHL:CMC  | 2.42                     | 0.48              |
| 24:b:87:VAL:HB    | 24:b:174:VAL:HG21 | 1.95                     | 0.48              |
| 2:1:106:VAL:HG23  | 2:1:107:TYR:CD1   | 2.48                     | 0.48              |
| 31:1:304:CLA:H43  | 30:1:305:CHL:HBD  | 1.96                     | 0.48              |
| 9:A:723:LEU:HD21  | 38:A:842:PQN:H151 | 1.96                     | 0.48              |
| 10:B:228:GLY:HA3  | 14:G:86:LEU:HD13  | 1.94                     | 0.48              |
| 31:B:803:CLA:HMB1 | 31:B:803:CLA:HBB1 | 1.94                     | 0.48              |
| 21:O:127:GLY:O    | 31:O:203:CLA:CMA  | 2.61                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:f:167:ASN:HD22 | 26:f:176:HIS:HA   | 1.78                     | 0.48              |
| 29:e:173:GLY:C    | 29:e:174:GLU:HG3  | 2.38                     | 0.48              |
| 30:0:306:CHL:HHC  | 30:0:306:CHL:HBB1 | 1.95                     | 0.48              |
| 10:B:714:SER:HB2  | 41:B:849:DGD:HBH1 | 1.95                     | 0.48              |
| 25:d:14:PRO:HG3   | 42:h:523:NEX:H41  | 1.95                     | 0.48              |
| 25:d:130:TYR:HB3  | 30:d:608:CHL:CMC  | 2.44                     | 0.48              |
| 26:f:180:ILE:HG23 | 26:f:181:LEU:HD22 | 1.94                     | 0.48              |
| 42:g:523:NEX:C36  | 31:g:604:CLA:CHC  | 2.91                     | 0.48              |
| 28:i:153:ILE:HD13 | 28:i:173:ILE:HG22 | 1.95                     | 0.48              |
| 29:e:189:ALA:HA   | 29:e:192:LYS:HE2  | 1.95                     | 0.48              |
| 3:2:77:MET:HE1    | 16:J:5:LYS:HD3    | 1.95                     | 0.48              |
| 2:5:98:ASN:HB2    | 2:5:200:PRO:HD2   | 1.96                     | 0.48              |
| 31:A:853:CLA:H121 | 16:J:18:TRP:CD1   | 2.49                     | 0.48              |
| 13:F:93:ARG:NH2   | 13:F:142:ASP:O    | 2.42                     | 0.48              |
| 22:a:154:GLY:HA2  | 30:a:609:CHL:HAB  | 1.94                     | 0.48              |
| 24:b:114:LEU:HB2  | 24:b:117:THR:HG22 | 1.95                     | 0.48              |
| 42:i:523:NEX:C36  | 31:i:604:CLA:HAB  | 2.43                     | 0.48              |
| 1:0:48:GLY:N      | 1:0:53:ASP:OD2    | 2.43                     | 0.48              |
| 2:1:70:MET:HE2    | 31:B:841:CLA:HAB  | 1.95                     | 0.48              |
| 31:1:312:CLA:NC   | 31:1:312:CLA:H43  | 2.28                     | 0.48              |
| 2:5:207:HIS:HA    | 2:5:214:ALA:HB3   | 1.96                     | 0.48              |
| 30:8:301:CHL:H62  | 30:8:313:CHL:H2   | 1.96                     | 0.48              |
| 10:B:328:ASN:ND2  | 14:G:39:ASN:OD1   | 2.35                     | 0.48              |
| 10:B:653:GLY:HA3  | 10:B:720:THR:HG23 | 1.95                     | 0.48              |
| 31:B:817:CLA:HBC3 | 31:B:817:CLA:HHD  | 1.95                     | 0.48              |
| 24:b:177:GLY:O    | 24:b:178:GLU:HB2  | 2.12                     | 0.48              |
| 22:h:42:GLY:HA3   | 30:h:601:CHL:HBB1 | 1.94                     | 0.48              |
| 28:i:69:ARG:HD2   | 28:i:86:GLY:HA3   | 1.95                     | 0.48              |
| 30:e:601:CHL:H3A  | 30:e:601:CHL:HBA1 | 1.61                     | 0.48              |
| 1:0:79:GLY:O      | 1:0:83:MET:HG3    | 2.14                     | 0.48              |
| 4:3:74:GLY:HA3    | 4:3:230:ILE:HG21  | 1.95                     | 0.48              |
| 8:9:143:THR:HB    | 8:9:145:MET:HE3   | 1.96                     | 0.48              |
| 31:A:814:CLA:H8   | 31:A:816:CLA:HAB  | 1.94                     | 0.48              |
| 10:B:524:ALA:HB2  | 31:B:837:CLA:HMA1 | 1.95                     | 0.48              |
| 11:D:102:ILE:HG23 | 11:D:129:LEU:HB3  | 1.95                     | 0.48              |
| 24:b:121:LYS:O    | 24:b:124:SER:OG   | 2.24                     | 0.48              |
| 28:i:61:SER:HG    | 28:i:65:TYR:HB2   | 1.78                     | 0.48              |
| 28:i:90:GLY:H     | 28:i:228:VAL:HG22 | 1.78                     | 0.48              |
| 2:1:91:GLN:HE22   | 2:1:96:PHE:HD2    | 1.62                     | 0.48              |
| 10:B:134:ASP:N    | 10:B:134:ASP:OD1  | 2.47                     | 0.48              |
| 15:I:32:LYS:HD2   | 15:I:35:ILE:HG22  | 1.96                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:a:159:TYR:HB3  | 30:a:608:CHL:CMC  | 2.44                     | 0.48              |
| 23:c:56:LEU:HD13  | 23:c:65:GLY:HA2   | 1.94                     | 0.48              |
| 26:f:194:ILE:CD1  | 42:f:523:NEX:H34  | 2.43                     | 0.48              |
| 42:f:523:NEX:C17  | 28:i:76:LEU:HD11  | 2.43                     | 0.48              |
| 28:i:116:HIS:HE1  | 31:i:603:CLA:NA   | 2.11                     | 0.48              |
| 34:1:601:LHG:HC91 | 32:4:402:8CT:C05  | 2.44                     | 0.48              |
| 5:6:114:ARG:NH2   | 5:6:125:VAL:HG12  | 2.28                     | 0.48              |
| 9:A:34:TRP:HE1    | 31:A:811:CLA:CHB  | 2.26                     | 0.48              |
| 10:B:290:MET:HE1  | 31:B:820:CLA:CAD  | 2.44                     | 0.48              |
| 21:O:65:TRP:CH2   | 21:O:113:TRP:HA   | 2.48                     | 0.48              |
| 23:c:215:TYR:OH   | 33:c:520:0UR:O42  | 2.26                     | 0.48              |
| 24:b:42:PRO:HB3   | 30:b:601:CHL:HBC1 | 1.94                     | 0.48              |
| 25:g:58:ARG:NH1   | 30:g:608:CHL:OBD  | 2.46                     | 0.48              |
| 30:2:301:CHL:C1C  | 34:2:601:LHG:HC81 | 2.43                     | 0.48              |
| 31:2:310:CLA:H91  | 31:2:310:CLA:H111 | 1.68                     | 0.48              |
| 31:2:310:CLA:HED2 | 31:2:310:CLA:H2A  | 1.96                     | 0.48              |
| 9:A:436:ILE:O     | 9:A:439:ARG:HG3   | 2.14                     | 0.48              |
| 9:A:695:ARG:NH1   | 9:A:722:ALA:O     | 2.47                     | 0.48              |
| 11:D:154:PHE:CE2  | 11:D:167:HIS:HB2  | 2.49                     | 0.48              |
| 17:L:141:LEU:HD23 | 27:H:96:LEU:HD13  | 1.96                     | 0.48              |
| 30:c:601:CHL:H61  | 30:c:601:CHL:H41  | 1.51                     | 0.48              |
| 25:d:12:LEU:O     | 30:d:601:CHL:HBB1 | 2.14                     | 0.48              |
| 26:f:253:THR:HG21 | 31:f:613:CLA:HAC2 | 1.95                     | 0.48              |
| 5:6:114:ARG:CZ    | 5:6:125:VAL:HG12  | 2.44                     | 0.48              |
| 10:B:123:TRP:O    | 10:B:127:ILE:HG12 | 2.13                     | 0.48              |
| 31:B:806:CLA:HBC2 | 31:B:806:CLA:HHD  | 1.95                     | 0.48              |
| 31:B:823:CLA:H41  | 31:B:823:CLA:H62  | 1.55                     | 0.48              |
| 13:F:199:ILE:O    | 16:J:11:ALA:N     | 2.47                     | 0.48              |
| 19:K:66:PHE:CE2   | 31:K:105:CLA:HAB  | 2.49                     | 0.48              |
| 26:f:104:MET:SD   | 29:e:78:LEU:HD13  | 2.54                     | 0.48              |
| 42:i:523:NEX:C22  | 31:i:604:CLA:CHC  | 2.91                     | 0.48              |
| 5:6:64:TRP:CE2    | 30:6:307:CHL:HED2 | 2.48                     | 0.47              |
| 9:A:310:PHE:HE1   | 31:A:821:CLA:HAB  | 1.78                     | 0.47              |
| 9:A:658:GLN:HB3   | 9:A:751:ARG:HD2   | 1.95                     | 0.47              |
| 10:B:415:LYS:O    | 10:B:419:ILE:HG12 | 2.14                     | 0.47              |
| 31:B:824:CLA:HHB  | 31:B:841:CLA:O1D  | 2.14                     | 0.47              |
| 25:g:118:TRP:HZ2  | 30:h:614:CHL:HBD  | 1.79                     | 0.47              |
| 29:e:83:ALA:O     | 29:e:87:MET:HG3   | 2.13                     | 0.47              |
| 29:e:85:TRP:CE2   | 30:e:608:CHL:HED2 | 2.49                     | 0.47              |
| 29:e:156:TYR:HB3  | 30:e:608:CHL:CMC  | 2.44                     | 0.47              |
| 30:4:319:CHL:H62  | 30:4:319:CHL:H41  | 1.54                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:1:114:TRP:CD1   | 2:1:119:MET:HG2   | 2.49                     | 0.47              |
| 31:7:318:CLA:H3A  | 31:7:318:CLA:HBA1 | 1.60                     | 0.47              |
| 9:A:686:PHE:HZ    | 31:A:840:CLA:HBC2 | 1.79                     | 0.47              |
| 13:F:172:TYR:OH   | 13:F:214:ALA:O    | 2.25                     | 0.47              |
| 18:C:3:HIS:HE1    | 18:C:76:SER:HB2   | 1.79                     | 0.47              |
| 22:a:57:PHE:HB3   | 22:a:58:PRO:HD2   | 1.96                     | 0.47              |
| 23:c:83:GLU:HA    | 23:c:176:LEU:HD11 | 1.96                     | 0.47              |
| 24:b:41:ARG:NH2   | 24:b:57:LEU:O     | 2.47                     | 0.47              |
| 25:d:164:GLU:O    | 25:d:168:LYS:HG2  | 2.13                     | 0.47              |
| 42:h:523:NEX:C39  | 30:h:606:CHL:HBB  | 2.44                     | 0.47              |
| 7:4:145:ILE:HG21  | 30:4:319:CHL:HBA1 | 1.96                     | 0.47              |
| 1:0:58:PRO:O      | 1:0:241:ARG:NH1   | 2.38                     | 0.47              |
| 2:1:46:PRO:HD2    | 2:1:49:LEU:HD11   | 1.96                     | 0.47              |
| 31:2:304:CLA:H111 | 31:2:304:CLA:H142 | 1.73                     | 0.47              |
| 6:7:210:LEU:HD12  | 31:7:312:CLA:HAC2 | 1.96                     | 0.47              |
| 31:9:308:CLA:H203 | 31:9:308:CLA:H141 | 1.95                     | 0.47              |
| 9:A:60:ASP:O      | 9:A:67:HIS:NE2    | 2.36                     | 0.47              |
| 10:B:519:VAL:HG21 | 10:B:593:TYR:HB2  | 1.96                     | 0.47              |
| 25:g:2:GLU:O      | 25:g:9:ALA:N      | 2.48                     | 0.47              |
| 22:h:34:GLY:O     | 22:h:37:ARG:NE    | 2.47                     | 0.47              |
| 22:h:189:PHE:HE1  | 31:h:610:CLA:H2A  | 1.79                     | 0.47              |
| 4:3:55:ASP:OD1    | 4:3:55:ASP:N      | 2.47                     | 0.47              |
| 4:3:192:LEU:HD21  | 6:7:65:MET:HE3    | 1.95                     | 0.47              |
| 8:9:155:ASP:O     | 8:9:156:PRO:C     | 2.58                     | 0.47              |
| 31:A:807:CLA:HMB1 | 31:A:807:CLA:HBB1 | 1.96                     | 0.47              |
| 31:A:828:CLA:H41  | 31:A:828:CLA:H61  | 1.55                     | 0.47              |
| 31:A:831:CLA:HAB  | 31:A:838:CLA:HBB2 | 1.95                     | 0.47              |
| 10:B:29:HIS:ND1   | 31:B:809:CLA:O1A  | 2.31                     | 0.47              |
| 10:B:359:ALA:O    | 10:B:360:PHE:HB2  | 2.15                     | 0.47              |
| 31:B:836:CLA:HMB1 | 31:B:836:CLA:HBB1 | 1.97                     | 0.47              |
| 24:b:133:ASP:N    | 24:b:133:ASP:OD1  | 2.47                     | 0.47              |
| 30:b:601:CHL:H122 | 30:b:601:CHL:H162 | 1.46                     | 0.47              |
| 42:h:523:NEX:H31  | 30:h:606:CHL:HBA2 | 1.97                     | 0.47              |
| 1:0:150:ASP:O     | 1:0:152:LEU:N     | 2.48                     | 0.47              |
| 4:3:246:GLN:O     | 4:3:250:THR:OG1   | 2.26                     | 0.47              |
| 31:A:840:CLA:H101 | 31:A:840:CLA:H61  | 1.50                     | 0.47              |
| 31:B:823:CLA:HHC  | 31:B:841:CLA:HED1 | 1.97                     | 0.47              |
| 31:B:832:CLA:H12  | 13:F:177:THR:HB   | 1.97                     | 0.47              |
| 17:L:10:ILE:HA    | 17:L:20:GLU:HG2   | 1.97                     | 0.47              |
| 25:g:110:ALA:HB1  | 25:g:116:ILE:HD11 | 1.96                     | 0.47              |
| 22:h:82:GLU:HB2   | 30:h:602:CHL:C1B  | 2.44                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:i:64:TRP:CZ2   | 31:i:611:CLA:H2A  | 2.47                     | 0.47              |
| 28:i:175:ASN:HB3  | 30:i:605:CHL:HBC3 | 1.96                     | 0.47              |
| 31:1:309:CLA:H41  | 31:1:309:CLA:H62  | 1.68                     | 0.47              |
| 31:7:304:CLA:H62  | 31:7:304:CLA:H41  | 1.68                     | 0.47              |
| 7:8:108:ILE:C     | 7:8:110:LEU:H     | 2.22                     | 0.47              |
| 9:A:333:SER:OG    | 31:A:823:CLA:O1D  | 2.30                     | 0.47              |
| 9:A:443:ILE:HG13  | 9:A:561:TYR:HE1   | 1.79                     | 0.47              |
| 10:B:382:MET:HE3  | 31:B:809:CLA:HMB1 | 1.96                     | 0.47              |
| 31:B:839:CLA:H122 | 31:B:840:CLA:H13  | 1.97                     | 0.47              |
| 14:G:11:SER:HB2   | 14:G:82:ALA:HB2   | 1.97                     | 0.47              |
| 30:f:601:CHL:H162 | 30:f:601:CHL:H121 | 1.65                     | 0.47              |
| 31:g:612:CLA:HED2 | 31:g:612:CLA:H2A  | 1.97                     | 0.47              |
| 22:h:114:VAL:HB   | 22:h:117:LYS:HB2  | 1.96                     | 0.47              |
| 22:h:126:GLY:O    | 22:h:140:GLN:NE2  | 2.48                     | 0.47              |
| 22:h:159:TYR:HB3  | 30:h:608:CHL:CMC  | 2.44                     | 0.47              |
| 1:0:180:GLN:HB3   | 1:0:191:ASN:ND2   | 2.30                     | 0.47              |
| 1:0:243:ILE:O     | 1:0:245:TRP:N     | 2.47                     | 0.47              |
| 30:3:307:CHL:HBA1 | 32:7:404:8CT:C24  | 2.45                     | 0.47              |
| 5:6:97:ILE:HG13   | 5:6:98:ILE:HD12   | 1.96                     | 0.47              |
| 7:8:166:LYS:O     | 7:8:168:PRO:HD3   | 2.14                     | 0.47              |
| 8:9:76:ALA:O      | 8:9:80:ASN:ND2    | 2.37                     | 0.47              |
| 9:A:366:GLY:HA2   | 9:A:403:GLY:HA2   | 1.96                     | 0.47              |
| 9:A:435:VAL:HA    | 9:A:438:HIS:CE1   | 2.50                     | 0.47              |
| 9:A:700:GLU:OE2   | 10:B:550:LYS:NZ   | 2.45                     | 0.47              |
| 10:B:441:ASP:OD1  | 10:B:616:LEU:N    | 2.41                     | 0.47              |
| 22:a:166:LEU:HG   | 22:a:176:ALA:HB3  | 1.97                     | 0.47              |
| 23:c:87:ILE:HG22  | 30:c:609:CHL:HMD2 | 1.97                     | 0.47              |
| 24:b:197:VAL:HA   | 24:b:200:ILE:HG22 | 1.97                     | 0.47              |
| 30:b:606:CHL:HBC2 | 30:b:607:CHL:HHD  | 1.96                     | 0.47              |
| 26:f:191:MET:HE2  | 30:f:606:CHL:HMA1 | 1.96                     | 0.47              |
| 25:g:51:GLU:HG3   | 25:g:144:LEU:HD21 | 1.97                     | 0.47              |
| 22:h:178:ASP:OD1  | 33:h:520:0UR:O40  | 2.32                     | 0.47              |
| 37:i:521:0IE:C30  | 30:i:606:CHL:HBB2 | 2.45                     | 0.47              |
| 29:e:82:HIS:HD2   | 30:e:602:CHL:HBB2 | 1.79                     | 0.47              |
| 31:4:304:CLA:H51  | 30:4:305:CHL:HBD  | 1.96                     | 0.47              |
| 1:0:76:LEU:O      | 1:0:80:ARG:HG3    | 2.15                     | 0.47              |
| 1:0:192:LEU:O     | 1:0:196:ILE:HG12  | 2.15                     | 0.47              |
| 31:0:321:CLA:HMA3 | 34:M:104:LHG:H241 | 1.97                     | 0.47              |
| 3:2:229:PRO:O     | 33:2:501:0UR:O39  | 2.33                     | 0.47              |
| 4:3:153:TRP:CD1   | 4:3:153:TRP:H     | 2.32                     | 0.47              |
| 31:3:303:CLA:H2   | 31:3:303:CLA:H61  | 1.54                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:6:302:CHL:HBC1 | 34:6:601:LHG:H282 | 1.97                     | 0.47              |
| 7:8:159:VAL:HG22  | 7:8:168:PRO:HD2   | 1.96                     | 0.47              |
| 8:9:161:SER:OG    | 8:9:162:GLU:N     | 2.48                     | 0.47              |
| 31:9:308:CLA:H62  | 31:9:308:CLA:H2   | 1.59                     | 0.47              |
| 31:A:808:CLA:CHC  | 31:A:809:CLA:HMD2 | 2.45                     | 0.47              |
| 31:A:853:CLA:H93  | 31:A:853:CLA:H61  | 1.65                     | 0.47              |
| 10:B:283:LEU:HD22 | 31:B:818:CLA:HMC1 | 1.97                     | 0.47              |
| 10:B:571:SER:OG   | 10:B:574:ASP:OD2  | 2.32                     | 0.47              |
| 30:c:607:CHL:HHC  | 30:c:607:CHL:HBB1 | 1.95                     | 0.47              |
| 26:f:84:PHE:HA    | 29:e:159:SER:HB3  | 1.97                     | 0.47              |
| 42:i:523:NEX:H241 | 31:i:604:CLA:C1   | 2.45                     | 0.47              |
| 4:3:169:PHE:O     | 4:3:173:ARG:HB2   | 2.15                     | 0.47              |
| 2:5:127:LEU:HD11  | 30:5:305:CHL:C2D  | 2.45                     | 0.47              |
| 30:5:301:CHL:HED3 | 7:8:146:ARG:HD2   | 1.97                     | 0.47              |
| 31:7:308:CLA:H11  | 31:7:317:CLA:HBC2 | 1.95                     | 0.47              |
| 31:9:308:CLA:H142 | 31:9:308:CLA:H111 | 1.63                     | 0.47              |
| 9:A:215:SER:OG    | 9:A:303:HIS:O     | 2.33                     | 0.47              |
| 26:f:194:ILE:HD12 | 42:f:523:NEX:H34  | 1.97                     | 0.47              |
| 25:g:10:LEU:HD13  | 25:g:20:VAL:HG21  | 1.96                     | 0.47              |
| 29:e:59:GLY:N     | 30:e:602:CHL:OBD  | 2.48                     | 0.47              |
| 7:4:88:ARG:HA     | 7:4:91:MET:HE3    | 1.96                     | 0.47              |
| 4:3:189:PHE:N     | 4:3:193:GLU:OE1   | 2.39                     | 0.47              |
| 5:6:95:PHE:HB3    | 7:8:234:TRP:CG    | 2.50                     | 0.47              |
| 9:A:178:MET:HE1   | 31:A:813:CLA:H71  | 1.96                     | 0.47              |
| 9:A:302:HIS:CE1   | 9:A:306:ILE:HD13  | 2.50                     | 0.47              |
| 9:A:361:ASN:O     | 9:A:365:PHE:HB2   | 2.15                     | 0.47              |
| 23:c:160:GLU:OE1  | 23:c:163:ARG:NH2  | 2.48                     | 0.47              |
| 25:d:59:TRP:CE2   | 30:d:608:CHL:HED2 | 2.50                     | 0.47              |
| 22:h:195:LYS:HD3  | 31:h:612:CLA:HBD  | 1.97                     | 0.47              |
| 1:0:204:ILE:HD11  | 1:0:213:VAL:HG21  | 1.97                     | 0.46              |
| 3:2:236:HIS:CG    | 31:2:312:CLA:HAA2 | 2.50                     | 0.46              |
| 30:5:306:CHL:HHC  | 30:5:306:CHL:HBB1 | 1.97                     | 0.46              |
| 31:5:314:CLA:H3A  | 31:5:314:CLA:HBA1 | 1.58                     | 0.46              |
| 6:7:89:MET:HE3    | 6:7:198:GLY:N     | 2.30                     | 0.46              |
| 7:8:144:GLU:HG3   | 7:8:147:ARG:NH1   | 2.30                     | 0.46              |
| 9:A:44:LEU:HD13   | 9:A:57:LEU:HA     | 1.97                     | 0.46              |
| 31:A:818:CLA:HBA2 | 31:A:818:CLA:H3A  | 1.66                     | 0.46              |
| 10:B:716:GLY:O    | 10:B:720:THR:OG1  | 2.30                     | 0.46              |
| 18:C:25:VAL:HG21  | 18:C:48:CYS:HA    | 1.97                     | 0.46              |
| 25:d:92:GLN:HB2   | 25:d:99:LEU:HD23  | 1.96                     | 0.46              |
| 25:d:156:ALA:HB2  | 25:d:165:LEU:HD12 | 1.97                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 42:f:523:NEX:H35  | 42:f:523:NEX:H401 | 1.58                     | 0.46              |
| 29:e:212:GLN:O    | 29:e:216:THR:OG1  | 2.20                     | 0.46              |
| 1:0:102:GLU:HA    | 30:0:306:CHL:HED1 | 1.96                     | 0.46              |
| 31:7:312:CLA:H92  | 31:7:312:CLA:H61  | 1.73                     | 0.46              |
| 9:A:589:CYS:HB2   | 10:B:667:TRP:HB3  | 1.97                     | 0.46              |
| 31:A:840:CLA:H62  | 31:A:840:CLA:H41  | 1.46                     | 0.46              |
| 31:B:806:CLA:H72  | 31:B:806:CLA:H112 | 1.73                     | 0.46              |
| 22:a:110:PHE:HE1  | 22:a:131:LEU:H    | 1.64                     | 0.46              |
| 22:h:131:LEU:HD21 | 31:h:604:CLA:HMD3 | 1.97                     | 0.46              |
| 31:0:309:CLA:H92  | 31:0:309:CLA:H61  | 1.78                     | 0.46              |
| 2:5:198:LYS:HE2   | 2:5:202:GLN:HG3   | 1.97                     | 0.46              |
| 7:8:97:MET:O      | 7:8:100:PRO:HD2   | 2.15                     | 0.46              |
| 9:A:206:HIS:ND1   | 31:A:825:CLA:OBD  | 2.48                     | 0.46              |
| 31:A:841:CLA:H62  | 31:A:841:CLA:H41  | 1.60                     | 0.46              |
| 31:B:809:CLA:HED1 | 31:B:830:CLA:H2   | 1.98                     | 0.46              |
| 31:B:831:CLA:HBB2 | 31:B:838:CLA:HMC1 | 1.97                     | 0.46              |
| 31:L:202:CLA:HBA2 | 31:L:202:CLA:H3A  | 1.60                     | 0.46              |
| 22:a:136:LEU:O    | 22:a:138:HIS:N    | 2.48                     | 0.46              |
| 30:f:609:CHL:H91  | 30:f:609:CHL:H112 | 1.77                     | 0.46              |
| 7:4:190:VAL:HG12  | 7:4:194:LYS:HE3   | 1.98                     | 0.46              |
| 2:1:88:MET:HE1    | 2:1:186:PHE:CD1   | 2.50                     | 0.46              |
| 3:2:248:ASN:OD1   | 3:2:249:GLY:N     | 2.48                     | 0.46              |
| 31:3:309:CLA:HBA2 | 31:3:309:CLA:H3A  | 1.50                     | 0.46              |
| 8:9:95:GLU:HG3    | 8:9:101:THR:HA    | 1.96                     | 0.46              |
| 8:9:145:MET:SD    | 8:9:153:PRO:HG3   | 2.55                     | 0.46              |
| 10:B:128:GLY:HA2  | 10:B:130:ARG:NH1  | 2.30                     | 0.46              |
| 10:B:558:PRO:HB3  | 10:B:702:ILE:HB   | 1.97                     | 0.46              |
| 31:B:834:CLA:HBC2 | 31:B:835:CLA:HAB  | 1.97                     | 0.46              |
| 14:G:81:VAL:O     | 14:G:85:ILE:HG12  | 2.15                     | 0.46              |
| 22:a:90:MET:SD    | 31:a:610:CLA:HAB  | 2.55                     | 0.46              |
| 25:d:61:MET:HE3   | 25:d:173:GLY:N    | 2.31                     | 0.46              |
| 25:g:61:MET:HE1   | 31:g:610:CLA:HHC  | 1.97                     | 0.46              |
| 7:4:54:LEU:HD12   | 7:4:54:LEU:HA     | 1.80                     | 0.46              |
| 31:0:312:CLA:H121 | 34:0:601:LHG:H101 | 1.96                     | 0.46              |
| 30:1:305:CHL:HMB1 | 31:1:308:CLA:HBC2 | 1.97                     | 0.46              |
| 30:2:313:CHL:H12  | 30:3:305:CHL:H42  | 1.96                     | 0.46              |
| 30:6:301:CHL:H12  | 34:6:601:LHG:H131 | 1.97                     | 0.46              |
| 30:6:302:CHL:H93  | 30:6:302:CHL:H61  | 1.74                     | 0.46              |
| 31:6:312:CLA:H101 | 34:6:601:LHG:H142 | 1.96                     | 0.46              |
| 6:7:87:TRP:CE2    | 31:7:308:CLA:HBC3 | 2.50                     | 0.46              |
| 7:8:86:HIS:HB3    | 7:8:205:MET:HE3   | 1.96                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:B:374:HIS:HB2  | 31:B:828:CLA:C1B  | 2.46                     | 0.46              |
| 31:B:810:CLA:HHD  | 31:B:810:CLA:HBC2 | 1.97                     | 0.46              |
| 14:G:38:GLN:N     | 14:G:41:LEU:O     | 2.44                     | 0.46              |
| 16:J:2:GLN:O      | 16:J:6:ILE:HG13   | 2.16                     | 0.46              |
| 17:L:38:ALA:O     | 17:L:48:ARG:NH2   | 2.48                     | 0.46              |
| 22:a:53:LEU:HD11  | 22:a:64:ASP:HB2   | 1.97                     | 0.46              |
| 30:b:602:CHL:H91  | 30:b:602:CHL:H111 | 1.70                     | 0.46              |
| 7:4:146:ARG:HA    | 30:4:319:CHL:HED3 | 1.98                     | 0.46              |
| 31:1:312:CLA:H41  | 31:1:312:CLA:H61  | 1.46                     | 0.46              |
| 7:8:144:GLU:HG3   | 7:8:147:ARG:HH12  | 1.79                     | 0.46              |
| 30:8:307:CHL:HBA2 | 30:8:307:CHL:H3A  | 1.64                     | 0.46              |
| 24:b:198:LYS:HD3  | 31:b:612:CLA:HAA2 | 1.97                     | 0.46              |
| 22:h:164:GLY:N    | 22:h:167:GLY:O    | 2.48                     | 0.46              |
| 29:e:174:GLU:CD   | 29:e:175:ALA:H    | 2.23                     | 0.46              |
| 7:4:88:ARG:HB3    | 31:4:309:CLA:CAC  | 2.46                     | 0.46              |
| 2:1:104:SER:HA    | 2:1:108:GLU:OE1   | 2.15                     | 0.46              |
| 7:8:191:ASP:N     | 7:8:191:ASP:OD1   | 2.46                     | 0.46              |
| 7:8:196:LYS:HD3   | 31:8:311:CLA:HBD  | 1.97                     | 0.46              |
| 30:8:313:CHL:H62  | 30:8:313:CHL:H41  | 1.57                     | 0.46              |
| 34:A:855:LHG:H242 | 34:A:855:LHG:HC61 | 1.76                     | 0.46              |
| 10:B:15:ASP:HB3   | 10:B:20:ARG:HB2   | 1.97                     | 0.46              |
| 10:B:84:ILE:HD13  | 27:H:145:ILE:HB   | 1.97                     | 0.46              |
| 28:i:61:SER:OG    | 28:i:65:TYR:HB2   | 2.16                     | 0.46              |
| 28:i:146:TRP:CE2  | 28:i:147:PHE:HD1  | 2.34                     | 0.46              |
| 31:i:603:CLA:HED2 | 31:i:603:CLA:H2A  | 1.98                     | 0.46              |
| 29:e:133:LEU:HD23 | 30:e:605:CHL:HED2 | 1.98                     | 0.46              |
| 7:4:136:GLN:O     | 7:4:140:MET:HB2   | 2.15                     | 0.46              |
| 31:0:309:CLA:H62  | 31:0:309:CLA:H41  | 1.61                     | 0.46              |
| 31:5:303:CLA:H42  | 7:4:166:LYS:HG3   | 1.96                     | 0.46              |
| 6:7:259:CYS:O     | 34:7:602:LHG:HC62 | 2.16                     | 0.46              |
| 9:A:697:TYR:CE2   | 10:B:536:LYS:HD2  | 2.51                     | 0.46              |
| 31:B:828:CLA:HBA2 | 31:B:828:CLA:H3A  | 1.39                     | 0.46              |
| 16:J:24:SER:CB    | 31:J:103:CLA:HAB  | 2.45                     | 0.46              |
| 21:O:127:GLY:C    | 31:O:203:CLA:HMA3 | 2.40                     | 0.46              |
| 22:a:182:MET:HB2  | 31:a:610:CLA:O1A  | 2.16                     | 0.46              |
| 30:a:601:CHL:H3A  | 30:a:601:CHL:HBA1 | 1.34                     | 0.46              |
| 25:g:52:LEU:HD23  | 31:g:603:CLA:HAA2 | 1.98                     | 0.46              |
| 25:g:145:TYR:CZ   | 25:g:166:LYS:HD2  | 2.50                     | 0.46              |
| 22:h:146:VAL:HB   | 30:h:607:CHL:HBC1 | 1.97                     | 0.46              |
| 42:i:523:NEX:C22  | 31:i:604:CLA:NC   | 2.78                     | 0.46              |
| 7:4:114:GLY:O     | 7:4:116:GLU:N     | 2.49                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:A:431:LEU:HD13  | 31:A:824:CLA:C1C  | 2.45                     | 0.46              |
| 31:A:806:CLA:H41  | 34:A:844:LHG:H271 | 1.97                     | 0.46              |
| 11:D:78:THR:HG23  | 11:D:126:PRO:HB2  | 1.98                     | 0.46              |
| 42:a:523:NEX:H201 | 42:a:523:NEX:H15  | 1.62                     | 0.46              |
| 25:d:12:LEU:HB2   | 25:d:16:SER:HB3   | 1.97                     | 0.46              |
| 25:g:173:GLY:O    | 25:g:177:MET:HG2  | 2.16                     | 0.46              |
| 6:7:240:GLY:O     | 6:7:264:GLN:N     | 2.49                     | 0.46              |
| 7:8:55:ASP:N      | 7:8:55:ASP:OD1    | 2.47                     | 0.46              |
| 7:8:56:GLY:HA2    | 7:8:61:ASP:HB3    | 1.98                     | 0.46              |
| 34:9:601:LHG:O3   | 34:9:601:LHG:O1   | 2.26                     | 0.46              |
| 9:A:15:ILE:HG13   | 9:A:16:LYS:H      | 1.80                     | 0.46              |
| 25:d:194:PRO:O    | 33:d:520:O:UR:O39 | 2.34                     | 0.46              |
| 29:e:85:TRP:CD1   | 30:e:609:CHL:HMD3 | 2.51                     | 0.46              |
| 7:4:122:ALA:C     | 7:4:124:PRO:HD3   | 2.40                     | 0.46              |
| 2:1:148:MET:O     | 2:1:152:VAL:HG23  | 2.15                     | 0.45              |
| 31:7:308:CLA:H42  | 31:7:317:CLA:HBC1 | 1.97                     | 0.45              |
| 30:9:306:CHL:H3A  | 30:9:306:CHL:HBA1 | 1.64                     | 0.45              |
| 9:A:699:GLN:O     | 9:A:703:GLU:HG3   | 2.17                     | 0.45              |
| 10:B:22:TRP:CG    | 10:B:704:GLN:HE22 | 2.34                     | 0.45              |
| 10:B:585:ASN:HB2  | 31:B:803:CLA:HBC2 | 1.98                     | 0.45              |
| 24:b:207:MET:HE2  | 30:b:602:CHL:OMC  | 2.16                     | 0.45              |
| 25:d:73:LEU:HD23  | 25:d:81:PHE:HZ    | 1.81                     | 0.45              |
| 25:g:128:GLU:HA   | 25:g:131:ARG:HG2  | 1.97                     | 0.45              |
| 1:0:150:ASP:OD2   | 1:0:154:MET:HB2   | 2.16                     | 0.45              |
| 1:0:162:LYS:HD3   | 31:0:311:CLA:HBA1 | 1.99                     | 0.45              |
| 30:0:301:CHL:H51  | 30:0:301:CHL:H12  | 1.78                     | 0.45              |
| 2:1:49:LEU:HD22   | 2:1:71:ILE:HD11   | 1.97                     | 0.45              |
| 2:1:61:SER:OG     | 2:1:61:SER:O      | 2.33                     | 0.45              |
| 2:5:63:ASN:HB3    | 2:5:66:ASN:HB2    | 1.98                     | 0.45              |
| 31:A:830:CLA:H42  | 34:A:844:LHG:H241 | 1.98                     | 0.45              |
| 10:B:203:ARG:NH2  | 10:B:253:ALA:O    | 2.43                     | 0.45              |
| 31:B:806:CLA:H142 | 31:B:806:CLA:H111 | 1.64                     | 0.45              |
| 12:E:11:VAL:HB    | 12:E:61:VAL:HG13  | 1.98                     | 0.45              |
| 17:L:6:VAL:HG13   | 21:O:50:TRP:HB2   | 1.97                     | 0.45              |
| 42:d:523:NEX:H11  | 42:d:523:NEX:H191 | 1.82                     | 0.45              |
| 30:f:609:CHL:HHC  | 30:f:609:CHL:HBB1 | 1.97                     | 0.45              |
| 22:h:91:MET:HB3   | 31:h:604:CLA:HBB2 | 1.97                     | 0.45              |
| 28:i:64:TRP:NE1   | 31:i:611:CLA:O1D  | 2.49                     | 0.45              |
| 31:4:310:CLA:H92  | 31:4:310:CLA:H61  | 1.77                     | 0.45              |
| 2:5:127:LEU:HD21  | 30:5:305:CHL:C4D  | 2.46                     | 0.45              |
| 31:7:304:CLA:H71  | 30:7:305:CHL:HBD  | 1.98                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:A:124:TRP:CD2   | 31:A:809:CLA:HED3 | 2.51                     | 0.45              |
| 9:A:439:ARG:NH1   | 9:A:564:SER:O     | 2.49                     | 0.45              |
| 31:A:825:CLA:H203 | 31:A:825:CLA:H162 | 1.75                     | 0.45              |
| 31:A:832:CLA:H141 | 31:A:832:CLA:H161 | 1.77                     | 0.45              |
| 10:B:340:SER:O    | 10:B:344:ILE:HG12 | 2.17                     | 0.45              |
| 22:a:65:SER:O     | 23:c:80:GLN:NE2   | 2.49                     | 0.45              |
| 31:i:604:CLA:C4   | 30:i:606:CHL:O1A  | 2.65                     | 0.45              |
| 7:4:97:MET:HE1    | 7:4:208:THR:HG23  | 1.97                     | 0.45              |
| 7:4:179:ILE:HG23  | 7:4:179:ILE:O     | 2.15                     | 0.45              |
| 3:2:206:LYS:NZ    | 34:2:601:LHG:O4   | 2.32                     | 0.45              |
| 31:6:303:CLA:H61  | 31:6:303:CLA:H41  | 1.57                     | 0.45              |
| 31:6:304:CLA:HMB1 | 30:6:305:CHL:HBB1 | 1.98                     | 0.45              |
| 30:6:308:CHL:H2   | 30:6:308:CHL:H62  | 1.73                     | 0.45              |
| 31:9:300:CLA:HBA2 | 14:G:50:ARG:HD3   | 1.97                     | 0.45              |
| 31:9:309:CLA:HMB3 | 31:9:311:CLA:HAA1 | 1.98                     | 0.45              |
| 9:A:18:VAL:HG21   | 9:A:319:THR:HB    | 1.98                     | 0.45              |
| 31:A:809:CLA:H91  | 31:A:809:CLA:H111 | 1.67                     | 0.45              |
| 10:B:415:LYS:NZ   | 10:B:540:ASP:OD1  | 2.38                     | 0.45              |
| 10:B:415:LYS:NZ   | 13:F:238:VAL:HG21 | 2.29                     | 0.45              |
| 31:B:839:CLA:H2A  | 15:I:27:PHE:HE2   | 1.82                     | 0.45              |
| 26:f:187:GLN:OE1  | 30:f:607:CHL:HMC  | 2.17                     | 0.45              |
| 28:i:145:VAL:HB   | 28:i:148:LYS:HE2  | 1.98                     | 0.45              |
| 30:1:313:CHL:HAA2 | 7:4:135:MET:HE2   | 1.98                     | 0.45              |
| 30:2:319:CHL:H112 | 30:2:319:CHL:H91  | 1.60                     | 0.45              |
| 8:9:157:LEU:O     | 8:9:158:GLY:C     | 2.59                     | 0.45              |
| 9:A:685:ALA:O     | 9:A:686:PHE:C     | 2.57                     | 0.45              |
| 31:A:810:CLA:HBB2 | 31:A:813:CLA:HMA3 | 1.99                     | 0.45              |
| 38:A:842:PQN:H161 | 38:A:842:PQN:H141 | 1.72                     | 0.45              |
| 22:a:82:GLU:HB2   | 30:a:602:CHL:CHB  | 2.47                     | 0.45              |
| 30:a:607:CHL:H3A  | 30:a:607:CHL:HBA1 | 1.42                     | 0.45              |
| 28:i:69:ARG:NH2   | 28:i:91:ASP:O     | 2.50                     | 0.45              |
| 28:i:135:LYS:HE3  | 28:i:135:LYS:HB3  | 1.86                     | 0.45              |
| 29:e:107:PHE:CE2  | 29:e:128:LEU:HA   | 2.52                     | 0.45              |
| 7:4:159:VAL:HG13  | 7:4:162:ILE:HB    | 1.99                     | 0.45              |
| 7:4:217:VAL:HG11  | 7:4:241:ILE:HD13  | 1.98                     | 0.45              |
| 1:0:110:PRO:HB2   | 28:i:162:LEU:HD23 | 1.99                     | 0.45              |
| 2:5:160:PRO:HD2   | 33:5:501:OUR:O40  | 2.13                     | 0.45              |
| 30:7:307:CHL:CBB  | 31:7:315:CLA:HMC2 | 2.47                     | 0.45              |
| 7:8:161:PRO:HB3   | 30:8:315:CHL:C1C  | 2.46                     | 0.45              |
| 10:B:101:VAL:O    | 10:B:105:THR:HG23 | 2.17                     | 0.45              |
| 10:B:286:ILE:O    | 31:B:822:CLA:HBC1 | 2.16                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:B:809:CLA:HBB  | 31:B:830:CLA:HAB  | 1.98                     | 0.45              |
| 31:B:822:CLA:H143 | 14:G:81:VAL:HB    | 1.99                     | 0.45              |
| 14:G:54:TYR:CG    | 14:G:55:VAL:N     | 2.85                     | 0.45              |
| 23:c:40:ARG:NE    | 23:c:63:ASP:O     | 2.36                     | 0.45              |
| 42:c:523:NEX:H222 | 31:c:604:CLA:CHC  | 2.47                     | 0.45              |
| 24:b:65:TYR:HB2   | 30:b:602:CHL:HMD3 | 1.98                     | 0.45              |
| 30:d:606:CHL:HBC2 | 30:d:607:CHL:HHD  | 1.99                     | 0.45              |
| 22:h:228:HIS:CG   | 31:h:613:CLA:HAA2 | 2.52                     | 0.45              |
| 31:4:310:CLA:H43  | 31:4:311:CLA:HMD2 | 1.97                     | 0.45              |
| 30:1:306:CHL:HHC  | 30:1:306:CHL:HBB1 | 1.99                     | 0.45              |
| 31:3:313:CLA:HBA2 | 31:3:313:CLA:H3A  | 1.57                     | 0.45              |
| 9:A:594:TRP:NE1   | 31:A:830:CLA:HMD3 | 2.31                     | 0.45              |
| 31:A:831:CLA:HAB  | 31:A:838:CLA:CBB  | 2.47                     | 0.45              |
| 23:c:89:SER:HB2   | 23:c:205:GLY:HA3  | 1.99                     | 0.45              |
| 30:b:608:CHL:H143 | 30:b:608:CHL:H162 | 1.70                     | 0.45              |
| 30:e:608:CHL:H62  | 30:e:608:CHL:H101 | 1.64                     | 0.45              |
| 1:0:72:ARG:NH1    | 1:0:75:GLU:OE1    | 2.50                     | 0.45              |
| 2:1:85:VAL:HG13   | 2:1:189:PHE:CE2   | 2.52                     | 0.45              |
| 30:2:302:CHL:H93  | 30:2:302:CHL:H111 | 1.70                     | 0.45              |
| 4:3:215:LEU:HB2   | 31:3:309:CLA:HBA1 | 1.98                     | 0.45              |
| 7:8:103:LEU:HD13  | 7:8:111:PRO:HG2   | 1.99                     | 0.45              |
| 7:8:149:GLN:CB    | 7:8:158:ASN:HD21  | 2.29                     | 0.45              |
| 9:A:119:SER:HB2   | 9:A:136:VAL:HG11  | 1.99                     | 0.45              |
| 9:A:121:GLN:NE2   | 31:A:809:CLA:OBD  | 2.47                     | 0.45              |
| 9:A:603:TRP:HE1   | 31:B:806:CLA:C1D  | 2.30                     | 0.45              |
| 9:A:610:ILE:HD12  | 39:A:857:CL0:H53  | 1.98                     | 0.45              |
| 9:A:665:SER:O     | 9:A:671:SER:HA    | 2.17                     | 0.45              |
| 31:A:817:CLA:H41  | 31:A:817:CLA:H61  | 1.71                     | 0.45              |
| 31:A:837:CLA:HBB1 | 31:A:838:CLA:CHD  | 2.47                     | 0.45              |
| 31:B:819:CLA:H61  | 31:B:819:CLA:H93  | 1.84                     | 0.45              |
| 42:g:523:NEX:H35  | 42:g:523:NEX:H401 | 1.57                     | 0.45              |
| 22:h:158:ALA:HB1  | 28:i:76:LEU:HB3   | 1.98                     | 0.45              |
| 22:h:183:ALA:HB2  | 22:h:192:LEU:HD12 | 1.99                     | 0.45              |
| 22:h:212:THR:HG21 | 31:h:613:CLA:HAC2 | 1.99                     | 0.45              |
| 28:i:134:GLU:HA   | 28:i:139:ALA:HB2  | 1.98                     | 0.45              |
| 42:e:523:NEX:H35  | 42:e:523:NEX:H401 | 1.75                     | 0.45              |
| 4:3:168:GLN:NE2   | 31:3:318:CLA:O1D  | 2.50                     | 0.45              |
| 4:3:230:ILE:HD12  | 4:3:230:ILE:HA    | 1.87                     | 0.45              |
| 9:A:133:ASN:HB3   | 9:A:141:GLN:HB3   | 1.99                     | 0.45              |
| 9:A:295:TRP:HB2   | 9:A:298:ASP:OD2   | 2.17                     | 0.45              |
| 9:A:434:ARG:O     | 9:A:438:HIS:ND1   | 2.48                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 38:A:842:PQN:H141 | 31:A:853:CLA:HBB2 | 1.99                     | 0.45              |
| 10:B:658:ALA:HB3  | 31:B:806:CLA:HBB2 | 1.99                     | 0.45              |
| 34:2:601:LHG:H272 | 34:2:601:LHG:H242 | 1.79                     | 0.45              |
| 9:A:440:ASP:OD1   | 9:A:561:TYR:OH    | 2.29                     | 0.45              |
| 31:A:826:CLA:H62  | 31:A:826:CLA:H101 | 1.60                     | 0.45              |
| 31:A:843:CLA:HBA2 | 21:O:122:THR:HG23 | 1.98                     | 0.45              |
| 31:B:819:CLA:H62  | 31:B:819:CLA:H41  | 1.57                     | 0.45              |
| 22:a:33:TYR:CE2   | 22:a:190:ALA:HB1  | 2.52                     | 0.45              |
| 22:a:159:TYR:HB3  | 30:a:608:CHL:OMC  | 2.17                     | 0.45              |
| 23:c:152:GLN:HE22 | 30:c:607:CHL:HAC1 | 1.82                     | 0.45              |
| 24:b:107:ASN:HB2  | 24:b:117:THR:HG21 | 1.99                     | 0.45              |
| 24:b:176:PRO:HD2  | 31:b:610:CLA:OBD  | 2.16                     | 0.45              |
| 29:e:227:HIS:CG   | 31:e:613:CLA:HAA2 | 2.52                     | 0.45              |
| 1:0:200:LEU:HD21  | 8:9:114:VAL:HG23  | 1.99                     | 0.44              |
| 2:5:161:ALA:O     | 2:5:163:PHE:N     | 2.50                     | 0.44              |
| 9:A:703:GLU:CD    | 10:B:545:LYS:HB2  | 2.41                     | 0.44              |
| 9:A:705:ILE:HD13  | 31:A:839:CLA:HMD1 | 1.99                     | 0.44              |
| 31:A:822:CLA:HBA2 | 31:A:822:CLA:H3A  | 1.21                     | 0.44              |
| 31:A:839:CLA:H172 | 13:F:181:GLY:HA2  | 1.99                     | 0.44              |
| 29:e:54:PHE:O     | 29:e:57:ASP:HB2   | 2.16                     | 0.44              |
| 2:5:167:ASN:OD1   | 2:5:167:ASN:N     | 2.50                     | 0.44              |
| 5:6:203:THR:HG22  | 5:6:205:PHE:N     | 2.26                     | 0.44              |
| 8:9:95:GLU:CD     | 8:9:194:VAL:HG12  | 2.42                     | 0.44              |
| 9:A:225:LEU:C     | 9:A:228:PRO:HD2   | 2.43                     | 0.44              |
| 31:A:831:CLA:HBA2 | 34:A:845:LHG:HC92 | 1.98                     | 0.44              |
| 31:B:831:CLA:HBA2 | 31:B:831:CLA:H3A  | 1.34                     | 0.44              |
| 22:a:116:PHE:CD2  | 22:a:117:LYS:HG3  | 2.52                     | 0.44              |
| 30:c:601:CHL:H3A  | 30:c:601:CHL:HBA1 | 1.59                     | 0.44              |
| 37:b:521:OIE:C19  | 30:b:602:CHL:H2   | 2.47                     | 0.44              |
| 30:f:601:CHL:HBA1 | 30:f:601:CHL:H3A  | 1.73                     | 0.44              |
| 31:g:613:CLA:H3A  | 31:g:613:CLA:HBA2 | 1.72                     | 0.44              |
| 31:e:610:CLA:HMB3 | 31:e:612:CLA:HAA1 | 1.98                     | 0.44              |
| 7:4:229:HIS:CG    | 31:4:312:CLA:HAA2 | 2.52                     | 0.44              |
| 31:5:303:CLA:H111 | 31:5:303:CLA:H91  | 1.76                     | 0.44              |
| 31:6:310:CLA:HED2 | 31:6:310:CLA:H2A  | 1.97                     | 0.44              |
| 9:A:33:LYS:HB2    | 31:A:811:CLA:HAA2 | 1.99                     | 0.44              |
| 9:A:401:TRP:CD1   | 31:A:828:CLA:HAB  | 2.53                     | 0.44              |
| 9:A:458:PHE:O     | 9:A:462:ILE:HG12  | 2.18                     | 0.44              |
| 9:A:484:LEU:H     | 9:A:535:THR:HG22  | 1.81                     | 0.44              |
| 31:B:808:CLA:HBB1 | 31:B:808:CLA:HMB1 | 2.00                     | 0.44              |
| 31:B:825:CLA:H111 | 31:B:825:CLA:H151 | 1.76                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:c:608:CHL:H43  | 30:c:608:CHL:H203 | 2.00                     | 0.44              |
| 25:d:64:THR:HG23  | 25:d:180:MET:HG2  | 1.99                     | 0.44              |
| 30:f:601:CHL:H12  | 30:f:601:CHL:H51  | 1.74                     | 0.44              |
| 1:0:241:ARG:HH22  | 35:0:603:SQD:H5   | 1.83                     | 0.44              |
| 30:0:301:CHL:HBA2 | 30:0:301:CHL:H3A  | 1.70                     | 0.44              |
| 2:5:130:ILE:HA    | 2:5:133:VAL:HG12  | 1.99                     | 0.44              |
| 5:6:212:LEU:O     | 6:7:256:PRO:HD3   | 2.17                     | 0.44              |
| 8:9:145:MET:HE3   | 8:9:145:MET:HB2   | 1.62                     | 0.44              |
| 9:A:337:PRO:HB2   | 17:L:6:VAL:HG23   | 1.99                     | 0.44              |
| 31:A:819:CLA:HBA2 | 31:A:819:CLA:H3A  | 1.42                     | 0.44              |
| 31:A:822:CLA:H12  | 31:K:105:CLA:HMB2 | 1.98                     | 0.44              |
| 31:A:832:CLA:H62  | 31:A:832:CLA:H93  | 1.70                     | 0.44              |
| 31:A:852:CLA:HMC1 | 31:B:838:CLA:HAC1 | 2.00                     | 0.44              |
| 12:E:54:ASN:ND2   | 18:C:61:ASP:HB2   | 2.32                     | 0.44              |
| 14:G:26:PHE:O     | 14:G:30:ASN:ND2   | 2.31                     | 0.44              |
| 16:J:26:ILE:HG21  | 32:J:104:8CT:C29  | 2.48                     | 0.44              |
| 17:L:40:ARG:HD2   | 27:H:80:ARG:HH11  | 1.82                     | 0.44              |
| 42:d:523:NEX:H401 | 42:d:523:NEX:H35  | 1.57                     | 0.44              |
| 26:f:128:MET:SD   | 31:f:610:CLA:HAB  | 2.58                     | 0.44              |
| 26:f:220:PRO:O    | 28:i:50:ARG:NH2   | 2.42                     | 0.44              |
| 28:i:259:TRP:CE2  | 28:i:263:ILE:HD11 | 2.51                     | 0.44              |
| 29:e:194:LYS:NZ   | 31:e:612:CLA:O1D  | 2.41                     | 0.44              |
| 30:e:608:CHL:H143 | 30:e:608:CHL:H161 | 1.77                     | 0.44              |
| 7:4:243:LEU:HD22  | 7:4:244:ALA:N     | 2.33                     | 0.44              |
| 1:0:161:LEU:HD23  | 31:0:310:CLA:HED2 | 1.99                     | 0.44              |
| 2:1:133:VAL:HG22  | 14:G:14:LEU:HD13  | 1.99                     | 0.44              |
| 4:3:218:THR:C     | 4:3:220:GLU:H     | 2.25                     | 0.44              |
| 31:7:315:CLA:H11  | 31:7:315:CLA:HBA1 | 1.78                     | 0.44              |
| 31:A:803:CLA:H193 | 31:B:803:CLA:H192 | 2.00                     | 0.44              |
| 31:A:826:CLA:HBA2 | 31:A:826:CLA:H3A  | 1.78                     | 0.44              |
| 10:B:430:GLY:HA2  | 10:B:525:LEU:HD22 | 1.99                     | 0.44              |
| 31:B:801:CLA:H111 | 31:B:801:CLA:H143 | 1.65                     | 0.44              |
| 25:d:120:GLN:HE22 | 30:d:607:CHL:CMC  | 2.31                     | 0.44              |
| 26:f:264:GLN:NE2  | 26:f:268:ASP:OD1  | 2.50                     | 0.44              |
| 30:f:601:CHL:H202 | 30:f:601:CHL:H161 | 1.71                     | 0.44              |
| 30:h:602:CHL:H91  | 30:h:602:CHL:H111 | 1.79                     | 0.44              |
| 27:H:76:GLU:OE1   | 27:H:76:GLU:N     | 2.49                     | 0.44              |
| 28:i:184:MET:CE   | 42:i:523:NEX:H30  | 2.40                     | 0.44              |
| 29:e:101:LYS:NZ   | 29:e:225:ALA:HB2  | 2.32                     | 0.44              |
| 7:4:98:LEU:HD13   | 7:4:211:PHE:HZ    | 1.82                     | 0.44              |
| 4:3:168:GLN:HE22  | 31:3:318:CLA:CHA  | 2.31                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:5:309:CLA:H102 | 31:5:311:CLA:HBC1 | 2.00                     | 0.44              |
| 31:A:803:CLA:H72  | 31:A:803:CLA:H112 | 1.75                     | 0.44              |
| 31:B:806:CLA:H92  | 31:B:806:CLA:H62  | 1.84                     | 0.44              |
| 31:B:818:CLA:H3A  | 31:B:818:CLA:HBA2 | 1.27                     | 0.44              |
| 22:a:217:THR:OG1  | 22:a:218:GLY:N    | 2.50                     | 0.44              |
| 31:c:613:CLA:H2   | 31:c:613:CLA:H61  | 1.55                     | 0.44              |
| 34:d:630:LHG:O3   | 34:d:630:LHG:O1   | 2.31                     | 0.44              |
| 25:g:101:TYR:HD2  | 25:g:107:LEU:HD13 | 1.82                     | 0.44              |
| 22:h:208:PHE:HD2  | 31:h:613:CLA:HMC1 | 1.83                     | 0.44              |
| 29:e:66:SER:O     | 29:e:66:SER:OG    | 2.27                     | 0.44              |
| 1:0:109:VAL:HG12  | 1:0:111:ILE:H     | 1.82                     | 0.44              |
| 2:1:114:TRP:HD1   | 2:1:118:GLY:O     | 2.01                     | 0.44              |
| 3:2:83:GLN:HE21   | 3:2:83:GLN:HB2    | 1.57                     | 0.44              |
| 31:6:317:CLA:HMB1 | 31:6:317:CLA:HBB1 | 2.00                     | 0.44              |
| 30:8:305:CHL:HBA1 | 32:8:402:8CT:C15  | 2.48                     | 0.44              |
| 8:9:213:VAL:HG11  | 34:G:105:LHG:H251 | 2.00                     | 0.44              |
| 10:B:86:PRO:HB3   | 10:B:121:TYR:CG   | 2.53                     | 0.44              |
| 23:c:109:GLY:HA2  | 29:e:132:GLN:HG3  | 2.00                     | 0.44              |
| 42:c:523:NEX:H11  | 42:c:523:NEX:H191 | 1.82                     | 0.44              |
| 24:b:140:VAL:HG21 | 24:b:148:ILE:HD12 | 1.99                     | 0.44              |
| 26:f:197:TYR:HB3  | 30:f:608:CHL:CMC  | 2.47                     | 0.44              |
| 42:f:523:NEX:H11  | 42:f:523:NEX:H191 | 1.82                     | 0.44              |
| 30:f:607:CHL:HHC  | 30:f:607:CHL:HBB1 | 1.99                     | 0.44              |
| 28:i:69:ARG:H     | 28:i:69:ARG:CD    | 2.28                     | 0.44              |
| 28:i:140:ASN:ND2  | 28:i:162:LEU:O    | 2.45                     | 0.44              |
| 28:i:230:GLU:HB3  | 31:i:610:CLA:C1B  | 2.48                     | 0.44              |
| 3:2:103:GLY:C     | 3:2:230:VAL:HG11  | 2.43                     | 0.44              |
| 30:2:319:CHL:HBB1 | 30:2:319:CHL:CHC  | 2.45                     | 0.44              |
| 31:A:821:CLA:H192 | 31:A:821:CLA:H162 | 1.84                     | 0.44              |
| 31:A:841:CLA:H112 | 31:A:841:CLA:H72  | 1.60                     | 0.44              |
| 10:B:397:ASP:HA   | 11:D:198:ILE:HD13 | 2.00                     | 0.44              |
| 10:B:582:TRP:O    | 10:B:586:THR:HG22 | 2.17                     | 0.44              |
| 31:B:820:CLA:HBC2 | 31:B:824:CLA:H72  | 2.00                     | 0.44              |
| 31:B:830:CLA:H42  | 41:B:849:DGD:HB42 | 1.99                     | 0.44              |
| 22:a:116:PHE:HD2  | 22:a:117:LYS:HG3  | 1.82                     | 0.44              |
| 25:d:119:THR:HG21 | 30:d:605:CHL:HBC1 | 1.99                     | 0.44              |
| 26:f:197:TYR:OH   | 42:f:523:NEX:H191 | 2.17                     | 0.44              |
| 22:h:52:TYR:OH    | 22:h:64:ASP:OD2   | 2.26                     | 0.44              |
| 7:4:98:LEU:O      | 7:4:102:LEU:N     | 2.43                     | 0.44              |
| 7:4:222:PRO:O     | 33:4:501:0UR:O39  | 2.36                     | 0.44              |
| 1:0:128:GLU:HG3   | 31:0:308:CLA:NB   | 2.32                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:1:219:ASN:ND2   | 31:1:312:CLA:OBD  | 2.50                     | 0.44              |
| 31:1:311:CLA:H41  | 31:1:311:CLA:H61  | 1.83                     | 0.44              |
| 3:2:185:ASP:OD1   | 33:2:501:0UR:O40  | 2.36                     | 0.44              |
| 8:9:45:PRO:HG3    | 14:G:54:TYR:HE1   | 1.83                     | 0.44              |
| 9:A:302:HIS:HB2   | 31:A:818:CLA:CHB  | 2.48                     | 0.44              |
| 10:B:352:MET:HE2  | 10:B:352:MET:HB3  | 1.87                     | 0.44              |
| 31:B:825:CLA:H18  | 31:B:825:CLA:H152 | 1.84                     | 0.44              |
| 24:b:88:MET:HE2   | 24:b:163:ARG:NH1  | 2.32                     | 0.44              |
| 30:g:609:CHL:HHC  | 30:g:609:CHL:HBB1 | 2.00                     | 0.44              |
| 2:5:158:PHE:HE1   | 30:5:307:CHL:HBA2 | 1.83                     | 0.43              |
| 30:8:315:CHL:HHC  | 30:8:315:CHL:HBB1 | 2.00                     | 0.43              |
| 8:9:159:MET:HG3   | 31:9:309:CLA:O1A  | 2.18                     | 0.43              |
| 9:A:519:ILE:HD13  | 9:A:632:VAL:HG21  | 1.99                     | 0.43              |
| 31:A:813:CLA:H93  | 31:A:813:CLA:H111 | 1.73                     | 0.43              |
| 10:B:174:ARG:HH11 | 31:B:808:CLA:H141 | 1.82                     | 0.43              |
| 10:B:325:THR:HG21 | 10:B:403:ASN:OD1  | 2.18                     | 0.43              |
| 10:B:378:ILE:O    | 10:B:382:MET:HG3  | 2.18                     | 0.43              |
| 31:B:811:CLA:CGA  | 31:B:811:CLA:C1A  | 2.97                     | 0.43              |
| 31:B:816:CLA:H51  | 31:B:816:CLA:H11  | 1.73                     | 0.43              |
| 31:B:826:CLA:HMA1 | 32:B:847:8CT:C17  | 2.47                     | 0.43              |
| 23:c:218:GLN:O    | 23:c:222:THR:N    | 2.52                     | 0.43              |
| 24:b:70:MET:HB3   | 24:b:72:LEU:HG    | 1.99                     | 0.43              |
| 33:b:520:0UR:C13  | 31:b:610:CLA:HAB  | 2.48                     | 0.43              |
| 42:b:523:NEX:H401 | 42:b:523:NEX:H35  | 1.58                     | 0.43              |
| 30:d:601:CHL:HBB1 | 30:d:601:CHL:HHC  | 1.99                     | 0.43              |
| 31:d:603:CLA:HBB1 | 30:d:609:CHL:H161 | 2.00                     | 0.43              |
| 42:f:523:NEX:H201 | 42:f:523:NEX:H15  | 1.62                     | 0.43              |
| 30:f:606:CHL:HMB1 | 30:f:609:CHL:HMC  | 1.99                     | 0.43              |
| 22:h:195:LYS:NZ   | 31:h:612:CLA:O1D  | 2.44                     | 0.43              |
| 29:e:151:GLY:HA2  | 30:e:609:CHL:HAB  | 2.00                     | 0.43              |
| 1:0:145:SER:OG    | 28:i:213:PRO:HA   | 2.18                     | 0.43              |
| 34:1:601:LHG:H151 | 34:1:601:LHG:H322 | 1.98                     | 0.43              |
| 4:3:76:TYR:HD2    | 30:3:302:CHL:HMD2 | 1.83                     | 0.43              |
| 2:5:44:TYR:OH     | 2:5:59:GLY:HA2    | 2.18                     | 0.43              |
| 7:8:222:PRO:O     | 33:8:501:0UR:O39  | 2.36                     | 0.43              |
| 9:A:700:GLU:OE1   | 10:B:536:LYS:NZ   | 2.48                     | 0.43              |
| 31:A:811:CLA:H202 | 31:A:811:CLA:H162 | 1.77                     | 0.43              |
| 31:A:828:CLA:H93  | 31:A:828:CLA:H62  | 1.77                     | 0.43              |
| 10:B:134:ASP:OD2  | 10:B:208:ARG:NE   | 2.49                     | 0.43              |
| 10:B:290:MET:CB   | 31:B:822:CLA:HBC3 | 2.46                     | 0.43              |
| 10:B:700:LEU:HD22 | 10:B:704:GLN:NE2  | 2.34                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:c:43:TRP:N     | 23:c:64:TYR:O     | 2.51                     | 0.43              |
| 25:g:185:VAL:HG11 | 31:g:613:CLA:HAC2 | 1.99                     | 0.43              |
| 42:g:523:NEX:H201 | 42:g:523:NEX:H15  | 1.62                     | 0.43              |
| 42:i:523:NEX:H383 | 31:i:604:CLA:C2B  | 2.46                     | 0.43              |
| 7:4:159:VAL:HG22  | 7:4:161:PRO:HD2   | 2.00                     | 0.43              |
| 7:4:171:ASN:HB2   | 7:4:178:GLY:HA2   | 1.99                     | 0.43              |
| 2:1:112:PRO:HG2   | 2:1:114:TRP:CZ2   | 2.53                     | 0.43              |
| 8:9:61:LEU:O      | 31:B:813:CLA:HBA1 | 2.18                     | 0.43              |
| 9:A:343:HIS:HB3   | 9:A:346:LEU:HD12  | 2.00                     | 0.43              |
| 10:B:347:MET:O    | 10:B:351:HIS:ND1  | 2.51                     | 0.43              |
| 31:B:825:CLA:H143 | 31:B:825:CLA:H161 | 1.80                     | 0.43              |
| 17:L:23:VAL:O     | 17:L:29:VAL:HG11  | 2.18                     | 0.43              |
| 31:K:102:CLA:C1D  | 34:K:106:LHG:H262 | 2.48                     | 0.43              |
| 24:b:148:ILE:HD13 | 30:b:606:CHL:HMD2 | 2.00                     | 0.43              |
| 25:g:160:GLU:CD   | 25:g:160:GLU:H    | 2.26                     | 0.43              |
| 22:h:33:TYR:CZ    | 22:h:190:ALA:HB1  | 2.53                     | 0.43              |
| 7:4:162:ILE:HD13  | 7:4:162:ILE:HA    | 1.87                     | 0.43              |
| 2:1:72:GLU:HG3    | 2:1:152:VAL:HG22  | 1.98                     | 0.43              |
| 30:6:315:CHL:HBB1 | 30:6:315:CHL:HHC  | 2.00                     | 0.43              |
| 6:7:246:ASP:OD1   | 6:7:246:ASP:N     | 2.52                     | 0.43              |
| 30:7:301:CHL:HHC  | 30:7:301:CHL:HBB1 | 1.99                     | 0.43              |
| 7:8:45:LEU:HB3    | 7:8:48:ALA:HB2    | 1.99                     | 0.43              |
| 7:8:136:GLN:HG3   | 7:8:137:PHE:N     | 2.33                     | 0.43              |
| 30:8:301:CHL:HBB2 | 30:8:302:CHL:HBC2 | 2.01                     | 0.43              |
| 10:B:128:GLY:O    | 10:B:208:ARG:NH2  | 2.51                     | 0.43              |
| 10:B:451:LYS:HB3  | 31:B:833:CLA:HED3 | 2.00                     | 0.43              |
| 10:B:697:PRO:HB3  | 31:B:839:CLA:C1C  | 2.49                     | 0.43              |
| 14:G:2:LEU:HD23   | 14:G:2:LEU:HA     | 1.92                     | 0.43              |
| 17:L:28:ILE:H     | 17:L:28:ILE:HD12  | 1.83                     | 0.43              |
| 17:L:69:PRO:HG3   | 31:H:201:CLA:HBA2 | 1.99                     | 0.43              |
| 23:c:91:TRP:CD1   | 30:c:609:CHL:HMD2 | 2.54                     | 0.43              |
| 26:f:241:GLY:O    | 26:f:245:MET:HG3  | 2.18                     | 0.43              |
| 25:g:51:GLU:HA    | 25:g:144:LEU:HD11 | 2.01                     | 0.43              |
| 31:3:306:CLA:H3A  | 31:3:306:CLA:HBA2 | 1.65                     | 0.43              |
| 2:5:225:PHE:HD1   | 2:5:225:PHE:H     | 1.66                     | 0.43              |
| 31:6:310:CLA:HAB  | 6:7:158:VAL:HG12  | 2.00                     | 0.43              |
| 6:7:136:MET:HA    | 6:7:139:VAL:HG22  | 2.00                     | 0.43              |
| 8:9:77:GLU:HB2    | 31:9:302:CLA:C1B  | 2.48                     | 0.43              |
| 31:9:303:CLA:HED2 | 31:9:303:CLA:H12  | 1.99                     | 0.43              |
| 9:A:540:VAL:HG11  | 9:A:614:HIS:CG    | 2.54                     | 0.43              |
| 10:B:282:VAL:HG21 | 31:B:817:CLA:HAB  | 2.01                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:B:652:PHE:O    | 10:B:656:VAL:HG23 | 2.19                     | 0.43              |
| 31:L:203:CLA:H143 | 31:L:203:CLA:H162 | 1.74                     | 0.43              |
| 42:g:523:NEX:H362 | 31:g:604:CLA:C3B  | 2.49                     | 0.43              |
| 7:4:58:ILE:HG22   | 7:4:59:PRO:HD2    | 2.00                     | 0.43              |
| 30:2:302:CHL:H161 | 30:2:302:CHL:H122 | 1.45                     | 0.43              |
| 4:3:195:VAL:HG23  | 4:3:208:ALA:HB3   | 1.99                     | 0.43              |
| 5:6:47:ASN:OD1    | 5:6:47:ASN:N      | 2.48                     | 0.43              |
| 5:6:204:ILE:HD13  | 31:6:312:CLA:HMD3 | 2.00                     | 0.43              |
| 9:A:458:PHE:CE1   | 31:A:802:CLA:HHB  | 2.54                     | 0.43              |
| 31:A:808:CLA:HBA2 | 31:A:808:CLA:H3A  | 1.38                     | 0.43              |
| 25:d:53:GLU:HB2   | 30:d:602:CHL:C1B  | 2.48                     | 0.43              |
| 22:h:110:PHE:CE1  | 22:h:131:LEU:HD23 | 2.54                     | 0.43              |
| 28:i:188:GLU:OE1  | 28:i:191:ARG:NE   | 2.39                     | 0.43              |
| 42:i:523:NEX:H222 | 31:i:604:CLA:NC   | 2.34                     | 0.43              |
| 30:0:302:CHL:H161 | 30:0:302:CHL:H122 | 1.54                     | 0.43              |
| 3:2:113:PRO:HG3   | 3:2:121:VAL:HG21  | 1.99                     | 0.43              |
| 3:2:135:MET:HB2   | 30:4:313:CHL:HED1 | 2.00                     | 0.43              |
| 4:3:137:TRP:C     | 4:3:139:ARG:H     | 2.27                     | 0.43              |
| 4:3:189:PHE:CZ    | 30:3:307:CHL:HBB2 | 2.54                     | 0.43              |
| 31:3:308:CLA:H3A  | 31:3:308:CLA:HBA2 | 1.32                     | 0.43              |
| 30:6:313:CHL:HAA2 | 6:7:131:PHE:HA    | 2.00                     | 0.43              |
| 6:7:142:ARG:NE    | 30:7:307:CHL:OMC  | 2.46                     | 0.43              |
| 9:A:145:ILE:HD12  | 31:A:808:CLA:CAD  | 2.48                     | 0.43              |
| 9:A:513:LEU:HB2   | 9:A:528:MET:HG3   | 1.99                     | 0.43              |
| 9:A:731:VAL:O     | 9:A:735:HIS:ND1   | 2.52                     | 0.43              |
| 10:B:275:HIS:HB3  | 31:B:818:CLA:HMB2 | 2.00                     | 0.43              |
| 10:B:290:MET:HE1  | 31:B:820:CLA:C3D  | 2.48                     | 0.43              |
| 17:L:40:ARG:HD2   | 27:H:80:ARG:NH1   | 2.33                     | 0.43              |
| 31:K:102:CLA:C4B  | 34:K:106:LHG:H311 | 2.49                     | 0.43              |
| 34:K:106:LHG:H172 | 34:K:106:LHG:H141 | 1.75                     | 0.43              |
| 30:a:602:CHL:HBC1 | 34:a:630:LHG:H262 | 2.00                     | 0.43              |
| 23:c:139:PHE:O    | 23:c:141:HIS:N    | 2.49                     | 0.43              |
| 26:f:59:ARG:N     | 27:H:72:MET:O     | 2.52                     | 0.43              |
| 22:h:40:TRP:HB3   | 22:h:61:TYR:HB3   | 2.00                     | 0.43              |
| 29:e:194:LYS:NZ   | 31:e:612:CLA:O1A  | 2.39                     | 0.43              |
| 2:5:42:PRO:HB2    | 2:5:44:TYR:CE2    | 2.53                     | 0.43              |
| 2:5:213:GLY:HA2   | 2:5:218:THR:HG21  | 1.98                     | 0.43              |
| 30:5:301:CHL:OBD  | 7:8:146:ARG:NH1   | 2.52                     | 0.43              |
| 7:8:181:ASP:OD1   | 33:8:501:OUR:O40  | 2.37                     | 0.43              |
| 8:9:152:PHE:CB    | 8:9:153:PRO:CD    | 2.95                     | 0.43              |
| 9:A:135:ASP:OD2   | 13:F:107:LYS:NZ   | 2.47                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:A:601:LEU:HB3   | 9:A:737:ILE:HD11  | 1.99                     | 0.43              |
| 10:B:378:ILE:HD13 | 31:B:829:CLA:CBB  | 2.48                     | 0.43              |
| 10:B:444:LEU:HD22 | 10:B:615:TYR:CZ   | 2.54                     | 0.43              |
| 10:B:686:PRO:HD2  | 31:L:201:CLA:HBA1 | 1.99                     | 0.43              |
| 18:C:55:GLU:HB3   | 18:C:63:LEU:HD13  | 2.01                     | 0.43              |
| 24:b:119:TRP:HD1  | 24:b:224:PRO:HD3  | 1.84                     | 0.43              |
| 25:d:110:ALA:HA   | 30:d:605:CHL:HHC  | 2.01                     | 0.43              |
| 25:g:53:GLU:HB2   | 30:g:602:CHL:CHB  | 2.49                     | 0.43              |
| 30:e:608:CHL:C4A  | 30:e:608:CHL:HBA2 | 2.49                     | 0.43              |
| 30:e:609:CHL:H91  | 30:e:609:CHL:H111 | 1.80                     | 0.43              |
| 7:4:137:PHE:CD2   | 30:4:308:CHL:HBB2 | 2.53                     | 0.43              |
| 31:1:303:CLA:H62  | 31:1:303:CLA:H41  | 1.59                     | 0.43              |
| 31:1:312:CLA:H42  | 30:1:313:CHL:HMD1 | 2.01                     | 0.43              |
| 3:2:107:ARG:NH1   | 3:2:231:ASP:OD1   | 2.49                     | 0.43              |
| 30:6:308:CHL:H111 | 30:6:308:CHL:H91  | 1.75                     | 0.43              |
| 8:9:94:CYS:HB3    | 8:9:99:ILE:O      | 2.19                     | 0.43              |
| 9:A:125:PRO:HA    | 9:A:130:GLU:HG3   | 2.01                     | 0.43              |
| 9:A:126:ILE:HG12  | 9:A:127:VAL:H     | 1.83                     | 0.43              |
| 9:A:183:TRP:HB2   | 31:A:811:CLA:HMC2 | 2.00                     | 0.43              |
| 9:A:729:ARG:NH2   | 40:B:802:SF4:S4   | 2.92                     | 0.43              |
| 31:A:826:CLA:H141 | 31:A:826:CLA:H161 | 1.70                     | 0.43              |
| 31:A:839:CLA:C4C  | 31:A:839:CLA:H51  | 2.48                     | 0.43              |
| 36:L:211:LMG:H111 | 36:L:211:LMG:H142 | 1.72                     | 0.43              |
| 25:d:125:GLY:HA2  | 30:d:609:CHL:HAB  | 2.01                     | 0.43              |
| 26:f:167:ASN:HB3  | 26:f:171:ASN:O    | 2.19                     | 0.43              |
| 25:g:130:TYR:O    | 25:g:134:GLY:N    | 2.52                     | 0.43              |
| 22:h:40:TRP:CE2   | 22:h:41:LEU:HG    | 2.53                     | 0.43              |
| 22:h:86:ALA:O     | 22:h:90:MET:HG2   | 2.19                     | 0.43              |
| 34:e:630:LHG:H292 | 34:e:630:LHG:HC92 | 1.99                     | 0.43              |
| 7:4:116:GLU:CD    | 7:4:116:GLU:H     | 2.25                     | 0.43              |
| 30:0:301:CHL:H43  | 31:0:312:CLA:H52  | 2.01                     | 0.43              |
| 2:1:145:GLU:HB3   | 2:1:151:ARG:HG3   | 2.00                     | 0.43              |
| 31:3:304:CLA:H112 | 31:3:304:CLA:H72  | 1.87                     | 0.43              |
| 31:6:318:CLA:HBA1 | 31:6:318:CLA:H3A  | 1.34                     | 0.43              |
| 9:A:716:PRO:HG2   | 9:A:720:PRO:HD3   | 2.00                     | 0.43              |
| 31:A:818:CLA:H122 | 31:A:818:CLA:H161 | 1.72                     | 0.43              |
| 39:A:857:CL0:H14  | 31:B:805:CLA:C1A  | 2.48                     | 0.43              |
| 24:b:199:GLU:HB2  | 31:b:610:CLA:C1B  | 2.49                     | 0.43              |
| 31:b:603:CLA:HED2 | 31:b:603:CLA:H2A  | 2.00                     | 0.43              |
| 25:d:131:ARG:HG3  | 30:d:608:CHL:C1D  | 2.49                     | 0.43              |
| 28:i:167:LEU:O    | 28:i:169:HIS:N    | 2.51                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:4:193:LEU:HD13  | 31:4:309:CLA:O1A  | 2.19                     | 0.43              |
| 4:3:92:GLY:O      | 4:3:95:ASN:ND2    | 2.52                     | 0.42              |
| 31:3:308:CLA:H92  | 31:3:308:CLA:H62  | 1.72                     | 0.42              |
| 5:6:235:THR:HA    | 30:6:306:CHL:O1A  | 2.19                     | 0.42              |
| 6:7:144:TRP:HB2   | 31:7:308:CLA:CMA  | 2.48                     | 0.42              |
| 31:7:308:CLA:H162 | 31:7:308:CLA:H121 | 1.41                     | 0.42              |
| 31:9:311:CLA:HBB1 | 31:9:311:CLA:HHC  | 2.01                     | 0.42              |
| 9:A:291:ASN:HB3   | 9:A:383:PRO:HA    | 2.01                     | 0.42              |
| 9:A:536:SER:O     | 9:A:540:VAL:HG23  | 2.18                     | 0.42              |
| 9:A:719:GLN:NE2   | 12:E:19:TYR:OH    | 2.52                     | 0.42              |
| 31:A:809:CLA:H62  | 31:A:809:CLA:H101 | 1.65                     | 0.42              |
| 10:B:240:ILE:HA   | 10:B:263:PRO:HG2  | 2.00                     | 0.42              |
| 31:B:812:CLA:HBA2 | 31:B:812:CLA:H3A  | 1.87                     | 0.42              |
| 14:G:41:LEU:HD12  | 14:G:45:GLU:HB3   | 2.01                     | 0.42              |
| 17:L:3:GLN:OE1    | 21:O:131:ARG:HB2  | 2.18                     | 0.42              |
| 20:M:23:LEU:HD11  | 34:M:104:LHG:H371 | 2.00                     | 0.42              |
| 22:a:48:ALA:HB2   | 23:c:164:CYS:HB3  | 2.01                     | 0.42              |
| 22:a:98:THR:HB    | 22:a:99:PRO:HD3   | 2.01                     | 0.42              |
| 22:a:169:ASP:HB3  | 22:a:173:PRO:HA   | 2.01                     | 0.42              |
| 22:a:202:LEU:HA   | 34:a:630:LHG:H272 | 2.01                     | 0.42              |
| 23:c:86:VAL:HG21  | 23:c:176:LEU:HD13 | 2.01                     | 0.42              |
| 26:f:174:LEU:O    | 26:f:176:HIS:N    | 2.52                     | 0.42              |
| 26:f:191:MET:HE1  | 42:f:523:NEX:H30  | 2.01                     | 0.42              |
| 30:h:609:CHL:H2A  | 28:i:96:THR:HG21  | 2.01                     | 0.42              |
| 29:e:133:LEU:O    | 29:e:135:HIS:N    | 2.52                     | 0.42              |
| 1:0:74:ALA:O      | 1:0:78:ASN:ND2    | 2.37                     | 0.42              |
| 2:1:80:TRP:CD1    | 31:1:308:CLA:HMD3 | 2.54                     | 0.42              |
| 9:A:120:ALA:N     | 9:A:145:ILE:HG12  | 2.34                     | 0.42              |
| 10:B:583:MET:HG2  | 31:B:826:CLA:HBC1 | 2.00                     | 0.42              |
| 31:B:832:CLA:H62  | 31:B:832:CLA:H2   | 1.70                     | 0.42              |
| 18:C:73:THR:N     | 18:C:76:SER:OG    | 2.44                     | 0.42              |
| 24:b:157:GLY:CA   | 30:b:609:CHL:HAB  | 2.49                     | 0.42              |
| 34:b:630:LHG:H242 | 34:b:630:LHG:HC62 | 1.68                     | 0.42              |
| 28:i:121:MET:HB2  | 33:i:520:OUR:C10  | 2.48                     | 0.42              |
| 28:i:208:GLY:O    | 28:i:212:ASP:N    | 2.41                     | 0.42              |
| 29:e:111:VAL:HG23 | 29:e:113:PHE:O    | 2.19                     | 0.42              |
| 4:3:189:PHE:CE2   | 30:3:307:CHL:HBB2 | 2.53                     | 0.42              |
| 2:5:85:VAL:HG13   | 2:5:189:PHE:CE2   | 2.53                     | 0.42              |
| 9:A:27:THR:O      | 9:A:187:HIS:ND1   | 2.42                     | 0.42              |
| 9:A:296:LEU:HD23  | 9:A:299:ILE:HD12  | 2.00                     | 0.42              |
| 9:A:548:ILE:HD11  | 31:A:836:CLA:HBB1 | 2.01                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:A:818:CLA:H203 | 31:A:818:CLA:H162 | 1.81                     | 0.42              |
| 32:B:804:8CT:C20  | 31:B:832:CLA:H3A  | 2.49                     | 0.42              |
| 15:I:4:ALA:O      | 15:I:7:PRO:HD2    | 2.20                     | 0.42              |
| 31:a:603:CLA:HAC2 | 30:a:607:CHL:H152 | 2.01                     | 0.42              |
| 42:c:523:NEX:C39  | 30:c:606:CHL:HMB2 | 2.47                     | 0.42              |
| 30:c:609:CHL:H61  | 30:c:609:CHL:H92  | 1.81                     | 0.42              |
| 26:f:79:LEU:HD23  | 26:f:85:THR:HB    | 2.01                     | 0.42              |
| 30:e:601:CHL:H12  | 34:e:630:LHG:H161 | 2.00                     | 0.42              |
| 1:0:175:VAL:HG12  | 31:0:312:CLA:HAC1 | 2.01                     | 0.42              |
| 2:5:60:ILE:HB     | 30:5:302:CHL:O1A  | 2.19                     | 0.42              |
| 6:7:142:ARG:HE    | 30:7:307:CHL:CMC  | 2.29                     | 0.42              |
| 34:A:844:LHG:O3   | 34:A:844:LHG:O1   | 2.28                     | 0.42              |
| 31:B:811:CLA:H91  | 31:B:811:CLA:H112 | 1.72                     | 0.42              |
| 13:F:216:TRP:CG   | 13:F:217:PRO:HD3  | 2.54                     | 0.42              |
| 14:G:5:SER:HA     | 31:G:102:CLA:OBD  | 2.20                     | 0.42              |
| 22:a:163:GLY:HA3  | 22:a:168:GLU:HG2  | 2.02                     | 0.42              |
| 30:c:608:CHL:C4A  | 30:c:608:CHL:HBA2 | 2.49                     | 0.42              |
| 24:b:76:PRO:O     | 24:b:80:GLU:HG2   | 2.20                     | 0.42              |
| 30:d:602:CHL:H143 | 30:d:602:CHL:H112 | 1.66                     | 0.42              |
| 31:f:613:CLA:H2   | 31:f:613:CLA:H61  | 1.74                     | 0.42              |
| 28:i:119:TRP:CD1  | 30:i:609:CHL:HMD3 | 2.53                     | 0.42              |
| 28:i:183:LEU:HB3  | 42:i:523:NEX:C15  | 2.50                     | 0.42              |
| 1:0:169:LEU:HD13  | 31:0:310:CLA:HBC1 | 2.02                     | 0.42              |
| 2:5:139:GLU:HG3   | 31:5:308:CLA:NB   | 2.34                     | 0.42              |
| 8:9:212:ASN:ND2   | 31:9:312:CLA:OBD  | 2.51                     | 0.42              |
| 31:A:815:CLA:H161 | 31:A:815:CLA:H141 | 1.60                     | 0.42              |
| 31:A:832:CLA:H151 | 31:A:832:CLA:H112 | 1.83                     | 0.42              |
| 10:B:280:ILE:HD13 | 10:B:280:ILE:HA   | 1.90                     | 0.42              |
| 10:B:662:MET:HB2  | 31:B:806:CLA:C1C  | 2.49                     | 0.42              |
| 31:B:810:CLA:HMA1 | 31:B:811:CLA:CHB  | 2.49                     | 0.42              |
| 31:B:811:CLA:H111 | 31:B:811:CLA:H142 | 1.77                     | 0.42              |
| 31:B:833:CLA:H92  | 16:J:25:LEU:HD21  | 2.02                     | 0.42              |
| 13:F:222:ASN:HB3  | 7:4:75:THR:HG21   | 2.00                     | 0.42              |
| 24:b:86:GLU:HB2   | 30:b:602:CHL:CHB  | 2.49                     | 0.42              |
| 25:g:183:PHE:CE1  | 25:g:194:PRO:HB3  | 2.54                     | 0.42              |
| 31:2:312:CLA:H2   | 30:2:313:CHL:HMD1 | 2.01                     | 0.42              |
| 31:3:303:CLA:H42  | 31:A:810:CLA:H11  | 2.00                     | 0.42              |
| 31:7:309:CLA:H3A  | 31:7:309:CLA:HBA2 | 1.51                     | 0.42              |
| 31:A:829:CLA:H91  | 31:A:829:CLA:H111 | 1.69                     | 0.42              |
| 38:A:842:PQN:H222 | 31:A:853:CLA:C1B  | 2.50                     | 0.42              |
| 10:B:276:HIS:HB2  | 31:B:818:CLA:CHB  | 2.50                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:B:817:CLA:H61  | 31:B:817:CLA:H41  | 1.77                     | 0.42              |
| 31:B:827:CLA:H162 | 31:B:827:CLA:H202 | 1.74                     | 0.42              |
| 31:L:204:CLA:HBA1 | 31:L:204:CLA:H3A  | 1.78                     | 0.42              |
| 18:C:32:ASP:N     | 18:C:32:ASP:OD1   | 2.51                     | 0.42              |
| 23:c:222:THR:HA   | 23:c:247:VAL:HG13 | 2.01                     | 0.42              |
| 25:g:12:LEU:HB2   | 25:g:16:SER:HA    | 2.00                     | 0.42              |
| 28:i:117:ALA:O    | 28:i:121:MET:HG2  | 2.18                     | 0.42              |
| 2:1:88:MET:HE1    | 2:1:186:PHE:HD1   | 1.85                     | 0.42              |
| 4:3:249:LEU:O     | 4:3:277:VAL:HA    | 2.19                     | 0.42              |
| 31:7:317:CLA:CGD  | 31:7:317:CLA:HBA2 | 2.49                     | 0.42              |
| 7:8:138:LEU:HD13  | 7:8:138:LEU:HA    | 1.93                     | 0.42              |
| 31:A:843:CLA:CHC  | 34:A:845:LHG:HC32 | 2.49                     | 0.42              |
| 10:B:181:GLY:HA3  | 31:B:814:CLA:HBB1 | 2.00                     | 0.42              |
| 10:B:257:PHE:HZ   | 31:B:818:CLA:H71  | 1.83                     | 0.42              |
| 42:a:523:NEX:H401 | 42:a:523:NEX:H35  | 1.58                     | 0.42              |
| 24:b:83:ARG:O     | 24:b:87:VAL:HG23  | 2.18                     | 0.42              |
| 26:f:72:TRP:HH2   | 31:f:611:CLA:HMA3 | 1.84                     | 0.42              |
| 22:h:115:TRP:CD1  | 22:h:221:PRO:HD3  | 2.51                     | 0.42              |
| 22:h:202:LEU:HD23 | 34:h:630:LHG:H271 | 2.01                     | 0.42              |
| 7:4:72:ASP:HB2    | 7:4:75:THR:OG1    | 2.20                     | 0.42              |
| 31:0:321:CLA:HAB  | 15:I:21:ILE:CG2   | 2.49                     | 0.42              |
| 2:1:82:MET:SD     | 31:1:309:CLA:HAB  | 2.60                     | 0.42              |
| 31:2:314:CLA:HBC1 | 4:3:161:PHE:HB2   | 2.02                     | 0.42              |
| 8:9:157:LEU:O     | 8:9:159:MET:HG2   | 2.19                     | 0.42              |
| 9:A:325:HIS:HB3   | 9:A:330:ILE:HD11  | 2.02                     | 0.42              |
| 9:A:330:ILE:O     | 9:A:334:HIS:ND1   | 2.52                     | 0.42              |
| 31:A:828:CLA:H3A  | 31:A:828:CLA:HBA2 | 1.88                     | 0.42              |
| 31:A:840:CLA:H142 | 31:A:840:CLA:H111 | 1.71                     | 0.42              |
| 31:A:843:CLA:HED2 | 21:O:125:GLN:NE2  | 2.35                     | 0.42              |
| 10:B:427:LEU:HD23 | 31:B:801:CLA:HBA2 | 2.02                     | 0.42              |
| 10:B:507:SER:HA   | 10:B:510:LEU:HD21 | 2.02                     | 0.42              |
| 13:F:232:LYS:HG3  | 13:F:234:GLU:OE1  | 2.20                     | 0.42              |
| 19:K:2:PHE:CD2    | 34:K:106:LHG:HC61 | 2.55                     | 0.42              |
| 34:a:630:LHG:H291 | 34:a:630:LHG:H261 | 1.87                     | 0.42              |
| 24:b:68:ASP:O     | 24:b:69:THR:C     | 2.63                     | 0.42              |
| 42:i:523:NEX:H201 | 42:i:523:NEX:H15  | 1.62                     | 0.42              |
| 30:i:602:CHL:H92  | 30:i:602:CHL:H62  | 1.71                     | 0.42              |
| 30:e:602:CHL:H92  | 30:e:602:CHL:H62  | 1.77                     | 0.42              |
| 30:4:308:CHL:H3A  | 30:4:308:CHL:HBA1 | 1.78                     | 0.42              |
| 1:0:107:VAL:HG22  | 31:0:304:CLA:HED3 | 2.02                     | 0.42              |
| 30:1:302:CHL:H143 | 30:1:302:CHL:H162 | 1.72                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:2:310:CLA:H61  | 31:2:310:CLA:H92  | 1.62                     | 0.42              |
| 4:3:254:PRO:O     | 33:3:501:OUR:O39  | 2.37                     | 0.42              |
| 7:8:172:ILE:HD13  | 7:8:172:ILE:HA    | 1.88                     | 0.42              |
| 9:A:364:LEU:HD21  | 31:A:821:CLA:H71  | 2.01                     | 0.42              |
| 9:A:681:HIS:HB3   | 31:B:803:CLA:HBD  | 2.02                     | 0.42              |
| 10:B:175:LEU:HD21 | 31:B:820:CLA:HMA2 | 2.02                     | 0.42              |
| 31:B:819:CLA:HBA2 | 31:B:819:CLA:H3A  | 1.48                     | 0.42              |
| 31:B:826:CLA:HMB3 | 31:B:827:CLA:H193 | 2.01                     | 0.42              |
| 31:B:833:CLA:HMA2 | 36:J:105:LMG:H332 | 2.01                     | 0.42              |
| 13:F:135:SER:HB2  | 16:J:38:ILE:HD11  | 2.01                     | 0.42              |
| 14:G:28:ARG:NH2   | 14:G:70:ASP:OD2   | 2.43                     | 0.42              |
| 17:L:10:ILE:HB    | 17:L:18:MET:HB3   | 2.02                     | 0.42              |
| 22:a:142:ILE:HA   | 22:a:145:ILE:HG12 | 2.02                     | 0.42              |
| 23:c:146:LEU:H    | 23:c:146:LEU:HD12 | 1.85                     | 0.42              |
| 24:b:240:GLY:N    | 31:b:613:CLA:O1A  | 2.53                     | 0.42              |
| 25:d:87:PHE:HE1   | 25:d:88:LYS:HE3   | 1.85                     | 0.42              |
| 42:d:523:NEX:H31  | 30:d:606:CHL:CBA  | 2.47                     | 0.42              |
| 42:i:523:NEX:H11  | 42:i:523:NEX:H191 | 1.82                     | 0.42              |
| 31:i:604:CLA:H43  | 30:i:606:CHL:O1A  | 2.20                     | 0.42              |
| 30:i:606:CHL:CMB  | 30:i:609:CHL:HAC1 | 2.48                     | 0.42              |
| 7:4:181:ASP:OD1   | 7:4:185:PHE:HB2   | 2.20                     | 0.42              |
| 1:0:198:ASP:OD1   | 1:0:198:ASP:N     | 2.53                     | 0.42              |
| 2:1:113:THR:HG21  | 30:1:305:CHL:CMD  | 2.47                     | 0.42              |
| 3:2:143:TRP:O     | 3:2:147:MET:HG3   | 2.20                     | 0.42              |
| 3:2:178:TYR:HB3   | 31:2:309:CLA:HED2 | 2.01                     | 0.42              |
| 30:5:301:CHL:HBB2 | 30:5:302:CHL:HHB  | 2.01                     | 0.42              |
| 6:7:129:LEU:HD13  | 30:7:306:CHL:HBC3 | 2.02                     | 0.42              |
| 30:7:302:CHL:H101 | 30:7:302:CHL:H62  | 1.86                     | 0.42              |
| 7:8:167:LEU:HD23  | 7:8:169:ASP:H     | 1.85                     | 0.42              |
| 7:8:229:HIS:ND1   | 7:8:236:ASN:O     | 2.37                     | 0.42              |
| 30:9:301:CHL:CGA  | 34:9:601:LHG:H142 | 2.50                     | 0.42              |
| 31:A:820:CLA:H92  | 31:A:820:CLA:H61  | 1.82                     | 0.42              |
| 31:A:837:CLA:H62  | 31:A:837:CLA:H41  | 1.66                     | 0.42              |
| 31:A:843:CLA:HBD  | 21:O:125:GLN:HG3  | 2.01                     | 0.42              |
| 10:B:105:THR:OG1  | 27:H:137:GLY:HA2  | 2.19                     | 0.42              |
| 22:a:143:LEU:O    | 22:a:147:TRP:HD1  | 2.03                     | 0.42              |
| 22:a:192:LEU:HG   | 31:a:610:CLA:HHB  | 2.02                     | 0.42              |
| 26:f:142:LYS:NZ   | 26:f:264:GLN:OE1  | 2.51                     | 0.42              |
| 30:f:601:CHL:HMD2 | 34:f:630:LHG:H251 | 2.02                     | 0.42              |
| 28:i:58:ASP:OD1   | 28:i:58:ASP:N     | 2.53                     | 0.42              |
| 42:i:523:NEX:H362 | 31:i:604:CLA:HAB  | 2.02                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 29:e:134:VAL:N    | 30:e:605:CHL:O1D  | 2.41                     | 0.42              |
| 30:e:606:CHL:HBC2 | 30:e:607:CHL:HHD  | 2.01                     | 0.42              |
| 31:0:312:CLA:H93  | 31:0:312:CLA:H62  | 1.79                     | 0.41              |
| 2:1:65:ALA:O      | 2:1:68:GLU:HG3    | 2.20                     | 0.41              |
| 34:5:601:LHG:H132 | 34:5:601:LHG:H322 | 2.02                     | 0.41              |
| 9:A:661:GLN:O     | 9:A:665:SER:HB3   | 2.19                     | 0.41              |
| 31:A:830:CLA:H62  | 31:A:830:CLA:H41  | 1.74                     | 0.41              |
| 10:B:35:ASP:OD1   | 10:B:36:SER:N     | 2.53                     | 0.41              |
| 10:B:183:PHE:CE2  | 31:B:814:CLA:H72  | 2.55                     | 0.41              |
| 31:B:809:CLA:H43  | 41:B:849:DGD:HB51 | 2.01                     | 0.41              |
| 31:B:829:CLA:HBA2 | 31:B:829:CLA:H3A  | 1.70                     | 0.41              |
| 11:D:156:ARG:HB2  | 11:D:166:LEU:HD11 | 2.01                     | 0.41              |
| 34:G:105:LHG:H271 | 34:G:105:LHG:H241 | 1.85                     | 0.41              |
| 21:O:55:PRO:HB3   | 31:O:206:CLA:OBD  | 2.20                     | 0.41              |
| 23:c:233:HIS:ND1  | 31:c:613:CLA:HAA2 | 2.35                     | 0.41              |
| 42:d:523:NEX:H28  | 30:d:606:CHL:HBA2 | 2.02                     | 0.41              |
| 30:d:609:CHL:H91  | 30:d:609:CHL:H111 | 1.77                     | 0.41              |
| 22:h:88:TRP:O     | 37:h:521:OIE:O29  | 2.38                     | 0.41              |
| 28:i:99:LEU:HB2   | 30:i:602:CHL:H11  | 2.02                     | 0.41              |
| 2:1:63:ASN:HD22   | 10:B:311:PRO:HB2  | 1.85                     | 0.41              |
| 5:6:164:LEU:HD23  | 5:6:164:LEU:HA    | 1.91                     | 0.41              |
| 6:7:257:LEU:HA    | 30:7:306:CHL:O1A  | 2.20                     | 0.41              |
| 30:7:307:CHL:HBA2 | 30:7:307:CHL:H3A  | 1.65                     | 0.41              |
| 7:8:137:PHE:CD2   | 30:8:308:CHL:HBB2 | 2.55                     | 0.41              |
| 31:A:821:CLA:H141 | 31:A:821:CLA:H161 | 1.75                     | 0.41              |
| 11:D:137:CYS:O    | 11:D:141:THR:HG23 | 2.20                     | 0.41              |
| 12:E:15:ARG:HD2   | 12:E:18:SER:HB2   | 2.02                     | 0.41              |
| 14:G:38:GLN:O     | 14:G:40:GLY:N     | 2.53                     | 0.41              |
| 23:c:117:VAL:HG23 | 23:c:120:SER:HB2  | 2.02                     | 0.41              |
| 30:c:601:CHL:C1D  | 34:c:630:LHG:HC81 | 2.50                     | 0.41              |
| 31:c:603:CLA:HBB1 | 30:c:609:CHL:H161 | 2.02                     | 0.41              |
| 34:d:630:LHG:H271 | 34:d:630:LHG:H242 | 1.75                     | 0.41              |
| 26:f:125:ARG:HA   | 26:f:128:MET:HE3  | 2.02                     | 0.41              |
| 42:h:523:NEX:H15  | 42:h:523:NEX:H201 | 1.62                     | 0.41              |
| 28:i:150:GLY:HA2  | 30:i:606:CHL:HBC1 | 2.03                     | 0.41              |
| 6:7:193:LYS:O     | 6:7:197:ASN:ND2   | 2.27                     | 0.41              |
| 8:9:193:PRO:O     | 33:9:501:OUR:O39  | 2.38                     | 0.41              |
| 9:A:195:TRP:CZ2   | 31:A:810:CLA:HMA1 | 2.54                     | 0.41              |
| 9:A:222:GLN:HA    | 9:A:226:SER:HB2   | 2.03                     | 0.41              |
| 9:A:225:LEU:HD11  | 31:A:814:CLA:C2D  | 2.50                     | 0.41              |
| 10:B:90:ALA:HA    | 10:B:113:VAL:HG12 | 2.03                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:B:808:CLA:H62  | 31:B:814:CLA:H2   | 2.02                     | 0.41              |
| 15:I:21:ILE:HD11  | 27:H:107:PHE:HD1  | 1.85                     | 0.41              |
| 24:b:102:VAL:HG11 | 31:b:604:CLA:HAC2 | 2.00                     | 0.41              |
| 42:b:523:NEX:H201 | 42:b:523:NEX:H15  | 1.62                     | 0.41              |
| 29:e:36:LEU:HD22  | 29:e:46:VAL:HG21  | 2.01                     | 0.41              |
| 31:0:321:CLA:HBA1 | 31:0:321:CLA:H3A  | 1.33                     | 0.41              |
| 31:1:312:CLA:H93  | 31:1:312:CLA:H111 | 1.72                     | 0.41              |
| 2:5:191:LEU:HD12  | 31:5:312:CLA:HAC2 | 2.01                     | 0.41              |
| 6:7:156:ASP:OD1   | 6:7:158:VAL:N     | 2.52                     | 0.41              |
| 31:9:309:CLA:H92  | 31:9:309:CLA:H61  | 1.73                     | 0.41              |
| 9:A:99:HIS:CE1    | 31:A:807:CLA:NA   | 2.88                     | 0.41              |
| 31:B:801:CLA:H162 | 31:B:801:CLA:H193 | 1.83                     | 0.41              |
| 23:c:65:GLY:N     | 30:c:602:CHL:OBD  | 2.54                     | 0.41              |
| 31:i:611:CLA:HAC1 | 34:i:630:LHG:H291 | 2.02                     | 0.41              |
| 1:0:148:PRO:O     | 1:0:150:ASP:N     | 2.54                     | 0.41              |
| 31:3:304:CLA:H172 | 30:7:302:CHL:H161 | 2.03                     | 0.41              |
| 31:5:304:CLA:C4A  | 31:5:304:CLA:HBA2 | 2.50                     | 0.41              |
| 31:7:309:CLA:H61  | 31:7:309:CLA:H41  | 1.81                     | 0.41              |
| 30:8:308:CHL:HHC  | 30:8:308:CHL:HBB1 | 2.02                     | 0.41              |
| 9:A:412:ALA:HB2   | 9:A:597:VAL:HG11  | 2.01                     | 0.41              |
| 9:A:481:THR:O     | 9:A:483:GLN:HG3   | 2.19                     | 0.41              |
| 31:A:827:CLA:H61  | 31:A:827:CLA:H2   | 1.76                     | 0.41              |
| 10:B:497:TRP:CD1  | 31:B:818:CLA:H11  | 2.56                     | 0.41              |
| 11:D:104:TRP:NE1  | 11:D:122:MET:SD   | 2.88                     | 0.41              |
| 31:L:203:CLA:HBA2 | 31:L:203:CLA:H3A  | 1.65                     | 0.41              |
| 18:C:15:THR:HG22  | 18:C:28:MET:HG3   | 2.03                     | 0.41              |
| 30:a:608:CHL:C4A  | 30:a:608:CHL:HBA2 | 2.50                     | 0.41              |
| 23:c:217:VAL:HG12 | 31:c:613:CLA:HMD3 | 2.02                     | 0.41              |
| 30:c:608:CHL:H2   | 30:c:608:CHL:H61  | 1.65                     | 0.41              |
| 30:b:602:CHL:H143 | 30:b:602:CHL:H112 | 1.85                     | 0.41              |
| 30:b:608:CHL:HAA2 | 30:b:608:CHL:H172 | 2.03                     | 0.41              |
| 25:d:90:GLY:HA2   | 30:d:606:CHL:HAC2 | 2.02                     | 0.41              |
| 25:d:153:MET:HE2  | 25:d:153:MET:HB2  | 1.97                     | 0.41              |
| 25:g:38:GLY:HA3   | 28:i:108:ARG:HG3  | 2.02                     | 0.41              |
| 31:H:201:CLA:O1D  | 31:H:201:CLA:H2   | 2.21                     | 0.41              |
| 31:0:312:CLA:H2   | 31:0:313:CLA:CMC  | 2.51                     | 0.41              |
| 4:3:270:ILE:HD13  | 31:3:312:CLA:H42  | 2.02                     | 0.41              |
| 5:6:149:ALA:HB2   | 31:6:309:CLA:HBD  | 2.02                     | 0.41              |
| 8:9:61:LEU:HB3    | 31:B:813:CLA:HBA1 | 2.03                     | 0.41              |
| 9:A:310:PHE:CE1   | 31:A:821:CLA:HAB  | 2.55                     | 0.41              |
| 31:A:819:CLA:CAD  | 31:A:829:CLA:H41  | 2.51                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:A:828:CLA:H72  | 32:A:850:8CT:C28  | 2.51                     | 0.41              |
| 31:A:841:CLA:H191 | 17:L:56:HIS:HD2   | 1.85                     | 0.41              |
| 10:B:157:LEU:HD12 | 10:B:157:LEU:HA   | 1.76                     | 0.41              |
| 10:B:533:ILE:HG12 | 31:B:801:CLA:HMD3 | 2.03                     | 0.41              |
| 31:B:817:CLA:C1D  | 31:B:818:CLA:HBB2 | 2.50                     | 0.41              |
| 42:a:523:NEX:H191 | 42:a:523:NEX:H11  | 1.82                     | 0.41              |
| 24:b:128:ASP:OD1  | 24:b:129:SER:N    | 2.45                     | 0.41              |
| 30:b:601:CHL:H112 | 30:b:601:CHL:H91  | 1.66                     | 0.41              |
| 25:g:109:HIS:HB3  | 30:g:605:CHL:HMA3 | 2.03                     | 0.41              |
| 22:h:40:TRP:N     | 22:h:61:TYR:HB3   | 2.35                     | 0.41              |
| 22:h:136:LEU:O    | 22:h:138:HIS:N    | 2.54                     | 0.41              |
| 28:i:150:GLY:HA3  | 30:i:607:CHL:C3D  | 2.51                     | 0.41              |
| 29:e:101:LYS:HZ2  | 29:e:225:ALA:HB2  | 1.85                     | 0.41              |
| 1:0:150:ASP:C     | 1:0:152:LEU:N     | 2.79                     | 0.41              |
| 31:0:312:CLA:H42  | 31:0:312:CLA:C4C  | 2.50                     | 0.41              |
| 31:0:321:CLA:HAB  | 15:I:21:ILE:HG21  | 2.02                     | 0.41              |
| 2:1:106:VAL:HG12  | 2:1:114:TRP:HZ3   | 1.86                     | 0.41              |
| 4:3:225:MET:HE1   | 31:3:311:CLA:HBA2 | 2.03                     | 0.41              |
| 4:3:261:HIS:ND1   | 4:3:268:ASN:O     | 2.36                     | 0.41              |
| 31:5:312:CLA:HMB1 | 30:5:313:CHL:HAC2 | 2.03                     | 0.41              |
| 7:8:161:PRO:HD2   | 7:8:164:GLY:O     | 2.20                     | 0.41              |
| 9:A:582:GLY:HA2   | 10:B:562:PRO:HD3  | 2.02                     | 0.41              |
| 31:A:818:CLA:H3A  | 31:A:818:CLA:CGA  | 2.48                     | 0.41              |
| 31:A:821:CLA:H62  | 31:A:821:CLA:H2   | 1.77                     | 0.41              |
| 31:B:818:CLA:H43  | 31:B:834:CLA:HED3 | 2.02                     | 0.41              |
| 31:F:301:CLA:HBA1 | 31:F:301:CLA:H3A  | 1.60                     | 0.41              |
| 31:K:104:CLA:CAC  | 30:c:601:CHL:HMC  | 2.45                     | 0.41              |
| 36:O:207:LMG:H142 | 36:O:207:LMG:H292 | 2.01                     | 0.41              |
| 22:a:93:VAL:HG11  | 33:a:520:0UR:C6   | 2.51                     | 0.41              |
| 23:c:230:TRP:NE1  | 30:c:614:CHL:HMC  | 2.35                     | 0.41              |
| 30:c:602:CHL:H111 | 30:c:602:CHL:H91  | 1.72                     | 0.41              |
| 25:g:29:PRO:HG2   | 25:g:166:LYS:HE2  | 2.02                     | 0.41              |
| 25:g:69:THR:OG1   | 25:g:70:PRO:HD3   | 2.20                     | 0.41              |
| 22:h:63:TRP:HZ3   | 30:h:602:CHL:HBC2 | 1.83                     | 0.41              |
| 27:H:76:GLU:H     | 27:H:76:GLU:CD    | 2.27                     | 0.41              |
| 2:1:83:LEU:HD23   | 2:1:83:LEU:HA     | 1.92                     | 0.41              |
| 31:6:317:CLA:H151 | 6:7:129:LEU:HD11  | 2.02                     | 0.41              |
| 30:7:305:CHL:HMB1 | 31:7:308:CLA:HBC2 | 2.03                     | 0.41              |
| 31:7:308:CLA:H91  | 31:7:308:CLA:H111 | 1.68                     | 0.41              |
| 31:A:813:CLA:C3B  | 31:A:813:CLA:H142 | 2.51                     | 0.41              |
| 31:A:825:CLA:H161 | 31:A:825:CLA:H141 | 1.78                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:A:852:CLA:H122 | 31:A:852:CLA:H161 | 1.89                     | 0.41              |
| 10:B:439:HIS:CD2  | 10:B:453:ILE:HG13 | 2.56                     | 0.41              |
| 10:B:548:PRO:HD2  | 18:C:62:PHE:CE1   | 2.56                     | 0.41              |
| 31:B:834:CLA:HBA2 | 31:B:834:CLA:H3A  | 1.49                     | 0.41              |
| 31:O:206:CLA:OBD  | 31:f:611:CLA:HBA1 | 2.21                     | 0.41              |
| 22:a:37:ARG:HB3   | 22:a:38:ALA:H     | 1.70                     | 0.41              |
| 25:d:8:ARG:NH2    | 25:d:31:ASP:OD1   | 2.53                     | 0.41              |
| 25:g:73:LEU:O     | 25:g:78:GLY:N     | 2.47                     | 0.41              |
| 30:g:602:CHL:HAC2 | 34:g:630:LHG:H252 | 2.02                     | 0.41              |
| 1:0:162:LYS:O     | 1:0:166:ASN:ND2   | 2.26                     | 0.41              |
| 31:0:303:CLA:H141 | 31:0:303:CLA:H162 | 1.76                     | 0.41              |
| 2:1:53:TYR:HB2    | 30:1:302:CHL:HMD3 | 2.03                     | 0.41              |
| 30:1:307:CHL:H2   | 30:1:307:CHL:H61  | 1.79                     | 0.41              |
| 2:5:140:ALA:O     | 2:5:144:SER:OG    | 2.25                     | 0.41              |
| 5:6:21:PRO:HD2    | 30:6:301:CHL:O2D  | 2.21                     | 0.41              |
| 5:6:93:LEU:HD13   | 5:6:97:ILE:HG23   | 2.03                     | 0.41              |
| 6:7:124:ASN:O     | 6:7:125:LEU:HB2   | 2.21                     | 0.41              |
| 7:8:94:LEU:HD22   | 33:8:501:0UR:C6   | 2.51                     | 0.41              |
| 8:9:148:LEU:O     | 8:9:150:ASP:N     | 2.54                     | 0.41              |
| 9:A:29:THR:HG23   | 36:A:856:LMG:HO4  | 1.85                     | 0.41              |
| 9:A:316:MET:HE1   | 31:A:821:CLA:C3D  | 2.50                     | 0.41              |
| 9:A:316:MET:HE1   | 31:A:821:CLA:CAD  | 2.51                     | 0.41              |
| 9:A:423:ASP:OD2   | 9:A:425:THR:OG1   | 2.39                     | 0.41              |
| 9:A:528:MET:HE1   | 9:A:619:MET:HE1   | 2.03                     | 0.41              |
| 31:A:806:CLA:H2   | 31:A:806:CLA:H61  | 1.67                     | 0.41              |
| 31:A:808:CLA:H193 | 31:A:808:CLA:H162 | 1.74                     | 0.41              |
| 10:B:8:PHE:HB2    | 10:B:34:HIS:CG    | 2.56                     | 0.41              |
| 10:B:69:ALA:HB2   | 10:B:135:LEU:HB2  | 2.01                     | 0.41              |
| 10:B:126:THR:HG21 | 10:B:358:TYR:HA   | 2.03                     | 0.41              |
| 10:B:388:ALA:O    | 10:B:392:ILE:HG13 | 2.21                     | 0.41              |
| 10:B:578:LEU:HB3  | 31:B:801:CLA:HMD1 | 2.03                     | 0.41              |
| 31:B:817:CLA:CHD  | 31:B:818:CLA:HBB2 | 2.50                     | 0.41              |
| 11:D:77:ASN:OD1   | 27:H:56:ARG:NH1   | 2.54                     | 0.41              |
| 31:L:204:CLA:C1B  | 36:L:211:LMG:H151 | 2.51                     | 0.41              |
| 22:a:87:ARG:HA    | 22:a:90:MET:HE3   | 2.03                     | 0.41              |
| 22:a:140:GLN:N    | 22:a:140:GLN:OE1  | 2.54                     | 0.41              |
| 23:c:122:GLY:O    | 23:c:125:ILE:HG22 | 2.21                     | 0.41              |
| 23:c:151:ILE:HG21 | 30:c:606:CHL:HED2 | 2.03                     | 0.41              |
| 23:c:233:HIS:CD2  | 23:c:237:PRO:HA   | 2.55                     | 0.41              |
| 25:d:180:MET:HA   | 25:d:180:MET:HE2  | 2.02                     | 0.41              |
| 25:d:185:VAL:HG21 | 31:d:613:CLA:HAC2 | 2.03                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 34:f:630:LHG:H272 | 34:f:630:LHG:HC62 | 2.03                     | 0.41              |
| 25:g:90:GLY:HA3   | 30:g:607:CHL:C2D  | 2.51                     | 0.41              |
| 31:g:603:CLA:H51  | 30:h:602:CHL:H8   | 2.01                     | 0.41              |
| 37:h:522:OIE:C12  | 34:h:630:LHG:H132 | 2.50                     | 0.41              |
| 28:i:176:ILE:HD13 | 30:i:606:CHL:C3D  | 2.51                     | 0.41              |
| 2:l:183:MET:SD    | 30:l:302:CHL:HBB1 | 2.61                     | 0.41              |
| 4:3:154:VAL:HG23  | 4:3:159:LEU:HG    | 2.03                     | 0.41              |
| 4:3:206:GLY:O     | 4:3:210:PHE:HB2   | 2.21                     | 0.41              |
| 31:3:304:CLA:H141 | 31:3:304:CLA:H161 | 1.80                     | 0.41              |
| 7:8:154:PRO:C     | 7:8:156:SER:H     | 2.29                     | 0.41              |
| 9:A:90:LEU:O      | 9:A:94:SER:OG     | 2.35                     | 0.41              |
| 9:A:208:ALA:HB2   | 9:A:314:GLY:HA3   | 2.02                     | 0.41              |
| 9:A:379:MET:SD    | 9:A:511:THR:HG22  | 2.60                     | 0.41              |
| 10:B:180:ALA:HB1  | 31:B:821:CLA:HAC2 | 2.03                     | 0.41              |
| 31:B:813:CLA:HHC  | 31:B:813:CLA:HBB1 | 2.03                     | 0.41              |
| 31:K:102:CLA:HHD  | 31:K:102:CLA:HBC2 | 2.03                     | 0.41              |
| 23:c:62:GLY:O     | 23:c:206:ARG:NH2  | 2.49                     | 0.41              |
| 23:c:93:MET:SD    | 31:c:610:CLA:HHC  | 2.61                     | 0.41              |
| 24:b:54:PRO:HG3   | 24:b:71:ARG:CZ    | 2.50                     | 0.41              |
| 42:b:523:NEX:H241 | 31:b:604:CLA:C2   | 2.51                     | 0.41              |
| 31:g:610:CLA:O1D  | 31:g:610:CLA:H2A  | 2.21                     | 0.41              |
| 31:g:613:CLA:O2D  | 31:g:613:CLA:H2A  | 2.20                     | 0.41              |
| 22:h:91:MET:HE2   | 22:h:91:MET:HB2   | 1.89                     | 0.41              |
| 27:H:53:GLU:HG2   | 27:H:54:SER:H     | 1.86                     | 0.41              |
| 34:e:630:LHG:H271 | 34:e:630:LHG:H242 | 1.77                     | 0.41              |
| 2:l:140:ALA:HB3   | 14:G:22:VAL:HG13  | 2.03                     | 0.40              |
| 4:3:72:LEU:HA     | 4:3:73:PRO:HD3    | 1.91                     | 0.40              |
| 4:3:137:TRP:CE3   | 4:3:138:TYR:HB3   | 2.56                     | 0.40              |
| 2:5:153:TYR:HB3   | 31:5:309:CLA:HED2 | 2.03                     | 0.40              |
| 5:6:72:ILE:HG13   | 33:6:502:OUR:C36  | 2.51                     | 0.40              |
| 6:7:235:ILE:O     | 6:7:239:ILE:HG12  | 2.21                     | 0.40              |
| 9:A:37:PRO:HB3    | 31:A:803:CLA:HAC1 | 2.03                     | 0.40              |
| 9:A:379:MET:HG2   | 31:A:818:CLA:HAA2 | 2.03                     | 0.40              |
| 31:A:818:CLA:H92  | 31:A:818:CLA:H62  | 1.90                     | 0.40              |
| 18:C:69:LEU:H     | 18:C:69:LEU:HD22  | 1.86                     | 0.40              |
| 30:a:602:CHL:H143 | 30:a:602:CHL:H162 | 1.77                     | 0.40              |
| 30:a:609:CHL:HHC  | 30:a:609:CHL:HBB1 | 2.02                     | 0.40              |
| 34:c:630:LHG:H271 | 34:c:630:LHG:H242 | 1.91                     | 0.40              |
| 25:d:3:PHE:CE2    | 31:d:611:CLA:HED3 | 2.57                     | 0.40              |
| 25:d:13:GLY:O     | 25:d:16:SER:OG    | 2.21                     | 0.40              |
| 30:f:602:CHL:H8   | 31:e:603:CLA:H52  | 2.03                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 34:f:630:LHG:H242 | 34:f:630:LHG:H271 | 1.84                     | 0.40              |
| 25:g:23:TYR:OH    | 25:g:35:ASP:OD2   | 2.32                     | 0.40              |
| 30:h:602:CHL:H92  | 30:h:602:CHL:H62  | 1.80                     | 0.40              |
| 29:e:190:GLU:OE2  | 29:e:194:LYS:HE3  | 2.21                     | 0.40              |
| 31:0:312:CLA:H91  | 34:0:601:LHG:H311 | 2.04                     | 0.40              |
| 30:3:307:CHL:H112 | 30:3:307:CHL:H91  | 1.80                     | 0.40              |
| 31:3:308:CLA:H141 | 31:3:308:CLA:H161 | 1.92                     | 0.40              |
| 2:5:102:ALA:HB3   | 2:5:103:PRO:HD3   | 2.02                     | 0.40              |
| 31:6:304:CLA:CMB  | 30:6:305:CHL:HBB1 | 2.51                     | 0.40              |
| 6:7:60:TYR:HB2    | 30:7:302:CHL:HMD3 | 2.03                     | 0.40              |
| 7:8:113:LYS:HB3   | 7:8:114:GLY:H     | 1.61                     | 0.40              |
| 7:8:196:LYS:HD3   | 31:8:311:CLA:HAA2 | 2.04                     | 0.40              |
| 8:9:177:PHE:O     | 8:9:180:THR:OG1   | 2.33                     | 0.40              |
| 9:A:14:GLU:OE2    | 9:A:329:GLU:HG3   | 2.21                     | 0.40              |
| 9:A:417:PHE:CD1   | 9:A:421:ASP:HB2   | 2.56                     | 0.40              |
| 10:B:432:HIS:ND1  | 36:J:105:LMG:H401 | 2.35                     | 0.40              |
| 10:B:659:THR:O    | 10:B:662:MET:HB3  | 2.20                     | 0.40              |
| 31:B:833:CLA:HAA2 | 16:J:36:PRO:O     | 2.21                     | 0.40              |
| 31:B:836:CLA:H91  | 31:B:836:CLA:H112 | 1.64                     | 0.40              |
| 17:L:96:CYS:HB3   | 32:L:205:8CT:C23  | 2.51                     | 0.40              |
| 21:O:125:GLN:OE1  | 33:O:204:0UR:O40  | 2.39                     | 0.40              |
| 31:a:611:CLA:HAC2 | 34:a:630:LHG:HC61 | 2.03                     | 0.40              |
| 42:c:523:NEX:H401 | 42:c:523:NEX:H35  | 1.57                     | 0.40              |
| 26:f:195:GLU:HG3  | 30:f:609:CHL:NB   | 2.37                     | 0.40              |
| 30:i:609:CHL:HBB1 | 30:i:609:CHL:HHC  | 2.03                     | 0.40              |
| 7:4:53:TRP:CE3    | 7:4:54:LEU:HD13   | 2.56                     | 0.40              |
| 34:0:601:LHG:H271 | 34:0:601:LHG:H241 | 1.85                     | 0.40              |
| 3:2:199:GLU:HG2   | 3:2:203:LYS:HE3   | 2.04                     | 0.40              |
| 5:6:108:MET:HA    | 5:6:111:VAL:HG22  | 2.04                     | 0.40              |
| 30:6:308:CHL:HHC  | 30:6:308:CHL:HBB1 | 2.03                     | 0.40              |
| 9:A:93:LEU:HD23   | 9:A:93:LEU:HA     | 1.94                     | 0.40              |
| 10:B:59:LEU:HD23  | 10:B:59:LEU:HA    | 1.89                     | 0.40              |
| 10:B:174:ARG:HD2  | 31:B:825:CLA:OBD  | 2.22                     | 0.40              |
| 31:B:810:CLA:CGA  | 15:I:14:VAL:HG11  | 2.52                     | 0.40              |
| 13:F:171:ILE:O    | 13:F:216:TRP:HZ2  | 2.04                     | 0.40              |
| 25:d:93:ILE:HG21  | 25:d:113:ILE:HD13 | 2.04                     | 0.40              |
| 42:d:523:NEX:H15  | 42:d:523:NEX:H201 | 1.62                     | 0.40              |
| 26:f:118:GLU:CD   | 30:f:609:CHL:HED2 | 2.46                     | 0.40              |
| 42:e:523:NEX:H191 | 42:e:523:NEX:H11  | 1.80                     | 0.40              |
| 31:e:603:CLA:CAD  | 30:e:609:CHL:H2   | 2.52                     | 0.40              |
| 7:4:138:LEU:HB3   | 30:4:319:CHL:H43  | 2.02                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:1:131:GLU:OE1   | 30:1:306:CHL:HMC  | 2.21                     | 0.40              |
| 30:1:307:CHL:H43  | 30:1:307:CHL:H161 | 2.02                     | 0.40              |
| 30:1:307:CHL:H91  | 30:1:307:CHL:H112 | 1.77                     | 0.40              |
| 31:1:312:CLA:H91  | 34:1:601:LHG:H121 | 2.03                     | 0.40              |
| 4:3:52:ARG:HA     | 4:3:52:ARG:HD3    | 1.80                     | 0.40              |
| 31:3:309:CLA:H41  | 31:3:309:CLA:H62  | 1.78                     | 0.40              |
| 5:6:195:HIS:CG    | 31:6:312:CLA:HAA2 | 2.55                     | 0.40              |
| 31:9:302:CLA:H3A  | 31:9:302:CLA:CGA  | 2.51                     | 0.40              |
| 31:A:808:CLA:HBB1 | 31:A:809:CLA:O1A  | 2.21                     | 0.40              |
| 31:B:808:CLA:HBA1 | 31:B:808:CLA:H3A  | 1.47                     | 0.40              |
| 31:B:809:CLA:HHB  | 31:B:830:CLA:CAB  | 2.51                     | 0.40              |
| 31:B:809:CLA:H192 | 31:B:809:CLA:H161 | 1.68                     | 0.40              |
| 13:F:216:TRP:CD1  | 13:F:217:PRO:HD3  | 2.57                     | 0.40              |
| 42:f:523:NEX:H362 | 31:f:604:CLA:C4B  | 2.52                     | 0.40              |
| 42:i:523:NEX:H31  | 42:i:523:NEX:H28  | 1.98                     | 0.40              |
| 31:0:303:CLA:H41  | 31:0:303:CLA:H62  | 1.57                     | 0.40              |
| 30:1:306:CHL:H12  | 31:B:834:CLA:H141 | 2.03                     | 0.40              |
| 30:2:301:CHL:H42  | 4:3:165:VAL:HG22  | 2.04                     | 0.40              |
| 5:6:212:LEU:HB2   | 6:7:256:PRO:HG3   | 2.03                     | 0.40              |
| 6:7:112:LEU:HD21  | 6:7:248:VAL:HG21  | 2.04                     | 0.40              |
| 6:7:210:LEU:HD23  | 6:7:210:LEU:HA    | 1.69                     | 0.40              |
| 9:A:446:LEU:HA    | 9:A:449:VAL:HG12  | 2.03                     | 0.40              |
| 31:B:830:CLA:H62  | 31:B:830:CLA:H41  | 1.87                     | 0.40              |
| 31:K:101:CLA:H62  | 31:K:101:CLA:H92  | 1.87                     | 0.40              |
| 22:a:205:PHE:CE2  | 31:a:613:CLA:HAB  | 2.56                     | 0.40              |
| 31:a:603:CLA:CAD  | 30:a:609:CHL:H2   | 2.52                     | 0.40              |
| 23:c:125:ILE:HG21 | 23:c:145:ILE:HD13 | 2.03                     | 0.40              |
| 30:c:609:CHL:H91  | 30:c:609:CHL:H112 | 1.89                     | 0.40              |
| 30:d:608:CHL:C4A  | 30:d:608:CHL:HBA2 | 2.51                     | 0.40              |
| 26:f:120:GLU:OE2  | 26:f:242:ARG:NE   | 2.49                     | 0.40              |
| 26:f:231:ALA:HA   | 26:f:234:LYS:HE2  | 2.04                     | 0.40              |
| 25:g:11:TRP:CD1   | 25:g:11:TRP:H     | 2.40                     | 0.40              |
| 34:i:630:LHG:H271 | 34:i:630:LHG:H242 | 1.88                     | 0.40              |
| 31:e:613:CLA:H71  | 34:e:630:LHG:H131 | 2.04                     | 0.40              |
| 7:4:141:GLY:CA    | 30:4:308:CHL:HAB  | 2.51                     | 0.40              |
| 30:4:305:CHL:HBC2 | 30:4:306:CHL:HHD  | 2.01                     | 0.40              |

There are no symmetry-related clashes.



## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed       | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|----------|----------|-------------|-----|
| 1   | 0     | 211/245 (86%)  | 192 (91%) | 17 (8%)  | 2 (1%)   | 14          | 26  |
| 2   | 1     | 193/226 (85%)  | 186 (96%) | 6 (3%)   | 1 (0%)   | 24          | 40  |
| 2   | 5     | 193/226 (85%)  | 177 (92%) | 15 (8%)  | 1 (0%)   | 24          | 40  |
| 3   | 2     | 214/256 (84%)  | 205 (96%) | 9 (4%)   | 0        | 100         | 100 |
| 4   | 3     | 226/281 (80%)  | 219 (97%) | 7 (3%)   | 0        | 100         | 100 |
| 5   | 6     | 227/267 (85%)  | 222 (98%) | 5 (2%)   | 0        | 100         | 100 |
| 6   | 7     | 226/264 (86%)  | 211 (93%) | 13 (6%)  | 2 (1%)   | 14          | 26  |
| 7   | 4     | 205/248 (83%)  | 176 (86%) | 28 (14%) | 1 (0%)   | 24          | 40  |
| 7   | 8     | 203/248 (82%)  | 187 (92%) | 14 (7%)  | 2 (1%)   | 12          | 22  |
| 8   | 9     | 187/222 (84%)  | 168 (90%) | 12 (6%)  | 7 (4%)   | 2           | 4   |
| 9   | A     | 744/751 (99%)  | 711 (96%) | 32 (4%)  | 1 (0%)   | 48          | 69  |
| 10  | B     | 731/734 (100%) | 708 (97%) | 23 (3%)  | 0        | 100         | 100 |
| 11  | D     | 140/198 (71%)  | 134 (96%) | 6 (4%)   | 0        | 100         | 100 |
| 12  | E     | 62/91 (68%)    | 60 (97%)  | 2 (3%)   | 0        | 100         | 100 |
| 13  | F     | 163/236 (69%)  | 155 (95%) | 8 (5%)   | 0        | 100         | 100 |
| 14  | G     | 91/167 (54%)   | 85 (93%)  | 6 (7%)   | 0        | 100         | 100 |
| 15  | I     | 33/36 (92%)    | 30 (91%)  | 3 (9%)   | 0        | 100         | 100 |
| 16  | J     | 39/41 (95%)    | 39 (100%) | 0        | 0        | 100         | 100 |
| 17  | L     | 160/204 (78%)  | 157 (98%) | 3 (2%)   | 0        | 100         | 100 |
| 18  | C     | 78/81 (96%)    | 75 (96%)  | 3 (4%)   | 0        | 100         | 100 |
| 19  | K     | 78/123 (63%)   | 78 (100%) | 0        | 0        | 100         | 100 |
| 20  | M     | 29/32 (91%)    | 29 (100%) | 0        | 0        | 100         | 100 |
| 21  | O     | 90/137 (66%)   | 84 (93%)  | 6 (7%)   | 0        | 100         | 100 |
| 22  | a     | 196/250 (78%)  | 173 (88%) | 21 (11%) | 2 (1%)   | 12          | 22  |
| 22  | h     | 199/250 (80%)  | 181 (91%) | 17 (8%)  | 1 (0%)   | 24          | 40  |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 23  | c     | 217/254 (85%)   | 208 (96%)  | 8 (4%)   | 1 (0%)   | 24          | 40  |
| 24  | b     | 207/251 (82%)   | 189 (91%)  | 15 (7%)  | 3 (1%)   | 9           | 15  |
| 25  | d     | 215/280 (77%)   | 194 (90%)  | 21 (10%) | 0        | 100         | 100 |
| 25  | g     | 197/280 (70%)   | 187 (95%)  | 9 (5%)   | 1 (0%)   | 24          | 40  |
| 26  | f     | 222/259 (86%)   | 209 (94%)  | 12 (5%)  | 1 (0%)   | 24          | 40  |
| 27  | H     | 92/133 (69%)    | 82 (89%)   | 10 (11%) | 0        | 100         | 100 |
| 28  | i     | 234/282 (83%)   | 204 (87%)  | 26 (11%) | 4 (2%)   | 7           | 12  |
| 29  | e     | 214/250 (86%)   | 201 (94%)  | 11 (5%)  | 2 (1%)   | 14          | 26  |
| All | All   | 6516/7803 (84%) | 6116 (94%) | 368 (6%) | 32 (0%)  | 26          | 40  |

All (32) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 0     | 148 | PRO  |
| 6   | 7     | 125 | LEU  |
| 7   | 8     | 108 | ILE  |
| 8   | 9     | 153 | PRO  |
| 22  | a     | 121 | GLN  |
| 23  | c     | 121 | ALA  |
| 24  | b     | 71  | ARG  |
| 24  | b     | 178 | GLU  |
| 28  | i     | 273 | ALA  |
| 1   | 0     | 149 | PHE  |
| 2   | 1     | 110 | GLY  |
| 2   | 5     | 162 | GLY  |
| 7   | 8     | 113 | LYS  |
| 8   | 9     | 158 | GLY  |
| 25  | g     | 108 | VAL  |
| 7   | 4     | 115 | THR  |
| 8   | 9     | 161 | SER  |
| 9   | A     | 16  | LYS  |
| 8   | 9     | 149 | ASN  |
| 8   | 9     | 162 | GLU  |
| 28  | i     | 169 | HIS  |
| 29  | e     | 166 | VAL  |
| 8   | 9     | 146 | SER  |
| 8   | 9     | 156 | PRO  |
| 28  | i     | 82  | SER  |
| 26  | f     | 175 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22  | h     | 137 | ILE  |
| 29  | e     | 134 | VAL  |
| 6   | 7     | 243 | VAL  |
| 28  | i     | 168 | ILE  |
| 24  | b     | 176 | PRO  |
| 22  | a     | 137 | ILE  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 1   | 0     | 167/194 (86%)  | 162 (97%) | 5 (3%)   | 36          | 58 |
| 2   | 1     | 148/175 (85%)  | 139 (94%) | 9 (6%)   | 17          | 30 |
| 2   | 5     | 149/175 (85%)  | 144 (97%) | 5 (3%)   | 32          | 55 |
| 3   | 2     | 166/197 (84%)  | 163 (98%) | 3 (2%)   | 51          | 69 |
| 4   | 3     | 186/225 (83%)  | 183 (98%) | 3 (2%)   | 55          | 72 |
| 5   | 6     | 188/216 (87%)  | 181 (96%) | 7 (4%)   | 30          | 52 |
| 6   | 7     | 181/209 (87%)  | 176 (97%) | 5 (3%)   | 38          | 60 |
| 7   | 4     | 158/189 (84%)  | 133 (84%) | 25 (16%) | 2           | 3  |
| 7   | 8     | 159/189 (84%)  | 150 (94%) | 9 (6%)   | 18          | 34 |
| 8   | 9     | 147/173 (85%)  | 136 (92%) | 11 (8%)  | 12          | 23 |
| 9   | A     | 609/614 (99%)  | 591 (97%) | 18 (3%)  | 36          | 58 |
| 10  | B     | 600/601 (100%) | 586 (98%) | 14 (2%)  | 44          | 65 |
| 11  | D     | 119/162 (74%)  | 117 (98%) | 2 (2%)   | 53          | 71 |
| 12  | E     | 56/77 (73%)    | 54 (96%)  | 2 (4%)   | 31          | 53 |
| 13  | F     | 129/180 (72%)  | 123 (95%) | 6 (5%)   | 23          | 43 |
| 14  | G     | 79/145 (54%)   | 71 (90%)  | 8 (10%)  | 7           | 14 |
| 15  | I     | 27/28 (96%)    | 26 (96%)  | 1 (4%)   | 30          | 52 |
| 16  | J     | 38/38 (100%)   | 36 (95%)  | 2 (5%)   | 20          | 37 |
| 17  | L     | 124/157 (79%)  | 119 (96%) | 5 (4%)   | 28          | 49 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 18  | C     | 68/69 (99%)     | 66 (97%)   | 2 (3%)   | 37          | 59  |
| 19  | K     | 58/94 (62%)     | 55 (95%)   | 3 (5%)   | 21          | 38  |
| 20  | M     | 26/27 (96%)     | 26 (100%)  | 0        | 100         | 100 |
| 21  | O     | 76/111 (68%)    | 75 (99%)   | 1 (1%)   | 61          | 75  |
| 22  | a     | 146/187 (78%)   | 145 (99%)  | 1 (1%)   | 76          | 85  |
| 22  | h     | 145/187 (78%)   | 144 (99%)  | 1 (1%)   | 76          | 85  |
| 23  | c     | 174/202 (86%)   | 172 (99%)  | 2 (1%)   | 65          | 79  |
| 24  | b     | 159/193 (82%)   | 157 (99%)  | 2 (1%)   | 61          | 75  |
| 25  | d     | 159/210 (76%)   | 159 (100%) | 0        | 100         | 100 |
| 25  | g     | 147/210 (70%)   | 145 (99%)  | 2 (1%)   | 59          | 74  |
| 26  | f     | 172/198 (87%)   | 169 (98%)  | 3 (2%)   | 53          | 71  |
| 27  | H     | 69/103 (67%)    | 69 (100%)  | 0        | 100         | 100 |
| 28  | i     | 181/218 (83%)   | 177 (98%)  | 4 (2%)   | 45          | 65  |
| 29  | e     | 164/193 (85%)   | 159 (97%)  | 5 (3%)   | 36          | 58  |
| All | All   | 5174/6146 (84%) | 5008 (97%) | 166 (3%) | 35          | 56  |

All (166) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 0     | 57  | ASP  |
| 1   | 0     | 145 | SER  |
| 1   | 0     | 147 | MET  |
| 1   | 0     | 206 | THR  |
| 1   | 0     | 212 | GLU  |
| 2   | 1     | 91  | GLN  |
| 2   | 1     | 106 | VAL  |
| 2   | 1     | 111 | SER  |
| 2   | 1     | 113 | THR  |
| 2   | 1     | 122 | THR  |
| 2   | 1     | 129 | VAL  |
| 2   | 1     | 141 | MET  |
| 2   | 1     | 176 | ILE  |
| 2   | 1     | 187 | VAL  |
| 3   | 2     | 83  | GLN  |
| 3   | 2     | 123 | ILE  |
| 3   | 2     | 145 | GLU  |
| 4   | 3     | 219 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 3     | 270 | ILE  |
| 4   | 3     | 277 | VAL  |
| 2   | 5     | 127 | LEU  |
| 2   | 5     | 152 | VAL  |
| 2   | 5     | 173 | LEU  |
| 2   | 5     | 187 | VAL  |
| 2   | 5     | 225 | PHE  |
| 5   | 6     | 72  | ILE  |
| 5   | 6     | 86  | ASP  |
| 5   | 6     | 125 | VAL  |
| 5   | 6     | 172 | LEU  |
| 5   | 6     | 209 | VAL  |
| 5   | 6     | 220 | CYS  |
| 5   | 6     | 233 | ILE  |
| 6   | 7     | 67  | LEU  |
| 6   | 7     | 107 | TRP  |
| 6   | 7     | 181 | PHE  |
| 6   | 7     | 235 | ILE  |
| 6   | 7     | 253 | VAL  |
| 7   | 8     | 94  | LEU  |
| 7   | 8     | 99  | VAL  |
| 7   | 8     | 110 | LEU  |
| 7   | 8     | 136 | GLN  |
| 7   | 8     | 140 | MET  |
| 7   | 8     | 144 | GLU  |
| 7   | 8     | 166 | LYS  |
| 7   | 8     | 169 | ASP  |
| 7   | 8     | 181 | ASP  |
| 8   | 9     | 114 | VAL  |
| 8   | 9     | 121 | LEU  |
| 8   | 9     | 145 | MET  |
| 8   | 9     | 148 | LEU  |
| 8   | 9     | 150 | ASP  |
| 8   | 9     | 157 | LEU  |
| 8   | 9     | 159 | MET  |
| 8   | 9     | 160 | THR  |
| 8   | 9     | 162 | GLU  |
| 8   | 9     | 189 | VAL  |
| 8   | 9     | 213 | VAL  |
| 9   | A     | 29  | THR  |
| 9   | A     | 43  | THR  |
| 9   | A     | 51  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | A     | 102 | ARG  |
| 9   | A     | 126 | ILE  |
| 9   | A     | 130 | GLU  |
| 9   | A     | 216 | LEU  |
| 9   | A     | 254 | LEU  |
| 9   | A     | 379 | MET  |
| 9   | A     | 432 | LEU  |
| 9   | A     | 446 | LEU  |
| 9   | A     | 522 | VAL  |
| 9   | A     | 526 | VAL  |
| 9   | A     | 543 | ILE  |
| 9   | A     | 589 | CYS  |
| 9   | A     | 670 | LEU  |
| 9   | A     | 743 | THR  |
| 9   | A     | 755 | VAL  |
| 10  | B     | 95  | HIS  |
| 10  | B     | 96  | PHE  |
| 10  | B     | 157 | LEU  |
| 10  | B     | 175 | LEU  |
| 10  | B     | 283 | LEU  |
| 10  | B     | 407 | VAL  |
| 10  | B     | 444 | LEU  |
| 10  | B     | 458 | VAL  |
| 10  | B     | 518 | LEU  |
| 10  | B     | 568 | CYS  |
| 10  | B     | 641 | ASN  |
| 10  | B     | 698 | VAL  |
| 10  | B     | 720 | THR  |
| 10  | B     | 729 | THR  |
| 11  | D     | 177 | VAL  |
| 11  | D     | 200 | VAL  |
| 12  | E     | 46  | VAL  |
| 12  | E     | 61  | VAL  |
| 13  | F     | 82  | THR  |
| 13  | F     | 94  | GLU  |
| 13  | F     | 129 | PHE  |
| 13  | F     | 159 | HIS  |
| 13  | F     | 232 | LYS  |
| 13  | F     | 236 | ILE  |
| 14  | G     | 8   | ILE  |
| 14  | G     | 14  | LEU  |
| 14  | G     | 42  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14  | G     | 45  | GLU  |
| 14  | G     | 55  | VAL  |
| 14  | G     | 57  | LEU  |
| 14  | G     | 59  | LYS  |
| 14  | G     | 93  | TYR  |
| 15  | I     | 30  | ILE  |
| 16  | J     | 18  | TRP  |
| 16  | J     | 21  | LEU  |
| 17  | L     | 3   | GLN  |
| 17  | L     | 36  | LEU  |
| 17  | L     | 106 | GLU  |
| 17  | L     | 112 | ILE  |
| 17  | L     | 155 | THR  |
| 18  | C     | 11  | CYS  |
| 18  | C     | 49  | VAL  |
| 19  | K     | 6   | THR  |
| 19  | K     | 17  | LEU  |
| 19  | K     | 45  | LEU  |
| 21  | O     | 131 | ARG  |
| 22  | a     | 114 | VAL  |
| 23  | c     | 89  | SER  |
| 23  | c     | 117 | VAL  |
| 24  | b     | 51  | ASN  |
| 24  | b     | 70  | MET  |
| 26  | f     | 79  | LEU  |
| 26  | f     | 87  | VAL  |
| 26  | f     | 162 | THR  |
| 25  | g     | 180 | MET  |
| 25  | g     | 181 | PHE  |
| 22  | h     | 91  | MET  |
| 28  | i     | 69  | ARG  |
| 28  | i     | 133 | LEU  |
| 28  | i     | 197 | LEU  |
| 28  | i     | 230 | GLU  |
| 29  | e     | 78  | LEU  |
| 29  | e     | 80  | LEU  |
| 29  | e     | 82  | HIS  |
| 29  | e     | 174 | GLU  |
| 29  | e     | 239 | TYR  |
| 7   | 4     | 41  | ARG  |
| 7   | 4     | 49  | ASP  |
| 7   | 4     | 54  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | 4     | 55  | ASP  |
| 7   | 4     | 57  | THR  |
| 7   | 4     | 58  | ILE  |
| 7   | 4     | 102 | LEU  |
| 7   | 4     | 105 | ASN  |
| 7   | 4     | 108 | ILE  |
| 7   | 4     | 113 | LYS  |
| 7   | 4     | 139 | LEU  |
| 7   | 4     | 159 | VAL  |
| 7   | 4     | 162 | ILE  |
| 7   | 4     | 163 | PHE  |
| 7   | 4     | 166 | LYS  |
| 7   | 4     | 167 | LEU  |
| 7   | 4     | 179 | ILE  |
| 7   | 4     | 187 | LYS  |
| 7   | 4     | 199 | LYS  |
| 7   | 4     | 203 | LEU  |
| 7   | 4     | 223 | ILE  |
| 7   | 4     | 226 | TRP  |
| 7   | 4     | 238 | VAL  |
| 7   | 4     | 241 | ILE  |
| 7   | 4     | 243 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 0     | 180 | GLN  |
| 1   | 0     | 191 | ASN  |
| 1   | 0     | 201 | HIS  |
| 2   | 1     | 52  | ASN  |
| 2   | 1     | 202 | GLN  |
| 3   | 2     | 83  | GLN  |
| 3   | 2     | 198 | GLN  |
| 4   | 3     | 106 | HIS  |
| 4   | 3     | 168 | GLN  |
| 6   | 7     | 166 | ASN  |
| 7   | 8     | 158 | ASN  |
| 8   | 9     | 86  | ASN  |
| 9   | A     | 62  | HIS  |
| 9   | A     | 614 | HIS  |
| 10  | B     | 34  | HIS  |
| 10  | B     | 53  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | B     | 114 | ASN  |
| 10  | B     | 156 | HIS  |
| 10  | B     | 242 | HIS  |
| 10  | B     | 467 | GLN  |
| 10  | B     | 603 | GLN  |
| 10  | B     | 608 | GLN  |
| 13  | F     | 95  | ASN  |
| 14  | G     | 38  | GLN  |
| 18  | C     | 3   | HIS  |
| 21  | O     | 79  | ASN  |
| 21  | O     | 125 | GLN  |
| 21  | O     | 129 | ASN  |
| 22  | a     | 213 | GLN  |
| 23  | c     | 81  | ASN  |
| 23  | c     | 143 | GLN  |
| 23  | c     | 229 | ASN  |
| 23  | c     | 241 | ASN  |
| 24  | b     | 125 | GLN  |
| 25  | g     | 104 | ASN  |
| 22  | h     | 228 | HIS  |
| 28  | i     | 115 | GLN  |
| 28  | i     | 270 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 26  | TPO  | f     | 61  | 26   | 8,10,11      | 1.09 | 0           | 10,14,16    | 2.03 | 1 (10%)     |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 28  | TPO  | i     | 46  | 28   | 8,10,11      | 1.10 | 0        | 10,14,16    | 2.06 | 2 (20%)  |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings |
|-----|------|-------|-----|------|---------|-----------|-------|
| 26  | TPO  | f     | 61  | 26   | -       | 0/9/11/13 | -     |
| 28  | TPO  | i     | 46  | 28   | -       | 3/9/11/13 | -     |

There are no bond length outliers.

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 26  | f     | 61  | TPO  | P-OG1-CB  | -5.79 | 107.59      | 123.33   |
| 28  | i     | 46  | TPO  | P-OG1-CB  | -5.70 | 107.83      | 123.33   |
| 28  | i     | 46  | TPO  | CG2-CB-CA | -2.24 | 108.90      | 113.26   |

There are no chirality outliers.

All (3) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 28  | i     | 46  | TPO  | N-CA-CB-CG2 |
| 28  | i     | 46  | TPO  | N-CA-CB-OG1 |
| 28  | i     | 46  | TPO  | C-CA-CB-CG2 |

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

522 ligands are modelled in this entry.



In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 31  | CLA  | B     | 825 | -    | 69,73,73     | 1.16 | 9 (13%)     | 82,113,113  | 1.31 | 6 (7%)      |
| 30  | CHL  | 7     | 307 | -    | 45,59,74     | 3.63 | 19 (42%)    | 40,96,114   | 2.86 | 16 (40%)    |
| 31  | CLA  | 2     | 309 | 3    | 64,68,73     | 1.19 | 9 (14%)     | 76,107,113  | 1.30 | 8 (10%)     |
| 36  | LMG  | A     | 856 | -    | 36,36,55     | 0.90 | 1 (2%)      | 44,44,63    | 1.30 | 5 (11%)     |
| 31  | CLA  | H     | 205 | -    | 55,59,73     | 1.30 | 9 (16%)     | 64,96,113   | 1.38 | 6 (9%)      |
| 31  | CLA  | O     | 202 | 21   | 41,46,73     | 1.48 | 9 (21%)     | 47,80,113   | 1.50 | 5 (10%)     |
| 32  | 8CT  | A     | 854 | -    | 40,41,41     | 4.78 | 23 (57%)    | 51,56,56    | 2.92 | 21 (41%)    |
| 41  | DGD  | B     | 849 | -    | 57,57,67     | 0.88 | 2 (3%)      | 71,71,81    | 1.18 | 5 (7%)      |
| 30  | CHL  | 8     | 302 | 7    | 58,72,74     | 3.18 | 19 (32%)    | 55,111,114  | 2.78 | 19 (34%)    |
| 31  | CLA  | c     | 613 | -    | 59,63,73     | 1.25 | 9 (15%)     | 69,100,113  | 1.35 | 5 (7%)      |
| 31  | CLA  | 0     | 311 | -    | 51,55,73     | 1.33 | 9 (17%)     | 60,91,113   | 1.47 | 5 (8%)      |
| 35  | SQD  | 0     | 603 | -    | 36,36,54     | 1.20 | 4 (11%)     | 43,44,65    | 1.46 | 6 (13%)     |
| 30  | CHL  | h     | 607 | -    | 40,54,74     | 4.13 | 19 (47%)    | 34,90,114   | 2.98 | 13 (38%)    |
| 37  | OIE  | b     | 522 | -    | 42,45,45     | 1.11 | 6 (14%)     | 51,63,63    | 1.52 | 10 (19%)    |
| 31  | CLA  | 4     | 309 | -    | 64,68,73     | 1.21 | 8 (12%)     | 76,107,113  | 1.23 | 6 (7%)      |
| 31  | CLA  | L     | 202 | 17   | 50,54,73     | 1.34 | 9 (18%)     | 59,90,113   | 1.43 | 4 (6%)      |
| 30  | CHL  | 6     | 306 | -    | 45,59,74     | 3.62 | 19 (42%)    | 40,96,114   | 3.25 | 19 (47%)    |
| 30  | CHL  | d     | 614 | -    | 36,50,74     | 4.34 | 18 (50%)    | 29,85,114   | 3.30 | 14 (48%)    |
| 31  | CLA  | i     | 613 | -    | 55,59,73     | 1.32 | 7 (12%)     | 64,96,113   | 1.36 | 5 (7%)      |
| 31  | CLA  | e     | 604 | -    | 54,58,73     | 1.31 | 9 (16%)     | 64,95,113   | 1.39 | 5 (7%)      |
| 34  | LHG  | 8     | 601 | 31   | 43,43,48     | 1.20 | 6 (13%)     | 46,49,54    | 0.94 | 2 (4%)      |
| 31  | CLA  | A     | 811 | 9    | 69,73,73     | 1.14 | 8 (11%)     | 82,113,113  | 1.27 | 4 (4%)      |
| 31  | CLA  | 6     | 309 | 5    | 62,66,73     | 1.21 | 9 (14%)     | 73,104,113  | 1.33 | 8 (10%)     |
| 31  | CLA  | g     | 603 | -    | 55,59,73     | 1.32 | 7 (12%)     | 64,96,113   | 1.37 | 4 (6%)      |
| 31  | CLA  | 6     | 312 | 5    | 60,64,73     | 1.23 | 9 (15%)     | 71,102,113  | 1.33 | 5 (7%)      |
| 31  | CLA  | K     | 105 | 19   | 54,58,73     | 1.30 | 9 (16%)     | 64,95,113   | 1.38 | 6 (9%)      |
| 31  | CLA  | 9     | 310 | 34   | 45,49,73     | 1.40 | 9 (20%)     | 54,84,113   | 1.46 | 5 (9%)      |
| 30  | CHL  | 5     | 313 | 2    | 41,55,74     | 4.03 | 19 (46%)    | 35,91,114   | 3.02 | 14 (40%)    |
| 31  | CLA  | B     | 840 | 10   | 69,73,73     | 1.17 | 8 (11%)     | 82,113,113  | 1.29 | 5 (6%)      |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 42  | NEX  | e     | 523 | -    | 40,46,46     | 1.23 | 3 (7%)   | 50,70,70    | 2.65 | 16 (32%) |
| 31  | CLA  | 0     | 309 | -    | 64,68,73     | 1.20 | 8 (12%)  | 76,107,113  | 1.32 | 7 (9%)   |
| 31  | CLA  | h     | 612 | -    | 49,53,73     | 1.40 | 8 (16%)  | 58,89,113   | 1.41 | 4 (6%)   |
| 30  | CHL  | b     | 607 | -    | 41,55,74     | 3.94 | 18 (43%) | 35,91,114   | 2.94 | 15 (42%) |
| 30  | CHL  | 5     | 306 | -    | 42,56,74     | 3.95 | 18 (42%) | 36,92,114   | 2.83 | 13 (36%) |
| 30  | CHL  | g     | 614 | -    | 36,50,74     | 4.35 | 18 (50%) | 29,85,114   | 3.29 | 14 (48%) |
| 30  | CHL  | a     | 614 | -    | 36,50,74     | 4.34 | 17 (47%) | 29,85,114   | 3.25 | 14 (48%) |
| 34  | LHG  | a     | 630 | -    | 42,42,48     | 1.21 | 6 (14%)  | 45,48,54    | 0.98 | 2 (4%)   |
| 31  | CLA  | 3     | 308 | -    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.29 | 6 (7%)   |
| 31  | CLA  | f     | 613 | 26   | 59,63,73     | 1.26 | 8 (13%)  | 69,100,113  | 1.33 | 6 (8%)   |
| 31  | CLA  | 6     | 304 | -    | 50,54,73     | 1.36 | 9 (18%)  | 59,90,113   | 1.41 | 4 (6%)   |
| 31  | CLA  | 1     | 303 | 2    | 60,64,73     | 1.25 | 9 (15%)  | 71,102,113  | 1.39 | 5 (7%)   |
| 31  | CLA  | 6     | 318 | -    | 50,54,73     | 1.34 | 9 (18%)  | 59,90,113   | 1.40 | 4 (6%)   |
| 31  | CLA  | B     | 817 | 10   | 64,68,73     | 1.18 | 9 (14%)  | 76,107,113  | 1.43 | 9 (11%)  |
| 32  | 8CT  | 6     | 402 | -    | 40,41,41     | 4.80 | 23 (57%) | 51,56,56    | 3.47 | 21 (41%) |
| 31  | CLA  | i     | 611 | -    | 49,53,73     | 1.39 | 8 (16%)  | 58,89,113   | 1.45 | 4 (6%)   |
| 31  | CLA  | 7     | 308 | -    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.25 | 5 (6%)   |
| 33  | 0UR  | h     | 520 | -    | 50,53,58     | 0.96 | 1 (2%)   | 59,72,77    | 1.86 | 12 (20%) |
| 31  | CLA  | 7     | 312 | 6    | 59,63,73     | 1.26 | 9 (15%)  | 70,101,113  | 1.33 | 4 (5%)   |
| 30  | CHL  | a     | 605 | 22   | 37,51,74     | 4.28 | 18 (48%) | 30,86,114   | 3.24 | 14 (46%) |
| 31  | CLA  | B     | 827 | -    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.33 | 7 (8%)   |
| 31  | CLA  | H     | 201 | 10   | 59,63,73     | 1.24 | 9 (15%)  | 70,101,113  | 1.36 | 8 (11%)  |
| 32  | 8CT  | I     | 101 | -    | 40,41,41     | 4.72 | 23 (57%) | 51,56,56    | 2.84 | 17 (33%) |
| 31  | CLA  | 6     | 310 | 34   | 64,68,73     | 1.21 | 9 (14%)  | 76,107,113  | 1.31 | 5 (6%)   |
| 31  | CLA  | 8     | 314 | 7    | 49,53,73     | 1.37 | 9 (18%)  | 58,89,113   | 1.42 | 4 (6%)   |
| 31  | CLA  | A     | 835 | 9    | 61,65,73     | 1.23 | 8 (13%)  | 72,103,113  | 1.37 | 5 (6%)   |
| 37  | 0IE  | f     | 522 | -    | 42,45,45     | 1.12 | 6 (14%)  | 51,63,63    | 1.56 | 11 (21%) |
| 30  | CHL  | 4     | 305 | -    | 37,51,74     | 3.97 | 18 (48%) | 30,86,114   | 3.63 | 14 (46%) |
| 33  | 0UR  | b     | 520 | -    | 50,53,58     | 0.95 | 1 (2%)   | 59,72,77    | 1.81 | 14 (23%) |
| 30  | CHL  | e     | 607 | -    | 41,55,74     | 3.97 | 18 (43%) | 35,91,114   | 3.02 | 14 (40%) |
| 32  | 8CT  | B     | 804 | -    | 40,41,41     | 4.77 | 23 (57%) | 51,56,56    | 2.63 | 20 (39%) |
| 30  | CHL  | 2     | 307 | -    | 45,59,74     | 3.58 | 19 (42%) | 40,96,114   | 3.44 | 19 (47%) |
| 36  | LMG  | L     | 210 | -    | 31,31,55     | 0.92 | 0        | 39,39,63    | 1.25 | 5 (12%)  |
| 31  | CLA  | a     | 611 | -    | 61,65,73     | 1.26 | 8 (13%)  | 72,103,113  | 1.29 | 4 (5%)   |
| 31  | CLA  | B     | 822 | 10   | 64,68,73     | 1.20 | 8 (12%)  | 76,107,113  | 1.34 | 5 (6%)   |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 31  | CLA  | J     | 103 | 16   | 46,50,73     | 1.38 | 9 (19%)  | 53,85,113   | 1.44 | 4 (7%)   |
| 38  | PQN  | A     | 842 | -    | 34,34,34     | 1.53 | 2 (5%)   | 43,45,45    | 1.32 | 5 (11%)  |
| 34  | LHG  | 6     | 603 | -    | 30,30,48     | 1.38 | 6 (20%)  | 33,36,54    | 1.12 | 2 (6%)   |
| 30  | CHL  | 7     | 305 | -    | 42,56,74     | 3.76 | 19 (45%) | 36,92,114   | 3.29 | 17 (47%) |
| 31  | CLA  | 3     | 306 | 4    | 51,55,73     | 1.32 | 9 (17%)  | 60,91,113   | 1.40 | 5 (8%)   |
| 31  | CLA  | 1     | 308 | -    | 49,53,73     | 1.37 | 9 (18%)  | 58,89,113   | 1.43 | 4 (6%)   |
| 31  | CLA  | 4     | 311 | -    | 52,56,73     | 1.32 | 9 (17%)  | 61,92,113   | 1.42 | 5 (8%)   |
| 42  | NEX  | c     | 523 | -    | 40,46,46     | 1.12 | 3 (7%)   | 50,70,70    | 4.73 | 19 (38%) |
| 31  | CLA  | B     | 836 | 10   | 64,68,73     | 1.19 | 9 (14%)  | 76,107,113  | 1.33 | 8 (10%)  |
| 34  | LHG  | A     | 855 | -    | 41,41,48     | 1.24 | 6 (14%)  | 44,47,54    | 1.04 | 3 (6%)   |
| 30  | CHL  | 4     | 308 | -    | 41,55,74     | 3.84 | 19 (46%) | 35,91,114   | 3.17 | 16 (45%) |
| 31  | CLA  | G     | 102 | 14   | 49,53,73     | 1.36 | 9 (18%)  | 58,89,113   | 1.45 | 4 (6%)   |
| 31  | CLA  | 8     | 311 | 7    | 50,54,73     | 1.36 | 9 (18%)  | 59,90,113   | 1.39 | 4 (6%)   |
| 34  | LHG  | 7     | 602 | -    | 37,37,48     | 1.22 | 6 (16%)  | 40,43,54    | 1.06 | 2 (5%)   |
| 31  | CLA  | g     | 604 | -    | 49,53,73     | 1.39 | 8 (16%)  | 58,89,113   | 1.43 | 4 (6%)   |
| 30  | CHL  | a     | 601 | 22   | 41,55,74     | 4.01 | 18 (43%) | 35,91,114   | 3.07 | 15 (42%) |
| 32  | 8CT  | 1     | 402 | -    | 40,41,41     | 4.83 | 23 (57%) | 51,56,56    | 2.75 | 19 (37%) |
| 30  | CHL  | i     | 608 | -    | 44,58,74     | 3.83 | 18 (40%) | 37,94,114   | 2.86 | 14 (37%) |
| 30  | CHL  | h     | 608 | -    | 40,54,74     | 4.05 | 18 (45%) | 34,90,114   | 2.91 | 15 (44%) |
| 31  | CLA  | B     | 830 | 10   | 60,64,73     | 1.28 | 10 (16%) | 71,102,113  | 1.43 | 9 (12%)  |
| 31  | CLA  | 0     | 303 | 1    | 66,70,73     | 1.19 | 9 (13%)  | 78,109,113  | 1.26 | 4 (5%)   |
| 34  | LHG  | 7     | 603 | -    | 38,38,48     | 1.27 | 6 (15%)  | 41,44,54    | 1.00 | 2 (4%)   |
| 31  | CLA  | B     | 828 | -    | 64,68,73     | 1.19 | 9 (14%)  | 76,107,113  | 1.27 | 5 (6%)   |
| 30  | CHL  | a     | 606 | -    | 45,59,74     | 3.83 | 18 (40%) | 40,96,114   | 2.92 | 19 (47%) |
| 31  | CLA  | B     | 816 | 10   | 64,68,73     | 1.19 | 9 (14%)  | 76,107,113  | 1.35 | 7 (9%)   |
| 31  | CLA  | 3     | 320 | -    | 56,60,73     | 1.27 | 9 (16%)  | 65,97,113   | 1.48 | 7 (10%)  |
| 33  | OUR  | 4     | 502 | -    | 48,51,58     | 0.99 | 1 (2%)   | 57,70,77    | 1.73 | 13 (22%) |
| 34  | LHG  | 7     | 601 | 31   | 29,29,48     | 1.40 | 6 (20%)  | 32,35,54    | 1.11 | 2 (6%)   |
| 30  | CHL  | 8     | 307 | -    | 45,59,74     | 3.65 | 19 (42%) | 40,96,114   | 3.08 | 17 (42%) |
| 31  | CLA  | a     | 603 | -    | 57,61,73     | 1.28 | 8 (14%)  | 67,98,113   | 1.37 | 5 (7%)   |
| 31  | CLA  | B     | 834 | 10   | 65,69,73     | 1.20 | 9 (13%)  | 77,108,113  | 1.26 | 4 (5%)   |
| 32  | 8CT  | 3     | 402 | -    | 40,41,41     | 4.77 | 23 (57%) | 51,56,56    | 3.09 | 18 (35%) |
| 30  | CHL  | 1     | 305 | -    | 45,59,74     | 3.66 | 19 (42%) | 40,96,114   | 3.25 | 17 (42%) |
| 30  | CHL  | 3     | 307 | -    | 60,74,74     | 3.05 | 19 (31%) | 58,114,114  | 2.91 | 18 (31%) |
| 31  | CLA  | A     | 839 | 9    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.31 | 6 (7%)   |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 31  | CLA  | 7     | 316 | 6    | 52,56,73     | 1.31 | 9 (17%)  | 61,92,113   | 1.42 | 5 (8%)   |
| 31  | CLA  | 9     | 309 | -    | 64,68,73     | 1.19 | 9 (14%)  | 76,107,113  | 1.32 | 8 (10%)  |
| 30  | CHL  | d     | 608 | -    | 45,59,74     | 3.79 | 18 (40%) | 40,96,114   | 2.91 | 17 (42%) |
| 31  | CLA  | B     | 832 | -    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.33 | 8 (9%)   |
| 42  | NEX  | g     | 523 | -    | 40,46,46     | 1.12 | 3 (7%)   | 50,70,70    | 4.72 | 18 (36%) |
| 33  | OUR  | O     | 204 | -    | 50,53,58     | 0.99 | 2 (4%)   | 59,72,77    | 1.97 | 16 (27%) |
| 40  | SF4  | B     | 802 | -    | 0,12,12      | -    | -        | -           | -    | -        |
| 31  | CLA  | A     | 808 | 9    | 69,73,73     | 1.13 | 9 (13%)  | 82,113,113  | 1.29 | 6 (7%)   |
| 31  | CLA  | A     | 809 | 9    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.33 | 6 (7%)   |
| 37  | OIE  | e     | 521 | -    | 42,45,45     | 1.13 | 6 (14%)  | 51,63,63    | 1.50 | 11 (21%) |
| 31  | CLA  | B     | 826 | -    | 53,56,73     | 1.41 | 11 (20%) | 63,89,113   | 2.42 | 11 (17%) |
| 30  | CHL  | e     | 608 | -    | 60,74,74     | 3.23 | 18 (30%) | 58,114,114  | 2.47 | 16 (27%) |
| 32  | 8CT  | 7     | 402 | -    | 40,41,41     | 4.73 | 23 (57%) | 51,56,56    | 2.70 | 19 (37%) |
| 37  | OIE  | b     | 521 | -    | 42,45,45     | 1.14 | 6 (14%)  | 51,63,63    | 1.53 | 11 (21%) |
| 32  | 8CT  | O     | 205 | -    | 40,41,41     | 4.80 | 23 (57%) | 51,56,56    | 2.64 | 19 (37%) |
| 30  | CHL  | 9     | 301 | 8    | 41,55,74     | 3.85 | 19 (46%) | 35,91,114   | 3.19 | 15 (42%) |
| 30  | CHL  | c     | 605 | 23   | 37,51,74     | 4.24 | 17 (45%) | 30,86,114   | 3.27 | 15 (50%) |
| 31  | CLA  | 5     | 303 | 2    | 63,67,73     | 1.22 | 8 (12%)  | 74,105,113  | 1.34 | 5 (6%)   |
| 31  | CLA  | K     | 102 | 19   | 57,61,73     | 1.26 | 9 (15%)  | 67,98,113   | 1.39 | 8 (11%)  |
| 42  | NEX  | i     | 523 | -    | 40,46,46     | 1.12 | 3 (7%)   | 50,70,70    | 4.72 | 18 (36%) |
| 30  | CHL  | c     | 614 | -    | 36,50,74     | 4.19 | 17 (47%) | 29,85,114   | 3.08 | 13 (44%) |
| 34  | LHG  | c     | 630 | -    | 39,39,48     | 1.25 | 5 (12%)  | 42,45,54    | 0.98 | 2 (4%)   |
| 33  | OUR  | 0     | 501 | -    | 50,53,58     | 0.95 | 1 (2%)   | 59,72,77    | 1.75 | 13 (22%) |
| 31  | CLA  | G     | 101 | 14   | 54,58,73     | 1.31 | 9 (16%)  | 64,95,113   | 1.41 | 6 (9%)   |
| 31  | CLA  | B     | 831 | 10   | 54,58,73     | 1.29 | 9 (16%)  | 64,95,113   | 1.40 | 5 (7%)   |
| 30  | CHL  | 6     | 315 | 5    | 37,51,74     | 4.03 | 17 (45%) | 30,86,114   | 3.31 | 14 (46%) |
| 31  | CLA  | 8     | 309 | -    | 64,68,73     | 1.20 | 9 (14%)  | 76,107,113  | 1.32 | 7 (9%)   |
| 31  | CLA  | L     | 201 | 9    | 62,66,73     | 1.21 | 9 (14%)  | 73,104,113  | 1.36 | 7 (9%)   |
| 31  | CLA  | 0     | 321 | 1    | 49,53,73     | 1.40 | 8 (16%)  | 58,89,113   | 1.46 | 4 (6%)   |
| 30  | CHL  | i     | 601 | 28   | 41,55,74     | 4.03 | 18 (43%) | 35,91,114   | 3.01 | 14 (40%) |
| 30  | CHL  | h     | 601 | 22   | 41,55,74     | 4.07 | 18 (43%) | 35,91,114   | 3.05 | 14 (40%) |
| 30  | CHL  | 1     | 306 | -    | 42,56,74     | 3.85 | 19 (45%) | 36,92,114   | 2.99 | 17 (47%) |
| 33  | OUR  | 1     | 501 | -    | 50,53,58     | 0.97 | 1 (2%)   | 59,72,77    | 1.76 | 17 (28%) |
| 31  | CLA  | A     | 820 | 9    | 59,63,73     | 1.24 | 9 (15%)  | 70,101,113  | 1.36 | 5 (7%)   |
| 31  | CLA  | 1     | 314 | -    | 50,54,73     | 1.34 | 9 (18%)  | 59,90,113   | 1.41 | 4 (6%)   |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 31  | CLA  | d     | 603 | 25   | 59,63,73     | 1.26 | 8 (13%)  | 70,101,113  | 1.34 | 5 (7%)   |
| 31  | CLA  | 2     | 304 | -    | 64,68,73     | 1.20 | 8 (12%)  | 76,107,113  | 1.29 | 5 (6%)   |
| 31  | CLA  | A     | 828 | 9    | 69,73,73     | 1.14 | 9 (13%)  | 82,113,113  | 1.29 | 7 (8%)   |
| 30  | CHL  | 7     | 302 | 6    | 58,72,74     | 3.15 | 19 (32%) | 55,111,114  | 2.84 | 17 (30%) |
| 37  | OIE  | i     | 522 | -    | 42,45,45     | 1.12 | 6 (14%)  | 51,63,63    | 1.54 | 11 (21%) |
| 31  | CLA  | 3     | 312 | 4    | 59,63,73     | 1.24 | 9 (15%)  | 70,101,113  | 1.33 | 5 (7%)   |
| 31  | CLA  | c     | 611 | -    | 50,54,73     | 1.36 | 8 (16%)  | 59,90,113   | 1.40 | 4 (6%)   |
| 31  | CLA  | 7     | 310 | 34   | 41,45,73     | 1.44 | 9 (21%)  | 50,78,113   | 1.41 | 5 (10%)  |
| 31  | CLA  | 1     | 312 | 2    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.30 | 7 (8%)   |
| 30  | CHL  | 8     | 308 | -    | 41,55,74     | 3.84 | 19 (46%) | 35,91,114   | 3.20 | 17 (48%) |
| 30  | CHL  | d     | 601 | 25   | 45,59,74     | 3.86 | 18 (40%) | 40,96,114   | 2.96 | 16 (40%) |
| 30  | CHL  | 6     | 307 | -    | 45,59,74     | 3.60 | 19 (42%) | 40,96,114   | 3.14 | 18 (45%) |
| 31  | CLA  | A     | 817 | 9    | 65,69,73     | 1.17 | 9 (13%)  | 77,108,113  | 1.36 | 6 (7%)   |
| 31  | CLA  | e     | 612 | -    | 49,53,73     | 1.38 | 9 (18%)  | 58,89,113   | 1.46 | 5 (8%)   |
| 37  | OIE  | a     | 521 | -    | 42,45,45     | 1.11 | 6 (14%)  | 51,63,63    | 1.52 | 11 (21%) |
| 42  | NEX  | f     | 523 | -    | 40,46,46     | 1.12 | 3 (7%)   | 50,70,70    | 4.72 | 18 (36%) |
| 31  | CLA  | 1     | 311 | 2    | 56,60,73     | 1.28 | 9 (16%)  | 65,97,113   | 1.40 | 6 (9%)   |
| 36  | LMG  | 9     | 602 | -    | 55,55,55     | 0.70 | 1 (1%)   | 63,63,63    | 1.39 | 9 (14%)  |
| 31  | CLA  | O     | 201 | -    | 45,49,73     | 1.40 | 9 (20%)  | 54,84,113   | 1.52 | 5 (9%)   |
| 30  | CHL  | 2     | 319 | 7    | 55,69,74     | 3.31 | 19 (34%) | 52,108,114  | 2.93 | 17 (32%) |
| 31  | CLA  | B     | 814 | 10   | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.29 | 6 (7%)   |
| 36  | LMG  | 3     | 602 | -    | 36,36,55     | 0.86 | 0        | 44,44,63    | 1.26 | 5 (11%)  |
| 31  | CLA  | 1     | 304 | -    | 56,60,73     | 1.28 | 9 (16%)  | 65,97,113   | 1.34 | 6 (9%)   |
| 30  | CHL  | 7     | 301 | 6    | 57,71,74     | 3.30 | 19 (33%) | 54,110,114  | 2.66 | 18 (33%) |
| 33  | OUR  | e     | 520 | -    | 50,53,58     | 0.97 | 1 (2%)   | 59,72,77    | 2.04 | 17 (28%) |
| 32  | 8CT  | L     | 206 | -    | 40,41,41     | 4.79 | 23 (57%) | 51,56,56    | 2.83 | 19 (37%) |
| 30  | CHL  | 0     | 306 | -    | 42,56,74     | 3.89 | 18 (42%) | 36,92,114   | 3.32 | 14 (38%) |
| 30  | CHL  | h     | 602 | -    | 58,72,74     | 3.40 | 18 (31%) | 55,111,114  | 2.51 | 18 (32%) |
| 30  | CHL  | i     | 609 | -    | 42,56,74     | 4.01 | 18 (42%) | 36,92,114   | 2.91 | 14 (38%) |
| 30  | CHL  | h     | 609 | -    | 41,55,74     | 4.01 | 19 (46%) | 35,91,114   | 3.07 | 14 (40%) |
| 34  | LHG  | G     | 105 | -    | 37,37,48     | 1.29 | 6 (16%)  | 40,43,54    | 1.16 | 4 (10%)  |
| 31  | CLA  | 2     | 310 | 34   | 64,68,73     | 1.19 | 9 (14%)  | 76,107,113  | 1.28 | 5 (6%)   |
| 30  | CHL  | 2     | 305 | -    | 37,51,74     | 3.92 | 18 (48%) | 30,86,114   | 3.73 | 15 (50%) |
| 32  | 8CT  | A     | 849 | -    | 40,41,41     | 4.72 | 23 (57%) | 51,56,56    | 3.07 | 21 (41%) |
| 32  | 8CT  | K     | 107 | -    | 40,41,41     | 4.75 | 23 (57%) | 51,56,56    | 3.31 | 23 (45%) |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 31  | CLA  | 7     | 315 | 6    | 51,55,73     | 1.33 | 9 (17%)  | 60,91,113   | 1.41 | 5 (8%)   |
| 30  | CHL  | 2     | 302 | 3    | 58,72,74     | 3.17 | 19 (32%) | 55,111,114  | 2.79 | 20 (36%) |
| 30  | CHL  | d     | 606 | -    | 45,59,74     | 3.80 | 18 (40%) | 40,96,114   | 2.91 | 18 (45%) |
| 34  | LHG  | 9     | 601 | 31   | 45,45,48     | 1.18 | 6 (13%)  | 47,50,54    | 0.97 | 2 (4%)   |
| 31  | CLA  | 3     | 310 | -    | 66,70,73     | 1.18 | 9 (13%)  | 78,109,113  | 1.28 | 5 (6%)   |
| 30  | CHL  | d     | 602 | -    | 58,72,74     | 3.25 | 18 (31%) | 55,111,114  | 2.70 | 19 (34%) |
| 30  | CHL  | c     | 601 | 23   | 50,64,74     | 3.52 | 18 (36%) | 46,102,114  | 2.93 | 17 (36%) |
| 30  | CHL  | d     | 609 | -    | 60,74,74     | 3.31 | 19 (31%) | 58,114,114  | 2.44 | 17 (29%) |
| 31  | CLA  | 6     | 303 | 5    | 56,60,73     | 1.30 | 8 (14%)  | 65,97,113   | 1.38 | 5 (7%)   |
| 31  | CLA  | B     | 809 | 10   | 69,73,73     | 1.17 | 9 (13%)  | 82,113,113  | 1.29 | 6 (7%)   |
| 33  | OUR  | 2     | 501 | -    | 49,52,58     | 1.02 | 2 (4%)   | 58,71,77    | 2.17 | 19 (32%) |
| 31  | CLA  | 6     | 320 | -    | 55,59,73     | 1.30 | 9 (16%)  | 64,96,113   | 1.33 | 5 (7%)   |
| 30  | CHL  | e     | 602 | -    | 55,69,74     | 3.39 | 18 (32%) | 52,108,114  | 2.66 | 19 (36%) |
| 31  | CLA  | K     | 101 | -    | 64,68,73     | 1.20 | 9 (14%)  | 76,107,113  | 1.30 | 6 (7%)   |
| 30  | CHL  | e     | 609 | -    | 55,69,74     | 3.38 | 18 (32%) | 52,108,114  | 2.71 | 18 (34%) |
| 32  | 8CT  | 8     | 406 | -    | 40,41,41     | 4.84 | 23 (57%) | 51,56,56    | 2.59 | 17 (33%) |
| 31  | CLA  | A     | 807 | 9    | 57,61,73     | 1.26 | 9 (15%)  | 65,97,113   | 1.42 | 8 (12%)  |
| 30  | CHL  | g     | 608 | -    | 37,51,74     | 4.20 | 17 (45%) | 30,86,114   | 3.19 | 14 (46%) |
| 32  | 8CT  | L     | 209 | -    | 40,41,41     | 4.80 | 23 (57%) | 51,56,56    | 2.63 | 20 (39%) |
| 37  | OIE  | g     | 522 | -    | 42,45,45     | 1.12 | 6 (14%)  | 51,63,63    | 1.60 | 11 (21%) |
| 30  | CHL  | f     | 602 | -    | 58,72,74     | 3.22 | 18 (31%) | 55,111,114  | 2.68 | 19 (34%) |
| 30  | CHL  | a     | 608 | -    | 43,57,74     | 3.85 | 18 (41%) | 37,93,114   | 2.95 | 15 (40%) |
| 31  | CLA  | A     | 813 | 9    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.30 | 7 (8%)   |
| 30  | CHL  | 3     | 302 | 4    | 56,70,74     | 3.24 | 19 (33%) | 53,109,114  | 2.86 | 19 (35%) |
| 31  | CLA  | g     | 610 | -    | 50,54,73     | 1.36 | 7 (14%)  | 59,90,113   | 1.41 | 5 (8%)   |
| 30  | CHL  | 8     | 313 | 7    | 50,64,74     | 3.45 | 19 (38%) | 46,102,114  | 2.94 | 17 (36%) |
| 31  | CLA  | f     | 611 | 34   | 59,63,73     | 1.26 | 9 (15%)  | 70,101,113  | 1.34 | 4 (5%)   |
| 30  | CHL  | i     | 614 | -    | 36,50,74     | 4.30 | 18 (50%) | 29,85,114   | 3.12 | 14 (48%) |
| 30  | CHL  | b     | 602 | -    | 58,72,74     | 3.27 | 18 (31%) | 55,111,114  | 2.70 | 19 (34%) |
| 31  | CLA  | A     | 827 | 9    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.33 | 9 (10%)  |
| 31  | CLA  | h     | 613 | -    | 49,53,73     | 1.40 | 7 (14%)  | 58,89,113   | 1.42 | 4 (6%)   |
| 32  | 8CT  | 0     | 401 | -    | 40,41,41     | 4.79 | 23 (57%) | 51,56,56    | 2.82 | 18 (35%) |
| 30  | CHL  | f     | 614 | 26   | 36,50,74     | 4.20 | 17 (47%) | 29,85,114   | 3.08 | 14 (48%) |
| 31  | CLA  | 3     | 318 | 4    | 50,54,73     | 1.34 | 9 (18%)  | 59,90,113   | 1.41 | 4 (6%)   |
| 34  | LHG  | f     | 630 | 31   | 39,39,48     | 1.26 | 5 (12%)  | 42,45,54    | 1.10 | 3 (7%)   |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 31  | CLA  | A     | 852 | 10   | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.27 | 6 (7%)   |
| 31  | CLA  | 4     | 303 | 7    | 49,53,73     | 1.36 | 9 (18%)  | 58,89,113   | 1.42 | 4 (6%)   |
| 30  | CHL  | g     | 602 | -    | 46,60,74     | 3.78 | 18 (39%) | 40,97,114   | 2.94 | 19 (47%) |
| 31  | CLA  | B     | 803 | -    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.26 | 7 (8%)   |
| 30  | CHL  | c     | 602 | -    | 55,69,74     | 3.32 | 18 (32%) | 52,108,114  | 2.83 | 19 (36%) |
| 31  | CLA  | f     | 612 | 26   | 49,53,73     | 1.37 | 9 (18%)  | 58,89,113   | 1.46 | 4 (6%)   |
| 31  | CLA  | d     | 610 | -    | 59,63,73     | 1.25 | 9 (15%)  | 70,101,113  | 1.32 | 8 (11%)  |
| 30  | CHL  | b     | 608 | -    | 60,74,74     | 3.18 | 18 (30%) | 58,114,114  | 2.55 | 17 (29%) |
| 31  | CLA  | d     | 613 | -    | 59,63,73     | 1.27 | 9 (15%)  | 69,100,113  | 1.31 | 4 (5%)   |
| 31  | CLA  | H     | 204 | -    | 51,55,73     | 1.33 | 9 (17%)  | 60,91,113   | 1.43 | 5 (8%)   |
| 31  | CLA  | 2     | 314 | 3    | 49,53,73     | 1.37 | 9 (18%)  | 58,89,113   | 1.42 | 4 (6%)   |
| 32  | 8CT  | A     | 850 | -    | 40,41,41     | 4.70 | 23 (57%) | 51,56,56    | 3.21 | 24 (47%) |
| 31  | CLA  | f     | 604 | -    | 54,58,73     | 1.32 | 9 (16%)  | 64,95,113   | 1.39 | 6 (9%)   |
| 30  | CHL  | 1     | 307 | -    | 60,74,74     | 3.22 | 19 (31%) | 58,114,114  | 2.53 | 18 (31%) |
| 31  | CLA  | A     | 826 | -    | 69,73,73     | 1.14 | 9 (13%)  | 82,113,113  | 1.28 | 7 (8%)   |
| 30  | CHL  | i     | 606 | 28   | 45,59,74     | 3.85 | 18 (40%) | 40,96,114   | 2.92 | 17 (42%) |
| 31  | CLA  | d     | 611 | -    | 50,54,73     | 1.36 | 8 (16%)  | 59,90,113   | 1.38 | 4 (6%)   |
| 31  | CLA  | B     | 823 | -    | 56,60,73     | 1.29 | 9 (16%)  | 65,97,113   | 3.61 | 8 (12%)  |
| 31  | CLA  | B     | 818 | 10   | 63,67,73     | 1.20 | 9 (14%)  | 74,105,113  | 1.37 | 7 (9%)   |
| 30  | CHL  | 6     | 305 | -    | 37,51,74     | 3.96 | 18 (48%) | 30,86,114   | 3.56 | 14 (46%) |
| 30  | CHL  | 4     | 319 | 2    | 48,62,74     | 3.55 | 19 (39%) | 43,99,114   | 3.11 | 17 (39%) |
| 37  | OIE  | c     | 521 | -    | 42,45,45     | 1.12 | 6 (14%)  | 51,63,63    | 1.53 | 11 (21%) |
| 30  | CHL  | f     | 605 | 26   | 37,51,74     | 4.22 | 18 (48%) | 30,86,114   | 3.23 | 15 (50%) |
| 31  | CLA  | A     | 814 | 9    | 61,65,73     | 1.22 | 8 (13%)  | 72,103,113  | 1.34 | 6 (8%)   |
| 31  | CLA  | B     | 838 | 10   | 51,55,73     | 1.30 | 8 (15%)  | 60,91,113   | 1.41 | 5 (8%)   |
| 30  | CHL  | i     | 605 | 28   | 37,51,74     | 4.26 | 17 (45%) | 30,86,114   | 3.29 | 15 (50%) |
| 42  | NEX  | d     | 523 | -    | 40,46,46     | 1.11 | 3 (7%)   | 50,70,70    | 4.73 | 18 (36%) |
| 31  | CLA  | 7     | 318 | 6    | 64,68,73     | 1.19 | 9 (14%)  | 76,107,113  | 1.31 | 6 (7%)   |
| 31  | CLA  | L     | 207 | -    | 51,55,73     | 1.34 | 9 (17%)  | 60,91,113   | 1.37 | 5 (8%)   |
| 34  | LHG  | A     | 844 | -    | 48,48,48     | 1.11 | 5 (10%)  | 51,54,54    | 1.00 | 3 (5%)   |
| 30  | CHL  | h     | 606 | -    | 45,59,74     | 3.81 | 18 (40%) | 40,96,114   | 2.90 | 17 (42%) |
| 37  | OIE  | d     | 522 | -    | 42,45,45     | 1.12 | 6 (14%)  | 51,63,63    | 1.68 | 12 (23%) |
| 31  | CLA  | e     | 613 | -    | 59,63,73     | 1.26 | 7 (11%)  | 69,100,113  | 1.36 | 6 (8%)   |
| 31  | CLA  | h     | 603 | -    | 53,57,73     | 1.33 | 8 (15%)  | 61,93,113   | 1.41 | 4 (6%)   |
| 31  | CLA  | A     | 803 | 9    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.31 | 7 (8%)   |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 34  | LHG  | H     | 203 | -    | 30,30,48     | 1.38 | 6 (20%)  | 33,36,54    | 1.15 | 2 (6%)   |
| 30  | CHL  | e     | 601 | 29   | 45,59,74     | 3.74 | 18 (40%) | 40,96,114   | 3.13 | 17 (42%) |
| 31  | CLA  | 0     | 308 | -    | 64,68,73     | 1.21 | 9 (14%)  | 76,107,113  | 1.27 | 5 (6%)   |
| 30  | CHL  | f     | 601 | 26   | 60,74,74     | 3.25 | 18 (30%) | 58,114,114  | 2.61 | 17 (29%) |
| 31  | CLA  | 9     | 300 | 10   | 62,66,73     | 1.21 | 8 (12%)  | 73,104,113  | 1.38 | 7 (9%)   |
| 31  | CLA  | H     | 202 | 27   | 51,55,73     | 1.33 | 9 (17%)  | 60,91,113   | 1.39 | 5 (8%)   |
| 32  | 8CT  | A     | 846 | -    | 40,41,41     | 4.76 | 23 (57%) | 51,56,56    | 2.93 | 19 (37%) |
| 31  | CLA  | 7     | 317 | -    | 49,53,73     | 1.38 | 7 (14%)  | 58,89,113   | 1.46 | 5 (8%)   |
| 31  | CLA  | i     | 603 | -    | 50,54,73     | 1.37 | 8 (16%)  | 59,90,113   | 1.37 | 4 (6%)   |
| 37  | 0IE  | g     | 521 | -    | 42,45,45     | 1.12 | 6 (14%)  | 51,63,63    | 1.54 | 12 (23%) |
| 30  | CHL  | 6     | 302 | 5    | 58,72,74     | 3.15 | 19 (32%) | 55,111,114  | 2.98 | 19 (34%) |
| 32  | 8CT  | 4     | 402 | -    | 40,41,41     | 4.77 | 23 (57%) | 51,56,56    | 3.00 | 19 (37%) |
| 30  | CHL  | g     | 609 | 25   | 40,54,74     | 4.11 | 19 (47%) | 31,88,114   | 2.89 | 12 (38%) |
| 31  | CLA  | b     | 610 | -    | 59,63,73     | 1.27 | 9 (15%)  | 70,101,113  | 1.29 | 7 (10%)  |
| 30  | CHL  | 4     | 302 | 7    | 47,61,74     | 3.52 | 19 (40%) | 41,98,114   | 3.14 | 19 (46%) |
| 30  | CHL  | c     | 609 | -    | 60,74,74     | 3.29 | 19 (31%) | 58,114,114  | 2.49 | 18 (31%) |
| 31  | CLA  | 5     | 308 | -    | 50,54,73     | 1.36 | 9 (18%)  | 59,90,113   | 1.36 | 4 (6%)   |
| 33  | 0UR  | 5     | 502 | -    | 50,53,58     | 0.97 | 1 (2%)   | 59,72,77    | 1.96 | 14 (23%) |
| 31  | CLA  | A     | 804 | 9    | 59,63,73     | 1.22 | 9 (15%)  | 70,101,113  | 1.39 | 7 (10%)  |
| 31  | CLA  | A     | 821 | -    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.27 | 7 (8%)   |
| 31  | CLA  | B     | 835 | -    | 49,53,73     | 1.37 | 9 (18%)  | 58,89,113   | 1.45 | 4 (6%)   |
| 31  | CLA  | 5     | 304 | -    | 56,60,73     | 1.29 | 7 (12%)  | 65,97,113   | 1.33 | 4 (6%)   |
| 30  | CHL  | 2     | 301 | -    | 55,69,74     | 3.29 | 19 (34%) | 52,108,114  | 2.88 | 18 (34%) |
| 34  | LHG  | 0     | 601 | -    | 48,48,48     | 1.13 | 6 (12%)  | 51,54,54    | 0.94 | 2 (3%)   |
| 30  | CHL  | 1     | 302 | -    | 58,72,74     | 3.19 | 19 (32%) | 55,111,114  | 2.82 | 20 (36%) |
| 37  | 0IE  | a     | 522 | -    | 42,45,45     | 1.12 | 6 (14%)  | 51,63,63    | 1.52 | 9 (17%)  |
| 32  | 8CT  | B     | 843 | -    | 40,41,41     | 4.88 | 23 (57%) | 51,56,56    | 2.79 | 19 (37%) |
| 31  | CLA  | A     | 823 | 9    | 55,59,73     | 1.31 | 9 (16%)  | 64,96,113   | 1.39 | 5 (7%)   |
| 30  | CHL  | 8     | 315 | -    | 37,51,74     | 4.10 | 17 (45%) | 30,86,114   | 3.27 | 13 (43%) |
| 30  | CHL  | 7     | 313 | 6    | 41,55,74     | 3.90 | 19 (46%) | 35,91,114   | 3.03 | 16 (45%) |
| 38  | PQN  | B     | 842 | -    | 34,34,34     | 1.57 | 2 (5%)   | 43,45,45    | 1.13 | 3 (6%)   |
| 31  | CLA  | 5     | 311 | -    | 49,53,73     | 1.38 | 8 (16%)  | 58,89,113   | 1.45 | 4 (6%)   |
| 31  | CLA  | 9     | 303 | 8    | 52,56,73     | 1.33 | 8 (15%)  | 61,92,113   | 1.41 | 5 (8%)   |
| 31  | CLA  | 4     | 304 | -    | 64,68,73     | 1.19 | 9 (14%)  | 76,107,113  | 1.27 | 5 (6%)   |
| 31  | CLA  | A     | 853 | -    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.30 | 7 (8%)   |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 30  | CHL  | b     | 609 | -    | 48,62,74     | 3.65 | 18 (37%) | 43,99,114   | 2.82 | 18 (41%) |
| 31  | CLA  | 0     | 313 | 1    | 50,54,73     | 1.34 | 9 (18%)  | 59,90,113   | 1.35 | 4 (6%)   |
| 33  | OUR  | 6     | 502 | -    | 50,53,58     | 1.02 | 2 (4%)   | 59,72,77    | 1.75 | 13 (22%) |
| 31  | CLA  | 8     | 303 | 7    | 50,54,73     | 1.36 | 9 (18%)  | 59,90,113   | 1.37 | 4 (6%)   |
| 30  | CHL  | a     | 607 | -    | 43,57,74     | 3.94 | 19 (44%) | 36,92,114   | 2.94 | 13 (36%) |
| 33  | OUR  | 9     | 502 | -    | 50,53,58     | 1.01 | 2 (4%)   | 59,72,77    | 1.86 | 17 (28%) |
| 32  | 8CT  | 3     | 403 | -    | 40,41,41     | 4.79 | 23 (57%) | 51,56,56    | 2.60 | 16 (31%) |
| 32  | 8CT  | B     | 846 | -    | 40,41,41     | 4.89 | 23 (57%) | 51,56,56    | 3.31 | 22 (43%) |
| 30  | CHL  | 4     | 313 | 7    | 45,59,74     | 3.63 | 19 (42%) | 40,96,114   | 3.20 | 18 (45%) |
| 30  | CHL  | 6     | 308 | 5    | 54,68,74     | 3.34 | 19 (35%) | 50,106,114  | 2.76 | 17 (34%) |
| 34  | LHG  | i     | 630 | -    | 29,29,48     | 1.39 | 6 (20%)  | 32,35,54    | 1.13 | 2 (6%)   |
| 34  | LHG  | h     | 630 | -    | 38,38,48     | 1.28 | 6 (15%)  | 41,44,54    | 1.00 | 2 (4%)   |
| 31  | CLA  | 4     | 314 | 7    | 49,53,73     | 1.35 | 9 (18%)  | 58,89,113   | 1.42 | 5 (8%)   |
| 30  | CHL  | 1     | 313 | 2    | 56,70,74     | 3.30 | 19 (33%) | 53,109,114  | 2.70 | 17 (32%) |
| 30  | CHL  | 9     | 305 | -    | 45,59,74     | 3.63 | 19 (42%) | 40,96,114   | 3.16 | 17 (42%) |
| 31  | CLA  | F     | 301 | -    | 49,53,73     | 1.36 | 9 (18%)  | 58,89,113   | 1.43 | 4 (6%)   |
| 30  | CHL  | 9     | 306 | -    | 42,56,74     | 3.80 | 19 (45%) | 36,92,114   | 3.36 | 16 (44%) |
| 31  | CLA  | M     | 101 | -    | 50,54,73     | 1.33 | 8 (16%)  | 59,90,113   | 1.40 | 4 (6%)   |
| 31  | CLA  | A     | 818 | 9    | 69,73,73     | 1.14 | 7 (10%)  | 82,113,113  | 1.33 | 9 (10%)  |
| 30  | CHL  | 5     | 301 | 2    | 46,60,74     | 3.74 | 19 (41%) | 40,97,114   | 2.94 | 16 (40%) |
| 31  | CLA  | 6     | 314 | -    | 49,53,73     | 1.36 | 9 (18%)  | 58,89,113   | 1.45 | 5 (8%)   |
| 34  | LHG  | d     | 630 | -    | 35,35,48     | 1.31 | 6 (17%)  | 38,41,54    | 1.06 | 2 (5%)   |
| 31  | CLA  | B     | 813 | 10   | 59,63,73     | 1.26 | 9 (15%)  | 70,101,113  | 1.34 | 5 (7%)   |
| 34  | LHG  | M     | 104 | -    | 45,45,48     | 1.17 | 6 (13%)  | 48,51,54    | 0.98 | 3 (6%)   |
| 31  | CLA  | h     | 610 | -    | 50,54,73     | 1.36 | 8 (16%)  | 59,90,113   | 1.41 | 4 (6%)   |
| 31  | CLA  | 9     | 312 | 8    | 60,64,73     | 1.23 | 9 (15%)  | 71,102,113  | 1.32 | 5 (7%)   |
| 31  | CLA  | 0     | 312 | 1    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.26 | 5 (6%)   |
| 31  | CLA  | A     | 832 | 9    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.27 | 5 (6%)   |
| 37  | OIE  | i     | 521 | -    | 42,45,45     | 1.12 | 6 (14%)  | 51,63,63    | 1.51 | 10 (19%) |
| 34  | LHG  | e     | 630 | 31   | 42,42,48     | 1.22 | 6 (14%)  | 45,48,54    | 0.98 | 2 (4%)   |
| 33  | OUR  | a     | 520 | -    | 45,48,58     | 0.77 | 1 (2%)   | 55,67,77    | 1.72 | 16 (29%) |
| 34  | LHG  | 3     | 603 | -    | 35,35,48     | 1.31 | 6 (17%)  | 38,41,54    | 1.07 | 2 (5%)   |
| 31  | CLA  | 1     | 310 | 34   | 67,71,73     | 1.17 | 9 (13%)  | 79,110,113  | 1.28 | 4 (5%)   |
| 37  | OIE  | 3     | 502 | -    | 42,45,45     | 1.16 | 5 (11%)  | 51,63,63    | 1.51 | 11 (21%) |
| 31  | CLA  | B     | 807 | 10   | 49,53,73     | 1.35 | 9 (18%)  | 58,89,113   | 1.51 | 7 (12%)  |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 30  | CHL  | i     | 607 | -    | 41,55,74     | 4.05 | 18 (43%) | 35,91,114   | 3.03 | 16 (45%) |
| 31  | CLA  | B     | 837 | -    | 69,73,73     | 1.14 | 9 (13%)  | 82,113,113  | 1.30 | 7 (8%)   |
| 34  | LHG  | 2     | 601 | 31   | 31,31,48     | 1.38 | 5 (16%)  | 34,37,54    | 1.13 | 3 (8%)   |
| 37  | OIE  | 7     | 502 | -    | 42,45,45     | 1.16 | 5 (11%)  | 51,63,63    | 1.49 | 11 (21%) |
| 31  | CLA  | A     | 841 | -    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.32 | 6 (7%)   |
| 31  | CLA  | h     | 611 | -    | 45,49,73     | 1.42 | 7 (15%)  | 54,84,113   | 1.47 | 5 (9%)   |
| 31  | CLA  | A     | 838 | 9    | 60,64,73     | 1.24 | 9 (15%)  | 71,102,113  | 1.32 | 6 (8%)   |
| 30  | CHL  | h     | 605 | 22   | 37,51,74     | 4.27 | 18 (48%) | 30,86,114   | 3.18 | 13 (43%) |
| 31  | CLA  | e     | 610 | -    | 59,63,73     | 1.26 | 9 (15%)  | 70,101,113  | 1.34 | 8 (11%)  |
| 31  | CLA  | 9     | 311 | 8    | 56,60,73     | 1.29 | 9 (16%)  | 65,97,113   | 1.37 | 6 (9%)   |
| 30  | CHL  | 4     | 306 | -    | 42,56,74     | 3.84 | 19 (45%) | 36,92,114   | 3.25 | 16 (44%) |
| 31  | CLA  | K     | 104 | 19   | 50,54,73     | 1.35 | 9 (18%)  | 59,90,113   | 1.43 | 4 (6%)   |
| 33  | OUR  | 4     | 501 | -    | 49,52,58     | 0.99 | 2 (4%)   | 58,71,77    | 2.18 | 22 (37%) |
| 30  | CHL  | h     | 614 | -    | 36,50,74     | 4.32 | 18 (50%) | 29,85,114   | 3.05 | 12 (41%) |
| 30  | CHL  | f     | 609 | -    | 60,74,74     | 3.30 | 18 (30%) | 58,114,114  | 2.43 | 17 (29%) |
| 32  | 8CT  | 7     | 405 | -    | 40,41,41     | 4.75 | 23 (57%) | 51,56,56    | 2.77 | 20 (39%) |
| 30  | CHL  | 5     | 305 | -    | 40,54,74     | 3.99 | 18 (45%) | 34,90,114   | 3.21 | 15 (44%) |
| 31  | CLA  | g     | 612 | -    | 49,53,73     | 1.39 | 7 (14%)  | 58,89,113   | 1.43 | 4 (6%)   |
| 31  | CLA  | B     | 820 | -    | 60,64,73     | 1.24 | 9 (15%)  | 71,102,113  | 1.36 | 5 (7%)   |
| 30  | CHL  | d     | 605 | 25   | 37,51,74     | 4.29 | 17 (45%) | 30,86,114   | 3.34 | 15 (50%) |
| 36  | LMG  | 2     | 602 | -    | 36,36,55     | 0.89 | 1 (2%)   | 44,44,63    | 1.24 | 5 (11%)  |
| 37  | OIE  | f     | 521 | -    | 42,45,45     | 1.13 | 6 (14%)  | 51,63,63    | 1.51 | 10 (19%) |
| 32  | 8CT  | 9     | 401 | -    | 40,41,41     | 4.80 | 23 (57%) | 51,56,56    | 2.78 | 19 (37%) |
| 37  | OIE  | c     | 522 | -    | 42,45,45     | 1.11 | 6 (14%)  | 51,63,63    | 1.66 | 13 (25%) |
| 31  | CLA  | 3     | 309 | 4    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.29 | 7 (8%)   |
| 33  | OUR  | 8     | 502 | -    | 50,53,58     | 0.98 | 1 (2%)   | 59,72,77    | 1.95 | 13 (22%) |
| 31  | CLA  | B     | 824 | 10   | 64,68,73     | 1.21 | 9 (14%)  | 76,107,113  | 1.29 | 6 (7%)   |
| 30  | CHL  | b     | 614 | -    | 36,50,74     | 4.26 | 17 (47%) | 29,85,114   | 3.13 | 16 (55%) |
| 30  | CHL  | a     | 609 | -    | 53,67,74     | 3.55 | 18 (33%) | 49,105,114  | 2.63 | 18 (36%) |
| 31  | CLA  | B     | 806 | -    | 69,73,73     | 1.15 | 10 (14%) | 82,113,113  | 1.34 | 7 (8%)   |
| 33  | OUR  | 9     | 501 | -    | 50,53,58     | 0.97 | 1 (2%)   | 59,72,77    | 1.76 | 16 (27%) |
| 31  | CLA  | B     | 810 | 10   | 66,70,73     | 1.16 | 9 (13%)  | 78,109,113  | 1.32 | 7 (8%)   |
| 34  | LHG  | 3     | 601 | -    | 35,35,48     | 1.32 | 6 (17%)  | 38,41,54    | 1.13 | 2 (5%)   |
| 31  | CLA  | 9     | 302 | -    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.26 | 5 (6%)   |
| 30  | CHL  | b     | 606 | -    | 45,59,74     | 3.72 | 18 (40%) | 40,96,114   | 2.99 | 18 (45%) |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 31  | CLA  | G     | 103 | 14   | 50,54,73     | 1.35 | 8 (16%)  | 59,90,113   | 1.38 | 4 (6%)   |
| 30  | CHL  | 6     | 301 | 5    | 55,69,74     | 3.31 | 19 (34%) | 52,108,114  | 2.77 | 18 (34%) |
| 30  | CHL  | c     | 607 | -    | 41,55,74     | 4.00 | 18 (43%) | 35,91,114   | 3.01 | 15 (42%) |
| 31  | CLA  | b     | 603 | 24   | 59,63,73     | 1.27 | 9 (15%)  | 70,101,113  | 1.31 | 4 (5%)   |
| 30  | CHL  | 0     | 305 | -    | 45,59,74     | 3.74 | 18 (40%) | 40,96,114   | 3.07 | 19 (47%) |
| 31  | CLA  | A     | 843 | 34   | 56,60,73     | 1.27 | 9 (16%)  | 65,97,113   | 1.41 | 8 (12%)  |
| 39  | CL0  | A     | 857 | 9    | 58,73,73     | 2.15 | 13 (22%) | 60,113,113  | 1.56 | 11 (18%) |
| 30  | CHL  | 0     | 302 | 1    | 58,72,74     | 3.19 | 19 (32%) | 55,111,114  | 2.74 | 18 (32%) |
| 30  | CHL  | g     | 601 | 25   | 46,60,74     | 3.87 | 19 (41%) | 40,97,114   | 3.00 | 18 (45%) |
| 32  | 8CT  | B     | 848 | -    | 40,41,41     | 4.81 | 23 (57%) | 51,56,56    | 2.63 | 19 (37%) |
| 31  | CLA  | a     | 604 | -    | 54,58,73     | 1.32 | 9 (16%)  | 64,95,113   | 1.36 | 6 (9%)   |
| 34  | LHG  | A     | 845 | 31   | 26,26,48     | 1.30 | 4 (15%)  | 29,32,54    | 1.20 | 2 (6%)   |
| 31  | CLA  | 0     | 310 | -    | 45,49,73     | 1.38 | 9 (20%)  | 54,84,113   | 1.48 | 5 (9%)   |
| 31  | CLA  | B     | 811 | 10   | 69,73,73     | 1.14 | 9 (13%)  | 82,113,113  | 1.35 | 7 (8%)   |
| 30  | CHL  | b     | 601 | 24   | 60,74,74     | 3.31 | 18 (30%) | 58,114,114  | 2.50 | 16 (27%) |
| 30  | CHL  | d     | 607 | -    | 41,55,74     | 4.04 | 18 (43%) | 35,91,114   | 3.01 | 14 (40%) |
| 30  | CHL  | 4     | 307 | -    | 45,59,74     | 3.63 | 19 (42%) | 40,96,114   | 3.19 | 17 (42%) |
| 31  | CLA  | d     | 612 | 25   | 49,53,73     | 1.39 | 9 (18%)  | 58,89,113   | 1.42 | 4 (6%)   |
| 30  | CHL  | 5     | 302 | 2    | 58,72,74     | 3.17 | 19 (32%) | 55,111,114  | 2.79 | 18 (32%) |
| 32  | 8CT  | B     | 844 | -    | 40,41,41     | 4.86 | 23 (57%) | 51,56,56    | 2.73 | 22 (43%) |
| 31  | CLA  | c     | 610 | -    | 59,63,73     | 1.25 | 9 (15%)  | 70,101,113  | 1.34 | 6 (8%)   |
| 31  | CLA  | 8     | 310 | 34   | 50,54,73     | 1.33 | 9 (18%)  | 59,90,113   | 1.36 | 4 (6%)   |
| 33  | 0UR  | 0     | 502 | -    | 50,53,58     | 0.98 | 1 (2%)   | 59,72,77    | 1.96 | 18 (30%) |
| 40  | SF4  | C     | 102 | 18   | 0,12,12      | -    | -        | -           | -    | -        |
| 31  | CLA  | 6     | 317 | 5    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.32 | 7 (8%)   |
| 31  | CLA  | c     | 612 | 23   | 49,53,73     | 1.38 | 9 (18%)  | 58,89,113   | 1.45 | 4 (6%)   |
| 31  | CLA  | 5     | 310 | 34   | 49,53,73     | 1.37 | 9 (18%)  | 58,89,113   | 1.40 | 4 (6%)   |
| 31  | CLA  | f     | 610 | -    | 59,63,73     | 1.26 | 9 (15%)  | 70,101,113  | 1.32 | 7 (10%)  |
| 31  | CLA  | A     | 816 | -    | 49,53,73     | 1.39 | 9 (18%)  | 58,89,113   | 1.45 | 4 (6%)   |
| 32  | 8CT  | J     | 101 | -    | 40,41,41     | 4.75 | 23 (57%) | 51,56,56    | 2.88 | 18 (35%) |
| 31  | CLA  | 1     | 309 | 2    | 59,63,73     | 1.25 | 9 (15%)  | 70,101,113  | 1.31 | 6 (8%)   |
| 31  | CLA  | 7     | 309 | -    | 63,67,73     | 1.20 | 9 (14%)  | 74,105,113  | 1.33 | 7 (9%)   |
| 30  | CHL  | f     | 606 | -    | 45,59,74     | 3.78 | 18 (40%) | 40,96,114   | 3.08 | 19 (47%) |
| 30  | CHL  | g     | 607 | -    | 45,59,74     | 3.90 | 18 (40%) | 40,96,114   | 2.90 | 19 (47%) |
| 30  | CHL  | 8     | 301 | 7    | 55,69,74     | 3.35 | 19 (34%) | 52,108,114  | 2.89 | 19 (36%) |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 34  | LHG  | g     | 630 | -    | 29,29,48     | 1.39 | 6 (20%)  | 32,35,54    | 1.17 | 3 (9%)   |
| 33  | OUR  | g     | 520 | -    | 50,53,58     | 0.95 | 1 (2%)   | 59,72,77    | 1.99 | 12 (20%) |
| 31  | CLA  | b     | 613 | -    | 59,63,73     | 1.27 | 9 (15%)  | 69,100,113  | 1.35 | 5 (7%)   |
| 36  | LMG  | J     | 102 | -    | 29,29,55     | 0.97 | 1 (3%)   | 37,37,63    | 1.28 | 4 (10%)  |
| 32  | 8CT  | B     | 851 | -    | 40,41,41     | 4.76 | 23 (57%) | 51,56,56    | 2.52 | 17 (33%) |
| 30  | CHL  | 8     | 305 | -    | 41,55,74     | 3.86 | 19 (46%) | 35,91,114   | 3.21 | 16 (45%) |
| 31  | CLA  | 7     | 303 | 6    | 49,53,73     | 1.37 | 9 (18%)  | 58,89,113   | 1.42 | 4 (6%)   |
| 31  | CLA  | A     | 822 | -    | 53,57,73     | 1.29 | 9 (16%)  | 61,93,113   | 1.39 | 4 (6%)   |
| 33  | OUR  | 5     | 501 | -    | 49,52,58     | 0.97 | 1 (2%)   | 58,71,77    | 1.82 | 13 (22%) |
| 31  | CLA  | 9     | 308 | -    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.28 | 5 (6%)   |
| 32  | 8CT  | B     | 847 | -    | 40,41,41     | 4.75 | 23 (57%) | 51,56,56    | 3.16 | 20 (39%) |
| 31  | CLA  | B     | 815 | 10   | 59,63,73     | 1.24 | 9 (15%)  | 70,101,113  | 1.36 | 8 (11%)  |
| 31  | CLA  | A     | 819 | 9    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.30 | 9 (10%)  |
| 31  | CLA  | a     | 613 | 22   | 59,63,73     | 1.28 | 9 (15%)  | 69,100,113  | 1.36 | 6 (8%)   |
| 31  | CLA  | B     | 850 | 13   | 51,55,73     | 1.33 | 9 (17%)  | 60,91,113   | 1.37 | 5 (8%)   |
| 34  | LHG  | 6     | 601 | 31   | 36,36,48     | 1.30 | 6 (16%)  | 39,42,54    | 1.06 | 2 (5%)   |
| 33  | OUR  | d     | 520 | -    | 47,50,58     | 0.99 | 1 (2%)   | 56,69,77    | 1.78 | 13 (23%) |
| 31  | CLA  | a     | 610 | -    | 59,63,73     | 1.26 | 7 (11%)  | 70,101,113  | 1.35 | 7 (10%)  |
| 31  | CLA  | O     | 206 | -    | 55,59,73     | 1.30 | 9 (16%)  | 64,96,113   | 1.32 | 5 (7%)   |
| 31  | CLA  | B     | 805 | 10   | 69,73,73     | 1.14 | 9 (13%)  | 82,113,113  | 1.26 | 6 (7%)   |
| 31  | CLA  | B     | 808 | 10   | 69,73,73     | 1.14 | 9 (13%)  | 82,113,113  | 1.34 | 9 (10%)  |
| 31  | CLA  | a     | 612 | -    | 49,53,73     | 1.38 | 7 (14%)  | 58,89,113   | 1.45 | 4 (6%)   |
| 32  | 8CT  | G     | 104 | -    | 40,41,41     | 4.80 | 23 (57%) | 51,56,56    | 3.09 | 20 (39%) |
| 37  | OIE  | h     | 521 | -    | 42,45,45     | 1.12 | 6 (14%)  | 51,63,63    | 1.52 | 10 (19%) |
| 31  | CLA  | B     | 812 | 10   | 56,60,73     | 1.28 | 8 (14%)  | 65,97,113   | 1.41 | 7 (10%)  |
| 30  | CHL  | 2     | 308 | -    | 41,55,74     | 3.81 | 19 (46%) | 35,91,114   | 3.10 | 15 (42%) |
| 31  | CLA  | 5     | 314 | 2    | 50,54,73     | 1.35 | 8 (16%)  | 59,90,113   | 1.35 | 4 (6%)   |
| 32  | 8CT  | 2     | 402 | -    | 40,41,41     | 4.79 | 23 (57%) | 51,56,56    | 3.05 | 19 (37%) |
| 31  | CLA  | B     | 801 | -    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.35 | 9 (10%)  |
| 31  | CLA  | 4     | 312 | 7    | 57,61,73     | 1.27 | 9 (15%)  | 67,98,113   | 1.35 | 4 (5%)   |
| 36  | LMG  | O     | 207 | -    | 39,39,55     | 0.82 | 1 (2%)   | 47,47,63    | 1.27 | 5 (10%)  |
| 30  | CHL  | e     | 614 | -    | 36,50,74     | 4.30 | 17 (47%) | 29,85,114   | 3.08 | 15 (51%) |
| 31  | CLA  | f     | 603 | -    | 59,63,73     | 1.26 | 8 (13%)  | 70,101,113  | 1.32 | 5 (7%)   |
| 37  | OIE  | e     | 522 | -    | 42,45,45     | 1.11 | 6 (14%)  | 51,63,63    | 1.58 | 11 (21%) |
| 30  | CHL  | e     | 605 | 29   | 37,51,74     | 4.18 | 17 (45%) | 30,86,114   | 3.19 | 16 (53%) |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 31  | CLA  | 3     | 303 | -    | 59,63,73     | 1.24 | 9 (15%)  | 70,101,113  | 1.35 | 8 (11%)  |
| 37  | OIE  | d     | 521 | -    | 42,45,45     | 1.13 | 6 (14%)  | 51,63,63    | 1.53 | 12 (23%) |
| 30  | CHL  | 6     | 313 | 5    | 46,60,74     | 3.62 | 19 (41%) | 40,97,114   | 3.27 | 19 (47%) |
| 31  | CLA  | 2     | 303 | 3    | 60,64,73     | 1.25 | 9 (15%)  | 71,102,113  | 1.35 | 5 (7%)   |
| 31  | CLA  | h     | 604 | -    | 50,54,73     | 1.36 | 8 (16%)  | 59,90,113   | 1.42 | 5 (8%)   |
| 31  | CLA  | 8     | 304 | -    | 69,73,73     | 1.16 | 8 (11%)  | 82,113,113  | 1.24 | 6 (7%)   |
| 33  | OUR  | 1     | 502 | -    | 50,53,58     | 1.01 | 1 (2%)   | 59,72,77    | 1.88 | 12 (20%) |
| 31  | CLA  | 3     | 313 | 4    | 49,53,73     | 1.37 | 9 (18%)  | 58,89,113   | 1.42 | 4 (6%)   |
| 33  | OUR  | c     | 520 | -    | 50,53,58     | 1.02 | 2 (4%)   | 59,72,77    | 1.87 | 16 (27%) |
| 31  | CLA  | L     | 203 | 17   | 67,71,73     | 1.17 | 9 (13%)  | 79,110,113  | 1.33 | 5 (6%)   |
| 31  | CLA  | A     | 836 | -    | 55,59,73     | 1.27 | 9 (16%)  | 64,96,113   | 1.43 | 8 (12%)  |
| 30  | CHL  | 9     | 313 | 8    | 41,55,74     | 3.86 | 18 (43%) | 35,91,114   | 3.34 | 16 (45%) |
| 36  | LMG  | B     | 853 | -    | 42,42,55     | 0.79 | 0        | 50,50,63    | 1.31 | 6 (12%)  |
| 31  | CLA  | 7     | 304 | -    | 59,63,73     | 1.25 | 9 (15%)  | 70,101,113  | 1.36 | 7 (10%)  |
| 32  | 8CT  | F     | 302 | -    | 40,41,41     | 4.78 | 23 (57%) | 51,56,56    | 2.76 | 17 (33%) |
| 31  | CLA  | e     | 603 | 29   | 61,65,73     | 1.24 | 8 (13%)  | 72,103,113  | 1.31 | 4 (5%)   |
| 30  | CHL  | 8     | 306 | -    | 45,59,74     | 3.70 | 18 (40%) | 40,96,114   | 3.02 | 19 (47%) |
| 30  | CHL  | c     | 608 | -    | 60,74,74     | 3.25 | 18 (30%) | 58,114,114  | 2.42 | 18 (31%) |
| 32  | 8CT  | A     | 847 | -    | 40,41,41     | 4.73 | 23 (57%) | 51,56,56    | 3.14 | 20 (39%) |
| 31  | CLA  | A     | 815 | 9    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.32 | 6 (7%)   |
| 30  | CHL  | 2     | 313 | 3    | 45,59,74     | 3.63 | 19 (42%) | 40,96,114   | 3.05 | 17 (42%) |
| 31  | CLA  | e     | 611 | 34   | 59,63,73     | 1.27 | 9 (15%)  | 70,101,113  | 1.32 | 6 (8%)   |
| 31  | CLA  | B     | 833 | 10   | 59,63,73     | 1.25 | 9 (15%)  | 70,101,113  | 1.36 | 8 (11%)  |
| 30  | CHL  | f     | 608 | -    | 45,59,74     | 3.69 | 18 (40%) | 40,96,114   | 3.22 | 17 (42%) |
| 31  | CLA  | O     | 203 | -    | 41,46,73     | 1.59 | 9 (21%)  | 51,81,113   | 1.53 | 7 (13%)  |
| 31  | CLA  | A     | 829 | 9    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.30 | 6 (7%)   |
| 31  | CLA  | i     | 610 | -    | 59,63,73     | 1.25 | 8 (13%)  | 70,101,113  | 1.32 | 6 (8%)   |
| 34  | LHG  | B     | 854 | -    | 42,42,48     | 1.22 | 6 (14%)  | 45,48,54    | 0.98 | 2 (4%)   |
| 30  | CHL  | 2     | 306 | -    | 42,56,74     | 3.82 | 19 (45%) | 36,92,114   | 3.24 | 16 (44%) |
| 30  | CHL  | 5     | 307 | -    | 41,55,74     | 3.95 | 19 (46%) | 35,91,114   | 3.04 | 16 (45%) |
| 33  | OUR  | 8     | 501 | -    | 49,52,58     | 0.97 | 1 (2%)   | 58,71,77    | 1.83 | 16 (27%) |
| 31  | CLA  | c     | 604 | -    | 54,58,73     | 1.31 | 9 (16%)  | 64,95,113   | 1.41 | 7 (10%)  |
| 31  | CLA  | A     | 805 | 9    | 69,73,73     | 1.17 | 9 (13%)  | 82,113,113  | 1.29 | 5 (6%)   |
| 31  | CLA  | 5     | 309 | -    | 64,68,73     | 1.21 | 9 (14%)  | 76,107,113  | 1.29 | 8 (10%)  |
| 32  | 8CT  | L     | 205 | -    | 40,41,41     | 4.76 | 23 (57%) | 51,56,56    | 3.01 | 19 (37%) |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 31  | CLA  | A     | 802 | -    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.23 | 4 (4%)   |
| 31  | CLA  | A     | 812 | 9    | 58,62,73     | 1.27 | 9 (15%)  | 68,99,113   | 1.32 | 6 (8%)   |
| 31  | CLA  | 2     | 312 | 3    | 64,68,73     | 1.19 | 9 (14%)  | 76,107,113  | 1.34 | 6 (7%)   |
| 34  | LHG  | B     | 852 | 31   | 22,22,48     | 1.33 | 3 (13%)  | 25,28,54    | 1.09 | 1 (4%)   |
| 34  | LHG  | 5     | 601 | 31   | 36,36,48     | 1.29 | 6 (16%)  | 39,42,54    | 1.09 | 3 (7%)   |
| 34  | LHG  | 1     | 601 | 31   | 48,48,48     | 1.14 | 5 (10%)  | 51,54,54    | 0.98 | 2 (3%)   |
| 31  | CLA  | A     | 810 | 9    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.30 | 5 (6%)   |
| 36  | LMG  | L     | 211 | -    | 37,37,55     | 0.88 | 1 (2%)   | 45,45,63    | 1.26 | 4 (8%)   |
| 34  | LHG  | 4     | 601 | 31   | 31,31,48     | 1.37 | 5 (16%)  | 34,37,54    | 1.16 | 3 (8%)   |
| 31  | CLA  | b     | 604 | -    | 54,58,73     | 1.32 | 8 (14%)  | 64,95,113   | 1.37 | 5 (7%)   |
| 32  | 8CT  | B     | 845 | -    | 40,41,41     | 4.76 | 23 (57%) | 51,56,56    | 3.28 | 22 (43%) |
| 31  | CLA  | A     | 824 | 9    | 59,63,73     | 1.24 | 9 (15%)  | 70,101,113  | 1.32 | 5 (7%)   |
| 31  | CLA  | B     | 819 | 10   | 64,68,73     | 1.19 | 9 (14%)  | 76,107,113  | 1.31 | 7 (9%)   |
| 34  | LHG  | K     | 106 | -    | 42,42,48     | 1.20 | 6 (14%)  | 45,47,54    | 1.06 | 4 (8%)   |
| 30  | CHL  | f     | 607 | -    | 41,55,74     | 3.99 | 18 (43%) | 35,91,114   | 3.04 | 15 (42%) |
| 33  | OUR  | i     | 520 | -    | 48,51,58     | 0.98 | 1 (2%)   | 57,70,77    | 1.91 | 13 (22%) |
| 31  | CLA  | 4     | 310 | 34   | 64,68,73     | 1.20 | 9 (14%)  | 76,107,113  | 1.29 | 5 (6%)   |
| 30  | CHL  | e     | 606 | -    | 45,59,74     | 3.77 | 18 (40%) | 40,96,114   | 3.01 | 18 (45%) |
| 30  | CHL  | c     | 606 | -    | 38,52,74     | 4.00 | 17 (44%) | 31,87,114   | 3.20 | 14 (45%) |
| 31  | CLA  | 3     | 304 | -    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.34 | 6 (7%)   |
| 31  | CLA  | A     | 831 | 9    | 54,58,73     | 1.29 | 9 (16%)  | 64,95,113   | 1.44 | 6 (9%)   |
| 31  | CLA  | 2     | 311 | 3    | 52,56,73     | 1.31 | 8 (15%)  | 61,92,113   | 1.45 | 6 (9%)   |
| 31  | CLA  | A     | 830 | 9    | 69,73,73     | 1.17 | 10 (14%) | 82,113,113  | 1.42 | 9 (10%)  |
| 31  | CLA  | B     | 829 | -    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.21 | 4 (4%)   |
| 42  | NEX  | b     | 523 | -    | 40,46,46     | 1.12 | 3 (7%)   | 50,70,70    | 4.72 | 18 (36%) |
| 32  | 8CT  | 7     | 404 | -    | 40,41,41     | 4.76 | 23 (57%) | 51,56,56    | 3.69 | 24 (47%) |
| 32  | 8CT  | M     | 102 | -    | 40,41,41     | 4.76 | 23 (57%) | 51,56,56    | 2.90 | 19 (37%) |
| 31  | CLA  | B     | 839 | -    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.28 | 5 (6%)   |
| 30  | CHL  | 7     | 306 | -    | 55,69,74     | 3.33 | 19 (34%) | 51,107,114  | 2.73 | 18 (35%) |
| 33  | OUR  | 7     | 501 | -    | 49,52,58     | 1.01 | 1 (2%)   | 58,71,77    | 2.14 | 18 (31%) |
| 42  | NEX  | a     | 523 | -    | 40,46,46     | 1.11 | 3 (7%)   | 50,70,70    | 4.73 | 18 (36%) |
| 31  | CLA  | i     | 612 | -    | 49,53,73     | 1.39 | 7 (14%)  | 58,89,113   | 1.42 | 5 (8%)   |
| 31  | CLA  | L     | 204 | -    | 50,54,73     | 1.33 | 9 (18%)  | 59,90,113   | 1.37 | 4 (6%)   |
| 36  | LMG  | J     | 105 | -    | 46,46,55     | 0.88 | 2 (4%)   | 54,54,63    | 1.36 | 7 (12%)  |
| 31  | CLA  | A     | 833 | 9    | 69,73,73     | 1.14 | 9 (13%)  | 82,113,113  | 1.29 | 5 (6%)   |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 31  | CLA  | 0     | 304 | -    | 56,60,73     | 1.29 | 9 (16%)  | 65,97,113   | 1.37 | 6 (9%)   |
| 30  | CHL  | 0     | 301 | 1    | 46,60,74     | 3.62 | 19 (41%) | 40,97,114   | 3.06 | 16 (40%) |
| 31  | CLA  | A     | 825 | -    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.31 | 8 (9%)   |
| 31  | CLA  | 6     | 311 | 5    | 52,56,73     | 1.34 | 9 (17%)  | 61,92,113   | 1.37 | 5 (8%)   |
| 31  | CLA  | i     | 604 | -    | 54,58,73     | 1.33 | 8 (14%)  | 64,95,113   | 1.39 | 6 (9%)   |
| 31  | CLA  | 8     | 312 | 7    | 60,64,73     | 1.25 | 9 (15%)  | 71,102,113  | 1.32 | 4 (5%)   |
| 31  | CLA  | A     | 837 | 9    | 65,69,73     | 1.18 | 9 (13%)  | 77,108,113  | 1.35 | 7 (9%)   |
| 31  | CLA  | B     | 821 | 10   | 54,58,73     | 1.29 | 9 (16%)  | 64,95,113   | 1.45 | 8 (12%)  |
| 31  | CLA  | g     | 613 | 25   | 51,55,73     | 1.36 | 9 (17%)  | 60,91,113   | 1.45 | 6 (10%)  |
| 33  | OUR  | 2     | 502 | -    | 48,51,58     | 1.01 | 1 (2%)   | 57,70,77    | 1.99 | 12 (21%) |
| 30  | CHL  | g     | 605 | -    | 37,51,74     | 4.30 | 18 (48%) | 30,86,114   | 3.26 | 15 (50%) |
| 31  | CLA  | 5     | 312 | 2    | 60,64,73     | 1.24 | 9 (15%)  | 71,102,113  | 1.34 | 4 (5%)   |
| 31  | CLA  | A     | 834 | 9    | 50,54,73     | 1.32 | 9 (18%)  | 59,90,113   | 1.42 | 4 (6%)   |
| 33  | OUR  | f     | 520 | -    | 47,50,58     | 1.02 | 1 (2%)   | 56,69,77    | 1.91 | 16 (28%) |
| 42  | NEX  | h     | 523 | -    | 40,46,46     | 1.11 | 3 (7%)   | 50,70,70    | 4.72 | 18 (36%) |
| 32  | 8CT  | A     | 848 | -    | 40,41,41     | 4.73 | 23 (57%) | 51,56,56    | 2.84 | 23 (45%) |
| 31  | CLA  | b     | 612 | -    | 49,53,73     | 1.39 | 9 (18%)  | 58,89,113   | 1.43 | 4 (6%)   |
| 31  | CLA  | c     | 603 | -    | 56,60,73     | 1.30 | 8 (14%)  | 65,97,113   | 1.39 | 6 (9%)   |
| 32  | 8CT  | 8     | 402 | -    | 40,41,41     | 4.80 | 23 (57%) | 51,56,56    | 2.76 | 19 (37%) |
| 31  | CLA  | A     | 806 | -    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.31 | 6 (7%)   |
| 30  | CHL  | 3     | 305 | -    | 45,59,74     | 3.64 | 19 (42%) | 40,96,114   | 3.14 | 17 (42%) |
| 31  | CLA  | 3     | 311 | 4    | 50,54,73     | 1.35 | 9 (18%)  | 59,90,113   | 1.46 | 5 (8%)   |
| 31  | CLA  | 9     | 304 | -    | 55,59,73     | 1.30 | 9 (16%)  | 64,96,113   | 1.37 | 5 (7%)   |
| 33  | OUR  | 6     | 501 | -    | 49,52,58     | 1.00 | 2 (4%)   | 58,71,77    | 1.92 | 15 (25%) |
| 31  | CLA  | 7     | 311 | 6    | 56,60,73     | 1.28 | 9 (16%)  | 65,97,113   | 1.38 | 6 (9%)   |
| 30  | CHL  | g     | 606 | -    | 45,59,74     | 3.84 | 18 (40%) | 40,96,114   | 2.97 | 18 (45%) |
| 33  | OUR  | 3     | 501 | -    | 49,52,58     | 1.02 | 2 (4%)   | 58,71,77    | 2.12 | 21 (36%) |
| 31  | CLA  | A     | 840 | 9    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.32 | 6 (7%)   |
| 30  | CHL  | i     | 602 | -    | 55,69,74     | 3.42 | 18 (32%) | 52,108,114  | 2.72 | 19 (36%) |
| 40  | SF4  | C     | 101 | -    | 0,12,12      | -    | -        | -           | -    | -        |
| 30  | CHL  | a     | 602 | -    | 58,72,74     | 3.34 | 18 (31%) | 55,111,114  | 2.62 | 19 (34%) |
| 31  | CLA  | b     | 611 | -    | 64,68,73     | 1.21 | 8 (12%)  | 76,107,113  | 1.28 | 5 (6%)   |
| 31  | CLA  | B     | 841 | 34   | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.31 | 6 (7%)   |
| 37  | OIE  | h     | 522 | -    | 42,45,45     | 1.12 | 6 (14%)  | 51,63,63    | 1.52 | 9 (17%)  |
| 31  | CLA  | g     | 611 | -    | 50,54,73     | 1.36 | 7 (14%)  | 59,90,113   | 1.40 | 5 (8%)   |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 31  | CLA  | d     | 604 | -    | 54,58,73     | 1.32 | 8 (14%)  | 64,95,113   | 1.38 | 5 (7%)   |
| 34  | LHG  | b     | 630 | -    | 40,40,48     | 1.24 | 6 (15%)  | 43,46,54    | 0.99 | 2 (4%)   |
| 32  | 8CT  | J     | 104 | -    | 40,41,41     | 4.80 | 23 (57%) | 51,56,56    | 3.45 | 23 (45%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 31  | CLA  | B     | 825 | -    | 1/1/15/20 | 7/39/115/115  | -       |
| 30  | CHL  | 7     | 307 | -    | 3/3/17/26 | 4/21/119/137  | -       |
| 31  | CLA  | 2     | 309 | 3    | 1/1/14/20 | 3/33/109/115  | -       |
| 36  | LMG  | A     | 856 | -    | -         | 13/31/51/70   | 0/1/1/1 |
| 31  | CLA  | H     | 205 | -    | 1/1/12/20 | 9/23/99/115   | -       |
| 31  | CLA  | O     | 202 | 21   | 1/1/9/20  | 2/6/78/115    | -       |
| 32  | 8CT  | A     | 854 | -    | -         | 10/29/63/63   | 0/2/2/2 |
| 41  | DGD  | B     | 849 | -    | -         | 27/45/85/95   | 0/2/2/2 |
| 30  | CHL  | 8     | 302 | 7    | 3/3/19/26 | 17/37/135/137 | -       |
| 31  | CLA  | c     | 613 | -    | 1/1/12/20 | 6/27/103/115  | -       |
| 31  | CLA  | 0     | 311 | -    | 1/1/11/20 | 8/18/94/115   | -       |
| 35  | SQD  | 0     | 603 | -    | -         | 17/31/51/69   | 0/1/1/1 |
| 30  | CHL  | h     | 607 | -    | 3/3/16/26 | 5/15/113/137  | -       |
| 37  | 0IE  | b     | 522 | -    | -         | 3/33/72/72    | 0/2/2/2 |
| 31  | CLA  | 4     | 309 | -    | 1/1/14/20 | 5/33/109/115  | -       |
| 31  | CLA  | L     | 202 | 17   | 1/1/11/20 | 5/17/93/115   | -       |
| 30  | CHL  | 6     | 306 | -    | 3/3/17/26 | 7/21/119/137  | -       |
| 30  | CHL  | d     | 614 | -    | 3/3/15/26 | 0/10/108/137  | -       |
| 31  | CLA  | i     | 613 | -    | 1/1/12/20 | 5/23/99/115   | -       |
| 31  | CLA  | e     | 604 | -    | 1/1/12/20 | 7/21/97/115   | -       |
| 34  | LHG  | 8     | 601 | 31   | -         | 30/48/48/53   | -       |
| 31  | CLA  | A     | 811 | 9    | 1/1/15/20 | 12/39/115/115 | -       |
| 31  | CLA  | 6     | 309 | 5    | 1/1/13/20 | 2/31/107/115  | -       |
| 31  | CLA  | g     | 603 | -    | 1/1/12/20 | 4/23/99/115   | -       |
| 31  | CLA  | 6     | 312 | 5    | 1/1/13/20 | 7/29/105/115  | -       |
| 31  | CLA  | K     | 105 | 19   | 1/1/12/20 | 11/21/97/115  | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 31  | CLA  | 9     | 310 | 34   | 1/1/10/20 | 4/10/86/115   | -       |
| 30  | CHL  | 5     | 313 | 2    | 3/3/16/26 | 9/17/115/137  | -       |
| 31  | CLA  | B     | 840 | 10   | 1/1/15/20 | 10/39/115/115 | -       |
| 42  | NEX  | e     | 523 | -    | -         | 4/27/83/83    | 0/3/3/3 |
| 31  | CLA  | 0     | 309 | -    | 1/1/14/20 | 9/33/109/115  | -       |
| 31  | CLA  | h     | 612 | -    | 1/1/11/20 | 6/15/91/115   | -       |
| 30  | CHL  | b     | 607 | -    | 3/3/16/26 | 4/17/115/137  | -       |
| 30  | CHL  | 5     | 306 | -    | 3/3/16/26 | 11/18/116/137 | -       |
| 30  | CHL  | g     | 614 | -    | 3/3/15/26 | 2/10/108/137  | -       |
| 30  | CHL  | a     | 614 | -    | 3/3/15/26 | 0/10/108/137  | -       |
| 34  | LHG  | a     | 630 | -    | -         | 27/47/47/53   | -       |
| 31  | CLA  | 3     | 308 | -    | 1/1/15/20 | 16/39/115/115 | -       |
| 31  | CLA  | f     | 613 | 26   | 1/1/12/20 | 8/27/103/115  | -       |
| 31  | CLA  | 6     | 304 | -    | 1/1/11/20 | 6/17/93/115   | -       |
| 31  | CLA  | 1     | 303 | 2    | 1/1/13/20 | 14/29/105/115 | -       |
| 31  | CLA  | 6     | 318 | -    | 1/1/11/20 | 11/17/93/115  | -       |
| 31  | CLA  | B     | 817 | 10   | 1/1/14/20 | 18/33/109/115 | -       |
| 32  | 8CT  | 6     | 402 | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 31  | CLA  | i     | 611 | -    | 1/1/11/20 | 5/15/91/115   | -       |
| 31  | CLA  | 7     | 308 | -    | 1/1/15/20 | 15/39/115/115 | -       |
| 33  | 0UR  | h     | 520 | -    | -         | 9/42/81/86    | 0/2/2/2 |
| 31  | CLA  | 7     | 312 | 6    | 1/1/13/20 | 10/27/103/115 | -       |
| 30  | CHL  | a     | 605 | 22   | 3/3/15/26 | 4/12/110/137  | -       |
| 31  | CLA  | B     | 827 | -    | 1/1/15/20 | 10/39/115/115 | -       |
| 31  | CLA  | H     | 201 | 10   | 1/1/13/20 | 7/27/103/115  | -       |
| 32  | 8CT  | I     | 101 | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 31  | CLA  | 6     | 310 | 34   | 1/1/14/20 | 11/33/109/115 | -       |
| 31  | CLA  | 8     | 314 | 7    | 1/1/11/20 | 9/15/91/115   | -       |
| 31  | CLA  | A     | 835 | 9    | 1/1/13/20 | 12/30/106/115 | -       |
| 37  | 0IE  | f     | 522 | -    | -         | 0/33/72/72    | 0/2/2/2 |
| 30  | CHL  | 4     | 305 | -    | 3/3/15/26 | 0/12/110/137  | -       |
| 33  | 0UR  | b     | 520 | -    | -         | 10/42/81/86   | 0/2/2/2 |
| 30  | CHL  | e     | 607 | -    | 3/3/16/26 | 4/17/115/137  | -       |
| 32  | 8CT  | B     | 804 | -    | -         | 14/29/63/63   | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 30  | CHL  | 2     | 307 | -    | 3/3/17/26 | 6/21/119/137  | -       |
| 36  | LMG  | L     | 210 | -    | -         | 13/26/46/70   | 0/1/1/1 |
| 31  | CLA  | a     | 611 | -    | 1/1/13/20 | 8/30/106/115  | -       |
| 31  | CLA  | B     | 822 | 10   | 1/1/14/20 | 11/33/109/115 | -       |
| 31  | CLA  | J     | 103 | 16   | 1/1/10/20 | 3/12/88/115   | -       |
| 38  | PQN  | A     | 842 | -    | -         | 7/23/43/43    | 0/2/2/2 |
| 34  | LHG  | 6     | 603 | -    | -         | 12/35/35/53   | -       |
| 30  | CHL  | 7     | 305 | -    | 3/3/16/26 | 7/18/116/137  | -       |
| 31  | CLA  | 3     | 306 | 4    | 1/1/11/20 | 5/18/94/115   | -       |
| 31  | CLA  | 1     | 308 | -    | 1/1/11/20 | 6/15/91/115   | -       |
| 31  | CLA  | 4     | 311 | -    | 1/1/11/20 | 4/19/95/115   | -       |
| 42  | NEX  | c     | 523 | -    | -         | 5/27/83/83    | 0/3/3/3 |
| 31  | CLA  | B     | 836 | 10   | 1/1/14/20 | 11/33/109/115 | -       |
| 34  | LHG  | A     | 855 | -    | -         | 26/46/46/53   | -       |
| 30  | CHL  | 4     | 308 | -    | 3/3/16/26 | 3/17/115/137  | -       |
| 31  | CLA  | G     | 102 | 14   | 1/1/11/20 | 4/15/91/115   | -       |
| 31  | CLA  | 8     | 311 | 7    | 1/1/11/20 | 8/17/93/115   | -       |
| 34  | LHG  | 7     | 602 | -    | -         | 20/42/42/53   | -       |
| 31  | CLA  | g     | 604 | -    | 1/1/11/20 | 5/15/91/115   | -       |
| 30  | CHL  | a     | 601 | 22   | 3/3/16/26 | 7/17/115/137  | -       |
| 32  | 8CT  | 1     | 402 | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 30  | CHL  | i     | 608 | -    | 3/3/16/26 | 8/20/118/137  | -       |
| 30  | CHL  | h     | 608 | -    | 3/3/16/26 | 6/15/113/137  | -       |
| 31  | CLA  | B     | 830 | 10   | 1/1/13/20 | 7/29/105/115  | -       |
| 31  | CLA  | 0     | 303 | 1    | 1/1/14/20 | 10/36/112/115 | -       |
| 34  | LHG  | 7     | 603 | -    | -         | 20/43/43/53   | -       |
| 31  | CLA  | B     | 828 | -    | 1/1/14/20 | 6/33/109/115  | -       |
| 30  | CHL  | a     | 606 | -    | 3/3/17/26 | 7/21/119/137  | -       |
| 31  | CLA  | B     | 816 | 10   | 1/1/14/20 | 8/33/109/115  | -       |
| 31  | CLA  | 3     | 320 | -    | 1/1/12/20 | 5/24/100/115  | -       |
| 33  | OUR  | 4     | 502 | -    | -         | 13/40/79/86   | 0/2/2/2 |
| 34  | LHG  | 7     | 601 | 31   | -         | 10/34/34/53   | -       |
| 30  | CHL  | 8     | 307 | -    | 3/3/17/26 | 9/21/119/137  | -       |
| 31  | CLA  | a     | 603 | -    | 1/1/12/20 | 4/25/101/115  | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 31  | CLA  | B     | 834 | 10   | 1/1/14/20 | 15/35/111/115 | -       |
| 32  | 8CT  | 3     | 402 | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 30  | CHL  | 1     | 305 | -    | 3/3/17/26 | 7/21/119/137  | -       |
| 30  | CHL  | 3     | 307 | -    | 3/3/20/26 | 26/39/137/137 | -       |
| 31  | CLA  | A     | 839 | 9    | 1/1/15/20 | 12/39/115/115 | -       |
| 31  | CLA  | 7     | 316 | 6    | 1/1/12/20 | 2/15/91/115   | -       |
| 31  | CLA  | 9     | 309 | -    | 1/1/14/20 | 7/33/109/115  | -       |
| 30  | CHL  | d     | 608 | -    | 3/3/17/26 | 5/21/119/137  | -       |
| 31  | CLA  | B     | 832 | -    | 1/1/15/20 | 8/39/115/115  | -       |
| 42  | NEX  | g     | 523 | -    | -         | 5/27/83/83    | 0/3/3/3 |
| 33  | OUR  | O     | 204 | -    | -         | 5/42/81/86    | 0/2/2/2 |
| 40  | SF4  | B     | 802 | -    | -         | -             | 0/6/5/5 |
| 31  | CLA  | A     | 808 | 9    | 1/1/15/20 | 21/39/115/115 | -       |
| 31  | CLA  | A     | 809 | 9    | 1/1/15/20 | 9/39/115/115  | -       |
| 37  | OIE  | e     | 521 | -    | -         | 2/33/72/72    | 0/2/2/2 |
| 31  | CLA  | B     | 826 | -    | 1/1/10/20 | 1/23/87/115   | -       |
| 30  | CHL  | e     | 608 | -    | 3/3/20/26 | 16/39/137/137 | -       |
| 32  | 8CT  | 7     | 402 | -    | -         | 15/29/63/63   | 0/2/2/2 |
| 37  | OIE  | b     | 521 | -    | -         | 2/33/72/72    | 0/2/2/2 |
| 32  | 8CT  | O     | 205 | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 30  | CHL  | 9     | 301 | 8    | 3/3/16/26 | 8/17/115/137  | -       |
| 30  | CHL  | c     | 605 | 23   | 3/3/15/26 | 2/12/110/137  | -       |
| 31  | CLA  | 5     | 303 | 2    | 1/1/13/20 | 13/32/108/115 | -       |
| 31  | CLA  | K     | 102 | 19   | 1/1/12/20 | 11/25/101/115 | -       |
| 42  | NEX  | i     | 523 | -    | -         | 5/27/83/83    | 0/3/3/3 |
| 30  | CHL  | c     | 614 | -    | 3/3/15/26 | 4/10/108/137  | -       |
| 34  | LHG  | c     | 630 | -    | -         | 19/44/44/53   | -       |
| 33  | OUR  | 0     | 501 | -    | -         | 3/42/81/86    | 0/2/2/2 |
| 31  | CLA  | G     | 101 | 14   | 1/1/12/20 | 7/21/97/115   | -       |
| 31  | CLA  | B     | 831 | 10   | 1/1/12/20 | 7/21/97/115   | -       |
| 30  | CHL  | 6     | 315 | 5    | 3/3/15/26 | 4/12/110/137  | -       |
| 31  | CLA  | 8     | 309 | -    | 1/1/14/20 | 6/33/109/115  | -       |
| 31  | CLA  | L     | 201 | 9    | 1/1/13/20 | 7/31/107/115  | -       |
| 31  | CLA  | 0     | 321 | 1    | 1/1/11/20 | 11/15/91/115  | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 30  | CHL  | i     | 601 | 28   | 3/3/16/26 | 7/17/115/137  | -       |
| 30  | CHL  | h     | 601 | 22   | 3/3/16/26 | 6/17/115/137  | -       |
| 30  | CHL  | 1     | 306 | -    | 3/3/16/26 | 7/18/116/137  | -       |
| 33  | OUR  | 1     | 501 | -    | -         | 3/42/81/86    | 0/2/2/2 |
| 31  | CLA  | A     | 820 | 9    | 1/1/13/20 | 8/27/103/115  | -       |
| 31  | CLA  | 1     | 314 | -    | 1/1/11/20 | 4/17/93/115   | -       |
| 31  | CLA  | d     | 603 | 25   | 1/1/13/20 | 9/27/103/115  | -       |
| 31  | CLA  | 2     | 304 | -    | 1/1/14/20 | 11/33/109/115 | -       |
| 31  | CLA  | A     | 828 | 9    | 1/1/15/20 | 18/39/115/115 | -       |
| 30  | CHL  | 7     | 302 | 6    | 3/3/19/26 | 16/37/135/137 | -       |
| 37  | OIE  | i     | 522 | -    | -         | 0/33/72/72    | 0/2/2/2 |
| 31  | CLA  | 3     | 312 | 4    | 1/1/13/20 | 5/27/103/115  | -       |
| 31  | CLA  | c     | 611 | -    | 1/1/11/20 | 4/17/93/115   | -       |
| 31  | CLA  | 7     | 310 | 34   | 1/1/8/20  | 2/4/76/115    | -       |
| 31  | CLA  | 1     | 312 | 2    | 1/1/15/20 | 12/39/115/115 | -       |
| 30  | CHL  | 8     | 308 | -    | 3/3/16/26 | 2/17/115/137  | -       |
| 30  | CHL  | d     | 601 | 25   | 3/3/17/26 | 5/21/119/137  | -       |
| 30  | CHL  | 6     | 307 | -    | 3/3/17/26 | 7/21/119/137  | -       |
| 31  | CLA  | A     | 817 | 9    | 1/1/14/20 | 16/35/111/115 | -       |
| 31  | CLA  | e     | 612 | -    | 1/1/11/20 | 4/15/91/115   | -       |
| 37  | OIE  | a     | 521 | -    | -         | 2/33/72/72    | 0/2/2/2 |
| 42  | NEX  | f     | 523 | -    | -         | 5/27/83/83    | 0/3/3/3 |
| 31  | CLA  | 1     | 311 | 2    | 1/1/12/20 | 6/24/100/115  | -       |
| 36  | LMG  | 9     | 602 | -    | -         | 31/50/70/70   | 0/1/1/1 |
| 31  | CLA  | O     | 201 | -    | 1/1/10/20 | 6/10/86/115   | -       |
| 30  | CHL  | 2     | 319 | 7    | 3/3/19/26 | 16/33/131/137 | -       |
| 31  | CLA  | B     | 814 | 10   | 1/1/15/20 | 15/39/115/115 | -       |
| 36  | LMG  | 3     | 602 | -    | -         | 16/31/51/70   | 0/1/1/1 |
| 31  | CLA  | 1     | 304 | -    | 1/1/12/20 | 3/24/100/115  | -       |
| 30  | CHL  | 7     | 301 | 6    | 3/3/19/26 | 14/36/134/137 | -       |
| 33  | OUR  | e     | 520 | -    | -         | 10/42/81/86   | 0/2/2/2 |
| 32  | 8CT  | L     | 206 | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 30  | CHL  | 0     | 306 | -    | 3/3/16/26 | 8/18/116/137  | -       |
| 30  | CHL  | h     | 602 | -    | 3/3/19/26 | 16/37/135/137 | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 30  | CHL  | i     | 609 | -    | 3/3/16/26 | 4/18/116/137  | -       |
| 30  | CHL  | h     | 609 | -    | 3/3/16/26 | 3/17/115/137  | -       |
| 34  | LHG  | G     | 105 | -    | -         | 27/42/42/53   | -       |
| 31  | CLA  | 2     | 310 | 34   | 1/1/14/20 | 14/33/109/115 | -       |
| 30  | CHL  | 2     | 305 | -    | 3/3/15/26 | 0/12/110/137  | -       |
| 32  | 8CT  | A     | 849 | -    | -         | 7/29/63/63    | 0/2/2/2 |
| 32  | 8CT  | K     | 107 | -    | -         | 12/29/63/63   | 0/2/2/2 |
| 31  | CLA  | 7     | 315 | 6    | 1/1/11/20 | 8/18/94/115   | -       |
| 30  | CHL  | 2     | 302 | 3    | 3/3/19/26 | 26/37/135/137 | -       |
| 30  | CHL  | d     | 606 | -    | 3/3/17/26 | 9/21/119/137  | -       |
| 34  | LHG  | 9     | 601 | 31   | -         | 18/48/48/53   | -       |
| 31  | CLA  | 3     | 310 | -    | 1/1/14/20 | 13/36/112/115 | -       |
| 30  | CHL  | d     | 602 | -    | 3/3/19/26 | 16/37/135/137 | -       |
| 30  | CHL  | c     | 601 | 23   | 3/3/18/26 | 13/27/125/137 | -       |
| 30  | CHL  | d     | 609 | -    | 3/3/20/26 | 19/39/137/137 | -       |
| 31  | CLA  | 6     | 303 | 5    | 1/1/12/20 | 6/24/100/115  | -       |
| 31  | CLA  | B     | 809 | 10   | 1/1/15/20 | 11/39/115/115 | -       |
| 33  | OUR  | 2     | 501 | -    | -         | 7/41/80/86    | 0/2/2/2 |
| 31  | CLA  | 6     | 320 | -    | 1/1/12/20 | 10/23/99/115  | -       |
| 30  | CHL  | e     | 602 | -    | 3/3/19/26 | 18/33/131/137 | -       |
| 31  | CLA  | K     | 101 | -    | 1/1/14/20 | 10/33/109/115 | -       |
| 30  | CHL  | e     | 609 | -    | 3/3/19/26 | 15/33/131/137 | -       |
| 32  | 8CT  | 8     | 406 | -    | -         | 11/29/63/63   | 0/2/2/2 |
| 31  | CLA  | A     | 807 | 9    | 1/1/12/20 | 4/23/99/115   | -       |
| 30  | CHL  | g     | 608 | -    | 3/3/15/26 | 5/12/110/137  | -       |
| 32  | 8CT  | L     | 209 | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 37  | OIE  | g     | 522 | -    | -         | 1/33/72/72    | 0/2/2/2 |
| 30  | CHL  | f     | 602 | -    | 3/3/19/26 | 19/37/135/137 | -       |
| 30  | CHL  | a     | 608 | -    | 3/3/16/26 | 6/19/117/137  | -       |
| 31  | CLA  | A     | 813 | 9    | 1/1/15/20 | 7/39/115/115  | -       |
| 30  | CHL  | 3     | 302 | 4    | 3/3/19/26 | 18/35/133/137 | -       |
| 31  | CLA  | g     | 610 | -    | 1/1/11/20 | 3/17/93/115   | -       |
| 30  | CHL  | 8     | 313 | 7    | 3/3/18/26 | 9/27/125/137  | -       |
| 31  | CLA  | f     | 611 | 34   | 1/1/13/20 | 5/27/103/115  | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 30  | CHL  | i     | 614 | -    | 3/3/15/26 | 4/10/108/137  | -       |
| 30  | CHL  | b     | 602 | -    | 3/3/19/26 | 19/37/135/137 | -       |
| 31  | CLA  | A     | 827 | 9    | 1/1/15/20 | 2/39/115/115  | -       |
| 31  | CLA  | h     | 613 | -    | 1/1/11/20 | 5/15/91/115   | -       |
| 32  | 8CT  | 0     | 401 | -    | -         | 5/29/63/63    | 0/2/2/2 |
| 30  | CHL  | f     | 614 | 26   | 3/3/15/26 | 6/10/108/137  | -       |
| 31  | CLA  | 3     | 318 | 4    | 1/1/11/20 | 0/17/93/115   | -       |
| 34  | LHG  | f     | 630 | 31   | -         | 26/44/44/53   | -       |
| 31  | CLA  | A     | 852 | 10   | 1/1/15/20 | 13/39/115/115 | -       |
| 31  | CLA  | 4     | 303 | 7    | 1/1/11/20 | 4/15/91/115   | -       |
| 30  | CHL  | g     | 602 | -    | 3/3/17/26 | 10/23/121/137 | -       |
| 31  | CLA  | B     | 803 | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 30  | CHL  | c     | 602 | -    | 3/3/19/26 | 18/33/131/137 | -       |
| 31  | CLA  | f     | 612 | 26   | 1/1/11/20 | 6/15/91/115   | -       |
| 31  | CLA  | d     | 610 | -    | 1/1/13/20 | 5/27/103/115  | -       |
| 30  | CHL  | b     | 608 | -    | 3/3/20/26 | 19/39/137/137 | -       |
| 31  | CLA  | d     | 613 | -    | 1/1/12/20 | 8/27/103/115  | -       |
| 31  | CLA  | H     | 204 | -    | 1/1/11/20 | 3/18/94/115   | -       |
| 31  | CLA  | 2     | 314 | 3    | 1/1/11/20 | 5/15/91/115   | -       |
| 32  | 8CT  | A     | 850 | -    | -         | 10/29/63/63   | 0/2/2/2 |
| 31  | CLA  | f     | 604 | -    | 1/1/12/20 | 6/21/97/115   | -       |
| 30  | CHL  | 1     | 307 | -    | 3/3/20/26 | 22/39/137/137 | -       |
| 31  | CLA  | A     | 826 | -    | 1/1/15/20 | 10/39/115/115 | -       |
| 30  | CHL  | i     | 606 | 28   | 3/3/17/26 | 7/21/119/137  | -       |
| 31  | CLA  | d     | 611 | -    | 1/1/11/20 | 4/17/93/115   | -       |
| 31  | CLA  | B     | 823 | -    | 1/1/12/20 | 10/24/100/115 | -       |
| 31  | CLA  | B     | 818 | 10   | 1/1/13/20 | 8/32/108/115  | -       |
| 30  | CHL  | 6     | 305 | -    | 3/3/15/26 | 0/12/110/137  | -       |
| 30  | CHL  | 4     | 319 | 2    | 3/3/17/26 | 11/25/123/137 | -       |
| 37  | 0IE  | c     | 521 | -    | -         | 2/33/72/72    | 0/2/2/2 |
| 30  | CHL  | f     | 605 | 26   | 3/3/15/26 | 2/12/110/137  | -       |
| 31  | CLA  | A     | 814 | 9    | 1/1/13/20 | 10/30/106/115 | -       |
| 31  | CLA  | B     | 838 | 10   | 1/1/11/20 | 2/18/94/115   | -       |
| 30  | CHL  | i     | 605 | 28   | 3/3/15/26 | 2/12/110/137  | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 42  | NEX  | d     | 523 | -    | -         | 5/27/83/83    | 0/3/3/3 |
| 31  | CLA  | 7     | 318 | 6    | 1/1/14/20 | 9/33/109/115  | -       |
| 31  | CLA  | L     | 207 | -    | 1/1/11/20 | 7/18/94/115   | -       |
| 34  | LHG  | A     | 844 | -    | -         | 19/53/53/53   | -       |
| 30  | CHL  | h     | 606 | -    | 3/3/17/26 | 6/21/119/137  | -       |
| 37  | OIE  | d     | 522 | -    | -         | 3/33/72/72    | 0/2/2/2 |
| 31  | CLA  | e     | 613 | -    | 1/1/12/20 | 9/27/103/115  | -       |
| 31  | CLA  | h     | 603 | -    | 1/1/11/20 | 4/20/96/115   | -       |
| 31  | CLA  | A     | 803 | 9    | 1/1/15/20 | 9/39/115/115  | -       |
| 34  | LHG  | H     | 203 | -    | -         | 13/35/35/53   | -       |
| 30  | CHL  | e     | 601 | 29   | 3/3/17/26 | 6/21/119/137  | -       |
| 31  | CLA  | 0     | 308 | -    | 1/1/14/20 | 12/33/109/115 | -       |
| 30  | CHL  | f     | 601 | 26   | 3/3/20/26 | 15/39/137/137 | -       |
| 31  | CLA  | 9     | 300 | 10   | 1/1/13/20 | 13/31/107/115 | -       |
| 31  | CLA  | H     | 202 | 27   | 1/1/11/20 | 6/18/94/115   | -       |
| 32  | 8CT  | A     | 846 | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 31  | CLA  | 7     | 317 | -    | 1/1/11/20 | 13/15/91/115  | -       |
| 31  | CLA  | i     | 603 | -    | 1/1/11/20 | 4/17/93/115   | -       |
| 37  | OIE  | g     | 521 | -    | -         | 3/33/72/72    | 0/2/2/2 |
| 30  | CHL  | 6     | 302 | 5    | 3/3/19/26 | 19/37/135/137 | -       |
| 32  | 8CT  | 4     | 402 | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 30  | CHL  | g     | 609 | 25   | 3/3/15/26 | 5/12/110/137  | -       |
| 31  | CLA  | b     | 610 | -    | 1/1/13/20 | 4/27/103/115  | -       |
| 30  | CHL  | 4     | 302 | 7    | 3/3/17/26 | 13/24/122/137 | -       |
| 30  | CHL  | c     | 609 | -    | 3/3/20/26 | 23/39/137/137 | -       |
| 31  | CLA  | 5     | 308 | -    | 1/1/11/20 | 7/17/93/115   | -       |
| 33  | OUR  | 5     | 502 | -    | -         | 10/42/81/86   | 0/2/2/2 |
| 31  | CLA  | A     | 804 | 9    | 1/1/13/20 | 8/27/103/115  | -       |
| 31  | CLA  | A     | 821 | -    | 1/1/15/20 | 10/39/115/115 | -       |
| 31  | CLA  | B     | 835 | -    | 1/1/11/20 | 0/15/91/115   | -       |
| 31  | CLA  | 5     | 304 | -    | 1/1/12/20 | 7/24/100/115  | -       |
| 30  | CHL  | 2     | 301 | -    | 3/3/19/26 | 9/33/131/137  | -       |
| 34  | LHG  | 0     | 601 | -    | -         | 30/53/53/53   | -       |
| 30  | CHL  | 1     | 302 | -    | 3/3/19/26 | 16/37/135/137 | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 37  | OIE  | a     | 522 | -    | -         | 0/33/72/72    | 0/2/2/2 |
| 32  | 8CT  | B     | 843 | -    | -         | 14/29/63/63   | 0/2/2/2 |
| 31  | CLA  | A     | 823 | 9    | 1/1/12/20 | 4/23/99/115   | -       |
| 30  | CHL  | 8     | 315 | -    | 3/3/15/26 | 4/12/110/137  | -       |
| 30  | CHL  | 7     | 313 | 6    | 3/3/16/26 | 9/17/115/137  | -       |
| 38  | PQN  | B     | 842 | -    | -         | 6/23/43/43    | 0/2/2/2 |
| 31  | CLA  | 5     | 311 | -    | 1/1/11/20 | 8/15/91/115   | -       |
| 31  | CLA  | 9     | 303 | 8    | 1/1/11/20 | 5/19/95/115   | -       |
| 31  | CLA  | 4     | 304 | -    | 1/1/14/20 | 8/33/109/115  | -       |
| 31  | CLA  | A     | 853 | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 30  | CHL  | b     | 609 | -    | 3/3/17/26 | 11/25/123/137 | -       |
| 31  | CLA  | 0     | 313 | 1    | 1/1/11/20 | 10/17/93/115  | -       |
| 33  | OUR  | 6     | 502 | -    | -         | 11/42/81/86   | 0/2/2/2 |
| 31  | CLA  | 8     | 303 | 7    | 1/1/11/20 | 6/17/93/115   | -       |
| 30  | CHL  | a     | 607 | -    | 3/3/16/26 | 7/17/115/137  | -       |
| 33  | OUR  | 9     | 502 | -    | -         | 8/42/81/86    | 0/2/2/2 |
| 32  | 8CT  | 3     | 403 | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 32  | 8CT  | B     | 846 | -    | -         | 13/29/63/63   | 0/2/2/2 |
| 30  | CHL  | 4     | 313 | 7    | 3/3/17/26 | 5/21/119/137  | -       |
| 30  | CHL  | 6     | 308 | 5    | 3/3/18/26 | 8/32/130/137  | -       |
| 34  | LHG  | i     | 630 | -    | -         | 9/34/34/53    | -       |
| 34  | LHG  | h     | 630 | -    | -         | 18/43/43/53   | -       |
| 31  | CLA  | 4     | 314 | 7    | 1/1/11/20 | 4/15/91/115   | -       |
| 30  | CHL  | 1     | 313 | 2    | 3/3/19/26 | 21/35/133/137 | -       |
| 30  | CHL  | 9     | 305 | -    | 3/3/17/26 | 7/21/119/137  | -       |
| 31  | CLA  | F     | 301 | -    | 1/1/11/20 | 6/15/91/115   | -       |
| 30  | CHL  | 9     | 306 | -    | 3/3/16/26 | 7/18/116/137  | -       |
| 31  | CLA  | M     | 101 | -    | 1/1/11/20 | 1/17/93/115   | -       |
| 31  | CLA  | A     | 818 | 9    | 1/1/15/20 | 12/39/115/115 | -       |
| 30  | CHL  | 5     | 301 | 2    | 3/3/17/26 | 10/23/121/137 | -       |
| 31  | CLA  | 6     | 314 | -    | 1/1/11/20 | 2/15/91/115   | -       |
| 34  | LHG  | d     | 630 | -    | -         | 17/40/40/53   | -       |
| 31  | CLA  | B     | 813 | 10   | 1/1/13/20 | 10/27/103/115 | -       |
| 34  | LHG  | M     | 104 | -    | -         | 20/50/50/53   | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 31  | CLA  | h     | 610 | -    | 1/1/11/20 | 3/17/93/115   | -       |
| 31  | CLA  | 9     | 312 | 8    | 1/1/13/20 | 6/29/105/115  | -       |
| 31  | CLA  | 0     | 312 | 1    | 1/1/15/20 | 12/39/115/115 | -       |
| 31  | CLA  | A     | 832 | 9    | 1/1/15/20 | 10/39/115/115 | -       |
| 37  | 0IE  | i     | 521 | -    | -         | 4/33/72/72    | 0/2/2/2 |
| 34  | LHG  | e     | 630 | 31   | -         | 20/47/47/53   | -       |
| 33  | 0UR  | a     | 520 | -    | -         | 7/36/75/86    | 0/2/2/2 |
| 34  | LHG  | 3     | 603 | -    | -         | 18/40/40/53   | -       |
| 31  | CLA  | 1     | 310 | 34   | 1/1/14/20 | 10/37/113/115 | -       |
| 37  | 0IE  | 3     | 502 | -    | -         | 2/33/72/72    | 0/2/2/2 |
| 31  | CLA  | B     | 807 | 10   | 1/1/11/20 | 5/15/91/115   | -       |
| 30  | CHL  | i     | 607 | -    | 3/3/16/26 | 11/17/115/137 | -       |
| 31  | CLA  | B     | 837 | -    | 1/1/15/20 | 4/39/115/115  | -       |
| 34  | LHG  | 2     | 601 | 31   | -         | 17/36/36/53   | -       |
| 37  | 0IE  | 7     | 502 | -    | -         | 2/33/72/72    | 0/2/2/2 |
| 31  | CLA  | A     | 841 | -    | 1/1/15/20 | 10/39/115/115 | -       |
| 31  | CLA  | h     | 611 | -    | 1/1/10/20 | 2/10/86/115   | -       |
| 31  | CLA  | A     | 838 | 9    | 1/1/13/20 | 3/29/105/115  | -       |
| 30  | CHL  | h     | 605 | 22   | 3/3/15/26 | 4/12/110/137  | -       |
| 31  | CLA  | e     | 610 | -    | 1/1/13/20 | 4/27/103/115  | -       |
| 31  | CLA  | 9     | 311 | 8    | 1/1/12/20 | 6/24/100/115  | -       |
| 30  | CHL  | 4     | 306 | -    | 3/3/16/26 | 6/18/116/137  | -       |
| 31  | CLA  | K     | 104 | 19   | 1/1/11/20 | 5/17/93/115   | -       |
| 33  | 0UR  | 4     | 501 | -    | -         | 9/41/80/86    | 0/2/2/2 |
| 30  | CHL  | h     | 614 | -    | 3/3/15/26 | 4/10/108/137  | -       |
| 30  | CHL  | f     | 609 | -    | 3/3/20/26 | 19/39/137/137 | -       |
| 32  | 8CT  | 7     | 405 | -    | -         | 10/29/63/63   | 0/2/2/2 |
| 30  | CHL  | 5     | 305 | -    | 3/3/16/26 | 9/15/113/137  | -       |
| 31  | CLA  | g     | 612 | -    | 1/1/11/20 | 6/15/91/115   | -       |
| 31  | CLA  | B     | 820 | -    | 1/1/13/20 | 10/29/105/115 | -       |
| 30  | CHL  | d     | 605 | 25   | 3/3/15/26 | 3/12/110/137  | -       |
| 36  | LMG  | 2     | 602 | -    | -         | 14/31/51/70   | 0/1/1/1 |
| 37  | 0IE  | f     | 521 | -    | -         | 2/33/72/72    | 0/2/2/2 |
| 32  | 8CT  | 9     | 401 | -    | -         | 11/29/63/63   | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 37  | 0IE  | c     | 522 | -    | -         | 12/33/72/72   | 0/2/2/2 |
| 31  | CLA  | 3     | 309 | 4    | 1/1/15/20 | 12/39/115/115 | -       |
| 33  | 0UR  | 8     | 502 | -    | -         | 8/42/81/86    | 0/2/2/2 |
| 31  | CLA  | B     | 824 | 10   | 1/1/14/20 | 8/33/109/115  | -       |
| 30  | CHL  | b     | 614 | -    | 3/3/15/26 | 4/10/108/137  | -       |
| 30  | CHL  | a     | 609 | -    | 3/3/18/26 | 11/31/129/137 | -       |
| 31  | CLA  | B     | 806 | -    | 1/1/15/20 | 11/39/115/115 | -       |
| 33  | 0UR  | 9     | 501 | -    | -         | 3/42/81/86    | 0/2/2/2 |
| 31  | CLA  | B     | 810 | 10   | 1/1/14/20 | 6/36/112/115  | -       |
| 34  | LHG  | 3     | 601 | -    | -         | 15/40/40/53   | -       |
| 31  | CLA  | 9     | 302 | -    | 1/1/15/20 | 15/39/115/115 | -       |
| 30  | CHL  | b     | 606 | -    | 3/3/17/26 | 3/21/119/137  | -       |
| 31  | CLA  | G     | 103 | 14   | 1/1/11/20 | 5/17/93/115   | -       |
| 30  | CHL  | 6     | 301 | 5    | 3/3/19/26 | 14/33/131/137 | -       |
| 30  | CHL  | c     | 607 | -    | 3/3/16/26 | 9/17/115/137  | -       |
| 31  | CLA  | b     | 603 | 24   | 1/1/13/20 | 6/27/103/115  | -       |
| 30  | CHL  | 0     | 305 | -    | 3/3/17/26 | 7/21/119/137  | -       |
| 31  | CLA  | A     | 843 | 34   | 1/1/12/20 | 6/24/100/115  | -       |
| 39  | CL0  | A     | 857 | 9    | 3/3/20/25 | 10/37/135/135 | -       |
| 30  | CHL  | 0     | 302 | 1    | 3/3/19/26 | 14/37/135/137 | -       |
| 30  | CHL  | g     | 601 | 25   | 3/3/17/26 | 7/23/121/137  | -       |
| 32  | 8CT  | B     | 848 | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 31  | CLA  | a     | 604 | -    | 1/1/12/20 | 3/21/97/115   | -       |
| 34  | LHG  | A     | 845 | 31   | -         | 17/31/31/53   | -       |
| 31  | CLA  | 0     | 310 | -    | 1/1/10/20 | 2/10/86/115   | -       |
| 31  | CLA  | B     | 811 | 10   | 1/1/15/20 | 9/39/115/115  | -       |
| 30  | CHL  | b     | 601 | 24   | 3/3/20/26 | 22/39/137/137 | -       |
| 30  | CHL  | d     | 607 | -    | 3/3/16/26 | 11/17/115/137 | -       |
| 30  | CHL  | 4     | 307 | -    | 3/3/17/26 | 10/21/119/137 | -       |
| 31  | CLA  | d     | 612 | 25   | 1/1/11/20 | 7/15/91/115   | -       |
| 30  | CHL  | 5     | 302 | 2    | 3/3/19/26 | 18/37/135/137 | -       |
| 32  | 8CT  | B     | 844 | -    | -         | 11/29/63/63   | 0/2/2/2 |
| 31  | CLA  | c     | 610 | -    | 1/1/13/20 | 3/27/103/115  | -       |
| 31  | CLA  | 8     | 310 | 34   | 1/1/11/20 | 4/17/93/115   | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 33  | OUR  | 0     | 502 | -    | -         | 12/42/81/86   | 0/2/2/2 |
| 40  | SF4  | C     | 102 | 18   | -         | -             | 0/6/5/5 |
| 31  | CLA  | 6     | 317 | 5    | 1/1/15/20 | 15/39/115/115 | -       |
| 31  | CLA  | c     | 612 | 23   | 1/1/11/20 | 4/15/91/115   | -       |
| 31  | CLA  | 5     | 310 | 34   | 1/1/11/20 | 5/15/91/115   | -       |
| 31  | CLA  | f     | 610 | -    | 1/1/13/20 | 3/27/103/115  | -       |
| 31  | CLA  | A     | 816 | -    | 1/1/11/20 | 5/15/91/115   | -       |
| 32  | 8CT  | J     | 101 | -    | -         | 11/29/63/63   | 0/2/2/2 |
| 31  | CLA  | 1     | 309 | 2    | 1/1/13/20 | 6/27/103/115  | -       |
| 31  | CLA  | 7     | 309 | -    | 1/1/13/20 | 11/32/108/115 | -       |
| 30  | CHL  | f     | 606 | -    | 3/3/17/26 | 5/21/119/137  | -       |
| 30  | CHL  | g     | 607 | -    | 3/3/17/26 | 7/21/119/137  | -       |
| 30  | CHL  | 8     | 301 | 7    | 3/3/19/26 | 5/33/131/137  | -       |
| 34  | LHG  | g     | 630 | -    | -         | 15/34/34/53   | -       |
| 33  | OUR  | g     | 520 | -    | -         | 9/42/81/86    | 0/2/2/2 |
| 31  | CLA  | b     | 613 | -    | 1/1/12/20 | 6/27/103/115  | -       |
| 36  | LMG  | J     | 102 | -    | -         | 12/24/44/70   | 0/1/1/1 |
| 32  | 8CT  | B     | 851 | -    | -         | 13/29/63/63   | 0/2/2/2 |
| 30  | CHL  | 8     | 305 | -    | 3/3/16/26 | 6/17/115/137  | -       |
| 31  | CLA  | 7     | 303 | 6    | 1/1/11/20 | 6/15/91/115   | -       |
| 31  | CLA  | A     | 822 | -    | 1/1/11/20 | 5/20/96/115   | -       |
| 33  | OUR  | 5     | 501 | -    | -         | 11/41/80/86   | 0/2/2/2 |
| 31  | CLA  | 9     | 308 | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 32  | 8CT  | B     | 847 | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 31  | CLA  | B     | 815 | 10   | 1/1/13/20 | 3/27/103/115  | -       |
| 31  | CLA  | A     | 819 | 9    | 1/1/15/20 | 18/39/115/115 | -       |
| 31  | CLA  | a     | 613 | 22   | 1/1/12/20 | 8/27/103/115  | -       |
| 31  | CLA  | B     | 850 | 13   | 1/1/11/20 | 4/18/94/115   | -       |
| 34  | LHG  | 6     | 601 | 31   | -         | 17/41/41/53   | -       |
| 33  | OUR  | d     | 520 | -    | -         | 10/39/78/86   | 0/2/2/2 |
| 31  | CLA  | a     | 610 | -    | 1/1/13/20 | 4/27/103/115  | -       |
| 31  | CLA  | O     | 206 | -    | 1/1/12/20 | 9/23/99/115   | -       |
| 31  | CLA  | B     | 805 | 10   | 1/1/15/20 | 9/39/115/115  | -       |
| 31  | CLA  | B     | 808 | 10   | 1/1/15/20 | 10/39/115/115 | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 31  | CLA  | a     | 612 | -    | 1/1/11/20 | 2/15/91/115   | -       |
| 32  | 8CT  | G     | 104 | -    | -         | 13/29/63/63   | 0/2/2/2 |
| 37  | 0IE  | h     | 521 | -    | -         | 4/33/72/72    | 0/2/2/2 |
| 31  | CLA  | B     | 812 | 10   | 1/1/12/20 | 3/24/100/115  | -       |
| 30  | CHL  | 2     | 308 | -    | 3/3/16/26 | 4/17/115/137  | -       |
| 31  | CLA  | 5     | 314 | 2    | 1/1/11/20 | 9/17/93/115   | -       |
| 32  | 8CT  | 2     | 402 | -    | -         | 12/29/63/63   | 0/2/2/2 |
| 31  | CLA  | B     | 801 | -    | 1/1/15/20 | 10/39/115/115 | -       |
| 31  | CLA  | 4     | 312 | 7    | 1/1/12/20 | 6/25/101/115  | -       |
| 36  | LMG  | O     | 207 | -    | -         | 10/34/54/70   | 0/1/1/1 |
| 30  | CHL  | e     | 614 | -    | 3/3/15/26 | 4/10/108/137  | -       |
| 31  | CLA  | f     | 603 | -    | 1/1/13/20 | 7/27/103/115  | -       |
| 37  | 0IE  | e     | 522 | -    | -         | 0/33/72/72    | 0/2/2/2 |
| 30  | CHL  | e     | 605 | 29   | 3/3/15/26 | 4/12/110/137  | -       |
| 31  | CLA  | 3     | 303 | -    | 1/1/13/20 | 7/27/103/115  | -       |
| 37  | 0IE  | d     | 521 | -    | -         | 2/33/72/72    | 0/2/2/2 |
| 30  | CHL  | 6     | 313 | 5    | 3/3/17/26 | 6/23/121/137  | -       |
| 31  | CLA  | 2     | 303 | 3    | 1/1/13/20 | 9/29/105/115  | -       |
| 31  | CLA  | h     | 604 | -    | 1/1/11/20 | 7/17/93/115   | -       |
| 31  | CLA  | 8     | 304 | -    | 1/1/15/20 | 10/39/115/115 | -       |
| 33  | 0UR  | 1     | 502 | -    | -         | 10/42/81/86   | 0/2/2/2 |
| 31  | CLA  | 3     | 313 | 4    | 1/1/11/20 | 7/15/91/115   | -       |
| 33  | 0UR  | c     | 520 | -    | -         | 9/42/81/86    | 0/2/2/2 |
| 31  | CLA  | L     | 203 | 17   | 1/1/14/20 | 19/37/113/115 | -       |
| 31  | CLA  | A     | 836 | -    | 1/1/12/20 | 8/23/99/115   | -       |
| 30  | CHL  | 9     | 313 | 8    | 3/3/16/26 | 9/17/115/137  | -       |
| 36  | LMG  | B     | 853 | -    | -         | 23/37/57/70   | 0/1/1/1 |
| 31  | CLA  | 7     | 304 | -    | 1/1/13/20 | 7/27/103/115  | -       |
| 32  | 8CT  | F     | 302 | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 31  | CLA  | e     | 603 | 29   | 1/1/13/20 | 4/30/106/115  | -       |
| 30  | CHL  | 8     | 306 | -    | 3/3/17/26 | 13/21/119/137 | -       |
| 30  | CHL  | c     | 608 | -    | 3/3/20/26 | 22/39/137/137 | -       |
| 32  | 8CT  | A     | 847 | -    | -         | 10/29/63/63   | 0/2/2/2 |
| 31  | CLA  | A     | 815 | 9    | 1/1/15/20 | 8/39/115/115  | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 30  | CHL  | 2     | 313 | 3    | 3/3/17/26 | 3/21/119/137  | -       |
| 31  | CLA  | e     | 611 | 34   | 1/1/13/20 | 6/27/103/115  | -       |
| 31  | CLA  | B     | 833 | 10   | 1/1/13/20 | 9/27/103/115  | -       |
| 30  | CHL  | f     | 608 | -    | 3/3/17/26 | 4/21/119/137  | -       |
| 31  | CLA  | O     | 203 | -    | 1/1/10/20 | 1/4/80/115    | -       |
| 31  | CLA  | A     | 829 | 9    | 1/1/15/20 | 13/39/115/115 | -       |
| 31  | CLA  | i     | 610 | -    | 1/1/13/20 | 3/27/103/115  | -       |
| 34  | LHG  | B     | 854 | -    | -         | 17/47/47/53   | -       |
| 30  | CHL  | 2     | 306 | -    | 3/3/16/26 | 5/18/116/137  | -       |
| 30  | CHL  | 5     | 307 | -    | 3/3/16/26 | 7/17/115/137  | -       |
| 33  | OUR  | 8     | 501 | -    | -         | 7/41/80/86    | 0/2/2/2 |
| 31  | CLA  | c     | 604 | -    | 1/1/12/20 | 3/21/97/115   | -       |
| 31  | CLA  | A     | 805 | 9    | 1/1/15/20 | 13/39/115/115 | -       |
| 31  | CLA  | 5     | 309 | -    | 1/1/14/20 | 8/33/109/115  | -       |
| 32  | 8CT  | L     | 205 | -    | -         | 7/29/63/63    | 0/2/2/2 |
| 31  | CLA  | A     | 802 | -    | 1/1/15/20 | 4/39/115/115  | -       |
| 31  | CLA  | A     | 812 | 9    | 1/1/12/20 | 1/26/102/115  | -       |
| 31  | CLA  | 2     | 312 | 3    | 1/1/14/20 | 10/33/109/115 | -       |
| 34  | LHG  | B     | 852 | 31   | -         | 17/26/26/53   | -       |
| 34  | LHG  | 5     | 601 | 31   | -         | 13/41/41/53   | -       |
| 34  | LHG  | 1     | 601 | 31   | -         | 21/53/53/53   | -       |
| 31  | CLA  | A     | 810 | 9    | 1/1/15/20 | 3/39/115/115  | -       |
| 36  | LMG  | L     | 211 | -    | -         | 15/32/52/70   | 0/1/1/1 |
| 34  | LHG  | 4     | 601 | 31   | -         | 12/36/36/53   | -       |
| 31  | CLA  | b     | 604 | -    | 1/1/12/20 | 7/21/97/115   | -       |
| 32  | 8CT  | B     | 845 | -    | -         | 10/29/63/63   | 0/2/2/2 |
| 31  | CLA  | A     | 824 | 9    | 1/1/13/20 | 8/27/103/115  | -       |
| 31  | CLA  | B     | 819 | 10   | 1/1/14/20 | 14/33/109/115 | -       |
| 34  | LHG  | K     | 106 | -    | -         | 23/46/46/53   | -       |
| 30  | CHL  | f     | 607 | -    | 3/3/16/26 | 7/17/115/137  | -       |
| 33  | OUR  | i     | 520 | -    | -         | 5/40/79/86    | 0/2/2/2 |
| 31  | CLA  | 4     | 310 | 34   | 1/1/14/20 | 14/33/109/115 | -       |
| 30  | CHL  | e     | 606 | -    | 3/3/17/26 | 6/21/119/137  | -       |
| 30  | CHL  | c     | 606 | -    | 3/3/15/26 | 3/13/111/137  | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 31  | CLA  | 3     | 304 | -    | 1/1/15/20 | 7/39/115/115  | -       |
| 31  | CLA  | A     | 831 | 9    | 1/1/12/20 | 3/21/97/115   | -       |
| 31  | CLA  | 2     | 311 | 3    | 1/1/11/20 | 5/19/95/115   | -       |
| 31  | CLA  | A     | 830 | 9    | 1/1/15/20 | 12/39/115/115 | -       |
| 31  | CLA  | B     | 829 | -    | 1/1/15/20 | 9/39/115/115  | -       |
| 42  | NEX  | b     | 523 | -    | -         | 5/27/83/83    | 0/3/3/3 |
| 32  | 8CT  | 7     | 404 | -    | -         | 7/29/63/63    | 0/2/2/2 |
| 32  | 8CT  | M     | 102 | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 31  | CLA  | B     | 839 | -    | 1/1/15/20 | 8/39/115/115  | -       |
| 30  | CHL  | 7     | 306 | -    | 3/3/18/26 | 17/33/131/137 | -       |
| 33  | OUR  | 7     | 501 | -    | -         | 9/41/80/86    | 0/2/2/2 |
| 42  | NEX  | a     | 523 | -    | -         | 5/27/83/83    | 0/3/3/3 |
| 31  | CLA  | i     | 612 | -    | 1/1/11/20 | 2/15/91/115   | -       |
| 31  | CLA  | L     | 204 | -    | 1/1/11/20 | 6/17/93/115   | -       |
| 36  | LMG  | J     | 105 | -    | -         | 15/41/61/70   | 0/1/1/1 |
| 31  | CLA  | A     | 833 | 9    | 1/1/15/20 | 12/39/115/115 | -       |
| 31  | CLA  | 0     | 304 | -    | 1/1/12/20 | 4/24/100/115  | -       |
| 30  | CHL  | 0     | 301 | 1    | 3/3/17/26 | 12/23/121/137 | -       |
| 31  | CLA  | A     | 825 | -    | 1/1/15/20 | 8/39/115/115  | -       |
| 31  | CLA  | 6     | 311 | 5    | 1/1/11/20 | 3/19/95/115   | -       |
| 31  | CLA  | i     | 604 | -    | 1/1/12/20 | 6/21/97/115   | -       |
| 31  | CLA  | 8     | 312 | 7    | 1/1/13/20 | 8/29/105/115  | -       |
| 31  | CLA  | A     | 837 | 9    | 1/1/14/20 | 12/35/111/115 | -       |
| 31  | CLA  | B     | 821 | 10   | 1/1/12/20 | 0/21/97/115   | -       |
| 31  | CLA  | g     | 613 | 25   | 1/1/11/20 | 3/18/94/115   | -       |
| 33  | OUR  | 2     | 502 | -    | -         | 11/40/79/86   | 0/2/2/2 |
| 30  | CHL  | g     | 605 | -    | 3/3/15/26 | 4/12/110/137  | -       |
| 31  | CLA  | 5     | 312 | 2    | 1/1/13/20 | 10/29/105/115 | -       |
| 31  | CLA  | A     | 834 | 9    | 1/1/11/20 | 0/17/93/115   | -       |
| 33  | OUR  | f     | 520 | -    | -         | 9/39/78/86    | 0/2/2/2 |
| 42  | NEX  | h     | 523 | -    | -         | 5/27/83/83    | 0/3/3/3 |
| 32  | 8CT  | A     | 848 | -    | -         | 7/29/63/63    | 0/2/2/2 |
| 31  | CLA  | b     | 612 | -    | 1/1/11/20 | 4/15/91/115   | -       |
| 31  | CLA  | c     | 603 | -    | 1/1/12/20 | 5/24/100/115  | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 32  | 8CT  | 8     | 402 | -    | -         | 10/29/63/63   | 0/2/2/2 |
| 31  | CLA  | A     | 806 | -    | 1/1/15/20 | 19/39/115/115 | -       |
| 30  | CHL  | 3     | 305 | -    | 3/3/17/26 | 4/21/119/137  | -       |
| 31  | CLA  | 3     | 311 | 4    | 1/1/11/20 | 1/17/93/115   | -       |
| 31  | CLA  | 9     | 304 | -    | 1/1/12/20 | 0/23/99/115   | -       |
| 33  | OUR  | 6     | 501 | -    | -         | 11/41/80/86   | 0/2/2/2 |
| 31  | CLA  | 7     | 311 | 6    | 1/1/12/20 | 8/24/100/115  | -       |
| 30  | CHL  | g     | 606 | -    | 3/3/17/26 | 5/21/119/137  | -       |
| 33  | OUR  | 3     | 501 | -    | -         | 9/41/80/86    | 0/2/2/2 |
| 31  | CLA  | A     | 840 | 9    | 1/1/15/20 | 17/39/115/115 | -       |
| 30  | CHL  | i     | 602 | -    | 3/3/19/26 | 19/33/131/137 | -       |
| 40  | SF4  | C     | 101 | -    | -         | -             | 0/6/5/5 |
| 30  | CHL  | a     | 602 | -    | 3/3/19/26 | 18/37/135/137 | -       |
| 31  | CLA  | b     | 611 | -    | 1/1/14/20 | 4/33/109/115  | -       |
| 31  | CLA  | B     | 841 | 34   | 1/1/15/20 | 7/39/115/115  | -       |
| 37  | OIE  | h     | 522 | -    | -         | 0/33/72/72    | 0/2/2/2 |
| 31  | CLA  | g     | 611 | -    | 1/1/11/20 | 0/17/93/115   | -       |
| 31  | CLA  | d     | 604 | -    | 1/1/12/20 | 5/21/97/115   | -       |
| 34  | LHG  | b     | 630 | -    | -         | 29/45/45/53   | -       |
| 32  | 8CT  | J     | 104 | -    | -         | 8/29/63/63    | 0/2/2/2 |

All (5807) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 32  | B     | 844 | 8CT  | C02-C03 | 14.92 | 1.59        | 1.34     |
| 32  | J     | 104 | 8CT  | C02-C03 | 14.91 | 1.59        | 1.34     |
| 32  | 8     | 406 | 8CT  | C02-C03 | 14.82 | 1.59        | 1.34     |
| 32  | B     | 848 | 8CT  | C02-C03 | 14.79 | 1.59        | 1.34     |
| 32  | A     | 846 | 8CT  | C02-C03 | 14.79 | 1.59        | 1.34     |
| 32  | G     | 104 | 8CT  | C02-C03 | 14.74 | 1.59        | 1.34     |
| 32  | A     | 849 | 8CT  | C02-C03 | 14.74 | 1.59        | 1.34     |
| 32  | F     | 302 | 8CT  | C02-C03 | 14.72 | 1.59        | 1.34     |
| 32  | B     | 804 | 8CT  | C02-C03 | 14.70 | 1.59        | 1.34     |
| 32  | O     | 205 | 8CT  | C02-C03 | 14.70 | 1.59        | 1.34     |
| 32  | 1     | 402 | 8CT  | C02-C03 | 14.68 | 1.59        | 1.34     |
| 32  | 7     | 404 | 8CT  | C02-C03 | 14.64 | 1.59        | 1.34     |
| 32  | 6     | 402 | 8CT  | C02-C03 | 14.63 | 1.59        | 1.34     |
| 32  | 8     | 402 | 8CT  | C02-C03 | 14.63 | 1.59        | 1.34     |
| 32  | B     | 843 | 8CT  | C02-C03 | 14.62 | 1.59        | 1.34     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 32  | M     | 102 | 8CT  | C02-C03 | 14.62 | 1.59        | 1.34     |
| 32  | L     | 209 | 8CT  | C02-C03 | 14.61 | 1.59        | 1.34     |
| 32  | 2     | 402 | 8CT  | C02-C03 | 14.60 | 1.59        | 1.34     |
| 32  | A     | 854 | 8CT  | C02-C03 | 14.58 | 1.59        | 1.34     |
| 32  | 7     | 405 | 8CT  | C02-C03 | 14.57 | 1.58        | 1.34     |
| 32  | L     | 206 | 8CT  | C02-C03 | 14.56 | 1.58        | 1.34     |
| 32  | A     | 847 | 8CT  | C02-C03 | 14.56 | 1.58        | 1.34     |
| 32  | A     | 848 | 8CT  | C02-C03 | 14.54 | 1.58        | 1.34     |
| 32  | B     | 847 | 8CT  | C02-C03 | 14.54 | 1.58        | 1.34     |
| 32  | K     | 107 | 8CT  | C02-C03 | 14.53 | 1.58        | 1.34     |
| 32  | I     | 101 | 8CT  | C02-C03 | 14.48 | 1.58        | 1.34     |
| 32  | B     | 851 | 8CT  | C02-C03 | 14.48 | 1.58        | 1.34     |
| 32  | B     | 846 | 8CT  | C02-C03 | 14.47 | 1.58        | 1.34     |
| 32  | L     | 205 | 8CT  | C02-C03 | 14.47 | 1.58        | 1.34     |
| 32  | 3     | 403 | 8CT  | C02-C03 | 14.46 | 1.58        | 1.34     |
| 32  | 3     | 402 | 8CT  | C02-C03 | 14.46 | 1.58        | 1.34     |
| 32  | 9     | 401 | 8CT  | C02-C03 | 14.45 | 1.58        | 1.34     |
| 32  | 4     | 402 | 8CT  | C02-C03 | 14.44 | 1.58        | 1.34     |
| 32  | B     | 845 | 8CT  | C02-C03 | 14.43 | 1.58        | 1.34     |
| 32  | 0     | 401 | 8CT  | C02-C03 | 14.42 | 1.58        | 1.34     |
| 32  | J     | 101 | 8CT  | C02-C03 | 14.39 | 1.58        | 1.34     |
| 32  | 1     | 402 | 8CT  | C32-C31 | 14.33 | 1.60        | 1.32     |
| 32  | 7     | 402 | 8CT  | C02-C03 | 14.32 | 1.58        | 1.34     |
| 32  | B     | 843 | 8CT  | C32-C31 | 14.32 | 1.59        | 1.32     |
| 32  | 3     | 403 | 8CT  | C32-C31 | 14.31 | 1.59        | 1.32     |
| 32  | B     | 846 | 8CT  | C32-C31 | 14.31 | 1.59        | 1.32     |
| 32  | 8     | 406 | 8CT  | C32-C31 | 14.30 | 1.59        | 1.32     |
| 32  | A     | 850 | 8CT  | C02-C03 | 14.29 | 1.58        | 1.34     |
| 32  | 9     | 401 | 8CT  | C32-C31 | 14.29 | 1.59        | 1.32     |
| 32  | 7     | 402 | 8CT  | C32-C31 | 14.29 | 1.59        | 1.32     |
| 32  | L     | 206 | 8CT  | C32-C31 | 14.29 | 1.59        | 1.32     |
| 32  | O     | 205 | 8CT  | C32-C31 | 14.27 | 1.59        | 1.32     |
| 32  | B     | 804 | 8CT  | C32-C31 | 14.27 | 1.59        | 1.32     |
| 32  | 6     | 402 | 8CT  | C32-C31 | 14.26 | 1.59        | 1.32     |
| 32  | 8     | 402 | 8CT  | C32-C31 | 14.17 | 1.59        | 1.32     |
| 32  | B     | 851 | 8CT  | C32-C31 | 14.17 | 1.59        | 1.32     |
| 32  | B     | 848 | 8CT  | C32-C31 | 14.16 | 1.59        | 1.32     |
| 32  | 7     | 405 | 8CT  | C32-C31 | 14.16 | 1.59        | 1.32     |
| 32  | L     | 209 | 8CT  | C32-C31 | 14.15 | 1.59        | 1.32     |
| 32  | F     | 302 | 8CT  | C32-C31 | 14.11 | 1.59        | 1.32     |
| 32  | A     | 846 | 8CT  | C32-C31 | 14.08 | 1.59        | 1.32     |
| 32  | 0     | 401 | 8CT  | C32-C31 | 14.08 | 1.59        | 1.32     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 32  | 3     | 402 | 8CT  | C32-C31 | 14.08 | 1.59        | 1.32     |
| 32  | B     | 847 | 8CT  | C32-C31 | 14.07 | 1.59        | 1.32     |
| 32  | A     | 848 | 8CT  | C32-C31 | 14.05 | 1.59        | 1.32     |
| 32  | 7     | 404 | 8CT  | C32-C31 | 14.04 | 1.59        | 1.32     |
| 32  | J     | 101 | 8CT  | C32-C31 | 14.03 | 1.59        | 1.32     |
| 32  | L     | 205 | 8CT  | C32-C31 | 14.02 | 1.59        | 1.32     |
| 32  | A     | 850 | 8CT  | C32-C31 | 14.00 | 1.59        | 1.32     |
| 32  | G     | 104 | 8CT  | C32-C31 | 14.00 | 1.59        | 1.32     |
| 32  | J     | 104 | 8CT  | C32-C31 | 13.97 | 1.59        | 1.32     |
| 32  | M     | 102 | 8CT  | C32-C31 | 13.97 | 1.59        | 1.32     |
| 32  | A     | 854 | 8CT  | C32-C31 | 13.95 | 1.59        | 1.32     |
| 32  | A     | 849 | 8CT  | C32-C31 | 13.94 | 1.59        | 1.32     |
| 32  | A     | 847 | 8CT  | C32-C31 | 13.93 | 1.59        | 1.32     |
| 32  | I     | 101 | 8CT  | C32-C31 | 13.92 | 1.59        | 1.32     |
| 32  | B     | 844 | 8CT  | C32-C31 | 13.91 | 1.59        | 1.32     |
| 32  | B     | 845 | 8CT  | C32-C31 | 13.90 | 1.59        | 1.32     |
| 32  | K     | 107 | 8CT  | C32-C31 | 13.87 | 1.59        | 1.32     |
| 32  | 2     | 402 | 8CT  | C32-C31 | 13.87 | 1.59        | 1.32     |
| 32  | 4     | 402 | 8CT  | C32-C31 | 13.81 | 1.59        | 1.32     |
| 30  | h     | 605 | CHL  | C2C-C3C | 11.70 | 1.47        | 1.36     |
| 30  | d     | 605 | CHL  | C2C-C3C | 11.69 | 1.47        | 1.36     |
| 30  | g     | 605 | CHL  | C2C-C3C | 11.66 | 1.47        | 1.36     |
| 30  | h     | 614 | CHL  | C2C-C3C | 11.62 | 1.47        | 1.36     |
| 30  | d     | 614 | CHL  | C2C-C3C | 11.61 | 1.47        | 1.36     |
| 30  | g     | 609 | CHL  | C2C-C3C | 11.60 | 1.47        | 1.36     |
| 30  | i     | 605 | CHL  | C2C-C3C | 11.58 | 1.47        | 1.36     |
| 30  | a     | 614 | CHL  | C2C-C3C | 11.56 | 1.47        | 1.36     |
| 30  | h     | 607 | CHL  | C2C-C3C | 11.56 | 1.47        | 1.36     |
| 30  | a     | 605 | CHL  | C2C-C3C | 11.54 | 1.47        | 1.36     |
| 30  | g     | 614 | CHL  | C2C-C3C | 11.54 | 1.47        | 1.36     |
| 30  | i     | 614 | CHL  | C2C-C3C | 11.53 | 1.47        | 1.36     |
| 30  | c     | 605 | CHL  | C2C-C3C | 11.53 | 1.47        | 1.36     |
| 30  | g     | 601 | CHL  | C2C-C3C | 11.52 | 1.47        | 1.36     |
| 30  | h     | 609 | CHL  | C2C-C3C | 11.48 | 1.47        | 1.36     |
| 30  | f     | 605 | CHL  | C2C-C3C | 11.46 | 1.47        | 1.36     |
| 30  | i     | 609 | CHL  | C2C-C3C | 11.46 | 1.47        | 1.36     |
| 30  | h     | 601 | CHL  | C2C-C3C | 11.39 | 1.47        | 1.36     |
| 30  | e     | 614 | CHL  | C2C-C3C | 11.37 | 1.47        | 1.36     |
| 30  | 0     | 306 | CHL  | C2C-C3C | 11.34 | 1.47        | 1.36     |
| 30  | i     | 607 | CHL  | C2C-C3C | 11.33 | 1.47        | 1.36     |
| 30  | h     | 602 | CHL  | C2C-C3C | 11.33 | 1.47        | 1.36     |
| 30  | 5     | 313 | CHL  | C2C-C3C | 11.32 | 1.47        | 1.36     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 30  | g     | 608 | CHL  | C2C-C3C | 11.27 | 1.47        | 1.36     |
| 30  | a     | 601 | CHL  | C2C-C3C | 11.26 | 1.47        | 1.36     |
| 30  | a     | 609 | CHL  | C2C-C3C | 11.26 | 1.47        | 1.36     |
| 30  | g     | 607 | CHL  | C2C-C3C | 11.26 | 1.47        | 1.36     |
| 30  | a     | 607 | CHL  | C2C-C3C | 11.26 | 1.47        | 1.36     |
| 30  | 5     | 306 | CHL  | C2C-C3C | 11.25 | 1.47        | 1.36     |
| 30  | i     | 601 | CHL  | C2C-C3C | 11.24 | 1.47        | 1.36     |
| 30  | d     | 607 | CHL  | C2C-C3C | 11.24 | 1.47        | 1.36     |
| 30  | i     | 606 | CHL  | C2C-C3C | 11.22 | 1.47        | 1.36     |
| 30  | e     | 605 | CHL  | C2C-C3C | 11.20 | 1.47        | 1.36     |
| 30  | b     | 614 | CHL  | C2C-C3C | 11.19 | 1.47        | 1.36     |
| 30  | c     | 609 | CHL  | C2C-C3C | 11.17 | 1.47        | 1.36     |
| 30  | d     | 609 | CHL  | C2C-C3C | 11.17 | 1.47        | 1.36     |
| 30  | a     | 606 | CHL  | C2C-C3C | 11.16 | 1.47        | 1.36     |
| 30  | d     | 601 | CHL  | C2C-C3C | 11.16 | 1.47        | 1.36     |
| 30  | b     | 601 | CHL  | C2C-C3C | 11.16 | 1.47        | 1.36     |
| 30  | g     | 606 | CHL  | C2C-C3C | 11.15 | 1.47        | 1.36     |
| 30  | c     | 607 | CHL  | C2C-C3C | 11.14 | 1.47        | 1.36     |
| 30  | f     | 609 | CHL  | C2C-C3C | 11.11 | 1.47        | 1.36     |
| 30  | e     | 607 | CHL  | C2C-C3C | 11.08 | 1.47        | 1.36     |
| 30  | 5     | 307 | CHL  | C2C-C3C | 11.07 | 1.47        | 1.36     |
| 30  | 5     | 301 | CHL  | C2C-C3C | 11.06 | 1.47        | 1.36     |
| 30  | h     | 608 | CHL  | C2C-C3C | 11.06 | 1.47        | 1.36     |
| 30  | f     | 607 | CHL  | C2C-C3C | 11.06 | 1.47        | 1.36     |
| 30  | f     | 606 | CHL  | C2C-C3C | 11.02 | 1.47        | 1.36     |
| 30  | f     | 614 | CHL  | C2C-C3C | 11.01 | 1.47        | 1.36     |
| 30  | d     | 608 | CHL  | C2C-C3C | 10.98 | 1.47        | 1.36     |
| 30  | d     | 606 | CHL  | C2C-C3C | 10.98 | 1.47        | 1.36     |
| 30  | g     | 602 | CHL  | C2C-C3C | 10.97 | 1.47        | 1.36     |
| 30  | b     | 609 | CHL  | C2C-C3C | 10.95 | 1.47        | 1.36     |
| 30  | h     | 606 | CHL  | C2C-C3C | 10.95 | 1.47        | 1.36     |
| 30  | c     | 614 | CHL  | C2C-C3C | 10.94 | 1.47        | 1.36     |
| 30  | i     | 602 | CHL  | C2C-C3C | 10.93 | 1.47        | 1.36     |
| 30  | f     | 601 | CHL  | C2C-C3C | 10.92 | 1.46        | 1.36     |
| 30  | e     | 609 | CHL  | C2C-C3C | 10.92 | 1.46        | 1.36     |
| 30  | b     | 607 | CHL  | C2C-C3C | 10.91 | 1.46        | 1.36     |
| 30  | 8     | 315 | CHL  | C2C-C3C | 10.90 | 1.46        | 1.36     |
| 30  | e     | 606 | CHL  | C2C-C3C | 10.90 | 1.46        | 1.36     |
| 30  | i     | 608 | CHL  | C2C-C3C | 10.89 | 1.46        | 1.36     |
| 30  | a     | 608 | CHL  | C2C-C3C | 10.88 | 1.46        | 1.36     |
| 30  | a     | 602 | CHL  | C2C-C3C | 10.86 | 1.46        | 1.36     |
| 30  | c     | 608 | CHL  | C2C-C3C | 10.84 | 1.46        | 1.36     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 30  | 5     | 305 | CHL  | C2C-C3C | 10.81 | 1.46        | 1.36     |
| 30  | e     | 601 | CHL  | C2C-C3C | 10.78 | 1.46        | 1.36     |
| 30  | 0     | 305 | CHL  | C2C-C3C | 10.77 | 1.46        | 1.36     |
| 30  | c     | 601 | CHL  | C2C-C3C | 10.77 | 1.46        | 1.36     |
| 30  | 1     | 307 | CHL  | C2C-C3C | 10.73 | 1.46        | 1.36     |
| 30  | 9     | 313 | CHL  | C2C-C3C | 10.73 | 1.46        | 1.36     |
| 30  | 8     | 301 | CHL  | C2C-C3C | 10.71 | 1.46        | 1.36     |
| 30  | 7     | 301 | CHL  | C2C-C3C | 10.64 | 1.46        | 1.36     |
| 30  | 8     | 308 | CHL  | C2C-C3C | 10.63 | 1.46        | 1.36     |
| 30  | b     | 606 | CHL  | C2C-C3C | 10.63 | 1.46        | 1.36     |
| 30  | 7     | 306 | CHL  | C2C-C3C | 10.62 | 1.46        | 1.36     |
| 30  | f     | 608 | CHL  | C2C-C3C | 10.61 | 1.46        | 1.36     |
| 30  | 7     | 313 | CHL  | C2C-C3C | 10.60 | 1.46        | 1.36     |
| 30  | 2     | 301 | CHL  | C2C-C3C | 10.59 | 1.46        | 1.36     |
| 30  | e     | 602 | CHL  | C2C-C3C | 10.59 | 1.46        | 1.36     |
| 30  | 1     | 306 | CHL  | C2C-C3C | 10.58 | 1.46        | 1.36     |
| 30  | c     | 606 | CHL  | C2C-C3C | 10.56 | 1.46        | 1.36     |
| 30  | e     | 608 | CHL  | C2C-C3C | 10.55 | 1.46        | 1.36     |
| 30  | 6     | 315 | CHL  | C2C-C3C | 10.55 | 1.46        | 1.36     |
| 30  | 8     | 305 | CHL  | C2C-C3C | 10.55 | 1.46        | 1.36     |
| 30  | 4     | 306 | CHL  | C2C-C3C | 10.52 | 1.46        | 1.36     |
| 30  | d     | 602 | CHL  | C2C-C3C | 10.51 | 1.46        | 1.36     |
| 30  | 2     | 308 | CHL  | C2C-C3C | 10.50 | 1.46        | 1.36     |
| 30  | 8     | 306 | CHL  | C2C-C3C | 10.50 | 1.46        | 1.36     |
| 30  | 4     | 308 | CHL  | C2C-C3C | 10.49 | 1.46        | 1.36     |
| 30  | 9     | 301 | CHL  | C2C-C3C | 10.49 | 1.46        | 1.36     |
| 30  | 4     | 319 | CHL  | C2C-C3C | 10.48 | 1.46        | 1.36     |
| 30  | 2     | 306 | CHL  | C2C-C3C | 10.47 | 1.46        | 1.36     |
| 30  | 0     | 301 | CHL  | C2C-C3C | 10.47 | 1.46        | 1.36     |
| 30  | 6     | 301 | CHL  | C2C-C3C | 10.44 | 1.46        | 1.36     |
| 30  | 9     | 306 | CHL  | C2C-C3C | 10.43 | 1.46        | 1.36     |
| 30  | 1     | 313 | CHL  | C2C-C3C | 10.42 | 1.46        | 1.36     |
| 30  | 6     | 313 | CHL  | C2C-C3C | 10.41 | 1.46        | 1.36     |
| 30  | b     | 602 | CHL  | C2C-C3C | 10.39 | 1.46        | 1.36     |
| 30  | 2     | 313 | CHL  | C2C-C3C | 10.39 | 1.46        | 1.36     |
| 30  | 2     | 319 | CHL  | C2C-C3C | 10.38 | 1.46        | 1.36     |
| 30  | 6     | 308 | CHL  | C2C-C3C | 10.38 | 1.46        | 1.36     |
| 30  | 4     | 307 | CHL  | C2C-C3C | 10.36 | 1.46        | 1.36     |
| 30  | 1     | 305 | CHL  | C2C-C3C | 10.34 | 1.46        | 1.36     |
| 30  | 8     | 313 | CHL  | C2C-C3C | 10.33 | 1.46        | 1.36     |
| 30  | b     | 608 | CHL  | C2C-C3C | 10.32 | 1.46        | 1.36     |
| 30  | 4     | 313 | CHL  | C2C-C3C | 10.32 | 1.46        | 1.36     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 30  | 6     | 305 | CHL  | C2C-C3C | 10.31 | 1.46        | 1.36     |
| 30  | 6     | 306 | CHL  | C2C-C3C | 10.26 | 1.46        | 1.36     |
| 30  | 4     | 305 | CHL  | C2C-C3C | 10.25 | 1.46        | 1.36     |
| 30  | 8     | 307 | CHL  | C2C-C3C | 10.22 | 1.46        | 1.36     |
| 30  | 3     | 305 | CHL  | C2C-C3C | 10.18 | 1.46        | 1.36     |
| 30  | 9     | 305 | CHL  | C2C-C3C | 10.14 | 1.46        | 1.36     |
| 30  | 2     | 305 | CHL  | C2C-C3C | 10.13 | 1.46        | 1.36     |
| 30  | c     | 602 | CHL  | C2C-C3C | 10.13 | 1.46        | 1.36     |
| 30  | 6     | 307 | CHL  | C2C-C3C | 10.12 | 1.46        | 1.36     |
| 30  | f     | 602 | CHL  | C2C-C3C | 10.06 | 1.46        | 1.36     |
| 30  | 7     | 305 | CHL  | C2C-C3C | 10.06 | 1.46        | 1.36     |
| 30  | 3     | 307 | CHL  | C2C-C3C | 10.04 | 1.46        | 1.36     |
| 30  | 4     | 302 | CHL  | C2C-C3C | 10.03 | 1.46        | 1.36     |
| 30  | 5     | 302 | CHL  | C2C-C3C | 10.03 | 1.46        | 1.36     |
| 30  | 0     | 302 | CHL  | C2C-C3C | 10.02 | 1.46        | 1.36     |
| 30  | 3     | 302 | CHL  | C2C-C3C | 10.00 | 1.46        | 1.36     |
| 30  | 7     | 307 | CHL  | C2C-C3C | 9.99  | 1.46        | 1.36     |
| 30  | 6     | 302 | CHL  | C2C-C3C | 9.99  | 1.46        | 1.36     |
| 30  | 2     | 302 | CHL  | C2C-C3C | 9.92  | 1.46        | 1.36     |
| 30  | 7     | 302 | CHL  | C2C-C3C | 9.91  | 1.46        | 1.36     |
| 30  | 2     | 307 | CHL  | C2C-C3C | 9.83  | 1.45        | 1.36     |
| 30  | 1     | 302 | CHL  | C2C-C3C | 9.81  | 1.45        | 1.36     |
| 30  | 8     | 302 | CHL  | C2C-C3C | 9.79  | 1.45        | 1.36     |
| 32  | A     | 848 | 8CT  | C34-C35 | -9.19 | 1.36        | 1.54     |
| 32  | B     | 804 | 8CT  | C34-C35 | -9.07 | 1.37        | 1.54     |
| 32  | B     | 848 | 8CT  | C34-C35 | -9.00 | 1.37        | 1.54     |
| 32  | B     | 846 | 8CT  | C34-C35 | -8.96 | 1.37        | 1.54     |
| 32  | L     | 209 | 8CT  | C34-C35 | -8.95 | 1.37        | 1.54     |
| 32  | B     | 851 | 8CT  | C34-C35 | -8.92 | 1.37        | 1.54     |
| 32  | 3     | 403 | 8CT  | C34-C35 | -8.92 | 1.37        | 1.54     |
| 32  | 8     | 406 | 8CT  | C34-C35 | -8.92 | 1.37        | 1.54     |
| 30  | g     | 614 | CHL  | C1A-CHA | 8.91  | 1.50        | 1.40     |
| 32  | A     | 850 | 8CT  | C34-C35 | -8.89 | 1.37        | 1.54     |
| 32  | B     | 843 | 8CT  | C34-C35 | -8.89 | 1.37        | 1.54     |
| 30  | g     | 605 | CHL  | C1A-CHA | 8.89  | 1.50        | 1.40     |
| 32  | A     | 854 | 8CT  | C34-C35 | -8.87 | 1.37        | 1.54     |
| 30  | a     | 605 | CHL  | C1A-CHA | 8.85  | 1.50        | 1.40     |
| 32  | F     | 302 | 8CT  | C34-C35 | -8.84 | 1.37        | 1.54     |
| 32  | O     | 205 | 8CT  | C34-C35 | -8.84 | 1.37        | 1.54     |
| 32  | 7     | 405 | 8CT  | C34-C35 | -8.84 | 1.37        | 1.54     |
| 32  | 1     | 402 | 8CT  | C34-C35 | -8.82 | 1.37        | 1.54     |
| 30  | i     | 605 | CHL  | C1A-CHA | 8.82  | 1.50        | 1.40     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 30  | g     | 607 | CHL  | C1A-CHA | 8.82  | 1.50        | 1.40     |
| 30  | d     | 605 | CHL  | C1A-CHA | 8.82  | 1.50        | 1.40     |
| 30  | g     | 601 | CHL  | C1A-CHA | 8.81  | 1.50        | 1.40     |
| 30  | a     | 614 | CHL  | C1A-CHA | 8.80  | 1.50        | 1.40     |
| 32  | 7     | 404 | 8CT  | C34-C35 | -8.80 | 1.37        | 1.54     |
| 32  | 6     | 402 | 8CT  | C34-C35 | -8.80 | 1.37        | 1.54     |
| 32  | 8     | 402 | 8CT  | C34-C35 | -8.80 | 1.37        | 1.54     |
| 32  | A     | 846 | 8CT  | C34-C35 | -8.80 | 1.37        | 1.54     |
| 30  | e     | 614 | CHL  | C1A-CHA | 8.79  | 1.50        | 1.40     |
| 32  | J     | 104 | 8CT  | C34-C35 | -8.78 | 1.37        | 1.54     |
| 30  | d     | 614 | CHL  | C1A-CHA | 8.78  | 1.50        | 1.40     |
| 32  | A     | 847 | 8CT  | C34-C35 | -8.76 | 1.37        | 1.54     |
| 32  | B     | 847 | 8CT  | C34-C35 | -8.75 | 1.37        | 1.54     |
| 32  | 7     | 402 | 8CT  | C34-C35 | -8.74 | 1.37        | 1.54     |
| 30  | a     | 601 | CHL  | C1A-CHA | 8.73  | 1.49        | 1.40     |
| 30  | c     | 605 | CHL  | C1A-CHA | 8.70  | 1.49        | 1.40     |
| 32  | L     | 206 | 8CT  | C34-C35 | -8.69 | 1.37        | 1.54     |
| 32  | M     | 102 | 8CT  | C34-C35 | -8.69 | 1.37        | 1.54     |
| 32  | L     | 205 | 8CT  | C34-C35 | -8.68 | 1.37        | 1.54     |
| 32  | B     | 844 | 8CT  | C34-C35 | -8.67 | 1.37        | 1.54     |
| 32  | 9     | 401 | 8CT  | C34-C35 | -8.66 | 1.37        | 1.54     |
| 30  | h     | 605 | CHL  | C1B-C2B | 8.66  | 1.49        | 1.39     |
| 30  | h     | 601 | CHL  | C1A-CHA | 8.64  | 1.49        | 1.40     |
| 32  | B     | 845 | 8CT  | C34-C35 | -8.63 | 1.37        | 1.54     |
| 30  | g     | 608 | CHL  | C1A-CHA | 8.63  | 1.49        | 1.40     |
| 30  | a     | 601 | CHL  | C1B-C2B | 8.62  | 1.49        | 1.39     |
| 30  | f     | 614 | CHL  | C1A-CHA | 8.61  | 1.49        | 1.40     |
| 32  | A     | 849 | 8CT  | C34-C35 | -8.58 | 1.38        | 1.54     |
| 30  | i     | 614 | CHL  | C1B-C2B | 8.58  | 1.49        | 1.39     |
| 32  | I     | 101 | 8CT  | C34-C35 | -8.58 | 1.38        | 1.54     |
| 30  | g     | 607 | CHL  | C1B-C2B | 8.57  | 1.49        | 1.39     |
| 30  | i     | 614 | CHL  | C1A-CHA | 8.56  | 1.49        | 1.40     |
| 30  | a     | 614 | CHL  | C1B-C2B | 8.56  | 1.49        | 1.39     |
| 30  | e     | 605 | CHL  | C1A-CHA | 8.55  | 1.49        | 1.40     |
| 30  | h     | 607 | CHL  | C1B-C2B | 8.55  | 1.49        | 1.39     |
| 30  | a     | 609 | CHL  | C1B-C2B | 8.55  | 1.49        | 1.39     |
| 30  | i     | 607 | CHL  | C1B-C2B | 8.55  | 1.49        | 1.39     |
| 32  | 2     | 402 | 8CT  | C34-C35 | -8.54 | 1.38        | 1.54     |
| 32  | 3     | 402 | 8CT  | C34-C35 | -8.53 | 1.38        | 1.54     |
| 30  | i     | 605 | CHL  | C1B-C2B | 8.53  | 1.49        | 1.39     |
| 30  | i     | 606 | CHL  | C1B-C2B | 8.53  | 1.49        | 1.39     |
| 30  | f     | 605 | CHL  | C1A-CHA | 8.52  | 1.49        | 1.40     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 30  | f     | 607 | CHL  | C1B-C2B | 8.52  | 1.49        | 1.39     |
| 32  | K     | 107 | 8CT  | C34-C35 | -8.52 | 1.38        | 1.54     |
| 30  | i     | 609 | CHL  | C1B-C2B | 8.52  | 1.49        | 1.39     |
| 30  | g     | 614 | CHL  | C1B-C2B | 8.52  | 1.49        | 1.39     |
| 30  | h     | 606 | CHL  | C1B-C2B | 8.52  | 1.49        | 1.39     |
| 30  | 8     | 315 | CHL  | C1B-C2B | 8.51  | 1.49        | 1.39     |
| 30  | a     | 605 | CHL  | C1B-C2B | 8.51  | 1.49        | 1.39     |
| 30  | d     | 605 | CHL  | C1B-C2B | 8.50  | 1.49        | 1.39     |
| 30  | g     | 602 | CHL  | C1B-C2B | 8.49  | 1.49        | 1.39     |
| 30  | g     | 605 | CHL  | C1B-C2B | 8.49  | 1.49        | 1.39     |
| 30  | a     | 607 | CHL  | C1B-C2B | 8.48  | 1.49        | 1.39     |
| 30  | e     | 614 | CHL  | C1B-C2B | 8.48  | 1.49        | 1.39     |
| 30  | i     | 607 | CHL  | C1A-CHA | 8.46  | 1.49        | 1.40     |
| 32  | J     | 101 | 8CT  | C34-C35 | -8.46 | 1.38        | 1.54     |
| 30  | g     | 601 | CHL  | C1B-C2B | 8.46  | 1.49        | 1.39     |
| 30  | b     | 614 | CHL  | C1A-CHA | 8.46  | 1.49        | 1.40     |
| 30  | d     | 601 | CHL  | C1B-C2B | 8.46  | 1.49        | 1.39     |
| 30  | h     | 614 | CHL  | C1B-C2B | 8.45  | 1.49        | 1.39     |
| 30  | c     | 605 | CHL  | C1B-C2B | 8.45  | 1.49        | 1.39     |
| 30  | 5     | 307 | CHL  | C1B-C2B | 8.45  | 1.49        | 1.39     |
| 30  | e     | 605 | CHL  | C1B-C2B | 8.45  | 1.49        | 1.39     |
| 30  | b     | 601 | CHL  | C1A-CHA | 8.45  | 1.49        | 1.40     |
| 30  | d     | 614 | CHL  | C1B-C2B | 8.44  | 1.49        | 1.39     |
| 30  | i     | 601 | CHL  | C1B-C2B | 8.43  | 1.49        | 1.39     |
| 30  | c     | 607 | CHL  | C1B-C2B | 8.43  | 1.49        | 1.39     |
| 30  | d     | 608 | CHL  | C1B-C2B | 8.43  | 1.49        | 1.39     |
| 30  | 6     | 313 | CHL  | C1B-C2B | 8.42  | 1.49        | 1.39     |
| 30  | h     | 601 | CHL  | C1B-C2B | 8.42  | 1.49        | 1.39     |
| 30  | d     | 609 | CHL  | C1B-C2B | 8.42  | 1.49        | 1.39     |
| 32  | G     | 104 | 8CT  | C34-C35 | -8.42 | 1.38        | 1.54     |
| 30  | e     | 607 | CHL  | C1B-C2B | 8.42  | 1.49        | 1.39     |
| 30  | b     | 614 | CHL  | C1B-C2B | 8.42  | 1.49        | 1.39     |
| 30  | a     | 608 | CHL  | C1B-C2B | 8.41  | 1.49        | 1.39     |
| 30  | f     | 605 | CHL  | C1B-C2B | 8.41  | 1.49        | 1.39     |
| 30  | g     | 609 | CHL  | C1B-C2B | 8.41  | 1.49        | 1.39     |
| 30  | f     | 614 | CHL  | C1B-C2B | 8.40  | 1.49        | 1.39     |
| 30  | f     | 608 | CHL  | C1B-C2B | 8.40  | 1.49        | 1.39     |
| 30  | d     | 606 | CHL  | C1B-C2B | 8.39  | 1.49        | 1.39     |
| 30  | i     | 602 | CHL  | C1B-C2B | 8.39  | 1.49        | 1.39     |
| 30  | b     | 609 | CHL  | C1B-C2B | 8.39  | 1.49        | 1.39     |
| 30  | 0     | 306 | CHL  | C1B-C2B | 8.38  | 1.49        | 1.39     |
| 30  | e     | 601 | CHL  | C1B-C2B | 8.38  | 1.49        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 30  | b     | 602 | CHL  | C1B-C2B | 8.37  | 1.49        | 1.39     |
| 30  | g     | 606 | CHL  | C1B-C2B | 8.37  | 1.49        | 1.39     |
| 30  | e     | 609 | CHL  | C1B-C2B | 8.37  | 1.49        | 1.39     |
| 30  | d     | 607 | CHL  | C1B-C2B | 8.37  | 1.49        | 1.39     |
| 30  | h     | 602 | CHL  | C1B-C2B | 8.36  | 1.49        | 1.39     |
| 30  | i     | 608 | CHL  | C1B-C2B | 8.36  | 1.49        | 1.39     |
| 30  | f     | 609 | CHL  | C1B-C2B | 8.35  | 1.49        | 1.39     |
| 30  | h     | 614 | CHL  | C1A-CHA | 8.34  | 1.49        | 1.40     |
| 32  | 0     | 401 | 8CT  | C34-C35 | -8.33 | 1.38        | 1.54     |
| 30  | h     | 609 | CHL  | C1B-C2B | 8.33  | 1.49        | 1.39     |
| 30  | 1     | 307 | CHL  | C1B-C2B | 8.32  | 1.49        | 1.39     |
| 30  | e     | 602 | CHL  | C3B-C4B | 8.31  | 1.49        | 1.41     |
| 30  | b     | 601 | CHL  | C1B-C2B | 8.31  | 1.49        | 1.39     |
| 30  | f     | 606 | CHL  | C1B-C2B | 8.31  | 1.49        | 1.39     |
| 30  | h     | 608 | CHL  | C1A-CHA | 8.31  | 1.49        | 1.40     |
| 30  | 1     | 306 | CHL  | C1B-C2B | 8.30  | 1.49        | 1.39     |
| 30  | h     | 606 | CHL  | C1A-CHA | 8.29  | 1.49        | 1.40     |
| 30  | 9     | 313 | CHL  | C1B-C2B | 8.29  | 1.49        | 1.39     |
| 30  | c     | 606 | CHL  | C1B-C2B | 8.29  | 1.49        | 1.39     |
| 30  | a     | 606 | CHL  | C1B-C2B | 8.28  | 1.49        | 1.39     |
| 30  | 5     | 313 | CHL  | C1B-C2B | 8.28  | 1.49        | 1.39     |
| 30  | e     | 608 | CHL  | C1B-C2B | 8.28  | 1.49        | 1.39     |
| 30  | f     | 601 | CHL  | C1B-C2B | 8.26  | 1.49        | 1.39     |
| 30  | c     | 601 | CHL  | C1B-C2B | 8.26  | 1.49        | 1.39     |
| 30  | 5     | 313 | CHL  | C1A-CHA | 8.26  | 1.49        | 1.40     |
| 30  | c     | 606 | CHL  | C1A-CHA | 8.25  | 1.49        | 1.40     |
| 30  | g     | 608 | CHL  | C1B-C2B | 8.25  | 1.48        | 1.39     |
| 30  | h     | 608 | CHL  | C1B-C2B | 8.25  | 1.48        | 1.39     |
| 30  | 8     | 305 | CHL  | C1B-C2B | 8.22  | 1.48        | 1.39     |
| 30  | b     | 608 | CHL  | C1B-C2B | 8.22  | 1.48        | 1.39     |
| 30  | a     | 608 | CHL  | C1A-CHA | 8.22  | 1.49        | 1.40     |
| 30  | 0     | 301 | CHL  | C1B-C2B | 8.21  | 1.48        | 1.39     |
| 30  | a     | 602 | CHL  | C1B-C2B | 8.20  | 1.48        | 1.39     |
| 30  | d     | 608 | CHL  | C1A-CHA | 8.20  | 1.49        | 1.40     |
| 30  | c     | 614 | CHL  | C1B-C2B | 8.20  | 1.48        | 1.39     |
| 30  | 5     | 306 | CHL  | C1B-C2B | 8.20  | 1.48        | 1.39     |
| 30  | a     | 606 | CHL  | C3B-C4B | 8.19  | 1.49        | 1.41     |
| 30  | d     | 601 | CHL  | C1A-CHA | 8.19  | 1.49        | 1.40     |
| 30  | 6     | 315 | CHL  | C1B-C2B | 8.19  | 1.48        | 1.39     |
| 30  | d     | 607 | CHL  | C1A-CHA | 8.19  | 1.49        | 1.40     |
| 30  | c     | 614 | CHL  | C1A-CHA | 8.17  | 1.49        | 1.40     |
| 30  | c     | 608 | CHL  | C1B-C2B | 8.17  | 1.48        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 30  | b     | 607 | CHL  | C1B-C2B | 8.17  | 1.48        | 1.39     |
| 30  | 5     | 301 | CHL  | C3B-C4B | 8.17  | 1.49        | 1.41     |
| 30  | 8     | 313 | CHL  | C1B-C2B | 8.17  | 1.48        | 1.39     |
| 30  | 1     | 313 | CHL  | C1B-C2B | 8.16  | 1.48        | 1.39     |
| 30  | c     | 609 | CHL  | C1B-C2B | 8.16  | 1.48        | 1.39     |
| 30  | 8     | 301 | CHL  | C1B-C2B | 8.16  | 1.48        | 1.39     |
| 30  | 8     | 306 | CHL  | C1B-C2B | 8.16  | 1.48        | 1.39     |
| 30  | i     | 608 | CHL  | C1A-CHA | 8.15  | 1.49        | 1.40     |
| 30  | 6     | 306 | CHL  | C1B-C2B | 8.14  | 1.48        | 1.39     |
| 30  | 6     | 301 | CHL  | C1B-C2B | 8.14  | 1.48        | 1.39     |
| 30  | 5     | 305 | CHL  | C1B-C2B | 8.14  | 1.48        | 1.39     |
| 30  | 7     | 313 | CHL  | C1B-C2B | 8.14  | 1.48        | 1.39     |
| 30  | e     | 606 | CHL  | C1B-C2B | 8.13  | 1.48        | 1.39     |
| 30  | 7     | 313 | CHL  | C1A-CHA | 8.13  | 1.49        | 1.40     |
| 30  | c     | 602 | CHL  | C1B-C2B | 8.13  | 1.48        | 1.39     |
| 30  | a     | 607 | CHL  | C1A-CHA | 8.12  | 1.49        | 1.40     |
| 32  | 4     | 402 | 8CT  | C34-C35 | -8.12 | 1.38        | 1.54     |
| 30  | h     | 608 | CHL  | C3B-C4B | 8.12  | 1.49        | 1.41     |
| 30  | h     | 605 | CHL  | C1A-CHA | 8.11  | 1.49        | 1.40     |
| 30  | a     | 602 | CHL  | C3B-C4B | 8.11  | 1.49        | 1.41     |
| 30  | g     | 606 | CHL  | C3B-C4B | 8.11  | 1.49        | 1.41     |
| 30  | 4     | 308 | CHL  | C1B-C2B | 8.11  | 1.48        | 1.39     |
| 30  | 6     | 308 | CHL  | C1B-C2B | 8.10  | 1.48        | 1.39     |
| 30  | 2     | 308 | CHL  | C1B-C2B | 8.10  | 1.48        | 1.39     |
| 30  | 0     | 306 | CHL  | C1A-CHA | 8.10  | 1.49        | 1.40     |
| 30  | 4     | 307 | CHL  | C1B-C2B | 8.10  | 1.48        | 1.39     |
| 30  | h     | 602 | CHL  | C3B-C4B | 8.09  | 1.49        | 1.41     |
| 30  | g     | 605 | CHL  | C3B-C4B | 8.09  | 1.49        | 1.41     |
| 30  | a     | 609 | CHL  | C1A-CHA | 8.09  | 1.49        | 1.40     |
| 30  | c     | 608 | CHL  | C1A-CHA | 8.08  | 1.49        | 1.40     |
| 30  | 8     | 308 | CHL  | C1B-C2B | 8.07  | 1.48        | 1.39     |
| 30  | 9     | 301 | CHL  | C1A-CHA | 8.06  | 1.49        | 1.40     |
| 30  | 4     | 313 | CHL  | C1B-C2B | 8.05  | 1.48        | 1.39     |
| 30  | 8     | 307 | CHL  | C1B-C2B | 8.05  | 1.48        | 1.39     |
| 30  | e     | 608 | CHL  | C1A-CHA | 8.04  | 1.49        | 1.40     |
| 30  | d     | 602 | CHL  | C1B-C2B | 8.04  | 1.48        | 1.39     |
| 30  | 9     | 306 | CHL  | C1B-C2B | 8.04  | 1.48        | 1.39     |
| 30  | g     | 608 | CHL  | C3B-C4B | 8.03  | 1.49        | 1.41     |
| 30  | 2     | 313 | CHL  | C1B-C2B | 8.03  | 1.48        | 1.39     |
| 30  | 6     | 305 | CHL  | C1B-C2B | 8.02  | 1.48        | 1.39     |
| 30  | 1     | 302 | CHL  | C3B-C4B | 8.02  | 1.49        | 1.41     |
| 30  | 7     | 305 | CHL  | C1B-C2B | 8.01  | 1.48        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 30  | 2     | 306 | CHL  | C1B-C2B | 8.01 | 1.48        | 1.39     |
| 30  | g     | 614 | CHL  | C3B-C4B | 8.01 | 1.49        | 1.41     |
| 30  | 1     | 307 | CHL  | C1A-CHA | 8.00 | 1.49        | 1.40     |
| 30  | 5     | 302 | CHL  | C1B-C2B | 8.00 | 1.48        | 1.39     |
| 30  | d     | 605 | CHL  | C3B-C4B | 8.00 | 1.49        | 1.41     |
| 30  | e     | 614 | CHL  | C3B-C4B | 7.99 | 1.49        | 1.41     |
| 30  | f     | 607 | CHL  | C1A-CHA | 7.99 | 1.49        | 1.40     |
| 30  | i     | 601 | CHL  | C1A-CHA | 7.98 | 1.49        | 1.40     |
| 30  | 4     | 306 | CHL  | C1B-C2B | 7.98 | 1.48        | 1.39     |
| 30  | d     | 614 | CHL  | C3B-C4B | 7.97 | 1.49        | 1.41     |
| 30  | 6     | 302 | CHL  | C1B-C2B | 7.97 | 1.48        | 1.39     |
| 30  | 0     | 302 | CHL  | C1B-C2B | 7.97 | 1.48        | 1.39     |
| 30  | 4     | 305 | CHL  | C1B-C2B | 7.97 | 1.48        | 1.39     |
| 30  | i     | 608 | CHL  | C3B-C4B | 7.96 | 1.49        | 1.41     |
| 30  | f     | 602 | CHL  | C1B-C2B | 7.96 | 1.48        | 1.39     |
| 30  | 9     | 301 | CHL  | C1B-C2B | 7.96 | 1.48        | 1.39     |
| 30  | g     | 609 | CHL  | C3B-C4B | 7.96 | 1.49        | 1.41     |
| 30  | 0     | 305 | CHL  | C3B-C4B | 7.95 | 1.49        | 1.41     |
| 30  | i     | 602 | CHL  | C1A-CHA | 7.95 | 1.49        | 1.40     |
| 30  | 4     | 306 | CHL  | C3B-C4B | 7.95 | 1.49        | 1.41     |
| 30  | a     | 605 | CHL  | C3B-C4B | 7.95 | 1.49        | 1.41     |
| 30  | 1     | 306 | CHL  | C1A-CHA | 7.95 | 1.49        | 1.40     |
| 30  | 7     | 301 | CHL  | C1B-C2B | 7.94 | 1.48        | 1.39     |
| 30  | 0     | 305 | CHL  | C1B-C2B | 7.94 | 1.48        | 1.39     |
| 30  | i     | 609 | CHL  | C1A-CHA | 7.94 | 1.49        | 1.40     |
| 30  | 3     | 305 | CHL  | C1B-C2B | 7.93 | 1.48        | 1.39     |
| 30  | h     | 607 | CHL  | C1A-CHA | 7.92 | 1.49        | 1.40     |
| 30  | b     | 606 | CHL  | C1B-C2B | 7.92 | 1.48        | 1.39     |
| 30  | b     | 606 | CHL  | C3B-C4B | 7.92 | 1.49        | 1.41     |
| 30  | a     | 614 | CHL  | C3B-C4B | 7.92 | 1.49        | 1.41     |
| 30  | 5     | 301 | CHL  | C1B-C2B | 7.91 | 1.48        | 1.39     |
| 30  | 7     | 307 | CHL  | C3B-C4B | 7.91 | 1.49        | 1.41     |
| 30  | e     | 606 | CHL  | C3B-C4B | 7.91 | 1.49        | 1.41     |
| 30  | b     | 607 | CHL  | C1A-CHA | 7.90 | 1.49        | 1.40     |
| 30  | h     | 607 | CHL  | C3B-C4B | 7.89 | 1.49        | 1.41     |
| 30  | 6     | 307 | CHL  | C1B-C2B | 7.89 | 1.48        | 1.39     |
| 30  | 2     | 307 | CHL  | C1B-C2B | 7.88 | 1.48        | 1.39     |
| 30  | i     | 614 | CHL  | C3B-C4B | 7.88 | 1.49        | 1.41     |
| 30  | c     | 607 | CHL  | C1A-CHA | 7.88 | 1.49        | 1.40     |
| 30  | d     | 608 | CHL  | C3B-C4B | 7.87 | 1.49        | 1.41     |
| 30  | g     | 607 | CHL  | C3B-C4B | 7.87 | 1.49        | 1.41     |
| 30  | 8     | 306 | CHL  | C1A-CHA | 7.86 | 1.48        | 1.40     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 30  | d     | 601 | CHL  | C3B-C4B | 7.86 | 1.49        | 1.41     |
| 30  | h     | 609 | CHL  | C1A-CHA | 7.85 | 1.48        | 1.40     |
| 30  | 2     | 313 | CHL  | C1A-CHA | 7.84 | 1.48        | 1.40     |
| 30  | a     | 607 | CHL  | C3B-C4B | 7.84 | 1.49        | 1.41     |
| 30  | g     | 601 | CHL  | C3B-C4B | 7.84 | 1.49        | 1.41     |
| 30  | b     | 608 | CHL  | C1A-CHA | 7.84 | 1.48        | 1.40     |
| 30  | g     | 609 | CHL  | C1A-CHA | 7.84 | 1.48        | 1.40     |
| 30  | 4     | 319 | CHL  | C3B-C4B | 7.84 | 1.49        | 1.41     |
| 30  | i     | 601 | CHL  | C3B-C4B | 7.84 | 1.49        | 1.41     |
| 30  | 7     | 307 | CHL  | C1A-CHA | 7.83 | 1.48        | 1.40     |
| 30  | i     | 607 | CHL  | C3B-C4B | 7.83 | 1.49        | 1.41     |
| 30  | 2     | 305 | CHL  | C1B-C2B | 7.82 | 1.48        | 1.39     |
| 30  | b     | 607 | CHL  | C3B-C4B | 7.82 | 1.49        | 1.41     |
| 30  | h     | 605 | CHL  | C3B-C4B | 7.82 | 1.49        | 1.41     |
| 30  | f     | 601 | CHL  | C1A-CHA | 7.81 | 1.48        | 1.40     |
| 30  | 4     | 307 | CHL  | C1A-CHA | 7.81 | 1.48        | 1.40     |
| 30  | 2     | 301 | CHL  | C1B-C2B | 7.81 | 1.48        | 1.39     |
| 30  | i     | 606 | CHL  | C1A-CHA | 7.81 | 1.48        | 1.40     |
| 30  | 9     | 305 | CHL  | C3B-C4B | 7.81 | 1.49        | 1.41     |
| 30  | 4     | 305 | CHL  | C3B-C4B | 7.81 | 1.49        | 1.41     |
| 30  | 2     | 319 | CHL  | C1B-C2B | 7.81 | 1.48        | 1.39     |
| 30  | 8     | 307 | CHL  | C3B-C4B | 7.80 | 1.49        | 1.41     |
| 30  | 2     | 302 | CHL  | C1B-C2B | 7.80 | 1.48        | 1.39     |
| 30  | i     | 609 | CHL  | C3B-C4B | 7.80 | 1.49        | 1.41     |
| 30  | 3     | 305 | CHL  | C1A-CHA | 7.80 | 1.48        | 1.40     |
| 30  | b     | 614 | CHL  | C3B-C4B | 7.79 | 1.49        | 1.41     |
| 30  | i     | 606 | CHL  | C3B-C4B | 7.79 | 1.49        | 1.41     |
| 30  | 7     | 301 | CHL  | C3B-C4B | 7.79 | 1.49        | 1.41     |
| 30  | 4     | 302 | CHL  | C1B-C2B | 7.79 | 1.48        | 1.39     |
| 30  | 8     | 301 | CHL  | C3B-C4B | 7.79 | 1.49        | 1.41     |
| 30  | h     | 601 | CHL  | C3B-C4B | 7.79 | 1.49        | 1.41     |
| 30  | c     | 601 | CHL  | C1A-CHA | 7.78 | 1.48        | 1.40     |
| 30  | f     | 605 | CHL  | C3B-C4B | 7.78 | 1.49        | 1.41     |
| 30  | 8     | 315 | CHL  | C1A-CHA | 7.77 | 1.48        | 1.40     |
| 30  | 8     | 305 | CHL  | C3B-C4B | 7.77 | 1.49        | 1.41     |
| 30  | i     | 605 | CHL  | C3B-C4B | 7.77 | 1.49        | 1.41     |
| 30  | h     | 614 | CHL  | C3B-C4B | 7.77 | 1.49        | 1.41     |
| 30  | 2     | 306 | CHL  | C3B-C4B | 7.77 | 1.49        | 1.41     |
| 30  | b     | 609 | CHL  | C1A-CHA | 7.77 | 1.48        | 1.40     |
| 30  | f     | 602 | CHL  | C3B-C4B | 7.76 | 1.48        | 1.41     |
| 30  | e     | 608 | CHL  | C3B-C4B | 7.76 | 1.48        | 1.41     |
| 30  | e     | 605 | CHL  | C3B-C4B | 7.76 | 1.48        | 1.41     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 30  | 7     | 302 | CHL  | C1B-C2B | 7.76 | 1.48        | 1.39     |
| 30  | a     | 608 | CHL  | C3B-C4B | 7.76 | 1.48        | 1.41     |
| 30  | 4     | 319 | CHL  | C1B-C2B | 7.76 | 1.48        | 1.39     |
| 30  | 7     | 306 | CHL  | C1B-C2B | 7.76 | 1.48        | 1.39     |
| 30  | i     | 602 | CHL  | C3B-C4B | 7.76 | 1.48        | 1.41     |
| 30  | g     | 602 | CHL  | C3B-C4B | 7.75 | 1.48        | 1.41     |
| 30  | 2     | 319 | CHL  | C3B-C4B | 7.75 | 1.48        | 1.41     |
| 30  | 3     | 302 | CHL  | C3B-C4B | 7.75 | 1.48        | 1.41     |
| 30  | c     | 607 | CHL  | C3B-C4B | 7.75 | 1.48        | 1.41     |
| 30  | 5     | 305 | CHL  | C1A-CHA | 7.75 | 1.48        | 1.40     |
| 30  | f     | 608 | CHL  | C1A-CHA | 7.75 | 1.48        | 1.40     |
| 30  | g     | 602 | CHL  | C1A-CHA | 7.74 | 1.48        | 1.40     |
| 30  | 8     | 301 | CHL  | C1A-CHA | 7.73 | 1.48        | 1.40     |
| 30  | d     | 606 | CHL  | C3B-C4B | 7.73 | 1.48        | 1.41     |
| 30  | 1     | 313 | CHL  | C1A-CHA | 7.73 | 1.48        | 1.40     |
| 30  | a     | 606 | CHL  | C1A-CHA | 7.73 | 1.48        | 1.40     |
| 30  | 7     | 306 | CHL  | C3B-C4B | 7.73 | 1.48        | 1.41     |
| 30  | 8     | 302 | CHL  | C3B-C4B | 7.73 | 1.48        | 1.41     |
| 30  | f     | 609 | CHL  | C1A-CHA | 7.72 | 1.48        | 1.40     |
| 30  | c     | 614 | CHL  | C3B-C4B | 7.72 | 1.48        | 1.41     |
| 30  | 5     | 306 | CHL  | C3B-C4B | 7.72 | 1.48        | 1.41     |
| 30  | d     | 607 | CHL  | C3B-C4B | 7.71 | 1.48        | 1.41     |
| 30  | 5     | 306 | CHL  | C1A-CHA | 7.71 | 1.48        | 1.40     |
| 30  | 1     | 305 | CHL  | C1B-C2B | 7.70 | 1.48        | 1.39     |
| 30  | e     | 601 | CHL  | C1A-CHA | 7.70 | 1.48        | 1.40     |
| 38  | B     | 842 | PQN  | C3-C2   | 7.70 | 1.49        | 1.35     |
| 30  | h     | 602 | CHL  | C1A-CHA | 7.70 | 1.48        | 1.40     |
| 30  | f     | 614 | CHL  | C3B-C4B | 7.70 | 1.48        | 1.41     |
| 30  | c     | 605 | CHL  | C3B-C4B | 7.70 | 1.48        | 1.41     |
| 30  | b     | 606 | CHL  | C1A-CHA | 7.69 | 1.48        | 1.40     |
| 30  | 7     | 301 | CHL  | C1A-CHA | 7.68 | 1.48        | 1.40     |
| 30  | 0     | 301 | CHL  | C1A-CHA | 7.68 | 1.48        | 1.40     |
| 30  | 1     | 302 | CHL  | C1B-C2B | 7.68 | 1.48        | 1.39     |
| 30  | b     | 601 | CHL  | C3B-C4B | 7.68 | 1.48        | 1.41     |
| 30  | 6     | 308 | CHL  | C1A-CHA | 7.67 | 1.48        | 1.40     |
| 30  | 7     | 307 | CHL  | C1B-C2B | 7.67 | 1.48        | 1.39     |
| 30  | g     | 606 | CHL  | C1A-CHA | 7.66 | 1.48        | 1.40     |
| 30  | 8     | 313 | CHL  | C1A-CHA | 7.66 | 1.48        | 1.40     |
| 30  | h     | 606 | CHL  | C3B-C4B | 7.66 | 1.48        | 1.41     |
| 30  | c     | 608 | CHL  | C3B-C4B | 7.65 | 1.48        | 1.41     |
| 30  | b     | 602 | CHL  | C3B-C4B | 7.64 | 1.48        | 1.41     |
| 30  | 9     | 306 | CHL  | C3B-C4B | 7.64 | 1.48        | 1.41     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 30  | d     | 606 | CHL  | C1A-CHA | 7.64 | 1.48        | 1.40     |
| 30  | 6     | 315 | CHL  | C1A-CHA | 7.64 | 1.48        | 1.40     |
| 30  | 4     | 305 | CHL  | C1A-CHA | 7.64 | 1.48        | 1.40     |
| 30  | 2     | 307 | CHL  | C3B-C4B | 7.63 | 1.48        | 1.41     |
| 30  | b     | 608 | CHL  | C3B-C4B | 7.63 | 1.48        | 1.41     |
| 39  | A     | 857 | CL0  | C1B-C2B | 7.62 | 1.48        | 1.39     |
| 30  | c     | 606 | CHL  | C3B-C4B | 7.62 | 1.48        | 1.41     |
| 30  | e     | 607 | CHL  | C3B-C4B | 7.62 | 1.48        | 1.41     |
| 30  | e     | 607 | CHL  | C1A-CHA | 7.62 | 1.48        | 1.40     |
| 30  | 8     | 302 | CHL  | C1B-C2B | 7.62 | 1.48        | 1.39     |
| 30  | f     | 601 | CHL  | C3B-C4B | 7.61 | 1.48        | 1.41     |
| 30  | 6     | 306 | CHL  | C1A-CHA | 7.61 | 1.48        | 1.40     |
| 30  | 5     | 305 | CHL  | C3B-C4B | 7.60 | 1.48        | 1.41     |
| 30  | 3     | 302 | CHL  | C1B-C2B | 7.60 | 1.48        | 1.39     |
| 30  | 5     | 307 | CHL  | C1A-CHA | 7.60 | 1.48        | 1.40     |
| 30  | 3     | 307 | CHL  | C1B-C2B | 7.60 | 1.48        | 1.39     |
| 30  | f     | 609 | CHL  | C3B-C4B | 7.59 | 1.48        | 1.41     |
| 30  | e     | 602 | CHL  | C1A-CHA | 7.59 | 1.48        | 1.40     |
| 30  | 6     | 313 | CHL  | C1A-CHA | 7.59 | 1.48        | 1.40     |
| 30  | e     | 606 | CHL  | C1A-CHA | 7.59 | 1.48        | 1.40     |
| 30  | d     | 602 | CHL  | C3B-C4B | 7.59 | 1.48        | 1.41     |
| 30  | e     | 601 | CHL  | C3B-C4B | 7.59 | 1.48        | 1.41     |
| 30  | 0     | 302 | CHL  | C1A-CHA | 7.59 | 1.48        | 1.40     |
| 30  | d     | 609 | CHL  | C1A-CHA | 7.59 | 1.48        | 1.40     |
| 30  | 2     | 305 | CHL  | C3B-C4B | 7.58 | 1.48        | 1.41     |
| 30  | 9     | 305 | CHL  | C1B-C2B | 7.58 | 1.48        | 1.39     |
| 30  | f     | 606 | CHL  | C3B-C4B | 7.58 | 1.48        | 1.41     |
| 30  | 7     | 305 | CHL  | C1A-CHA | 7.57 | 1.48        | 1.40     |
| 30  | c     | 602 | CHL  | C1A-CHA | 7.57 | 1.48        | 1.40     |
| 30  | 6     | 305 | CHL  | C3B-C4B | 7.57 | 1.48        | 1.41     |
| 30  | 4     | 306 | CHL  | C1A-CHA | 7.57 | 1.48        | 1.40     |
| 30  | 1     | 307 | CHL  | C3B-C4B | 7.56 | 1.48        | 1.41     |
| 30  | a     | 609 | CHL  | C3B-C4B | 7.56 | 1.48        | 1.41     |
| 30  | f     | 607 | CHL  | C3B-C4B | 7.55 | 1.48        | 1.41     |
| 30  | 0     | 305 | CHL  | C1A-CHA | 7.55 | 1.48        | 1.40     |
| 30  | d     | 609 | CHL  | C3B-C4B | 7.54 | 1.48        | 1.41     |
| 30  | 2     | 308 | CHL  | C1A-CHA | 7.54 | 1.48        | 1.40     |
| 30  | e     | 609 | CHL  | C1A-CHA | 7.54 | 1.48        | 1.40     |
| 30  | 7     | 313 | CHL  | C3B-C4B | 7.54 | 1.48        | 1.41     |
| 30  | 5     | 313 | CHL  | C3B-C4B | 7.54 | 1.48        | 1.41     |
| 30  | 8     | 307 | CHL  | C1A-CHA | 7.54 | 1.48        | 1.40     |
| 30  | 4     | 308 | CHL  | C1A-CHA | 7.54 | 1.48        | 1.40     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 30  | f     | 608 | CHL  | C3B-C4B | 7.53 | 1.48        | 1.41     |
| 30  | 0     | 306 | CHL  | C3B-C4B | 7.53 | 1.48        | 1.41     |
| 30  | e     | 602 | CHL  | C1B-C2B | 7.52 | 1.48        | 1.39     |
| 30  | 8     | 315 | CHL  | C3B-C4B | 7.52 | 1.48        | 1.41     |
| 30  | 6     | 307 | CHL  | C1A-CHA | 7.51 | 1.48        | 1.40     |
| 30  | a     | 602 | CHL  | C1A-CHA | 7.51 | 1.48        | 1.40     |
| 30  | 8     | 308 | CHL  | C1A-CHA | 7.50 | 1.48        | 1.40     |
| 30  | 1     | 306 | CHL  | C3B-C4B | 7.50 | 1.48        | 1.41     |
| 30  | b     | 602 | CHL  | C1A-CHA | 7.50 | 1.48        | 1.40     |
| 30  | 5     | 307 | CHL  | C3B-C4B | 7.48 | 1.48        | 1.41     |
| 30  | c     | 602 | CHL  | C3B-C4B | 7.48 | 1.48        | 1.41     |
| 30  | 9     | 306 | CHL  | C1A-CHA | 7.47 | 1.48        | 1.40     |
| 30  | 8     | 306 | CHL  | C3B-C4B | 7.47 | 1.48        | 1.41     |
| 30  | a     | 601 | CHL  | C3B-C4B | 7.47 | 1.48        | 1.41     |
| 30  | 4     | 319 | CHL  | C1A-CHA | 7.44 | 1.48        | 1.40     |
| 30  | 5     | 301 | CHL  | C1A-CHA | 7.44 | 1.48        | 1.40     |
| 30  | 1     | 305 | CHL  | C1A-CHA | 7.44 | 1.48        | 1.40     |
| 30  | 1     | 305 | CHL  | C3B-C4B | 7.44 | 1.48        | 1.41     |
| 30  | 1     | 313 | CHL  | C3B-C4B | 7.43 | 1.48        | 1.41     |
| 30  | 8     | 305 | CHL  | C1A-CHA | 7.43 | 1.48        | 1.40     |
| 30  | c     | 609 | CHL  | C1A-CHA | 7.43 | 1.48        | 1.40     |
| 30  | f     | 606 | CHL  | C1A-CHA | 7.43 | 1.48        | 1.40     |
| 30  | f     | 602 | CHL  | C1A-CHA | 7.43 | 1.48        | 1.40     |
| 30  | c     | 609 | CHL  | C3B-C4B | 7.43 | 1.48        | 1.41     |
| 30  | h     | 609 | CHL  | C3B-C4B | 7.42 | 1.48        | 1.41     |
| 30  | 6     | 305 | CHL  | C1A-CHA | 7.41 | 1.48        | 1.40     |
| 30  | 0     | 301 | CHL  | C3B-C4B | 7.40 | 1.48        | 1.41     |
| 30  | 5     | 302 | CHL  | C1A-CHA | 7.40 | 1.48        | 1.40     |
| 30  | 6     | 315 | CHL  | C3B-C4B | 7.40 | 1.48        | 1.41     |
| 30  | 4     | 313 | CHL  | C1A-CHA | 7.39 | 1.48        | 1.40     |
| 30  | 9     | 301 | CHL  | C3B-C4B | 7.37 | 1.48        | 1.41     |
| 30  | 2     | 302 | CHL  | C1A-CHA | 7.36 | 1.48        | 1.40     |
| 30  | 2     | 319 | CHL  | C1A-CHA | 7.36 | 1.48        | 1.40     |
| 30  | c     | 601 | CHL  | C3B-C4B | 7.35 | 1.48        | 1.41     |
| 38  | A     | 842 | PQN  | C3-C2   | 7.35 | 1.48        | 1.35     |
| 30  | 9     | 313 | CHL  | C1A-CHA | 7.34 | 1.48        | 1.40     |
| 30  | 4     | 307 | CHL  | C3B-C4B | 7.33 | 1.48        | 1.41     |
| 30  | 2     | 306 | CHL  | C1A-CHA | 7.33 | 1.48        | 1.40     |
| 30  | 9     | 305 | CHL  | C1A-CHA | 7.33 | 1.48        | 1.40     |
| 30  | 9     | 313 | CHL  | C3B-C4B | 7.32 | 1.48        | 1.41     |
| 30  | 6     | 301 | CHL  | C1A-CHA | 7.32 | 1.48        | 1.40     |
| 30  | 4     | 302 | CHL  | C3B-C4B | 7.32 | 1.48        | 1.41     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 30  | 7     | 305 | CHL  | C3B-C4B | 7.32  | 1.48        | 1.41     |
| 30  | 2     | 305 | CHL  | C1A-CHA | 7.31  | 1.48        | 1.40     |
| 30  | 6     | 307 | CHL  | C3B-C4B | 7.31  | 1.48        | 1.41     |
| 30  | 2     | 307 | CHL  | C1A-CHA | 7.31  | 1.48        | 1.40     |
| 30  | 7     | 302 | CHL  | C3B-C4B | 7.30  | 1.48        | 1.41     |
| 30  | e     | 609 | CHL  | C3B-C4B | 7.29  | 1.48        | 1.41     |
| 30  | 1     | 302 | CHL  | C1A-CHA | 7.29  | 1.48        | 1.40     |
| 30  | d     | 602 | CHL  | C1A-CHA | 7.29  | 1.48        | 1.40     |
| 30  | 2     | 308 | CHL  | C3B-C4B | 7.28  | 1.48        | 1.41     |
| 30  | 6     | 308 | CHL  | C3B-C4B | 7.27  | 1.48        | 1.41     |
| 30  | 3     | 307 | CHL  | C1A-CHA | 7.26  | 1.48        | 1.40     |
| 39  | A     | 857 | CL0  | C1D-C2D | 7.26  | 1.47        | 1.39     |
| 30  | 4     | 302 | CHL  | C1A-CHA | 7.26  | 1.48        | 1.40     |
| 30  | 3     | 305 | CHL  | C3B-C4B | 7.25  | 1.48        | 1.41     |
| 30  | 2     | 302 | CHL  | C3B-C4B | 7.24  | 1.48        | 1.41     |
| 30  | 2     | 301 | CHL  | C3B-C4B | 7.22  | 1.48        | 1.41     |
| 30  | 2     | 301 | CHL  | C1A-CHA | 7.22  | 1.48        | 1.40     |
| 30  | 6     | 302 | CHL  | C1A-CHA | 7.21  | 1.48        | 1.40     |
| 30  | 2     | 313 | CHL  | C3B-C4B | 7.20  | 1.48        | 1.41     |
| 30  | 4     | 313 | CHL  | C3B-C4B | 7.20  | 1.48        | 1.41     |
| 30  | 8     | 308 | CHL  | C3B-C4B | 7.19  | 1.48        | 1.41     |
| 30  | b     | 609 | CHL  | C3B-C4B | 7.18  | 1.48        | 1.41     |
| 30  | 7     | 302 | CHL  | C1A-CHA | 7.17  | 1.48        | 1.40     |
| 30  | 0     | 302 | CHL  | C3B-C4B | 7.15  | 1.48        | 1.41     |
| 30  | 7     | 306 | CHL  | C1A-CHA | 7.15  | 1.48        | 1.40     |
| 30  | 6     | 301 | CHL  | C3B-C4B | 7.14  | 1.48        | 1.41     |
| 30  | 6     | 313 | CHL  | C3B-C4B | 7.13  | 1.48        | 1.41     |
| 30  | 5     | 302 | CHL  | C3B-C4B | 7.10  | 1.48        | 1.41     |
| 30  | 8     | 302 | CHL  | C1A-CHA | 7.09  | 1.48        | 1.40     |
| 30  | 6     | 302 | CHL  | C3B-C4B | 7.08  | 1.48        | 1.41     |
| 30  | h     | 605 | CHL  | C1D-C2D | 7.08  | 1.47        | 1.39     |
| 30  | h     | 614 | CHL  | C1D-C2D | 7.07  | 1.47        | 1.39     |
| 30  | 8     | 313 | CHL  | C3B-C4B | 7.06  | 1.48        | 1.41     |
| 30  | i     | 606 | CHL  | C1D-C2D | 7.04  | 1.47        | 1.39     |
| 30  | 6     | 306 | CHL  | C3B-C4B | 7.04  | 1.48        | 1.41     |
| 30  | h     | 609 | CHL  | C1D-C2D | 7.04  | 1.47        | 1.39     |
| 30  | g     | 614 | CHL  | C1D-C2D | 7.03  | 1.47        | 1.39     |
| 30  | c     | 609 | CHL  | C1D-C2D | 7.02  | 1.47        | 1.39     |
| 30  | 4     | 308 | CHL  | C3B-C4B | 6.99  | 1.48        | 1.41     |
| 30  | h     | 607 | CHL  | C1D-C2D | 6.99  | 1.47        | 1.39     |
| 32  | J     | 104 | 8CT  | C05-C06 | -6.98 | 1.36        | 1.52     |
| 32  | B     | 848 | 8CT  | C05-C06 | -6.98 | 1.36        | 1.52     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 32  | B     | 804 | 8CT  | C05-C06 | -6.97 | 1.36        | 1.52     |
| 30  | f     | 606 | CHL  | C1D-C2D | 6.97  | 1.47        | 1.39     |
| 30  | 3     | 302 | CHL  | C1A-CHA | 6.96  | 1.47        | 1.40     |
| 30  | a     | 609 | CHL  | C1D-C2D | 6.96  | 1.47        | 1.39     |
| 30  | g     | 609 | CHL  | C1D-C2D | 6.96  | 1.47        | 1.39     |
| 32  | G     | 104 | 8CT  | C05-C06 | -6.95 | 1.36        | 1.52     |
| 32  | B     | 846 | 8CT  | C15-C16 | 6.95  | 1.60        | 1.46     |
| 30  | a     | 605 | CHL  | C1D-C2D | 6.94  | 1.47        | 1.39     |
| 30  | i     | 609 | CHL  | C1D-C2D | 6.94  | 1.47        | 1.39     |
| 30  | d     | 605 | CHL  | C1D-C2D | 6.93  | 1.47        | 1.39     |
| 30  | g     | 605 | CHL  | C1D-C2D | 6.92  | 1.47        | 1.39     |
| 30  | d     | 614 | CHL  | C1D-C2D | 6.92  | 1.47        | 1.39     |
| 30  | i     | 605 | CHL  | C1D-C2D | 6.91  | 1.47        | 1.39     |
| 32  | A     | 849 | 8CT  | C05-C06 | -6.91 | 1.36        | 1.52     |
| 32  | F     | 302 | 8CT  | C05-C06 | -6.91 | 1.36        | 1.52     |
| 30  | a     | 614 | CHL  | C1D-C2D | 6.90  | 1.47        | 1.39     |
| 32  | B     | 844 | 8CT  | C15-C16 | 6.90  | 1.60        | 1.46     |
| 32  | 6     | 402 | 8CT  | C05-C06 | -6.90 | 1.36        | 1.52     |
| 30  | h     | 601 | CHL  | C1D-C2D | 6.89  | 1.47        | 1.39     |
| 32  | M     | 102 | 8CT  | C05-C06 | -6.88 | 1.36        | 1.52     |
| 32  | 8     | 406 | 8CT  | C05-C06 | -6.88 | 1.36        | 1.52     |
| 32  | 7     | 404 | 8CT  | C05-C06 | -6.88 | 1.36        | 1.52     |
| 32  | B     | 851 | 8CT  | C05-C06 | -6.88 | 1.36        | 1.52     |
| 30  | c     | 605 | CHL  | C1D-C2D | 6.88  | 1.47        | 1.39     |
| 32  | 1     | 402 | 8CT  | C05-C06 | -6.88 | 1.36        | 1.52     |
| 32  | A     | 854 | 8CT  | C05-C06 | -6.87 | 1.36        | 1.52     |
| 30  | d     | 607 | CHL  | C1D-C2D | 6.87  | 1.47        | 1.39     |
| 30  | f     | 605 | CHL  | C1D-C2D | 6.87  | 1.47        | 1.39     |
| 30  | d     | 606 | CHL  | C1D-C2D | 6.87  | 1.47        | 1.39     |
| 30  | d     | 609 | CHL  | C1D-C2D | 6.87  | 1.47        | 1.39     |
| 32  | B     | 847 | 8CT  | C05-C06 | -6.86 | 1.36        | 1.52     |
| 30  | i     | 601 | CHL  | C1D-C2D | 6.86  | 1.47        | 1.39     |
| 32  | 3     | 402 | 8CT  | C05-C06 | -6.86 | 1.36        | 1.52     |
| 30  | g     | 607 | CHL  | C1D-C2D | 6.86  | 1.47        | 1.39     |
| 32  | B     | 843 | 8CT  | C05-C06 | -6.85 | 1.36        | 1.52     |
| 32  | 7     | 405 | 8CT  | C05-C06 | -6.85 | 1.36        | 1.52     |
| 30  | a     | 607 | CHL  | C1D-C2D | 6.84  | 1.47        | 1.39     |
| 32  | I     | 101 | 8CT  | C05-C06 | -6.84 | 1.36        | 1.52     |
| 32  | 7     | 402 | 8CT  | C05-C06 | -6.84 | 1.36        | 1.52     |
| 30  | h     | 602 | CHL  | C1D-C2D | 6.83  | 1.47        | 1.39     |
| 32  | 8     | 402 | 8CT  | C05-C06 | -6.83 | 1.36        | 1.52     |
| 30  | g     | 606 | CHL  | C1D-C2D | 6.82  | 1.47        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 30  | 5     | 313 | CHL  | C1D-C2D | 6.82  | 1.47        | 1.39     |
| 32  | O     | 205 | 8CT  | C05-C06 | -6.81 | 1.36        | 1.52     |
| 30  | f     | 609 | CHL  | C1D-C2D | 6.81  | 1.47        | 1.39     |
| 32  | L     | 206 | 8CT  | C05-C06 | -6.81 | 1.36        | 1.52     |
| 32  | L     | 205 | 8CT  | C05-C06 | -6.81 | 1.36        | 1.52     |
| 30  | b     | 614 | CHL  | C1D-C2D | 6.80  | 1.47        | 1.39     |
| 32  | 9     | 401 | 8CT  | C05-C06 | -6.80 | 1.36        | 1.52     |
| 32  | B     | 844 | 8CT  | C05-C06 | -6.79 | 1.36        | 1.52     |
| 32  | J     | 101 | 8CT  | C05-C06 | -6.79 | 1.36        | 1.52     |
| 30  | e     | 607 | CHL  | C1D-C2D | 6.78  | 1.47        | 1.39     |
| 32  | A     | 847 | 8CT  | C05-C06 | -6.78 | 1.36        | 1.52     |
| 32  | L     | 209 | 8CT  | C05-C06 | -6.78 | 1.36        | 1.52     |
| 30  | g     | 608 | CHL  | C1D-C2D | 6.77  | 1.47        | 1.39     |
| 30  | a     | 606 | CHL  | C1D-C2D | 6.77  | 1.47        | 1.39     |
| 30  | i     | 614 | CHL  | C1D-C2D | 6.77  | 1.47        | 1.39     |
| 32  | 4     | 402 | 8CT  | C05-C06 | -6.77 | 1.36        | 1.52     |
| 32  | A     | 846 | 8CT  | C05-C06 | -6.77 | 1.36        | 1.52     |
| 32  | 0     | 401 | 8CT  | C05-C06 | -6.76 | 1.36        | 1.52     |
| 30  | 5     | 306 | CHL  | C1D-C2D | 6.76  | 1.47        | 1.39     |
| 32  | 3     | 403 | 8CT  | C05-C06 | -6.75 | 1.36        | 1.52     |
| 30  | g     | 601 | CHL  | C1D-C2D | 6.75  | 1.47        | 1.39     |
| 32  | B     | 845 | 8CT  | C05-C06 | -6.75 | 1.36        | 1.52     |
| 30  | i     | 607 | CHL  | C1D-C2D | 6.74  | 1.47        | 1.39     |
| 30  | h     | 608 | CHL  | C1D-C2D | 6.74  | 1.47        | 1.39     |
| 30  | 3     | 307 | CHL  | C3B-C4B | 6.74  | 1.48        | 1.41     |
| 30  | a     | 602 | CHL  | C1D-C2D | 6.74  | 1.47        | 1.39     |
| 32  | 2     | 402 | 8CT  | C05-C06 | -6.73 | 1.36        | 1.52     |
| 32  | A     | 850 | 8CT  | C05-C06 | -6.73 | 1.36        | 1.52     |
| 30  | i     | 602 | CHL  | C1D-C2D | 6.72  | 1.47        | 1.39     |
| 32  | B     | 843 | 8CT  | C15-C16 | 6.72  | 1.60        | 1.46     |
| 30  | e     | 605 | CHL  | C1D-C2D | 6.71  | 1.47        | 1.39     |
| 30  | e     | 601 | CHL  | C1D-C2D | 6.70  | 1.47        | 1.39     |
| 30  | c     | 607 | CHL  | C1D-C2D | 6.70  | 1.47        | 1.39     |
| 32  | B     | 846 | 8CT  | C05-C06 | -6.69 | 1.36        | 1.52     |
| 30  | 5     | 307 | CHL  | C1D-C2D | 6.68  | 1.47        | 1.39     |
| 32  | K     | 107 | 8CT  | C05-C06 | -6.68 | 1.36        | 1.52     |
| 30  | 5     | 305 | CHL  | C1D-C2D | 6.67  | 1.47        | 1.39     |
| 30  | c     | 608 | CHL  | C1D-C2D | 6.67  | 1.47        | 1.39     |
| 30  | g     | 602 | CHL  | C1D-C2D | 6.67  | 1.47        | 1.39     |
| 30  | i     | 608 | CHL  | C1D-C2D | 6.66  | 1.47        | 1.39     |
| 30  | b     | 609 | CHL  | C1D-C2D | 6.66  | 1.47        | 1.39     |
| 30  | e     | 614 | CHL  | C1D-C2D | 6.66  | 1.47        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 30  | 8     | 315 | CHL  | C1D-C2D | 6.66  | 1.47        | 1.39     |
| 32  | A     | 848 | 8CT  | C05-C06 | -6.65 | 1.36        | 1.52     |
| 30  | d     | 601 | CHL  | C1D-C2D | 6.65  | 1.47        | 1.39     |
| 30  | e     | 602 | CHL  | C1D-C2D | 6.63  | 1.47        | 1.39     |
| 30  | a     | 601 | CHL  | C1D-C2D | 6.63  | 1.47        | 1.39     |
| 30  | b     | 601 | CHL  | C1D-C2D | 6.62  | 1.47        | 1.39     |
| 30  | e     | 609 | CHL  | C1D-C2D | 6.61  | 1.47        | 1.39     |
| 30  | h     | 606 | CHL  | C1D-C2D | 6.61  | 1.47        | 1.39     |
| 32  | B     | 845 | 8CT  | C15-C16 | 6.59  | 1.60        | 1.46     |
| 30  | f     | 607 | CHL  | C1D-C2D | 6.58  | 1.47        | 1.39     |
| 30  | 8     | 305 | CHL  | C1D-C2D | 6.57  | 1.47        | 1.39     |
| 30  | d     | 608 | CHL  | C1D-C2D | 6.55  | 1.47        | 1.39     |
| 30  | f     | 601 | CHL  | C1D-C2D | 6.54  | 1.47        | 1.39     |
| 30  | e     | 606 | CHL  | C1D-C2D | 6.53  | 1.47        | 1.39     |
| 30  | 6     | 315 | CHL  | C1D-C2D | 6.51  | 1.47        | 1.39     |
| 30  | 0     | 305 | CHL  | C1D-C2D | 6.51  | 1.46        | 1.39     |
| 30  | c     | 614 | CHL  | C1D-C2D | 6.50  | 1.46        | 1.39     |
| 30  | c     | 601 | CHL  | C1D-C2D | 6.49  | 1.46        | 1.39     |
| 30  | b     | 607 | CHL  | C1D-C2D | 6.49  | 1.46        | 1.39     |
| 30  | f     | 614 | CHL  | C1D-C2D | 6.49  | 1.46        | 1.39     |
| 30  | d     | 602 | CHL  | C1D-C2D | 6.48  | 1.46        | 1.39     |
| 30  | e     | 608 | CHL  | C1D-C2D | 6.48  | 1.46        | 1.39     |
| 32  | A     | 850 | 8CT  | C04-C03 | -6.47 | 1.45        | 1.53     |
| 30  | 5     | 301 | CHL  | C1D-C2D | 6.46  | 1.46        | 1.39     |
| 30  | a     | 608 | CHL  | C1D-C2D | 6.46  | 1.46        | 1.39     |
| 32  | 3     | 402 | 8CT  | C15-C16 | 6.45  | 1.59        | 1.46     |
| 32  | 2     | 402 | 8CT  | C28-C26 | 6.44  | 1.59        | 1.46     |
| 30  | 9     | 313 | CHL  | C1D-C2D | 6.44  | 1.46        | 1.39     |
| 32  | 4     | 402 | 8CT  | C28-C26 | 6.44  | 1.59        | 1.46     |
| 30  | 8     | 306 | CHL  | C1D-C2D | 6.43  | 1.46        | 1.39     |
| 32  | B     | 846 | 8CT  | C28-C26 | 6.42  | 1.59        | 1.46     |
| 30  | 1     | 306 | CHL  | C1D-C2D | 6.42  | 1.46        | 1.39     |
| 30  | 1     | 305 | CHL  | C1D-C2D | 6.42  | 1.46        | 1.39     |
| 32  | G     | 104 | 8CT  | C15-C16 | 6.40  | 1.59        | 1.46     |
| 30  | b     | 602 | CHL  | C1D-C2D | 6.40  | 1.46        | 1.39     |
| 32  | 4     | 402 | 8CT  | C15-C16 | 6.39  | 1.59        | 1.46     |
| 32  | B     | 848 | 8CT  | C15-C16 | 6.39  | 1.59        | 1.46     |
| 30  | c     | 606 | CHL  | C1D-C2D | 6.38  | 1.46        | 1.39     |
| 30  | b     | 606 | CHL  | C1D-C2D | 6.38  | 1.46        | 1.39     |
| 30  | c     | 602 | CHL  | C1D-C2D | 6.37  | 1.46        | 1.39     |
| 32  | A     | 854 | 8CT  | C15-C16 | 6.37  | 1.59        | 1.46     |
| 30  | 6     | 301 | CHL  | C1D-C2D | 6.37  | 1.46        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 32  | 8     | 402 | 8CT  | C15-C16 | 6.36  | 1.59        | 1.46     |
| 32  | 0     | 401 | 8CT  | C28-C26 | 6.35  | 1.59        | 1.46     |
| 30  | 7     | 306 | CHL  | C1D-C2D | 6.35  | 1.46        | 1.39     |
| 32  | 8     | 406 | 8CT  | C15-C16 | 6.34  | 1.59        | 1.46     |
| 32  | B     | 843 | 8CT  | C28-C26 | 6.34  | 1.59        | 1.46     |
| 32  | L     | 209 | 8CT  | C15-C16 | 6.33  | 1.59        | 1.46     |
| 30  | f     | 608 | CHL  | C1D-C2D | 6.33  | 1.46        | 1.39     |
| 32  | 0     | 401 | 8CT  | C15-C16 | 6.33  | 1.59        | 1.46     |
| 30  | 8     | 313 | CHL  | C1D-C2D | 6.32  | 1.46        | 1.39     |
| 32  | K     | 107 | 8CT  | C15-C16 | 6.32  | 1.59        | 1.46     |
| 32  | 2     | 402 | 8CT  | C15-C16 | 6.30  | 1.59        | 1.46     |
| 30  | 6     | 313 | CHL  | C1D-C2D | 6.30  | 1.46        | 1.39     |
| 32  | 3     | 403 | 8CT  | C15-C16 | 6.30  | 1.59        | 1.46     |
| 30  | 0     | 306 | CHL  | C1D-C2D | 6.29  | 1.46        | 1.39     |
| 30  | 9     | 301 | CHL  | C1D-C2D | 6.29  | 1.46        | 1.39     |
| 30  | 1     | 307 | CHL  | C1D-C2D | 6.29  | 1.46        | 1.39     |
| 30  | 5     | 302 | CHL  | C1D-C2D | 6.29  | 1.46        | 1.39     |
| 32  | 8     | 406 | 8CT  | C28-C26 | 6.29  | 1.59        | 1.46     |
| 32  | L     | 206 | 8CT  | C15-C16 | 6.28  | 1.59        | 1.46     |
| 32  | 9     | 401 | 8CT  | C15-C16 | 6.28  | 1.59        | 1.46     |
| 30  | 7     | 313 | CHL  | C1D-C2D | 6.28  | 1.46        | 1.39     |
| 32  | A     | 846 | 8CT  | C15-C16 | 6.28  | 1.59        | 1.46     |
| 30  | 2     | 306 | CHL  | C1D-C2D | 6.28  | 1.46        | 1.39     |
| 30  | 4     | 308 | CHL  | C1D-C2D | 6.28  | 1.46        | 1.39     |
| 32  | 1     | 402 | 8CT  | C15-C16 | 6.28  | 1.59        | 1.46     |
| 32  | B     | 844 | 8CT  | C23-C21 | 6.28  | 1.59        | 1.46     |
| 30  | 2     | 319 | CHL  | C1D-C2D | 6.27  | 1.46        | 1.39     |
| 32  | 6     | 402 | 8CT  | C15-C16 | 6.27  | 1.59        | 1.46     |
| 32  | 7     | 404 | 8CT  | C15-C16 | 6.27  | 1.59        | 1.46     |
| 30  | 4     | 306 | CHL  | C1D-C2D | 6.27  | 1.46        | 1.39     |
| 30  | b     | 608 | CHL  | C1D-C2D | 6.26  | 1.46        | 1.39     |
| 32  | O     | 205 | 8CT  | C15-C16 | 6.25  | 1.59        | 1.46     |
| 32  | J     | 104 | 8CT  | C15-C16 | 6.25  | 1.59        | 1.46     |
| 32  | 1     | 402 | 8CT  | C28-C26 | 6.25  | 1.59        | 1.46     |
| 32  | 9     | 401 | 8CT  | C28-C26 | 6.24  | 1.59        | 1.46     |
| 32  | I     | 101 | 8CT  | C15-C16 | 6.23  | 1.59        | 1.46     |
| 32  | G     | 104 | 8CT  | C28-C26 | 6.23  | 1.59        | 1.46     |
| 30  | 2     | 301 | CHL  | C1D-C2D | 6.23  | 1.46        | 1.39     |
| 30  | f     | 602 | CHL  | C1D-C2D | 6.23  | 1.46        | 1.39     |
| 32  | F     | 302 | 8CT  | C15-C16 | 6.22  | 1.59        | 1.46     |
| 32  | J     | 101 | 8CT  | C04-C03 | -6.22 | 1.45        | 1.53     |
| 32  | A     | 847 | 8CT  | C15-C16 | 6.21  | 1.59        | 1.46     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 30  | 2     | 305 | CHL  | C1D-C2D | 6.21  | 1.46        | 1.39     |
| 30  | 7     | 305 | CHL  | C1D-C2D | 6.21  | 1.46        | 1.39     |
| 32  | A     | 854 | 8CT  | C28-C26 | 6.20  | 1.59        | 1.46     |
| 30  | 8     | 308 | CHL  | C1D-C2D | 6.19  | 1.46        | 1.39     |
| 32  | B     | 804 | 8CT  | C15-C16 | 6.18  | 1.59        | 1.46     |
| 32  | 7     | 402 | 8CT  | C04-C03 | -6.18 | 1.45        | 1.53     |
| 30  | 3     | 302 | CHL  | C1D-C2D | 6.18  | 1.46        | 1.39     |
| 30  | 9     | 306 | CHL  | C1D-C2D | 6.18  | 1.46        | 1.39     |
| 30  | 0     | 302 | CHL  | C1D-C2D | 6.18  | 1.46        | 1.39     |
| 32  | B     | 847 | 8CT  | C15-C16 | 6.18  | 1.59        | 1.46     |
| 30  | 7     | 301 | CHL  | C1D-C2D | 6.17  | 1.46        | 1.39     |
| 30  | 4     | 302 | CHL  | C1D-C2D | 6.17  | 1.46        | 1.39     |
| 32  | 8     | 402 | 8CT  | C28-C26 | 6.16  | 1.59        | 1.46     |
| 32  | M     | 102 | 8CT  | C15-C16 | 6.16  | 1.59        | 1.46     |
| 30  | 8     | 302 | CHL  | C1D-C2D | 6.16  | 1.46        | 1.39     |
| 30  | 0     | 301 | CHL  | C1D-C2D | 6.16  | 1.46        | 1.39     |
| 32  | L     | 209 | 8CT  | C28-C26 | 6.16  | 1.59        | 1.46     |
| 32  | L     | 205 | 8CT  | C15-C16 | 6.15  | 1.59        | 1.46     |
| 30  | 8     | 301 | CHL  | C1D-C2D | 6.15  | 1.46        | 1.39     |
| 32  | J     | 104 | 8CT  | C28-C26 | 6.14  | 1.59        | 1.46     |
| 30  | 8     | 307 | CHL  | C1D-C2D | 6.14  | 1.46        | 1.39     |
| 32  | B     | 844 | 8CT  | C28-C26 | 6.14  | 1.59        | 1.46     |
| 32  | A     | 847 | 8CT  | C04-C03 | -6.13 | 1.45        | 1.53     |
| 30  | 1     | 313 | CHL  | C1D-C2D | 6.13  | 1.46        | 1.39     |
| 32  | F     | 302 | 8CT  | C28-C26 | 6.13  | 1.59        | 1.46     |
| 32  | 9     | 401 | 8CT  | C04-C03 | -6.12 | 1.45        | 1.53     |
| 30  | 4     | 319 | CHL  | C1D-C2D | 6.12  | 1.46        | 1.39     |
| 30  | 6     | 305 | CHL  | C1D-C2D | 6.11  | 1.46        | 1.39     |
| 30  | 4     | 313 | CHL  | C1D-C2D | 6.11  | 1.46        | 1.39     |
| 32  | O     | 205 | 8CT  | C28-C26 | 6.11  | 1.59        | 1.46     |
| 32  | 3     | 402 | 8CT  | C28-C26 | 6.11  | 1.59        | 1.46     |
| 30  | 9     | 305 | CHL  | C1D-C2D | 6.11  | 1.46        | 1.39     |
| 32  | L     | 206 | 8CT  | C28-C26 | 6.10  | 1.59        | 1.46     |
| 30  | 1     | 302 | CHL  | C1D-C2D | 6.10  | 1.46        | 1.39     |
| 32  | K     | 107 | 8CT  | C28-C26 | 6.10  | 1.59        | 1.46     |
| 30  | 2     | 302 | CHL  | C1D-C2D | 6.09  | 1.46        | 1.39     |
| 30  | 4     | 305 | CHL  | C1D-C2D | 6.09  | 1.46        | 1.39     |
| 32  | B     | 851 | 8CT  | C15-C16 | 6.08  | 1.59        | 1.46     |
| 32  | B     | 845 | 8CT  | C04-C03 | -6.07 | 1.46        | 1.53     |
| 32  | 3     | 403 | 8CT  | C28-C26 | 6.07  | 1.59        | 1.46     |
| 30  | 2     | 308 | CHL  | C1D-C2D | 6.07  | 1.46        | 1.39     |
| 32  | I     | 101 | 8CT  | C04-C03 | -6.07 | 1.46        | 1.53     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 30  | 3     | 305 | CHL  | C1D-C2D | 6.06  | 1.46        | 1.39     |
| 32  | J     | 101 | 8CT  | C15-C16 | 6.06  | 1.58        | 1.46     |
| 30  | 6     | 306 | CHL  | C1D-C2D | 6.06  | 1.46        | 1.39     |
| 30  | 7     | 302 | CHL  | C1D-C2D | 6.05  | 1.46        | 1.39     |
| 32  | B     | 851 | 8CT  | C04-C03 | -6.05 | 1.46        | 1.53     |
| 32  | J     | 101 | 8CT  | C28-C26 | 6.04  | 1.58        | 1.46     |
| 32  | 7     | 405 | 8CT  | C15-C16 | 6.04  | 1.58        | 1.46     |
| 32  | A     | 849 | 8CT  | C04-C03 | -6.04 | 1.46        | 1.53     |
| 32  | M     | 102 | 8CT  | C28-C26 | 6.04  | 1.58        | 1.46     |
| 30  | 7     | 307 | CHL  | C1D-C2D | 6.04  | 1.46        | 1.39     |
| 32  | 3     | 403 | 8CT  | C04-C03 | -6.04 | 1.46        | 1.53     |
| 32  | 0     | 401 | 8CT  | C04-C03 | -6.04 | 1.46        | 1.53     |
| 32  | 6     | 402 | 8CT  | C28-C26 | 6.04  | 1.58        | 1.46     |
| 30  | 6     | 308 | CHL  | C1D-C2D | 6.03  | 1.46        | 1.39     |
| 32  | B     | 843 | 8CT  | C23-C21 | 6.03  | 1.58        | 1.46     |
| 32  | B     | 851 | 8CT  | C28-C26 | 6.02  | 1.58        | 1.46     |
| 30  | 3     | 307 | CHL  | C1D-C2D | 6.02  | 1.46        | 1.39     |
| 30  | 4     | 307 | CHL  | C1D-C2D | 6.02  | 1.46        | 1.39     |
| 32  | L     | 205 | 8CT  | C28-C26 | 6.01  | 1.58        | 1.46     |
| 32  | B     | 846 | 8CT  | C04-C03 | -6.01 | 1.46        | 1.53     |
| 32  | 7     | 402 | 8CT  | C15-C16 | 6.00  | 1.58        | 1.46     |
| 32  | B     | 848 | 8CT  | C28-C26 | 5.99  | 1.58        | 1.46     |
| 32  | A     | 849 | 8CT  | C15-C16 | 5.99  | 1.58        | 1.46     |
| 32  | M     | 102 | 8CT  | C04-C03 | -5.98 | 1.46        | 1.53     |
| 32  | A     | 848 | 8CT  | C04-C03 | -5.98 | 1.46        | 1.53     |
| 30  | 2     | 313 | CHL  | C1D-C2D | 5.98  | 1.46        | 1.39     |
| 32  | B     | 804 | 8CT  | C28-C26 | 5.98  | 1.58        | 1.46     |
| 30  | 6     | 307 | CHL  | C1D-C2D | 5.97  | 1.46        | 1.39     |
| 32  | A     | 850 | 8CT  | C15-C16 | 5.97  | 1.58        | 1.46     |
| 32  | A     | 848 | 8CT  | C15-C16 | 5.96  | 1.58        | 1.46     |
| 32  | B     | 846 | 8CT  | C23-C21 | 5.96  | 1.58        | 1.46     |
| 32  | 2     | 402 | 8CT  | C23-C21 | 5.96  | 1.58        | 1.46     |
| 32  | 7     | 405 | 8CT  | C28-C26 | 5.94  | 1.58        | 1.46     |
| 30  | 2     | 307 | CHL  | C1D-C2D | 5.94  | 1.46        | 1.39     |
| 32  | B     | 843 | 8CT  | C04-C03 | -5.93 | 1.46        | 1.53     |
| 32  | I     | 101 | 8CT  | C28-C26 | 5.92  | 1.58        | 1.46     |
| 32  | 4     | 402 | 8CT  | C23-C21 | 5.91  | 1.58        | 1.46     |
| 32  | 7     | 402 | 8CT  | C28-C26 | 5.91  | 1.58        | 1.46     |
| 32  | B     | 804 | 8CT  | C04-C03 | -5.91 | 1.46        | 1.53     |
| 32  | 4     | 402 | 8CT  | C04-C03 | -5.91 | 1.46        | 1.53     |
| 32  | 4     | 402 | 8CT  | C34-C33 | 5.90  | 1.65        | 1.52     |
| 32  | B     | 847 | 8CT  | C28-C26 | 5.90  | 1.58        | 1.46     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 32  | A     | 846 | 8CT  | C04-C03 | -5.89 | 1.46        | 1.53     |
| 32  | O     | 205 | 8CT  | C04-C03 | -5.89 | 1.46        | 1.53     |
| 32  | A     | 846 | 8CT  | C28-C26 | 5.88  | 1.58        | 1.46     |
| 32  | L     | 206 | 8CT  | C04-C03 | -5.88 | 1.46        | 1.53     |
| 32  | 0     | 401 | 8CT  | C23-C21 | 5.88  | 1.58        | 1.46     |
| 32  | A     | 854 | 8CT  | C04-C03 | -5.87 | 1.46        | 1.53     |
| 32  | A     | 847 | 8CT  | C28-C26 | 5.87  | 1.58        | 1.46     |
| 32  | 2     | 402 | 8CT  | C04-C03 | -5.87 | 1.46        | 1.53     |
| 32  | L     | 205 | 8CT  | C04-C03 | -5.87 | 1.46        | 1.53     |
| 32  | 7     | 404 | 8CT  | C28-C26 | 5.86  | 1.58        | 1.46     |
| 32  | A     | 848 | 8CT  | C28-C26 | 5.86  | 1.58        | 1.46     |
| 32  | A     | 849 | 8CT  | C28-C26 | 5.85  | 1.58        | 1.46     |
| 32  | 0     | 401 | 8CT  | C34-C33 | 5.83  | 1.65        | 1.52     |
| 32  | 6     | 402 | 8CT  | C23-C21 | 5.83  | 1.58        | 1.46     |
| 32  | J     | 104 | 8CT  | C23-C21 | 5.82  | 1.58        | 1.46     |
| 30  | 6     | 302 | CHL  | C1D-C2D | 5.82  | 1.46        | 1.39     |
| 32  | 1     | 402 | 8CT  | C04-C03 | -5.82 | 1.46        | 1.53     |
| 32  | 6     | 402 | 8CT  | C04-C03 | -5.81 | 1.46        | 1.53     |
| 32  | B     | 845 | 8CT  | C28-C26 | 5.80  | 1.58        | 1.46     |
| 32  | 2     | 402 | 8CT  | C34-C33 | 5.80  | 1.65        | 1.52     |
| 32  | G     | 104 | 8CT  | C23-C21 | 5.80  | 1.58        | 1.46     |
| 32  | 8     | 402 | 8CT  | C04-C03 | -5.80 | 1.46        | 1.53     |
| 32  | 8     | 406 | 8CT  | C23-C21 | 5.79  | 1.58        | 1.46     |
| 32  | 7     | 405 | 8CT  | C04-C03 | -5.79 | 1.46        | 1.53     |
| 32  | B     | 845 | 8CT  | C23-C21 | 5.78  | 1.58        | 1.46     |
| 32  | J     | 101 | 8CT  | C34-C33 | 5.78  | 1.65        | 1.52     |
| 32  | 3     | 402 | 8CT  | C04-C03 | -5.78 | 1.46        | 1.53     |
| 32  | 9     | 401 | 8CT  | C23-C21 | 5.77  | 1.58        | 1.46     |
| 39  | A     | 857 | CL0  | C3B-C4B | 5.77  | 1.47        | 1.41     |
| 32  | A     | 854 | 8CT  | C34-C33 | 5.77  | 1.65        | 1.52     |
| 32  | I     | 101 | 8CT  | C34-C33 | 5.77  | 1.65        | 1.52     |
| 32  | B     | 847 | 8CT  | C04-C03 | -5.77 | 1.46        | 1.53     |
| 32  | B     | 844 | 8CT  | C34-C33 | 5.76  | 1.65        | 1.52     |
| 32  | 3     | 402 | 8CT  | C34-C33 | 5.76  | 1.65        | 1.52     |
| 32  | L     | 206 | 8CT  | C23-C21 | 5.76  | 1.58        | 1.46     |
| 32  | 3     | 402 | 8CT  | C23-C21 | 5.75  | 1.58        | 1.46     |
| 32  | A     | 854 | 8CT  | C23-C21 | 5.73  | 1.58        | 1.46     |
| 32  | 9     | 401 | 8CT  | C34-C33 | 5.72  | 1.65        | 1.52     |
| 32  | 1     | 402 | 8CT  | C23-C21 | 5.72  | 1.58        | 1.46     |
| 32  | B     | 847 | 8CT  | C23-C21 | 5.72  | 1.58        | 1.46     |
| 32  | L     | 209 | 8CT  | C04-C03 | -5.71 | 1.46        | 1.53     |
| 32  | B     | 848 | 8CT  | C23-C21 | 5.71  | 1.58        | 1.46     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 32  | 7     | 404 | 8CT  | C04-C03 | -5.71 | 1.46        | 1.53     |
| 32  | 7     | 402 | 8CT  | C34-C33 | 5.70  | 1.65        | 1.52     |
| 32  | F     | 302 | 8CT  | C04-C03 | -5.70 | 1.46        | 1.53     |
| 32  | B     | 844 | 8CT  | C04-C03 | -5.68 | 1.46        | 1.53     |
| 32  | A     | 849 | 8CT  | C34-C33 | 5.67  | 1.65        | 1.52     |
| 32  | K     | 107 | 8CT  | C04-C03 | -5.65 | 1.46        | 1.53     |
| 32  | 8     | 402 | 8CT  | C23-C21 | 5.65  | 1.58        | 1.46     |
| 32  | J     | 104 | 8CT  | C34-C33 | 5.65  | 1.65        | 1.52     |
| 32  | A     | 850 | 8CT  | C28-C26 | 5.65  | 1.58        | 1.46     |
| 32  | F     | 302 | 8CT  | C23-C21 | 5.64  | 1.58        | 1.46     |
| 32  | O     | 205 | 8CT  | C23-C21 | 5.64  | 1.58        | 1.46     |
| 32  | O     | 205 | 8CT  | C34-C33 | 5.63  | 1.65        | 1.52     |
| 32  | 8     | 402 | 8CT  | C34-C33 | 5.63  | 1.65        | 1.52     |
| 32  | 7     | 405 | 8CT  | C23-C21 | 5.63  | 1.58        | 1.46     |
| 32  | J     | 101 | 8CT  | C23-C21 | 5.62  | 1.58        | 1.46     |
| 32  | L     | 209 | 8CT  | C23-C21 | 5.61  | 1.58        | 1.46     |
| 32  | L     | 206 | 8CT  | C34-C33 | 5.61  | 1.65        | 1.52     |
| 32  | K     | 107 | 8CT  | C23-C21 | 5.60  | 1.57        | 1.46     |
| 32  | B     | 851 | 8CT  | C23-C21 | 5.60  | 1.57        | 1.46     |
| 32  | K     | 107 | 8CT  | C34-C33 | 5.58  | 1.65        | 1.52     |
| 32  | G     | 104 | 8CT  | C34-C33 | 5.58  | 1.65        | 1.52     |
| 32  | G     | 104 | 8CT  | C04-C03 | -5.58 | 1.46        | 1.53     |
| 32  | 7     | 404 | 8CT  | C23-C21 | 5.58  | 1.57        | 1.46     |
| 32  | M     | 102 | 8CT  | C34-C33 | 5.57  | 1.65        | 1.52     |
| 32  | 8     | 406 | 8CT  | C34-C33 | 5.57  | 1.65        | 1.52     |
| 32  | F     | 302 | 8CT  | C34-C33 | 5.57  | 1.65        | 1.52     |
| 32  | I     | 101 | 8CT  | C23-C21 | 5.57  | 1.57        | 1.46     |
| 32  | L     | 205 | 8CT  | C23-C21 | 5.56  | 1.57        | 1.46     |
| 32  | 3     | 403 | 8CT  | C23-C21 | 5.56  | 1.57        | 1.46     |
| 32  | M     | 102 | 8CT  | C23-C21 | 5.55  | 1.57        | 1.46     |
| 32  | B     | 846 | 8CT  | C34-C33 | 5.54  | 1.65        | 1.52     |
| 32  | 6     | 402 | 8CT  | C34-C33 | 5.54  | 1.65        | 1.52     |
| 32  | A     | 846 | 8CT  | C34-C33 | 5.54  | 1.65        | 1.52     |
| 32  | 7     | 404 | 8CT  | C34-C33 | 5.53  | 1.65        | 1.52     |
| 32  | A     | 847 | 8CT  | C34-C33 | 5.53  | 1.65        | 1.52     |
| 32  | B     | 845 | 8CT  | C34-C33 | 5.53  | 1.65        | 1.52     |
| 32  | B     | 851 | 8CT  | C34-C33 | 5.52  | 1.65        | 1.52     |
| 32  | 1     | 402 | 8CT  | C34-C33 | 5.52  | 1.65        | 1.52     |
| 32  | B     | 848 | 8CT  | C34-C33 | 5.52  | 1.65        | 1.52     |
| 32  | 7     | 402 | 8CT  | C23-C21 | 5.51  | 1.57        | 1.46     |
| 32  | L     | 205 | 8CT  | C34-C33 | 5.50  | 1.65        | 1.52     |
| 30  | h     | 614 | CHL  | C3B-C2B | 5.49  | 1.47        | 1.40     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 32  | 8     | 406 | 8CT  | C04-C03 | -5.49 | 1.46        | 1.53     |
| 32  | B     | 847 | 8CT  | C34-C33 | 5.47  | 1.64        | 1.52     |
| 30  | g     | 614 | CHL  | C3B-C2B | 5.46  | 1.47        | 1.40     |
| 30  | d     | 614 | CHL  | CHC-C4B | 5.46  | 1.48        | 1.39     |
| 32  | J     | 104 | 8CT  | C04-C03 | -5.46 | 1.46        | 1.53     |
| 32  | A     | 846 | 8CT  | C23-C21 | 5.46  | 1.57        | 1.46     |
| 32  | 3     | 403 | 8CT  | C34-C33 | 5.46  | 1.64        | 1.52     |
| 32  | B     | 804 | 8CT  | C34-C33 | 5.46  | 1.64        | 1.52     |
| 30  | h     | 602 | CHL  | CHC-C4B | 5.45  | 1.48        | 1.39     |
| 30  | h     | 614 | CHL  | CHC-C4B | 5.45  | 1.48        | 1.39     |
| 32  | B     | 804 | 8CT  | C23-C21 | 5.45  | 1.57        | 1.46     |
| 30  | g     | 605 | CHL  | CHC-C4B | 5.45  | 1.48        | 1.39     |
| 32  | B     | 843 | 8CT  | C34-C33 | 5.45  | 1.64        | 1.52     |
| 30  | d     | 605 | CHL  | CHC-C4B | 5.45  | 1.48        | 1.39     |
| 30  | 9     | 305 | CHL  | C3A-C2A | -5.44 | 1.50        | 1.54     |
| 30  | h     | 605 | CHL  | C3B-C2B | 5.44  | 1.47        | 1.40     |
| 32  | 7     | 405 | 8CT  | C34-C33 | 5.43  | 1.64        | 1.52     |
| 30  | h     | 607 | CHL  | CHC-C4B | 5.43  | 1.48        | 1.39     |
| 32  | L     | 209 | 8CT  | C34-C33 | 5.43  | 1.64        | 1.52     |
| 30  | 7     | 302 | CHL  | C3A-C2A | -5.41 | 1.50        | 1.54     |
| 30  | d     | 605 | CHL  | C3B-C2B | 5.41  | 1.47        | 1.40     |
| 30  | d     | 614 | CHL  | C3B-C2B | 5.41  | 1.47        | 1.40     |
| 30  | g     | 614 | CHL  | CHC-C4B | 5.40  | 1.48        | 1.39     |
| 30  | i     | 605 | CHL  | C3B-C2B | 5.40  | 1.47        | 1.40     |
| 30  | i     | 607 | CHL  | CHC-C4B | 5.39  | 1.48        | 1.39     |
| 30  | g     | 605 | CHL  | C3B-C2B | 5.39  | 1.47        | 1.40     |
| 30  | 1     | 305 | CHL  | C3A-C2A | -5.39 | 1.50        | 1.54     |
| 30  | g     | 602 | CHL  | CHC-C4B | 5.38  | 1.48        | 1.39     |
| 30  | a     | 605 | CHL  | CHC-C4B | 5.38  | 1.48        | 1.39     |
| 30  | g     | 601 | CHL  | CHC-C4B | 5.38  | 1.48        | 1.39     |
| 30  | e     | 614 | CHL  | CHC-C4B | 5.37  | 1.48        | 1.39     |
| 30  | h     | 605 | CHL  | CHC-C4B | 5.37  | 1.48        | 1.39     |
| 30  | a     | 614 | CHL  | CHC-C4B | 5.37  | 1.48        | 1.39     |
| 32  | A     | 847 | 8CT  | C23-C21 | 5.37  | 1.57        | 1.46     |
| 30  | i     | 605 | CHL  | CHC-C4B | 5.37  | 1.48        | 1.39     |
| 32  | A     | 849 | 8CT  | C23-C21 | 5.36  | 1.57        | 1.46     |
| 30  | a     | 614 | CHL  | C3B-C2B | 5.36  | 1.47        | 1.40     |
| 30  | 2     | 319 | CHL  | C3A-C2A | -5.36 | 1.50        | 1.54     |
| 30  | c     | 605 | CHL  | C3B-C2B | 5.36  | 1.47        | 1.40     |
| 30  | d     | 601 | CHL  | CHC-C4B | 5.35  | 1.48        | 1.39     |
| 32  | B     | 848 | 8CT  | C04-C03 | -5.35 | 1.46        | 1.53     |
| 30  | g     | 609 | CHL  | CHC-C4B | 5.35  | 1.48        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 30  | i     | 614 | CHL  | CHC-C4B | 5.35  | 1.48        | 1.39     |
| 32  | A     | 848 | 8CT  | C23-C21 | 5.35  | 1.57        | 1.46     |
| 30  | i     | 601 | CHL  | CHC-C4B | 5.34  | 1.48        | 1.39     |
| 30  | a     | 605 | CHL  | C3B-C2B | 5.33  | 1.47        | 1.40     |
| 32  | A     | 850 | 8CT  | C34-C33 | 5.33  | 1.64        | 1.52     |
| 30  | i     | 601 | CHL  | C3B-C2B | 5.33  | 1.47        | 1.40     |
| 30  | g     | 608 | CHL  | CHC-C4B | 5.33  | 1.48        | 1.39     |
| 30  | 4     | 319 | CHL  | C3A-C2A | -5.33 | 1.50        | 1.54     |
| 32  | A     | 848 | 8CT  | C34-C33 | 5.33  | 1.64        | 1.52     |
| 30  | d     | 605 | CHL  | CHD-C1D | 5.33  | 1.48        | 1.39     |
| 30  | g     | 614 | CHL  | CHD-C1D | 5.33  | 1.48        | 1.39     |
| 30  | g     | 607 | CHL  | C3B-C2B | 5.32  | 1.47        | 1.40     |
| 30  | i     | 614 | CHL  | C3B-C2B | 5.32  | 1.47        | 1.40     |
| 30  | 3     | 302 | CHL  | C3A-C2A | -5.31 | 1.50        | 1.54     |
| 30  | h     | 607 | CHL  | C3D-C2D | 5.31  | 1.48        | 1.39     |
| 30  | h     | 605 | CHL  | C3D-C2D | 5.31  | 1.48        | 1.39     |
| 30  | d     | 607 | CHL  | CHC-C4B | 5.31  | 1.48        | 1.39     |
| 30  | g     | 609 | CHL  | C3D-C2D | 5.31  | 1.48        | 1.39     |
| 30  | 1     | 302 | CHL  | CHB-C4A | -5.31 | 1.32        | 1.38     |
| 30  | g     | 606 | CHL  | CHC-C4B | 5.30  | 1.48        | 1.39     |
| 30  | i     | 609 | CHL  | C3B-C2B | 5.30  | 1.47        | 1.40     |
| 30  | g     | 605 | CHL  | C3D-C2D | 5.30  | 1.48        | 1.39     |
| 30  | g     | 601 | CHL  | C3B-C2B | 5.30  | 1.47        | 1.40     |
| 30  | 3     | 307 | CHL  | C3A-C2A | -5.30 | 1.50        | 1.54     |
| 30  | d     | 607 | CHL  | C3B-C2B | 5.29  | 1.47        | 1.40     |
| 30  | a     | 606 | CHL  | CHC-C4B | 5.29  | 1.48        | 1.39     |
| 30  | a     | 607 | CHL  | CHC-C4B | 5.29  | 1.48        | 1.39     |
| 30  | h     | 605 | CHL  | CHD-C1D | 5.29  | 1.48        | 1.39     |
| 30  | 5     | 301 | CHL  | CHC-C4B | 5.29  | 1.48        | 1.39     |
| 30  | g     | 605 | CHL  | CHD-C1D | 5.29  | 1.48        | 1.39     |
| 30  | f     | 605 | CHL  | C3B-C2B | 5.29  | 1.47        | 1.40     |
| 30  | 2     | 307 | CHL  | C3A-C2A | -5.28 | 1.50        | 1.54     |
| 30  | h     | 607 | CHL  | C3B-C2B | 5.28  | 1.47        | 1.40     |
| 30  | a     | 605 | CHL  | C3D-C2D | 5.28  | 1.48        | 1.39     |
| 30  | i     | 605 | CHL  | CHD-C1D | 5.28  | 1.48        | 1.39     |
| 30  | d     | 601 | CHL  | C3B-C2B | 5.28  | 1.47        | 1.40     |
| 30  | 5     | 302 | CHL  | C3A-C2A | -5.27 | 1.50        | 1.54     |
| 30  | d     | 605 | CHL  | C3D-C2D | 5.27  | 1.48        | 1.39     |
| 30  | e     | 614 | CHL  | C3B-C2B | 5.27  | 1.47        | 1.40     |
| 30  | e     | 605 | CHL  | CHC-C4B | 5.27  | 1.48        | 1.39     |
| 32  | A     | 850 | 8CT  | C23-C21 | 5.27  | 1.57        | 1.46     |
| 30  | i     | 605 | CHL  | C3D-C2D | 5.26  | 1.48        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 30  | g     | 609 | CHL  | C3B-C2B | 5.26  | 1.47        | 1.40     |
| 30  | g     | 608 | CHL  | C3B-C2B | 5.25  | 1.47        | 1.40     |
| 30  | a     | 605 | CHL  | CHD-C1D | 5.25  | 1.48        | 1.39     |
| 30  | a     | 614 | CHL  | C3D-C2D | 5.25  | 1.48        | 1.39     |
| 32  | K     | 107 | 8CT  | C05-C04 | 5.25  | 1.66        | 1.54     |
| 30  | h     | 602 | CHL  | C3D-C2D | 5.25  | 1.48        | 1.39     |
| 30  | f     | 605 | CHL  | CHC-C4B | 5.25  | 1.48        | 1.39     |
| 30  | g     | 607 | CHL  | CHC-C4B | 5.25  | 1.48        | 1.39     |
| 30  | g     | 601 | CHL  | CHD-C1D | 5.24  | 1.48        | 1.39     |
| 30  | i     | 609 | CHL  | CHC-C4B | 5.24  | 1.48        | 1.39     |
| 30  | c     | 605 | CHL  | CHC-C4B | 5.24  | 1.48        | 1.39     |
| 30  | a     | 614 | CHL  | CHD-C1D | 5.24  | 1.48        | 1.39     |
| 30  | g     | 614 | CHL  | C3D-C2D | 5.24  | 1.48        | 1.39     |
| 30  | g     | 607 | CHL  | C3D-C2D | 5.24  | 1.48        | 1.39     |
| 30  | a     | 609 | CHL  | C3B-C2B | 5.24  | 1.47        | 1.40     |
| 30  | 7     | 305 | CHL  | C3A-C2A | -5.24 | 1.50        | 1.54     |
| 30  | b     | 614 | CHL  | CHC-C4B | 5.24  | 1.48        | 1.39     |
| 30  | i     | 609 | CHL  | C3D-C2D | 5.24  | 1.48        | 1.39     |
| 30  | 4     | 305 | CHL  | C3A-C2A | -5.23 | 1.50        | 1.54     |
| 30  | 8     | 302 | CHL  | CHB-C4A | -5.23 | 1.32        | 1.38     |
| 30  | i     | 601 | CHL  | C3D-C2D | 5.23  | 1.48        | 1.39     |
| 30  | i     | 606 | CHL  | CHC-C4B | 5.23  | 1.48        | 1.39     |
| 30  | c     | 605 | CHL  | CHD-C1D | 5.23  | 1.48        | 1.39     |
| 30  | f     | 605 | CHL  | CHD-C1D | 5.23  | 1.48        | 1.39     |
| 30  | f     | 607 | CHL  | C3B-C2B | 5.22  | 1.47        | 1.40     |
| 30  | d     | 607 | CHL  | C3D-C2D | 5.22  | 1.48        | 1.39     |
| 30  | g     | 601 | CHL  | C3D-C2D | 5.22  | 1.48        | 1.39     |
| 30  | f     | 607 | CHL  | C3D-C2D | 5.22  | 1.48        | 1.39     |
| 30  | 5     | 306 | CHL  | CHC-C4B | 5.22  | 1.48        | 1.39     |
| 30  | 0     | 302 | CHL  | C3A-C2A | -5.21 | 1.50        | 1.54     |
| 30  | 5     | 313 | CHL  | C3D-C2D | 5.21  | 1.48        | 1.39     |
| 30  | 8     | 302 | CHL  | C3A-C2A | -5.21 | 1.50        | 1.54     |
| 30  | h     | 601 | CHL  | CHC-C4B | 5.21  | 1.48        | 1.39     |
| 30  | h     | 601 | CHL  | C3B-C2B | 5.20  | 1.47        | 1.40     |
| 30  | 0     | 302 | CHL  | CHB-C4A | -5.20 | 1.32        | 1.38     |
| 30  | 3     | 302 | CHL  | CHB-C4A | -5.20 | 1.32        | 1.38     |
| 30  | i     | 609 | CHL  | CHD-C1D | 5.20  | 1.48        | 1.39     |
| 30  | 2     | 302 | CHL  | C3A-C2A | -5.20 | 1.50        | 1.54     |
| 30  | d     | 614 | CHL  | CHD-C1D | 5.20  | 1.48        | 1.39     |
| 30  | i     | 614 | CHL  | C3D-C2D | 5.20  | 1.48        | 1.39     |
| 30  | g     | 602 | CHL  | C3D-C2D | 5.20  | 1.48        | 1.39     |
| 30  | c     | 605 | CHL  | C3D-C2D | 5.19  | 1.48        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 32  | L     | 205 | 8CT  | C05-C04 | 5.19  | 1.66        | 1.54     |
| 30  | 5     | 313 | CHL  | CHC-C4B | 5.19  | 1.48        | 1.39     |
| 30  | 1     | 305 | CHL  | CHB-C4A | -5.19 | 1.32        | 1.38     |
| 30  | i     | 607 | CHL  | C3B-C2B | 5.19  | 1.47        | 1.40     |
| 30  | g     | 609 | CHL  | CHD-C1D | 5.19  | 1.48        | 1.39     |
| 30  | h     | 614 | CHL  | O2D-CGD | 5.19  | 1.46        | 1.33     |
| 30  | f     | 602 | CHL  | CHC-C4B | 5.19  | 1.48        | 1.39     |
| 32  | A     | 848 | 8CT  | C05-C04 | 5.19  | 1.66        | 1.54     |
| 30  | d     | 601 | CHL  | C3D-C2D | 5.19  | 1.48        | 1.39     |
| 30  | i     | 607 | CHL  | C3D-C2D | 5.19  | 1.48        | 1.39     |
| 30  | b     | 614 | CHL  | C3B-C2B | 5.19  | 1.47        | 1.40     |
| 30  | e     | 614 | CHL  | C3D-C2D | 5.19  | 1.48        | 1.39     |
| 30  | e     | 606 | CHL  | CHC-C4B | 5.19  | 1.48        | 1.39     |
| 30  | d     | 614 | CHL  | C3D-C2D | 5.19  | 1.48        | 1.39     |
| 30  | 5     | 307 | CHL  | CHC-C4B | 5.18  | 1.48        | 1.39     |
| 30  | h     | 614 | CHL  | CHD-C1D | 5.18  | 1.48        | 1.39     |
| 32  | 2     | 402 | 8CT  | C05-C04 | 5.18  | 1.66        | 1.54     |
| 30  | h     | 609 | CHL  | C3B-C2B | 5.18  | 1.47        | 1.40     |
| 30  | c     | 607 | CHL  | CHC-C4B | 5.18  | 1.48        | 1.39     |
| 30  | f     | 609 | CHL  | CHC-C4B | 5.18  | 1.48        | 1.39     |
| 30  | 9     | 305 | CHL  | CHB-C4A | -5.18 | 1.32        | 1.38     |
| 30  | a     | 609 | CHL  | CHD-C1D | 5.18  | 1.48        | 1.39     |
| 30  | b     | 614 | CHL  | C3D-C2D | 5.18  | 1.48        | 1.39     |
| 30  | 1     | 302 | CHL  | C3A-C2A | -5.17 | 1.50        | 1.54     |
| 32  | O     | 205 | 8CT  | C05-C04 | 5.17  | 1.65        | 1.54     |
| 30  | 2     | 305 | CHL  | C3A-C2A | -5.17 | 1.50        | 1.54     |
| 30  | e     | 614 | CHL  | O2D-CGD | 5.17  | 1.45        | 1.33     |
| 30  | g     | 607 | CHL  | CHD-C1D | 5.17  | 1.48        | 1.39     |
| 32  | L     | 209 | 8CT  | C05-C04 | 5.16  | 1.65        | 1.54     |
| 30  | b     | 601 | CHL  | CHC-C4B | 5.16  | 1.48        | 1.39     |
| 30  | g     | 606 | CHL  | C3B-C2B | 5.16  | 1.47        | 1.40     |
| 30  | c     | 614 | CHL  | CHC-C4B | 5.16  | 1.48        | 1.39     |
| 30  | b     | 606 | CHL  | CHC-C4B | 5.16  | 1.48        | 1.39     |
| 30  | 2     | 301 | CHL  | C3A-C2A | -5.16 | 1.50        | 1.54     |
| 30  | 4     | 306 | CHL  | C3A-C2A | -5.16 | 1.50        | 1.54     |
| 30  | i     | 614 | CHL  | CHD-C1D | 5.16  | 1.48        | 1.39     |
| 30  | g     | 605 | CHL  | O2D-CGD | 5.16  | 1.45        | 1.33     |
| 30  | h     | 606 | CHL  | O2D-CGD | 5.15  | 1.45        | 1.33     |
| 30  | 1     | 313 | CHL  | C3A-C2A | -5.15 | 1.50        | 1.54     |
| 30  | f     | 605 | CHL  | C3D-C2D | 5.15  | 1.48        | 1.39     |
| 30  | g     | 614 | CHL  | O2D-CGD | 5.15  | 1.45        | 1.33     |
| 30  | f     | 605 | CHL  | O2D-CGD | 5.15  | 1.45        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 30  | e     | 605 | CHL  | C3B-C2B | 5.15  | 1.47        | 1.40     |
| 30  | a     | 614 | CHL  | O2D-CGD | 5.15  | 1.45        | 1.33     |
| 30  | a     | 609 | CHL  | CHC-C4B | 5.15  | 1.48        | 1.39     |
| 30  | b     | 607 | CHL  | CHC-C4B | 5.15  | 1.48        | 1.39     |
| 30  | f     | 607 | CHL  | CHC-C4B | 5.15  | 1.48        | 1.39     |
| 30  | h     | 609 | CHL  | CHD-C1D | 5.15  | 1.48        | 1.39     |
| 30  | 5     | 313 | CHL  | C3B-C2B | 5.14  | 1.47        | 1.40     |
| 30  | 4     | 307 | CHL  | C3A-C2A | -5.14 | 1.50        | 1.54     |
| 30  | f     | 607 | CHL  | O2D-CGD | 5.14  | 1.45        | 1.33     |
| 30  | 7     | 307 | CHL  | CHC-C4B | 5.14  | 1.47        | 1.39     |
| 30  | g     | 605 | CHL  | OBD-CAD | 5.14  | 1.29        | 1.22     |
| 30  | e     | 601 | CHL  | O2D-CGD | 5.14  | 1.45        | 1.33     |
| 30  | c     | 607 | CHL  | C3B-C2B | 5.14  | 1.47        | 1.40     |
| 30  | f     | 609 | CHL  | C3B-C2B | 5.14  | 1.47        | 1.40     |
| 30  | 4     | 313 | CHL  | C3A-C2A | -5.14 | 1.50        | 1.54     |
| 30  | a     | 609 | CHL  | C3D-C2D | 5.14  | 1.48        | 1.39     |
| 30  | 5     | 306 | CHL  | C3D-C2D | 5.14  | 1.48        | 1.39     |
| 30  | c     | 609 | CHL  | CHD-C1D | 5.14  | 1.47        | 1.39     |
| 30  | 6     | 305 | CHL  | C3A-C2A | -5.14 | 1.50        | 1.54     |
| 30  | 7     | 307 | CHL  | CHB-C4A | -5.14 | 1.32        | 1.38     |
| 30  | c     | 607 | CHL  | C3D-C2D | 5.13  | 1.48        | 1.39     |
| 30  | a     | 607 | CHL  | C3B-C2B | 5.13  | 1.47        | 1.40     |
| 30  | h     | 601 | CHL  | C3D-C2D | 5.13  | 1.48        | 1.39     |
| 30  | d     | 606 | CHL  | CHC-C4B | 5.13  | 1.47        | 1.39     |
| 30  | 3     | 302 | CHL  | CHC-C4B | 5.13  | 1.47        | 1.39     |
| 30  | d     | 609 | CHL  | C3B-C2B | 5.13  | 1.47        | 1.40     |
| 30  | i     | 605 | CHL  | O2D-CGD | 5.13  | 1.45        | 1.33     |
| 30  | i     | 609 | CHL  | O2D-CGD | 5.13  | 1.45        | 1.33     |
| 30  | a     | 605 | CHL  | OBD-CAD | 5.13  | 1.29        | 1.22     |
| 30  | g     | 608 | CHL  | O2D-CGD | 5.13  | 1.45        | 1.33     |
| 30  | e     | 605 | CHL  | C3D-C2D | 5.13  | 1.48        | 1.39     |
| 30  | d     | 607 | CHL  | O2D-CGD | 5.13  | 1.45        | 1.33     |
| 30  | i     | 606 | CHL  | O2D-CGD | 5.13  | 1.45        | 1.33     |
| 32  | L     | 206 | 8CT  | C05-C04 | 5.13  | 1.65        | 1.54     |
| 30  | 8     | 307 | CHL  | C3A-C2A | -5.12 | 1.50        | 1.54     |
| 30  | e     | 607 | CHL  | CHC-C4B | 5.12  | 1.47        | 1.39     |
| 30  | 5     | 306 | CHL  | O2D-CGD | 5.12  | 1.45        | 1.33     |
| 30  | d     | 602 | CHL  | O2D-CGD | 5.12  | 1.45        | 1.33     |
| 30  | d     | 614 | CHL  | O2D-CGD | 5.12  | 1.45        | 1.33     |
| 30  | h     | 609 | CHL  | C3D-C2D | 5.12  | 1.48        | 1.39     |
| 30  | b     | 609 | CHL  | O2D-CGD | 5.12  | 1.45        | 1.33     |
| 30  | g     | 601 | CHL  | O2D-CGD | 5.12  | 1.45        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 30  | g     | 607 | CHL  | O2D-CGD | 5.12  | 1.45        | 1.33     |
| 30  | d     | 606 | CHL  | C3D-C2D | 5.12  | 1.48        | 1.39     |
| 30  | b     | 601 | CHL  | C3B-C2B | 5.12  | 1.47        | 1.40     |
| 30  | h     | 601 | CHL  | CHD-C1D | 5.12  | 1.47        | 1.39     |
| 30  | f     | 614 | CHL  | CHC-C4B | 5.12  | 1.47        | 1.39     |
| 30  | i     | 606 | CHL  | CHD-C1D | 5.12  | 1.47        | 1.39     |
| 30  | h     | 614 | CHL  | C3D-C2D | 5.12  | 1.48        | 1.39     |
| 30  | i     | 607 | CHL  | O2D-CGD | 5.12  | 1.45        | 1.33     |
| 30  | c     | 602 | CHL  | CHC-C4B | 5.12  | 1.47        | 1.39     |
| 30  | h     | 602 | CHL  | O2D-CGD | 5.12  | 1.45        | 1.33     |
| 30  | e     | 614 | CHL  | CHD-C1D | 5.11  | 1.47        | 1.39     |
| 30  | d     | 609 | CHL  | C3D-C2D | 5.11  | 1.48        | 1.39     |
| 30  | a     | 607 | CHL  | O2D-CGD | 5.11  | 1.45        | 1.33     |
| 30  | h     | 601 | CHL  | O2D-CGD | 5.11  | 1.45        | 1.33     |
| 30  | e     | 602 | CHL  | O2D-CGD | 5.11  | 1.45        | 1.33     |
| 30  | a     | 605 | CHL  | O2D-CGD | 5.11  | 1.45        | 1.33     |
| 30  | 3     | 305 | CHL  | C3A-C2A | -5.11 | 1.50        | 1.54     |
| 30  | a     | 602 | CHL  | O2D-CGD | 5.11  | 1.45        | 1.33     |
| 30  | a     | 607 | CHL  | CHD-C1D | 5.11  | 1.47        | 1.39     |
| 30  | d     | 609 | CHL  | CHD-C1D | 5.11  | 1.47        | 1.39     |
| 30  | g     | 608 | CHL  | CHD-C1D | 5.11  | 1.47        | 1.39     |
| 30  | 2     | 306 | CHL  | CHB-C4A | -5.11 | 1.32        | 1.38     |
| 30  | f     | 606 | CHL  | CHC-C4B | 5.11  | 1.47        | 1.39     |
| 30  | a     | 602 | CHL  | CHC-C4B | 5.10  | 1.47        | 1.39     |
| 30  | d     | 605 | CHL  | O2D-CGD | 5.10  | 1.45        | 1.33     |
| 32  | 1     | 402 | 8CT  | C05-C04 | 5.10  | 1.65        | 1.54     |
| 30  | 2     | 305 | CHL  | CHB-C4A | -5.10 | 1.32        | 1.38     |
| 32  | 9     | 401 | 8CT  | C05-C04 | 5.10  | 1.65        | 1.54     |
| 30  | 0     | 305 | CHL  | CHC-C4B | 5.10  | 1.47        | 1.39     |
| 30  | g     | 602 | CHL  | O2D-CGD | 5.10  | 1.45        | 1.33     |
| 30  | h     | 614 | CHL  | OBD-CAD | 5.10  | 1.29        | 1.22     |
| 30  | 5     | 307 | CHL  | C3B-C2B | 5.10  | 1.47        | 1.40     |
| 30  | h     | 609 | CHL  | CHC-C4B | 5.10  | 1.47        | 1.39     |
| 30  | 4     | 302 | CHL  | C3A-C2A | -5.10 | 1.50        | 1.54     |
| 30  | d     | 606 | CHL  | OBD-CAD | 5.10  | 1.29        | 1.22     |
| 30  | c     | 606 | CHL  | O2D-CGD | 5.10  | 1.45        | 1.33     |
| 30  | i     | 606 | CHL  | C3B-C2B | 5.10  | 1.47        | 1.40     |
| 30  | d     | 608 | CHL  | O2D-CGD | 5.10  | 1.45        | 1.33     |
| 30  | c     | 614 | CHL  | C3D-C2D | 5.10  | 1.48        | 1.39     |
| 30  | h     | 606 | CHL  | C3D-C2D | 5.10  | 1.48        | 1.39     |
| 30  | g     | 606 | CHL  | O2D-CGD | 5.09  | 1.45        | 1.33     |
| 30  | a     | 607 | CHL  | C3D-C2D | 5.09  | 1.48        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 30  | c     | 614 | CHL  | C3B-C2B | 5.09  | 1.47        | 1.40     |
| 30  | a     | 609 | CHL  | O2D-CGD | 5.09  | 1.45        | 1.33     |
| 30  | b     | 609 | CHL  | C3D-C2D | 5.09  | 1.48        | 1.39     |
| 30  | d     | 614 | CHL  | OBD-CAD | 5.09  | 1.29        | 1.22     |
| 30  | i     | 602 | CHL  | CHC-C4B | 5.09  | 1.47        | 1.39     |
| 30  | e     | 605 | CHL  | O2D-CGD | 5.09  | 1.45        | 1.33     |
| 30  | a     | 601 | CHL  | CHC-C4B | 5.09  | 1.47        | 1.39     |
| 30  | h     | 607 | CHL  | O2D-CGD | 5.09  | 1.45        | 1.33     |
| 30  | i     | 607 | CHL  | CHD-C1D | 5.09  | 1.47        | 1.39     |
| 30  | 4     | 302 | CHL  | CHB-C4A | -5.09 | 1.32        | 1.38     |
| 30  | 6     | 307 | CHL  | CHB-C4A | -5.09 | 1.32        | 1.38     |
| 30  | c     | 605 | CHL  | O2D-CGD | 5.09  | 1.45        | 1.33     |
| 30  | d     | 606 | CHL  | O2D-CGD | 5.09  | 1.45        | 1.33     |
| 30  | 8     | 302 | CHL  | CHC-C4B | 5.08  | 1.47        | 1.39     |
| 32  | 7     | 405 | 8CT  | C05-C04 | 5.08  | 1.65        | 1.54     |
| 30  | d     | 601 | CHL  | O2D-CGD | 5.08  | 1.45        | 1.33     |
| 30  | 5     | 313 | CHL  | CHD-C1D | 5.08  | 1.47        | 1.39     |
| 30  | b     | 602 | CHL  | CHC-C4B | 5.08  | 1.47        | 1.39     |
| 30  | h     | 607 | CHL  | CHD-C1D | 5.08  | 1.47        | 1.39     |
| 30  | h     | 605 | CHL  | O2D-CGD | 5.08  | 1.45        | 1.33     |
| 30  | i     | 601 | CHL  | O2D-CGD | 5.08  | 1.45        | 1.33     |
| 30  | d     | 607 | CHL  | CHD-C1D | 5.08  | 1.47        | 1.39     |
| 30  | h     | 608 | CHL  | C3B-C2B | 5.08  | 1.47        | 1.40     |
| 30  | 7     | 313 | CHL  | CHC-C4B | 5.08  | 1.47        | 1.39     |
| 30  | g     | 608 | CHL  | C3D-C2D | 5.08  | 1.48        | 1.39     |
| 30  | e     | 602 | CHL  | CHC-C4B | 5.08  | 1.47        | 1.39     |
| 30  | 7     | 302 | CHL  | CHB-C4A | -5.08 | 1.32        | 1.38     |
| 30  | i     | 614 | CHL  | O2D-CGD | 5.08  | 1.45        | 1.33     |
| 30  | i     | 601 | CHL  | CHD-C1D | 5.08  | 1.47        | 1.39     |
| 30  | d     | 609 | CHL  | O2D-CGD | 5.08  | 1.45        | 1.33     |
| 30  | i     | 608 | CHL  | O2D-CGD | 5.08  | 1.45        | 1.33     |
| 30  | i     | 602 | CHL  | O2D-CGD | 5.07  | 1.45        | 1.33     |
| 30  | 5     | 305 | CHL  | O2D-CGD | 5.07  | 1.45        | 1.33     |
| 30  | e     | 602 | CHL  | CHB-C4A | -5.07 | 1.32        | 1.38     |
| 30  | 1     | 302 | CHL  | CHC-C4B | 5.07  | 1.47        | 1.39     |
| 30  | d     | 601 | CHL  | CHD-C1D | 5.07  | 1.47        | 1.39     |
| 30  | b     | 601 | CHL  | O2D-CGD | 5.07  | 1.45        | 1.33     |
| 30  | f     | 609 | CHL  | C3D-C2D | 5.07  | 1.48        | 1.39     |
| 30  | i     | 606 | CHL  | C3D-C2D | 5.07  | 1.48        | 1.39     |
| 30  | c     | 605 | CHL  | OBD-CAD | 5.06  | 1.28        | 1.22     |
| 30  | 8     | 315 | CHL  | CHC-C4B | 5.06  | 1.47        | 1.39     |
| 30  | 8     | 315 | CHL  | C3B-C2B | 5.06  | 1.47        | 1.40     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 30  | b     | 606 | CHL  | O2D-CGD | 5.06  | 1.45        | 1.33     |
| 30  | h     | 602 | CHL  | C3B-C2B | 5.06  | 1.47        | 1.40     |
| 30  | h     | 608 | CHL  | O2D-CGD | 5.06  | 1.45        | 1.33     |
| 30  | d     | 608 | CHL  | C3B-C2B | 5.06  | 1.47        | 1.40     |
| 30  | h     | 605 | CHL  | CHB-C1B | 5.06  | 1.47        | 1.39     |
| 30  | 0     | 305 | CHL  | O2D-CGD | 5.06  | 1.45        | 1.33     |
| 30  | a     | 608 | CHL  | CHC-C4B | 5.06  | 1.47        | 1.39     |
| 30  | a     | 601 | CHL  | C3B-C2B | 5.06  | 1.47        | 1.40     |
| 30  | h     | 609 | CHL  | O2D-CGD | 5.06  | 1.45        | 1.33     |
| 30  | f     | 609 | CHL  | O2D-CGD | 5.06  | 1.45        | 1.33     |
| 32  | J     | 101 | 8CT  | C05-C04 | 5.06  | 1.65        | 1.54     |
| 30  | g     | 614 | CHL  | OBD-CAD | 5.06  | 1.28        | 1.22     |
| 30  | 8     | 301 | CHL  | CHC-C4B | 5.06  | 1.47        | 1.39     |
| 30  | d     | 609 | CHL  | CHC-C4B | 5.06  | 1.47        | 1.39     |
| 30  | 6     | 306 | CHL  | C3A-C2A | -5.05 | 1.50        | 1.54     |
| 33  | d     | 520 | 0UR  | O44-C45 | 5.05  | 1.45        | 1.34     |
| 30  | a     | 606 | CHL  | C3D-C2D | 5.05  | 1.48        | 1.39     |
| 30  | f     | 606 | CHL  | O2D-CGD | 5.05  | 1.45        | 1.33     |
| 30  | a     | 606 | CHL  | O2D-CGD | 5.05  | 1.45        | 1.33     |
| 30  | c     | 607 | CHL  | O2D-CGD | 5.05  | 1.45        | 1.33     |
| 32  | 0     | 401 | 8CT  | C05-C04 | 5.05  | 1.65        | 1.54     |
| 30  | c     | 608 | CHL  | O2D-CGD | 5.05  | 1.45        | 1.33     |
| 30  | f     | 607 | CHL  | CHD-C1D | 5.05  | 1.47        | 1.39     |
| 30  | d     | 605 | CHL  | OBD-CAD | 5.05  | 1.28        | 1.22     |
| 30  | 3     | 305 | CHL  | CHB-C4A | -5.05 | 1.32        | 1.38     |
| 30  | 4     | 306 | CHL  | CHB-C4A | -5.05 | 1.32        | 1.38     |
| 30  | e     | 607 | CHL  | O2D-CGD | 5.05  | 1.45        | 1.33     |
| 30  | f     | 602 | CHL  | O2D-CGD | 5.05  | 1.45        | 1.33     |
| 30  | e     | 608 | CHL  | O2D-CGD | 5.04  | 1.45        | 1.33     |
| 30  | 5     | 306 | CHL  | C3B-C2B | 5.04  | 1.47        | 1.40     |
| 30  | h     | 614 | CHL  | CHB-C1B | 5.04  | 1.47        | 1.39     |
| 30  | f     | 602 | CHL  | CHB-C4A | -5.04 | 1.32        | 1.38     |
| 30  | h     | 608 | CHL  | CHC-C4B | 5.04  | 1.47        | 1.39     |
| 30  | f     | 607 | CHL  | OBD-CAD | 5.04  | 1.28        | 1.22     |
| 33  | 3     | 501 | 0UR  | O44-C45 | 5.04  | 1.45        | 1.34     |
| 30  | c     | 609 | CHL  | C3D-C2D | 5.04  | 1.48        | 1.39     |
| 30  | e     | 607 | CHL  | C3D-C2D | 5.04  | 1.48        | 1.39     |
| 30  | a     | 606 | CHL  | OBD-CAD | 5.04  | 1.28        | 1.22     |
| 30  | g     | 606 | CHL  | OBD-CAD | 5.04  | 1.28        | 1.22     |
| 30  | 6     | 302 | CHL  | CHB-C4A | -5.04 | 1.32        | 1.38     |
| 30  | 8     | 315 | CHL  | C3D-C2D | 5.04  | 1.48        | 1.39     |
| 32  | 8     | 406 | 8CT  | C05-C04 | 5.04  | 1.65        | 1.54     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 30  | h     | 605 | CHL  | OBD-CAD | 5.04  | 1.28        | 1.22     |
| 30  | g     | 609 | CHL  | O2D-CGD | 5.04  | 1.45        | 1.33     |
| 30  | g     | 607 | CHL  | OBD-CAD | 5.04  | 1.28        | 1.22     |
| 30  | g     | 606 | CHL  | C3D-C2D | 5.04  | 1.48        | 1.39     |
| 30  | 6     | 315 | CHL  | O2D-CGD | 5.03  | 1.45        | 1.33     |
| 30  | h     | 608 | CHL  | OBD-CAD | 5.03  | 1.28        | 1.22     |
| 30  | e     | 609 | CHL  | O2D-CGD | 5.03  | 1.45        | 1.33     |
| 30  | c     | 602 | CHL  | O2D-CGD | 5.03  | 1.45        | 1.33     |
| 30  | b     | 608 | CHL  | O2D-CGD | 5.03  | 1.45        | 1.33     |
| 30  | 2     | 302 | CHL  | CHB-C4A | -5.03 | 1.32        | 1.38     |
| 30  | b     | 607 | CHL  | C3D-C2D | 5.03  | 1.48        | 1.39     |
| 32  | G     | 104 | 8CT  | C05-C04 | 5.03  | 1.65        | 1.54     |
| 30  | a     | 614 | CHL  | OBD-CAD | 5.03  | 1.28        | 1.22     |
| 30  | g     | 601 | CHL  | OBD-CAD | 5.03  | 1.28        | 1.22     |
| 30  | a     | 601 | CHL  | C3D-C2D | 5.03  | 1.48        | 1.39     |
| 30  | e     | 609 | CHL  | CHC-C4B | 5.03  | 1.47        | 1.39     |
| 32  | B     | 846 | 8CT  | C05-C04 | 5.03  | 1.65        | 1.54     |
| 30  | b     | 607 | CHL  | O2D-CGD | 5.03  | 1.45        | 1.33     |
| 33  | h     | 520 | 0UR  | O44-C45 | 5.03  | 1.45        | 1.34     |
| 33  | 2     | 501 | 0UR  | O44-C45 | 5.03  | 1.45        | 1.34     |
| 30  | 5     | 306 | CHL  | CHD-C1D | 5.03  | 1.47        | 1.39     |
| 33  | 0     | 501 | 0UR  | O44-C45 | 5.03  | 1.45        | 1.34     |
| 30  | 5     | 305 | CHL  | OBD-CAD | 5.03  | 1.28        | 1.22     |
| 30  | d     | 607 | CHL  | OBD-CAD | 5.03  | 1.28        | 1.22     |
| 32  | 8     | 402 | 8CT  | C05-C04 | 5.02  | 1.65        | 1.54     |
| 33  | O     | 204 | 0UR  | O44-C45 | 5.02  | 1.45        | 1.34     |
| 33  | 7     | 501 | 0UR  | O44-C45 | 5.02  | 1.45        | 1.34     |
| 30  | e     | 606 | CHL  | O2D-CGD | 5.02  | 1.45        | 1.33     |
| 30  | i     | 606 | CHL  | OBD-CAD | 5.02  | 1.28        | 1.22     |
| 30  | f     | 614 | CHL  | O2D-CGD | 5.02  | 1.45        | 1.33     |
| 32  | B     | 847 | 8CT  | C05-C04 | 5.02  | 1.65        | 1.54     |
| 30  | b     | 614 | CHL  | OBD-CAD | 5.02  | 1.28        | 1.22     |
| 30  | 8     | 315 | CHL  | O2D-CGD | 5.02  | 1.45        | 1.33     |
| 30  | f     | 608 | CHL  | O2D-CGD | 5.02  | 1.45        | 1.33     |
| 30  | 4     | 305 | CHL  | CHB-C4A | -5.02 | 1.32        | 1.38     |
| 30  | h     | 607 | CHL  | OBD-CAD | 5.02  | 1.28        | 1.22     |
| 30  | f     | 614 | CHL  | C3B-C2B | 5.02  | 1.47        | 1.40     |
| 30  | 8     | 305 | CHL  | O2D-CGD | 5.02  | 1.45        | 1.33     |
| 30  | 2     | 308 | CHL  | C3A-C2A | -5.02 | 1.50        | 1.54     |
| 30  | 9     | 313 | CHL  | O2D-CGD | 5.02  | 1.45        | 1.33     |
| 30  | i     | 608 | CHL  | CHC-C4B | 5.02  | 1.47        | 1.39     |
| 30  | a     | 602 | CHL  | C3D-C2D | 5.01  | 1.48        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 30  | 8     | 315 | CHL  | OBD-CAD | 5.01  | 1.28        | 1.22     |
| 30  | g     | 602 | CHL  | OBD-CAD | 5.01  | 1.28        | 1.22     |
| 30  | f     | 602 | CHL  | C3A-C2A | -5.01 | 1.50        | 1.54     |
| 30  | 6     | 315 | CHL  | CHC-C4B | 5.01  | 1.47        | 1.39     |
| 30  | f     | 609 | CHL  | CHD-C1D | 5.01  | 1.47        | 1.39     |
| 30  | f     | 601 | CHL  | O2D-CGD | 5.01  | 1.45        | 1.33     |
| 30  | h     | 606 | CHL  | CHC-C4B | 5.01  | 1.47        | 1.39     |
| 30  | e     | 605 | CHL  | CHD-C1D | 5.01  | 1.47        | 1.39     |
| 30  | 2     | 301 | CHL  | CHB-C4A | -5.01 | 1.32        | 1.38     |
| 30  | c     | 609 | CHL  | O2D-CGD | 5.01  | 1.45        | 1.33     |
| 30  | a     | 606 | CHL  | CHD-C1D | 5.01  | 1.47        | 1.39     |
| 30  | a     | 601 | CHL  | O2D-CGD | 5.01  | 1.45        | 1.33     |
| 30  | i     | 607 | CHL  | OBD-CAD | 5.01  | 1.28        | 1.22     |
| 30  | b     | 602 | CHL  | O2D-CGD | 5.01  | 1.45        | 1.33     |
| 30  | 0     | 301 | CHL  | CHB-C4A | -5.01 | 1.32        | 1.38     |
| 30  | 0     | 305 | CHL  | OBD-CAD | 5.01  | 1.28        | 1.22     |
| 30  | 9     | 305 | CHL  | CHC-C4B | 5.01  | 1.47        | 1.39     |
| 30  | b     | 607 | CHL  | C3B-C2B | 5.01  | 1.47        | 1.40     |
| 30  | i     | 605 | CHL  | OBD-CAD | 5.01  | 1.28        | 1.22     |
| 30  | 4     | 319 | CHL  | CHB-C4A | -5.00 | 1.32        | 1.38     |
| 30  | c     | 609 | CHL  | CHC-C4B | 5.00  | 1.47        | 1.39     |
| 32  | 7     | 404 | 8CT  | C05-C04 | 5.00  | 1.65        | 1.54     |
| 32  | M     | 102 | 8CT  | C05-C04 | 5.00  | 1.65        | 1.54     |
| 30  | a     | 608 | CHL  | C3B-C2B | 5.00  | 1.47        | 1.40     |
| 30  | 8     | 307 | CHL  | CHB-C4A | -5.00 | 1.32        | 1.38     |
| 30  | b     | 614 | CHL  | CHD-C1D | 5.00  | 1.47        | 1.39     |
| 32  | 6     | 402 | 8CT  | C05-C04 | 5.00  | 1.65        | 1.54     |
| 30  | i     | 614 | CHL  | OBD-CAD | 5.00  | 1.28        | 1.22     |
| 32  | B     | 844 | 8CT  | C05-C04 | 5.00  | 1.65        | 1.54     |
| 30  | 6     | 307 | CHL  | CHC-C4B | 5.00  | 1.47        | 1.39     |
| 30  | g     | 614 | CHL  | CHB-C1B | 5.00  | 1.47        | 1.39     |
| 30  | 1     | 305 | CHL  | O2D-CGD | 5.00  | 1.45        | 1.33     |
| 30  | i     | 608 | CHL  | C3B-C2B | 5.00  | 1.47        | 1.40     |
| 30  | a     | 607 | CHL  | OBD-CAD | 5.00  | 1.28        | 1.22     |
| 30  | e     | 608 | CHL  | CHC-C4B | 5.00  | 1.47        | 1.39     |
| 30  | 6     | 305 | CHL  | O2D-CGD | 5.00  | 1.45        | 1.33     |
| 30  | 3     | 307 | CHL  | CHB-C4A | -5.00 | 1.32        | 1.38     |
| 30  | c     | 602 | CHL  | OBD-CAD | 4.99  | 1.28        | 1.22     |
| 30  | c     | 607 | CHL  | OBD-CAD | 4.99  | 1.28        | 1.22     |
| 30  | d     | 605 | CHL  | CHB-C1B | 4.99  | 1.47        | 1.39     |
| 30  | e     | 614 | CHL  | OBD-CAD | 4.99  | 1.28        | 1.22     |
| 30  | h     | 602 | CHL  | CHD-C1D | 4.99  | 1.47        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 30  | b     | 614 | CHL  | O2D-CGD | 4.99  | 1.45        | 1.33     |
| 30  | b     | 609 | CHL  | CHD-C1D | 4.99  | 1.47        | 1.39     |
| 30  | d     | 608 | CHL  | CHC-C4B | 4.99  | 1.47        | 1.39     |
| 30  | a     | 606 | CHL  | C3B-C2B | 4.99  | 1.47        | 1.40     |
| 32  | B     | 848 | 8CT  | C05-C04 | 4.99  | 1.65        | 1.54     |
| 30  | b     | 609 | CHL  | C3B-C2B | 4.99  | 1.47        | 1.40     |
| 30  | b     | 601 | CHL  | CHD-C1D | 4.99  | 1.47        | 1.39     |
| 30  | c     | 614 | CHL  | OBD-CAD | 4.99  | 1.28        | 1.22     |
| 30  | g     | 602 | CHL  | C3B-C2B | 4.99  | 1.47        | 1.40     |
| 30  | 4     | 302 | CHL  | O2D-CGD | 4.99  | 1.45        | 1.33     |
| 30  | a     | 608 | CHL  | O2D-CGD | 4.98  | 1.45        | 1.33     |
| 30  | b     | 601 | CHL  | C3D-C2D | 4.98  | 1.48        | 1.39     |
| 30  | 8     | 313 | CHL  | O2D-CGD | 4.98  | 1.45        | 1.33     |
| 33  | 5     | 501 | 0UR  | O44-C45 | 4.98  | 1.45        | 1.34     |
| 30  | h     | 606 | CHL  | OBD-CAD | 4.98  | 1.28        | 1.22     |
| 30  | i     | 601 | CHL  | OBD-CAD | 4.98  | 1.28        | 1.22     |
| 32  | A     | 847 | 8CT  | C05-C04 | 4.98  | 1.65        | 1.54     |
| 30  | 2     | 319 | CHL  | CHB-C4A | -4.98 | 1.32        | 1.38     |
| 30  | h     | 601 | CHL  | OBD-CAD | 4.98  | 1.28        | 1.22     |
| 30  | i     | 608 | CHL  | C3D-C2D | 4.98  | 1.48        | 1.39     |
| 30  | 0     | 301 | CHL  | O2D-CGD | 4.98  | 1.45        | 1.33     |
| 30  | 6     | 305 | CHL  | CHB-C4A | -4.98 | 1.32        | 1.38     |
| 30  | a     | 601 | CHL  | CHD-C1D | 4.98  | 1.47        | 1.39     |
| 30  | d     | 602 | CHL  | CHC-C4B | 4.98  | 1.47        | 1.39     |
| 30  | i     | 609 | CHL  | CHB-C1B | 4.97  | 1.47        | 1.39     |
| 30  | e     | 605 | CHL  | OBD-CAD | 4.97  | 1.28        | 1.22     |
| 30  | 6     | 307 | CHL  | C3A-C2A | -4.97 | 1.50        | 1.54     |
| 30  | 9     | 305 | CHL  | O2D-CGD | 4.97  | 1.45        | 1.33     |
| 30  | f     | 605 | CHL  | OBD-CAD | 4.97  | 1.28        | 1.22     |
| 30  | e     | 606 | CHL  | OBD-CAD | 4.97  | 1.28        | 1.22     |
| 33  | g     | 520 | 0UR  | O44-C45 | 4.97  | 1.45        | 1.34     |
| 30  | 6     | 306 | CHL  | O2D-CGD | 4.97  | 1.45        | 1.33     |
| 32  | 3     | 403 | 8CT  | C05-C04 | 4.97  | 1.65        | 1.54     |
| 30  | 8     | 306 | CHL  | CHB-C4A | -4.97 | 1.32        | 1.38     |
| 30  | i     | 609 | CHL  | OBD-CAD | 4.97  | 1.28        | 1.22     |
| 30  | 1     | 313 | CHL  | O2D-CGD | 4.97  | 1.45        | 1.33     |
| 30  | 7     | 306 | CHL  | CHB-C4A | -4.97 | 1.32        | 1.38     |
| 30  | c     | 601 | CHL  | O2D-CGD | 4.97  | 1.45        | 1.33     |
| 30  | 4     | 306 | CHL  | CHC-C4B | 4.97  | 1.47        | 1.39     |
| 33  | i     | 520 | 0UR  | O44-C45 | 4.97  | 1.45        | 1.34     |
| 30  | d     | 601 | CHL  | OBD-CAD | 4.96  | 1.28        | 1.22     |
| 30  | 4     | 306 | CHL  | O2D-CGD | 4.96  | 1.45        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 30  | c     | 601 | CHL  | CHB-C4A | -4.96 | 1.32        | 1.38     |
| 30  | 6     | 315 | CHL  | OBD-CAD | 4.96  | 1.28        | 1.22     |
| 30  | d     | 607 | CHL  | CHB-C1B | 4.96  | 1.47        | 1.39     |
| 30  | 4     | 305 | CHL  | O2D-CGD | 4.96  | 1.45        | 1.33     |
| 32  | B     | 843 | 8CT  | C05-C04 | 4.96  | 1.65        | 1.54     |
| 30  | e     | 607 | CHL  | CHD-C1D | 4.96  | 1.47        | 1.39     |
| 30  | 5     | 306 | CHL  | OBD-CAD | 4.96  | 1.28        | 1.22     |
| 30  | e     | 607 | CHL  | C3B-C2B | 4.96  | 1.47        | 1.40     |
| 30  | i     | 602 | CHL  | C3D-C2D | 4.96  | 1.48        | 1.39     |
| 32  | A     | 854 | 8CT  | C05-C04 | 4.96  | 1.65        | 1.54     |
| 30  | 6     | 313 | CHL  | O2D-CGD | 4.96  | 1.45        | 1.33     |
| 30  | a     | 601 | CHL  | OBD-CAD | 4.96  | 1.28        | 1.22     |
| 32  | 4     | 402 | 8CT  | C05-C04 | 4.96  | 1.65        | 1.54     |
| 30  | d     | 614 | CHL  | CHB-C1B | 4.96  | 1.47        | 1.39     |
| 32  | 3     | 402 | 8CT  | C05-C04 | 4.95  | 1.65        | 1.54     |
| 30  | 5     | 313 | CHL  | O2D-CGD | 4.95  | 1.45        | 1.33     |
| 30  | h     | 602 | CHL  | OBD-CAD | 4.95  | 1.28        | 1.22     |
| 30  | 5     | 302 | CHL  | CHB-C4A | -4.95 | 1.32        | 1.38     |
| 30  | 2     | 302 | CHL  | CHC-C4B | 4.95  | 1.47        | 1.39     |
| 32  | B     | 845 | 8CT  | C05-C04 | 4.95  | 1.65        | 1.54     |
| 33  | c     | 520 | 0UR  | O44-C45 | 4.95  | 1.45        | 1.34     |
| 30  | 9     | 306 | CHL  | O2D-CGD | 4.95  | 1.45        | 1.33     |
| 30  | f     | 614 | CHL  | CHD-C1D | 4.95  | 1.47        | 1.39     |
| 30  | 8     | 313 | CHL  | C3A-C2A | -4.95 | 1.50        | 1.54     |
| 33  | 0     | 502 | 0UR  | O44-C45 | 4.95  | 1.45        | 1.34     |
| 30  | f     | 606 | CHL  | CHD-C1D | 4.95  | 1.47        | 1.39     |
| 30  | g     | 606 | CHL  | CHD-C1D | 4.95  | 1.47        | 1.39     |
| 30  | 7     | 313 | CHL  | O2D-CGD | 4.95  | 1.45        | 1.33     |
| 30  | g     | 609 | CHL  | OBD-CAD | 4.95  | 1.28        | 1.22     |
| 30  | c     | 606 | CHL  | CHC-C4B | 4.95  | 1.47        | 1.39     |
| 30  | 6     | 313 | CHL  | C3A-C2A | -4.94 | 1.50        | 1.54     |
| 30  | h     | 608 | CHL  | C3D-C2D | 4.94  | 1.48        | 1.39     |
| 30  | 4     | 313 | CHL  | CHB-C4A | -4.94 | 1.32        | 1.38     |
| 30  | 7     | 305 | CHL  | CHC-C4B | 4.94  | 1.47        | 1.39     |
| 30  | h     | 606 | CHL  | CHD-C1D | 4.94  | 1.47        | 1.39     |
| 30  | b     | 601 | CHL  | OBD-CAD | 4.94  | 1.28        | 1.22     |
| 30  | 5     | 307 | CHL  | O2D-CGD | 4.94  | 1.45        | 1.33     |
| 30  | 2     | 307 | CHL  | CHC-C4B | 4.94  | 1.47        | 1.39     |
| 30  | 6     | 307 | CHL  | O2D-CGD | 4.94  | 1.45        | 1.33     |
| 33  | 9     | 501 | 0UR  | O44-C45 | 4.94  | 1.45        | 1.34     |
| 30  | i     | 601 | CHL  | CHB-C1B | 4.94  | 1.47        | 1.39     |
| 30  | h     | 606 | CHL  | C3B-C2B | 4.94  | 1.47        | 1.40     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 30  | e     | 609 | CHL  | C3B-C2B | 4.94  | 1.47        | 1.40     |
| 30  | 4     | 319 | CHL  | CHC-C4B | 4.94  | 1.47        | 1.39     |
| 30  | c     | 606 | CHL  | OBD-CAD | 4.94  | 1.28        | 1.22     |
| 33  | e     | 520 | OUR  | O44-C45 | 4.94  | 1.45        | 1.34     |
| 30  | f     | 601 | CHL  | CHC-C4B | 4.94  | 1.47        | 1.39     |
| 30  | 9     | 301 | CHL  | O2D-CGD | 4.94  | 1.45        | 1.33     |
| 30  | 8     | 308 | CHL  | CHC-C4B | 4.94  | 1.47        | 1.39     |
| 30  | 0     | 302 | CHL  | O2D-CGD | 4.93  | 1.45        | 1.33     |
| 30  | f     | 614 | CHL  | OBD-CAD | 4.93  | 1.28        | 1.22     |
| 30  | a     | 605 | CHL  | CHB-C1B | 4.93  | 1.47        | 1.39     |
| 30  | c     | 608 | CHL  | CHC-C4B | 4.93  | 1.47        | 1.39     |
| 30  | b     | 609 | CHL  | CHC-C4B | 4.93  | 1.47        | 1.39     |
| 30  | c     | 609 | CHL  | C3B-C2B | 4.93  | 1.47        | 1.40     |
| 30  | g     | 608 | CHL  | OBD-CAD | 4.93  | 1.28        | 1.22     |
| 30  | 5     | 305 | CHL  | C3D-C2D | 4.93  | 1.48        | 1.39     |
| 30  | 7     | 301 | CHL  | CHC-C4B | 4.93  | 1.47        | 1.39     |
| 30  | b     | 608 | CHL  | OBD-CAD | 4.93  | 1.28        | 1.22     |
| 30  | e     | 607 | CHL  | OBD-CAD | 4.93  | 1.28        | 1.22     |
| 30  | 7     | 301 | CHL  | CHB-C4A | -4.93 | 1.32        | 1.38     |
| 32  | B     | 851 | 8CT  | C05-C04 | 4.93  | 1.65        | 1.54     |
| 30  | f     | 606 | CHL  | OBD-CAD | 4.93  | 1.28        | 1.22     |
| 30  | f     | 614 | CHL  | C3D-C2D | 4.93  | 1.48        | 1.39     |
| 32  | J     | 104 | 8CT  | C05-C04 | 4.93  | 1.65        | 1.54     |
| 30  | 7     | 301 | CHL  | C3A-C2A | -4.93 | 1.50        | 1.54     |
| 30  | b     | 606 | CHL  | CHB-C4A | -4.93 | 1.32        | 1.38     |
| 30  | 4     | 307 | CHL  | CHB-C4A | -4.93 | 1.32        | 1.38     |
| 30  | 5     | 305 | CHL  | CHC-C4B | 4.93  | 1.47        | 1.39     |
| 30  | i     | 608 | CHL  | CHD-C1D | 4.93  | 1.47        | 1.39     |
| 30  | 9     | 301 | CHL  | CHB-C4A | -4.93 | 1.32        | 1.38     |
| 30  | 2     | 306 | CHL  | O2D-CGD | 4.93  | 1.45        | 1.33     |
| 30  | 7     | 307 | CHL  | O2D-CGD | 4.93  | 1.45        | 1.33     |
| 30  | e     | 602 | CHL  | C3D-C2D | 4.93  | 1.48        | 1.39     |
| 30  | d     | 602 | CHL  | CHB-C4A | -4.93 | 1.32        | 1.38     |
| 30  | 8     | 306 | CHL  | O2D-CGD | 4.93  | 1.45        | 1.33     |
| 30  | 0     | 306 | CHL  | CHC-C4B | 4.93  | 1.47        | 1.39     |
| 30  | 1     | 313 | CHL  | CHC-C4B | 4.92  | 1.47        | 1.39     |
| 30  | 7     | 301 | CHL  | O2D-CGD | 4.92  | 1.45        | 1.33     |
| 32  | I     | 101 | 8CT  | C05-C04 | 4.92  | 1.65        | 1.54     |
| 30  | 3     | 305 | CHL  | O2D-CGD | 4.92  | 1.45        | 1.33     |
| 30  | 1     | 307 | CHL  | O2D-CGD | 4.92  | 1.45        | 1.33     |
| 30  | 5     | 301 | CHL  | O2D-CGD | 4.92  | 1.45        | 1.33     |
| 30  | 3     | 302 | CHL  | O2D-CGD | 4.92  | 1.45        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 30  | 9     | 313 | CHL  | CHC-C4B | 4.92  | 1.47        | 1.39     |
| 30  | 6     | 315 | CHL  | C3D-C2D | 4.92  | 1.48        | 1.39     |
| 33  | 5     | 502 | OUR  | O44-C45 | 4.92  | 1.45        | 1.34     |
| 30  | 2     | 313 | CHL  | O2D-CGD | 4.92  | 1.45        | 1.33     |
| 30  | a     | 614 | CHL  | CHB-C1B | 4.92  | 1.47        | 1.39     |
| 30  | 7     | 305 | CHL  | CHB-C4A | -4.92 | 1.32        | 1.38     |
| 30  | d     | 601 | CHL  | CHB-C1B | 4.92  | 1.47        | 1.39     |
| 30  | 2     | 307 | CHL  | CHB-C4A | -4.92 | 1.32        | 1.38     |
| 30  | 1     | 307 | CHL  | CHC-C4B | 4.92  | 1.47        | 1.39     |
| 30  | a     | 609 | CHL  | OBD-CAD | 4.92  | 1.28        | 1.22     |
| 30  | 2     | 305 | CHL  | O2D-CGD | 4.92  | 1.45        | 1.33     |
| 30  | c     | 607 | CHL  | CHD-C1D | 4.92  | 1.47        | 1.39     |
| 30  | f     | 601 | CHL  | OBD-CAD | 4.91  | 1.28        | 1.22     |
| 30  | e     | 601 | CHL  | OBD-CAD | 4.91  | 1.28        | 1.22     |
| 30  | 2     | 313 | CHL  | CHC-C4B | 4.91  | 1.47        | 1.39     |
| 30  | 7     | 305 | CHL  | O2D-CGD | 4.91  | 1.45        | 1.33     |
| 30  | c     | 605 | CHL  | CHB-C1B | 4.91  | 1.47        | 1.39     |
| 30  | h     | 607 | CHL  | CHB-C1B | 4.91  | 1.47        | 1.39     |
| 30  | d     | 608 | CHL  | C3D-C2D | 4.91  | 1.48        | 1.39     |
| 30  | 4     | 308 | CHL  | CHC-C4B | 4.91  | 1.47        | 1.39     |
| 30  | h     | 608 | CHL  | CHD-C1D | 4.91  | 1.47        | 1.39     |
| 33  | f     | 520 | OUR  | O44-C45 | 4.91  | 1.45        | 1.34     |
| 30  | 3     | 307 | CHL  | O2D-CGD | 4.91  | 1.45        | 1.33     |
| 30  | d     | 606 | CHL  | CHD-C1D | 4.91  | 1.47        | 1.39     |
| 30  | g     | 602 | CHL  | CHD-C1D | 4.91  | 1.47        | 1.39     |
| 30  | 6     | 306 | CHL  | CHB-C4A | -4.91 | 1.32        | 1.38     |
| 30  | 2     | 307 | CHL  | O2D-CGD | 4.91  | 1.45        | 1.33     |
| 30  | 5     | 301 | CHL  | C3D-C2D | 4.91  | 1.48        | 1.39     |
| 32  | A     | 846 | 8CT  | C05-C04 | 4.91  | 1.65        | 1.54     |
| 30  | 2     | 306 | CHL  | CHC-C4B | 4.91  | 1.47        | 1.39     |
| 30  | b     | 602 | CHL  | C3D-C2D | 4.91  | 1.48        | 1.39     |
| 30  | 4     | 307 | CHL  | O2D-CGD | 4.91  | 1.45        | 1.33     |
| 30  | 6     | 301 | CHL  | CHB-C4A | -4.91 | 1.32        | 1.38     |
| 30  | 9     | 301 | CHL  | OBD-CAD | 4.91  | 1.28        | 1.22     |
| 30  | 5     | 307 | CHL  | CHD-C1D | 4.90  | 1.47        | 1.39     |
| 30  | 8     | 305 | CHL  | OBD-CAD | 4.90  | 1.28        | 1.22     |
| 30  | 1     | 306 | CHL  | CHC-C4B | 4.90  | 1.47        | 1.39     |
| 30  | 0     | 306 | CHL  | OBD-CAD | 4.90  | 1.28        | 1.22     |
| 32  | 7     | 402 | 8CT  | C05-C04 | 4.90  | 1.65        | 1.54     |
| 30  | 4     | 306 | CHL  | OBD-CAD | 4.90  | 1.28        | 1.22     |
| 33  | 8     | 501 | OUR  | O44-C45 | 4.90  | 1.45        | 1.34     |
| 30  | 2     | 302 | CHL  | O2D-CGD | 4.90  | 1.45        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 30  | i     | 605 | CHL  | CHB-C1B | 4.90  | 1.47        | 1.39     |
| 30  | 7     | 306 | CHL  | O2D-CGD | 4.90  | 1.45        | 1.33     |
| 30  | i     | 608 | CHL  | OBD-CAD | 4.90  | 1.28        | 1.22     |
| 32  | B     | 804 | 8CT  | C05-C04 | 4.90  | 1.65        | 1.54     |
| 30  | 4     | 308 | CHL  | C3D-C2D | 4.89  | 1.48        | 1.39     |
| 30  | e     | 601 | CHL  | CHC-C4B | 4.89  | 1.47        | 1.39     |
| 30  | 2     | 306 | CHL  | C3A-C2A | -4.89 | 1.50        | 1.54     |
| 30  | 0     | 306 | CHL  | C3B-C2B | 4.89  | 1.47        | 1.40     |
| 32  | F     | 302 | 8CT  | C05-C04 | 4.89  | 1.65        | 1.54     |
| 30  | d     | 602 | CHL  | C3D-C2D | 4.89  | 1.48        | 1.39     |
| 30  | g     | 601 | CHL  | CHB-C1B | 4.89  | 1.47        | 1.39     |
| 33  | b     | 520 | 0UR  | O44-C45 | 4.89  | 1.45        | 1.34     |
| 30  | d     | 608 | CHL  | OBD-CAD | 4.89  | 1.28        | 1.22     |
| 30  | 2     | 319 | CHL  | CHC-C4B | 4.89  | 1.47        | 1.39     |
| 30  | 1     | 305 | CHL  | CHC-C4B | 4.89  | 1.47        | 1.39     |
| 33  | 2     | 502 | 0UR  | O44-C45 | 4.89  | 1.45        | 1.34     |
| 30  | 8     | 315 | CHL  | CHD-C1D | 4.89  | 1.47        | 1.39     |
| 30  | 0     | 302 | CHL  | OBD-CAD | 4.89  | 1.28        | 1.22     |
| 30  | 2     | 305 | CHL  | CHC-C4B | 4.88  | 1.47        | 1.39     |
| 30  | 8     | 306 | CHL  | OBD-CAD | 4.88  | 1.28        | 1.22     |
| 30  | 8     | 308 | CHL  | O2D-CGD | 4.88  | 1.45        | 1.33     |
| 30  | d     | 609 | CHL  | OBD-CAD | 4.88  | 1.28        | 1.22     |
| 33  | 8     | 502 | 0UR  | O44-C45 | 4.88  | 1.45        | 1.34     |
| 30  | 8     | 306 | CHL  | C3A-C2A | -4.88 | 1.50        | 1.54     |
| 30  | e     | 602 | CHL  | OBD-CAD | 4.88  | 1.28        | 1.22     |
| 30  | d     | 606 | CHL  | C3B-C2B | 4.88  | 1.47        | 1.40     |
| 30  | 8     | 307 | CHL  | CHC-C4B | 4.88  | 1.47        | 1.39     |
| 30  | 5     | 305 | CHL  | CHD-C1D | 4.88  | 1.47        | 1.39     |
| 30  | c     | 614 | CHL  | C2A-C3A | -4.88 | 1.50        | 1.54     |
| 30  | 6     | 305 | CHL  | CHC-C4B | 4.88  | 1.47        | 1.39     |
| 30  | 6     | 308 | CHL  | CHC-C4B | 4.88  | 1.47        | 1.39     |
| 30  | 5     | 305 | CHL  | CHB-C4A | -4.88 | 1.32        | 1.38     |
| 33  | 1     | 501 | 0UR  | O44-C45 | 4.88  | 1.45        | 1.34     |
| 30  | h     | 609 | CHL  | OBD-CAD | 4.88  | 1.28        | 1.22     |
| 30  | 9     | 313 | CHL  | OBD-CAD | 4.88  | 1.28        | 1.22     |
| 30  | b     | 607 | CHL  | OBD-CAD | 4.88  | 1.28        | 1.22     |
| 30  | i     | 602 | CHL  | OBD-CAD | 4.88  | 1.28        | 1.22     |
| 30  | 5     | 301 | CHL  | C3B-C2B | 4.88  | 1.47        | 1.40     |
| 30  | 8     | 301 | CHL  | CHB-C4A | -4.88 | 1.32        | 1.38     |
| 30  | 7     | 302 | CHL  | CHC-C4B | 4.88  | 1.47        | 1.39     |
| 30  | 1     | 306 | CHL  | C3D-C2D | 4.87  | 1.48        | 1.39     |
| 30  | 7     | 313 | CHL  | C3D-C2D | 4.87  | 1.48        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 30  | 4     | 313 | CHL  | O2D-CGD | 4.87  | 1.45        | 1.33     |
| 30  | 4     | 302 | CHL  | CHC-C4B | 4.87  | 1.47        | 1.39     |
| 30  | c     | 602 | CHL  | C3D-C2D | 4.87  | 1.48        | 1.39     |
| 33  | 4     | 501 | 0UR  | O44-C45 | 4.87  | 1.45        | 1.34     |
| 33  | 6     | 502 | 0UR  | O44-C45 | 4.87  | 1.45        | 1.34     |
| 30  | 4     | 308 | CHL  | O2D-CGD | 4.87  | 1.45        | 1.33     |
| 30  | a     | 602 | CHL  | OBD-CAD | 4.87  | 1.28        | 1.22     |
| 30  | c     | 602 | CHL  | CHB-C4A | -4.87 | 1.32        | 1.38     |
| 30  | a     | 609 | CHL  | CHB-C1B | 4.87  | 1.47        | 1.39     |
| 30  | 2     | 308 | CHL  | CHC-C4B | 4.87  | 1.47        | 1.39     |
| 30  | 3     | 305 | CHL  | CHC-C4B | 4.87  | 1.47        | 1.39     |
| 30  | 9     | 306 | CHL  | CHC-C4B | 4.87  | 1.47        | 1.39     |
| 30  | c     | 601 | CHL  | OBD-CAD | 4.87  | 1.28        | 1.22     |
| 30  | 6     | 301 | CHL  | CHC-C4B | 4.87  | 1.47        | 1.39     |
| 30  | 3     | 305 | CHL  | OBD-CAD | 4.86  | 1.28        | 1.22     |
| 30  | e     | 602 | CHL  | C3A-C2A | -4.86 | 1.50        | 1.54     |
| 30  | 8     | 302 | CHL  | O2D-CGD | 4.86  | 1.45        | 1.33     |
| 30  | 4     | 305 | CHL  | OBD-CAD | 4.86  | 1.28        | 1.22     |
| 30  | 2     | 301 | CHL  | CHC-C4B | 4.86  | 1.47        | 1.39     |
| 30  | i     | 606 | CHL  | CHB-C1B | 4.86  | 1.47        | 1.39     |
| 30  | 1     | 302 | CHL  | O2D-CGD | 4.86  | 1.45        | 1.33     |
| 30  | g     | 605 | CHL  | CHB-C1B | 4.86  | 1.47        | 1.39     |
| 30  | c     | 614 | CHL  | CHD-C1D | 4.86  | 1.47        | 1.39     |
| 30  | 9     | 306 | CHL  | C3D-C2D | 4.86  | 1.47        | 1.39     |
| 30  | 5     | 302 | CHL  | O2D-CGD | 4.86  | 1.45        | 1.33     |
| 30  | 6     | 313 | CHL  | CHC-C4B | 4.86  | 1.47        | 1.39     |
| 30  | c     | 614 | CHL  | O2D-CGD | 4.86  | 1.45        | 1.33     |
| 30  | 9     | 306 | CHL  | CHB-C4A | -4.86 | 1.32        | 1.38     |
| 30  | f     | 608 | CHL  | CHC-C4B | 4.86  | 1.47        | 1.39     |
| 30  | 7     | 306 | CHL  | C3D-C2D | 4.86  | 1.47        | 1.39     |
| 30  | e     | 614 | CHL  | CHB-C1B | 4.86  | 1.47        | 1.39     |
| 30  | c     | 602 | CHL  | C3A-C2A | -4.86 | 1.50        | 1.54     |
| 30  | 2     | 308 | CHL  | O2D-CGD | 4.85  | 1.45        | 1.33     |
| 30  | a     | 601 | CHL  | CHB-C1B | 4.85  | 1.47        | 1.39     |
| 30  | 1     | 306 | CHL  | O2D-CGD | 4.85  | 1.45        | 1.33     |
| 30  | 6     | 302 | CHL  | OBD-CAD | 4.85  | 1.28        | 1.22     |
| 30  | i     | 614 | CHL  | CHB-C1B | 4.85  | 1.47        | 1.39     |
| 30  | 4     | 305 | CHL  | CHC-C4B | 4.85  | 1.47        | 1.39     |
| 32  | A     | 850 | 8CT  | C05-C04 | 4.85  | 1.65        | 1.54     |
| 30  | c     | 606 | CHL  | C3D-C2D | 4.85  | 1.47        | 1.39     |
| 30  | 6     | 308 | CHL  | O2D-CGD | 4.85  | 1.45        | 1.33     |
| 30  | 7     | 306 | CHL  | CHC-C4B | 4.85  | 1.47        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 30  | 8     | 306 | CHL  | C3D-C2D | 4.85  | 1.47        | 1.39     |
| 30  | 6     | 305 | CHL  | OBD-CAD | 4.85  | 1.28        | 1.22     |
| 30  | 6     | 302 | CHL  | CHC-C4B | 4.85  | 1.47        | 1.39     |
| 30  | 6     | 301 | CHL  | OBD-CAD | 4.85  | 1.28        | 1.22     |
| 30  | b     | 606 | CHL  | C3D-C2D | 4.85  | 1.47        | 1.39     |
| 30  | 2     | 313 | CHL  | CHB-C4A | -4.85 | 1.32        | 1.38     |
| 30  | e     | 609 | CHL  | C3D-C2D | 4.84  | 1.47        | 1.39     |
| 30  | e     | 606 | CHL  | C3B-C2B | 4.84  | 1.46        | 1.40     |
| 33  | 1     | 502 | OUR  | O44-C45 | 4.84  | 1.45        | 1.34     |
| 30  | 1     | 307 | CHL  | C3B-C2B | 4.84  | 1.46        | 1.40     |
| 30  | 8     | 301 | CHL  | O2D-CGD | 4.84  | 1.45        | 1.33     |
| 30  | 6     | 301 | CHL  | O2D-CGD | 4.84  | 1.45        | 1.33     |
| 30  | 0     | 301 | CHL  | C3A-C2A | -4.84 | 1.50        | 1.54     |
| 30  | g     | 602 | CHL  | CHB-C1B | 4.84  | 1.47        | 1.39     |
| 30  | a     | 608 | CHL  | OBD-CAD | 4.84  | 1.28        | 1.22     |
| 30  | g     | 609 | CHL  | CHB-C1B | 4.84  | 1.47        | 1.39     |
| 30  | 7     | 305 | CHL  | OBD-CAD | 4.84  | 1.28        | 1.22     |
| 30  | a     | 608 | CHL  | C3D-C2D | 4.84  | 1.47        | 1.39     |
| 32  | A     | 849 | 8CT  | C05-C04 | 4.84  | 1.65        | 1.54     |
| 30  | h     | 602 | CHL  | CHB-C1B | 4.84  | 1.47        | 1.39     |
| 30  | f     | 602 | CHL  | C3D-C2D | 4.84  | 1.47        | 1.39     |
| 30  | 1     | 305 | CHL  | OBD-CAD | 4.84  | 1.28        | 1.22     |
| 30  | 5     | 313 | CHL  | OBD-CAD | 4.84  | 1.28        | 1.22     |
| 30  | 4     | 308 | CHL  | C3A-C2A | -4.84 | 1.50        | 1.54     |
| 30  | 8     | 307 | CHL  | O2D-CGD | 4.84  | 1.45        | 1.33     |
| 30  | 5     | 307 | CHL  | C3D-C2D | 4.84  | 1.47        | 1.39     |
| 30  | 6     | 301 | CHL  | C3A-C2A | -4.84 | 1.50        | 1.54     |
| 30  | 7     | 306 | CHL  | C3A-C2A | -4.84 | 1.50        | 1.54     |
| 30  | 8     | 305 | CHL  | CHC-C4B | 4.84  | 1.47        | 1.39     |
| 30  | 1     | 313 | CHL  | OBD-CAD | 4.83  | 1.28        | 1.22     |
| 30  | 2     | 313 | CHL  | C3A-C2A | -4.83 | 1.50        | 1.54     |
| 30  | 1     | 313 | CHL  | CHB-C4A | -4.83 | 1.32        | 1.38     |
| 30  | b     | 614 | CHL  | CHB-C1B | 4.83  | 1.47        | 1.39     |
| 30  | c     | 609 | CHL  | OBD-CAD | 4.83  | 1.28        | 1.22     |
| 30  | 2     | 319 | CHL  | O2D-CGD | 4.83  | 1.45        | 1.33     |
| 30  | a     | 602 | CHL  | CHD-C1D | 4.83  | 1.47        | 1.39     |
| 30  | c     | 608 | CHL  | C3D-C2D | 4.83  | 1.47        | 1.39     |
| 30  | 9     | 301 | CHL  | C3A-C2A | -4.83 | 1.50        | 1.54     |
| 30  | 2     | 306 | CHL  | OBD-CAD | 4.83  | 1.28        | 1.22     |
| 30  | 5     | 305 | CHL  | C3B-C2B | 4.83  | 1.46        | 1.40     |
| 30  | f     | 608 | CHL  | C3A-C2A | -4.83 | 1.50        | 1.54     |
| 30  | b     | 608 | CHL  | CHC-C4B | 4.82  | 1.47        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 30  | 6     | 301 | CHL  | C3D-C2D | 4.82  | 1.47        | 1.39     |
| 30  | c     | 601 | CHL  | C3D-C2D | 4.82  | 1.47        | 1.39     |
| 30  | g     | 607 | CHL  | CHB-C1B | 4.82  | 1.47        | 1.39     |
| 30  | b     | 602 | CHL  | OBD-CAD | 4.82  | 1.28        | 1.22     |
| 30  | e     | 606 | CHL  | C3D-C2D | 4.82  | 1.47        | 1.39     |
| 30  | 5     | 302 | CHL  | OBD-CAD | 4.82  | 1.28        | 1.22     |
| 30  | h     | 609 | CHL  | CHB-C1B | 4.82  | 1.47        | 1.39     |
| 30  | 7     | 301 | CHL  | OBD-CAD | 4.82  | 1.28        | 1.22     |
| 30  | 5     | 302 | CHL  | CHC-C4B | 4.82  | 1.47        | 1.39     |
| 30  | f     | 601 | CHL  | C3D-C2D | 4.82  | 1.47        | 1.39     |
| 30  | 0     | 302 | CHL  | CHC-C4B | 4.82  | 1.47        | 1.39     |
| 30  | 8     | 315 | CHL  | CHB-C1B | 4.82  | 1.47        | 1.39     |
| 30  | c     | 608 | CHL  | OBD-CAD | 4.82  | 1.28        | 1.22     |
| 30  | 6     | 302 | CHL  | C3A-C2A | -4.81 | 1.50        | 1.54     |
| 30  | 5     | 301 | CHL  | OBD-CAD | 4.81  | 1.28        | 1.22     |
| 30  | d     | 609 | CHL  | CHB-C1B | 4.81  | 1.47        | 1.39     |
| 30  | 4     | 319 | CHL  | O2D-CGD | 4.81  | 1.45        | 1.33     |
| 30  | f     | 609 | CHL  | CHB-C1B | 4.81  | 1.47        | 1.39     |
| 30  | i     | 602 | CHL  | CHD-C1D | 4.81  | 1.47        | 1.39     |
| 30  | d     | 608 | CHL  | CHD-C1D | 4.81  | 1.47        | 1.39     |
| 30  | i     | 602 | CHL  | C3B-C2B | 4.81  | 1.46        | 1.40     |
| 30  | b     | 607 | CHL  | CHD-C1D | 4.81  | 1.47        | 1.39     |
| 30  | 4     | 313 | CHL  | OBD-CAD | 4.81  | 1.28        | 1.22     |
| 30  | 1     | 307 | CHL  | CHB-C4A | -4.80 | 1.32        | 1.38     |
| 30  | 1     | 306 | CHL  | OBD-CAD | 4.80  | 1.28        | 1.22     |
| 30  | a     | 608 | CHL  | CHD-C1D | 4.80  | 1.47        | 1.39     |
| 30  | i     | 607 | CHL  | CHB-C1B | 4.80  | 1.47        | 1.39     |
| 30  | a     | 602 | CHL  | CHB-C4A | -4.80 | 1.32        | 1.38     |
| 30  | f     | 607 | CHL  | CHB-C1B | 4.80  | 1.47        | 1.39     |
| 30  | 1     | 307 | CHL  | C3A-C2A | -4.80 | 1.50        | 1.54     |
| 30  | 9     | 306 | CHL  | C3A-C2A | -4.80 | 1.50        | 1.54     |
| 30  | d     | 602 | CHL  | C3A-C2A | -4.80 | 1.50        | 1.54     |
| 30  | f     | 608 | CHL  | CHB-C4A | -4.80 | 1.32        | 1.38     |
| 30  | 6     | 315 | CHL  | C3B-C2B | 4.80  | 1.46        | 1.40     |
| 30  | c     | 607 | CHL  | CHB-C1B | 4.80  | 1.47        | 1.39     |
| 30  | 6     | 308 | CHL  | OBD-CAD | 4.80  | 1.28        | 1.22     |
| 30  | c     | 606 | CHL  | C3B-C2B | 4.79  | 1.46        | 1.40     |
| 30  | 4     | 302 | CHL  | OBD-CAD | 4.79  | 1.28        | 1.22     |
| 33  | 9     | 502 | OUR  | O44-C45 | 4.79  | 1.45        | 1.34     |
| 30  | 8     | 301 | CHL  | OBD-CAD | 4.79  | 1.28        | 1.22     |
| 30  | b     | 609 | CHL  | CHB-C1B | 4.79  | 1.47        | 1.39     |
| 30  | c     | 608 | CHL  | CHB-C4A | -4.79 | 1.32        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 30  | 0     | 301 | CHL  | CHC-C4B | 4.79  | 1.47        | 1.39     |
| 30  | b     | 602 | CHL  | CHB-C4A | -4.79 | 1.32        | 1.38     |
| 30  | 6     | 308 | CHL  | CHB-C4A | -4.79 | 1.32        | 1.38     |
| 30  | 6     | 308 | CHL  | C3D-C2D | 4.79  | 1.47        | 1.39     |
| 33  | 4     | 502 | OUR  | O44-C45 | 4.79  | 1.45        | 1.34     |
| 30  | 7     | 313 | CHL  | OBD-CAD | 4.79  | 1.28        | 1.22     |
| 30  | 2     | 302 | CHL  | C3D-C2D | 4.78  | 1.47        | 1.39     |
| 30  | 7     | 302 | CHL  | O2D-CGD | 4.78  | 1.45        | 1.33     |
| 30  | 0     | 306 | CHL  | O2D-CGD | 4.78  | 1.45        | 1.33     |
| 30  | 2     | 305 | CHL  | OBD-CAD | 4.78  | 1.28        | 1.22     |
| 30  | 2     | 306 | CHL  | C3D-C2D | 4.78  | 1.47        | 1.39     |
| 30  | 4     | 313 | CHL  | C3D-C2D | 4.78  | 1.47        | 1.39     |
| 30  | 1     | 306 | CHL  | C3B-C2B | 4.78  | 1.46        | 1.40     |
| 30  | c     | 608 | CHL  | C3B-C2B | 4.78  | 1.46        | 1.40     |
| 30  | e     | 605 | CHL  | CHB-C1B | 4.78  | 1.47        | 1.39     |
| 30  | a     | 607 | CHL  | CHB-C1B | 4.78  | 1.47        | 1.39     |
| 30  | d     | 606 | CHL  | CHB-C1B | 4.78  | 1.47        | 1.39     |
| 30  | f     | 602 | CHL  | OBD-CAD | 4.78  | 1.28        | 1.22     |
| 30  | 2     | 308 | CHL  | CHB-C4A | -4.77 | 1.32        | 1.38     |
| 30  | 8     | 308 | CHL  | C3D-C2D | 4.77  | 1.47        | 1.39     |
| 30  | b     | 606 | CHL  | C3A-C2A | -4.77 | 1.50        | 1.54     |
| 33  | 6     | 501 | OUR  | O44-C45 | 4.77  | 1.45        | 1.34     |
| 30  | 8     | 313 | CHL  | OBD-CAD | 4.77  | 1.28        | 1.22     |
| 30  | 6     | 302 | CHL  | C3D-C2D | 4.77  | 1.47        | 1.39     |
| 30  | h     | 601 | CHL  | CHB-C1B | 4.77  | 1.47        | 1.39     |
| 30  | 8     | 306 | CHL  | CHC-C4B | 4.77  | 1.47        | 1.39     |
| 30  | 0     | 305 | CHL  | C3D-C2D | 4.77  | 1.47        | 1.39     |
| 30  | e     | 609 | CHL  | CHD-C1D | 4.77  | 1.47        | 1.39     |
| 30  | 2     | 319 | CHL  | OBD-CAD | 4.77  | 1.28        | 1.22     |
| 30  | 7     | 301 | CHL  | C3D-C2D | 4.76  | 1.47        | 1.39     |
| 30  | 1     | 302 | CHL  | C3D-C2D | 4.76  | 1.47        | 1.39     |
| 30  | 2     | 308 | CHL  | C3D-C2D | 4.76  | 1.47        | 1.39     |
| 30  | e     | 608 | CHL  | CHB-C4A | -4.76 | 1.32        | 1.38     |
| 30  | f     | 601 | CHL  | CHB-C4A | -4.76 | 1.32        | 1.38     |
| 30  | g     | 608 | CHL  | CHB-C1B | 4.76  | 1.47        | 1.39     |
| 30  | 6     | 306 | CHL  | OBD-CAD | 4.76  | 1.28        | 1.22     |
| 30  | f     | 605 | CHL  | CHB-C1B | 4.76  | 1.47        | 1.39     |
| 30  | 0     | 305 | CHL  | CHB-C4A | -4.76 | 1.32        | 1.38     |
| 30  | 7     | 313 | CHL  | CHB-C4A | -4.76 | 1.32        | 1.38     |
| 30  | e     | 608 | CHL  | OBD-CAD | 4.76  | 1.28        | 1.22     |
| 30  | e     | 608 | CHL  | C3B-C2B | 4.75  | 1.46        | 1.40     |
| 30  | e     | 602 | CHL  | CHD-C1D | 4.75  | 1.47        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 30  | 0     | 306 | CHL  | C3D-C2D | 4.75  | 1.47        | 1.39     |
| 30  | b     | 608 | CHL  | CHB-C4A | -4.75 | 1.32        | 1.38     |
| 30  | 9     | 301 | CHL  | CHC-C4B | 4.75  | 1.47        | 1.39     |
| 30  | 8     | 302 | CHL  | C3D-C2D | 4.75  | 1.47        | 1.39     |
| 30  | 2     | 301 | CHL  | O2D-CGD | 4.75  | 1.44        | 1.33     |
| 30  | e     | 601 | CHL  | C3B-C2B | 4.75  | 1.46        | 1.40     |
| 30  | 8     | 308 | CHL  | CHB-C4A | -4.74 | 1.32        | 1.38     |
| 30  | 9     | 306 | CHL  | OBD-CAD | 4.74  | 1.28        | 1.22     |
| 30  | c     | 601 | CHL  | CHC-C4B | 4.74  | 1.47        | 1.39     |
| 30  | e     | 606 | CHL  | CHB-C4A | -4.74 | 1.32        | 1.38     |
| 30  | g     | 606 | CHL  | CHB-C1B | 4.74  | 1.47        | 1.39     |
| 30  | 9     | 313 | CHL  | CHB-C4A | -4.74 | 1.32        | 1.38     |
| 30  | 0     | 302 | CHL  | C3D-C2D | 4.74  | 1.47        | 1.39     |
| 30  | 6     | 313 | CHL  | OBD-CAD | 4.74  | 1.28        | 1.22     |
| 30  | c     | 601 | CHL  | C3A-C2A | -4.74 | 1.50        | 1.54     |
| 30  | c     | 608 | CHL  | CHD-C1D | 4.74  | 1.47        | 1.39     |
| 30  | f     | 601 | CHL  | CHD-C1D | 4.74  | 1.47        | 1.39     |
| 30  | 5     | 306 | CHL  | CHB-C1B | 4.74  | 1.47        | 1.39     |
| 30  | 6     | 306 | CHL  | CHC-C4B | 4.74  | 1.47        | 1.39     |
| 30  | f     | 601 | CHL  | C3B-C2B | 4.74  | 1.46        | 1.40     |
| 30  | f     | 608 | CHL  | OBD-CAD | 4.73  | 1.28        | 1.22     |
| 30  | d     | 602 | CHL  | OBD-CAD | 4.73  | 1.28        | 1.22     |
| 30  | 3     | 302 | CHL  | C3D-C2D | 4.73  | 1.47        | 1.39     |
| 30  | 6     | 313 | CHL  | CHB-C4A | -4.73 | 1.32        | 1.38     |
| 30  | e     | 601 | CHL  | CHD-C1D | 4.73  | 1.47        | 1.39     |
| 30  | 4     | 308 | CHL  | CHB-C4A | -4.72 | 1.32        | 1.38     |
| 30  | 9     | 301 | CHL  | C3D-C2D | 4.72  | 1.47        | 1.39     |
| 30  | 8     | 313 | CHL  | CHB-C4A | -4.72 | 1.32        | 1.38     |
| 30  | e     | 608 | CHL  | C3D-C2D | 4.72  | 1.47        | 1.39     |
| 30  | b     | 602 | CHL  | C3A-C2A | -4.72 | 1.50        | 1.54     |
| 30  | b     | 606 | CHL  | OBD-CAD | 4.72  | 1.28        | 1.22     |
| 30  | f     | 606 | CHL  | C3B-C2B | 4.72  | 1.46        | 1.40     |
| 30  | 7     | 313 | CHL  | C3A-C2A | -4.72 | 1.50        | 1.54     |
| 30  | 5     | 301 | CHL  | CHB-C4A | -4.72 | 1.32        | 1.38     |
| 30  | 7     | 302 | CHL  | OBD-CAD | 4.71  | 1.28        | 1.22     |
| 30  | 4     | 308 | CHL  | C3B-C2B | 4.71  | 1.46        | 1.40     |
| 30  | 1     | 306 | CHL  | CHB-C4A | -4.71 | 1.32        | 1.38     |
| 30  | 2     | 301 | CHL  | C3D-C2D | 4.71  | 1.47        | 1.39     |
| 30  | 8     | 313 | CHL  | CHC-C4B | 4.71  | 1.47        | 1.39     |
| 30  | e     | 601 | CHL  | C3A-C2A | -4.71 | 1.50        | 1.54     |
| 30  | 5     | 307 | CHL  | CHB-C1B | 4.71  | 1.47        | 1.39     |
| 30  | 9     | 313 | CHL  | C3A-C2A | -4.71 | 1.50        | 1.54     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 32  | B     | 848 | 8CT  | C19-C20 | 4.70  | 1.57        | 1.43     |
| 30  | 1     | 302 | CHL  | OBD-CAD | 4.70  | 1.28        | 1.22     |
| 30  | 4     | 302 | CHL  | C3D-C2D | 4.70  | 1.47        | 1.39     |
| 30  | 6     | 315 | CHL  | CHB-C4A | -4.70 | 1.33        | 1.38     |
| 30  | c     | 601 | CHL  | CHD-C1D | 4.70  | 1.47        | 1.39     |
| 30  | 1     | 313 | CHL  | C3D-C2D | 4.70  | 1.47        | 1.39     |
| 30  | 8     | 301 | CHL  | C3D-C2D | 4.70  | 1.47        | 1.39     |
| 30  | 4     | 313 | CHL  | CHC-C4B | 4.70  | 1.47        | 1.39     |
| 30  | 8     | 308 | CHL  | C3A-C2A | -4.70 | 1.50        | 1.54     |
| 30  | 9     | 313 | CHL  | C3D-C2D | 4.70  | 1.47        | 1.39     |
| 30  | f     | 609 | CHL  | OBD-CAD | 4.70  | 1.28        | 1.22     |
| 30  | 0     | 305 | CHL  | CHD-C1D | 4.70  | 1.47        | 1.39     |
| 30  | 7     | 307 | CHL  | OBD-CAD | 4.70  | 1.28        | 1.22     |
| 30  | 3     | 302 | CHL  | OBD-CAD | 4.70  | 1.28        | 1.22     |
| 30  | 0     | 305 | CHL  | C3A-C2A | -4.70 | 1.50        | 1.54     |
| 30  | 8     | 307 | CHL  | OBD-CAD | 4.69  | 1.28        | 1.22     |
| 30  | a     | 602 | CHL  | C3B-C2B | 4.69  | 1.46        | 1.40     |
| 30  | h     | 606 | CHL  | CHB-C1B | 4.69  | 1.47        | 1.39     |
| 30  | e     | 608 | CHL  | CHD-C1D | 4.69  | 1.47        | 1.39     |
| 30  | 8     | 305 | CHL  | C3D-C2D | 4.69  | 1.47        | 1.39     |
| 30  | 1     | 306 | CHL  | CHD-C1D | 4.69  | 1.47        | 1.39     |
| 30  | 8     | 306 | CHL  | CHD-C1D | 4.68  | 1.47        | 1.39     |
| 30  | 8     | 305 | CHL  | C3A-C2A | -4.68 | 1.50        | 1.54     |
| 32  | A     | 850 | 8CT  | C06-C07 | 4.68  | 1.67        | 1.52     |
| 30  | a     | 606 | CHL  | CHB-C1B | 4.68  | 1.47        | 1.39     |
| 30  | e     | 607 | CHL  | CHB-C1B | 4.68  | 1.47        | 1.39     |
| 30  | 6     | 308 | CHL  | C3B-C2B | 4.68  | 1.46        | 1.40     |
| 30  | b     | 609 | CHL  | OBD-CAD | 4.68  | 1.28        | 1.22     |
| 30  | f     | 614 | CHL  | CHB-C1B | 4.68  | 1.47        | 1.39     |
| 30  | e     | 601 | CHL  | CHB-C4A | -4.68 | 1.33        | 1.38     |
| 30  | 5     | 307 | CHL  | OBD-CAD | 4.68  | 1.28        | 1.22     |
| 30  | 7     | 313 | CHL  | C3B-C2B | 4.68  | 1.46        | 1.40     |
| 32  | B     | 846 | 8CT  | C06-C07 | 4.68  | 1.67        | 1.52     |
| 30  | 4     | 319 | CHL  | OBD-CAD | 4.68  | 1.28        | 1.22     |
| 30  | 1     | 307 | CHL  | OBD-CAD | 4.68  | 1.28        | 1.22     |
| 30  | 5     | 301 | CHL  | CHD-C1D | 4.67  | 1.47        | 1.39     |
| 30  | f     | 606 | CHL  | CHB-C4A | -4.67 | 1.33        | 1.38     |
| 30  | b     | 608 | CHL  | C3B-C2B | 4.67  | 1.46        | 1.40     |
| 30  | 3     | 307 | CHL  | CHC-C4B | 4.67  | 1.47        | 1.39     |
| 30  | c     | 606 | CHL  | CHD-C1D | 4.67  | 1.47        | 1.39     |
| 30  | e     | 606 | CHL  | CHD-C1D | 4.67  | 1.47        | 1.39     |
| 30  | 8     | 302 | CHL  | OBD-CAD | 4.67  | 1.28        | 1.22     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 30  | c     | 609 | CHL  | CHB-C4A | -4.67 | 1.33        | 1.38     |
| 30  | d     | 608 | CHL  | CHB-C4A | -4.67 | 1.33        | 1.38     |
| 30  | e     | 609 | CHL  | OBD-CAD | 4.67  | 1.28        | 1.22     |
| 30  | 2     | 302 | CHL  | OBD-CAD | 4.67  | 1.28        | 1.22     |
| 30  | 4     | 306 | CHL  | C3D-C2D | 4.67  | 1.47        | 1.39     |
| 30  | 9     | 306 | CHL  | C3B-C2B | 4.66  | 1.46        | 1.40     |
| 30  | 3     | 305 | CHL  | C3D-C2D | 4.66  | 1.47        | 1.39     |
| 30  | 2     | 313 | CHL  | OBD-CAD | 4.66  | 1.28        | 1.22     |
| 30  | 4     | 307 | CHL  | CHC-C4B | 4.66  | 1.47        | 1.39     |
| 30  | 0     | 306 | CHL  | CHB-C1B | 4.66  | 1.47        | 1.39     |
| 30  | c     | 609 | CHL  | CHB-C1B | 4.66  | 1.47        | 1.39     |
| 30  | b     | 606 | CHL  | C3B-C2B | 4.66  | 1.46        | 1.40     |
| 30  | c     | 606 | CHL  | CHB-C4A | -4.65 | 1.33        | 1.38     |
| 30  | 6     | 315 | CHL  | CHD-C1D | 4.65  | 1.47        | 1.39     |
| 30  | e     | 609 | CHL  | CHB-C1B | 4.65  | 1.47        | 1.39     |
| 30  | b     | 601 | CHL  | CHB-C1B | 4.65  | 1.47        | 1.39     |
| 30  | 8     | 305 | CHL  | CHB-C4A | -4.65 | 1.33        | 1.38     |
| 30  | b     | 608 | CHL  | C3D-C2D | 4.65  | 1.47        | 1.39     |
| 30  | 8     | 308 | CHL  | OBD-CAD | 4.65  | 1.28        | 1.22     |
| 30  | 0     | 301 | CHL  | C3D-C2D | 4.65  | 1.47        | 1.39     |
| 32  | 3     | 403 | 8CT  | C06-C07 | 4.65  | 1.67        | 1.52     |
| 30  | 2     | 301 | CHL  | OBD-CAD | 4.65  | 1.28        | 1.22     |
| 30  | 2     | 306 | CHL  | C3B-C2B | 4.65  | 1.46        | 1.40     |
| 30  | 4     | 308 | CHL  | CHD-C1D | 4.65  | 1.47        | 1.39     |
| 30  | 1     | 313 | CHL  | C3B-C2B | 4.65  | 1.46        | 1.40     |
| 30  | f     | 606 | CHL  | C3D-C2D | 4.64  | 1.47        | 1.39     |
| 30  | e     | 609 | CHL  | CHB-C4A | -4.64 | 1.33        | 1.38     |
| 30  | 9     | 305 | CHL  | C3D-C2D | 4.64  | 1.47        | 1.39     |
| 30  | 8     | 301 | CHL  | C3B-C2B | 4.64  | 1.46        | 1.40     |
| 30  | h     | 614 | CHL  | CHD-C4C | 4.64  | 1.48        | 1.39     |
| 30  | 6     | 305 | CHL  | C3D-C2D | 4.64  | 1.47        | 1.39     |
| 30  | 7     | 306 | CHL  | CHD-C1D | 4.64  | 1.47        | 1.39     |
| 30  | 4     | 307 | CHL  | OBD-CAD | 4.64  | 1.28        | 1.22     |
| 30  | 7     | 305 | CHL  | C3D-C2D | 4.64  | 1.47        | 1.39     |
| 30  | 6     | 308 | CHL  | C3A-C2A | -4.64 | 1.50        | 1.54     |
| 30  | g     | 605 | CHL  | CHD-C4C | 4.64  | 1.48        | 1.39     |
| 30  | 4     | 308 | CHL  | OBD-CAD | 4.64  | 1.28        | 1.22     |
| 30  | 6     | 307 | CHL  | OBD-CAD | 4.63  | 1.28        | 1.22     |
| 30  | 0     | 306 | CHL  | CHB-C4A | -4.63 | 1.33        | 1.38     |
| 30  | 0     | 301 | CHL  | OBD-CAD | 4.63  | 1.28        | 1.22     |
| 30  | d     | 605 | CHL  | CHD-C4C | 4.63  | 1.48        | 1.39     |
| 32  | 0     | 401 | 8CT  | C06-C07 | 4.63  | 1.67        | 1.52     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 30  | e     | 601 | CHL  | C3D-C2D | 4.63  | 1.47        | 1.39     |
| 30  | h     | 605 | CHL  | CHD-C4C | 4.62  | 1.48        | 1.39     |
| 30  | 5     | 313 | CHL  | CHB-C1B | 4.62  | 1.47        | 1.39     |
| 30  | 8     | 306 | CHL  | C3B-C2B | 4.62  | 1.46        | 1.40     |
| 30  | c     | 614 | CHL  | CHB-C4A | -4.62 | 1.33        | 1.38     |
| 30  | 8     | 308 | CHL  | CHD-C1D | 4.62  | 1.47        | 1.39     |
| 32  | J     | 101 | 8CT  | C06-C07 | 4.62  | 1.67        | 1.52     |
| 32  | A     | 847 | 8CT  | C06-C07 | 4.62  | 1.67        | 1.52     |
| 30  | 5     | 302 | CHL  | C3D-C2D | 4.62  | 1.47        | 1.39     |
| 30  | 2     | 313 | CHL  | C3B-C2B | 4.61  | 1.46        | 1.40     |
| 30  | 5     | 301 | CHL  | CHB-C1B | 4.61  | 1.47        | 1.39     |
| 30  | b     | 608 | CHL  | CHD-C1D | 4.61  | 1.47        | 1.39     |
| 30  | 1     | 307 | CHL  | CHD-C1D | 4.61  | 1.47        | 1.39     |
| 30  | 8     | 305 | CHL  | CHD-C1D | 4.61  | 1.47        | 1.39     |
| 32  | K     | 107 | 8CT  | C06-C07 | 4.61  | 1.66        | 1.52     |
| 30  | f     | 601 | CHL  | C3A-C2A | -4.61 | 1.50        | 1.54     |
| 30  | 4     | 319 | CHL  | C3D-C2D | 4.61  | 1.47        | 1.39     |
| 30  | b     | 602 | CHL  | C3B-C2B | 4.61  | 1.46        | 1.40     |
| 30  | c     | 614 | CHL  | CHB-C1B | 4.61  | 1.47        | 1.39     |
| 30  | f     | 614 | CHL  | CHB-C4A | -4.60 | 1.33        | 1.38     |
| 30  | 6     | 302 | CHL  | O2D-CGD | 4.60  | 1.44        | 1.33     |
| 30  | 3     | 307 | CHL  | OBD-CAD | 4.60  | 1.28        | 1.22     |
| 30  | a     | 602 | CHL  | CHB-C1B | 4.60  | 1.47        | 1.39     |
| 32  | 7     | 402 | 8CT  | C06-C07 | 4.60  | 1.66        | 1.52     |
| 32  | B     | 845 | 8CT  | C06-C07 | 4.60  | 1.66        | 1.52     |
| 30  | h     | 608 | CHL  | CHB-C1B | 4.60  | 1.47        | 1.39     |
| 30  | 8     | 313 | CHL  | C3D-C2D | 4.60  | 1.47        | 1.39     |
| 30  | 7     | 301 | CHL  | C3B-C2B | 4.60  | 1.46        | 1.40     |
| 32  | A     | 848 | 8CT  | C06-C07 | 4.60  | 1.66        | 1.52     |
| 30  | 0     | 306 | CHL  | CHD-C1D | 4.60  | 1.47        | 1.39     |
| 30  | g     | 609 | CHL  | CHD-C4C | 4.60  | 1.48        | 1.39     |
| 38  | A     | 842 | PQN  | C10-C5  | 4.60  | 1.48        | 1.40     |
| 30  | g     | 614 | CHL  | CHD-C4C | 4.60  | 1.48        | 1.39     |
| 30  | i     | 602 | CHL  | CHB-C4A | -4.60 | 1.33        | 1.38     |
| 30  | i     | 608 | CHL  | CHB-C4A | -4.59 | 1.33        | 1.38     |
| 30  | b     | 607 | CHL  | CHB-C1B | 4.59  | 1.47        | 1.39     |
| 30  | 2     | 313 | CHL  | C3D-C2D | 4.59  | 1.47        | 1.39     |
| 30  | 7     | 307 | CHL  | C3D-C2D | 4.59  | 1.47        | 1.39     |
| 30  | 1     | 305 | CHL  | C3D-C2D | 4.59  | 1.47        | 1.39     |
| 30  | 2     | 319 | CHL  | C3D-C2D | 4.59  | 1.47        | 1.39     |
| 30  | h     | 608 | CHL  | CHB-C4A | -4.59 | 1.33        | 1.38     |
| 30  | 8     | 301 | CHL  | C3A-C2A | -4.59 | 1.50        | 1.54     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 30  | 4     | 305 | CHL  | C3D-C2D | 4.59  | 1.47        | 1.39     |
| 30  | 9     | 301 | CHL  | C3B-C2B | 4.59  | 1.46        | 1.40     |
| 32  | A     | 846 | 8CT  | C06-C07 | 4.59  | 1.66        | 1.52     |
| 30  | a     | 614 | CHL  | CHD-C4C | 4.58  | 1.48        | 1.39     |
| 30  | i     | 602 | CHL  | CHB-C1B | 4.58  | 1.47        | 1.39     |
| 30  | f     | 606 | CHL  | CHB-C1B | 4.58  | 1.47        | 1.39     |
| 30  | 6     | 313 | CHL  | C3B-C2B | 4.58  | 1.46        | 1.40     |
| 32  | B     | 844 | 8CT  | C06-C07 | 4.58  | 1.66        | 1.52     |
| 30  | 7     | 313 | CHL  | CHD-C1D | 4.58  | 1.47        | 1.39     |
| 30  | h     | 608 | CHL  | O2A-CGA | 4.58  | 1.45        | 1.30     |
| 30  | 8     | 301 | CHL  | CHD-C1D | 4.58  | 1.47        | 1.39     |
| 30  | b     | 602 | CHL  | CHD-C1D | 4.58  | 1.47        | 1.39     |
| 30  | 6     | 306 | CHL  | C3D-C2D | 4.57  | 1.47        | 1.39     |
| 32  | 4     | 402 | 8CT  | C06-C07 | 4.57  | 1.66        | 1.52     |
| 32  | I     | 101 | 8CT  | C06-C07 | 4.57  | 1.66        | 1.52     |
| 30  | b     | 608 | CHL  | C3A-C2A | -4.57 | 1.50        | 1.54     |
| 32  | 1     | 402 | 8CT  | C19-C20 | 4.57  | 1.57        | 1.43     |
| 30  | b     | 601 | CHL  | CHB-C4A | -4.56 | 1.33        | 1.38     |
| 30  | f     | 608 | CHL  | C3B-C2B | 4.56  | 1.46        | 1.40     |
| 32  | 7     | 404 | 8CT  | C19-C20 | 4.56  | 1.57        | 1.43     |
| 30  | 8     | 307 | CHL  | C3D-C2D | 4.56  | 1.47        | 1.39     |
| 30  | c     | 605 | CHL  | CHD-C4C | 4.56  | 1.48        | 1.39     |
| 32  | L     | 209 | 8CT  | C06-C07 | 4.56  | 1.66        | 1.52     |
| 32  | B     | 843 | 8CT  | C19-C20 | 4.56  | 1.57        | 1.43     |
| 30  | g     | 602 | CHL  | CHB-C4A | -4.56 | 1.33        | 1.38     |
| 30  | f     | 608 | CHL  | C3D-C2D | 4.56  | 1.47        | 1.39     |
| 30  | f     | 605 | CHL  | CHD-C4C | 4.56  | 1.48        | 1.39     |
| 30  | 6     | 302 | CHL  | C3B-C2B | 4.56  | 1.46        | 1.40     |
| 30  | b     | 606 | CHL  | CHD-C1D | 4.56  | 1.47        | 1.39     |
| 30  | b     | 609 | CHL  | CHB-C4A | -4.56 | 1.33        | 1.38     |
| 32  | 0     | 401 | 8CT  | C19-C20 | 4.56  | 1.57        | 1.43     |
| 30  | d     | 602 | CHL  | CHD-C1D | 4.56  | 1.47        | 1.39     |
| 30  | e     | 606 | CHL  | CHB-C1B | 4.56  | 1.47        | 1.39     |
| 30  | 2     | 307 | CHL  | OBD-CAD | 4.56  | 1.28        | 1.22     |
| 30  | a     | 605 | CHL  | CHD-C4C | 4.56  | 1.48        | 1.39     |
| 30  | h     | 607 | CHL  | O2A-CGA | 4.55  | 1.45        | 1.30     |
| 32  | G     | 104 | 8CT  | C19-C20 | 4.55  | 1.57        | 1.43     |
| 30  | b     | 607 | CHL  | CHB-C4A | -4.55 | 1.33        | 1.38     |
| 30  | i     | 609 | CHL  | CHD-C4C | 4.55  | 1.48        | 1.39     |
| 30  | 7     | 301 | CHL  | CHD-C1D | 4.55  | 1.47        | 1.39     |
| 32  | 7     | 405 | 8CT  | C06-C07 | 4.55  | 1.66        | 1.52     |
| 30  | d     | 609 | CHL  | CHB-C4A | -4.55 | 1.33        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 32  | 8     | 406 | 8CT  | C19-C20 | 4.55  | 1.57        | 1.43     |
| 32  | B     | 844 | 8CT  | C19-C20 | 4.55  | 1.57        | 1.43     |
| 32  | 9     | 401 | 8CT  | C06-C07 | 4.55  | 1.66        | 1.52     |
| 30  | c     | 606 | CHL  | CHB-C1B | 4.55  | 1.47        | 1.39     |
| 30  | d     | 608 | CHL  | CHB-C1B | 4.54  | 1.47        | 1.39     |
| 30  | 9     | 305 | CHL  | OBD-CAD | 4.54  | 1.28        | 1.22     |
| 30  | g     | 607 | CHL  | CHD-C4C | 4.54  | 1.48        | 1.39     |
| 30  | 2     | 308 | CHL  | OBD-CAD | 4.54  | 1.28        | 1.22     |
| 30  | 9     | 313 | CHL  | C3B-C2B | 4.54  | 1.46        | 1.40     |
| 30  | e     | 602 | CHL  | C3B-C2B | 4.54  | 1.46        | 1.40     |
| 32  | B     | 845 | 8CT  | C19-C20 | 4.54  | 1.57        | 1.43     |
| 30  | 5     | 306 | CHL  | CHB-C4A | -4.54 | 1.33        | 1.38     |
| 30  | 2     | 319 | CHL  | CHD-C1D | 4.54  | 1.47        | 1.39     |
| 30  | 6     | 308 | CHL  | CHB-C1B | 4.53  | 1.47        | 1.39     |
| 30  | 6     | 315 | CHL  | CHB-C1B | 4.53  | 1.47        | 1.39     |
| 30  | d     | 614 | CHL  | CHD-C4C | 4.53  | 1.48        | 1.39     |
| 38  | B     | 842 | PQN  | C10-C5  | 4.53  | 1.48        | 1.40     |
| 32  | B     | 843 | 8CT  | C06-C07 | 4.53  | 1.66        | 1.52     |
| 30  | 9     | 301 | CHL  | CHD-C1D | 4.53  | 1.47        | 1.39     |
| 32  | O     | 205 | 8CT  | C06-C07 | 4.53  | 1.66        | 1.52     |
| 30  | 4     | 308 | CHL  | CHB-C1B | 4.53  | 1.46        | 1.39     |
| 30  | g     | 601 | CHL  | CHD-C4C | 4.52  | 1.48        | 1.39     |
| 32  | 3     | 402 | 8CT  | C06-C07 | 4.52  | 1.66        | 1.52     |
| 30  | 8     | 315 | CHL  | CHB-C4A | -4.52 | 1.33        | 1.38     |
| 30  | i     | 605 | CHL  | CHD-C4C | 4.52  | 1.48        | 1.39     |
| 30  | f     | 609 | CHL  | CHB-C4A | -4.52 | 1.33        | 1.38     |
| 30  | 8     | 301 | CHL  | CHB-C1B | 4.52  | 1.46        | 1.39     |
| 30  | a     | 608 | CHL  | CHB-C4A | -4.52 | 1.33        | 1.38     |
| 30  | 6     | 308 | CHL  | CHD-C1D | 4.52  | 1.46        | 1.39     |
| 30  | 6     | 315 | CHL  | C3A-C2A | -4.52 | 1.50        | 1.54     |
| 32  | 9     | 401 | 8CT  | C19-C20 | 4.52  | 1.57        | 1.43     |
| 30  | 1     | 306 | CHL  | CHB-C1B | 4.52  | 1.46        | 1.39     |
| 30  | 9     | 306 | CHL  | CHD-C1D | 4.52  | 1.46        | 1.39     |
| 30  | 5     | 305 | CHL  | O2A-CGA | 4.51  | 1.45        | 1.30     |
| 30  | 8     | 308 | CHL  | C3B-C2B | 4.51  | 1.46        | 1.40     |
| 30  | 5     | 305 | CHL  | C3A-C2A | -4.51 | 1.50        | 1.54     |
| 32  | L     | 206 | 8CT  | C06-C07 | 4.51  | 1.66        | 1.52     |
| 30  | 4     | 307 | CHL  | C3D-C2D | 4.51  | 1.47        | 1.39     |
| 32  | A     | 854 | 8CT  | C06-C07 | 4.51  | 1.66        | 1.52     |
| 30  | 2     | 319 | CHL  | C3B-C2B | 4.51  | 1.46        | 1.40     |
| 30  | 6     | 307 | CHL  | C3D-C2D | 4.51  | 1.47        | 1.39     |
| 30  | a     | 608 | CHL  | CHB-C1B | 4.51  | 1.46        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 32  | L     | 205 | 8CT  | C06-C07 | 4.51  | 1.66        | 1.52     |
| 32  | 7     | 404 | 8CT  | C06-C07 | 4.51  | 1.66        | 1.52     |
| 30  | 0     | 305 | CHL  | CHB-C1B | 4.50  | 1.46        | 1.39     |
| 30  | e     | 607 | CHL  | CHB-C4A | -4.50 | 1.33        | 1.38     |
| 32  | A     | 850 | 8CT  | C19-C20 | 4.50  | 1.57        | 1.43     |
| 30  | 7     | 313 | CHL  | CHB-C1B | 4.50  | 1.46        | 1.39     |
| 32  | 2     | 402 | 8CT  | C06-C07 | 4.50  | 1.66        | 1.52     |
| 30  | 9     | 313 | CHL  | CHD-C1D | 4.50  | 1.46        | 1.39     |
| 32  | B     | 847 | 8CT  | C06-C07 | 4.50  | 1.66        | 1.52     |
| 30  | h     | 601 | CHL  | CHD-C4C | 4.49  | 1.48        | 1.39     |
| 30  | i     | 608 | CHL  | CHB-C1B | 4.49  | 1.46        | 1.39     |
| 32  | M     | 102 | 8CT  | C06-C07 | 4.49  | 1.66        | 1.52     |
| 30  | 0     | 305 | CHL  | C3B-C2B | 4.49  | 1.46        | 1.40     |
| 30  | 8     | 308 | CHL  | CHB-C1B | 4.49  | 1.46        | 1.39     |
| 30  | 6     | 313 | CHL  | C3D-C2D | 4.49  | 1.47        | 1.39     |
| 30  | d     | 605 | CHL  | CHC-C1C | 4.49  | 1.48        | 1.39     |
| 30  | h     | 607 | CHL  | CHD-C4C | 4.49  | 1.48        | 1.39     |
| 30  | f     | 608 | CHL  | CHD-C1D | 4.49  | 1.46        | 1.39     |
| 32  | B     | 851 | 8CT  | C06-C07 | 4.49  | 1.66        | 1.52     |
| 30  | 4     | 306 | CHL  | C3B-C2B | 4.49  | 1.46        | 1.40     |
| 32  | 8     | 402 | 8CT  | C06-C07 | 4.49  | 1.66        | 1.52     |
| 30  | 1     | 305 | CHL  | CHD-C1D | 4.49  | 1.46        | 1.39     |
| 30  | 4     | 306 | CHL  | CHD-C1D | 4.49  | 1.46        | 1.39     |
| 30  | d     | 602 | CHL  | C3B-C2B | 4.48  | 1.46        | 1.40     |
| 30  | 8     | 313 | CHL  | CHD-C1D | 4.48  | 1.46        | 1.39     |
| 32  | B     | 846 | 8CT  | C19-C20 | 4.48  | 1.57        | 1.43     |
| 30  | a     | 602 | CHL  | C3A-C2A | -4.48 | 1.50        | 1.54     |
| 30  | 2     | 306 | CHL  | CHD-C1D | 4.48  | 1.46        | 1.39     |
| 30  | 4     | 307 | CHL  | C3B-C2B | 4.48  | 1.46        | 1.40     |
| 30  | 9     | 313 | CHL  | CHB-C1B | 4.48  | 1.46        | 1.39     |
| 30  | i     | 614 | CHL  | CHD-C4C | 4.48  | 1.48        | 1.39     |
| 30  | h     | 602 | CHL  | CHC-C1C | 4.48  | 1.48        | 1.39     |
| 30  | a     | 609 | CHL  | CHD-C4C | 4.48  | 1.48        | 1.39     |
| 30  | c     | 602 | CHL  | CHD-C1D | 4.48  | 1.46        | 1.39     |
| 32  | 6     | 402 | 8CT  | C06-C07 | 4.47  | 1.66        | 1.52     |
| 32  | 6     | 402 | 8CT  | C19-C20 | 4.47  | 1.57        | 1.43     |
| 32  | 1     | 402 | 8CT  | C06-C07 | 4.47  | 1.66        | 1.52     |
| 30  | d     | 606 | CHL  | CHB-C4A | -4.47 | 1.33        | 1.38     |
| 32  | 8     | 402 | 8CT  | C19-C20 | 4.47  | 1.57        | 1.43     |
| 32  | J     | 104 | 8CT  | C06-C07 | 4.47  | 1.66        | 1.52     |
| 30  | h     | 609 | CHL  | CHD-C4C | 4.47  | 1.48        | 1.39     |
| 30  | i     | 606 | CHL  | CHD-C4C | 4.47  | 1.48        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 30  | 1     | 306 | CHL  | C3A-C2A | -4.47 | 1.50        | 1.54     |
| 30  | f     | 606 | CHL  | C3A-C2A | -4.47 | 1.50        | 1.54     |
| 30  | 8     | 313 | CHL  | C3B-C2B | 4.47  | 1.46        | 1.40     |
| 30  | c     | 607 | CHL  | CHB-C4A | -4.47 | 1.33        | 1.38     |
| 30  | 6     | 301 | CHL  | CHB-C1B | 4.47  | 1.46        | 1.39     |
| 30  | 7     | 307 | CHL  | C3A-C2A | -4.46 | 1.50        | 1.54     |
| 30  | 1     | 313 | CHL  | CHD-C1D | 4.46  | 1.46        | 1.39     |
| 30  | i     | 607 | CHL  | CHD-C4C | 4.46  | 1.47        | 1.39     |
| 30  | 5     | 307 | CHL  | CHB-C4A | -4.46 | 1.33        | 1.38     |
| 30  | 6     | 313 | CHL  | CHB-C1B | 4.46  | 1.46        | 1.39     |
| 30  | 2     | 308 | CHL  | C3B-C2B | 4.46  | 1.46        | 1.40     |
| 30  | h     | 609 | CHL  | CHB-C4A | -4.46 | 1.33        | 1.38     |
| 32  | 8     | 406 | 8CT  | C06-C07 | 4.46  | 1.66        | 1.52     |
| 30  | 0     | 301 | CHL  | C3B-C2B | 4.45  | 1.46        | 1.40     |
| 32  | A     | 849 | 8CT  | C06-C07 | 4.45  | 1.66        | 1.52     |
| 30  | 8     | 307 | CHL  | C3B-C2B | 4.45  | 1.46        | 1.40     |
| 32  | B     | 804 | 8CT  | C06-C07 | 4.45  | 1.66        | 1.52     |
| 30  | c     | 601 | CHL  | C3B-C2B | 4.45  | 1.46        | 1.40     |
| 32  | F     | 302 | 8CT  | C06-C07 | 4.45  | 1.66        | 1.52     |
| 32  | A     | 854 | 8CT  | C19-C20 | 4.45  | 1.57        | 1.43     |
| 30  | 7     | 302 | CHL  | C3D-C2D | 4.45  | 1.47        | 1.39     |
| 30  | e     | 606 | CHL  | C3A-C2A | -4.45 | 1.50        | 1.54     |
| 30  | 7     | 306 | CHL  | OBD-CAD | 4.45  | 1.28        | 1.22     |
| 32  | 3     | 402 | 8CT  | C19-C20 | 4.45  | 1.57        | 1.43     |
| 30  | e     | 608 | CHL  | C3A-C2A | -4.45 | 1.50        | 1.54     |
| 30  | 5     | 305 | CHL  | CHB-C1B | 4.44  | 1.46        | 1.39     |
| 32  | O     | 205 | 8CT  | C19-C20 | 4.44  | 1.57        | 1.43     |
| 30  | i     | 601 | CHL  | CHD-C4C | 4.44  | 1.47        | 1.39     |
| 30  | b     | 602 | CHL  | CHB-C1B | 4.44  | 1.46        | 1.39     |
| 30  | 4     | 313 | CHL  | C3B-C2B | 4.44  | 1.46        | 1.40     |
| 30  | h     | 605 | CHL  | CHC-C1C | 4.44  | 1.47        | 1.39     |
| 30  | h     | 602 | CHL  | CHD-C4C | 4.44  | 1.47        | 1.39     |
| 30  | 8     | 305 | CHL  | CHB-C1B | 4.44  | 1.46        | 1.39     |
| 32  | K     | 107 | 8CT  | C19-C20 | 4.44  | 1.57        | 1.43     |
| 30  | h     | 614 | CHL  | CHC-C1C | 4.44  | 1.47        | 1.39     |
| 30  | c     | 602 | CHL  | C3B-C2B | 4.44  | 1.46        | 1.40     |
| 30  | 7     | 307 | CHL  | CHD-C1D | 4.44  | 1.46        | 1.39     |
| 32  | L     | 209 | 8CT  | C19-C20 | 4.44  | 1.56        | 1.43     |
| 30  | 6     | 305 | CHL  | C3B-C2B | 4.44  | 1.46        | 1.40     |
| 30  | a     | 607 | CHL  | CHD-C4C | 4.44  | 1.47        | 1.39     |
| 32  | B     | 846 | 8CT  | C24-C25 | 4.44  | 1.56        | 1.43     |
| 32  | G     | 104 | 8CT  | C06-C07 | 4.43  | 1.66        | 1.52     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 30  | g     | 605 | CHL  | CHC-C1C | 4.43  | 1.47        | 1.39     |
| 32  | B     | 848 | 8CT  | C06-C07 | 4.43  | 1.66        | 1.52     |
| 30  | f     | 601 | CHL  | CHB-C1B | 4.43  | 1.46        | 1.39     |
| 30  | b     | 614 | CHL  | CHD-C4C | 4.43  | 1.47        | 1.39     |
| 30  | d     | 601 | CHL  | CHD-C4C | 4.43  | 1.47        | 1.39     |
| 30  | c     | 609 | CHL  | CHD-C4C | 4.42  | 1.47        | 1.39     |
| 32  | J     | 104 | 8CT  | C19-C20 | 4.42  | 1.56        | 1.43     |
| 30  | 1     | 307 | CHL  | CHB-C1B | 4.42  | 1.46        | 1.39     |
| 30  | d     | 609 | CHL  | CHD-C4C | 4.42  | 1.47        | 1.39     |
| 30  | d     | 607 | CHL  | CHD-C4C | 4.42  | 1.47        | 1.39     |
| 32  | L     | 205 | 8CT  | C19-C20 | 4.42  | 1.56        | 1.43     |
| 32  | B     | 847 | 8CT  | C19-C20 | 4.42  | 1.56        | 1.43     |
| 30  | a     | 606 | CHL  | CHB-C4A | -4.42 | 1.33        | 1.38     |
| 30  | e     | 605 | CHL  | CHD-C4C | 4.42  | 1.47        | 1.39     |
| 32  | M     | 102 | 8CT  | C19-C20 | 4.42  | 1.56        | 1.43     |
| 30  | 4     | 319 | CHL  | C3B-C2B | 4.42  | 1.46        | 1.40     |
| 30  | 6     | 301 | CHL  | CHD-C1D | 4.42  | 1.46        | 1.39     |
| 30  | 6     | 305 | CHL  | CHD-C1D | 4.42  | 1.46        | 1.39     |
| 30  | a     | 605 | CHL  | CHC-C1C | 4.42  | 1.47        | 1.39     |
| 30  | 5     | 313 | CHL  | CHD-C4C | 4.42  | 1.47        | 1.39     |
| 30  | 2     | 307 | CHL  | C3D-C2D | 4.42  | 1.47        | 1.39     |
| 30  | h     | 606 | CHL  | CHB-C4A | -4.41 | 1.33        | 1.38     |
| 32  | B     | 804 | 8CT  | C19-C20 | 4.41  | 1.56        | 1.43     |
| 32  | L     | 206 | 8CT  | C19-C20 | 4.41  | 1.56        | 1.43     |
| 30  | c     | 606 | CHL  | C3A-C2A | -4.41 | 1.50        | 1.54     |
| 30  | g     | 608 | CHL  | CHC-C1C | 4.41  | 1.47        | 1.39     |
| 30  | f     | 609 | CHL  | CHD-C4C | 4.41  | 1.47        | 1.39     |
| 30  | i     | 605 | CHL  | CHC-C1C | 4.41  | 1.47        | 1.39     |
| 30  | e     | 608 | CHL  | CHB-C1B | 4.41  | 1.46        | 1.39     |
| 30  | h     | 602 | CHL  | CHB-C4A | -4.41 | 1.33        | 1.38     |
| 30  | 2     | 301 | CHL  | C3B-C2B | 4.41  | 1.46        | 1.40     |
| 30  | a     | 614 | CHL  | CHC-C1C | 4.41  | 1.47        | 1.39     |
| 30  | b     | 601 | CHL  | CHD-C4C | 4.40  | 1.47        | 1.39     |
| 30  | g     | 614 | CHL  | CHC-C1C | 4.40  | 1.47        | 1.39     |
| 32  | 3     | 403 | 8CT  | C19-C20 | 4.40  | 1.56        | 1.43     |
| 30  | g     | 606 | CHL  | CHB-C4A | -4.40 | 1.33        | 1.38     |
| 30  | a     | 606 | CHL  | CHD-C4C | 4.40  | 1.47        | 1.39     |
| 30  | g     | 608 | CHL  | CHD-C4C | 4.40  | 1.47        | 1.39     |
| 30  | e     | 614 | CHL  | CHD-C4C | 4.40  | 1.47        | 1.39     |
| 30  | a     | 609 | CHL  | CHB-C4A | -4.40 | 1.33        | 1.38     |
| 30  | 6     | 301 | CHL  | C3B-C2B | 4.40  | 1.46        | 1.40     |
| 30  | 1     | 307 | CHL  | C3D-C2D | 4.40  | 1.47        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 30  | c     | 608 | CHL  | CHB-C1B | 4.40  | 1.46        | 1.39     |
| 30  | d     | 614 | CHL  | CHC-C1C | 4.39  | 1.47        | 1.39     |
| 30  | b     | 608 | CHL  | CHB-C1B | 4.39  | 1.46        | 1.39     |
| 30  | f     | 607 | CHL  | CHD-C4C | 4.39  | 1.47        | 1.39     |
| 30  | 5     | 306 | CHL  | CHD-C4C | 4.39  | 1.47        | 1.39     |
| 30  | g     | 608 | CHL  | CHB-C4A | -4.39 | 1.33        | 1.38     |
| 30  | 8     | 307 | CHL  | CHD-C1D | 4.39  | 1.46        | 1.39     |
| 30  | 6     | 306 | CHL  | CHD-C1D | 4.39  | 1.46        | 1.39     |
| 30  | 6     | 313 | CHL  | CHD-C1D | 4.39  | 1.46        | 1.39     |
| 32  | 4     | 402 | 8CT  | C19-C20 | 4.38  | 1.56        | 1.43     |
| 32  | 7     | 405 | 8CT  | C19-C20 | 4.38  | 1.56        | 1.43     |
| 30  | e     | 601 | CHL  | CHB-C1B | 4.38  | 1.46        | 1.39     |
| 32  | A     | 846 | 8CT  | C19-C20 | 4.38  | 1.56        | 1.43     |
| 30  | h     | 601 | CHL  | CHB-C4A | -4.38 | 1.33        | 1.38     |
| 30  | h     | 607 | CHL  | CHC-C1C | 4.38  | 1.47        | 1.39     |
| 30  | a     | 601 | CHL  | CHD-C4C | 4.38  | 1.47        | 1.39     |
| 30  | 3     | 305 | CHL  | CHD-C1D | 4.38  | 1.46        | 1.39     |
| 30  | g     | 606 | CHL  | CHD-C4C | 4.38  | 1.47        | 1.39     |
| 30  | 2     | 307 | CHL  | C3B-C2B | 4.38  | 1.46        | 1.40     |
| 30  | 7     | 305 | CHL  | CHD-C1D | 4.38  | 1.46        | 1.39     |
| 30  | c     | 607 | CHL  | CHD-C4C | 4.38  | 1.47        | 1.39     |
| 30  | a     | 607 | CHL  | CHB-C4A | -4.37 | 1.33        | 1.38     |
| 30  | f     | 606 | CHL  | CHD-C4C | 4.37  | 1.47        | 1.39     |
| 30  | e     | 609 | CHL  | C3A-C2A | -4.37 | 1.50        | 1.54     |
| 32  | B     | 851 | 8CT  | C19-C20 | 4.37  | 1.56        | 1.43     |
| 30  | 2     | 301 | CHL  | CHD-C1D | 4.37  | 1.46        | 1.39     |
| 32  | J     | 101 | 8CT  | C19-C20 | 4.37  | 1.56        | 1.43     |
| 30  | d     | 607 | CHL  | CHC-C1C | 4.37  | 1.47        | 1.39     |
| 32  | B     | 843 | 8CT  | C24-C25 | 4.36  | 1.56        | 1.43     |
| 30  | 0     | 306 | CHL  | C3A-C2A | -4.36 | 1.50        | 1.54     |
| 32  | I     | 101 | 8CT  | C19-C20 | 4.36  | 1.56        | 1.43     |
| 30  | f     | 605 | CHL  | CHC-C1C | 4.36  | 1.47        | 1.39     |
| 32  | F     | 302 | 8CT  | C19-C20 | 4.36  | 1.56        | 1.43     |
| 30  | 3     | 307 | CHL  | C3D-C2D | 4.36  | 1.47        | 1.39     |
| 30  | b     | 609 | CHL  | CHD-C4C | 4.36  | 1.47        | 1.39     |
| 30  | d     | 601 | CHL  | CHC-C1C | 4.36  | 1.47        | 1.39     |
| 30  | 2     | 308 | CHL  | CHD-C1D | 4.36  | 1.46        | 1.39     |
| 30  | 5     | 313 | CHL  | CHB-C4A | -4.35 | 1.33        | 1.38     |
| 30  | 0     | 301 | CHL  | CHD-C1D | 4.35  | 1.46        | 1.39     |
| 30  | g     | 602 | CHL  | CHD-C4C | 4.35  | 1.47        | 1.39     |
| 30  | h     | 606 | CHL  | C3A-C2A | -4.35 | 1.51        | 1.54     |
| 30  | 4     | 305 | CHL  | CHD-C1D | 4.35  | 1.46        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 30  | c     | 605 | CHL  | CHC-C1C | 4.35  | 1.47        | 1.39     |
| 30  | 5     | 313 | CHL  | C3A-C2A | -4.35 | 1.51        | 1.54     |
| 30  | a     | 606 | CHL  | O2A-CGA | 4.35  | 1.46        | 1.33     |
| 30  | 8     | 307 | CHL  | CHB-C1B | 4.35  | 1.46        | 1.39     |
| 30  | g     | 601 | CHL  | CHC-C1C | 4.35  | 1.47        | 1.39     |
| 30  | 7     | 306 | CHL  | CHB-C1B | 4.35  | 1.46        | 1.39     |
| 30  | 4     | 306 | CHL  | O2A-CGA | 4.34  | 1.46        | 1.33     |
| 32  | A     | 847 | 8CT  | C19-C20 | 4.34  | 1.56        | 1.43     |
| 30  | 6     | 306 | CHL  | C3B-C2B | 4.34  | 1.46        | 1.40     |
| 30  | f     | 602 | CHL  | CHD-C1D | 4.34  | 1.46        | 1.39     |
| 30  | g     | 607 | CHL  | CHB-C4A | -4.34 | 1.33        | 1.38     |
| 30  | i     | 606 | CHL  | O2A-CGA | 4.34  | 1.46        | 1.33     |
| 30  | 2     | 301 | CHL  | O2A-CGA | 4.34  | 1.46        | 1.33     |
| 30  | i     | 601 | CHL  | CHC-C1C | 4.34  | 1.47        | 1.39     |
| 30  | b     | 606 | CHL  | CHB-C1B | 4.34  | 1.46        | 1.39     |
| 30  | d     | 606 | CHL  | CHD-C4C | 4.34  | 1.47        | 1.39     |
| 30  | g     | 606 | CHL  | O2A-CGA | 4.33  | 1.46        | 1.33     |
| 30  | 4     | 302 | CHL  | CHD-C1D | 4.33  | 1.46        | 1.39     |
| 30  | a     | 602 | CHL  | CHD-C4C | 4.33  | 1.47        | 1.39     |
| 30  | 9     | 305 | CHL  | O2A-CGA | 4.33  | 1.46        | 1.33     |
| 30  | 5     | 306 | CHL  | O2A-CGA | 4.33  | 1.46        | 1.33     |
| 30  | 2     | 306 | CHL  | O2A-CGA | 4.33  | 1.46        | 1.33     |
| 30  | f     | 608 | CHL  | CHB-C1B | 4.33  | 1.46        | 1.39     |
| 30  | e     | 605 | CHL  | CHC-C1C | 4.33  | 1.47        | 1.39     |
| 30  | g     | 601 | CHL  | O2A-CGA | 4.33  | 1.46        | 1.33     |
| 30  | i     | 606 | CHL  | CHB-C4A | -4.33 | 1.33        | 1.38     |
| 32  | 2     | 402 | 8CT  | C19-C20 | 4.33  | 1.56        | 1.43     |
| 30  | f     | 614 | CHL  | C2A-C3A | -4.33 | 1.51        | 1.54     |
| 30  | 6     | 308 | CHL  | O2A-CGA | 4.32  | 1.46        | 1.33     |
| 30  | 5     | 301 | CHL  | C3A-C2A | -4.32 | 1.51        | 1.54     |
| 30  | e     | 602 | CHL  | O2A-CGA | 4.32  | 1.45        | 1.33     |
| 30  | 2     | 302 | CHL  | CHD-C1D | 4.32  | 1.46        | 1.39     |
| 30  | 2     | 305 | CHL  | CHD-C1D | 4.32  | 1.46        | 1.39     |
| 30  | 2     | 306 | CHL  | CHB-C1B | 4.32  | 1.46        | 1.39     |
| 30  | g     | 602 | CHL  | CHC-C1C | 4.32  | 1.47        | 1.39     |
| 30  | 0     | 301 | CHL  | O2A-CGA | 4.32  | 1.45        | 1.33     |
| 30  | b     | 609 | CHL  | C3A-C2A | -4.32 | 1.51        | 1.54     |
| 30  | 7     | 301 | CHL  | CHB-C1B | 4.32  | 1.46        | 1.39     |
| 30  | b     | 609 | CHL  | O2A-CGA | 4.32  | 1.45        | 1.33     |
| 30  | i     | 609 | CHL  | CHC-C1C | 4.32  | 1.47        | 1.39     |
| 30  | 2     | 308 | CHL  | CHB-C1B | 4.32  | 1.46        | 1.39     |
| 30  | d     | 606 | CHL  | O2A-CGA | 4.32  | 1.45        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 30  | 5     | 302 | CHL  | O2A-CGA | 4.32  | 1.45        | 1.33     |
| 32  | 4     | 402 | 8CT  | C24-C25 | 4.32  | 1.56        | 1.43     |
| 30  | 6     | 306 | CHL  | O2A-CGA | 4.31  | 1.45        | 1.33     |
| 30  | 8     | 305 | CHL  | C3B-C2B | 4.31  | 1.46        | 1.40     |
| 30  | 4     | 319 | CHL  | CHD-C1D | 4.31  | 1.46        | 1.39     |
| 30  | a     | 609 | CHL  | O2A-CGA | 4.31  | 1.45        | 1.33     |
| 30  | 7     | 305 | CHL  | O2A-CGA | 4.31  | 1.45        | 1.33     |
| 30  | 2     | 305 | CHL  | C3B-C2B | 4.31  | 1.46        | 1.40     |
| 30  | 8     | 306 | CHL  | O2A-CGA | 4.31  | 1.45        | 1.33     |
| 30  | e     | 614 | CHL  | CHB-C4A | -4.31 | 1.33        | 1.38     |
| 30  | f     | 614 | CHL  | CHD-C4C | 4.31  | 1.47        | 1.39     |
| 30  | 0     | 302 | CHL  | CHD-C1D | 4.31  | 1.46        | 1.39     |
| 30  | b     | 601 | CHL  | O2A-CGA | 4.31  | 1.45        | 1.33     |
| 30  | f     | 606 | CHL  | O2A-CGA | 4.31  | 1.45        | 1.33     |
| 30  | 1     | 313 | CHL  | CHB-C1B | 4.31  | 1.46        | 1.39     |
| 30  | g     | 609 | CHL  | CHC-C1C | 4.31  | 1.47        | 1.39     |
| 30  | i     | 607 | CHL  | CHB-C4A | -4.31 | 1.33        | 1.38     |
| 30  | b     | 606 | CHL  | O2A-CGA | 4.31  | 1.45        | 1.33     |
| 32  | 2     | 402 | 8CT  | C24-C25 | 4.31  | 1.56        | 1.43     |
| 30  | 9     | 305 | CHL  | CHD-C1D | 4.31  | 1.46        | 1.39     |
| 30  | i     | 608 | CHL  | O2A-CGA | 4.30  | 1.45        | 1.33     |
| 30  | c     | 602 | CHL  | CHB-C1B | 4.30  | 1.46        | 1.39     |
| 30  | 8     | 315 | CHL  | CHD-C4C | 4.30  | 1.47        | 1.39     |
| 30  | g     | 602 | CHL  | O2A-CGA | 4.30  | 1.45        | 1.33     |
| 30  | 1     | 306 | CHL  | O2A-CGA | 4.30  | 1.45        | 1.33     |
| 30  | e     | 605 | CHL  | CHB-C4A | -4.30 | 1.33        | 1.38     |
| 30  | f     | 609 | CHL  | O2A-CGA | 4.30  | 1.45        | 1.33     |
| 30  | 9     | 301 | CHL  | CHB-C1B | 4.30  | 1.46        | 1.39     |
| 30  | h     | 601 | CHL  | CHC-C1C | 4.30  | 1.47        | 1.39     |
| 30  | 7     | 301 | CHL  | O2A-CGA | 4.30  | 1.45        | 1.33     |
| 30  | e     | 607 | CHL  | C3A-C2A | -4.30 | 1.51        | 1.54     |
| 30  | 6     | 307 | CHL  | CHD-C1D | 4.30  | 1.46        | 1.39     |
| 30  | e     | 607 | CHL  | CHD-C4C | 4.30  | 1.47        | 1.39     |
| 30  | i     | 614 | CHL  | CHC-C1C | 4.30  | 1.47        | 1.39     |
| 30  | c     | 609 | CHL  | C3A-C2A | -4.30 | 1.51        | 1.54     |
| 30  | 4     | 305 | CHL  | C3B-C2B | 4.30  | 1.46        | 1.40     |
| 30  | 5     | 302 | CHL  | CHD-C1D | 4.29  | 1.46        | 1.39     |
| 30  | i     | 606 | CHL  | CHC-C1C | 4.29  | 1.47        | 1.39     |
| 32  | 7     | 402 | 8CT  | C19-C20 | 4.29  | 1.56        | 1.43     |
| 30  | 7     | 307 | CHL  | C3B-C2B | 4.29  | 1.46        | 1.40     |
| 30  | 9     | 306 | CHL  | CHB-C1B | 4.29  | 1.46        | 1.39     |
| 30  | d     | 609 | CHL  | O2A-CGA | 4.29  | 1.45        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 30  | 5     | 301 | CHL  | CHD-C4C | 4.29  | 1.47        | 1.39     |
| 30  | 1     | 305 | CHL  | O2A-CGA | 4.29  | 1.45        | 1.33     |
| 30  | e     | 608 | CHL  | O2A-CGA | 4.29  | 1.45        | 1.33     |
| 30  | g     | 607 | CHL  | O2A-CGA | 4.29  | 1.45        | 1.33     |
| 30  | 0     | 306 | CHL  | O2A-CGA | 4.29  | 1.45        | 1.33     |
| 30  | b     | 614 | CHL  | CHC-C1C | 4.29  | 1.47        | 1.39     |
| 30  | e     | 606 | CHL  | O2A-CGA | 4.29  | 1.45        | 1.33     |
| 30  | 2     | 313 | CHL  | CHD-C1D | 4.29  | 1.46        | 1.39     |
| 30  | 7     | 305 | CHL  | C3B-C2B | 4.29  | 1.46        | 1.40     |
| 30  | d     | 608 | CHL  | O2A-CGA | 4.29  | 1.45        | 1.33     |
| 30  | 9     | 305 | CHL  | C3B-C2B | 4.28  | 1.46        | 1.40     |
| 30  | b     | 614 | CHL  | CHB-C4A | -4.28 | 1.33        | 1.38     |
| 30  | f     | 605 | CHL  | CHB-C4A | -4.28 | 1.33        | 1.38     |
| 30  | i     | 602 | CHL  | O2A-CGA | 4.28  | 1.45        | 1.33     |
| 30  | h     | 608 | CHL  | CHD-C4C | 4.28  | 1.47        | 1.39     |
| 30  | c     | 602 | CHL  | O2A-CGA | 4.28  | 1.45        | 1.33     |
| 30  | g     | 609 | CHL  | CHB-C4A | -4.28 | 1.33        | 1.38     |
| 30  | d     | 602 | CHL  | CHB-C1B | 4.28  | 1.46        | 1.39     |
| 30  | c     | 608 | CHL  | O2A-CGA | 4.28  | 1.45        | 1.33     |
| 30  | c     | 614 | CHL  | CHD-C4C | 4.28  | 1.47        | 1.39     |
| 30  | d     | 601 | CHL  | O2A-CGA | 4.28  | 1.45        | 1.33     |
| 30  | e     | 614 | CHL  | CHC-C1C | 4.28  | 1.47        | 1.39     |
| 30  | b     | 608 | CHL  | O2A-CGA | 4.28  | 1.45        | 1.33     |
| 30  | 3     | 305 | CHL  | O2A-CGA | 4.28  | 1.45        | 1.33     |
| 30  | 1     | 313 | CHL  | O2A-CGA | 4.27  | 1.45        | 1.33     |
| 30  | 3     | 307 | CHL  | O2A-CGA | 4.27  | 1.45        | 1.33     |
| 30  | 5     | 301 | CHL  | O2A-CGA | 4.27  | 1.45        | 1.33     |
| 30  | h     | 602 | CHL  | O2A-CGA | 4.27  | 1.45        | 1.33     |
| 30  | 6     | 307 | CHL  | C3B-C2B | 4.27  | 1.46        | 1.40     |
| 30  | f     | 601 | CHL  | O2A-CGA | 4.27  | 1.45        | 1.33     |
| 30  | i     | 609 | CHL  | O2A-CGA | 4.27  | 1.45        | 1.33     |
| 30  | 2     | 313 | CHL  | CHB-C1B | 4.27  | 1.46        | 1.39     |
| 30  | 8     | 313 | CHL  | O2A-CGA | 4.27  | 1.45        | 1.33     |
| 30  | 0     | 305 | CHL  | O2A-CGA | 4.27  | 1.45        | 1.33     |
| 30  | 4     | 313 | CHL  | CHD-C1D | 4.27  | 1.46        | 1.39     |
| 30  | 4     | 306 | CHL  | CHB-C1B | 4.26  | 1.46        | 1.39     |
| 30  | i     | 608 | CHL  | CHD-C4C | 4.26  | 1.47        | 1.39     |
| 30  | f     | 602 | CHL  | O2A-CGA | 4.26  | 1.45        | 1.33     |
| 30  | 7     | 306 | CHL  | C3B-C2B | 4.26  | 1.46        | 1.40     |
| 30  | 8     | 302 | CHL  | CHD-C1D | 4.26  | 1.46        | 1.39     |
| 30  | a     | 602 | CHL  | O2A-CGA | 4.26  | 1.45        | 1.33     |
| 30  | e     | 609 | CHL  | O2A-CGA | 4.26  | 1.45        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 30  | h     | 606 | CHL  | CHD-C4C | 4.26  | 1.47        | 1.39     |
| 30  | 5     | 313 | CHL  | CHC-C1C | 4.26  | 1.47        | 1.39     |
| 30  | f     | 607 | CHL  | CHB-C4A | -4.26 | 1.33        | 1.38     |
| 30  | d     | 608 | CHL  | CHD-C4C | 4.26  | 1.47        | 1.39     |
| 30  | c     | 601 | CHL  | O2A-CGA | 4.25  | 1.45        | 1.33     |
| 30  | h     | 606 | CHL  | O2A-CGA | 4.25  | 1.45        | 1.33     |
| 30  | 9     | 306 | CHL  | O2A-CGA | 4.25  | 1.45        | 1.33     |
| 30  | 8     | 306 | CHL  | CHB-C1B | 4.25  | 1.46        | 1.39     |
| 30  | c     | 609 | CHL  | O2A-CGA | 4.25  | 1.45        | 1.33     |
| 30  | 7     | 302 | CHL  | CHD-C1D | 4.25  | 1.46        | 1.39     |
| 30  | a     | 609 | CHL  | CHC-C1C | 4.25  | 1.47        | 1.39     |
| 30  | g     | 607 | CHL  | CHC-C1C | 4.25  | 1.47        | 1.39     |
| 30  | f     | 608 | CHL  | O2A-CGA | 4.25  | 1.45        | 1.33     |
| 30  | i     | 602 | CHL  | CHD-C4C | 4.25  | 1.47        | 1.39     |
| 30  | e     | 609 | CHL  | CHD-C4C | 4.25  | 1.47        | 1.39     |
| 30  | 6     | 302 | CHL  | O2A-CGA | 4.25  | 1.45        | 1.33     |
| 30  | a     | 607 | CHL  | CHC-C1C | 4.25  | 1.47        | 1.39     |
| 30  | c     | 608 | CHL  | C3A-C2A | -4.25 | 1.51        | 1.54     |
| 30  | 6     | 307 | CHL  | O2A-CGA | 4.25  | 1.45        | 1.33     |
| 30  | 6     | 313 | CHL  | O2A-CGA | 4.25  | 1.45        | 1.33     |
| 30  | i     | 601 | CHL  | CHB-C4A | -4.24 | 1.33        | 1.38     |
| 30  | b     | 602 | CHL  | O2A-CGA | 4.24  | 1.45        | 1.33     |
| 30  | 7     | 306 | CHL  | O2A-CGA | 4.24  | 1.45        | 1.33     |
| 30  | 1     | 305 | CHL  | C3B-C2B | 4.24  | 1.46        | 1.40     |
| 30  | 2     | 313 | CHL  | O2A-CGA | 4.24  | 1.45        | 1.33     |
| 30  | 8     | 307 | CHL  | O2A-CGA | 4.24  | 1.45        | 1.33     |
| 30  | 1     | 302 | CHL  | CHD-C1D | 4.24  | 1.46        | 1.39     |
| 30  | 6     | 302 | CHL  | CHD-C1D | 4.24  | 1.46        | 1.39     |
| 30  | a     | 608 | CHL  | O2A-CGA | 4.24  | 1.45        | 1.33     |
| 30  | f     | 602 | CHL  | C3B-C2B | 4.24  | 1.46        | 1.40     |
| 30  | i     | 602 | CHL  | C3A-C2A | -4.24 | 1.51        | 1.54     |
| 30  | b     | 614 | CHL  | C2A-C3A | -4.24 | 1.51        | 1.54     |
| 30  | i     | 607 | CHL  | CHC-C1C | 4.23  | 1.47        | 1.39     |
| 30  | 6     | 307 | CHL  | CHB-C1B | 4.23  | 1.46        | 1.39     |
| 30  | d     | 602 | CHL  | O2A-CGA | 4.23  | 1.45        | 1.33     |
| 30  | 4     | 307 | CHL  | CHB-C1B | 4.23  | 1.46        | 1.39     |
| 30  | 2     | 307 | CHL  | CHB-C1B | 4.23  | 1.46        | 1.39     |
| 30  | i     | 614 | CHL  | CHB-C4A | -4.23 | 1.33        | 1.38     |
| 30  | 8     | 313 | CHL  | CHB-C1B | 4.23  | 1.46        | 1.39     |
| 30  | 4     | 319 | CHL  | O2A-CGA | 4.23  | 1.45        | 1.33     |
| 30  | 0     | 301 | CHL  | CHB-C1B | 4.23  | 1.46        | 1.39     |
| 30  | g     | 606 | CHL  | CHC-C1C | 4.23  | 1.47        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 30  | e     | 601 | CHL  | O2A-CGA | 4.23  | 1.45        | 1.33     |
| 30  | 4     | 307 | CHL  | O2A-CGA | 4.23  | 1.45        | 1.33     |
| 32  | A     | 848 | 8CT  | C19-C20 | 4.23  | 1.56        | 1.43     |
| 30  | 6     | 305 | CHL  | CHB-C1B | 4.23  | 1.46        | 1.39     |
| 30  | 5     | 307 | CHL  | CHD-C4C | 4.23  | 1.47        | 1.39     |
| 32  | B     | 844 | 8CT  | C24-C25 | 4.22  | 1.56        | 1.43     |
| 30  | 0     | 302 | CHL  | O2A-CGA | 4.22  | 1.45        | 1.33     |
| 30  | d     | 609 | CHL  | CHC-C1C | 4.22  | 1.47        | 1.39     |
| 30  | a     | 608 | CHL  | CHD-C4C | 4.22  | 1.47        | 1.39     |
| 30  | 2     | 305 | CHL  | C3D-C2D | 4.22  | 1.46        | 1.39     |
| 30  | e     | 606 | CHL  | CHD-C4C | 4.22  | 1.47        | 1.39     |
| 32  | A     | 849 | 8CT  | C19-C20 | 4.22  | 1.56        | 1.43     |
| 30  | 8     | 302 | CHL  | O2A-CGA | 4.22  | 1.45        | 1.33     |
| 30  | 3     | 305 | CHL  | C3B-C2B | 4.22  | 1.46        | 1.40     |
| 30  | 7     | 307 | CHL  | CHB-C1B | 4.22  | 1.46        | 1.39     |
| 30  | 4     | 305 | CHL  | CHB-C1B | 4.22  | 1.46        | 1.39     |
| 30  | 2     | 319 | CHL  | O2A-CGA | 4.21  | 1.45        | 1.33     |
| 30  | 2     | 302 | CHL  | C3B-C2B | 4.21  | 1.46        | 1.40     |
| 32  | B     | 845 | 8CT  | C24-C25 | 4.21  | 1.56        | 1.43     |
| 32  | B     | 848 | 8CT  | C24-C25 | 4.21  | 1.56        | 1.43     |
| 30  | b     | 601 | CHL  | CHC-C1C | 4.21  | 1.47        | 1.39     |
| 30  | 1     | 307 | CHL  | O2A-CGA | 4.21  | 1.45        | 1.33     |
| 30  | 4     | 313 | CHL  | O2A-CGA | 4.21  | 1.45        | 1.33     |
| 30  | 4     | 302 | CHL  | O2A-CGA | 4.21  | 1.45        | 1.33     |
| 30  | f     | 609 | CHL  | CHC-C1C | 4.20  | 1.47        | 1.39     |
| 30  | e     | 602 | CHL  | CHD-C4C | 4.20  | 1.47        | 1.39     |
| 32  | 0     | 401 | 8CT  | C24-C25 | 4.20  | 1.56        | 1.43     |
| 30  | 0     | 305 | CHL  | CHD-C4C | 4.20  | 1.47        | 1.39     |
| 30  | b     | 607 | CHL  | CHD-C4C | 4.20  | 1.47        | 1.39     |
| 30  | 5     | 305 | CHL  | CHD-C4C | 4.20  | 1.47        | 1.39     |
| 30  | 2     | 301 | CHL  | CHB-C1B | 4.20  | 1.46        | 1.39     |
| 30  | h     | 609 | CHL  | CHC-C1C | 4.19  | 1.47        | 1.39     |
| 30  | g     | 605 | CHL  | CHB-C4A | -4.19 | 1.33        | 1.38     |
| 30  | 6     | 306 | CHL  | CHB-C1B | 4.19  | 1.46        | 1.39     |
| 30  | d     | 601 | CHL  | CHB-C4A | -4.19 | 1.33        | 1.38     |
| 32  | 9     | 401 | 8CT  | C24-C25 | 4.19  | 1.56        | 1.43     |
| 30  | 3     | 302 | CHL  | O2A-CGA | 4.19  | 1.45        | 1.33     |
| 30  | 7     | 307 | CHL  | O2A-CGA | 4.19  | 1.45        | 1.33     |
| 30  | f     | 606 | CHL  | CHC-C1C | 4.19  | 1.47        | 1.39     |
| 32  | G     | 104 | 8CT  | C24-C25 | 4.19  | 1.56        | 1.43     |
| 30  | e     | 601 | CHL  | CHD-C4C | 4.19  | 1.47        | 1.39     |
| 30  | b     | 607 | CHL  | C3A-C2A | -4.19 | 1.51        | 1.54     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 30  | 5     | 301 | CHL  | CHC-C1C | 4.19  | 1.47        | 1.39     |
| 30  | f     | 607 | CHL  | CHC-C1C | 4.19  | 1.47        | 1.39     |
| 32  | L     | 209 | 8CT  | C24-C25 | 4.19  | 1.56        | 1.43     |
| 30  | c     | 608 | CHL  | CHD-C4C | 4.18  | 1.47        | 1.39     |
| 30  | e     | 606 | CHL  | CHC-C1C | 4.18  | 1.47        | 1.39     |
| 30  | 3     | 302 | CHL  | CHD-C1D | 4.18  | 1.46        | 1.39     |
| 30  | h     | 607 | CHL  | CHB-C4A | -4.18 | 1.33        | 1.38     |
| 30  | c     | 614 | CHL  | CHC-C1C | 4.18  | 1.47        | 1.39     |
| 30  | d     | 606 | CHL  | CHC-C1C | 4.18  | 1.47        | 1.39     |
| 32  | 1     | 402 | 8CT  | C24-C25 | 4.18  | 1.56        | 1.43     |
| 30  | 2     | 307 | CHL  | O2A-CGA | 4.17  | 1.45        | 1.33     |
| 30  | 4     | 307 | CHL  | CHD-C1D | 4.17  | 1.46        | 1.39     |
| 30  | 5     | 306 | CHL  | CHC-C1C | 4.17  | 1.47        | 1.39     |
| 32  | 8     | 406 | 8CT  | C24-C25 | 4.17  | 1.56        | 1.43     |
| 30  | a     | 601 | CHL  | CHB-C4A | -4.17 | 1.33        | 1.38     |
| 30  | a     | 606 | CHL  | CHC-C1C | 4.17  | 1.47        | 1.39     |
| 30  | f     | 601 | CHL  | CHD-C4C | 4.17  | 1.47        | 1.39     |
| 32  | J     | 104 | 8CT  | C24-C25 | 4.17  | 1.56        | 1.43     |
| 30  | 9     | 313 | CHL  | O2A-CGA | 4.16  | 1.45        | 1.33     |
| 30  | a     | 601 | CHL  | O2A-CGA | 4.16  | 1.45        | 1.33     |
| 30  | 6     | 301 | CHL  | O2A-CGA | 4.16  | 1.45        | 1.33     |
| 30  | 2     | 319 | CHL  | CHB-C1B | 4.16  | 1.46        | 1.39     |
| 30  | 7     | 302 | CHL  | O2A-CGA | 4.16  | 1.45        | 1.33     |
| 30  | b     | 602 | CHL  | CHC-C1C | 4.16  | 1.47        | 1.39     |
| 30  | 6     | 302 | CHL  | CHB-C1B | 4.16  | 1.46        | 1.39     |
| 30  | d     | 607 | CHL  | O2A-CGA | 4.16  | 1.45        | 1.33     |
| 30  | a     | 607 | CHL  | O2A-CGA | 4.16  | 1.45        | 1.33     |
| 30  | f     | 602 | CHL  | CHC-C1C | 4.16  | 1.47        | 1.39     |
| 30  | 2     | 302 | CHL  | O2A-CGA | 4.15  | 1.45        | 1.33     |
| 30  | a     | 614 | CHL  | CHB-C4A | -4.15 | 1.33        | 1.38     |
| 30  | f     | 614 | CHL  | CHC-C1C | 4.15  | 1.47        | 1.39     |
| 30  | 3     | 307 | CHL  | CHB-C1B | 4.15  | 1.46        | 1.39     |
| 30  | d     | 607 | CHL  | CHB-C4A | -4.15 | 1.33        | 1.38     |
| 30  | c     | 607 | CHL  | O2A-CGA | 4.15  | 1.45        | 1.33     |
| 30  | 7     | 307 | CHL  | CHC-C1C | 4.15  | 1.47        | 1.39     |
| 32  | A     | 854 | 8CT  | C24-C25 | 4.15  | 1.56        | 1.43     |
| 30  | 4     | 319 | CHL  | CHB-C1B | 4.15  | 1.46        | 1.39     |
| 30  | 3     | 302 | CHL  | CHC-C1C | 4.15  | 1.47        | 1.39     |
| 32  | L     | 206 | 8CT  | C24-C25 | 4.15  | 1.56        | 1.43     |
| 30  | 5     | 313 | CHL  | O2A-CGA | 4.15  | 1.45        | 1.33     |
| 30  | 9     | 301 | CHL  | O2A-CGA | 4.15  | 1.45        | 1.33     |
| 30  | c     | 601 | CHL  | CHB-C1B | 4.15  | 1.46        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 32  | 3     | 402 | 8CT  | C24-C25 | 4.14  | 1.56        | 1.43     |
| 30  | h     | 601 | CHL  | O2A-CGA | 4.14  | 1.45        | 1.33     |
| 30  | 5     | 307 | CHL  | O2A-CGA | 4.14  | 1.45        | 1.33     |
| 30  | i     | 605 | CHL  | CHB-C4A | -4.14 | 1.33        | 1.38     |
| 30  | 7     | 302 | CHL  | CHB-C1B | 4.14  | 1.46        | 1.39     |
| 30  | i     | 609 | CHL  | CHB-C4A | -4.14 | 1.33        | 1.38     |
| 30  | 8     | 302 | CHL  | C3B-C2B | 4.14  | 1.46        | 1.40     |
| 30  | 5     | 302 | CHL  | CHB-C1B | 4.14  | 1.46        | 1.39     |
| 32  | K     | 107 | 8CT  | C24-C25 | 4.14  | 1.56        | 1.43     |
| 30  | 7     | 313 | CHL  | O2A-CGA | 4.14  | 1.45        | 1.33     |
| 30  | 2     | 305 | CHL  | CHB-C1B | 4.14  | 1.46        | 1.39     |
| 30  | a     | 601 | CHL  | CHC-C1C | 4.13  | 1.47        | 1.39     |
| 30  | 4     | 313 | CHL  | CHB-C1B | 4.13  | 1.46        | 1.39     |
| 30  | 8     | 306 | CHL  | CHD-C4C | 4.13  | 1.47        | 1.39     |
| 30  | i     | 607 | CHL  | O2A-CGA | 4.13  | 1.45        | 1.33     |
| 30  | 2     | 302 | CHL  | CHB-C1B | 4.13  | 1.46        | 1.39     |
| 30  | g     | 601 | CHL  | CHB-C4A | -4.13 | 1.33        | 1.38     |
| 30  | 8     | 308 | CHL  | O2A-CGA | 4.13  | 1.45        | 1.33     |
| 30  | 8     | 315 | CHL  | CHC-C1C | 4.13  | 1.47        | 1.39     |
| 30  | e     | 602 | CHL  | CHB-C1B | 4.13  | 1.46        | 1.39     |
| 30  | h     | 609 | CHL  | O2A-CGA | 4.12  | 1.45        | 1.33     |
| 30  | d     | 614 | CHL  | CHB-C4A | -4.12 | 1.33        | 1.38     |
| 30  | e     | 607 | CHL  | CHC-C1C | 4.12  | 1.47        | 1.39     |
| 30  | d     | 608 | CHL  | CHC-C1C | 4.12  | 1.47        | 1.39     |
| 30  | 4     | 308 | CHL  | O2A-CGA | 4.12  | 1.45        | 1.33     |
| 30  | 7     | 306 | CHL  | CHD-C4C | 4.12  | 1.47        | 1.39     |
| 30  | e     | 607 | CHL  | O2A-CGA | 4.12  | 1.45        | 1.33     |
| 30  | 3     | 302 | CHL  | CHB-C1B | 4.12  | 1.46        | 1.39     |
| 30  | 5     | 307 | CHL  | CHC-C1C | 4.12  | 1.47        | 1.39     |
| 30  | f     | 607 | CHL  | O2A-CGA | 4.12  | 1.45        | 1.33     |
| 30  | c     | 606 | CHL  | CHD-C4C | 4.12  | 1.47        | 1.39     |
| 30  | 6     | 315 | CHL  | CHD-C4C | 4.11  | 1.47        | 1.39     |
| 30  | c     | 609 | CHL  | CHC-C1C | 4.11  | 1.47        | 1.39     |
| 30  | 8     | 302 | CHL  | CHB-C1B | 4.11  | 1.46        | 1.39     |
| 30  | b     | 602 | CHL  | CHD-C4C | 4.11  | 1.47        | 1.39     |
| 30  | 9     | 313 | CHL  | CHD-C4C | 4.11  | 1.47        | 1.39     |
| 30  | a     | 608 | CHL  | CHC-C1C | 4.11  | 1.47        | 1.39     |
| 30  | h     | 608 | CHL  | CHC-C1C | 4.11  | 1.47        | 1.39     |
| 30  | 3     | 305 | CHL  | CHB-C1B | 4.11  | 1.46        | 1.39     |
| 30  | 7     | 313 | CHL  | CHD-C4C | 4.11  | 1.47        | 1.39     |
| 30  | a     | 605 | CHL  | CHB-C4A | -4.10 | 1.33        | 1.38     |
| 30  | d     | 602 | CHL  | CHD-C4C | 4.10  | 1.47        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 32  | B     | 847 | 8CT  | C24-C25 | 4.10  | 1.55        | 1.43     |
| 30  | b     | 607 | CHL  | O2A-CGA | 4.10  | 1.45        | 1.33     |
| 30  | f     | 602 | CHL  | CHB-C1B | 4.10  | 1.46        | 1.39     |
| 30  | 0     | 302 | CHL  | CHB-C1B | 4.10  | 1.46        | 1.39     |
| 30  | g     | 602 | CHL  | C3A-C2A | -4.10 | 1.51        | 1.54     |
| 30  | d     | 608 | CHL  | C3A-C2A | -4.10 | 1.51        | 1.54     |
| 30  | 1     | 302 | CHL  | O2A-CGA | 4.10  | 1.45        | 1.33     |
| 30  | i     | 608 | CHL  | CHC-C1C | 4.10  | 1.47        | 1.39     |
| 30  | 1     | 306 | CHL  | CHD-C4C | 4.10  | 1.47        | 1.39     |
| 30  | 8     | 305 | CHL  | O2A-CGA | 4.10  | 1.45        | 1.33     |
| 30  | 0     | 306 | CHL  | CHD-C4C | 4.10  | 1.47        | 1.39     |
| 30  | h     | 606 | CHL  | CHC-C1C | 4.10  | 1.47        | 1.39     |
| 30  | c     | 602 | CHL  | CHC-C1C | 4.09  | 1.47        | 1.39     |
| 30  | i     | 601 | CHL  | O2A-CGA | 4.09  | 1.45        | 1.33     |
| 30  | 7     | 302 | CHL  | C3B-C2B | 4.09  | 1.45        | 1.40     |
| 32  | L     | 205 | 8CT  | C24-C25 | 4.09  | 1.55        | 1.43     |
| 30  | 2     | 308 | CHL  | O2A-CGA | 4.09  | 1.45        | 1.33     |
| 30  | e     | 608 | CHL  | CHD-C4C | 4.09  | 1.47        | 1.39     |
| 30  | 7     | 305 | CHL  | CHB-C1B | 4.09  | 1.46        | 1.39     |
| 30  | 8     | 301 | CHL  | O2A-CGA | 4.09  | 1.45        | 1.33     |
| 30  | 0     | 302 | CHL  | C3B-C2B | 4.09  | 1.45        | 1.40     |
| 30  | 3     | 302 | CHL  | C3B-C2B | 4.09  | 1.45        | 1.40     |
| 32  | B     | 844 | 8CT  | C14-C13 | 4.09  | 1.55        | 1.43     |
| 30  | 8     | 305 | CHL  | CHD-C4C | 4.09  | 1.47        | 1.39     |
| 32  | 7     | 405 | 8CT  | C24-C25 | 4.08  | 1.55        | 1.43     |
| 30  | b     | 606 | CHL  | CHD-C4C | 4.08  | 1.47        | 1.39     |
| 30  | 4     | 302 | CHL  | C3B-C2B | 4.08  | 1.45        | 1.40     |
| 30  | c     | 607 | CHL  | CHC-C1C | 4.08  | 1.47        | 1.39     |
| 30  | 8     | 302 | CHL  | CHC-C1C | 4.08  | 1.47        | 1.39     |
| 30  | 3     | 307 | CHL  | CHD-C1D | 4.08  | 1.46        | 1.39     |
| 30  | d     | 605 | CHL  | CHB-C4A | -4.08 | 1.33        | 1.38     |
| 30  | c     | 605 | CHL  | CHB-C4A | -4.08 | 1.33        | 1.38     |
| 32  | 3     | 403 | 8CT  | C24-C25 | 4.08  | 1.55        | 1.43     |
| 30  | a     | 602 | CHL  | CHC-C1C | 4.08  | 1.47        | 1.39     |
| 32  | O     | 205 | 8CT  | C24-C25 | 4.08  | 1.55        | 1.43     |
| 30  | 1     | 305 | CHL  | CHB-C1B | 4.07  | 1.46        | 1.39     |
| 30  | 8     | 308 | CHL  | CHD-C4C | 4.07  | 1.47        | 1.39     |
| 30  | 4     | 308 | CHL  | CHD-C4C | 4.07  | 1.47        | 1.39     |
| 42  | e     | 523 | NEX  | C7-C6   | -4.07 | 1.25        | 1.30     |
| 30  | 5     | 302 | CHL  | C3B-C2B | 4.06  | 1.45        | 1.40     |
| 32  | M     | 102 | 8CT  | C24-C25 | 4.06  | 1.55        | 1.43     |
| 32  | 8     | 402 | 8CT  | C24-C25 | 4.06  | 1.55        | 1.43     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 30  | a     | 608 | CHL  | C3A-C2A | -4.05 | 1.51        | 1.54     |
| 32  | B     | 851 | 8CT  | C24-C25 | 4.05  | 1.55        | 1.43     |
| 30  | 4     | 302 | CHL  | CHB-C1B | 4.05  | 1.46        | 1.39     |
| 30  | d     | 602 | CHL  | CHC-C1C | 4.05  | 1.47        | 1.39     |
| 30  | b     | 607 | CHL  | CHC-C1C | 4.05  | 1.47        | 1.39     |
| 32  | 6     | 402 | 8CT  | C24-C25 | 4.05  | 1.55        | 1.43     |
| 30  | c     | 608 | CHL  | CHC-C1C | 4.05  | 1.47        | 1.39     |
| 32  | F     | 302 | 8CT  | C24-C25 | 4.05  | 1.55        | 1.43     |
| 30  | 8     | 301 | CHL  | CHD-C4C | 4.05  | 1.47        | 1.39     |
| 30  | c     | 601 | CHL  | CHD-C4C | 4.05  | 1.47        | 1.39     |
| 30  | h     | 614 | CHL  | CHB-C4A | -4.04 | 1.33        | 1.38     |
| 32  | J     | 101 | 8CT  | C24-C25 | 4.04  | 1.55        | 1.43     |
| 30  | g     | 614 | CHL  | CHB-C4A | -4.04 | 1.33        | 1.38     |
| 30  | i     | 608 | CHL  | C3A-C2A | -4.04 | 1.51        | 1.54     |
| 30  | 1     | 302 | CHL  | CHB-C1B | 4.04  | 1.46        | 1.39     |
| 30  | 7     | 313 | CHL  | CHC-C1C | 4.04  | 1.47        | 1.39     |
| 32  | 7     | 404 | 8CT  | C24-C25 | 4.04  | 1.55        | 1.43     |
| 32  | B     | 804 | 8CT  | C24-C25 | 4.04  | 1.55        | 1.43     |
| 30  | h     | 605 | CHL  | CHB-C4A | -4.03 | 1.33        | 1.38     |
| 30  | i     | 602 | CHL  | CHC-C1C | 4.03  | 1.47        | 1.39     |
| 30  | b     | 608 | CHL  | CHD-C4C | 4.03  | 1.47        | 1.39     |
| 30  | f     | 609 | CHL  | C3A-C2A | -4.02 | 1.51        | 1.54     |
| 30  | e     | 609 | CHL  | CHC-C1C | 4.02  | 1.47        | 1.39     |
| 30  | b     | 606 | CHL  | CHC-C1C | 4.02  | 1.47        | 1.39     |
| 30  | b     | 609 | CHL  | CHC-C1C | 4.02  | 1.47        | 1.39     |
| 30  | e     | 602 | CHL  | CHC-C1C | 4.02  | 1.47        | 1.39     |
| 30  | 1     | 302 | CHL  | C3B-C2B | 4.02  | 1.45        | 1.40     |
| 30  | c     | 606 | CHL  | CHC-C1C | 4.02  | 1.47        | 1.39     |
| 30  | c     | 602 | CHL  | CHD-C4C | 4.01  | 1.47        | 1.39     |
| 30  | 1     | 305 | CHL  | CHD-C4C | 4.01  | 1.47        | 1.39     |
| 30  | 6     | 301 | CHL  | CHD-C4C | 4.01  | 1.47        | 1.39     |
| 30  | 3     | 305 | CHL  | CHC-C1C | 4.00  | 1.47        | 1.39     |
| 30  | 4     | 306 | CHL  | CHD-C4C | 4.00  | 1.47        | 1.39     |
| 32  | B     | 845 | 8CT  | C14-C13 | 4.00  | 1.55        | 1.43     |
| 30  | d     | 606 | CHL  | C3A-C2A | -4.00 | 1.51        | 1.54     |
| 30  | 9     | 301 | CHL  | CHD-C4C | 3.99  | 1.47        | 1.39     |
| 30  | 4     | 302 | CHL  | CHD-C4C | 3.99  | 1.47        | 1.39     |
| 32  | G     | 104 | 8CT  | C14-C13 | 3.99  | 1.55        | 1.43     |
| 30  | 2     | 307 | CHL  | CHD-C1D | 3.99  | 1.46        | 1.39     |
| 30  | 1     | 307 | CHL  | CHD-C4C | 3.99  | 1.47        | 1.39     |
| 32  | B     | 846 | 8CT  | C28-C29 | 3.99  | 1.41        | 1.32     |
| 30  | 7     | 307 | CHL  | CHD-C4C | 3.99  | 1.47        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 32  | I     | 101 | 8CT  | C24-C25 | 3.99  | 1.55        | 1.43     |
| 30  | 0     | 306 | CHL  | CHC-C1C | 3.98  | 1.47        | 1.39     |
| 30  | 2     | 301 | CHL  | CHD-C4C | 3.98  | 1.47        | 1.39     |
| 32  | 8     | 402 | 8CT  | C14-C13 | 3.98  | 1.55        | 1.43     |
| 30  | 7     | 305 | CHL  | CHC-C1C | 3.98  | 1.47        | 1.39     |
| 30  | 2     | 306 | CHL  | CHD-C4C | 3.98  | 1.47        | 1.39     |
| 30  | 7     | 301 | CHL  | CHD-C4C | 3.98  | 1.47        | 1.39     |
| 30  | 5     | 307 | CHL  | C3A-C2A | -3.98 | 1.51        | 1.54     |
| 32  | 7     | 402 | 8CT  | C24-C25 | 3.98  | 1.55        | 1.43     |
| 30  | 6     | 313 | CHL  | CHD-C4C | 3.98  | 1.47        | 1.39     |
| 30  | 7     | 302 | CHL  | CHC-C1C | 3.97  | 1.47        | 1.39     |
| 30  | 1     | 302 | CHL  | CHC-C1C | 3.97  | 1.47        | 1.39     |
| 30  | 2     | 319 | CHL  | CHD-C4C | 3.97  | 1.47        | 1.39     |
| 30  | f     | 601 | CHL  | CHC-C1C | 3.97  | 1.47        | 1.39     |
| 32  | A     | 846 | 8CT  | C24-C25 | 3.97  | 1.55        | 1.43     |
| 30  | e     | 614 | CHL  | C2A-C3A | -3.97 | 1.51        | 1.54     |
| 30  | d     | 609 | CHL  | C3A-C2A | -3.97 | 1.51        | 1.54     |
| 30  | c     | 607 | CHL  | C3A-C2A | -3.96 | 1.51        | 1.54     |
| 30  | 8     | 301 | CHL  | CHC-C1C | 3.96  | 1.47        | 1.39     |
| 30  | 8     | 313 | CHL  | CHD-C4C | 3.96  | 1.47        | 1.39     |
| 30  | 0     | 305 | CHL  | CHC-C1C | 3.96  | 1.47        | 1.39     |
| 30  | 4     | 319 | CHL  | CHD-C4C | 3.96  | 1.47        | 1.39     |
| 32  | B     | 843 | 8CT  | C14-C13 | 3.96  | 1.55        | 1.43     |
| 30  | f     | 602 | CHL  | CHD-C4C | 3.96  | 1.47        | 1.39     |
| 30  | f     | 608 | CHL  | CHD-C4C | 3.96  | 1.47        | 1.39     |
| 30  | 6     | 308 | CHL  | CHD-C4C | 3.96  | 1.47        | 1.39     |
| 30  | 6     | 307 | CHL  | CHC-C1C | 3.96  | 1.47        | 1.39     |
| 30  | 5     | 306 | CHL  | C3A-C2A | -3.95 | 1.51        | 1.54     |
| 30  | a     | 606 | CHL  | C3A-C2A | -3.95 | 1.51        | 1.54     |
| 30  | 1     | 313 | CHL  | CHD-C4C | 3.95  | 1.46        | 1.39     |
| 30  | 5     | 305 | CHL  | CHC-C1C | 3.95  | 1.46        | 1.39     |
| 30  | 1     | 307 | CHL  | CHC-C1C | 3.95  | 1.46        | 1.39     |
| 41  | B     | 849 | DGD  | O2G-C1B | 3.95  | 1.45        | 1.34     |
| 30  | 9     | 305 | CHL  | CHC-C1C | 3.95  | 1.46        | 1.39     |
| 30  | 6     | 315 | CHL  | CHC-C1C | 3.95  | 1.46        | 1.39     |
| 30  | g     | 609 | CHL  | C2A-C3A | -3.94 | 1.51        | 1.54     |
| 30  | 7     | 306 | CHL  | CHC-C1C | 3.93  | 1.46        | 1.39     |
| 30  | h     | 608 | CHL  | C3A-C2A | -3.92 | 1.51        | 1.54     |
| 30  | 2     | 305 | CHL  | CHD-C4C | 3.92  | 1.46        | 1.39     |
| 30  | e     | 608 | CHL  | CHC-C1C | 3.92  | 1.46        | 1.39     |
| 32  | A     | 847 | 8CT  | C24-C25 | 3.92  | 1.55        | 1.43     |
| 30  | i     | 607 | CHL  | C3A-C2A | -3.92 | 1.51        | 1.54     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 30  | 1     | 313 | CHL  | CHC-C1C | 3.92  | 1.46        | 1.39     |
| 32  | A     | 850 | 8CT  | C24-C25 | 3.92  | 1.55        | 1.43     |
| 30  | i     | 614 | CHL  | C2A-C3A | -3.91 | 1.51        | 1.54     |
| 30  | 8     | 302 | CHL  | CHD-C4C | 3.91  | 1.46        | 1.39     |
| 30  | 9     | 305 | CHL  | CHB-C1B | 3.91  | 1.46        | 1.39     |
| 30  | g     | 606 | CHL  | C3A-C2A | -3.91 | 1.51        | 1.54     |
| 30  | 2     | 302 | CHL  | CHD-C4C | 3.91  | 1.46        | 1.39     |
| 30  | 0     | 302 | CHL  | CHD-C4C | 3.90  | 1.46        | 1.39     |
| 32  | B     | 848 | 8CT  | C14-C13 | 3.90  | 1.55        | 1.43     |
| 39  | A     | 857 | CL0  | CMD-C2D | -3.90 | 1.43        | 1.51     |
| 30  | 6     | 306 | CHL  | CHD-C4C | 3.89  | 1.46        | 1.39     |
| 32  | B     | 846 | 8CT  | C14-C13 | 3.89  | 1.55        | 1.43     |
| 30  | 7     | 301 | CHL  | CHC-C1C | 3.89  | 1.46        | 1.39     |
| 30  | 2     | 308 | CHL  | CHD-C4C | 3.89  | 1.46        | 1.39     |
| 32  | 4     | 402 | 8CT  | C14-C13 | 3.89  | 1.55        | 1.43     |
| 30  | 0     | 301 | CHL  | CHD-C4C | 3.89  | 1.46        | 1.39     |
| 30  | 1     | 305 | CHL  | CHC-C1C | 3.89  | 1.46        | 1.39     |
| 30  | 8     | 308 | CHL  | CHC-C1C | 3.89  | 1.46        | 1.39     |
| 32  | 8     | 406 | 8CT  | C14-C13 | 3.89  | 1.55        | 1.43     |
| 30  | 0     | 302 | CHL  | CHC-C1C | 3.89  | 1.46        | 1.39     |
| 30  | e     | 601 | CHL  | CHC-C1C | 3.88  | 1.46        | 1.39     |
| 32  | A     | 849 | 8CT  | C24-C25 | 3.88  | 1.55        | 1.43     |
| 30  | 9     | 306 | CHL  | CHD-C4C | 3.88  | 1.46        | 1.39     |
| 32  | L     | 206 | 8CT  | C14-C13 | 3.88  | 1.55        | 1.43     |
| 30  | 1     | 306 | CHL  | CHC-C1C | 3.88  | 1.46        | 1.39     |
| 30  | 6     | 307 | CHL  | CHD-C4C | 3.88  | 1.46        | 1.39     |
| 32  | 7     | 404 | 8CT  | C28-C29 | 3.88  | 1.41        | 1.32     |
| 30  | 4     | 305 | CHL  | CHD-C4C | 3.88  | 1.46        | 1.39     |
| 32  | B     | 843 | 8CT  | C28-C29 | 3.88  | 1.41        | 1.32     |
| 32  | 6     | 402 | 8CT  | C14-C13 | 3.88  | 1.55        | 1.43     |
| 30  | 6     | 302 | CHL  | CHD-C4C | 3.87  | 1.46        | 1.39     |
| 32  | K     | 107 | 8CT  | C14-C13 | 3.87  | 1.55        | 1.43     |
| 30  | 8     | 306 | CHL  | CHC-C1C | 3.87  | 1.46        | 1.39     |
| 30  | 3     | 305 | CHL  | CHD-C4C | 3.87  | 1.46        | 1.39     |
| 30  | 7     | 302 | CHL  | CHD-C4C | 3.87  | 1.46        | 1.39     |
| 30  | 6     | 302 | CHL  | CHC-C1C | 3.87  | 1.46        | 1.39     |
| 32  | A     | 848 | 8CT  | C24-C25 | 3.86  | 1.55        | 1.43     |
| 30  | 6     | 308 | CHL  | CHC-C1C | 3.86  | 1.46        | 1.39     |
| 32  | 7     | 404 | 8CT  | C14-C13 | 3.86  | 1.55        | 1.43     |
| 30  | 1     | 302 | CHL  | CHD-C4C | 3.86  | 1.46        | 1.39     |
| 30  | b     | 601 | CHL  | C3A-C2A | -3.86 | 1.51        | 1.54     |
| 30  | 6     | 305 | CHL  | CHD-C4C | 3.86  | 1.46        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 30  | 9     | 305 | CHL  | CHD-C4C | 3.86  | 1.46        | 1.39     |
| 30  | 7     | 306 | CHL  | CHA-CBD | -3.86 | 1.47        | 1.51     |
| 30  | 3     | 302 | CHL  | CHD-C4C | 3.86  | 1.46        | 1.39     |
| 30  | 2     | 301 | CHL  | CHC-C1C | 3.86  | 1.46        | 1.39     |
| 32  | 4     | 402 | 8CT  | C28-C29 | 3.86  | 1.41        | 1.32     |
| 30  | 4     | 313 | CHL  | CHD-C4C | 3.85  | 1.46        | 1.39     |
| 30  | h     | 602 | CHL  | C3A-C2A | -3.85 | 1.51        | 1.54     |
| 30  | 8     | 307 | CHL  | CHD-C4C | 3.85  | 1.46        | 1.39     |
| 32  | 1     | 402 | 8CT  | C14-C13 | 3.85  | 1.55        | 1.43     |
| 30  | 5     | 302 | CHL  | CHD-C4C | 3.84  | 1.46        | 1.39     |
| 30  | 9     | 313 | CHL  | CHC-C1C | 3.84  | 1.46        | 1.39     |
| 30  | a     | 614 | CHL  | C2A-C3A | -3.84 | 1.51        | 1.54     |
| 30  | 4     | 308 | CHL  | CHC-C1C | 3.84  | 1.46        | 1.39     |
| 30  | 2     | 302 | CHL  | CHC-C1C | 3.84  | 1.46        | 1.39     |
| 32  | 0     | 401 | 8CT  | C14-C13 | 3.84  | 1.55        | 1.43     |
| 30  | 3     | 307 | CHL  | C3B-C2B | 3.84  | 1.45        | 1.40     |
| 32  | 2     | 402 | 8CT  | C14-C13 | 3.84  | 1.55        | 1.43     |
| 30  | 4     | 319 | CHL  | CHC-C1C | 3.83  | 1.46        | 1.39     |
| 30  | 4     | 302 | CHL  | CHC-C1C | 3.83  | 1.46        | 1.39     |
| 30  | f     | 607 | CHL  | C3A-C2A | -3.83 | 1.51        | 1.54     |
| 30  | e     | 605 | CHL  | C3A-C2A | -3.83 | 1.51        | 1.54     |
| 30  | 6     | 301 | CHL  | CHC-C1C | 3.82  | 1.46        | 1.39     |
| 30  | h     | 601 | CHL  | C3A-C2A | -3.82 | 1.51        | 1.54     |
| 30  | 8     | 315 | CHL  | C3A-C2A | -3.82 | 1.51        | 1.54     |
| 30  | 7     | 305 | CHL  | CHD-C4C | 3.82  | 1.46        | 1.39     |
| 30  | 2     | 307 | CHL  | CHC-C1C | 3.82  | 1.46        | 1.39     |
| 32  | B     | 844 | 8CT  | C28-C29 | 3.81  | 1.41        | 1.32     |
| 30  | d     | 601 | CHL  | C3A-C2A | -3.81 | 1.51        | 1.54     |
| 32  | J     | 104 | 8CT  | C14-C13 | 3.81  | 1.55        | 1.43     |
| 32  | 2     | 402 | 8CT  | C28-C29 | 3.81  | 1.40        | 1.32     |
| 32  | B     | 846 | 8CT  | C30-C29 | 3.81  | 1.56        | 1.50     |
| 32  | 9     | 401 | 8CT  | C14-C13 | 3.81  | 1.55        | 1.43     |
| 30  | 3     | 302 | CHL  | CHA-CBD | -3.81 | 1.47        | 1.51     |
| 30  | f     | 608 | CHL  | CHC-C1C | 3.80  | 1.46        | 1.39     |
| 30  | 3     | 307 | CHL  | CHD-C4C | 3.80  | 1.46        | 1.39     |
| 30  | 2     | 313 | CHL  | CHD-C4C | 3.80  | 1.46        | 1.39     |
| 30  | 2     | 319 | CHL  | CHC-C1C | 3.80  | 1.46        | 1.39     |
| 30  | 9     | 301 | CHL  | CHC-C1C | 3.80  | 1.46        | 1.39     |
| 30  | 4     | 306 | CHL  | CHC-C1C | 3.79  | 1.46        | 1.39     |
| 30  | 8     | 307 | CHL  | CHC-C1C | 3.79  | 1.46        | 1.39     |
| 30  | 5     | 302 | CHL  | CHC-C1C | 3.79  | 1.46        | 1.39     |
| 32  | A     | 854 | 8CT  | C14-C13 | 3.78  | 1.54        | 1.43     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 30  | 2     | 306 | CHL  | CHA-CBD | -3.78 | 1.47        | 1.51     |
| 32  | 8     | 402 | 8CT  | C11-C12 | 3.78  | 1.54        | 1.46     |
| 30  | 6     | 313 | CHL  | CHC-C1C | 3.78  | 1.46        | 1.39     |
| 32  | 3     | 403 | 8CT  | C14-C13 | 3.77  | 1.54        | 1.43     |
| 32  | A     | 847 | 8CT  | C14-C13 | 3.77  | 1.54        | 1.43     |
| 32  | A     | 846 | 8CT  | C14-C13 | 3.77  | 1.54        | 1.43     |
| 30  | i     | 601 | CHL  | C3A-C2A | -3.77 | 1.51        | 1.54     |
| 30  | 0     | 301 | CHL  | CHC-C1C | 3.76  | 1.46        | 1.39     |
| 30  | 2     | 308 | CHL  | CHC-C1C | 3.76  | 1.46        | 1.39     |
| 32  | O     | 205 | 8CT  | C14-C13 | 3.76  | 1.54        | 1.43     |
| 32  | 1     | 402 | 8CT  | C28-C29 | 3.76  | 1.40        | 1.32     |
| 30  | 2     | 313 | CHL  | CHC-C1C | 3.76  | 1.46        | 1.39     |
| 30  | 4     | 307 | CHL  | CHD-C4C | 3.76  | 1.46        | 1.39     |
| 30  | 8     | 305 | CHL  | CHC-C1C | 3.76  | 1.46        | 1.39     |
| 32  | B     | 848 | 8CT  | C28-C29 | 3.76  | 1.40        | 1.32     |
| 30  | 2     | 305 | CHL  | CHC-C1C | 3.76  | 1.46        | 1.39     |
| 30  | b     | 608 | CHL  | CHC-C1C | 3.76  | 1.46        | 1.39     |
| 32  | L     | 209 | 8CT  | C14-C13 | 3.75  | 1.54        | 1.43     |
| 30  | d     | 614 | CHL  | C2A-C3A | -3.75 | 1.51        | 1.54     |
| 30  | a     | 609 | CHL  | C3A-C2A | -3.75 | 1.51        | 1.54     |
| 30  | 2     | 306 | CHL  | CHC-C1C | 3.75  | 1.46        | 1.39     |
| 32  | F     | 302 | 8CT  | C14-C13 | 3.75  | 1.54        | 1.43     |
| 30  | d     | 607 | CHL  | C3A-C2A | -3.75 | 1.51        | 1.54     |
| 32  | J     | 101 | 8CT  | C14-C13 | 3.75  | 1.54        | 1.43     |
| 32  | L     | 205 | 8CT  | C14-C13 | 3.75  | 1.54        | 1.43     |
| 30  | c     | 601 | CHL  | CHC-C1C | 3.74  | 1.46        | 1.39     |
| 30  | 4     | 305 | CHL  | CHC-C1C | 3.74  | 1.46        | 1.39     |
| 30  | 9     | 306 | CHL  | CHC-C1C | 3.74  | 1.46        | 1.39     |
| 32  | G     | 104 | 8CT  | C28-C29 | 3.73  | 1.40        | 1.32     |
| 32  | B     | 843 | 8CT  | C11-C12 | 3.73  | 1.53        | 1.46     |
| 32  | B     | 845 | 8CT  | C11-C12 | 3.73  | 1.53        | 1.46     |
| 42  | e     | 523 | NEX  | C7-C8   | -3.73 | 1.25        | 1.31     |
| 30  | 6     | 305 | CHL  | CHC-C1C | 3.72  | 1.46        | 1.39     |
| 32  | B     | 851 | 8CT  | C14-C13 | 3.72  | 1.54        | 1.43     |
| 32  | 0     | 401 | 8CT  | C28-C29 | 3.72  | 1.40        | 1.32     |
| 32  | B     | 847 | 8CT  | C14-C13 | 3.72  | 1.54        | 1.43     |
| 42  | d     | 523 | NEX  | C7-C6   | -3.72 | 1.26        | 1.30     |
| 42  | i     | 523 | NEX  | C7-C6   | -3.72 | 1.26        | 1.30     |
| 32  | 7     | 405 | 8CT  | C14-C13 | 3.72  | 1.54        | 1.43     |
| 42  | a     | 523 | NEX  | C7-C6   | -3.71 | 1.26        | 1.30     |
| 32  | M     | 102 | 8CT  | C14-C13 | 3.71  | 1.54        | 1.43     |
| 30  | i     | 606 | CHL  | C3A-C2A | -3.71 | 1.51        | 1.54     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 30  | 4     | 313 | CHL  | CHC-C1C | 3.71  | 1.46        | 1.39     |
| 30  | h     | 609 | CHL  | C3A-C2A | -3.71 | 1.51        | 1.54     |
| 32  | 8     | 406 | 8CT  | C11-C12 | 3.71  | 1.53        | 1.46     |
| 30  | g     | 614 | CHL  | C2A-C3A | -3.70 | 1.51        | 1.54     |
| 32  | B     | 844 | 8CT  | C11-C12 | 3.70  | 1.53        | 1.46     |
| 32  | I     | 101 | 8CT  | C14-C13 | 3.70  | 1.54        | 1.43     |
| 30  | 9     | 306 | CHL  | CHA-CBD | -3.70 | 1.47        | 1.51     |
| 30  | 4     | 307 | CHL  | CHC-C1C | 3.70  | 1.46        | 1.39     |
| 32  | B     | 804 | 8CT  | C14-C13 | 3.70  | 1.54        | 1.43     |
| 42  | b     | 523 | NEX  | C7-C6   | -3.70 | 1.26        | 1.30     |
| 30  | 6     | 306 | CHL  | CHC-C1C | 3.70  | 1.46        | 1.39     |
| 31  | g     | 613 | CLA  | C1D-ND  | 3.70  | 1.42        | 1.37     |
| 32  | A     | 854 | 8CT  | C28-C29 | 3.69  | 1.40        | 1.32     |
| 32  | 3     | 403 | 8CT  | C28-C29 | 3.69  | 1.40        | 1.32     |
| 30  | 6     | 301 | CHL  | CHA-CBD | -3.69 | 1.47        | 1.51     |
| 30  | 4     | 313 | CHL  | CHA-CBD | -3.69 | 1.47        | 1.51     |
| 42  | f     | 523 | NEX  | C7-C6   | -3.68 | 1.26        | 1.30     |
| 42  | h     | 523 | NEX  | C7-C6   | -3.68 | 1.26        | 1.30     |
| 32  | 0     | 401 | 8CT  | C11-C12 | 3.68  | 1.53        | 1.46     |
| 32  | 9     | 401 | 8CT  | C28-C29 | 3.68  | 1.40        | 1.32     |
| 42  | c     | 523 | NEX  | C7-C6   | -3.68 | 1.26        | 1.30     |
| 30  | 2     | 307 | CHL  | CHD-C4C | 3.68  | 1.46        | 1.39     |
| 32  | 8     | 402 | 8CT  | C28-C29 | 3.68  | 1.40        | 1.32     |
| 32  | 4     | 402 | 8CT  | C11-C12 | 3.67  | 1.53        | 1.46     |
| 30  | 7     | 301 | CHL  | CHA-CBD | -3.67 | 1.47        | 1.51     |
| 30  | 2     | 302 | CHL  | CHA-CBD | -3.67 | 1.47        | 1.51     |
| 32  | 1     | 402 | 8CT  | C11-C12 | 3.67  | 1.53        | 1.46     |
| 32  | J     | 104 | 8CT  | C28-C29 | 3.67  | 1.40        | 1.32     |
| 41  | B     | 849 | DGD  | O1G-C1A | 3.67  | 1.44        | 1.33     |
| 32  | 3     | 402 | 8CT  | C11-C12 | 3.67  | 1.53        | 1.46     |
| 32  | B     | 846 | 8CT  | C11-C12 | 3.67  | 1.53        | 1.46     |
| 31  | h     | 611 | CLA  | C1D-ND  | 3.66  | 1.42        | 1.37     |
| 30  | 3     | 307 | CHL  | CHC-C1C | 3.66  | 1.46        | 1.39     |
| 32  | 7     | 402 | 8CT  | C14-C13 | 3.66  | 1.54        | 1.43     |
| 30  | 8     | 313 | CHL  | CHC-C1C | 3.66  | 1.46        | 1.39     |
| 32  | 8     | 406 | 8CT  | C28-C29 | 3.66  | 1.40        | 1.32     |
| 32  | L     | 205 | 8CT  | C28-C29 | 3.66  | 1.40        | 1.32     |
| 30  | 6     | 302 | CHL  | CHA-CBD | -3.66 | 1.47        | 1.51     |
| 32  | 6     | 402 | 8CT  | C28-C29 | 3.66  | 1.40        | 1.32     |
| 30  | 8     | 302 | CHL  | CHA-CBD | -3.66 | 1.47        | 1.51     |
| 30  | 2     | 301 | CHL  | CHA-CBD | -3.65 | 1.47        | 1.51     |
| 30  | f     | 605 | CHL  | C3A-C2A | -3.65 | 1.51        | 1.54     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 42  | g     | 523 | NEX  | C7-C6   | -3.65 | 1.26        | 1.30     |
| 32  | B     | 848 | 8CT  | C11-C12 | 3.65  | 1.53        | 1.46     |
| 30  | 4     | 319 | CHL  | CHA-CBD | -3.64 | 1.47        | 1.51     |
| 32  | 3     | 402 | 8CT  | C28-C29 | 3.64  | 1.40        | 1.32     |
| 30  | a     | 607 | CHL  | C3A-C2A | -3.64 | 1.51        | 1.54     |
| 30  | 5     | 301 | CHL  | CHA-CBD | -3.63 | 1.47        | 1.51     |
| 32  | J     | 101 | 8CT  | C28-C29 | 3.63  | 1.40        | 1.32     |
| 30  | a     | 601 | CHL  | C3A-C2A | -3.63 | 1.51        | 1.54     |
| 30  | 4     | 308 | CHL  | CHA-CBD | -3.63 | 1.47        | 1.51     |
| 32  | K     | 107 | 8CT  | C11-C12 | 3.62  | 1.53        | 1.46     |
| 32  | L     | 209 | 8CT  | C11-C12 | 3.62  | 1.53        | 1.46     |
| 32  | J     | 104 | 8CT  | C11-C12 | 3.62  | 1.53        | 1.46     |
| 32  | K     | 107 | 8CT  | C28-C29 | 3.61  | 1.40        | 1.32     |
| 32  | F     | 302 | 8CT  | C28-C29 | 3.61  | 1.40        | 1.32     |
| 32  | 3     | 402 | 8CT  | C14-C13 | 3.61  | 1.54        | 1.43     |
| 32  | 2     | 402 | 8CT  | C11-C12 | 3.61  | 1.53        | 1.46     |
| 30  | g     | 607 | CHL  | C3A-C2A | -3.61 | 1.51        | 1.54     |
| 30  | c     | 605 | CHL  | C3A-C2A | -3.60 | 1.51        | 1.54     |
| 30  | h     | 607 | CHL  | C3A-C2A | -3.60 | 1.51        | 1.54     |
| 31  | 0     | 321 | CLA  | C1D-ND  | 3.60  | 1.42        | 1.37     |
| 31  | a     | 611 | CLA  | C1D-ND  | 3.60  | 1.42        | 1.37     |
| 32  | A     | 848 | 8CT  | C14-C13 | 3.59  | 1.54        | 1.43     |
| 31  | g     | 611 | CLA  | C1D-ND  | 3.59  | 1.42        | 1.37     |
| 32  | L     | 206 | 8CT  | C28-C29 | 3.59  | 1.40        | 1.32     |
| 39  | A     | 857 | CL0  | C3D-C4D | 3.59  | 1.47        | 1.41     |
| 32  | L     | 209 | 8CT  | C28-C29 | 3.59  | 1.40        | 1.32     |
| 32  | J     | 101 | 8CT  | C11-C12 | 3.58  | 1.53        | 1.46     |
| 30  | 4     | 302 | CHL  | CHA-CBD | -3.58 | 1.47        | 1.51     |
| 32  | A     | 849 | 8CT  | C14-C13 | 3.58  | 1.54        | 1.43     |
| 32  | M     | 102 | 8CT  | C28-C29 | 3.57  | 1.40        | 1.32     |
| 32  | A     | 850 | 8CT  | C14-C13 | 3.57  | 1.54        | 1.43     |
| 32  | O     | 205 | 8CT  | C28-C29 | 3.56  | 1.40        | 1.32     |
| 31  | a     | 613 | CLA  | C1D-ND  | 3.56  | 1.42        | 1.37     |
| 30  | 5     | 302 | CHL  | CHA-CBD | -3.55 | 1.47        | 1.51     |
| 32  | 9     | 401 | 8CT  | C11-C12 | 3.55  | 1.53        | 1.46     |
| 32  | B     | 851 | 8CT  | C28-C29 | 3.55  | 1.40        | 1.32     |
| 32  | G     | 104 | 8CT  | C11-C12 | 3.55  | 1.53        | 1.46     |
| 31  | d     | 613 | CLA  | C1D-ND  | 3.55  | 1.42        | 1.37     |
| 31  | O     | 203 | CLA  | C1D-ND  | 3.55  | 1.42        | 1.37     |
| 31  | i     | 613 | CLA  | C1D-ND  | 3.55  | 1.42        | 1.37     |
| 39  | A     | 857 | CL0  | CBD-CGD | -3.55 | 1.48        | 1.52     |
| 30  | a     | 605 | CHL  | C3A-C2A | -3.55 | 1.51        | 1.54     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 30  | 4     | 306 | CHL  | CHA-CBD | -3.55 | 1.47        | 1.51     |
| 30  | 1     | 302 | CHL  | CHA-CBD | -3.54 | 1.47        | 1.51     |
| 30  | i     | 609 | CHL  | C3A-C2A | -3.54 | 1.51        | 1.54     |
| 31  | i     | 604 | CLA  | C1D-ND  | 3.54  | 1.42        | 1.37     |
| 31  | 5     | 311 | CLA  | C1D-ND  | 3.53  | 1.42        | 1.37     |
| 30  | 5     | 313 | CHL  | CHA-CBD | -3.53 | 1.47        | 1.51     |
| 31  | h     | 603 | CLA  | C1D-ND  | 3.53  | 1.42        | 1.37     |
| 32  | A     | 847 | 8CT  | C11-C12 | 3.53  | 1.53        | 1.46     |
| 31  | d     | 611 | CLA  | C1D-ND  | 3.52  | 1.42        | 1.37     |
| 31  | a     | 603 | CLA  | C1D-ND  | 3.52  | 1.42        | 1.37     |
| 32  | A     | 850 | 8CT  | C28-C29 | 3.52  | 1.40        | 1.32     |
| 32  | B     | 847 | 8CT  | C11-C12 | 3.52  | 1.53        | 1.46     |
| 31  | c     | 603 | CLA  | C1D-ND  | 3.52  | 1.42        | 1.37     |
| 31  | i     | 612 | CLA  | C1D-ND  | 3.52  | 1.42        | 1.37     |
| 30  | 8     | 308 | CHL  | CHA-CBD | -3.51 | 1.47        | 1.51     |
| 30  | g     | 608 | CHL  | C3A-C2A | -3.51 | 1.51        | 1.54     |
| 30  | h     | 614 | CHL  | C2A-C3A | -3.51 | 1.51        | 1.54     |
| 31  | h     | 612 | CLA  | C1D-ND  | 3.51  | 1.42        | 1.37     |
| 30  | 7     | 302 | CHL  | CHA-CBD | -3.51 | 1.47        | 1.51     |
| 32  | A     | 854 | 8CT  | C11-C12 | 3.51  | 1.53        | 1.46     |
| 31  | g     | 612 | CLA  | C1D-ND  | 3.51  | 1.42        | 1.37     |
| 31  | 5     | 308 | CLA  | C1D-ND  | 3.51  | 1.42        | 1.37     |
| 31  | a     | 612 | CLA  | C1D-ND  | 3.51  | 1.42        | 1.37     |
| 32  | B     | 844 | 8CT  | C01-C02 | 3.51  | 1.56        | 1.50     |
| 32  | A     | 846 | 8CT  | C11-C12 | 3.51  | 1.53        | 1.46     |
| 31  | g     | 604 | CLA  | C1D-ND  | 3.50  | 1.42        | 1.37     |
| 31  | g     | 603 | CLA  | C1D-ND  | 3.50  | 1.42        | 1.37     |
| 31  | h     | 610 | CLA  | C1D-ND  | 3.50  | 1.42        | 1.37     |
| 32  | 7     | 405 | 8CT  | C11-C12 | 3.50  | 1.53        | 1.46     |
| 30  | i     | 605 | CHL  | C3A-C2A | -3.50 | 1.51        | 1.54     |
| 31  | g     | 610 | CLA  | C1D-ND  | 3.50  | 1.42        | 1.37     |
| 32  | B     | 845 | 8CT  | C28-C29 | 3.50  | 1.40        | 1.32     |
| 31  | b     | 611 | CLA  | C1D-ND  | 3.50  | 1.42        | 1.37     |
| 31  | 1     | 308 | CLA  | C1D-ND  | 3.49  | 1.42        | 1.37     |
| 31  | d     | 612 | CLA  | C1D-ND  | 3.49  | 1.42        | 1.37     |
| 32  | A     | 849 | 8CT  | C28-C29 | 3.49  | 1.40        | 1.32     |
| 31  | i     | 603 | CLA  | C1D-ND  | 3.49  | 1.42        | 1.37     |
| 32  | 3     | 403 | 8CT  | C11-C12 | 3.49  | 1.53        | 1.46     |
| 31  | i     | 610 | CLA  | C1D-ND  | 3.48  | 1.42        | 1.37     |
| 31  | f     | 603 | CLA  | C1D-ND  | 3.48  | 1.42        | 1.37     |
| 32  | O     | 205 | 8CT  | C11-C12 | 3.48  | 1.53        | 1.46     |
| 32  | 6     | 402 | 8CT  | C11-C12 | 3.48  | 1.53        | 1.46     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 32  | L     | 206 | 8CT  | C11-C12 | 3.48  | 1.53        | 1.46     |
| 30  | c     | 609 | CHL  | CHA-CBD | -3.48 | 1.47        | 1.51     |
| 30  | 9     | 313 | CHL  | CHA-CBD | -3.47 | 1.47        | 1.51     |
| 31  | c     | 612 | CLA  | C1D-ND  | 3.47  | 1.42        | 1.37     |
| 31  | h     | 613 | CLA  | C1D-ND  | 3.47  | 1.42        | 1.37     |
| 31  | b     | 612 | CLA  | C1D-ND  | 3.47  | 1.42        | 1.37     |
| 31  | B     | 826 | CLA  | C4D-ND  | -3.47 | 1.33        | 1.37     |
| 31  | d     | 603 | CLA  | C1D-ND  | 3.47  | 1.42        | 1.37     |
| 31  | a     | 610 | CLA  | C1D-ND  | 3.47  | 1.42        | 1.37     |
| 31  | e     | 612 | CLA  | C1D-ND  | 3.47  | 1.42        | 1.37     |
| 30  | 0     | 305 | CHL  | CHA-CBD | -3.47 | 1.47        | 1.51     |
| 31  | e     | 611 | CLA  | C1D-ND  | 3.46  | 1.42        | 1.37     |
| 32  | 7     | 402 | 8CT  | C28-C29 | 3.46  | 1.40        | 1.32     |
| 31  | i     | 611 | CLA  | C1D-ND  | 3.46  | 1.42        | 1.37     |
| 31  | c     | 611 | CLA  | C1D-ND  | 3.46  | 1.42        | 1.37     |
| 32  | I     | 101 | 8CT  | C28-C29 | 3.46  | 1.40        | 1.32     |
| 32  | A     | 848 | 8CT  | C01-C02 | 3.45  | 1.56        | 1.50     |
| 32  | A     | 847 | 8CT  | C28-C29 | 3.45  | 1.40        | 1.32     |
| 31  | 5     | 304 | CLA  | C1D-ND  | 3.45  | 1.42        | 1.37     |
| 30  | 5     | 307 | CHL  | CHA-CBD | -3.45 | 1.47        | 1.51     |
| 31  | 5     | 312 | CLA  | C1D-ND  | 3.45  | 1.42        | 1.37     |
| 32  | G     | 104 | 8CT  | C01-C02 | 3.45  | 1.56        | 1.50     |
| 32  | B     | 804 | 8CT  | C28-C29 | 3.45  | 1.40        | 1.32     |
| 31  | d     | 604 | CLA  | C1D-ND  | 3.44  | 1.42        | 1.37     |
| 31  | G     | 103 | CLA  | C1D-ND  | 3.44  | 1.42        | 1.37     |
| 31  | e     | 603 | CLA  | C1D-ND  | 3.43  | 1.42        | 1.37     |
| 32  | 7     | 402 | 8CT  | C11-C12 | 3.43  | 1.53        | 1.46     |
| 31  | a     | 604 | CLA  | C1D-ND  | 3.43  | 1.42        | 1.37     |
| 31  | f     | 613 | CLA  | C1D-ND  | 3.43  | 1.42        | 1.37     |
| 31  | e     | 613 | CLA  | C1D-ND  | 3.43  | 1.42        | 1.37     |
| 31  | f     | 611 | CLA  | C1D-ND  | 3.43  | 1.42        | 1.37     |
| 32  | B     | 846 | 8CT  | C35-C30 | 3.43  | 1.65        | 1.56     |
| 30  | a     | 602 | CHL  | CHA-CBD | -3.43 | 1.47        | 1.51     |
| 30  | f     | 602 | CHL  | CHA-CBD | -3.43 | 1.47        | 1.51     |
| 32  | B     | 804 | 8CT  | C11-C12 | 3.43  | 1.53        | 1.46     |
| 42  | f     | 523 | NEX  | C7-C8   | -3.43 | 1.26        | 1.31     |
| 30  | 3     | 307 | CHL  | CHA-CBD | -3.43 | 1.47        | 1.51     |
| 32  | 3     | 402 | 8CT  | C30-C29 | 3.42  | 1.55        | 1.50     |
| 32  | F     | 302 | 8CT  | C11-C12 | 3.42  | 1.53        | 1.46     |
| 31  | b     | 610 | CLA  | C1D-ND  | 3.42  | 1.42        | 1.37     |
| 32  | L     | 205 | 8CT  | C35-C30 | 3.42  | 1.65        | 1.56     |
| 31  | 9     | 304 | CLA  | C1D-ND  | 3.42  | 1.42        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 4     | 309 | CLA  | C1D-ND  | 3.42  | 1.42        | 1.37     |
| 42  | c     | 523 | NEX  | C7-C8   | -3.42 | 1.26        | 1.31     |
| 31  | 8     | 303 | CLA  | C1D-ND  | 3.41  | 1.42        | 1.37     |
| 31  | h     | 604 | CLA  | C1D-ND  | 3.41  | 1.42        | 1.37     |
| 31  | f     | 604 | CLA  | C1D-ND  | 3.41  | 1.42        | 1.37     |
| 31  | H     | 204 | CLA  | C1D-ND  | 3.41  | 1.42        | 1.37     |
| 31  | c     | 610 | CLA  | C1D-ND  | 3.41  | 1.42        | 1.37     |
| 32  | A     | 846 | 8CT  | C01-C02 | 3.41  | 1.56        | 1.50     |
| 32  | 7     | 405 | 8CT  | C28-C29 | 3.41  | 1.40        | 1.32     |
| 42  | b     | 523 | NEX  | C7-C8   | -3.41 | 1.26        | 1.31     |
| 31  | e     | 604 | CLA  | C1D-ND  | 3.41  | 1.42        | 1.37     |
| 31  | 0     | 308 | CLA  | C1D-ND  | 3.41  | 1.42        | 1.37     |
| 32  | L     | 205 | 8CT  | C30-C29 | 3.41  | 1.55        | 1.50     |
| 31  | 7     | 317 | CLA  | C1D-ND  | 3.41  | 1.42        | 1.37     |
| 30  | g     | 601 | CHL  | C3A-C2A | -3.41 | 1.51        | 1.54     |
| 32  | B     | 846 | 8CT  | C01-C02 | 3.40  | 1.56        | 1.50     |
| 31  | c     | 604 | CLA  | C1D-ND  | 3.40  | 1.42        | 1.37     |
| 32  | A     | 848 | 8CT  | C11-C12 | 3.40  | 1.53        | 1.46     |
| 32  | L     | 205 | 8CT  | C11-C12 | 3.40  | 1.53        | 1.46     |
| 30  | c     | 602 | CHL  | CHA-CBD | -3.40 | 1.47        | 1.51     |
| 32  | G     | 104 | 8CT  | C35-C30 | 3.40  | 1.65        | 1.56     |
| 32  | J     | 101 | 8CT  | C35-C30 | 3.40  | 1.65        | 1.56     |
| 42  | i     | 523 | NEX  | C7-C8   | -3.40 | 1.26        | 1.31     |
| 32  | I     | 101 | 8CT  | C11-C12 | 3.40  | 1.53        | 1.46     |
| 32  | A     | 846 | 8CT  | C28-C29 | 3.40  | 1.40        | 1.32     |
| 30  | d     | 609 | CHL  | CHA-CBD | -3.40 | 1.47        | 1.51     |
| 32  | A     | 850 | 8CT  | C11-C12 | 3.39  | 1.53        | 1.46     |
| 30  | 6     | 315 | CHL  | CHA-CBD | -3.39 | 1.47        | 1.51     |
| 30  | d     | 602 | CHL  | CHA-CBD | -3.39 | 1.47        | 1.51     |
| 32  | 7     | 404 | 8CT  | C11-C12 | 3.39  | 1.53        | 1.46     |
| 32  | B     | 851 | 8CT  | C11-C12 | 3.39  | 1.53        | 1.46     |
| 32  | K     | 107 | 8CT  | C01-C02 | 3.39  | 1.56        | 1.50     |
| 31  | b     | 613 | CLA  | C1D-ND  | 3.39  | 1.42        | 1.37     |
| 31  | c     | 613 | CLA  | C1D-ND  | 3.39  | 1.42        | 1.37     |
| 30  | 0     | 302 | CHL  | CHA-CBD | -3.39 | 1.47        | 1.51     |
| 31  | 7     | 312 | CLA  | C1D-ND  | 3.39  | 1.42        | 1.37     |
| 32  | 8     | 406 | 8CT  | C01-C02 | 3.39  | 1.56        | 1.50     |
| 39  | A     | 857 | CL0  | CMB-C2B | -3.39 | 1.44        | 1.51     |
| 31  | e     | 610 | CLA  | C1D-ND  | 3.39  | 1.42        | 1.37     |
| 42  | a     | 523 | NEX  | C7-C8   | -3.39 | 1.26        | 1.31     |
| 30  | g     | 605 | CHL  | C3A-C2A | -3.39 | 1.51        | 1.54     |
| 42  | g     | 523 | NEX  | C7-C8   | -3.39 | 1.26        | 1.31     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 32  | B     | 847 | 8CT  | C28-C29 | 3.38  | 1.40        | 1.32     |
| 32  | A     | 849 | 8CT  | C01-C02 | 3.38  | 1.56        | 1.50     |
| 31  | B     | 840 | CLA  | C1D-ND  | 3.38  | 1.42        | 1.37     |
| 30  | b     | 602 | CHL  | CHA-CBD | -3.38 | 1.47        | 1.51     |
| 31  | b     | 603 | CLA  | C1D-ND  | 3.38  | 1.42        | 1.37     |
| 31  | 0     | 309 | CLA  | C1D-ND  | 3.38  | 1.42        | 1.37     |
| 31  | d     | 610 | CLA  | C1D-ND  | 3.38  | 1.42        | 1.37     |
| 31  | f     | 610 | CLA  | C1D-ND  | 3.38  | 1.42        | 1.37     |
| 30  | 2     | 305 | CHL  | CHA-CBD | -3.38 | 1.47        | 1.51     |
| 32  | 4     | 402 | 8CT  | C01-C02 | 3.38  | 1.56        | 1.50     |
| 32  | A     | 847 | 8CT  | C01-C02 | 3.38  | 1.56        | 1.50     |
| 31  | b     | 604 | CLA  | C1D-ND  | 3.37  | 1.42        | 1.37     |
| 30  | g     | 609 | CHL  | CHA-CBD | -3.37 | 1.47        | 1.51     |
| 42  | h     | 523 | NEX  | C7-C8   | -3.37 | 1.26        | 1.31     |
| 32  | 3     | 403 | 8CT  | C01-C02 | 3.37  | 1.56        | 1.50     |
| 30  | 2     | 308 | CHL  | CHA-CBD | -3.36 | 1.47        | 1.51     |
| 30  | 8     | 305 | CHL  | CHA-CBD | -3.36 | 1.47        | 1.51     |
| 31  | J     | 103 | CLA  | C1D-ND  | 3.36  | 1.42        | 1.37     |
| 31  | 0     | 313 | CLA  | C1D-ND  | 3.36  | 1.42        | 1.37     |
| 31  | H     | 202 | CLA  | C1D-ND  | 3.35  | 1.42        | 1.37     |
| 31  | 5     | 310 | CLA  | C1D-ND  | 3.35  | 1.42        | 1.37     |
| 31  | F     | 301 | CLA  | C1D-ND  | 3.35  | 1.42        | 1.37     |
| 31  | 9     | 310 | CLA  | C1D-ND  | 3.35  | 1.42        | 1.37     |
| 31  | O     | 206 | CLA  | C1D-ND  | 3.35  | 1.42        | 1.37     |
| 31  | 8     | 309 | CLA  | C1D-ND  | 3.35  | 1.42        | 1.37     |
| 30  | 4     | 305 | CHL  | CHA-CBD | -3.35 | 1.47        | 1.51     |
| 31  | 8     | 312 | CLA  | C1D-ND  | 3.35  | 1.42        | 1.37     |
| 31  | A     | 835 | CLA  | C1D-ND  | 3.35  | 1.42        | 1.37     |
| 31  | 6     | 310 | CLA  | C1D-ND  | 3.35  | 1.42        | 1.37     |
| 31  | 8     | 314 | CLA  | C1D-ND  | 3.35  | 1.42        | 1.37     |
| 32  | 3     | 402 | 8CT  | C35-C30 | 3.34  | 1.65        | 1.56     |
| 31  | 1     | 310 | CLA  | C1D-ND  | 3.34  | 1.42        | 1.37     |
| 32  | M     | 102 | 8CT  | C01-C02 | 3.34  | 1.56        | 1.50     |
| 30  | h     | 602 | CHL  | CHA-CBD | -3.34 | 1.47        | 1.51     |
| 32  | A     | 850 | 8CT  | C01-C02 | 3.34  | 1.56        | 1.50     |
| 31  | L     | 207 | CLA  | C1D-ND  | 3.34  | 1.42        | 1.37     |
| 32  | I     | 101 | 8CT  | C01-C02 | 3.34  | 1.56        | 1.50     |
| 32  | A     | 848 | 8CT  | C28-C29 | 3.33  | 1.39        | 1.32     |
| 30  | 9     | 305 | CHL  | CHA-CBD | -3.33 | 1.47        | 1.51     |
| 32  | 4     | 402 | 8CT  | C18-C17 | 3.33  | 1.53        | 1.43     |
| 31  | 7     | 304 | CLA  | C1D-ND  | 3.33  | 1.42        | 1.37     |
| 30  | 6     | 305 | CHL  | CHA-CBD | -3.33 | 1.47        | 1.51     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 30  | 7     | 305 | CHL  | CHA-CBD | -3.33 | 1.47        | 1.51     |
| 31  | H     | 205 | CLA  | C1D-ND  | 3.33  | 1.42        | 1.37     |
| 32  | O     | 205 | 8CT  | C01-C02 | 3.33  | 1.56        | 1.50     |
| 31  | A     | 833 | CLA  | C1D-ND  | 3.33  | 1.42        | 1.37     |
| 32  | F     | 302 | 8CT  | C01-C02 | 3.33  | 1.56        | 1.50     |
| 31  | 7     | 315 | CLA  | C1D-ND  | 3.33  | 1.42        | 1.37     |
| 31  | G     | 101 | CLA  | C1D-ND  | 3.33  | 1.42        | 1.37     |
| 31  | L     | 204 | CLA  | C1D-ND  | 3.33  | 1.42        | 1.37     |
| 42  | d     | 523 | NEX  | C7-C8   | -3.33 | 1.26        | 1.31     |
| 31  | A     | 824 | CLA  | C1D-ND  | 3.33  | 1.42        | 1.37     |
| 32  | 3     | 403 | 8CT  | C35-C30 | 3.33  | 1.65        | 1.56     |
| 31  | 1     | 309 | CLA  | C1D-ND  | 3.32  | 1.42        | 1.37     |
| 31  | 4     | 310 | CLA  | C1D-ND  | 3.32  | 1.42        | 1.37     |
| 31  | 1     | 311 | CLA  | C1D-ND  | 3.32  | 1.42        | 1.37     |
| 31  | 5     | 314 | CLA  | C1D-ND  | 3.32  | 1.42        | 1.37     |
| 31  | K     | 104 | CLA  | C1D-ND  | 3.32  | 1.42        | 1.37     |
| 30  | h     | 605 | CHL  | C3A-C2A | -3.32 | 1.51        | 1.54     |
| 30  | c     | 601 | CHL  | CHA-CBD | -3.32 | 1.47        | 1.51     |
| 31  | A     | 815 | CLA  | C1D-ND  | 3.32  | 1.42        | 1.37     |
| 31  | B     | 822 | CLA  | C1D-ND  | 3.32  | 1.42        | 1.37     |
| 31  | 9     | 308 | CLA  | C1D-ND  | 3.32  | 1.42        | 1.37     |
| 32  | 7     | 402 | 8CT  | C01-C02 | 3.32  | 1.56        | 1.50     |
| 31  | B     | 821 | CLA  | C1D-ND  | 3.32  | 1.42        | 1.37     |
| 32  | B     | 847 | 8CT  | C01-C02 | 3.32  | 1.56        | 1.50     |
| 32  | L     | 205 | 8CT  | C01-C02 | 3.32  | 1.56        | 1.50     |
| 31  | G     | 102 | CLA  | C1D-ND  | 3.32  | 1.42        | 1.37     |
| 31  | 0     | 304 | CLA  | C1D-ND  | 3.32  | 1.42        | 1.37     |
| 31  | A     | 825 | CLA  | C1D-ND  | 3.32  | 1.42        | 1.37     |
| 32  | 2     | 402 | 8CT  | C18-C17 | 3.31  | 1.53        | 1.43     |
| 32  | 6     | 402 | 8CT  | C35-C30 | 3.31  | 1.65        | 1.56     |
| 31  | 0     | 310 | CLA  | C1D-ND  | 3.31  | 1.42        | 1.37     |
| 31  | 2     | 303 | CLA  | C1D-ND  | 3.31  | 1.42        | 1.37     |
| 32  | M     | 102 | 8CT  | C11-C12 | 3.31  | 1.53        | 1.46     |
| 31  | 3     | 313 | CLA  | C1D-ND  | 3.31  | 1.42        | 1.37     |
| 31  | 1     | 312 | CLA  | C1D-ND  | 3.31  | 1.42        | 1.37     |
| 31  | 6     | 320 | CLA  | C1D-ND  | 3.31  | 1.42        | 1.37     |
| 30  | c     | 607 | CHL  | CHA-CBD | -3.31 | 1.47        | 1.51     |
| 32  | B     | 851 | 8CT  | C01-C02 | 3.31  | 1.56        | 1.50     |
| 30  | e     | 607 | CHL  | CHA-CBD | -3.30 | 1.47        | 1.51     |
| 31  | 3     | 311 | CLA  | C1D-ND  | 3.30  | 1.42        | 1.37     |
| 31  | 5     | 303 | CLA  | C1D-ND  | 3.30  | 1.42        | 1.37     |
| 31  | 6     | 309 | CLA  | C1D-ND  | 3.30  | 1.42        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | f     | 612 | CLA  | C1D-ND  | 3.30  | 1.42        | 1.37     |
| 31  | 4     | 312 | CLA  | C1D-ND  | 3.30  | 1.42        | 1.37     |
| 30  | d     | 605 | CHL  | C3A-C2A | -3.30 | 1.51        | 1.54     |
| 30  | 2     | 307 | CHL  | CHA-CBD | -3.30 | 1.47        | 1.51     |
| 30  | e     | 602 | CHL  | CHA-CBD | -3.30 | 1.47        | 1.51     |
| 32  | 0     | 401 | 8CT  | C01-C02 | 3.30  | 1.56        | 1.50     |
| 32  | 1     | 402 | 8CT  | C35-C30 | 3.30  | 1.65        | 1.56     |
| 30  | 2     | 319 | CHL  | CHA-CBD | -3.30 | 1.47        | 1.51     |
| 31  | 6     | 314 | CLA  | C1D-ND  | 3.30  | 1.42        | 1.37     |
| 31  | A     | 814 | CLA  | C1D-ND  | 3.30  | 1.42        | 1.37     |
| 31  | 8     | 310 | CLA  | C1D-ND  | 3.29  | 1.42        | 1.37     |
| 32  | L     | 209 | 8CT  | C01-C02 | 3.29  | 1.56        | 1.50     |
| 31  | 1     | 304 | CLA  | C1D-ND  | 3.29  | 1.42        | 1.37     |
| 31  | B     | 816 | CLA  | C1D-ND  | 3.29  | 1.42        | 1.37     |
| 30  | 3     | 305 | CHL  | CHA-CBD | -3.29 | 1.47        | 1.51     |
| 30  | g     | 606 | CHL  | CHA-CBD | -3.29 | 1.47        | 1.51     |
| 30  | f     | 609 | CHL  | CHA-CBD | -3.29 | 1.47        | 1.51     |
| 31  | 6     | 304 | CLA  | C1D-ND  | 3.29  | 1.42        | 1.37     |
| 32  | A     | 854 | 8CT  | C01-C02 | 3.29  | 1.56        | 1.50     |
| 32  | A     | 849 | 8CT  | C35-C30 | 3.29  | 1.65        | 1.56     |
| 32  | A     | 850 | 8CT  | C35-C30 | 3.28  | 1.65        | 1.56     |
| 32  | B     | 843 | 8CT  | C01-C02 | 3.28  | 1.56        | 1.50     |
| 31  | 5     | 309 | CLA  | C1D-ND  | 3.28  | 1.42        | 1.37     |
| 31  | 2     | 311 | CLA  | C1D-ND  | 3.28  | 1.42        | 1.37     |
| 32  | L     | 206 | 8CT  | C01-C02 | 3.28  | 1.56        | 1.50     |
| 32  | J     | 104 | 8CT  | C01-C02 | 3.28  | 1.56        | 1.50     |
| 30  | 9     | 301 | CHL  | CHA-CBD | -3.28 | 1.47        | 1.51     |
| 30  | h     | 607 | CHL  | CHA-CBD | -3.28 | 1.47        | 1.51     |
| 31  | 9     | 312 | CLA  | C1D-ND  | 3.28  | 1.42        | 1.37     |
| 32  | M     | 102 | 8CT  | C35-C30 | 3.28  | 1.65        | 1.56     |
| 30  | e     | 609 | CHL  | CHA-CBD | -3.28 | 1.47        | 1.51     |
| 31  | 1     | 314 | CLA  | C1D-ND  | 3.28  | 1.42        | 1.37     |
| 31  | A     | 837 | CLA  | C1D-ND  | 3.28  | 1.42        | 1.37     |
| 32  | G     | 104 | 8CT  | C30-C29 | 3.27  | 1.55        | 1.50     |
| 30  | f     | 601 | CHL  | CHA-CBD | -3.27 | 1.47        | 1.51     |
| 31  | 3     | 308 | CLA  | C1D-ND  | 3.27  | 1.42        | 1.37     |
| 31  | B     | 835 | CLA  | C1D-ND  | 3.27  | 1.42        | 1.37     |
| 32  | 1     | 402 | 8CT  | C01-C02 | 3.27  | 1.56        | 1.50     |
| 31  | 3     | 310 | CLA  | C1D-ND  | 3.27  | 1.42        | 1.37     |
| 30  | h     | 609 | CHL  | CHA-CBD | -3.27 | 1.47        | 1.51     |
| 31  | A     | 803 | CLA  | C1D-ND  | 3.27  | 1.42        | 1.37     |
| 31  | 9     | 311 | CLA  | C1D-ND  | 3.27  | 1.42        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | B     | 825 | CLA  | C1D-ND  | 3.27  | 1.42        | 1.37     |
| 31  | 8     | 311 | CLA  | C1D-ND  | 3.27  | 1.42        | 1.37     |
| 34  | 7     | 601 | LHG  | C26-C25 | -3.27 | 1.35        | 1.51     |
| 32  | 9     | 401 | 8CT  | C01-C02 | 3.27  | 1.56        | 1.50     |
| 31  | A     | 832 | CLA  | C1D-ND  | 3.27  | 1.42        | 1.37     |
| 31  | B     | 833 | CLA  | C1D-ND  | 3.26  | 1.42        | 1.37     |
| 31  | B     | 836 | CLA  | C1D-ND  | 3.26  | 1.42        | 1.37     |
| 30  | 8     | 315 | CHL  | CHA-CBD | -3.26 | 1.47        | 1.51     |
| 31  | B     | 832 | CLA  | C1D-ND  | 3.26  | 1.42        | 1.37     |
| 34  | 1     | 601 | LHG  | C26-C25 | -3.26 | 1.35        | 1.51     |
| 34  | 3     | 601 | LHG  | C26-C25 | -3.26 | 1.35        | 1.51     |
| 31  | O     | 202 | CLA  | C1D-ND  | 3.26  | 1.42        | 1.37     |
| 30  | 4     | 307 | CHL  | CHA-CBD | -3.26 | 1.47        | 1.51     |
| 32  | B     | 804 | 8CT  | C01-C02 | 3.26  | 1.56        | 1.50     |
| 31  | 7     | 310 | CLA  | C1D-ND  | 3.26  | 1.42        | 1.37     |
| 32  | L     | 209 | 8CT  | C35-C30 | 3.26  | 1.65        | 1.56     |
| 32  | 4     | 402 | 8CT  | C35-C30 | 3.26  | 1.65        | 1.56     |
| 31  | K     | 105 | CLA  | C1D-ND  | 3.26  | 1.42        | 1.37     |
| 32  | G     | 104 | 8CT  | C18-C17 | 3.26  | 1.53        | 1.43     |
| 30  | g     | 609 | CHL  | O2A-CGA | 3.26  | 1.45        | 1.33     |
| 32  | 7     | 404 | 8CT  | C18-C17 | 3.26  | 1.53        | 1.43     |
| 31  | B     | 827 | CLA  | C1D-ND  | 3.26  | 1.42        | 1.37     |
| 32  | 7     | 404 | 8CT  | C01-C02 | 3.26  | 1.56        | 1.50     |
| 34  | A     | 844 | LHG  | C26-C25 | -3.25 | 1.35        | 1.51     |
| 31  | 7     | 318 | CLA  | C1D-ND  | 3.25  | 1.42        | 1.37     |
| 31  | 0     | 312 | CLA  | C1D-ND  | 3.25  | 1.42        | 1.37     |
| 31  | 7     | 311 | CLA  | C1D-ND  | 3.25  | 1.42        | 1.37     |
| 31  | O     | 201 | CLA  | C1D-ND  | 3.25  | 1.42        | 1.37     |
| 31  | 0     | 311 | CLA  | C1D-ND  | 3.25  | 1.42        | 1.37     |
| 32  | B     | 843 | 8CT  | C30-C29 | 3.25  | 1.55        | 1.50     |
| 34  | 3     | 603 | LHG  | C26-C25 | -3.25 | 1.35        | 1.51     |
| 31  | A     | 816 | CLA  | C1D-ND  | 3.25  | 1.42        | 1.37     |
| 30  | e     | 606 | CHL  | CHA-CBD | -3.25 | 1.47        | 1.51     |
| 31  | 4     | 304 | CLA  | C1D-ND  | 3.25  | 1.42        | 1.37     |
| 30  | a     | 606 | CHL  | CHA-CBD | -3.24 | 1.47        | 1.51     |
| 31  | A     | 838 | CLA  | C1D-ND  | 3.24  | 1.42        | 1.37     |
| 31  | 4     | 311 | CLA  | C1D-ND  | 3.24  | 1.42        | 1.37     |
| 30  | 5     | 306 | CHL  | CHA-CBD | -3.24 | 1.47        | 1.51     |
| 31  | 2     | 314 | CLA  | C1D-ND  | 3.24  | 1.42        | 1.37     |
| 31  | 3     | 304 | CLA  | C1D-ND  | 3.24  | 1.42        | 1.37     |
| 32  | B     | 848 | 8CT  | C18-C17 | 3.24  | 1.53        | 1.43     |
| 32  | A     | 849 | 8CT  | C11-C12 | 3.24  | 1.52        | 1.46     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 34  | 8     | 601 | LHG  | C26-C25 | -3.24 | 1.35        | 1.51     |
| 32  | 0     | 401 | 8CT  | C35-C30 | 3.24  | 1.65        | 1.56     |
| 31  | 3     | 306 | CLA  | C1D-ND  | 3.24  | 1.42        | 1.37     |
| 32  | 8     | 406 | 8CT  | C35-C30 | 3.24  | 1.65        | 1.56     |
| 32  | B     | 843 | 8CT  | C35-C30 | 3.24  | 1.65        | 1.56     |
| 34  | 7     | 603 | LHG  | C26-C25 | -3.24 | 1.35        | 1.51     |
| 32  | 8     | 406 | 8CT  | C30-C29 | 3.24  | 1.55        | 1.50     |
| 34  | f     | 630 | LHG  | C26-C25 | -3.24 | 1.35        | 1.51     |
| 30  | 5     | 305 | CHL  | CHA-CBD | -3.24 | 1.47        | 1.51     |
| 31  | B     | 841 | CLA  | C1D-ND  | 3.24  | 1.42        | 1.37     |
| 34  | K     | 106 | LHG  | C26-C25 | -3.24 | 1.35        | 1.51     |
| 34  | M     | 104 | LHG  | C26-C25 | -3.23 | 1.35        | 1.51     |
| 34  | e     | 630 | LHG  | C26-C25 | -3.23 | 1.35        | 1.51     |
| 32  | 7     | 404 | 8CT  | C35-C30 | 3.23  | 1.65        | 1.56     |
| 31  | 6     | 303 | CLA  | C1D-ND  | 3.23  | 1.42        | 1.37     |
| 31  | A     | 810 | CLA  | C1D-ND  | 3.23  | 1.42        | 1.37     |
| 31  | B     | 815 | CLA  | C1D-ND  | 3.23  | 1.42        | 1.37     |
| 34  | 9     | 601 | LHG  | C26-C25 | -3.23 | 1.35        | 1.51     |
| 31  | A     | 819 | CLA  | C1D-ND  | 3.23  | 1.42        | 1.37     |
| 31  | A     | 843 | CLA  | C1D-ND  | 3.23  | 1.42        | 1.37     |
| 31  | B     | 813 | CLA  | C1D-ND  | 3.23  | 1.42        | 1.37     |
| 31  | 4     | 314 | CLA  | C1D-ND  | 3.23  | 1.42        | 1.37     |
| 31  | 4     | 303 | CLA  | C1D-ND  | 3.23  | 1.42        | 1.37     |
| 32  | B     | 845 | 8CT  | C01-C02 | 3.23  | 1.56        | 1.50     |
| 34  | c     | 630 | LHG  | C26-C25 | -3.23 | 1.35        | 1.51     |
| 32  | J     | 101 | 8CT  | C30-C29 | 3.23  | 1.55        | 1.50     |
| 31  | 0     | 303 | CLA  | C1D-ND  | 3.23  | 1.42        | 1.37     |
| 31  | 3     | 303 | CLA  | C1D-ND  | 3.23  | 1.42        | 1.37     |
| 31  | B     | 820 | CLA  | C1D-ND  | 3.23  | 1.42        | 1.37     |
| 32  | B     | 848 | 8CT  | C01-C02 | 3.23  | 1.56        | 1.50     |
| 34  | b     | 630 | LHG  | C26-C25 | -3.23 | 1.35        | 1.51     |
| 34  | 6     | 601 | LHG  | C26-C25 | -3.23 | 1.35        | 1.51     |
| 31  | 8     | 304 | CLA  | C1D-ND  | 3.23  | 1.42        | 1.37     |
| 34  | 2     | 601 | LHG  | C26-C25 | -3.23 | 1.35        | 1.51     |
| 31  | 7     | 303 | CLA  | C1D-ND  | 3.22  | 1.42        | 1.37     |
| 34  | 5     | 601 | LHG  | C26-C25 | -3.22 | 1.35        | 1.51     |
| 32  | J     | 101 | 8CT  | C01-C02 | 3.22  | 1.56        | 1.50     |
| 34  | 0     | 601 | LHG  | C26-C25 | -3.22 | 1.35        | 1.51     |
| 32  | B     | 845 | 8CT  | C18-C17 | 3.22  | 1.53        | 1.43     |
| 30  | h     | 605 | CHL  | CHA-CBD | -3.22 | 1.47        | 1.51     |
| 34  | 6     | 603 | LHG  | C26-C25 | -3.22 | 1.35        | 1.51     |
| 34  | B     | 854 | LHG  | C26-C25 | -3.22 | 1.35        | 1.51     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 34  | h     | 630 | LHG  | C26-C25 | -3.22 | 1.35        | 1.51     |
| 30  | i     | 606 | CHL  | CHA-CBD | -3.22 | 1.47        | 1.51     |
| 32  | 2     | 402 | 8CT  | C35-C30 | 3.22  | 1.65        | 1.56     |
| 31  | 9     | 302 | CLA  | C1D-ND  | 3.21  | 1.42        | 1.37     |
| 30  | 6     | 306 | CHL  | CHA-CBD | -3.21 | 1.47        | 1.51     |
| 31  | A     | 802 | CLA  | C1D-ND  | 3.21  | 1.42        | 1.37     |
| 30  | 6     | 308 | CHL  | CHA-CBD | -3.21 | 1.47        | 1.51     |
| 31  | 3     | 318 | CLA  | C1D-ND  | 3.21  | 1.42        | 1.37     |
| 31  | A     | 839 | CLA  | C1D-ND  | 3.21  | 1.42        | 1.37     |
| 34  | H     | 203 | LHG  | C26-C25 | -3.21 | 1.35        | 1.51     |
| 30  | 6     | 307 | CHL  | CHA-CBD | -3.21 | 1.47        | 1.51     |
| 34  | G     | 105 | LHG  | C26-C25 | -3.21 | 1.35        | 1.51     |
| 31  | 9     | 300 | CLA  | C1D-ND  | 3.21  | 1.42        | 1.37     |
| 34  | a     | 630 | LHG  | C26-C25 | -3.21 | 1.35        | 1.51     |
| 34  | d     | 630 | LHG  | C26-C25 | -3.21 | 1.35        | 1.51     |
| 34  | i     | 630 | LHG  | C26-C25 | -3.21 | 1.35        | 1.51     |
| 31  | 9     | 309 | CLA  | C1D-ND  | 3.20  | 1.42        | 1.37     |
| 30  | 1     | 313 | CHL  | CHA-CBD | -3.20 | 1.47        | 1.51     |
| 31  | A     | 827 | CLA  | C1D-ND  | 3.20  | 1.42        | 1.37     |
| 32  | 0     | 401 | 8CT  | C18-C17 | 3.20  | 1.53        | 1.43     |
| 35  | 0     | 603 | SQD  | O48-C23 | 3.20  | 1.42        | 1.33     |
| 31  | 2     | 312 | CLA  | C1D-ND  | 3.20  | 1.42        | 1.37     |
| 34  | 4     | 601 | LHG  | C26-C25 | -3.20 | 1.35        | 1.51     |
| 31  | B     | 850 | CLA  | C1D-ND  | 3.19  | 1.42        | 1.37     |
| 30  | d     | 606 | CHL  | CHA-CBD | -3.19 | 1.47        | 1.51     |
| 32  | 7     | 405 | 8CT  | C01-C02 | 3.19  | 1.56        | 1.50     |
| 31  | 2     | 309 | CLA  | C1D-ND  | 3.19  | 1.42        | 1.37     |
| 30  | b     | 607 | CHL  | CHA-CBD | -3.19 | 1.47        | 1.51     |
| 31  | A     | 812 | CLA  | C1D-ND  | 3.19  | 1.42        | 1.37     |
| 30  | 1     | 305 | CHL  | CHA-CBD | -3.19 | 1.47        | 1.51     |
| 30  | b     | 606 | CHL  | CHA-CBD | -3.19 | 1.47        | 1.51     |
| 30  | b     | 609 | CHL  | CHA-CBD | -3.19 | 1.47        | 1.51     |
| 31  | A     | 811 | CLA  | C1D-ND  | 3.19  | 1.42        | 1.37     |
| 31  | A     | 828 | CLA  | C1D-ND  | 3.19  | 1.42        | 1.37     |
| 30  | 0     | 301 | CHL  | CHA-CBD | -3.19 | 1.47        | 1.51     |
| 31  | 6     | 317 | CLA  | C1D-ND  | 3.19  | 1.42        | 1.37     |
| 30  | f     | 606 | CHL  | CHA-CBD | -3.19 | 1.47        | 1.51     |
| 30  | f     | 607 | CHL  | CHA-CBD | -3.19 | 1.47        | 1.51     |
| 32  | 9     | 401 | 8CT  | C18-C17 | 3.18  | 1.53        | 1.43     |
| 32  | 6     | 402 | 8CT  | C18-C17 | 3.18  | 1.53        | 1.43     |
| 31  | 1     | 303 | CLA  | C1D-ND  | 3.18  | 1.42        | 1.37     |
| 31  | A     | 808 | CLA  | C1D-ND  | 3.18  | 1.42        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | A     | 840 | CLA  | C1D-ND  | 3.18  | 1.42        | 1.37     |
| 31  | B     | 834 | CLA  | C1D-ND  | 3.18  | 1.42        | 1.37     |
| 34  | A     | 855 | LHG  | C26-C25 | -3.18 | 1.36        | 1.51     |
| 32  | 6     | 402 | 8CT  | C01-C02 | 3.18  | 1.56        | 1.50     |
| 32  | 8     | 406 | 8CT  | C18-C17 | 3.18  | 1.53        | 1.43     |
| 32  | J     | 104 | 8CT  | C18-C17 | 3.18  | 1.53        | 1.43     |
| 31  | B     | 807 | CLA  | C1D-ND  | 3.18  | 1.42        | 1.37     |
| 32  | 2     | 402 | 8CT  | C07-C02 | -3.18 | 1.45        | 1.51     |
| 31  | 6     | 311 | CLA  | C1D-ND  | 3.17  | 1.42        | 1.37     |
| 31  | B     | 818 | CLA  | C1D-ND  | 3.17  | 1.42        | 1.37     |
| 32  | 1     | 402 | 8CT  | C18-C17 | 3.17  | 1.53        | 1.43     |
| 31  | A     | 853 | CLA  | C1D-ND  | 3.17  | 1.42        | 1.37     |
| 32  | 3     | 402 | 8CT  | C01-C02 | 3.17  | 1.56        | 1.50     |
| 31  | 7     | 316 | CLA  | C1D-ND  | 3.17  | 1.42        | 1.37     |
| 30  | d     | 607 | CHL  | CHA-CBD | -3.17 | 1.48        | 1.51     |
| 31  | 6     | 318 | CLA  | C1D-ND  | 3.17  | 1.42        | 1.37     |
| 32  | B     | 847 | 8CT  | C35-C30 | 3.16  | 1.65        | 1.56     |
| 31  | 3     | 312 | CLA  | C1D-ND  | 3.16  | 1.42        | 1.37     |
| 31  | B     | 823 | CLA  | C1D-ND  | 3.16  | 1.42        | 1.37     |
| 31  | B     | 839 | CLA  | C1D-ND  | 3.16  | 1.42        | 1.37     |
| 31  | 7     | 308 | CLA  | C1D-ND  | 3.16  | 1.42        | 1.37     |
| 31  | 9     | 303 | CLA  | C1D-ND  | 3.16  | 1.42        | 1.37     |
| 34  | g     | 630 | LHG  | C26-C25 | -3.16 | 1.36        | 1.51     |
| 31  | 2     | 304 | CLA  | C1D-ND  | 3.16  | 1.42        | 1.37     |
| 31  | B     | 819 | CLA  | C1D-ND  | 3.16  | 1.42        | 1.37     |
| 30  | 8     | 307 | CHL  | CHA-CBD | -3.16 | 1.48        | 1.51     |
| 30  | 8     | 313 | CHL  | CHA-CBD | -3.16 | 1.48        | 1.51     |
| 31  | 3     | 309 | CLA  | C1D-ND  | 3.16  | 1.42        | 1.37     |
| 31  | A     | 852 | CLA  | C1D-ND  | 3.16  | 1.42        | 1.37     |
| 31  | A     | 805 | CLA  | C1D-ND  | 3.16  | 1.42        | 1.37     |
| 31  | B     | 838 | CLA  | C1D-ND  | 3.15  | 1.42        | 1.37     |
| 32  | B     | 843 | 8CT  | C10-C03 | 3.15  | 1.55        | 1.45     |
| 32  | B     | 847 | 8CT  | C07-C02 | -3.15 | 1.45        | 1.51     |
| 32  | B     | 844 | 8CT  | C10-C03 | 3.15  | 1.55        | 1.45     |
| 31  | L     | 203 | CLA  | C1D-ND  | 3.15  | 1.42        | 1.37     |
| 32  | I     | 101 | 8CT  | C35-C30 | 3.15  | 1.65        | 1.56     |
| 31  | B     | 828 | CLA  | C1D-ND  | 3.15  | 1.42        | 1.37     |
| 31  | L     | 202 | CLA  | C1D-ND  | 3.15  | 1.42        | 1.37     |
| 31  | B     | 837 | CLA  | C1D-ND  | 3.15  | 1.42        | 1.37     |
| 32  | 8     | 402 | 8CT  | C35-C30 | 3.15  | 1.65        | 1.56     |
| 31  | A     | 806 | CLA  | C1D-ND  | 3.15  | 1.42        | 1.37     |
| 31  | A     | 818 | CLA  | C1D-ND  | 3.15  | 1.42        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | B     | 811 | CLA  | C1D-ND  | 3.15  | 1.42        | 1.37     |
| 32  | L     | 206 | 8CT  | C18-C17 | 3.15  | 1.52        | 1.43     |
| 32  | J     | 104 | 8CT  | C30-C29 | 3.15  | 1.55        | 1.50     |
| 31  | 7     | 309 | CLA  | C1D-ND  | 3.14  | 1.42        | 1.37     |
| 31  | B     | 808 | CLA  | C1D-ND  | 3.14  | 1.42        | 1.37     |
| 31  | A     | 813 | CLA  | C1D-ND  | 3.14  | 1.42        | 1.37     |
| 31  | K     | 102 | CLA  | C1D-ND  | 3.14  | 1.42        | 1.37     |
| 32  | A     | 846 | 8CT  | C35-C30 | 3.14  | 1.65        | 1.56     |
| 32  | 2     | 402 | 8CT  | C01-C02 | 3.14  | 1.55        | 1.50     |
| 32  | K     | 107 | 8CT  | C35-C30 | 3.14  | 1.65        | 1.56     |
| 32  | 4     | 402 | 8CT  | C10-C03 | 3.14  | 1.55        | 1.45     |
| 32  | 7     | 405 | 8CT  | C35-C30 | 3.14  | 1.65        | 1.56     |
| 30  | 7     | 313 | CHL  | CHA-CBD | -3.14 | 1.48        | 1.51     |
| 31  | H     | 201 | CLA  | C1D-ND  | 3.13  | 1.42        | 1.37     |
| 32  | L     | 206 | 8CT  | C35-C30 | 3.13  | 1.65        | 1.56     |
| 32  | J     | 104 | 8CT  | C10-C03 | 3.13  | 1.55        | 1.45     |
| 31  | 6     | 311 | CLA  | C4B-NB  | 3.13  | 1.42        | 1.37     |
| 31  | 6     | 312 | CLA  | C1D-ND  | 3.13  | 1.42        | 1.37     |
| 31  | M     | 101 | CLA  | C1D-ND  | 3.13  | 1.42        | 1.37     |
| 31  | A     | 821 | CLA  | C1D-ND  | 3.13  | 1.42        | 1.37     |
| 32  | K     | 107 | 8CT  | C18-C17 | 3.13  | 1.52        | 1.43     |
| 32  | B     | 845 | 8CT  | C10-C03 | 3.12  | 1.55        | 1.45     |
| 32  | B     | 851 | 8CT  | C07-C02 | -3.12 | 1.45        | 1.51     |
| 31  | g     | 610 | CLA  | C4B-NB  | 3.12  | 1.42        | 1.37     |
| 31  | 3     | 320 | CLA  | C1D-ND  | 3.12  | 1.42        | 1.37     |
| 31  | A     | 831 | CLA  | C1D-ND  | 3.12  | 1.42        | 1.37     |
| 30  | 6     | 313 | CHL  | CHA-CBD | -3.12 | 1.48        | 1.51     |
| 31  | 2     | 310 | CLA  | C1D-ND  | 3.12  | 1.42        | 1.37     |
| 30  | g     | 602 | CHL  | CHA-CBD | -3.12 | 1.48        | 1.51     |
| 32  | B     | 846 | 8CT  | C18-C17 | 3.12  | 1.52        | 1.43     |
| 31  | h     | 612 | CLA  | C4B-NB  | 3.11  | 1.42        | 1.37     |
| 31  | B     | 803 | CLA  | C1D-ND  | 3.11  | 1.42        | 1.37     |
| 31  | B     | 812 | CLA  | C1D-ND  | 3.11  | 1.42        | 1.37     |
| 32  | L     | 209 | 8CT  | C18-C17 | 3.11  | 1.52        | 1.43     |
| 31  | A     | 820 | CLA  | C1D-ND  | 3.11  | 1.41        | 1.37     |
| 31  | 9     | 311 | CLA  | C4B-NB  | 3.11  | 1.41        | 1.37     |
| 31  | B     | 809 | CLA  | C1D-ND  | 3.11  | 1.41        | 1.37     |
| 32  | B     | 848 | 8CT  | C35-C30 | 3.11  | 1.65        | 1.56     |
| 31  | O     | 203 | CLA  | CAB-C3B | -3.11 | 1.44        | 1.50     |
| 32  | A     | 854 | 8CT  | C18-C17 | 3.11  | 1.52        | 1.43     |
| 32  | F     | 302 | 8CT  | C18-C17 | 3.11  | 1.52        | 1.43     |
| 32  | L     | 206 | 8CT  | C07-C02 | -3.11 | 1.45        | 1.51     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | B     | 829 | CLA  | C1D-ND  | 3.11  | 1.41        | 1.37     |
| 32  | 2     | 402 | 8CT  | C10-C03 | 3.11  | 1.55        | 1.45     |
| 32  | A     | 847 | 8CT  | C35-C30 | 3.11  | 1.65        | 1.56     |
| 30  | 1     | 306 | CHL  | CHA-CBD | -3.10 | 1.48        | 1.51     |
| 31  | A     | 822 | CLA  | C1D-ND  | 3.10  | 1.41        | 1.37     |
| 31  | a     | 604 | CLA  | C4B-NB  | 3.10  | 1.41        | 1.37     |
| 30  | d     | 601 | CHL  | CHA-CBD | -3.10 | 1.48        | 1.51     |
| 30  | c     | 614 | CHL  | CHA-CBD | -3.10 | 1.48        | 1.51     |
| 31  | A     | 836 | CLA  | C1D-ND  | 3.10  | 1.41        | 1.37     |
| 32  | M     | 102 | 8CT  | C18-C17 | 3.10  | 1.52        | 1.43     |
| 31  | B     | 824 | CLA  | C1D-ND  | 3.09  | 1.41        | 1.37     |
| 30  | i     | 609 | CHL  | CHA-CBD | -3.09 | 1.48        | 1.51     |
| 31  | A     | 807 | CLA  | C1D-ND  | 3.09  | 1.41        | 1.37     |
| 32  | 8     | 406 | 8CT  | C10-C03 | 3.09  | 1.55        | 1.45     |
| 31  | B     | 814 | CLA  | C1D-ND  | 3.09  | 1.41        | 1.37     |
| 31  | b     | 604 | CLA  | C4B-NB  | 3.09  | 1.41        | 1.37     |
| 31  | a     | 613 | CLA  | C4B-NB  | 3.09  | 1.41        | 1.37     |
| 32  | 8     | 402 | 8CT  | C18-C17 | 3.09  | 1.52        | 1.43     |
| 32  | F     | 302 | 8CT  | C35-C30 | 3.09  | 1.65        | 1.56     |
| 32  | A     | 848 | 8CT  | C35-C30 | 3.09  | 1.65        | 1.56     |
| 32  | B     | 844 | 8CT  | C18-C17 | 3.09  | 1.52        | 1.43     |
| 32  | B     | 846 | 8CT  | C10-C03 | 3.08  | 1.55        | 1.45     |
| 31  | A     | 823 | CLA  | C1D-ND  | 3.08  | 1.41        | 1.37     |
| 32  | 3     | 402 | 8CT  | C10-C03 | 3.08  | 1.55        | 1.45     |
| 30  | i     | 602 | CHL  | CHA-CBD | -3.08 | 1.48        | 1.51     |
| 31  | A     | 817 | CLA  | C1D-ND  | 3.08  | 1.41        | 1.37     |
| 32  | 8     | 402 | 8CT  | C10-C03 | 3.08  | 1.55        | 1.45     |
| 31  | g     | 603 | CLA  | C4B-NB  | 3.08  | 1.41        | 1.37     |
| 32  | L     | 205 | 8CT  | C07-C02 | -3.08 | 1.45        | 1.51     |
| 31  | d     | 611 | CLA  | C4B-NB  | 3.08  | 1.41        | 1.37     |
| 31  | h     | 613 | CLA  | C4B-NB  | 3.08  | 1.41        | 1.37     |
| 32  | B     | 848 | 8CT  | C10-C03 | 3.08  | 1.55        | 1.45     |
| 31  | B     | 817 | CLA  | C1D-ND  | 3.07  | 1.41        | 1.37     |
| 31  | A     | 809 | CLA  | C1D-ND  | 3.07  | 1.41        | 1.37     |
| 31  | L     | 201 | CLA  | C1D-ND  | 3.07  | 1.41        | 1.37     |
| 32  | B     | 848 | 8CT  | C07-C02 | -3.07 | 1.45        | 1.51     |
| 30  | 8     | 306 | CHL  | CHA-CBD | -3.07 | 1.48        | 1.51     |
| 31  | g     | 613 | CLA  | C4B-NB  | 3.07  | 1.41        | 1.37     |
| 32  | B     | 851 | 8CT  | C35-C30 | 3.07  | 1.64        | 1.56     |
| 32  | O     | 205 | 8CT  | C18-C17 | 3.07  | 1.52        | 1.43     |
| 32  | 1     | 402 | 8CT  | C30-C29 | 3.07  | 1.54        | 1.50     |
| 31  | A     | 841 | CLA  | C1D-ND  | 3.06  | 1.41        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | a     | 611 | CLA  | C4B-NB  | 3.06  | 1.41        | 1.37     |
| 31  | A     | 816 | CLA  | C4B-NB  | 3.06  | 1.41        | 1.37     |
| 30  | 2     | 313 | CHL  | CHA-CBD | -3.06 | 1.48        | 1.51     |
| 31  | i     | 611 | CLA  | C4B-NB  | 3.06  | 1.41        | 1.37     |
| 32  | B     | 843 | 8CT  | C18-C17 | 3.06  | 1.52        | 1.43     |
| 31  | B     | 826 | CLA  | C1D-ND  | 3.06  | 1.41        | 1.37     |
| 31  | i     | 603 | CLA  | C4B-NB  | 3.06  | 1.41        | 1.37     |
| 32  | 8     | 402 | 8CT  | C01-C02 | 3.06  | 1.55        | 1.50     |
| 32  | 3     | 403 | 8CT  | C18-C17 | 3.06  | 1.52        | 1.43     |
| 31  | B     | 830 | CLA  | CMB-C2B | -3.05 | 1.44        | 1.50     |
| 31  | O     | 203 | CLA  | C4B-NB  | 3.05  | 1.41        | 1.37     |
| 31  | A     | 830 | CLA  | C1D-ND  | 3.05  | 1.41        | 1.37     |
| 32  | A     | 847 | 8CT  | C10-C03 | 3.05  | 1.55        | 1.45     |
| 32  | K     | 107 | 8CT  | C10-C03 | 3.05  | 1.55        | 1.45     |
| 30  | i     | 601 | CHL  | CHA-CBD | -3.05 | 1.48        | 1.51     |
| 32  | A     | 846 | 8CT  | C18-C17 | 3.05  | 1.52        | 1.43     |
| 30  | a     | 607 | CHL  | CHA-CBD | -3.05 | 1.48        | 1.51     |
| 31  | i     | 613 | CLA  | C4B-NB  | 3.05  | 1.41        | 1.37     |
| 31  | g     | 612 | CLA  | C4B-NB  | 3.05  | 1.41        | 1.37     |
| 31  | K     | 101 | CLA  | C1D-ND  | 3.04  | 1.41        | 1.37     |
| 32  | 3     | 403 | 8CT  | C30-C29 | 3.04  | 1.54        | 1.50     |
| 32  | 0     | 401 | 8CT  | C10-C03 | 3.04  | 1.55        | 1.45     |
| 30  | 8     | 301 | CHL  | CHA-CBD | -3.04 | 1.48        | 1.51     |
| 32  | 3     | 402 | 8CT  | C07-C02 | -3.04 | 1.45        | 1.51     |
| 30  | b     | 614 | CHL  | CHA-CBD | -3.04 | 1.48        | 1.51     |
| 32  | M     | 102 | 8CT  | C07-C02 | -3.04 | 1.45        | 1.51     |
| 31  | A     | 804 | CLA  | C1D-ND  | 3.04  | 1.41        | 1.37     |
| 32  | 4     | 402 | 8CT  | C07-C02 | -3.04 | 1.45        | 1.51     |
| 32  | J     | 101 | 8CT  | C18-C17 | 3.03  | 1.52        | 1.43     |
| 31  | h     | 611 | CLA  | C4B-NB  | 3.03  | 1.41        | 1.37     |
| 31  | O     | 206 | CLA  | C4B-NB  | 3.03  | 1.41        | 1.37     |
| 31  | i     | 604 | CLA  | C4B-NB  | 3.03  | 1.41        | 1.37     |
| 32  | 3     | 403 | 8CT  | C10-C03 | 3.03  | 1.55        | 1.45     |
| 31  | 6     | 304 | CLA  | C4B-NB  | 3.03  | 1.41        | 1.37     |
| 31  | d     | 604 | CLA  | C4B-NB  | 3.03  | 1.41        | 1.37     |
| 32  | J     | 101 | 8CT  | C10-C03 | 3.02  | 1.55        | 1.45     |
| 31  | 8     | 311 | CLA  | C4B-NB  | 3.02  | 1.41        | 1.37     |
| 32  | B     | 851 | 8CT  | C18-C17 | 3.02  | 1.52        | 1.43     |
| 32  | B     | 847 | 8CT  | C30-C29 | 3.02  | 1.54        | 1.50     |
| 32  | 7     | 405 | 8CT  | C18-C17 | 3.02  | 1.52        | 1.43     |
| 32  | I     | 101 | 8CT  | C18-C17 | 3.02  | 1.52        | 1.43     |
| 32  | L     | 205 | 8CT  | C18-C17 | 3.02  | 1.52        | 1.43     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 32  | B     | 847 | 8CT  | C18-C17 | 3.02  | 1.52        | 1.43     |
| 31  | A     | 830 | CLA  | CMB-C2B | -3.02 | 1.44        | 1.50     |
| 32  | K     | 107 | 8CT  | C07-C02 | -3.02 | 1.45        | 1.51     |
| 32  | 3     | 402 | 8CT  | C18-C17 | 3.02  | 1.52        | 1.43     |
| 31  | 5     | 314 | CLA  | C4B-NB  | 3.02  | 1.41        | 1.37     |
| 32  | A     | 854 | 8CT  | C10-C03 | 3.02  | 1.55        | 1.45     |
| 32  | 9     | 401 | 8CT  | C35-C30 | 3.02  | 1.64        | 1.56     |
| 31  | h     | 603 | CLA  | C4B-NB  | 3.01  | 1.41        | 1.37     |
| 31  | h     | 610 | CLA  | C4B-NB  | 3.01  | 1.41        | 1.37     |
| 31  | A     | 834 | CLA  | C1D-ND  | 3.01  | 1.41        | 1.37     |
| 32  | B     | 804 | 8CT  | C18-C17 | 3.01  | 1.52        | 1.43     |
| 32  | 1     | 402 | 8CT  | C10-C03 | 3.01  | 1.55        | 1.45     |
| 32  | A     | 847 | 8CT  | C18-C17 | 3.01  | 1.52        | 1.43     |
| 32  | A     | 849 | 8CT  | C07-C02 | -3.01 | 1.45        | 1.51     |
| 31  | H     | 205 | CLA  | C4B-NB  | 3.01  | 1.41        | 1.37     |
| 30  | a     | 609 | CHL  | CHA-CBD | -3.00 | 1.48        | 1.51     |
| 32  | G     | 104 | 8CT  | C10-C03 | 3.00  | 1.55        | 1.45     |
| 32  | G     | 104 | 8CT  | C07-C02 | -3.00 | 1.45        | 1.51     |
| 32  | O     | 205 | 8CT  | C10-C03 | 3.00  | 1.55        | 1.45     |
| 31  | g     | 604 | CLA  | C4B-NB  | 3.00  | 1.41        | 1.37     |
| 32  | B     | 804 | 8CT  | C07-C02 | -3.00 | 1.45        | 1.51     |
| 31  | i     | 612 | CLA  | C4B-NB  | 3.00  | 1.41        | 1.37     |
| 32  | 7     | 402 | 8CT  | C10-C03 | 3.00  | 1.55        | 1.45     |
| 31  | A     | 826 | CLA  | C1D-ND  | 3.00  | 1.41        | 1.37     |
| 32  | A     | 846 | 8CT  | C10-C03 | 3.00  | 1.55        | 1.45     |
| 32  | L     | 209 | 8CT  | C10-C03 | 3.00  | 1.55        | 1.45     |
| 32  | B     | 844 | 8CT  | C35-C30 | 2.99  | 1.64        | 1.56     |
| 32  | L     | 206 | 8CT  | C10-C03 | 2.99  | 1.55        | 1.45     |
| 31  | d     | 612 | CLA  | C4B-NB  | 2.99  | 1.41        | 1.37     |
| 32  | F     | 302 | 8CT  | C10-C03 | 2.99  | 1.55        | 1.45     |
| 31  | B     | 805 | CLA  | C1D-ND  | 2.99  | 1.41        | 1.37     |
| 32  | 1     | 402 | 8CT  | C07-C02 | -2.99 | 1.45        | 1.51     |
| 31  | A     | 829 | CLA  | C1D-ND  | 2.99  | 1.41        | 1.37     |
| 32  | 9     | 401 | 8CT  | C07-C02 | -2.99 | 1.45        | 1.51     |
| 32  | A     | 848 | 8CT  | C07-C02 | -2.98 | 1.45        | 1.51     |
| 30  | e     | 601 | CHL  | CHA-CBD | -2.98 | 1.48        | 1.51     |
| 31  | L     | 207 | CLA  | C4B-NB  | 2.98  | 1.41        | 1.37     |
| 31  | b     | 613 | CLA  | C4B-NB  | 2.98  | 1.41        | 1.37     |
| 32  | B     | 843 | 8CT  | C07-C02 | -2.98 | 1.45        | 1.51     |
| 32  | B     | 847 | 8CT  | C10-C03 | 2.98  | 1.55        | 1.45     |
| 31  | f     | 604 | CLA  | C4B-NB  | 2.98  | 1.41        | 1.37     |
| 31  | a     | 610 | CLA  | C4B-NB  | 2.98  | 1.41        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 32  | 6     | 402 | 8CT  | C10-C03 | 2.98  | 1.55        | 1.45     |
| 30  | h     | 601 | CHL  | CHA-CBD | -2.98 | 1.48        | 1.51     |
| 31  | 0     | 321 | CLA  | C4B-NB  | 2.97  | 1.41        | 1.37     |
| 31  | d     | 613 | CLA  | C4B-NB  | 2.97  | 1.41        | 1.37     |
| 31  | h     | 604 | CLA  | C4B-NB  | 2.97  | 1.41        | 1.37     |
| 32  | J     | 101 | 8CT  | C07-C02 | -2.97 | 1.45        | 1.51     |
| 31  | f     | 603 | CLA  | C4B-NB  | 2.97  | 1.41        | 1.37     |
| 30  | 7     | 307 | CHL  | CHA-CBD | -2.97 | 1.48        | 1.51     |
| 32  | A     | 846 | 8CT  | C07-C02 | -2.97 | 1.45        | 1.51     |
| 30  | h     | 614 | CHL  | CHA-CBD | -2.96 | 1.48        | 1.51     |
| 32  | A     | 854 | 8CT  | C07-C02 | -2.96 | 1.45        | 1.51     |
| 32  | 7     | 404 | 8CT  | C10-C03 | 2.96  | 1.55        | 1.45     |
| 32  | 8     | 402 | 8CT  | C07-C02 | -2.96 | 1.45        | 1.51     |
| 32  | A     | 854 | 8CT  | C30-C29 | 2.96  | 1.54        | 1.50     |
| 31  | b     | 610 | CLA  | C4B-NB  | 2.96  | 1.41        | 1.37     |
| 31  | b     | 603 | CLA  | C4B-NB  | 2.96  | 1.41        | 1.37     |
| 31  | K     | 101 | CLA  | C4B-NB  | 2.96  | 1.41        | 1.37     |
| 32  | K     | 107 | 8CT  | C30-C29 | 2.96  | 1.54        | 1.50     |
| 32  | A     | 850 | 8CT  | C07-C02 | -2.96 | 1.45        | 1.51     |
| 30  | 1     | 307 | CHL  | CHA-CBD | -2.96 | 1.48        | 1.51     |
| 31  | B     | 810 | CLA  | C1D-ND  | 2.95  | 1.41        | 1.37     |
| 31  | A     | 805 | CLA  | C4B-NB  | 2.95  | 1.41        | 1.37     |
| 31  | c     | 603 | CLA  | C4B-NB  | 2.95  | 1.41        | 1.37     |
| 31  | 9     | 303 | CLA  | C4B-NB  | 2.95  | 1.41        | 1.37     |
| 32  | O     | 205 | 8CT  | C07-C02 | -2.95 | 1.45        | 1.51     |
| 32  | I     | 101 | 8CT  | C10-C03 | 2.95  | 1.55        | 1.45     |
| 32  | O     | 205 | 8CT  | C35-C30 | 2.95  | 1.64        | 1.56     |
| 32  | F     | 302 | 8CT  | C07-C02 | -2.95 | 1.45        | 1.51     |
| 31  | e     | 611 | CLA  | C4B-NB  | 2.95  | 1.41        | 1.37     |
| 32  | 8     | 402 | 8CT  | C30-C29 | 2.95  | 1.54        | 1.50     |
| 32  | 7     | 405 | 8CT  | C07-C02 | -2.95 | 1.45        | 1.51     |
| 32  | 9     | 401 | 8CT  | C10-C03 | 2.95  | 1.55        | 1.45     |
| 31  | a     | 612 | CLA  | C4B-NB  | 2.94  | 1.41        | 1.37     |
| 30  | e     | 608 | CHL  | CHA-CBD | -2.94 | 1.48        | 1.51     |
| 32  | 7     | 402 | 8CT  | C18-C17 | 2.94  | 1.52        | 1.43     |
| 32  | A     | 849 | 8CT  | C30-C29 | 2.94  | 1.54        | 1.50     |
| 31  | B     | 830 | CLA  | C1D-ND  | 2.94  | 1.41        | 1.37     |
| 32  | 8     | 406 | 8CT  | C07-C02 | -2.94 | 1.45        | 1.51     |
| 32  | L     | 209 | 8CT  | C07-C02 | -2.94 | 1.45        | 1.51     |
| 31  | c     | 604 | CLA  | C4B-NB  | 2.94  | 1.41        | 1.37     |
| 32  | A     | 848 | 8CT  | C10-C03 | 2.94  | 1.55        | 1.45     |
| 32  | B     | 845 | 8CT  | C35-C30 | 2.94  | 1.64        | 1.56     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | B     | 831 | CLA  | C1D-ND  | 2.94  | 1.41        | 1.37     |
| 31  | g     | 611 | CLA  | C4B-NB  | 2.93  | 1.41        | 1.37     |
| 32  | J     | 104 | 8CT  | C35-C30 | 2.93  | 1.64        | 1.56     |
| 32  | 6     | 402 | 8CT  | C07-C02 | -2.93 | 1.45        | 1.51     |
| 31  | b     | 612 | CLA  | C4B-NB  | 2.93  | 1.41        | 1.37     |
| 32  | A     | 850 | 8CT  | C18-C17 | 2.93  | 1.52        | 1.43     |
| 32  | L     | 205 | 8CT  | C10-C03 | 2.93  | 1.55        | 1.45     |
| 31  | e     | 613 | CLA  | C4B-NB  | 2.93  | 1.41        | 1.37     |
| 31  | b     | 611 | CLA  | C4B-NB  | 2.93  | 1.41        | 1.37     |
| 31  | 8     | 303 | CLA  | C4B-NB  | 2.92  | 1.41        | 1.37     |
| 32  | 7     | 404 | 8CT  | C07-C02 | -2.92 | 1.45        | 1.51     |
| 30  | c     | 608 | CHL  | CHA-CBD | -2.92 | 1.48        | 1.51     |
| 31  | c     | 611 | CLA  | C4B-NB  | 2.92  | 1.41        | 1.37     |
| 31  | f     | 611 | CLA  | C4B-NB  | 2.92  | 1.41        | 1.37     |
| 30  | a     | 601 | CHL  | CHA-CBD | -2.92 | 1.48        | 1.51     |
| 32  | 7     | 405 | 8CT  | C10-C03 | 2.92  | 1.55        | 1.45     |
| 31  | 5     | 308 | CLA  | C4B-NB  | 2.91  | 1.41        | 1.37     |
| 31  | d     | 603 | CLA  | C4B-NB  | 2.91  | 1.41        | 1.37     |
| 31  | 9     | 310 | CLA  | C4B-NB  | 2.91  | 1.41        | 1.37     |
| 32  | J     | 104 | 8CT  | C07-C02 | -2.91 | 1.45        | 1.51     |
| 31  | 0     | 303 | CLA  | C4B-NB  | 2.91  | 1.41        | 1.37     |
| 32  | A     | 854 | 8CT  | C35-C30 | 2.91  | 1.64        | 1.56     |
| 32  | A     | 849 | 8CT  | C18-C17 | 2.91  | 1.52        | 1.43     |
| 31  | 7     | 310 | CLA  | C4B-NB  | 2.91  | 1.41        | 1.37     |
| 31  | 4     | 309 | CLA  | C4B-NB  | 2.90  | 1.41        | 1.37     |
| 32  | A     | 848 | 8CT  | C18-C17 | 2.90  | 1.52        | 1.43     |
| 32  | M     | 102 | 8CT  | C10-C03 | 2.90  | 1.55        | 1.45     |
| 31  | 0     | 308 | CLA  | C4B-NB  | 2.90  | 1.41        | 1.37     |
| 31  | 8     | 304 | CLA  | C4B-NB  | 2.90  | 1.41        | 1.37     |
| 31  | B     | 822 | CLA  | C4B-NB  | 2.90  | 1.41        | 1.37     |
| 31  | e     | 610 | CLA  | C4B-NB  | 2.90  | 1.41        | 1.37     |
| 31  | 1     | 303 | CLA  | C4B-NB  | 2.90  | 1.41        | 1.37     |
| 32  | B     | 804 | 8CT  | C10-C03 | 2.90  | 1.55        | 1.45     |
| 31  | 2     | 314 | CLA  | C4B-NB  | 2.90  | 1.41        | 1.37     |
| 32  | B     | 851 | 8CT  | C10-C03 | 2.90  | 1.55        | 1.45     |
| 32  | B     | 845 | 8CT  | C07-C02 | -2.90 | 1.45        | 1.51     |
| 31  | 6     | 318 | CLA  | C4B-NB  | 2.90  | 1.41        | 1.37     |
| 31  | 7     | 315 | CLA  | C4B-NB  | 2.90  | 1.41        | 1.37     |
| 32  | F     | 302 | 8CT  | C30-C29 | 2.90  | 1.54        | 1.50     |
| 31  | A     | 853 | CLA  | C4B-NB  | 2.90  | 1.41        | 1.37     |
| 31  | B     | 806 | CLA  | C1D-ND  | 2.89  | 1.41        | 1.37     |
| 31  | c     | 612 | CLA  | C4B-NB  | 2.89  | 1.41        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | e     | 604 | CLA  | C4B-NB  | 2.89  | 1.41        | 1.37     |
| 31  | O     | 201 | CLA  | C4B-NB  | 2.89  | 1.41        | 1.37     |
| 30  | c     | 606 | CHL  | CHA-CBD | -2.89 | 1.48        | 1.51     |
| 31  | 5     | 304 | CLA  | C4B-NB  | 2.88  | 1.41        | 1.37     |
| 31  | f     | 612 | CLA  | C4B-NB  | 2.88  | 1.41        | 1.37     |
| 32  | 3     | 403 | 8CT  | C07-C02 | -2.88 | 1.45        | 1.51     |
| 31  | 5     | 309 | CLA  | C4B-NB  | 2.88  | 1.41        | 1.37     |
| 31  | a     | 603 | CLA  | C4B-NB  | 2.88  | 1.41        | 1.37     |
| 31  | 6     | 320 | CLA  | C4B-NB  | 2.88  | 1.41        | 1.37     |
| 31  | B     | 809 | CLA  | C4B-NB  | 2.88  | 1.41        | 1.37     |
| 31  | e     | 603 | CLA  | C4B-NB  | 2.88  | 1.41        | 1.37     |
| 35  | 0     | 603 | SQD  | O47-C7  | 2.88  | 1.42        | 1.34     |
| 32  | B     | 851 | 8CT  | C30-C29 | 2.88  | 1.54        | 1.50     |
| 31  | f     | 613 | CLA  | C4B-NB  | 2.88  | 1.41        | 1.37     |
| 31  | i     | 610 | CLA  | C4B-NB  | 2.88  | 1.41        | 1.37     |
| 32  | 7     | 402 | 8CT  | C07-C02 | -2.88 | 1.45        | 1.51     |
| 32  | B     | 804 | 8CT  | C35-C30 | 2.88  | 1.64        | 1.56     |
| 31  | B     | 829 | CLA  | C4B-NB  | 2.87  | 1.41        | 1.37     |
| 30  | h     | 606 | CHL  | CHA-CBD | -2.87 | 1.48        | 1.51     |
| 31  | 1     | 308 | CLA  | C4B-NB  | 2.87  | 1.41        | 1.37     |
| 31  | 7     | 317 | CLA  | C4B-NB  | 2.87  | 1.41        | 1.37     |
| 31  | e     | 612 | CLA  | C4B-NB  | 2.87  | 1.41        | 1.37     |
| 31  | A     | 823 | CLA  | C4B-NB  | 2.87  | 1.41        | 1.37     |
| 30  | c     | 605 | CHL  | CHA-CBD | -2.87 | 1.48        | 1.51     |
| 31  | 5     | 303 | CLA  | C4B-NB  | 2.87  | 1.41        | 1.37     |
| 31  | B     | 850 | CLA  | C4B-NB  | 2.87  | 1.41        | 1.37     |
| 31  | 8     | 312 | CLA  | C4B-NB  | 2.87  | 1.41        | 1.37     |
| 31  | M     | 101 | CLA  | C4B-NB  | 2.87  | 1.41        | 1.37     |
| 31  | 1     | 304 | CLA  | C4B-NB  | 2.86  | 1.41        | 1.37     |
| 31  | G     | 101 | CLA  | C4B-NB  | 2.86  | 1.41        | 1.37     |
| 31  | c     | 610 | CLA  | C4B-NB  | 2.86  | 1.41        | 1.37     |
| 31  | A     | 812 | CLA  | C4B-NB  | 2.86  | 1.41        | 1.37     |
| 30  | f     | 608 | CHL  | CHA-CBD | -2.86 | 1.48        | 1.51     |
| 31  | d     | 610 | CLA  | C4B-NB  | 2.86  | 1.41        | 1.37     |
| 32  | 0     | 401 | 8CT  | C30-C29 | 2.86  | 1.54        | 1.50     |
| 32  | A     | 850 | 8CT  | C10-C03 | 2.86  | 1.54        | 1.45     |
| 32  | I     | 101 | 8CT  | C07-C02 | -2.85 | 1.45        | 1.51     |
| 30  | b     | 608 | CHL  | CHA-CBD | -2.85 | 1.48        | 1.51     |
| 31  | 0     | 304 | CLA  | C4B-NB  | 2.85  | 1.41        | 1.37     |
| 32  | L     | 209 | 8CT  | C30-C29 | 2.85  | 1.54        | 1.50     |
| 31  | 3     | 313 | CLA  | C4B-NB  | 2.85  | 1.41        | 1.37     |
| 31  | 6     | 310 | CLA  | C4B-NB  | 2.85  | 1.41        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 0     | 312 | CLA  | C4B-NB  | 2.85  | 1.41        | 1.37     |
| 31  | B     | 801 | CLA  | C1D-ND  | 2.85  | 1.41        | 1.37     |
| 31  | B     | 835 | CLA  | C4B-NB  | 2.85  | 1.41        | 1.37     |
| 31  | H     | 202 | CLA  | C4B-NB  | 2.85  | 1.41        | 1.37     |
| 32  | A     | 847 | 8CT  | C07-C02 | -2.85 | 1.45        | 1.51     |
| 32  | 7     | 402 | 8CT  | C35-C30 | 2.85  | 1.64        | 1.56     |
| 32  | 0     | 401 | 8CT  | C07-C02 | -2.85 | 1.45        | 1.51     |
| 39  | A     | 857 | CL0  | C1A-CHA | -2.84 | 1.36        | 1.40     |
| 30  | h     | 608 | CHL  | CHA-CBD | -2.84 | 1.48        | 1.51     |
| 31  | c     | 613 | CLA  | C4B-NB  | 2.84  | 1.41        | 1.37     |
| 31  | 7     | 312 | CLA  | C4B-NB  | 2.83  | 1.41        | 1.37     |
| 31  | G     | 103 | CLA  | C4B-NB  | 2.83  | 1.41        | 1.37     |
| 31  | A     | 810 | CLA  | C4B-NB  | 2.83  | 1.41        | 1.37     |
| 31  | A     | 802 | CLA  | C4B-NB  | 2.83  | 1.41        | 1.37     |
| 31  | f     | 610 | CLA  | C4B-NB  | 2.82  | 1.41        | 1.37     |
| 31  | B     | 823 | CLA  | C4B-NB  | 2.82  | 1.41        | 1.37     |
| 30  | b     | 601 | CHL  | CHA-CBD | -2.82 | 1.48        | 1.51     |
| 31  | B     | 834 | CLA  | C4B-NB  | 2.82  | 1.41        | 1.37     |
| 31  | B     | 813 | CLA  | C4B-NB  | 2.81  | 1.41        | 1.37     |
| 31  | h     | 603 | CLA  | C1B-C2B | 2.81  | 1.49        | 1.43     |
| 31  | 6     | 303 | CLA  | C4B-NB  | 2.81  | 1.41        | 1.37     |
| 32  | B     | 846 | 8CT  | C07-C02 | -2.80 | 1.45        | 1.51     |
| 32  | A     | 849 | 8CT  | C10-C03 | 2.80  | 1.54        | 1.45     |
| 31  | A     | 838 | CLA  | C4B-NB  | 2.80  | 1.41        | 1.37     |
| 32  | B     | 844 | 8CT  | C30-C29 | 2.80  | 1.54        | 1.50     |
| 31  | 5     | 310 | CLA  | C4B-NB  | 2.80  | 1.41        | 1.37     |
| 31  | B     | 825 | CLA  | C4B-NB  | 2.80  | 1.41        | 1.37     |
| 31  | O     | 202 | CLA  | C4B-NB  | 2.80  | 1.41        | 1.37     |
| 31  | 3     | 312 | CLA  | C4B-NB  | 2.79  | 1.41        | 1.37     |
| 31  | b     | 611 | CLA  | C1B-C2B | 2.79  | 1.49        | 1.43     |
| 31  | L     | 202 | CLA  | C4B-NB  | 2.79  | 1.41        | 1.37     |
| 31  | 9     | 302 | CLA  | C4B-NB  | 2.79  | 1.41        | 1.37     |
| 31  | 2     | 304 | CLA  | C4B-NB  | 2.79  | 1.41        | 1.37     |
| 31  | 7     | 311 | CLA  | C4B-NB  | 2.79  | 1.41        | 1.37     |
| 31  | 4     | 310 | CLA  | C4B-NB  | 2.79  | 1.41        | 1.37     |
| 30  | i     | 607 | CHL  | CHA-CBD | -2.79 | 1.48        | 1.51     |
| 31  | h     | 613 | CLA  | C1B-C2B | 2.78  | 1.49        | 1.43     |
| 31  | 7     | 303 | CLA  | C4B-NB  | 2.78  | 1.41        | 1.37     |
| 31  | B     | 824 | CLA  | C4B-NB  | 2.78  | 1.41        | 1.37     |
| 31  | 0     | 310 | CLA  | C4B-NB  | 2.78  | 1.41        | 1.37     |
| 31  | 2     | 303 | CLA  | C4B-NB  | 2.78  | 1.41        | 1.37     |
| 31  | A     | 852 | CLA  | C4B-NB  | 2.78  | 1.41        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | A     | 806 | CLA  | C4B-NB  | 2.78  | 1.41        | 1.37     |
| 31  | 5     | 311 | CLA  | C4B-NB  | 2.78  | 1.41        | 1.37     |
| 31  | B     | 832 | CLA  | C4B-NB  | 2.78  | 1.41        | 1.37     |
| 32  | 6     | 402 | 8CT  | C30-C29 | 2.78  | 1.54        | 1.50     |
| 31  | g     | 603 | CLA  | C1B-C2B | 2.78  | 1.49        | 1.43     |
| 30  | a     | 605 | CHL  | CHA-CBD | -2.78 | 1.48        | 1.51     |
| 31  | L     | 203 | CLA  | C4B-NB  | 2.78  | 1.41        | 1.37     |
| 32  | B     | 844 | 8CT  | C07-C02 | -2.77 | 1.45        | 1.51     |
| 31  | K     | 105 | CLA  | C4B-NB  | 2.77  | 1.41        | 1.37     |
| 31  | 1     | 311 | CLA  | C4B-NB  | 2.77  | 1.41        | 1.37     |
| 31  | H     | 204 | CLA  | C4B-NB  | 2.77  | 1.41        | 1.37     |
| 30  | f     | 605 | CHL  | CHA-CBD | -2.77 | 1.48        | 1.51     |
| 31  | 4     | 303 | CLA  | C4B-NB  | 2.77  | 1.41        | 1.37     |
| 32  | B     | 848 | 8CT  | C30-C29 | 2.77  | 1.54        | 1.50     |
| 30  | i     | 608 | CHL  | CHA-CBD | -2.76 | 1.48        | 1.51     |
| 31  | 0     | 313 | CLA  | C4B-NB  | 2.76  | 1.41        | 1.37     |
| 31  | B     | 833 | CLA  | C4B-NB  | 2.76  | 1.41        | 1.37     |
| 31  | 3     | 306 | CLA  | C4B-NB  | 2.76  | 1.41        | 1.37     |
| 31  | h     | 612 | CLA  | C1B-C2B | 2.76  | 1.49        | 1.43     |
| 31  | J     | 103 | CLA  | C4B-NB  | 2.76  | 1.41        | 1.37     |
| 31  | 2     | 310 | CLA  | C4B-NB  | 2.76  | 1.41        | 1.37     |
| 31  | e     | 603 | CLA  | C1B-C2B | 2.76  | 1.49        | 1.43     |
| 32  | L     | 206 | 8CT  | C30-C29 | 2.76  | 1.54        | 1.50     |
| 31  | c     | 603 | CLA  | C1B-C2B | 2.76  | 1.49        | 1.43     |
| 31  | 9     | 304 | CLA  | C4B-NB  | 2.76  | 1.41        | 1.37     |
| 31  | a     | 612 | CLA  | C1B-C2B | 2.76  | 1.49        | 1.43     |
| 31  | g     | 613 | CLA  | C1B-C2B | 2.76  | 1.49        | 1.43     |
| 31  | i     | 603 | CLA  | C1B-C2B | 2.75  | 1.49        | 1.43     |
| 31  | 1     | 314 | CLA  | C4B-NB  | 2.75  | 1.41        | 1.37     |
| 31  | K     | 104 | CLA  | C4B-NB  | 2.75  | 1.41        | 1.37     |
| 31  | 3     | 320 | CLA  | C4B-NB  | 2.75  | 1.41        | 1.37     |
| 30  | g     | 605 | CHL  | CHA-CBD | -2.75 | 1.48        | 1.51     |
| 31  | 6     | 312 | CLA  | C4B-NB  | 2.75  | 1.41        | 1.37     |
| 31  | A     | 822 | CLA  | C4B-NB  | 2.75  | 1.41        | 1.37     |
| 31  | g     | 612 | CLA  | C1B-C2B | 2.75  | 1.49        | 1.43     |
| 31  | e     | 611 | CLA  | C1B-C2B | 2.75  | 1.49        | 1.43     |
| 31  | 5     | 312 | CLA  | C4B-NB  | 2.75  | 1.41        | 1.37     |
| 31  | h     | 611 | CLA  | C1B-C2B | 2.75  | 1.49        | 1.43     |
| 31  | i     | 612 | CLA  | C1B-C2B | 2.75  | 1.49        | 1.43     |
| 31  | 5     | 304 | CLA  | C1B-C2B | 2.75  | 1.49        | 1.43     |
| 31  | a     | 611 | CLA  | C1B-C2B | 2.75  | 1.49        | 1.43     |
| 31  | B     | 841 | CLA  | C4B-NB  | 2.75  | 1.41        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 8     | 310 | CLA  | C4B-NB  | 2.74  | 1.41        | 1.37     |
| 32  | 9     | 401 | 8CT  | C30-C29 | 2.74  | 1.54        | 1.50     |
| 31  | 3     | 310 | CLA  | C4B-NB  | 2.74  | 1.41        | 1.37     |
| 31  | 0     | 311 | CLA  | C4B-NB  | 2.74  | 1.41        | 1.37     |
| 31  | 7     | 317 | CLA  | C1B-C2B | 2.74  | 1.49        | 1.43     |
| 31  | 3     | 311 | CLA  | C4B-NB  | 2.74  | 1.41        | 1.37     |
| 31  | G     | 102 | CLA  | C4B-NB  | 2.74  | 1.41        | 1.37     |
| 31  | 4     | 311 | CLA  | C4B-NB  | 2.74  | 1.41        | 1.37     |
| 31  | B     | 837 | CLA  | C4B-NB  | 2.74  | 1.41        | 1.37     |
| 31  | i     | 611 | CLA  | C1B-C2B | 2.73  | 1.49        | 1.43     |
| 31  | 8     | 314 | CLA  | C4B-NB  | 2.73  | 1.41        | 1.37     |
| 31  | 7     | 304 | CLA  | C4B-NB  | 2.73  | 1.41        | 1.37     |
| 30  | e     | 605 | CHL  | CHA-CBD | -2.73 | 1.48        | 1.51     |
| 31  | i     | 613 | CLA  | C1B-C2B | 2.73  | 1.49        | 1.43     |
| 31  | B     | 812 | CLA  | C4B-NB  | 2.73  | 1.41        | 1.37     |
| 31  | B     | 828 | CLA  | C4B-NB  | 2.73  | 1.41        | 1.37     |
| 31  | a     | 603 | CLA  | C1B-C2B | 2.73  | 1.49        | 1.43     |
| 31  | d     | 613 | CLA  | C1B-C2B | 2.73  | 1.49        | 1.43     |
| 31  | 6     | 314 | CLA  | C4B-NB  | 2.73  | 1.41        | 1.37     |
| 32  | M     | 102 | 8CT  | C30-C29 | 2.73  | 1.54        | 1.50     |
| 31  | 1     | 310 | CLA  | C4B-NB  | 2.72  | 1.41        | 1.37     |
| 31  | g     | 604 | CLA  | C1B-C2B | 2.72  | 1.49        | 1.43     |
| 31  | B     | 808 | CLA  | C4B-NB  | 2.72  | 1.41        | 1.37     |
| 31  | A     | 835 | CLA  | C4B-NB  | 2.72  | 1.41        | 1.37     |
| 31  | B     | 805 | CLA  | C1B-C2B | 2.72  | 1.49        | 1.43     |
| 31  | e     | 612 | CLA  | C1B-C2B | 2.72  | 1.49        | 1.43     |
| 31  | 4     | 314 | CLA  | C4B-NB  | 2.72  | 1.41        | 1.37     |
| 31  | 3     | 318 | CLA  | C4B-NB  | 2.72  | 1.41        | 1.37     |
| 31  | A     | 826 | CLA  | C4B-NB  | 2.72  | 1.41        | 1.37     |
| 37  | 7     | 502 | 0IE  | C13-C12 | -2.72 | 1.40        | 1.46     |
| 39  | A     | 857 | CL0  | MG-NB   | -2.72 | 2.00        | 2.05     |
| 37  | 3     | 502 | 0IE  | C13-C12 | -2.71 | 1.40        | 1.46     |
| 31  | O     | 203 | CLA  | C1B-C2B | 2.71  | 1.49        | 1.43     |
| 32  | A     | 847 | 8CT  | C30-C29 | 2.71  | 1.54        | 1.50     |
| 31  | 0     | 309 | CLA  | C4B-NB  | 2.71  | 1.41        | 1.37     |
| 31  | g     | 611 | CLA  | C1B-C2B | 2.71  | 1.49        | 1.43     |
| 32  | B     | 804 | 8CT  | C30-C29 | 2.71  | 1.54        | 1.50     |
| 31  | B     | 830 | CLA  | C4B-NB  | 2.71  | 1.41        | 1.37     |
| 31  | L     | 204 | CLA  | C4B-NB  | 2.71  | 1.41        | 1.37     |
| 31  | 9     | 308 | CLA  | C4B-NB  | 2.71  | 1.41        | 1.37     |
| 31  | A     | 820 | CLA  | C4B-NB  | 2.71  | 1.41        | 1.37     |
| 31  | c     | 604 | CLA  | C1B-C2B | 2.71  | 1.49        | 1.43     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | O     | 203 | CLA  | C4B-C3B | 2.71  | 1.49        | 1.43     |
| 31  | b     | 603 | CLA  | C1B-C2B | 2.71  | 1.49        | 1.43     |
| 31  | i     | 604 | CLA  | C1B-C2B | 2.71  | 1.49        | 1.43     |
| 31  | A     | 841 | CLA  | C4B-NB  | 2.71  | 1.41        | 1.37     |
| 31  | B     | 821 | CLA  | C4B-NB  | 2.71  | 1.41        | 1.37     |
| 31  | h     | 610 | CLA  | C1B-C2B | 2.71  | 1.49        | 1.43     |
| 31  | 9     | 312 | CLA  | C4B-NB  | 2.70  | 1.41        | 1.37     |
| 31  | H     | 204 | CLA  | C1B-C2B | 2.70  | 1.49        | 1.43     |
| 31  | 3     | 303 | CLA  | C4B-NB  | 2.70  | 1.41        | 1.37     |
| 31  | d     | 611 | CLA  | C1B-C2B | 2.70  | 1.49        | 1.43     |
| 31  | a     | 613 | CLA  | C1B-C2B | 2.70  | 1.49        | 1.43     |
| 31  | b     | 613 | CLA  | C1B-C2B | 2.70  | 1.49        | 1.43     |
| 31  | c     | 612 | CLA  | C1B-C2B | 2.70  | 1.49        | 1.43     |
| 31  | b     | 612 | CLA  | C1B-C2B | 2.70  | 1.49        | 1.43     |
| 31  | A     | 814 | CLA  | C4B-NB  | 2.70  | 1.41        | 1.37     |
| 30  | g     | 601 | CHL  | CHA-CBD | -2.70 | 1.48        | 1.51     |
| 31  | 4     | 312 | CLA  | C4B-NB  | 2.69  | 1.41        | 1.37     |
| 31  | A     | 834 | CLA  | C4B-NB  | 2.69  | 1.41        | 1.37     |
| 31  | d     | 604 | CLA  | C1B-C2B | 2.69  | 1.49        | 1.43     |
| 31  | e     | 604 | CLA  | C1B-C2B | 2.69  | 1.49        | 1.43     |
| 31  | 8     | 309 | CLA  | C4B-NB  | 2.69  | 1.41        | 1.37     |
| 31  | d     | 603 | CLA  | C1B-C2B | 2.69  | 1.49        | 1.43     |
| 31  | B     | 820 | CLA  | C4B-NB  | 2.68  | 1.41        | 1.37     |
| 31  | a     | 610 | CLA  | C1B-C2B | 2.68  | 1.49        | 1.43     |
| 31  | d     | 612 | CLA  | C1B-C2B | 2.68  | 1.49        | 1.43     |
| 30  | d     | 605 | CHL  | CHA-CBD | -2.68 | 1.48        | 1.51     |
| 30  | 0     | 306 | CHL  | CHA-CBD | -2.68 | 1.48        | 1.51     |
| 31  | 1     | 310 | CLA  | C1B-C2B | 2.68  | 1.49        | 1.43     |
| 30  | d     | 614 | CHL  | CHA-CBD | -2.68 | 1.48        | 1.51     |
| 31  | B     | 840 | CLA  | C4B-NB  | 2.68  | 1.41        | 1.37     |
| 31  | 7     | 316 | CLA  | C4B-NB  | 2.68  | 1.41        | 1.37     |
| 31  | h     | 604 | CLA  | C1B-C2B | 2.68  | 1.49        | 1.43     |
| 31  | 7     | 308 | CLA  | C4B-NB  | 2.67  | 1.41        | 1.37     |
| 31  | A     | 843 | CLA  | C4B-NB  | 2.67  | 1.41        | 1.37     |
| 31  | A     | 817 | CLA  | C4B-NB  | 2.67  | 1.41        | 1.37     |
| 31  | B     | 831 | CLA  | C4B-NB  | 2.67  | 1.41        | 1.37     |
| 31  | f     | 603 | CLA  | C1B-C2B | 2.67  | 1.49        | 1.43     |
| 30  | i     | 614 | CHL  | CHA-CBD | -2.67 | 1.48        | 1.51     |
| 31  | 4     | 304 | CLA  | C4B-NB  | 2.67  | 1.41        | 1.37     |
| 30  | i     | 605 | CHL  | CHA-CBD | -2.67 | 1.48        | 1.51     |
| 31  | 6     | 303 | CLA  | C1B-C2B | 2.67  | 1.49        | 1.43     |
| 31  | 2     | 311 | CLA  | C4B-NB  | 2.67  | 1.41        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | B     | 838 | CLA  | C4B-NB  | 2.67  | 1.41        | 1.37     |
| 39  | A     | 857 | CL0  | CHC-C4B | -2.66 | 1.35        | 1.39     |
| 31  | 5     | 314 | CLA  | C1B-C2B | 2.66  | 1.49        | 1.43     |
| 31  | f     | 612 | CLA  | C1B-C2B | 2.66  | 1.49        | 1.43     |
| 37  | 3     | 502 | 0IE  | C17-C16 | -2.66 | 1.40        | 1.46     |
| 31  | A     | 840 | CLA  | C4B-NB  | 2.66  | 1.41        | 1.37     |
| 31  | B     | 839 | CLA  | C4B-NB  | 2.66  | 1.41        | 1.37     |
| 31  | B     | 816 | CLA  | C4B-NB  | 2.66  | 1.41        | 1.37     |
| 31  | B     | 826 | CLA  | C4B-NB  | 2.66  | 1.41        | 1.37     |
| 31  | G     | 102 | CLA  | C1B-C2B | 2.66  | 1.49        | 1.43     |
| 31  | e     | 613 | CLA  | C1B-C2B | 2.66  | 1.49        | 1.43     |
| 31  | A     | 811 | CLA  | C4B-NB  | 2.66  | 1.41        | 1.37     |
| 31  | c     | 613 | CLA  | C1B-C2B | 2.66  | 1.49        | 1.43     |
| 30  | f     | 614 | CHL  | CHA-CBD | -2.66 | 1.48        | 1.51     |
| 31  | 6     | 314 | CLA  | C1B-C2B | 2.66  | 1.49        | 1.43     |
| 31  | 5     | 310 | CLA  | C1B-C2B | 2.66  | 1.49        | 1.43     |
| 31  | L     | 202 | CLA  | C1B-C2B | 2.66  | 1.49        | 1.43     |
| 31  | F     | 301 | CLA  | C4B-NB  | 2.65  | 1.41        | 1.37     |
| 34  | 1     | 601 | LHG  | O8-C6   | -2.65 | 1.39        | 1.45     |
| 31  | 1     | 312 | CLA  | C4B-NB  | 2.65  | 1.41        | 1.37     |
| 31  | A     | 827 | CLA  | C4B-NB  | 2.65  | 1.41        | 1.37     |
| 31  | B     | 814 | CLA  | C4B-NB  | 2.65  | 1.41        | 1.37     |
| 31  | L     | 204 | CLA  | C1B-C2B | 2.65  | 1.49        | 1.43     |
| 31  | A     | 832 | CLA  | C4B-NB  | 2.65  | 1.41        | 1.37     |
| 31  | B     | 811 | CLA  | C4B-NB  | 2.65  | 1.41        | 1.37     |
| 31  | f     | 604 | CLA  | C1B-C2B | 2.65  | 1.49        | 1.43     |
| 32  | O     | 205 | 8CT  | C30-C29 | 2.65  | 1.54        | 1.50     |
| 31  | 0     | 321 | CLA  | C1B-C2B | 2.65  | 1.49        | 1.43     |
| 31  | M     | 101 | CLA  | C1B-C2B | 2.65  | 1.49        | 1.43     |
| 31  | A     | 819 | CLA  | C4B-NB  | 2.65  | 1.41        | 1.37     |
| 31  | B     | 819 | CLA  | C4B-NB  | 2.65  | 1.41        | 1.37     |
| 31  | 8     | 314 | CLA  | C1B-C2B | 2.64  | 1.49        | 1.43     |
| 31  | 7     | 315 | CLA  | C1B-C2B | 2.64  | 1.49        | 1.43     |
| 31  | i     | 610 | CLA  | C1B-C2B | 2.64  | 1.49        | 1.43     |
| 31  | 4     | 304 | CLA  | C1B-C2B | 2.64  | 1.49        | 1.43     |
| 31  | 5     | 308 | CLA  | C1B-C2B | 2.64  | 1.49        | 1.43     |
| 31  | B     | 821 | CLA  | C1B-C2B | 2.64  | 1.49        | 1.43     |
| 30  | a     | 614 | CHL  | CHA-CBD | -2.64 | 1.48        | 1.51     |
| 31  | f     | 611 | CLA  | C1B-C2B | 2.64  | 1.49        | 1.43     |
| 30  | g     | 607 | CHL  | CHA-CBD | -2.64 | 1.48        | 1.51     |
| 31  | 0     | 304 | CLA  | C1B-C2B | 2.64  | 1.49        | 1.43     |
| 31  | 1     | 309 | CLA  | C4B-NB  | 2.64  | 1.41        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 3     | 304 | CLA  | C4B-NB  | 2.64  | 1.41        | 1.37     |
| 31  | 7     | 318 | CLA  | C4B-NB  | 2.64  | 1.41        | 1.37     |
| 32  | A     | 846 | 8CT  | C30-C29 | 2.64  | 1.54        | 1.50     |
| 31  | B     | 803 | CLA  | C4B-NB  | 2.64  | 1.41        | 1.37     |
| 31  | B     | 817 | CLA  | C4B-NB  | 2.64  | 1.41        | 1.37     |
| 31  | 9     | 308 | CLA  | C1B-C2B | 2.64  | 1.49        | 1.43     |
| 31  | B     | 805 | CLA  | C4B-NB  | 2.64  | 1.41        | 1.37     |
| 31  | A     | 821 | CLA  | C4B-NB  | 2.63  | 1.41        | 1.37     |
| 31  | A     | 803 | CLA  | C4B-NB  | 2.63  | 1.41        | 1.37     |
| 31  | g     | 610 | CLA  | C1B-C2B | 2.63  | 1.49        | 1.43     |
| 31  | B     | 815 | CLA  | C4B-NB  | 2.63  | 1.41        | 1.37     |
| 31  | K     | 102 | CLA  | C4B-NB  | 2.63  | 1.41        | 1.37     |
| 37  | d     | 522 | 0IE  | C15-C16 | 2.63  | 1.41        | 1.35     |
| 30  | d     | 608 | CHL  | CHA-CBD | -2.63 | 1.48        | 1.51     |
| 31  | 6     | 320 | CLA  | C1B-C2B | 2.63  | 1.49        | 1.43     |
| 31  | L     | 207 | CLA  | C1B-C2B | 2.63  | 1.49        | 1.43     |
| 31  | 5     | 312 | CLA  | C1B-C2B | 2.62  | 1.49        | 1.43     |
| 31  | B     | 801 | CLA  | C4B-NB  | 2.62  | 1.41        | 1.37     |
| 31  | A     | 809 | CLA  | C4B-NB  | 2.62  | 1.41        | 1.37     |
| 31  | 7     | 309 | CLA  | C4B-NB  | 2.62  | 1.41        | 1.37     |
| 31  | 9     | 309 | CLA  | C4B-NB  | 2.62  | 1.41        | 1.37     |
| 37  | 7     | 502 | 0IE  | C17-C16 | -2.62 | 1.40        | 1.46     |
| 31  | K     | 104 | CLA  | C1B-C2B | 2.62  | 1.49        | 1.43     |
| 31  | A     | 804 | CLA  | C4B-NB  | 2.62  | 1.41        | 1.37     |
| 31  | A     | 830 | CLA  | C4B-NB  | 2.62  | 1.41        | 1.37     |
| 30  | g     | 608 | CHL  | CHA-CBD | -2.61 | 1.48        | 1.51     |
| 31  | 6     | 309 | CLA  | C4B-NB  | 2.61  | 1.41        | 1.37     |
| 34  | 7     | 602 | LHG  | O7-C5   | -2.61 | 1.40        | 1.46     |
| 31  | 3     | 320 | CLA  | C1B-C2B | 2.61  | 1.49        | 1.43     |
| 31  | 2     | 312 | CLA  | C4B-NB  | 2.61  | 1.41        | 1.37     |
| 31  | A     | 825 | CLA  | C4B-NB  | 2.61  | 1.41        | 1.37     |
| 31  | A     | 831 | CLA  | C4B-NB  | 2.61  | 1.41        | 1.37     |
| 31  | B     | 835 | CLA  | C1B-C2B | 2.61  | 1.49        | 1.43     |
| 31  | 0     | 312 | CLA  | C1B-C2B | 2.61  | 1.49        | 1.43     |
| 31  | f     | 613 | CLA  | C1B-C2B | 2.61  | 1.49        | 1.43     |
| 30  | e     | 614 | CHL  | CHA-CBD | -2.61 | 1.48        | 1.51     |
| 31  | B     | 810 | CLA  | C4B-NB  | 2.61  | 1.41        | 1.37     |
| 31  | 5     | 311 | CLA  | C1B-C2B | 2.60  | 1.49        | 1.43     |
| 39  | A     | 857 | CL0  | CAC-C3C | -2.60 | 1.47        | 1.51     |
| 31  | B     | 807 | CLA  | C4B-NB  | 2.60  | 1.41        | 1.37     |
| 31  | 0     | 313 | CLA  | C1B-C2B | 2.60  | 1.49        | 1.43     |
| 31  | A     | 837 | CLA  | C4B-NB  | 2.60  | 1.41        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 8     | 304 | CLA  | C1B-C2B | 2.60  | 1.49        | 1.43     |
| 31  | 9     | 302 | CLA  | C1B-C2B | 2.60  | 1.49        | 1.43     |
| 30  | a     | 608 | CHL  | CHA-CBD | -2.60 | 1.48        | 1.51     |
| 31  | A     | 807 | CLA  | C4B-NB  | 2.60  | 1.41        | 1.37     |
| 31  | a     | 604 | CLA  | C1B-C2B | 2.60  | 1.49        | 1.43     |
| 31  | L     | 201 | CLA  | C4B-NB  | 2.60  | 1.41        | 1.37     |
| 31  | 2     | 304 | CLA  | C1B-C2B | 2.60  | 1.49        | 1.43     |
| 31  | 9     | 300 | CLA  | C4B-NB  | 2.59  | 1.41        | 1.37     |
| 31  | 3     | 309 | CLA  | C4B-NB  | 2.59  | 1.41        | 1.37     |
| 31  | B     | 818 | CLA  | C4B-NB  | 2.59  | 1.41        | 1.37     |
| 31  | B     | 830 | CLA  | CMD-C2D | -2.59 | 1.45        | 1.50     |
| 31  | 5     | 303 | CLA  | C1B-C2B | 2.59  | 1.49        | 1.43     |
| 31  | H     | 202 | CLA  | C1B-C2B | 2.59  | 1.49        | 1.43     |
| 31  | B     | 840 | CLA  | C1B-C2B | 2.59  | 1.49        | 1.43     |
| 31  | 0     | 309 | CLA  | C1B-C2B | 2.59  | 1.49        | 1.43     |
| 31  | A     | 834 | CLA  | C1B-C2B | 2.58  | 1.49        | 1.43     |
| 31  | 4     | 311 | CLA  | C1B-C2B | 2.58  | 1.49        | 1.43     |
| 31  | A     | 833 | CLA  | C4B-NB  | 2.58  | 1.41        | 1.37     |
| 31  | 6     | 310 | CLA  | C1B-C2B | 2.58  | 1.49        | 1.43     |
| 31  | 1     | 314 | CLA  | C1B-C2B | 2.58  | 1.49        | 1.43     |
| 31  | 1     | 308 | CLA  | C1B-C2B | 2.58  | 1.49        | 1.43     |
| 33  | a     | 520 | OUR  | O44-C45 | 2.58  | 1.45        | 1.33     |
| 31  | 2     | 314 | CLA  | C1B-C2B | 2.58  | 1.49        | 1.43     |
| 31  | 9     | 304 | CLA  | C1B-C2B | 2.58  | 1.49        | 1.43     |
| 31  | 3     | 306 | CLA  | C1B-C2B | 2.58  | 1.49        | 1.43     |
| 31  | G     | 101 | CLA  | C1B-C2B | 2.58  | 1.49        | 1.43     |
| 31  | 3     | 308 | CLA  | C1B-C2B | 2.58  | 1.49        | 1.43     |
| 31  | c     | 610 | CLA  | C1B-C2B | 2.58  | 1.49        | 1.43     |
| 31  | B     | 830 | CLA  | MG-NB   | -2.57 | 2.00        | 2.05     |
| 31  | 7     | 311 | CLA  | C1B-C2B | 2.57  | 1.49        | 1.43     |
| 31  | O     | 202 | CLA  | C1B-C2B | 2.57  | 1.49        | 1.43     |
| 31  | 4     | 314 | CLA  | C1B-C2B | 2.57  | 1.49        | 1.43     |
| 31  | B     | 838 | CLA  | C1B-C2B | 2.57  | 1.49        | 1.43     |
| 31  | d     | 610 | CLA  | C1B-C2B | 2.57  | 1.49        | 1.43     |
| 31  | 2     | 312 | CLA  | C1B-C2B | 2.57  | 1.49        | 1.43     |
| 34  | A     | 845 | LHG  | O8-C6   | -2.57 | 1.39        | 1.45     |
| 34  | 7     | 602 | LHG  | C26-C25 | -2.57 | 1.35        | 1.51     |
| 31  | 3     | 308 | CLA  | C4B-NB  | 2.57  | 1.41        | 1.37     |
| 31  | 6     | 317 | CLA  | C4B-NB  | 2.57  | 1.41        | 1.37     |
| 31  | B     | 810 | CLA  | C1B-C2B | 2.57  | 1.49        | 1.43     |
| 31  | f     | 610 | CLA  | C1B-C2B | 2.57  | 1.49        | 1.43     |
| 31  | 2     | 309 | CLA  | C4B-NB  | 2.57  | 1.41        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 30  | g     | 614 | CHL  | CHA-CBD | -2.56 | 1.48        | 1.51     |
| 31  | H     | 201 | CLA  | C4B-NB  | 2.56  | 1.41        | 1.37     |
| 31  | 0     | 310 | CLA  | C1B-C2B | 2.56  | 1.49        | 1.43     |
| 31  | 2     | 311 | CLA  | C1B-C2B | 2.56  | 1.49        | 1.43     |
| 31  | A     | 837 | CLA  | C1B-C2B | 2.56  | 1.49        | 1.43     |
| 31  | A     | 814 | CLA  | C1B-C2B | 2.56  | 1.49        | 1.43     |
| 31  | O     | 201 | CLA  | C1B-C2B | 2.56  | 1.49        | 1.43     |
| 34  | K     | 106 | LHG  | O8-C6   | -2.56 | 1.39        | 1.45     |
| 31  | 8     | 303 | CLA  | C1B-C2B | 2.56  | 1.49        | 1.43     |
| 31  | K     | 102 | CLA  | C1B-C2B | 2.56  | 1.49        | 1.43     |
| 31  | 7     | 316 | CLA  | C1B-C2B | 2.56  | 1.49        | 1.43     |
| 31  | B     | 806 | CLA  | C4B-NB  | 2.56  | 1.41        | 1.37     |
| 31  | A     | 813 | CLA  | C4B-NB  | 2.56  | 1.41        | 1.37     |
| 31  | A     | 839 | CLA  | C4B-NB  | 2.56  | 1.41        | 1.37     |
| 31  | 6     | 318 | CLA  | C1B-C2B | 2.56  | 1.49        | 1.43     |
| 31  | B     | 834 | CLA  | C1B-C2B | 2.55  | 1.49        | 1.43     |
| 31  | A     | 829 | CLA  | C4B-NB  | 2.55  | 1.41        | 1.37     |
| 34  | B     | 852 | LHG  | O8-C6   | -2.55 | 1.39        | 1.45     |
| 31  | 0     | 303 | CLA  | C1B-C2B | 2.55  | 1.49        | 1.43     |
| 31  | 8     | 311 | CLA  | C1B-C2B | 2.55  | 1.49        | 1.43     |
| 31  | 1     | 311 | CLA  | C1B-C2B | 2.55  | 1.49        | 1.43     |
| 31  | A     | 822 | CLA  | C1B-C2B | 2.55  | 1.49        | 1.43     |
| 31  | 1     | 304 | CLA  | C1B-C2B | 2.55  | 1.49        | 1.43     |
| 31  | A     | 808 | CLA  | C1B-C2B | 2.55  | 1.49        | 1.43     |
| 31  | A     | 828 | CLA  | C4B-NB  | 2.55  | 1.41        | 1.37     |
| 31  | b     | 604 | CLA  | C1B-C2B | 2.55  | 1.49        | 1.43     |
| 31  | 3     | 313 | CLA  | C1B-C2B | 2.55  | 1.49        | 1.43     |
| 31  | J     | 103 | CLA  | C1B-C2B | 2.55  | 1.49        | 1.43     |
| 31  | 7     | 310 | CLA  | C1B-C2B | 2.54  | 1.49        | 1.43     |
| 37  | 7     | 502 | 0IE  | C6-C7   | -2.54 | 1.40        | 1.46     |
| 34  | A     | 844 | LHG  | O8-C6   | -2.54 | 1.39        | 1.45     |
| 31  | A     | 817 | CLA  | C1B-C2B | 2.54  | 1.49        | 1.43     |
| 31  | 4     | 310 | CLA  | C1B-C2B | 2.54  | 1.49        | 1.43     |
| 31  | A     | 810 | CLA  | C3B-C4B | 2.54  | 1.50        | 1.42     |
| 34  | 4     | 601 | LHG  | O7-C5   | -2.54 | 1.40        | 1.46     |
| 31  | 1     | 312 | CLA  | C1B-C2B | 2.54  | 1.49        | 1.43     |
| 32  | 7     | 405 | 8CT  | C30-C29 | 2.54  | 1.54        | 1.50     |
| 31  | 6     | 309 | CLA  | C1B-C2B | 2.54  | 1.49        | 1.43     |
| 31  | 4     | 312 | CLA  | C1B-C2B | 2.54  | 1.49        | 1.43     |
| 31  | H     | 201 | CLA  | C1B-C2B | 2.54  | 1.49        | 1.43     |
| 31  | 8     | 312 | CLA  | C1B-C2B | 2.53  | 1.49        | 1.43     |
| 39  | A     | 857 | CL0  | MG-ND   | -2.53 | 2.00        | 2.05     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | A     | 816 | CLA  | C1B-C2B | 2.53  | 1.49        | 1.43     |
| 34  | 1     | 601 | LHG  | O7-C5   | -2.53 | 1.40        | 1.46     |
| 31  | B     | 808 | CLA  | C1B-C2B | 2.53  | 1.49        | 1.43     |
| 31  | H     | 205 | CLA  | C1B-C2B | 2.53  | 1.49        | 1.43     |
| 31  | A     | 828 | CLA  | C1B-C2B | 2.52  | 1.49        | 1.43     |
| 31  | A     | 824 | CLA  | C4B-NB  | 2.52  | 1.41        | 1.37     |
| 34  | 2     | 601 | LHG  | O8-C6   | -2.52 | 1.39        | 1.45     |
| 31  | A     | 818 | CLA  | C1B-C2B | 2.52  | 1.49        | 1.43     |
| 31  | 9     | 310 | CLA  | C1B-C2B | 2.52  | 1.49        | 1.43     |
| 31  | 7     | 312 | CLA  | C1B-C2B | 2.52  | 1.49        | 1.43     |
| 31  | 3     | 311 | CLA  | C1B-C2B | 2.52  | 1.49        | 1.43     |
| 31  | 8     | 310 | CLA  | C1B-C2B | 2.52  | 1.49        | 1.43     |
| 31  | A     | 853 | CLA  | C3B-C4B | 2.51  | 1.50        | 1.42     |
| 31  | 6     | 304 | CLA  | CMB-C2B | -2.51 | 1.45        | 1.50     |
| 31  | 3     | 310 | CLA  | C1B-C2B | 2.51  | 1.49        | 1.43     |
| 31  | 9     | 309 | CLA  | C1B-C2B | 2.51  | 1.49        | 1.43     |
| 31  | B     | 850 | CLA  | C1B-C2B | 2.51  | 1.49        | 1.43     |
| 31  | c     | 611 | CLA  | C1B-C2B | 2.51  | 1.49        | 1.43     |
| 31  | B     | 837 | CLA  | C1B-C2B | 2.51  | 1.49        | 1.43     |
| 31  | A     | 811 | CLA  | C1B-C2B | 2.51  | 1.49        | 1.43     |
| 31  | 9     | 312 | CLA  | C1B-C2B | 2.51  | 1.49        | 1.43     |
| 34  | A     | 844 | LHG  | O7-C5   | -2.50 | 1.40        | 1.46     |
| 31  | A     | 805 | CLA  | C3B-C4B | 2.50  | 1.50        | 1.42     |
| 31  | A     | 843 | CLA  | C1B-C2B | 2.50  | 1.49        | 1.43     |
| 32  | A     | 850 | 8CT  | C33-C32 | -2.50 | 1.43        | 1.50     |
| 31  | A     | 836 | CLA  | C4B-NB  | 2.50  | 1.41        | 1.37     |
| 30  | 6     | 313 | CHL  | CBD-CGD | -2.50 | 1.49        | 1.52     |
| 31  | 4     | 309 | CLA  | C1B-C2B | 2.50  | 1.49        | 1.43     |
| 34  | 2     | 601 | LHG  | O7-C5   | -2.50 | 1.40        | 1.46     |
| 31  | A     | 829 | CLA  | C1B-C2B | 2.50  | 1.49        | 1.43     |
| 31  | 7     | 308 | CLA  | C1B-C2B | 2.50  | 1.49        | 1.43     |
| 31  | 7     | 304 | CLA  | C1B-C2B | 2.50  | 1.49        | 1.43     |
| 31  | G     | 103 | CLA  | C1B-C2B | 2.50  | 1.49        | 1.43     |
| 31  | B     | 826 | CLA  | C4D-CHA | 2.50  | 1.43        | 1.39     |
| 31  | B     | 824 | CLA  | C1B-C2B | 2.50  | 1.49        | 1.43     |
| 31  | 6     | 311 | CLA  | C1B-C2B | 2.50  | 1.49        | 1.43     |
| 31  | A     | 833 | CLA  | C1B-C2B | 2.50  | 1.49        | 1.43     |
| 37  | c     | 521 | 0IE  | C6-C7   | -2.50 | 1.40        | 1.46     |
| 31  | B     | 829 | CLA  | C3B-C4B | 2.50  | 1.50        | 1.42     |
| 31  | L     | 203 | CLA  | C1B-C2B | 2.49  | 1.49        | 1.43     |
| 31  | 0     | 311 | CLA  | C1B-C2B | 2.49  | 1.49        | 1.43     |
| 31  | 2     | 303 | CLA  | C1B-C2B | 2.49  | 1.49        | 1.43     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | A     | 818 | CLA  | C4B-NB  | 2.49  | 1.41        | 1.37     |
| 31  | B     | 823 | CLA  | C1B-C2B | 2.49  | 1.49        | 1.43     |
| 31  | A     | 820 | CLA  | C1B-C2B | 2.49  | 1.49        | 1.43     |
| 37  | 3     | 502 | 0IE  | C6-C7   | -2.49 | 1.40        | 1.46     |
| 32  | 4     | 402 | 8CT  | C30-C29 | 2.49  | 1.54        | 1.50     |
| 34  | 0     | 601 | LHG  | O7-C5   | -2.49 | 1.40        | 1.46     |
| 31  | K     | 105 | CLA  | C1B-C2B | 2.49  | 1.49        | 1.43     |
| 34  | B     | 854 | LHG  | O8-C6   | -2.49 | 1.39        | 1.45     |
| 31  | B     | 825 | CLA  | C1B-C2B | 2.49  | 1.49        | 1.43     |
| 34  | 9     | 601 | LHG  | O8-C6   | -2.49 | 1.39        | 1.45     |
| 34  | 6     | 601 | LHG  | O8-C6   | -2.49 | 1.39        | 1.45     |
| 32  | 2     | 402 | 8CT  | C30-C29 | 2.49  | 1.54        | 1.50     |
| 31  | A     | 826 | CLA  | C1B-C2B | 2.48  | 1.49        | 1.43     |
| 31  | 0     | 308 | CLA  | C1B-C2B | 2.48  | 1.49        | 1.43     |
| 31  | A     | 841 | CLA  | C1B-C2B | 2.48  | 1.49        | 1.43     |
| 31  | B     | 831 | CLA  | CMD-C2D | -2.48 | 1.45        | 1.50     |
| 31  | B     | 813 | CLA  | C3B-C4B | 2.48  | 1.50        | 1.42     |
| 32  | A     | 848 | 8CT  | C30-C29 | 2.48  | 1.54        | 1.50     |
| 31  | A     | 815 | CLA  | C4B-NB  | 2.48  | 1.41        | 1.37     |
| 31  | B     | 803 | CLA  | C1B-C2B | 2.48  | 1.48        | 1.43     |
| 34  | 5     | 601 | LHG  | O8-C6   | -2.48 | 1.39        | 1.45     |
| 31  | 6     | 312 | CLA  | C1B-C2B | 2.48  | 1.48        | 1.43     |
| 32  | I     | 101 | 8CT  | C30-C29 | 2.48  | 1.54        | 1.50     |
| 31  | B     | 827 | CLA  | C4B-NB  | 2.48  | 1.41        | 1.37     |
| 37  | d     | 521 | 0IE  | C13-C12 | -2.48 | 1.40        | 1.46     |
| 31  | A     | 839 | CLA  | C1B-C2B | 2.48  | 1.48        | 1.43     |
| 31  | B     | 841 | CLA  | C1B-C2B | 2.48  | 1.48        | 1.43     |
| 31  | A     | 809 | CLA  | C1B-C2B | 2.48  | 1.48        | 1.43     |
| 31  | 3     | 303 | CLA  | C1B-C2B | 2.48  | 1.48        | 1.43     |
| 31  | B     | 827 | CLA  | C1B-C2B | 2.47  | 1.48        | 1.43     |
| 34  | 0     | 601 | LHG  | O8-C6   | -2.47 | 1.39        | 1.45     |
| 31  | 3     | 312 | CLA  | C1B-C2B | 2.47  | 1.48        | 1.43     |
| 31  | 3     | 304 | CLA  | C1B-C2B | 2.47  | 1.48        | 1.43     |
| 31  | 7     | 318 | CLA  | C1B-C2B | 2.47  | 1.48        | 1.43     |
| 34  | 4     | 601 | LHG  | O8-C6   | -2.47 | 1.39        | 1.45     |
| 31  | 4     | 303 | CLA  | C1B-C2B | 2.47  | 1.48        | 1.43     |
| 31  | A     | 835 | CLA  | C1B-C2B | 2.47  | 1.48        | 1.43     |
| 31  | B     | 832 | CLA  | C1B-C2B | 2.47  | 1.48        | 1.43     |
| 34  | A     | 845 | LHG  | O7-C5   | -2.47 | 1.40        | 1.46     |
| 31  | 9     | 311 | CLA  | C3B-C4B | 2.47  | 1.49        | 1.42     |
| 31  | 6     | 304 | CLA  | C1B-C2B | 2.47  | 1.48        | 1.43     |
| 31  | B     | 817 | CLA  | C1B-C2B | 2.47  | 1.48        | 1.43     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | O     | 206 | CLA  | C1B-C2B | 2.47  | 1.48        | 1.43     |
| 37  | c     | 521 | 0IE  | C13-C12 | -2.47 | 1.40        | 1.46     |
| 31  | A     | 840 | CLA  | C1B-C2B | 2.47  | 1.48        | 1.43     |
| 34  | 7     | 601 | LHG  | O8-C6   | -2.47 | 1.39        | 1.45     |
| 31  | B     | 811 | CLA  | C1B-C2B | 2.46  | 1.48        | 1.43     |
| 31  | 6     | 311 | CLA  | C3B-C4B | 2.46  | 1.49        | 1.42     |
| 31  | A     | 819 | CLA  | MG-NB   | -2.46 | 2.00        | 2.05     |
| 31  | A     | 836 | CLA  | C1B-C2B | 2.46  | 1.48        | 1.43     |
| 31  | A     | 816 | CLA  | CMB-C2B | -2.46 | 1.45        | 1.50     |
| 31  | A     | 830 | CLA  | MG-NB   | -2.46 | 2.00        | 2.05     |
| 31  | 7     | 303 | CLA  | C1B-C2B | 2.46  | 1.48        | 1.43     |
| 31  | b     | 610 | CLA  | C1B-C2B | 2.46  | 1.48        | 1.43     |
| 34  | 7     | 602 | LHG  | O8-C6   | -2.46 | 1.39        | 1.45     |
| 31  | 2     | 310 | CLA  | C1B-C2B | 2.46  | 1.48        | 1.43     |
| 31  | B     | 816 | CLA  | C1B-C2B | 2.46  | 1.48        | 1.43     |
| 31  | A     | 808 | CLA  | C4B-NB  | 2.46  | 1.41        | 1.37     |
| 31  | A     | 803 | CLA  | C1B-C2B | 2.46  | 1.48        | 1.43     |
| 31  | B     | 836 | CLA  | C4B-NB  | 2.46  | 1.41        | 1.37     |
| 31  | B     | 833 | CLA  | C1B-C2B | 2.46  | 1.48        | 1.43     |
| 31  | 1     | 303 | CLA  | C1B-C2B | 2.46  | 1.48        | 1.43     |
| 31  | B     | 819 | CLA  | C1B-C2B | 2.46  | 1.48        | 1.43     |
| 31  | K     | 101 | CLA  | C1B-C2B | 2.46  | 1.48        | 1.43     |
| 31  | B     | 814 | CLA  | C1B-C2B | 2.46  | 1.48        | 1.43     |
| 32  | 7     | 404 | 8CT  | C30-C29 | 2.45  | 1.54        | 1.50     |
| 31  | B     | 812 | CLA  | C1B-C2B | 2.45  | 1.48        | 1.43     |
| 31  | A     | 823 | CLA  | C1B-C2B | 2.45  | 1.48        | 1.43     |
| 37  | b     | 521 | 0IE  | C6-C7   | -2.45 | 1.40        | 1.46     |
| 37  | b     | 522 | 0IE  | C15-C16 | 2.45  | 1.41        | 1.35     |
| 34  | f     | 630 | LHG  | O8-C6   | -2.45 | 1.39        | 1.45     |
| 31  | 8     | 309 | CLA  | C1B-C2B | 2.45  | 1.48        | 1.43     |
| 31  | A     | 815 | CLA  | C1B-C2B | 2.44  | 1.48        | 1.43     |
| 31  | B     | 815 | CLA  | C1B-C2B | 2.44  | 1.48        | 1.43     |
| 31  | B     | 812 | CLA  | CMB-C2B | -2.44 | 1.45        | 1.50     |
| 34  | f     | 630 | LHG  | O7-C5   | -2.44 | 1.40        | 1.46     |
| 31  | 2     | 309 | CLA  | C1B-C2B | 2.44  | 1.48        | 1.43     |
| 36  | J     | 105 | LMG  | O7-C8   | -2.44 | 1.40        | 1.46     |
| 31  | e     | 610 | CLA  | C1B-C2B | 2.44  | 1.48        | 1.43     |
| 31  | 9     | 303 | CLA  | C1B-C2B | 2.44  | 1.48        | 1.43     |
| 31  | 9     | 300 | CLA  | C1B-C2B | 2.44  | 1.48        | 1.43     |
| 34  | M     | 104 | LHG  | O7-C5   | -2.44 | 1.40        | 1.46     |
| 37  | i     | 521 | 0IE  | C11-C12 | 2.44  | 1.41        | 1.35     |
| 31  | B     | 831 | CLA  | MG-NB   | -2.44 | 2.01        | 2.05     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | B     | 820 | CLA  | CMB-C2B | -2.44 | 1.45        | 1.50     |
| 31  | B     | 840 | CLA  | CMB-C2B | -2.43 | 1.45        | 1.50     |
| 34  | e     | 630 | LHG  | O8-C6   | -2.43 | 1.39        | 1.45     |
| 31  | B     | 801 | CLA  | MG-NB   | -2.43 | 2.01        | 2.05     |
| 34  | 8     | 601 | LHG  | O8-C6   | -2.43 | 1.39        | 1.45     |
| 31  | A     | 825 | CLA  | C1B-C2B | 2.43  | 1.48        | 1.43     |
| 31  | g     | 610 | CLA  | C3B-C4B | 2.43  | 1.49        | 1.42     |
| 31  | 3     | 318 | CLA  | C1B-C2B | 2.43  | 1.48        | 1.43     |
| 31  | b     | 610 | CLA  | C3B-C4B | 2.43  | 1.49        | 1.42     |
| 37  | i     | 521 | 0IE  | C8-C7   | 2.43  | 1.41        | 1.35     |
| 31  | B     | 818 | CLA  | C1B-C2B | 2.43  | 1.48        | 1.43     |
| 31  | B     | 828 | CLA  | C1B-C2B | 2.43  | 1.48        | 1.43     |
| 31  | 1     | 309 | CLA  | C1B-C2B | 2.43  | 1.48        | 1.43     |
| 31  | A     | 802 | CLA  | C1B-C2B | 2.43  | 1.48        | 1.43     |
| 34  | 7     | 601 | LHG  | O7-C5   | -2.43 | 1.40        | 1.46     |
| 31  | A     | 821 | CLA  | MG-NB   | -2.43 | 2.01        | 2.05     |
| 31  | B     | 826 | CLA  | C1B-C2B | 2.43  | 1.48        | 1.43     |
| 37  | b     | 522 | 0IE  | C8-C7   | 2.43  | 1.41        | 1.35     |
| 37  | f     | 521 | 0IE  | C13-C12 | -2.43 | 1.40        | 1.46     |
| 31  | B     | 831 | CLA  | C1B-C2B | 2.43  | 1.48        | 1.43     |
| 34  | c     | 630 | LHG  | O8-C6   | -2.43 | 1.39        | 1.45     |
| 34  | 3     | 603 | LHG  | O7-C5   | -2.43 | 1.40        | 1.46     |
| 31  | A     | 832 | CLA  | C1B-C2B | 2.43  | 1.48        | 1.43     |
| 31  | 7     | 309 | CLA  | C1B-C2B | 2.42  | 1.48        | 1.43     |
| 31  | B     | 809 | CLA  | C1B-C2B | 2.42  | 1.48        | 1.43     |
| 31  | A     | 827 | CLA  | C1B-C2B | 2.42  | 1.48        | 1.43     |
| 31  | 9     | 311 | CLA  | C1B-C2B | 2.42  | 1.48        | 1.43     |
| 31  | g     | 610 | CLA  | CHC-C1C | 2.42  | 1.43        | 1.38     |
| 31  | A     | 804 | CLA  | C1B-C2B | 2.42  | 1.48        | 1.43     |
| 34  | K     | 106 | LHG  | O7-C5   | -2.42 | 1.40        | 1.46     |
| 34  | G     | 105 | LHG  | O8-C23  | 2.42  | 1.40        | 1.33     |
| 31  | B     | 822 | CLA  | C1B-C2B | 2.42  | 1.48        | 1.43     |
| 31  | 2     | 304 | CLA  | CMB-C2B | -2.42 | 1.45        | 1.50     |
| 37  | c     | 521 | 0IE  | C17-C16 | -2.42 | 1.40        | 1.46     |
| 34  | A     | 855 | LHG  | O8-C6   | -2.42 | 1.39        | 1.45     |
| 31  | A     | 823 | CLA  | CMB-C2B | -2.42 | 1.45        | 1.50     |
| 31  | A     | 824 | CLA  | C1B-C2B | 2.42  | 1.48        | 1.43     |
| 31  | B     | 836 | CLA  | C1B-C2B | 2.41  | 1.48        | 1.43     |
| 34  | b     | 630 | LHG  | O8-C6   | -2.41 | 1.39        | 1.45     |
| 31  | A     | 806 | CLA  | C1B-C2B | 2.41  | 1.48        | 1.43     |
| 31  | A     | 812 | CLA  | C3B-C4B | 2.41  | 1.49        | 1.42     |
| 37  | b     | 522 | 0IE  | C11-C12 | 2.41  | 1.41        | 1.35     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 34  | c     | 630 | LHG  | O7-C5   | -2.41 | 1.40        | 1.46     |
| 34  | 7     | 603 | LHG  | O8-C6   | -2.41 | 1.39        | 1.45     |
| 31  | A     | 836 | CLA  | MG-NB   | -2.41 | 2.01        | 2.05     |
| 42  | i     | 523 | NEX  | O24-C25 | -2.41 | 1.43        | 1.46     |
| 31  | A     | 852 | CLA  | C1B-C2B | 2.41  | 1.48        | 1.43     |
| 31  | F     | 301 | CLA  | C1B-C2B | 2.41  | 1.48        | 1.43     |
| 37  | h     | 521 | 0IE  | C11-C12 | 2.41  | 1.41        | 1.35     |
| 34  | 3     | 601 | LHG  | O7-C5   | -2.41 | 1.40        | 1.46     |
| 32  | A     | 848 | 8CT  | C33-C32 | -2.41 | 1.43        | 1.50     |
| 31  | A     | 821 | CLA  | C1B-C2B | 2.41  | 1.48        | 1.43     |
| 31  | B     | 829 | CLA  | CMD-C2D | -2.41 | 1.45        | 1.50     |
| 31  | A     | 818 | CLA  | MG-NB   | -2.41 | 2.01        | 2.05     |
| 42  | f     | 523 | NEX  | O24-C25 | -2.41 | 1.43        | 1.46     |
| 31  | B     | 823 | CLA  | CMD-C2D | -2.40 | 1.45        | 1.50     |
| 37  | g     | 521 | 0IE  | C13-C12 | -2.40 | 1.40        | 1.46     |
| 37  | d     | 522 | 0IE  | C8-C7   | 2.40  | 1.41        | 1.35     |
| 34  | 3     | 603 | LHG  | O8-C6   | -2.40 | 1.39        | 1.45     |
| 42  | d     | 523 | NEX  | O24-C25 | -2.40 | 1.43        | 1.46     |
| 37  | a     | 522 | 0IE  | C15-C16 | 2.40  | 1.41        | 1.35     |
| 31  | d     | 610 | CLA  | C3B-C4B | 2.40  | 1.49        | 1.42     |
| 31  | A     | 809 | CLA  | MG-NB   | -2.40 | 2.01        | 2.05     |
| 31  | 5     | 308 | CLA  | C3B-C4B | 2.40  | 1.49        | 1.42     |
| 31  | A     | 841 | CLA  | CMD-C2D | -2.40 | 1.45        | 1.50     |
| 42  | a     | 523 | NEX  | O24-C25 | -2.40 | 1.43        | 1.46     |
| 31  | B     | 819 | CLA  | MG-NB   | -2.40 | 2.01        | 2.05     |
| 37  | e     | 521 | 0IE  | C13-C12 | -2.40 | 1.40        | 1.46     |
| 34  | 3     | 601 | LHG  | O8-C6   | -2.40 | 1.39        | 1.45     |
| 31  | A     | 823 | CLA  | CMD-C2D | -2.40 | 1.45        | 1.50     |
| 34  | 8     | 601 | LHG  | O7-C5   | -2.40 | 1.41        | 1.46     |
| 42  | g     | 523 | NEX  | O24-C25 | -2.39 | 1.43        | 1.46     |
| 37  | c     | 522 | 0IE  | C11-C12 | 2.39  | 1.41        | 1.35     |
| 37  | b     | 521 | 0IE  | C13-C12 | -2.39 | 1.40        | 1.46     |
| 37  | h     | 522 | 0IE  | C11-C12 | 2.39  | 1.41        | 1.35     |
| 31  | L     | 201 | CLA  | MG-NB   | -2.39 | 2.01        | 2.05     |
| 37  | g     | 522 | 0IE  | C11-C12 | 2.39  | 1.41        | 1.35     |
| 37  | b     | 521 | 0IE  | C17-C16 | -2.39 | 1.40        | 1.46     |
| 34  | B     | 854 | LHG  | O7-C5   | -2.39 | 1.41        | 1.46     |
| 42  | c     | 523 | NEX  | O24-C25 | -2.39 | 1.43        | 1.46     |
| 31  | A     | 831 | CLA  | C1B-C2B | 2.39  | 1.48        | 1.43     |
| 37  | h     | 521 | 0IE  | C8-C7   | 2.39  | 1.41        | 1.35     |
| 31  | 2     | 303 | CLA  | CMB-C2B | -2.39 | 1.45        | 1.50     |
| 31  | 2     | 314 | CLA  | CMD-C2D | -2.39 | 1.45        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 36  | 2     | 602 | LMG  | O7-C8   | -2.39 | 1.41        | 1.46     |
| 34  | i     | 630 | LHG  | O8-C6   | -2.39 | 1.39        | 1.45     |
| 31  | 0     | 308 | CLA  | C3B-C4B | 2.39  | 1.49        | 1.42     |
| 37  | e     | 521 | 0IE  | C17-C16 | -2.39 | 1.40        | 1.46     |
| 31  | B     | 813 | CLA  | C1B-C2B | 2.39  | 1.48        | 1.43     |
| 37  | a     | 522 | 0IE  | C8-C7   | 2.39  | 1.41        | 1.35     |
| 31  | a     | 611 | CLA  | C3B-C4B | 2.39  | 1.49        | 1.42     |
| 34  | g     | 630 | LHG  | O8-C6   | -2.39 | 1.39        | 1.45     |
| 31  | 4     | 309 | CLA  | C3B-C4B | 2.39  | 1.49        | 1.42     |
| 37  | d     | 521 | 0IE  | C17-C16 | -2.38 | 1.40        | 1.46     |
| 42  | b     | 523 | NEX  | O24-C25 | -2.38 | 1.43        | 1.46     |
| 31  | B     | 839 | CLA  | C1B-C2B | 2.38  | 1.48        | 1.43     |
| 34  | h     | 630 | LHG  | O8-C6   | -2.38 | 1.39        | 1.45     |
| 37  | f     | 521 | 0IE  | C17-C16 | -2.38 | 1.40        | 1.46     |
| 34  | 6     | 601 | LHG  | O7-C5   | -2.38 | 1.41        | 1.46     |
| 34  | H     | 203 | LHG  | O7-C5   | -2.38 | 1.41        | 1.46     |
| 32  | B     | 845 | 8CT  | C30-C29 | 2.38  | 1.54        | 1.50     |
| 34  | A     | 855 | LHG  | O7-C7   | 2.38  | 1.41        | 1.34     |
| 37  | e     | 521 | 0IE  | C6-C7   | -2.38 | 1.40        | 1.46     |
| 34  | 6     | 603 | LHG  | O7-C5   | -2.38 | 1.41        | 1.46     |
| 37  | g     | 522 | 0IE  | C15-C16 | 2.38  | 1.41        | 1.35     |
| 31  | A     | 841 | CLA  | MG-NB   | -2.38 | 2.01        | 2.05     |
| 34  | d     | 630 | LHG  | O8-C23  | 2.38  | 1.40        | 1.33     |
| 34  | 6     | 603 | LHG  | O8-C6   | -2.38 | 1.39        | 1.45     |
| 34  | 9     | 601 | LHG  | O7-C5   | -2.38 | 1.41        | 1.46     |
| 34  | G     | 105 | LHG  | O7-C5   | -2.38 | 1.41        | 1.46     |
| 31  | A     | 819 | CLA  | CMB-C2B | -2.37 | 1.45        | 1.50     |
| 31  | A     | 839 | CLA  | MG-NB   | -2.37 | 2.01        | 2.05     |
| 31  | B     | 836 | CLA  | MG-NB   | -2.37 | 2.01        | 2.05     |
| 32  | 7     | 405 | 8CT  | C33-C32 | -2.37 | 1.43        | 1.50     |
| 32  | J     | 104 | 8CT  | C33-C32 | -2.37 | 1.43        | 1.50     |
| 32  | 7     | 402 | 8CT  | C30-C29 | 2.37  | 1.53        | 1.50     |
| 31  | A     | 813 | CLA  | C1B-C2B | 2.37  | 1.48        | 1.43     |
| 31  | 6     | 317 | CLA  | C1B-C2B | 2.37  | 1.48        | 1.43     |
| 31  | b     | 610 | CLA  | CHC-C1C | 2.37  | 1.43        | 1.38     |
| 37  | g     | 522 | 0IE  | C8-C7   | 2.37  | 1.41        | 1.35     |
| 31  | B     | 824 | CLA  | CMD-C2D | -2.37 | 1.45        | 1.50     |
| 31  | 6     | 303 | CLA  | MG-NB   | -2.37 | 2.01        | 2.05     |
| 31  | B     | 807 | CLA  | C1B-C2B | 2.37  | 1.48        | 1.43     |
| 31  | A     | 838 | CLA  | C3B-C4B | 2.37  | 1.49        | 1.42     |
| 37  | i     | 522 | 0IE  | C8-C7   | 2.37  | 1.41        | 1.35     |
| 31  | A     | 805 | CLA  | CMC-C2C | -2.37 | 1.45        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | B     | 806 | CLA  | C1B-C2B | 2.37  | 1.48        | 1.43     |
| 31  | 9     | 312 | CLA  | MG-NB   | -2.36 | 2.01        | 2.05     |
| 31  | 6     | 303 | CLA  | CMB-C2B | -2.36 | 1.45        | 1.50     |
| 32  | B     | 848 | 8CT  | C33-C32 | -2.36 | 1.43        | 1.50     |
| 31  | A     | 827 | CLA  | MG-NB   | -2.36 | 2.01        | 2.05     |
| 31  | A     | 832 | CLA  | MG-NB   | -2.36 | 2.01        | 2.05     |
| 31  | H     | 201 | CLA  | MG-NB   | -2.36 | 2.01        | 2.05     |
| 37  | h     | 521 | 0IE  | C15-C16 | 2.36  | 1.41        | 1.35     |
| 31  | a     | 613 | CLA  | C3B-C4B | 2.36  | 1.49        | 1.42     |
| 31  | e     | 610 | CLA  | C3B-C4B | 2.36  | 1.49        | 1.42     |
| 31  | B     | 807 | CLA  | C3B-C4B | 2.36  | 1.49        | 1.42     |
| 31  | h     | 613 | CLA  | C3B-C4B | 2.36  | 1.49        | 1.42     |
| 31  | B     | 818 | CLA  | MG-NB   | -2.36 | 2.01        | 2.05     |
| 32  | K     | 107 | 8CT  | C33-C32 | -2.36 | 1.44        | 1.50     |
| 37  | d     | 522 | 0IE  | C11-C12 | 2.36  | 1.41        | 1.35     |
| 37  | a     | 522 | 0IE  | C11-C12 | 2.36  | 1.41        | 1.35     |
| 32  | 7     | 404 | 8CT  | C33-C32 | -2.36 | 1.44        | 1.50     |
| 31  | A     | 853 | CLA  | CMD-C2D | -2.36 | 1.45        | 1.50     |
| 31  | B     | 827 | CLA  | MG-NB   | -2.36 | 2.01        | 2.05     |
| 37  | i     | 522 | 0IE  | C15-C16 | 2.36  | 1.41        | 1.35     |
| 34  | h     | 630 | LHG  | O8-C23  | 2.36  | 1.40        | 1.33     |
| 31  | d     | 611 | CLA  | C3B-C4B | 2.36  | 1.49        | 1.42     |
| 31  | A     | 838 | CLA  | C1B-C2B | 2.36  | 1.48        | 1.43     |
| 31  | 5     | 309 | CLA  | C3B-C4B | 2.36  | 1.49        | 1.42     |
| 31  | 1     | 303 | CLA  | C3B-C4B | 2.35  | 1.49        | 1.42     |
| 30  | 2     | 301 | CHL  | CBD-CGD | -2.35 | 1.49        | 1.52     |
| 34  | H     | 203 | LHG  | O8-C6   | -2.35 | 1.39        | 1.45     |
| 31  | L     | 201 | CLA  | C1B-C2B | 2.35  | 1.48        | 1.43     |
| 31  | A     | 841 | CLA  | CMB-C2B | -2.35 | 1.45        | 1.50     |
| 34  | d     | 630 | LHG  | O8-C6   | -2.35 | 1.39        | 1.45     |
| 34  | i     | 630 | LHG  | O8-C23  | 2.35  | 1.40        | 1.33     |
| 31  | A     | 827 | CLA  | CMC-C2C | -2.35 | 1.46        | 1.50     |
| 37  | f     | 522 | 0IE  | C11-C12 | 2.35  | 1.41        | 1.35     |
| 31  | B     | 831 | CLA  | CMB-C2B | -2.35 | 1.46        | 1.50     |
| 31  | 2     | 311 | CLA  | MG-NB   | -2.35 | 2.01        | 2.05     |
| 31  | A     | 805 | CLA  | C1B-C2B | 2.35  | 1.48        | 1.43     |
| 31  | A     | 807 | CLA  | C1B-C2B | 2.35  | 1.48        | 1.43     |
| 31  | h     | 604 | CLA  | C3B-C4B | 2.35  | 1.49        | 1.42     |
| 31  | h     | 610 | CLA  | C3B-C4B | 2.35  | 1.49        | 1.42     |
| 31  | a     | 604 | CLA  | C3B-C4B | 2.35  | 1.49        | 1.42     |
| 31  | A     | 829 | CLA  | CMD-C2D | -2.35 | 1.46        | 1.50     |
| 31  | B     | 818 | CLA  | CMC-C2C | -2.35 | 1.46        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 42  | e     | 523 | NEX  | O24-C25 | -2.35 | 1.43        | 1.46     |
| 31  | 3     | 309 | CLA  | C3B-C4B | 2.34  | 1.49        | 1.42     |
| 31  | H     | 205 | CLA  | C3B-C4B | 2.34  | 1.49        | 1.42     |
| 31  | 9     | 310 | CLA  | C3B-C4B | 2.34  | 1.49        | 1.42     |
| 31  | A     | 831 | CLA  | MG-NB   | -2.34 | 2.01        | 2.05     |
| 34  | a     | 630 | LHG  | O8-C6   | -2.34 | 1.39        | 1.45     |
| 31  | 4     | 303 | CLA  | MG-NB   | -2.34 | 2.01        | 2.05     |
| 34  | e     | 630 | LHG  | O7-C5   | -2.34 | 1.41        | 1.46     |
| 31  | 8     | 311 | CLA  | C3B-C4B | 2.34  | 1.49        | 1.42     |
| 31  | c     | 610 | CLA  | C3B-C4B | 2.34  | 1.49        | 1.42     |
| 37  | h     | 522 | 0IE  | C8-C7   | 2.34  | 1.41        | 1.35     |
| 31  | B     | 806 | CLA  | CHC-C1C | 2.34  | 1.43        | 1.38     |
| 37  | a     | 521 | 0IE  | C13-C12 | -2.34 | 1.40        | 1.46     |
| 31  | B     | 805 | CLA  | CMD-C2D | -2.34 | 1.46        | 1.50     |
| 32  | B     | 847 | 8CT  | C33-C32 | -2.34 | 1.44        | 1.50     |
| 34  | B     | 852 | LHG  | O7-C7   | 2.34  | 1.40        | 1.34     |
| 31  | e     | 610 | CLA  | CHC-C1C | 2.34  | 1.43        | 1.38     |
| 32  | F     | 302 | 8CT  | C33-C32 | -2.34 | 1.44        | 1.50     |
| 37  | f     | 521 | 0IE  | C11-C12 | 2.34  | 1.41        | 1.35     |
| 31  | A     | 825 | CLA  | MG-NB   | -2.34 | 2.01        | 2.05     |
| 37  | f     | 522 | 0IE  | C8-C7   | 2.34  | 1.41        | 1.35     |
| 32  | 2     | 402 | 8CT  | C33-C32 | -2.34 | 1.44        | 1.50     |
| 31  | 6     | 312 | CLA  | MG-NB   | -2.34 | 2.01        | 2.05     |
| 31  | B     | 838 | CLA  | MG-NB   | -2.34 | 2.01        | 2.05     |
| 31  | A     | 807 | CLA  | CMB-C2B | -2.34 | 1.46        | 1.50     |
| 31  | a     | 610 | CLA  | C3B-C4B | 2.34  | 1.49        | 1.42     |
| 31  | b     | 603 | CLA  | CMD-C2D | -2.34 | 1.46        | 1.50     |
| 31  | A     | 809 | CLA  | CMD-C2D | -2.34 | 1.46        | 1.50     |
| 31  | 2     | 311 | CLA  | CMC-C2C | -2.34 | 1.46        | 1.50     |
| 31  | B     | 820 | CLA  | C1B-C2B | 2.34  | 1.48        | 1.43     |
| 32  | L     | 209 | 8CT  | C33-C32 | -2.33 | 1.44        | 1.50     |
| 34  | M     | 104 | LHG  | O8-C6   | -2.33 | 1.39        | 1.45     |
| 31  | 7     | 318 | CLA  | MG-NB   | -2.33 | 2.01        | 2.05     |
| 31  | O     | 206 | CLA  | C3B-C4B | 2.33  | 1.49        | 1.42     |
| 31  | 7     | 303 | CLA  | CMD-C2D | -2.33 | 1.46        | 1.50     |
| 31  | a     | 613 | CLA  | CHC-C1C | 2.33  | 1.43        | 1.38     |
| 32  | 4     | 402 | 8CT  | C33-C32 | -2.33 | 1.44        | 1.50     |
| 31  | L     | 207 | CLA  | C3B-C4B | 2.33  | 1.49        | 1.42     |
| 34  | a     | 630 | LHG  | O8-C23  | 2.33  | 1.40        | 1.33     |
| 34  | g     | 630 | LHG  | O7-C7   | 2.33  | 1.40        | 1.34     |
| 31  | h     | 612 | CLA  | C3B-C4B | 2.33  | 1.49        | 1.42     |
| 34  | A     | 855 | LHG  | O8-C23  | 2.33  | 1.40        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 34  | H     | 203 | LHG  | O8-C23  | 2.33  | 1.40        | 1.33     |
| 34  | g     | 630 | LHG  | O8-C23  | 2.33  | 1.40        | 1.33     |
| 30  | 6     | 308 | CHL  | CBD-CGD | -2.33 | 1.49        | 1.52     |
| 31  | A     | 837 | CLA  | MG-NB   | -2.33 | 2.01        | 2.05     |
| 31  | 5     | 314 | CLA  | C3B-C4B | 2.33  | 1.49        | 1.42     |
| 37  | g     | 521 | 0IE  | C6-C7   | -2.33 | 1.41        | 1.46     |
| 32  | G     | 104 | 8CT  | C33-C32 | -2.33 | 1.44        | 1.50     |
| 30  | 2     | 306 | CHL  | CBD-CGD | -2.33 | 1.49        | 1.52     |
| 31  | 3     | 303 | CLA  | CMD-C2D | -2.33 | 1.46        | 1.50     |
| 31  | B     | 810 | CLA  | MG-NB   | -2.33 | 2.01        | 2.05     |
| 34  | G     | 105 | LHG  | O8-C6   | -2.33 | 1.40        | 1.45     |
| 31  | A     | 810 | CLA  | CMB-C2B | -2.33 | 1.46        | 1.50     |
| 31  | e     | 613 | CLA  | C3B-C4B | 2.33  | 1.49        | 1.42     |
| 31  | d     | 610 | CLA  | CHC-C1C | 2.33  | 1.43        | 1.38     |
| 31  | i     | 613 | CLA  | CHC-C1C | 2.33  | 1.43        | 1.38     |
| 34  | 5     | 601 | LHG  | O7-C5   | -2.33 | 1.41        | 1.46     |
| 31  | A     | 815 | CLA  | MG-NB   | -2.32 | 2.01        | 2.05     |
| 31  | B     | 841 | CLA  | MG-NB   | -2.32 | 2.01        | 2.05     |
| 31  | F     | 301 | CLA  | MG-NB   | -2.32 | 2.01        | 2.05     |
| 31  | O     | 202 | CLA  | MG-NB   | -2.32 | 2.01        | 2.05     |
| 34  | h     | 630 | LHG  | O7-C7   | 2.32  | 1.40        | 1.34     |
| 31  | f     | 610 | CLA  | C3B-C4B | 2.32  | 1.49        | 1.42     |
| 31  | O     | 203 | CLA  | CHC-C1C | 2.32  | 1.43        | 1.38     |
| 31  | B     | 822 | CLA  | C3B-C4B | 2.32  | 1.49        | 1.42     |
| 31  | K     | 101 | CLA  | C3B-C4B | 2.32  | 1.49        | 1.42     |
| 31  | h     | 613 | CLA  | CHC-C1C | 2.32  | 1.43        | 1.38     |
| 37  | i     | 521 | 0IE  | C15-C16 | 2.32  | 1.41        | 1.35     |
| 31  | 7     | 316 | CLA  | MG-NB   | -2.32 | 2.01        | 2.05     |
| 31  | 9     | 303 | CLA  | MG-NB   | -2.32 | 2.01        | 2.05     |
| 31  | A     | 826 | CLA  | CMD-C2D | -2.32 | 1.46        | 1.50     |
| 31  | 1     | 309 | CLA  | C3B-C4B | 2.32  | 1.49        | 1.42     |
| 31  | A     | 853 | CLA  | C1B-C2B | 2.32  | 1.48        | 1.43     |
| 31  | B     | 832 | CLA  | MG-NB   | -2.32 | 2.01        | 2.05     |
| 31  | B     | 811 | CLA  | CMD-C2D | -2.32 | 1.46        | 1.50     |
| 31  | A     | 806 | CLA  | MG-NB   | -2.32 | 2.01        | 2.05     |
| 31  | B     | 812 | CLA  | MG-NB   | -2.32 | 2.01        | 2.05     |
| 31  | 6     | 317 | CLA  | MG-NB   | -2.32 | 2.01        | 2.05     |
| 31  | 3     | 318 | CLA  | MG-NB   | -2.32 | 2.01        | 2.05     |
| 31  | B     | 820 | CLA  | MG-NB   | -2.32 | 2.01        | 2.05     |
| 31  | g     | 603 | CLA  | C3B-C4B | 2.32  | 1.49        | 1.42     |
| 31  | A     | 807 | CLA  | MG-NB   | -2.32 | 2.01        | 2.05     |
| 34  | i     | 630 | LHG  | O7-C5   | -2.32 | 1.41        | 1.46     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 32  | M     | 102 | 8CT  | C33-C32 | -2.32 | 1.44        | 1.50     |
| 39  | A     | 857 | CL0  | C3B-C2B | -2.32 | 1.37        | 1.40     |
| 31  | A     | 804 | CLA  | C3B-C4B | 2.32  | 1.49        | 1.42     |
| 30  | 8     | 308 | CHL  | CBD-CGD | -2.32 | 1.49        | 1.52     |
| 37  | d     | 521 | 0IE  | C6-C7   | -2.32 | 1.41        | 1.46     |
| 37  | i     | 521 | 0IE  | C17-C16 | -2.32 | 1.41        | 1.46     |
| 31  | A     | 823 | CLA  | MG-NB   | -2.32 | 2.01        | 2.05     |
| 31  | a     | 610 | CLA  | CHC-C1C | 2.32  | 1.43        | 1.38     |
| 31  | B     | 833 | CLA  | CMB-C2B | -2.32 | 1.46        | 1.50     |
| 34  | e     | 630 | LHG  | O8-C23  | 2.32  | 1.40        | 1.33     |
| 42  | h     | 523 | NEX  | O24-C25 | -2.32 | 1.43        | 1.46     |
| 31  | g     | 611 | CLA  | C3B-C4B | 2.31  | 1.49        | 1.42     |
| 31  | B     | 809 | CLA  | MG-NB   | -2.31 | 2.01        | 2.05     |
| 31  | A     | 810 | CLA  | C1B-C2B | 2.31  | 1.48        | 1.43     |
| 31  | d     | 612 | CLA  | C3B-C4B | 2.31  | 1.49        | 1.42     |
| 31  | B     | 801 | CLA  | CMB-C2B | -2.31 | 1.46        | 1.50     |
| 31  | A     | 803 | CLA  | MG-NB   | -2.31 | 2.01        | 2.05     |
| 31  | A     | 805 | CLA  | CHC-C1C | 2.31  | 1.43        | 1.38     |
| 37  | e     | 522 | 0IE  | C15-C16 | 2.31  | 1.41        | 1.35     |
| 30  | 7     | 306 | CHL  | CBD-CGD | -2.31 | 1.49        | 1.52     |
| 31  | e     | 611 | CLA  | C3B-C4B | 2.31  | 1.49        | 1.42     |
| 34  | 3     | 601 | LHG  | O8-C23  | 2.31  | 1.40        | 1.33     |
| 34  | b     | 630 | LHG  | O8-C23  | 2.31  | 1.40        | 1.33     |
| 37  | g     | 521 | 0IE  | C8-C7   | 2.31  | 1.41        | 1.35     |
| 31  | e     | 612 | CLA  | C3B-C4B | 2.31  | 1.49        | 1.42     |
| 31  | i     | 610 | CLA  | C3B-C4B | 2.31  | 1.49        | 1.42     |
| 31  | 2     | 304 | CLA  | MG-NB   | -2.31 | 2.01        | 2.05     |
| 31  | i     | 604 | CLA  | C3B-C4B | 2.31  | 1.49        | 1.42     |
| 34  | 7     | 603 | LHG  | O7-C7   | 2.31  | 1.40        | 1.34     |
| 31  | B     | 815 | CLA  | CMD-C2D | -2.31 | 1.46        | 1.50     |
| 31  | B     | 850 | CLA  | C3B-C4B | 2.31  | 1.49        | 1.42     |
| 31  | 5     | 309 | CLA  | MG-NB   | -2.31 | 2.01        | 2.05     |
| 31  | A     | 831 | CLA  | CMB-C2B | -2.31 | 1.46        | 1.50     |
| 31  | 4     | 312 | CLA  | MG-NB   | -2.31 | 2.01        | 2.05     |
| 31  | 4     | 309 | CLA  | CHC-C1C | 2.31  | 1.43        | 1.38     |
| 34  | b     | 630 | LHG  | O7-C5   | -2.31 | 1.41        | 1.46     |
| 32  | 3     | 403 | 8CT  | C33-C32 | -2.31 | 1.44        | 1.50     |
| 37  | a     | 521 | 0IE  | C17-C16 | -2.31 | 1.41        | 1.46     |
| 31  | 7     | 312 | CLA  | C3B-C4B | 2.31  | 1.49        | 1.42     |
| 31  | B     | 819 | CLA  | CMB-C2B | -2.31 | 1.46        | 1.50     |
| 31  | B     | 827 | CLA  | CMC-C2C | -2.31 | 1.46        | 1.50     |
| 31  | B     | 801 | CLA  | CHC-C1C | 2.31  | 1.43        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 7     | 303 | CLA  | MG-NB   | -2.31 | 2.01        | 2.05     |
| 31  | 9     | 309 | CLA  | C3B-C4B | 2.31  | 1.49        | 1.42     |
| 31  | g     | 612 | CLA  | C3B-C4B | 2.30  | 1.49        | 1.42     |
| 34  | i     | 630 | LHG  | O7-C7   | 2.30  | 1.40        | 1.34     |
| 31  | h     | 604 | CLA  | CHC-C1C | 2.30  | 1.43        | 1.38     |
| 31  | 7     | 304 | CLA  | CMB-C2B | -2.30 | 1.46        | 1.50     |
| 31  | g     | 604 | CLA  | C3B-C4B | 2.30  | 1.49        | 1.42     |
| 31  | 7     | 304 | CLA  | MG-NB   | -2.30 | 2.01        | 2.05     |
| 31  | 1     | 314 | CLA  | MG-NB   | -2.30 | 2.01        | 2.05     |
| 31  | 7     | 309 | CLA  | MG-NB   | -2.30 | 2.01        | 2.05     |
| 31  | 2     | 303 | CLA  | CMC-C2C | -2.30 | 1.46        | 1.50     |
| 32  | L     | 205 | 8CT  | C33-C32 | -2.30 | 1.44        | 1.50     |
| 31  | 6     | 318 | CLA  | C3B-C4B | 2.30  | 1.49        | 1.42     |
| 31  | A     | 802 | CLA  | CMD-C2D | -2.30 | 1.46        | 1.50     |
| 34  | a     | 630 | LHG  | O7-C7   | 2.30  | 1.40        | 1.34     |
| 37  | i     | 522 | 0IE  | C11-C12 | 2.30  | 1.41        | 1.35     |
| 31  | f     | 603 | CLA  | C3B-C4B | 2.30  | 1.49        | 1.42     |
| 31  | h     | 611 | CLA  | C3B-C4B | 2.30  | 1.49        | 1.42     |
| 37  | g     | 521 | 0IE  | C11-C12 | 2.30  | 1.41        | 1.35     |
| 31  | K     | 105 | CLA  | MG-NB   | -2.30 | 2.01        | 2.05     |
| 31  | H     | 202 | CLA  | C3B-C4B | 2.30  | 1.49        | 1.42     |
| 34  | d     | 630 | LHG  | O7-C5   | -2.30 | 1.41        | 1.46     |
| 31  | 6     | 314 | CLA  | MG-NB   | -2.30 | 2.01        | 2.05     |
| 31  | B     | 829 | CLA  | CMB-C2B | -2.30 | 1.46        | 1.50     |
| 37  | b     | 521 | 0IE  | C11-C12 | 2.30  | 1.41        | 1.35     |
| 31  | L     | 203 | CLA  | MG-NB   | -2.30 | 2.01        | 2.05     |
| 34  | h     | 630 | LHG  | O7-C5   | -2.30 | 1.41        | 1.46     |
| 31  | A     | 829 | CLA  | MG-NB   | -2.30 | 2.01        | 2.05     |
| 31  | A     | 812 | CLA  | C1B-C2B | 2.30  | 1.48        | 1.43     |
| 31  | A     | 812 | CLA  | CMB-C2B | -2.30 | 1.46        | 1.50     |
| 31  | A     | 805 | CLA  | CMB-C2B | -2.30 | 1.46        | 1.50     |
| 31  | B     | 806 | CLA  | CMC-C2C | -2.30 | 1.46        | 1.50     |
| 31  | 0     | 303 | CLA  | C3B-C4B | 2.30  | 1.49        | 1.42     |
| 31  | 7     | 303 | CLA  | C3B-C4B | 2.30  | 1.49        | 1.42     |
| 31  | A     | 817 | CLA  | MG-NB   | -2.30 | 2.01        | 2.05     |
| 34  | 7     | 603 | LHG  | O7-C5   | -2.30 | 1.41        | 1.46     |
| 31  | 5     | 309 | CLA  | C1B-C2B | 2.30  | 1.48        | 1.43     |
| 31  | 7     | 315 | CLA  | C3B-C4B | 2.30  | 1.49        | 1.42     |
| 31  | d     | 604 | CLA  | C3B-C4B | 2.30  | 1.49        | 1.42     |
| 30  | 2     | 308 | CHL  | CBD-CGD | -2.30 | 1.49        | 1.52     |
| 31  | 8     | 311 | CLA  | CHC-C1C | 2.30  | 1.43        | 1.38     |
| 31  | e     | 613 | CLA  | CHC-C1C | 2.30  | 1.43        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 37  | i     | 522 | 0IE  | C17-C16 | -2.29 | 1.41        | 1.46     |
| 31  | a     | 604 | CLA  | CHC-C1C | 2.29  | 1.43        | 1.38     |
| 31  | A     | 840 | CLA  | MG-NB   | -2.29 | 2.01        | 2.05     |
| 32  | A     | 850 | 8CT  | C30-C29 | 2.29  | 1.53        | 1.50     |
| 37  | a     | 521 | 0IE  | C6-C7   | -2.29 | 1.41        | 1.46     |
| 30  | 4     | 319 | CHL  | CBD-CGD | -2.29 | 1.49        | 1.52     |
| 31  | A     | 802 | CLA  | CMB-C2B | -2.29 | 1.46        | 1.50     |
| 34  | 3     | 601 | LHG  | O7-C7   | 2.29  | 1.40        | 1.34     |
| 31  | A     | 840 | CLA  | CMB-C2B | -2.29 | 1.46        | 1.50     |
| 31  | 7     | 309 | CLA  | C3B-C4B | 2.29  | 1.49        | 1.42     |
| 31  | 2     | 312 | CLA  | MG-NB   | -2.29 | 2.01        | 2.05     |
| 34  | d     | 630 | LHG  | O7-C7   | 2.29  | 1.40        | 1.34     |
| 31  | 2     | 310 | CLA  | MG-NB   | -2.29 | 2.01        | 2.05     |
| 31  | d     | 613 | CLA  | CHC-C1C | 2.29  | 1.43        | 1.38     |
| 31  | B     | 809 | CLA  | C3B-C4B | 2.29  | 1.49        | 1.42     |
| 30  | 8     | 307 | CHL  | CBD-CGD | -2.29 | 1.49        | 1.52     |
| 31  | i     | 612 | CLA  | C3B-C4B | 2.29  | 1.49        | 1.42     |
| 30  | 5     | 302 | CHL  | CBD-CGD | -2.29 | 1.49        | 1.52     |
| 31  | A     | 814 | CLA  | MG-NB   | -2.29 | 2.01        | 2.05     |
| 31  | B     | 823 | CLA  | CMB-C2B | -2.29 | 1.46        | 1.50     |
| 34  | 8     | 601 | LHG  | O8-C23  | 2.29  | 1.40        | 1.33     |
| 37  | h     | 522 | 0IE  | C15-C16 | 2.29  | 1.41        | 1.35     |
| 31  | 3     | 303 | CLA  | MG-NB   | -2.29 | 2.01        | 2.05     |
| 31  | K     | 104 | CLA  | MG-NB   | -2.29 | 2.01        | 2.05     |
| 31  | B     | 814 | CLA  | C3B-C4B | 2.29  | 1.49        | 1.42     |
| 31  | B     | 824 | CLA  | CHC-C1C | 2.29  | 1.43        | 1.38     |
| 31  | 3     | 312 | CLA  | MG-NB   | -2.29 | 2.01        | 2.05     |
| 31  | 6     | 310 | CLA  | C3B-C4B | 2.29  | 1.49        | 1.42     |
| 31  | B     | 808 | CLA  | CMD-C2D | -2.29 | 1.46        | 1.50     |
| 31  | A     | 813 | CLA  | MG-NB   | -2.29 | 2.01        | 2.05     |
| 31  | 3     | 304 | CLA  | CMB-C2B | -2.29 | 1.46        | 1.50     |
| 31  | A     | 808 | CLA  | MG-NB   | -2.29 | 2.01        | 2.05     |
| 31  | 3     | 306 | CLA  | C3B-C4B | 2.29  | 1.49        | 1.42     |
| 31  | 7     | 318 | CLA  | CMB-C2B | -2.29 | 1.46        | 1.50     |
| 31  | A     | 821 | CLA  | CMD-C2D | -2.29 | 1.46        | 1.50     |
| 31  | B     | 833 | CLA  | MG-NB   | -2.29 | 2.01        | 2.05     |
| 31  | A     | 816 | CLA  | CMD-C2D | -2.28 | 1.46        | 1.50     |
| 31  | f     | 613 | CLA  | C3B-C4B | 2.28  | 1.49        | 1.42     |
| 31  | i     | 611 | CLA  | C3B-C4B | 2.28  | 1.49        | 1.42     |
| 34  | 5     | 601 | LHG  | O7-C7   | 2.28  | 1.40        | 1.34     |
| 31  | 3     | 308 | CLA  | CMD-C2D | -2.28 | 1.46        | 1.50     |
| 34  | K     | 106 | LHG  | O8-C23  | 2.28  | 1.40        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 8     | 304 | CLA  | C3B-C4B | 2.28  | 1.49        | 1.42     |
| 31  | A     | 823 | CLA  | C3B-C4B | 2.28  | 1.49        | 1.42     |
| 31  | h     | 610 | CLA  | CHC-C1C | 2.28  | 1.43        | 1.38     |
| 34  | 8     | 601 | LHG  | O7-C7   | 2.28  | 1.40        | 1.34     |
| 37  | f     | 522 | 0IE  | C15-C16 | 2.28  | 1.41        | 1.35     |
| 31  | A     | 824 | CLA  | MG-NB   | -2.28 | 2.01        | 2.05     |
| 31  | B     | 839 | CLA  | MG-NB   | -2.28 | 2.01        | 2.05     |
| 31  | 8     | 312 | CLA  | C3B-C4B | 2.28  | 1.49        | 1.42     |
| 34  | 6     | 603 | LHG  | O8-C23  | 2.28  | 1.40        | 1.33     |
| 31  | B     | 824 | CLA  | MG-NB   | -2.28 | 2.01        | 2.05     |
| 31  | 0     | 309 | CLA  | C3B-C4B | 2.28  | 1.49        | 1.42     |
| 31  | B     | 815 | CLA  | C3B-C4B | 2.28  | 1.49        | 1.42     |
| 30  | 5     | 301 | CHL  | CBD-CGD | -2.28 | 1.49        | 1.52     |
| 34  | g     | 630 | LHG  | O7-C5   | -2.28 | 1.41        | 1.46     |
| 31  | A     | 843 | CLA  | MG-NB   | -2.28 | 2.01        | 2.05     |
| 31  | b     | 613 | CLA  | C3B-C4B | 2.28  | 1.49        | 1.42     |
| 34  | e     | 630 | LHG  | O7-C7   | 2.28  | 1.40        | 1.34     |
| 31  | B     | 829 | CLA  | C1B-C2B | 2.28  | 1.48        | 1.43     |
| 31  | 2     | 310 | CLA  | C3B-C4B | 2.28  | 1.49        | 1.42     |
| 31  | b     | 611 | CLA  | C3B-C4B | 2.28  | 1.49        | 1.42     |
| 37  | h     | 522 | 0IE  | C17-C16 | -2.28 | 1.41        | 1.46     |
| 31  | 3     | 309 | CLA  | CHC-C1C | 2.28  | 1.43        | 1.38     |
| 31  | O     | 202 | CLA  | C3B-C4B | 2.28  | 1.49        | 1.42     |
| 31  | 3     | 308 | CLA  | MG-NB   | -2.28 | 2.01        | 2.05     |
| 31  | B     | 814 | CLA  | MG-NB   | -2.28 | 2.01        | 2.05     |
| 31  | B     | 814 | CLA  | CMC-C2C | -2.28 | 1.46        | 1.50     |
| 30  | 8     | 302 | CHL  | CBD-CGD | -2.28 | 1.49        | 1.52     |
| 37  | c     | 522 | 0IE  | C15-C16 | 2.28  | 1.41        | 1.35     |
| 31  | K     | 102 | CLA  | MG-NB   | -2.28 | 2.01        | 2.05     |
| 31  | 8     | 303 | CLA  | CMB-C2B | -2.28 | 1.46        | 1.50     |
| 31  | A     | 811 | CLA  | CMD-C2D | -2.28 | 1.46        | 1.50     |
| 31  | B     | 834 | CLA  | CMD-C2D | -2.28 | 1.46        | 1.50     |
| 31  | B     | 806 | CLA  | MG-NB   | -2.28 | 2.01        | 2.05     |
| 34  | 7     | 601 | LHG  | O8-C23  | 2.28  | 1.40        | 1.33     |
| 31  | f     | 610 | CLA  | CHC-C1C | 2.28  | 1.43        | 1.38     |
| 31  | A     | 841 | CLA  | CMC-C2C | -2.28 | 1.46        | 1.50     |
| 31  | B     | 839 | CLA  | CMD-C2D | -2.28 | 1.46        | 1.50     |
| 31  | 8     | 309 | CLA  | C3B-C4B | 2.28  | 1.49        | 1.42     |
| 31  | A     | 819 | CLA  | C3B-C4B | 2.27  | 1.49        | 1.42     |
| 31  | 9     | 303 | CLA  | CMD-C2D | -2.27 | 1.46        | 1.50     |
| 37  | h     | 522 | 0IE  | C13-C12 | -2.27 | 1.41        | 1.46     |
| 37  | e     | 522 | 0IE  | C8-C7   | 2.27  | 1.41        | 1.35     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 4     | 310 | CLA  | CMC-C2C | -2.27 | 1.46        | 1.50     |
| 31  | A     | 812 | CLA  | MG-NB   | -2.27 | 2.01        | 2.05     |
| 31  | A     | 852 | CLA  | MG-NB   | -2.27 | 2.01        | 2.05     |
| 31  | 3     | 309 | CLA  | MG-NB   | -2.27 | 2.01        | 2.05     |
| 30  | 6     | 307 | CHL  | CBD-CGD | -2.27 | 1.49        | 1.52     |
| 31  | A     | 834 | CLA  | CMB-C2B | -2.27 | 1.46        | 1.50     |
| 31  | 4     | 310 | CLA  | MG-NB   | -2.27 | 2.01        | 2.05     |
| 37  | d     | 521 | 0IE  | C8-C7   | 2.27  | 1.41        | 1.35     |
| 31  | B     | 841 | CLA  | C3B-C4B | 2.27  | 1.49        | 1.42     |
| 37  | g     | 521 | 0IE  | C17-C16 | -2.27 | 1.41        | 1.46     |
| 31  | A     | 833 | CLA  | MG-NB   | -2.27 | 2.01        | 2.05     |
| 31  | d     | 613 | CLA  | C3B-C4B | 2.27  | 1.49        | 1.42     |
| 37  | d     | 521 | 0IE  | C11-C12 | 2.27  | 1.41        | 1.35     |
| 31  | 3     | 312 | CLA  | CMB-C2B | -2.27 | 1.46        | 1.50     |
| 34  | 7     | 602 | LHG  | O8-C23  | 2.27  | 1.40        | 1.33     |
| 31  | A     | 840 | CLA  | C3B-C4B | 2.27  | 1.49        | 1.42     |
| 31  | 1     | 303 | CLA  | CMD-C2D | -2.27 | 1.46        | 1.50     |
| 31  | 7     | 310 | CLA  | C3B-C4B | 2.27  | 1.49        | 1.42     |
| 31  | 6     | 320 | CLA  | CMD-C2D | -2.27 | 1.46        | 1.50     |
| 31  | A     | 820 | CLA  | CMD-C2D | -2.27 | 1.46        | 1.50     |
| 32  | A     | 849 | 8CT  | C33-C32 | -2.27 | 1.44        | 1.50     |
| 34  | M     | 104 | LHG  | O8-C23  | 2.27  | 1.40        | 1.33     |
| 37  | b     | 521 | 0IE  | C8-C7   | 2.27  | 1.41        | 1.35     |
| 30  | 9     | 301 | CHL  | CBD-CGD | -2.27 | 1.49        | 1.52     |
| 32  | A     | 846 | 8CT  | C33-C32 | -2.27 | 1.44        | 1.50     |
| 31  | 0     | 304 | CLA  | MG-NB   | -2.27 | 2.01        | 2.05     |
| 31  | B     | 806 | CLA  | C3B-C4B | 2.27  | 1.49        | 1.42     |
| 31  | A     | 835 | CLA  | MG-NB   | -2.27 | 2.01        | 2.05     |
| 31  | i     | 613 | CLA  | C3B-C4B | 2.27  | 1.49        | 1.42     |
| 31  | B     | 824 | CLA  | C3B-C4B | 2.27  | 1.49        | 1.42     |
| 31  | 9     | 303 | CLA  | CMB-C2B | -2.27 | 1.46        | 1.50     |
| 31  | 3     | 310 | CLA  | MG-NB   | -2.27 | 2.01        | 2.05     |
| 31  | 2     | 309 | CLA  | CHC-C1C | 2.27  | 1.43        | 1.38     |
| 37  | g     | 522 | 0IE  | C17-C16 | -2.27 | 1.41        | 1.46     |
| 31  | A     | 826 | CLA  | MG-NB   | -2.27 | 2.01        | 2.05     |
| 31  | 2     | 309 | CLA  | CMC-C2C | -2.27 | 1.46        | 1.50     |
| 31  | B     | 801 | CLA  | CMD-C2D | -2.27 | 1.46        | 1.50     |
| 31  | B     | 840 | CLA  | CMD-C2D | -2.27 | 1.46        | 1.50     |
| 32  | B     | 845 | 8CT  | C33-C32 | -2.26 | 1.44        | 1.50     |
| 31  | 5     | 303 | CLA  | MG-NB   | -2.26 | 2.01        | 2.05     |
| 32  | 6     | 402 | 8CT  | C33-C32 | -2.26 | 1.44        | 1.50     |
| 31  | 0     | 312 | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 0     | 321 | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |
| 31  | 4     | 311 | CLA  | MG-NB   | -2.26 | 2.01        | 2.05     |
| 31  | A     | 807 | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |
| 31  | 8     | 310 | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |
| 31  | 8     | 309 | CLA  | MG-NB   | -2.26 | 2.01        | 2.05     |
| 31  | 5     | 309 | CLA  | CHC-C1C | 2.26  | 1.43        | 1.38     |
| 34  | H     | 203 | LHG  | O7-C7   | 2.26  | 1.40        | 1.34     |
| 31  | A     | 813 | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |
| 31  | A     | 812 | CLA  | CHC-C1C | 2.26  | 1.43        | 1.38     |
| 32  | B     | 844 | 8CT  | C33-C32 | -2.26 | 1.44        | 1.50     |
| 31  | 1     | 304 | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |
| 31  | 4     | 310 | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |
| 37  | a     | 521 | 0IE  | C11-C12 | 2.26  | 1.41        | 1.35     |
| 31  | 0     | 304 | CLA  | CMB-C2B | -2.26 | 1.46        | 1.50     |
| 37  | e     | 522 | 0IE  | C6-C7   | -2.26 | 1.41        | 1.46     |
| 34  | A     | 855 | LHG  | O7-C5   | -2.26 | 1.41        | 1.46     |
| 31  | L     | 202 | CLA  | CMD-C2D | -2.26 | 1.46        | 1.50     |
| 31  | K     | 101 | CLA  | CHC-C1C | 2.26  | 1.43        | 1.38     |
| 31  | i     | 610 | CLA  | CHC-C1C | 2.26  | 1.43        | 1.38     |
| 37  | f     | 521 | 0IE  | C6-C7   | -2.26 | 1.41        | 1.46     |
| 31  | O     | 201 | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |
| 31  | 5     | 304 | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |
| 31  | i     | 603 | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |
| 31  | G     | 102 | CLA  | MG-NB   | -2.26 | 2.01        | 2.05     |
| 31  | B     | 834 | CLA  | CMB-C2B | -2.26 | 1.46        | 1.50     |
| 31  | 9     | 303 | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |
| 31  | J     | 103 | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |
| 31  | 0     | 313 | CLA  | MG-NB   | -2.26 | 2.01        | 2.05     |
| 31  | 0     | 303 | CLA  | CMD-C2D | -2.26 | 1.46        | 1.50     |
| 31  | 0     | 308 | CLA  | CMB-C2B | -2.26 | 1.46        | 1.50     |
| 34  | 5     | 601 | LHG  | O8-C23  | 2.26  | 1.39        | 1.33     |
| 34  | A     | 845 | LHG  | O7-C7   | 2.26  | 1.40        | 1.34     |
| 31  | 6     | 318 | CLA  | MG-NB   | -2.26 | 2.01        | 2.05     |
| 31  | c     | 613 | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |
| 31  | 1     | 309 | CLA  | CHC-C1C | 2.26  | 1.43        | 1.38     |
| 31  | c     | 611 | CLA  | CHC-C1C | 2.26  | 1.43        | 1.38     |
| 37  | h     | 521 | 0IE  | C17-C16 | -2.26 | 1.41        | 1.46     |
| 31  | 1     | 311 | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |
| 37  | a     | 521 | 0IE  | C8-C7   | 2.26  | 1.41        | 1.35     |
| 34  | 7     | 603 | LHG  | O8-C23  | 2.26  | 1.39        | 1.33     |
| 31  | B     | 811 | CLA  | CMB-C2B | -2.26 | 1.46        | 1.50     |
| 31  | A     | 834 | CLA  | MG-NB   | -2.26 | 2.01        | 2.05     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | B     | 801 | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |
| 31  | O     | 206 | CLA  | CHC-C1C | 2.26  | 1.43        | 1.38     |
| 31  | f     | 613 | CLA  | CHC-C1C | 2.26  | 1.43        | 1.38     |
| 31  | B     | 823 | CLA  | MG-NB   | -2.26 | 2.01        | 2.05     |
| 31  | h     | 612 | CLA  | CHC-C1C | 2.26  | 1.43        | 1.38     |
| 31  | c     | 612 | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |
| 31  | 5     | 303 | CLA  | CMD-C2D | -2.26 | 1.46        | 1.50     |
| 31  | a     | 612 | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |
| 34  | 7     | 601 | LHG  | O7-C7   | 2.26  | 1.40        | 1.34     |
| 31  | 0     | 311 | CLA  | CMB-C2B | -2.26 | 1.46        | 1.50     |
| 31  | G     | 103 | CLA  | MG-NB   | -2.26 | 2.01        | 2.05     |
| 31  | 5     | 314 | CLA  | CHC-C1C | 2.26  | 1.43        | 1.38     |
| 30  | 4     | 313 | CHL  | CBD-CGD | -2.26 | 1.49        | 1.52     |
| 31  | K     | 101 | CLA  | MG-NB   | -2.26 | 2.01        | 2.05     |
| 31  | 3     | 310 | CLA  | CMB-C2B | -2.25 | 1.46        | 1.50     |
| 31  | A     | 821 | CLA  | CMB-C2B | -2.25 | 1.46        | 1.50     |
| 31  | h     | 603 | CLA  | C3B-C4B | 2.25  | 1.49        | 1.42     |
| 31  | 3     | 309 | CLA  | CMB-C2B | -2.25 | 1.46        | 1.50     |
| 31  | 2     | 303 | CLA  | MG-NB   | -2.25 | 2.01        | 2.05     |
| 31  | 3     | 313 | CLA  | C3B-C4B | 2.25  | 1.49        | 1.42     |
| 31  | B     | 833 | CLA  | CMC-C2C | -2.25 | 1.46        | 1.50     |
| 32  | B     | 846 | 8CT  | C33-C32 | -2.25 | 1.44        | 1.50     |
| 31  | A     | 834 | CLA  | CMD-C2D | -2.25 | 1.46        | 1.50     |
| 37  | f     | 521 | 0IE  | C8-C7   | 2.25  | 1.41        | 1.35     |
| 31  | A     | 802 | CLA  | MG-NB   | -2.25 | 2.01        | 2.05     |
| 31  | g     | 612 | CLA  | CHC-C1C | 2.25  | 1.43        | 1.38     |
| 31  | 8     | 303 | CLA  | C3B-C4B | 2.25  | 1.49        | 1.42     |
| 31  | b     | 604 | CLA  | C3B-C4B | 2.25  | 1.49        | 1.42     |
| 31  | A     | 840 | CLA  | CMD-C2D | -2.25 | 1.46        | 1.50     |
| 31  | b     | 612 | CLA  | C3B-C4B | 2.25  | 1.49        | 1.42     |
| 31  | a     | 611 | CLA  | CHC-C1C | 2.25  | 1.43        | 1.38     |
| 34  | f     | 630 | LHG  | O8-C23  | 2.25  | 1.39        | 1.33     |
| 31  | 4     | 311 | CLA  | CMD-C2D | -2.25 | 1.46        | 1.50     |
| 31  | 3     | 310 | CLA  | C3B-C4B | 2.25  | 1.49        | 1.42     |
| 31  | G     | 103 | CLA  | C3B-C4B | 2.25  | 1.49        | 1.42     |
| 31  | g     | 613 | CLA  | C3B-C4B | 2.25  | 1.49        | 1.42     |
| 34  | a     | 630 | LHG  | O7-C5   | -2.25 | 1.41        | 1.46     |
| 31  | g     | 603 | CLA  | CHC-C1C | 2.25  | 1.43        | 1.38     |
| 34  | c     | 630 | LHG  | O7-C7   | 2.25  | 1.40        | 1.34     |
| 31  | b     | 604 | CLA  | CMB-C2B | -2.25 | 1.46        | 1.50     |
| 31  | 3     | 304 | CLA  | MG-NB   | -2.25 | 2.01        | 2.05     |
| 31  | A     | 817 | CLA  | CMD-C2D | -2.25 | 1.46        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 4     | 303 | CLA  | CMD-C2D | -2.25 | 1.46        | 1.50     |
| 31  | 0     | 311 | CLA  | MG-NB   | -2.25 | 2.01        | 2.05     |
| 31  | B     | 825 | CLA  | MG-NB   | -2.25 | 2.01        | 2.05     |
| 31  | 7     | 311 | CLA  | C3B-C4B | 2.25  | 1.49        | 1.42     |
| 31  | A     | 831 | CLA  | CMD-C2D | -2.25 | 1.46        | 1.50     |
| 31  | B     | 807 | CLA  | CHC-C1C | 2.25  | 1.43        | 1.38     |
| 31  | c     | 603 | CLA  | C3B-C4B | 2.25  | 1.49        | 1.42     |
| 37  | c     | 522 | 0IE  | C8-C7   | 2.25  | 1.41        | 1.35     |
| 31  | 4     | 314 | CLA  | C3B-C4B | 2.25  | 1.49        | 1.42     |
| 37  | e     | 522 | 0IE  | C11-C12 | 2.25  | 1.41        | 1.35     |
| 31  | 1     | 304 | CLA  | MG-NB   | -2.25 | 2.01        | 2.05     |
| 31  | B     | 826 | CLA  | MG-NB   | -2.25 | 2.01        | 2.05     |
| 31  | B     | 840 | CLA  | MG-NB   | -2.25 | 2.01        | 2.05     |
| 31  | c     | 611 | CLA  | C3B-C4B | 2.25  | 1.49        | 1.42     |
| 30  | 7     | 305 | CHL  | CBD-CGD | -2.25 | 1.49        | 1.52     |
| 37  | e     | 522 | 0IE  | C17-C16 | -2.25 | 1.41        | 1.46     |
| 32  | B     | 851 | 8CT  | C33-C32 | -2.25 | 1.44        | 1.50     |
| 31  | 9     | 300 | CLA  | MG-NB   | -2.25 | 2.01        | 2.05     |
| 31  | B     | 805 | CLA  | MG-NB   | -2.25 | 2.01        | 2.05     |
| 31  | 9     | 300 | CLA  | CMD-C2D | -2.25 | 1.46        | 1.50     |
| 31  | 3     | 312 | CLA  | C3B-C4B | 2.25  | 1.49        | 1.42     |
| 31  | 6     | 309 | CLA  | C3B-C4B | 2.24  | 1.49        | 1.42     |
| 31  | A     | 826 | CLA  | C3B-C4B | 2.24  | 1.49        | 1.42     |
| 31  | A     | 827 | CLA  | CMD-C2D | -2.24 | 1.46        | 1.50     |
| 34  | 6     | 601 | LHG  | O8-C23  | 2.24  | 1.39        | 1.33     |
| 31  | A     | 810 | CLA  | CHC-C1C | 2.24  | 1.43        | 1.38     |
| 31  | A     | 826 | CLA  | CHC-C1C | 2.24  | 1.43        | 1.38     |
| 31  | 9     | 304 | CLA  | MG-NB   | -2.24 | 2.01        | 2.05     |
| 31  | B     | 811 | CLA  | MG-NB   | -2.24 | 2.01        | 2.05     |
| 37  | c     | 522 | 0IE  | C6-C7   | -2.24 | 1.41        | 1.46     |
| 31  | b     | 613 | CLA  | CHC-C1C | 2.24  | 1.43        | 1.38     |
| 31  | M     | 101 | CLA  | MG-NB   | -2.24 | 2.01        | 2.05     |
| 31  | O     | 201 | CLA  | MG-NB   | -2.24 | 2.01        | 2.05     |
| 31  | G     | 101 | CLA  | CHC-C1C | 2.24  | 1.43        | 1.38     |
| 31  | 7     | 311 | CLA  | CMC-C2C | -2.24 | 1.46        | 1.50     |
| 31  | K     | 101 | CLA  | CMD-C2D | -2.24 | 1.46        | 1.50     |
| 31  | 6     | 304 | CLA  | MG-NB   | -2.24 | 2.01        | 2.05     |
| 31  | 6     | 309 | CLA  | MG-NB   | -2.24 | 2.01        | 2.05     |
| 31  | 0     | 310 | CLA  | MG-NB   | -2.24 | 2.01        | 2.05     |
| 31  | 7     | 312 | CLA  | MG-NB   | -2.24 | 2.01        | 2.05     |
| 31  | B     | 835 | CLA  | MG-NB   | -2.24 | 2.01        | 2.05     |
| 31  | O     | 202 | CLA  | CHC-C1C | 2.24  | 1.43        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 5     | 309 | CLA  | CMB-C2B | -2.24 | 1.46        | 1.50     |
| 37  | f     | 522 | 0IE  | C13-C12 | -2.24 | 1.41        | 1.46     |
| 31  | K     | 102 | CLA  | CMD-C2D | -2.24 | 1.46        | 1.50     |
| 37  | h     | 521 | 0IE  | C13-C12 | -2.24 | 1.41        | 1.46     |
| 31  | A     | 838 | CLA  | CMB-C2B | -2.24 | 1.46        | 1.50     |
| 31  | B     | 809 | CLA  | CMB-C2B | -2.24 | 1.46        | 1.50     |
| 31  | G     | 102 | CLA  | CMD-C2D | -2.24 | 1.46        | 1.50     |
| 30  | 3     | 302 | CHL  | CBD-CGD | -2.24 | 1.49        | 1.52     |
| 31  | A     | 822 | CLA  | MG-NB   | -2.24 | 2.01        | 2.05     |
| 31  | B     | 828 | CLA  | MG-NB   | -2.24 | 2.01        | 2.05     |
| 31  | c     | 604 | CLA  | C3B-C4B | 2.24  | 1.49        | 1.42     |
| 31  | 2     | 304 | CLA  | CMD-C2D | -2.24 | 1.46        | 1.50     |
| 31  | 3     | 308 | CLA  | CMB-C2B | -2.24 | 1.46        | 1.50     |
| 31  | B     | 803 | CLA  | CMD-C2D | -2.24 | 1.46        | 1.50     |
| 31  | 9     | 309 | CLA  | CHC-C1C | 2.24  | 1.43        | 1.38     |
| 30  | 7     | 307 | CHL  | CBD-CGD | -2.24 | 1.49        | 1.52     |
| 34  | B     | 854 | LHG  | O8-C23  | 2.24  | 1.39        | 1.33     |
| 31  | L     | 202 | CLA  | MG-NB   | -2.24 | 2.01        | 2.05     |
| 31  | 8     | 310 | CLA  | MG-NB   | -2.24 | 2.01        | 2.05     |
| 31  | 7     | 315 | CLA  | CMC-C2C | -2.24 | 1.46        | 1.50     |
| 31  | A     | 803 | CLA  | CMC-C2C | -2.24 | 1.46        | 1.50     |
| 31  | B     | 834 | CLA  | MG-NB   | -2.24 | 2.01        | 2.05     |
| 31  | B     | 825 | CLA  | CMD-C2D | -2.24 | 1.46        | 1.50     |
| 31  | 1     | 304 | CLA  | CHC-C1C | 2.24  | 1.43        | 1.38     |
| 31  | B     | 808 | CLA  | MG-NB   | -2.24 | 2.01        | 2.05     |
| 31  | 2     | 309 | CLA  | C3B-C4B | 2.24  | 1.49        | 1.42     |
| 31  | f     | 604 | CLA  | C3B-C4B | 2.24  | 1.49        | 1.42     |
| 31  | 8     | 309 | CLA  | CMD-C2D | -2.24 | 1.46        | 1.50     |
| 34  | c     | 630 | LHG  | O8-C23  | 2.24  | 1.39        | 1.33     |
| 31  | 0     | 303 | CLA  | MG-NB   | -2.24 | 2.01        | 2.05     |
| 31  | B     | 837 | CLA  | MG-NB   | -2.24 | 2.01        | 2.05     |
| 34  | 9     | 601 | LHG  | O8-C23  | 2.24  | 1.39        | 1.33     |
| 31  | 0     | 310 | CLA  | C3B-C4B | 2.24  | 1.49        | 1.42     |
| 31  | 7     | 304 | CLA  | CMD-C2D | -2.24 | 1.46        | 1.50     |
| 31  | A     | 812 | CLA  | CMD-C2D | -2.24 | 1.46        | 1.50     |
| 31  | B     | 829 | CLA  | CHC-C1C | 2.24  | 1.43        | 1.38     |
| 36  | L     | 211 | LMG  | O7-C8   | -2.23 | 1.41        | 1.46     |
| 32  | A     | 847 | 8CT  | C33-C32 | -2.23 | 1.44        | 1.50     |
| 31  | A     | 835 | CLA  | C3B-C4B | 2.23  | 1.49        | 1.42     |
| 31  | 7     | 308 | CLA  | CMD-C2D | -2.23 | 1.46        | 1.50     |
| 31  | 1     | 308 | CLA  | C3B-C4B | 2.23  | 1.49        | 1.42     |
| 31  | 5     | 310 | CLA  | C3B-C4B | 2.23  | 1.49        | 1.42     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | L     | 201 | CLA  | CMB-C2B | -2.23 | 1.46        | 1.50     |
| 31  | A     | 803 | CLA  | CMD-C2D | -2.23 | 1.46        | 1.50     |
| 34  | b     | 630 | LHG  | O7-C7   | 2.23  | 1.40        | 1.34     |
| 31  | A     | 806 | CLA  | C3B-C4B | 2.23  | 1.49        | 1.42     |
| 30  | 7     | 302 | CHL  | CBD-CGD | -2.23 | 1.49        | 1.52     |
| 37  | i     | 522 | 0IE  | C6-C7   | -2.23 | 1.41        | 1.46     |
| 31  | 8     | 303 | CLA  | MG-NB   | -2.23 | 2.01        | 2.05     |
| 31  | A     | 835 | CLA  | CMB-C2B | -2.23 | 1.46        | 1.50     |
| 31  | 2     | 303 | CLA  | C3B-C4B | 2.23  | 1.49        | 1.42     |
| 31  | 3     | 309 | CLA  | CMD-C2D | -2.23 | 1.46        | 1.50     |
| 31  | A     | 814 | CLA  | CMB-C2B | -2.23 | 1.46        | 1.50     |
| 31  | A     | 824 | CLA  | CMB-C2B | -2.23 | 1.46        | 1.50     |
| 31  | 7     | 308 | CLA  | MG-NB   | -2.23 | 2.01        | 2.05     |
| 31  | G     | 101 | CLA  | MG-NB   | -2.23 | 2.01        | 2.05     |
| 31  | A     | 811 | CLA  | CMB-C2B | -2.23 | 1.46        | 1.50     |
| 31  | A     | 813 | CLA  | CMC-C2C | -2.23 | 1.46        | 1.50     |
| 31  | 4     | 314 | CLA  | MG-NB   | -2.23 | 2.01        | 2.05     |
| 31  | 0     | 309 | CLA  | CHC-C1C | 2.23  | 1.43        | 1.38     |
| 31  | d     | 611 | CLA  | CHC-C1C | 2.23  | 1.43        | 1.38     |
| 31  | d     | 604 | CLA  | CHC-C1C | 2.23  | 1.43        | 1.38     |
| 31  | f     | 611 | CLA  | C3B-C4B | 2.23  | 1.49        | 1.42     |
| 34  | 6     | 603 | LHG  | O7-C7   | 2.23  | 1.40        | 1.34     |
| 31  | A     | 815 | CLA  | CMD-C2D | -2.23 | 1.46        | 1.50     |
| 31  | B     | 837 | CLA  | C3B-C4B | 2.23  | 1.49        | 1.42     |
| 31  | 1     | 312 | CLA  | CMD-C2D | -2.23 | 1.46        | 1.50     |
| 31  | 6     | 303 | CLA  | CMC-C2C | -2.23 | 1.46        | 1.50     |
| 31  | 9     | 302 | CLA  | MG-NB   | -2.23 | 2.01        | 2.05     |
| 31  | A     | 808 | CLA  | CMB-C2B | -2.23 | 1.46        | 1.50     |
| 31  | 4     | 311 | CLA  | CMC-C2C | -2.23 | 1.46        | 1.50     |
| 32  | I     | 101 | 8CT  | C33-C32 | -2.23 | 1.44        | 1.50     |
| 37  | f     | 522 | 0IE  | C6-C7   | -2.23 | 1.41        | 1.46     |
| 31  | 7     | 311 | CLA  | CMB-C2B | -2.23 | 1.46        | 1.50     |
| 31  | A     | 805 | CLA  | CMD-C2D | -2.23 | 1.46        | 1.50     |
| 37  | e     | 521 | 0IE  | C8-C7   | 2.23  | 1.40        | 1.35     |
| 31  | 5     | 311 | CLA  | MG-NB   | -2.23 | 2.01        | 2.05     |
| 31  | 6     | 310 | CLA  | MG-NB   | -2.23 | 2.01        | 2.05     |
| 31  | L     | 204 | CLA  | MG-NB   | -2.23 | 2.01        | 2.05     |
| 31  | 7     | 304 | CLA  | C3B-C4B | 2.23  | 1.49        | 1.42     |
| 31  | g     | 611 | CLA  | CHC-C1C | 2.23  | 1.42        | 1.38     |
| 31  | 5     | 314 | CLA  | CMD-C2D | -2.23 | 1.46        | 1.50     |
| 31  | 2     | 314 | CLA  | C3B-C4B | 2.23  | 1.49        | 1.42     |
| 31  | 7     | 309 | CLA  | CHC-C1C | 2.23  | 1.42        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | J     | 103 | CLA  | CHC-C1C | 2.23  | 1.42        | 1.38     |
| 31  | c     | 610 | CLA  | CHC-C1C | 2.23  | 1.42        | 1.38     |
| 31  | g     | 604 | CLA  | CHC-C1C | 2.23  | 1.42        | 1.38     |
| 37  | e     | 521 | 0IE  | C15-C16 | 2.23  | 1.40        | 1.35     |
| 31  | 5     | 310 | CLA  | MG-NB   | -2.23 | 2.01        | 2.05     |
| 31  | A     | 803 | CLA  | C3B-C4B | 2.22  | 1.49        | 1.42     |
| 31  | B     | 826 | CLA  | C3B-C4B | 2.22  | 1.49        | 1.42     |
| 37  | g     | 521 | 0IE  | C15-C16 | 2.22  | 1.40        | 1.35     |
| 31  | A     | 804 | CLA  | CHC-C1C | 2.22  | 1.42        | 1.38     |
| 31  | 0     | 309 | CLA  | MG-NB   | -2.22 | 2.01        | 2.05     |
| 31  | A     | 838 | CLA  | CMD-C2D | -2.22 | 1.46        | 1.50     |
| 37  | i     | 521 | 0IE  | C13-C12 | -2.22 | 1.41        | 1.46     |
| 31  | i     | 612 | CLA  | CHC-C1C | 2.22  | 1.42        | 1.38     |
| 31  | 6     | 311 | CLA  | CMD-C2D | -2.22 | 1.46        | 1.50     |
| 31  | B     | 841 | CLA  | CHC-C1C | 2.22  | 1.42        | 1.38     |
| 31  | B     | 832 | CLA  | CMB-C2B | -2.22 | 1.46        | 1.50     |
| 31  | 1     | 309 | CLA  | MG-NB   | -2.22 | 2.01        | 2.05     |
| 34  | 6     | 601 | LHG  | O7-C7   | 2.22  | 1.40        | 1.34     |
| 31  | 0     | 308 | CLA  | MG-NB   | -2.22 | 2.01        | 2.05     |
| 31  | 1     | 312 | CLA  | MG-NB   | -2.22 | 2.01        | 2.05     |
| 31  | B     | 807 | CLA  | MG-NB   | -2.22 | 2.01        | 2.05     |
| 31  | 3     | 318 | CLA  | C3B-C4B | 2.22  | 1.49        | 1.42     |
| 31  | O     | 202 | CLA  | CMD-C2D | -2.22 | 1.46        | 1.50     |
| 34  | G     | 105 | LHG  | O7-C7   | 2.22  | 1.40        | 1.34     |
| 31  | 6     | 309 | CLA  | CMD-C2D | -2.22 | 1.46        | 1.50     |
| 31  | A     | 852 | CLA  | CMB-C2B | -2.22 | 1.46        | 1.50     |
| 31  | A     | 825 | CLA  | CMD-C2D | -2.22 | 1.46        | 1.50     |
| 31  | i     | 603 | CLA  | CHC-C1C | 2.22  | 1.42        | 1.38     |
| 32  | L     | 206 | 8CT  | C33-C32 | -2.22 | 1.44        | 1.50     |
| 34  | 9     | 601 | LHG  | O7-C7   | 2.22  | 1.40        | 1.34     |
| 31  | A     | 816 | CLA  | C3B-C4B | 2.22  | 1.49        | 1.42     |
| 31  | 3     | 313 | CLA  | MG-NB   | -2.22 | 2.01        | 2.05     |
| 31  | A     | 828 | CLA  | MG-NB   | -2.22 | 2.01        | 2.05     |
| 31  | B     | 803 | CLA  | MG-NB   | -2.22 | 2.01        | 2.05     |
| 31  | B     | 814 | CLA  | CMD-C2D | -2.22 | 1.46        | 1.50     |
| 30  | 0     | 301 | CHL  | CBD-CGD | -2.22 | 1.49        | 1.52     |
| 30  | 2     | 307 | CHL  | CBD-CGD | -2.22 | 1.49        | 1.52     |
| 31  | 3     | 311 | CLA  | MG-NB   | -2.22 | 2.01        | 2.05     |
| 31  | 6     | 312 | CLA  | CMD-C2D | -2.22 | 1.46        | 1.50     |
| 31  | A     | 853 | CLA  | CMB-C2B | -2.22 | 1.46        | 1.50     |
| 31  | B     | 810 | CLA  | CMD-C2D | -2.22 | 1.46        | 1.50     |
| 31  | B     | 838 | CLA  | CMD-C2D | -2.22 | 1.46        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 3     | 320 | CLA  | MG-NB   | -2.22 | 2.01        | 2.05     |
| 31  | A     | 813 | CLA  | CMB-C2B | -2.22 | 1.46        | 1.50     |
| 31  | A     | 839 | CLA  | CMB-C2B | -2.22 | 1.46        | 1.50     |
| 31  | H     | 204 | CLA  | CMB-C2B | -2.22 | 1.46        | 1.50     |
| 37  | e     | 522 | 0IE  | C13-C12 | -2.22 | 1.41        | 1.46     |
| 31  | G     | 103 | CLA  | CHC-C1C | 2.22  | 1.42        | 1.38     |
| 31  | 3     | 311 | CLA  | C3B-C4B | 2.22  | 1.49        | 1.42     |
| 31  | 6     | 317 | CLA  | C3B-C4B | 2.22  | 1.49        | 1.42     |
| 30  | 4     | 307 | CHL  | CBD-CGD | -2.22 | 1.49        | 1.52     |
| 31  | 0     | 321 | CLA  | CMB-C2B | -2.22 | 1.46        | 1.50     |
| 31  | f     | 612 | CLA  | C3B-C4B | 2.22  | 1.49        | 1.42     |
| 31  | F     | 301 | CLA  | C3B-C4B | 2.22  | 1.49        | 1.42     |
| 31  | A     | 806 | CLA  | CMD-C2D | -2.22 | 1.46        | 1.50     |
| 31  | K     | 105 | CLA  | CMB-C2B | -2.22 | 1.46        | 1.50     |
| 31  | A     | 827 | CLA  | C3B-C4B | 2.22  | 1.49        | 1.42     |
| 31  | 1     | 311 | CLA  | MG-NB   | -2.22 | 2.01        | 2.05     |
| 31  | 3     | 304 | CLA  | CMD-C2D | -2.22 | 1.46        | 1.50     |
| 30  | 6     | 306 | CHL  | CBD-CGD | -2.22 | 1.49        | 1.52     |
| 31  | c     | 611 | CLA  | CMB-C2B | -2.21 | 1.46        | 1.50     |
| 31  | G     | 101 | CLA  | C3B-C4B | 2.21  | 1.49        | 1.42     |
| 31  | A     | 832 | CLA  | CMB-C2B | -2.21 | 1.46        | 1.50     |
| 31  | A     | 832 | CLA  | CMD-C2D | -2.21 | 1.46        | 1.50     |
| 31  | B     | 836 | CLA  | CMD-C2D | -2.21 | 1.46        | 1.50     |
| 31  | B     | 816 | CLA  | MG-NB   | -2.21 | 2.01        | 2.05     |
| 31  | 9     | 311 | CLA  | CHC-C1C | 2.21  | 1.42        | 1.38     |
| 31  | B     | 803 | CLA  | CHC-C1C | 2.21  | 1.42        | 1.38     |
| 31  | b     | 611 | CLA  | CHC-C1C | 2.21  | 1.42        | 1.38     |
| 31  | 9     | 302 | CLA  | C3B-C4B | 2.21  | 1.49        | 1.42     |
| 31  | A     | 824 | CLA  | C3B-C4B | 2.21  | 1.49        | 1.42     |
| 31  | 7     | 310 | CLA  | MG-NB   | -2.21 | 2.01        | 2.05     |
| 32  | 8     | 406 | 8CT  | C33-C32 | -2.21 | 1.44        | 1.50     |
| 31  | d     | 603 | CLA  | C3B-C4B | 2.21  | 1.49        | 1.42     |
| 31  | G     | 101 | CLA  | CMC-C2C | -2.21 | 1.46        | 1.50     |
| 31  | e     | 611 | CLA  | CHC-C1C | 2.21  | 1.42        | 1.38     |
| 37  | b     | 521 | 0IE  | C15-C16 | 2.21  | 1.40        | 1.35     |
| 31  | e     | 603 | CLA  | C3B-C4B | 2.21  | 1.49        | 1.42     |
| 37  | c     | 522 | 0IE  | C17-C16 | -2.21 | 1.41        | 1.46     |
| 31  | 3     | 318 | CLA  | CMD-C2D | -2.21 | 1.46        | 1.50     |
| 31  | B     | 826 | CLA  | C3D-C4D | 2.21  | 1.47        | 1.42     |
| 31  | B     | 826 | CLA  | CHC-C1C | 2.21  | 1.42        | 1.38     |
| 37  | d     | 522 | 0IE  | C17-C16 | -2.21 | 1.41        | 1.46     |
| 31  | K     | 105 | CLA  | C3B-C4B | 2.21  | 1.49        | 1.42     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | A     | 806 | CLA  | CHC-C1C | 2.21  | 1.42        | 1.38     |
| 31  | 3     | 311 | CLA  | CMD-C2D | -2.21 | 1.46        | 1.50     |
| 31  | 6     | 311 | CLA  | CMC-C2C | -2.21 | 1.46        | 1.50     |
| 31  | 0     | 310 | CLA  | CHC-C1C | 2.21  | 1.42        | 1.38     |
| 31  | 6     | 320 | CLA  | C3B-C4B | 2.21  | 1.49        | 1.42     |
| 31  | a     | 603 | CLA  | C3B-C4B | 2.21  | 1.49        | 1.42     |
| 31  | 3     | 310 | CLA  | CMD-C2D | -2.21 | 1.46        | 1.50     |
| 31  | 8     | 312 | CLA  | MG-NB   | -2.21 | 2.01        | 2.05     |
| 31  | B     | 850 | CLA  | CHC-C1C | 2.21  | 1.42        | 1.38     |
| 37  | i     | 522 | 0IE  | C13-C12 | -2.21 | 1.41        | 1.46     |
| 31  | B     | 825 | CLA  | C3B-C4B | 2.21  | 1.49        | 1.42     |
| 31  | 2     | 309 | CLA  | CMD-C2D | -2.21 | 1.46        | 1.50     |
| 31  | 9     | 312 | CLA  | CHC-C1C | 2.21  | 1.42        | 1.38     |
| 31  | c     | 603 | CLA  | CHC-C1C | 2.21  | 1.42        | 1.38     |
| 34  | 2     | 601 | LHG  | O7-C7   | 2.21  | 1.40        | 1.34     |
| 31  | B     | 813 | CLA  | CMB-C2B | -2.21 | 1.46        | 1.50     |
| 31  | B     | 832 | CLA  | CMD-C2D | -2.21 | 1.46        | 1.50     |
| 34  | 4     | 601 | LHG  | O8-C23  | 2.21  | 1.39        | 1.33     |
| 31  | 3     | 304 | CLA  | CMC-C2C | -2.21 | 1.46        | 1.50     |
| 31  | 3     | 313 | CLA  | CMD-C2D | -2.21 | 1.46        | 1.50     |
| 31  | 7     | 309 | CLA  | CMD-C2D | -2.21 | 1.46        | 1.50     |
| 31  | A     | 837 | CLA  | CMD-C2D | -2.21 | 1.46        | 1.50     |
| 31  | 1     | 303 | CLA  | MG-NB   | -2.21 | 2.01        | 2.05     |
| 31  | i     | 611 | CLA  | CHC-C1C | 2.21  | 1.42        | 1.38     |
| 34  | B     | 854 | LHG  | O7-C7   | 2.21  | 1.40        | 1.34     |
| 31  | B     | 818 | CLA  | CMB-C2B | -2.21 | 1.46        | 1.50     |
| 37  | f     | 521 | 0IE  | C15-C16 | 2.21  | 1.40        | 1.35     |
| 30  | 2     | 305 | CHL  | CBD-CGD | -2.21 | 1.49        | 1.52     |
| 31  | A     | 820 | CLA  | MG-NB   | -2.21 | 2.01        | 2.05     |
| 31  | B     | 833 | CLA  | C3B-C4B | 2.21  | 1.49        | 1.42     |
| 31  | 5     | 303 | CLA  | CMB-C2B | -2.21 | 1.46        | 1.50     |
| 31  | 7     | 312 | CLA  | CMB-C2B | -2.21 | 1.46        | 1.50     |
| 31  | A     | 830 | CLA  | CMC-C2C | -2.21 | 1.46        | 1.50     |
| 31  | B     | 811 | CLA  | CMC-C2C | -2.21 | 1.46        | 1.50     |
| 31  | b     | 613 | CLA  | MG-NB   | -2.21 | 2.01        | 2.05     |
| 31  | d     | 603 | CLA  | CHC-C1C | 2.21  | 1.42        | 1.38     |
| 31  | 3     | 311 | CLA  | CMC-C2C | -2.21 | 1.46        | 1.50     |
| 31  | 9     | 302 | CLA  | CHC-C1C | 2.21  | 1.42        | 1.38     |
| 31  | 8     | 312 | CLA  | CMB-C2B | -2.21 | 1.46        | 1.50     |
| 37  | a     | 522 | 0IE  | C6-C7   | -2.21 | 1.41        | 1.46     |
| 31  | B     | 817 | CLA  | MG-NB   | -2.21 | 2.01        | 2.05     |
| 31  | L     | 204 | CLA  | CHC-C1C | 2.21  | 1.42        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 32  | A     | 854 | 8CT  | C33-C32 | -2.21 | 1.44        | 1.50     |
| 31  | 7     | 309 | CLA  | CMB-C2B | -2.21 | 1.46        | 1.50     |
| 31  | B     | 816 | CLA  | CMB-C2B | -2.21 | 1.46        | 1.50     |
| 31  | B     | 819 | CLA  | CMD-C2D | -2.21 | 1.46        | 1.50     |
| 37  | i     | 521 | 0IE  | C6-C7   | -2.21 | 1.41        | 1.46     |
| 31  | 2     | 309 | CLA  | MG-NB   | -2.20 | 2.01        | 2.05     |
| 31  | B     | 815 | CLA  | CHC-C1C | 2.20  | 1.42        | 1.38     |
| 31  | H     | 205 | CLA  | CHC-C1C | 2.20  | 1.42        | 1.38     |
| 31  | e     | 612 | CLA  | CHC-C1C | 2.20  | 1.42        | 1.38     |
| 31  | 9     | 311 | CLA  | CMB-C2B | -2.20 | 1.46        | 1.50     |
| 31  | 8     | 311 | CLA  | MG-NB   | -2.20 | 2.01        | 2.05     |
| 31  | A     | 827 | CLA  | CHC-C1C | 2.20  | 1.42        | 1.38     |
| 31  | h     | 611 | CLA  | CHC-C1C | 2.20  | 1.42        | 1.38     |
| 34  | 4     | 601 | LHG  | O7-C7   | 2.20  | 1.40        | 1.34     |
| 31  | A     | 828 | CLA  | C3B-C4B | 2.20  | 1.49        | 1.42     |
| 31  | M     | 101 | CLA  | C3B-C4B | 2.20  | 1.49        | 1.42     |
| 31  | 6     | 320 | CLA  | MG-NB   | -2.20 | 2.01        | 2.05     |
| 31  | B     | 815 | CLA  | MG-NB   | -2.20 | 2.01        | 2.05     |
| 31  | 1     | 314 | CLA  | CMD-C2D | -2.20 | 1.46        | 1.50     |
| 32  | B     | 843 | 8CT  | C33-C32 | -2.20 | 1.44        | 1.50     |
| 34  | 3     | 603 | LHG  | O7-C7   | 2.20  | 1.40        | 1.34     |
| 37  | f     | 522 | 0IE  | C17-C16 | -2.20 | 1.41        | 1.46     |
| 31  | A     | 843 | CLA  | C3B-C4B | 2.20  | 1.49        | 1.42     |
| 31  | B     | 836 | CLA  | CHC-C1C | 2.20  | 1.42        | 1.38     |
| 31  | A     | 806 | CLA  | CMB-C2B | -2.20 | 1.46        | 1.50     |
| 31  | A     | 808 | CLA  | CMD-C2D | -2.20 | 1.46        | 1.50     |
| 31  | A     | 818 | CLA  | CMD-C2D | -2.20 | 1.46        | 1.50     |
| 31  | A     | 820 | CLA  | CMB-C2B | -2.20 | 1.46        | 1.50     |
| 31  | 6     | 304 | CLA  | C3B-C4B | 2.20  | 1.49        | 1.42     |
| 31  | K     | 102 | CLA  | C3B-C4B | 2.20  | 1.49        | 1.42     |
| 31  | 4     | 312 | CLA  | CMD-C2D | -2.20 | 1.46        | 1.50     |
| 31  | B     | 839 | CLA  | C3B-C4B | 2.20  | 1.49        | 1.42     |
| 34  | 0     | 601 | LHG  | O8-C23  | 2.20  | 1.39        | 1.33     |
| 31  | 9     | 310 | CLA  | MG-NB   | -2.20 | 2.01        | 2.05     |
| 31  | B     | 829 | CLA  | MG-NB   | -2.20 | 2.01        | 2.05     |
| 31  | 9     | 308 | CLA  | CMB-C2B | -2.20 | 1.46        | 1.50     |
| 31  | B     | 832 | CLA  | C3B-C4B | 2.20  | 1.49        | 1.42     |
| 31  | A     | 810 | CLA  | CMD-C2D | -2.20 | 1.46        | 1.50     |
| 31  | B     | 811 | CLA  | C3B-C4B | 2.20  | 1.49        | 1.42     |
| 31  | B     | 834 | CLA  | C3B-C4B | 2.20  | 1.49        | 1.42     |
| 32  | B     | 804 | 8CT  | C33-C32 | -2.20 | 1.44        | 1.50     |
| 31  | A     | 819 | CLA  | CMD-C2D | -2.20 | 1.46        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | A     | 819 | CLA  | C1B-C2B | 2.20  | 1.48        | 1.43     |
| 32  | 0     | 401 | 8CT  | C33-C32 | -2.20 | 1.44        | 1.50     |
| 31  | A     | 836 | CLA  | CMB-C2B | -2.20 | 1.46        | 1.50     |
| 31  | 4     | 304 | CLA  | MG-NB   | -2.20 | 2.01        | 2.05     |
| 34  | M     | 104 | LHG  | O7-C7   | 2.20  | 1.40        | 1.34     |
| 31  | B     | 839 | CLA  | CMB-C2B | -2.20 | 1.46        | 1.50     |
| 31  | B     | 828 | CLA  | C3B-C4B | 2.20  | 1.49        | 1.42     |
| 31  | B     | 824 | CLA  | CMB-C2B | -2.20 | 1.46        | 1.50     |
| 31  | K     | 104 | CLA  | CMD-C2D | -2.20 | 1.46        | 1.50     |
| 31  | 9     | 304 | CLA  | CMB-C2B | -2.20 | 1.46        | 1.50     |
| 31  | B     | 828 | CLA  | CMD-C2D | -2.20 | 1.46        | 1.50     |
| 31  | 6     | 309 | CLA  | CHC-C1C | 2.20  | 1.42        | 1.38     |
| 37  | a     | 521 | 0IE  | C15-C16 | 2.20  | 1.40        | 1.35     |
| 31  | 6     | 303 | CLA  | CMD-C2D | -2.20 | 1.46        | 1.50     |
| 31  | 6     | 311 | CLA  | CMB-C2B | -2.20 | 1.46        | 1.50     |
| 31  | B     | 816 | CLA  | CMC-C2C | -2.20 | 1.46        | 1.50     |
| 31  | e     | 604 | CLA  | C3B-C4B | 2.20  | 1.49        | 1.42     |
| 31  | f     | 613 | CLA  | CMD-C2D | -2.20 | 1.46        | 1.50     |
| 31  | 7     | 311 | CLA  | MG-NB   | -2.20 | 2.01        | 2.05     |
| 31  | A     | 829 | CLA  | C3B-C4B | 2.20  | 1.49        | 1.42     |
| 31  | 4     | 304 | CLA  | C3B-C4B | 2.20  | 1.49        | 1.42     |
| 34  | K     | 106 | LHG  | O7-C7   | 2.20  | 1.40        | 1.34     |
| 37  | e     | 521 | 0IE  | C11-C12 | 2.20  | 1.40        | 1.35     |
| 31  | B     | 833 | CLA  | CHC-C1C | 2.20  | 1.42        | 1.38     |
| 31  | A     | 815 | CLA  | CMB-C2B | -2.20 | 1.46        | 1.50     |
| 31  | 4     | 312 | CLA  | CMB-C2B | -2.20 | 1.46        | 1.50     |
| 31  | 5     | 312 | CLA  | MG-NB   | -2.20 | 2.01        | 2.05     |
| 31  | A     | 852 | CLA  | C3B-C4B | 2.20  | 1.49        | 1.42     |
| 31  | 5     | 312 | CLA  | CMC-C2C | -2.19 | 1.46        | 1.50     |
| 31  | 7     | 303 | CLA  | CMB-C2B | -2.19 | 1.46        | 1.50     |
| 31  | 9     | 308 | CLA  | CMD-C2D | -2.19 | 1.46        | 1.50     |
| 31  | A     | 829 | CLA  | CMB-C2B | -2.19 | 1.46        | 1.50     |
| 31  | b     | 613 | CLA  | CMD-C2D | -2.19 | 1.46        | 1.50     |
| 37  | a     | 522 | 0IE  | C17-C16 | -2.19 | 1.41        | 1.46     |
| 31  | K     | 104 | CLA  | C3B-C4B | 2.19  | 1.49        | 1.42     |
| 31  | 0     | 312 | CLA  | CMB-C2B | -2.19 | 1.46        | 1.50     |
| 31  | H     | 205 | CLA  | MG-NB   | -2.19 | 2.01        | 2.05     |
| 32  | 8     | 402 | 8CT  | C33-C32 | -2.19 | 1.44        | 1.50     |
| 31  | 1     | 310 | CLA  | CMD-C2D | -2.19 | 1.46        | 1.50     |
| 31  | 8     | 314 | CLA  | CMD-C2D | -2.19 | 1.46        | 1.50     |
| 31  | B     | 809 | CLA  | CMD-C2D | -2.19 | 1.46        | 1.50     |
| 31  | 4     | 310 | CLA  | CMB-C2B | -2.19 | 1.46        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 5     | 312 | CLA  | C3B-C4B | 2.19  | 1.49        | 1.42     |
| 31  | F     | 301 | CLA  | CMB-C2B | -2.19 | 1.46        | 1.50     |
| 34  | 3     | 603 | LHG  | O8-C23  | 2.19  | 1.39        | 1.33     |
| 34  | 0     | 601 | LHG  | O7-C7   | 2.19  | 1.40        | 1.34     |
| 31  | A     | 821 | CLA  | C3B-C4B | 2.19  | 1.49        | 1.42     |
| 31  | G     | 102 | CLA  | C3B-C4B | 2.19  | 1.49        | 1.42     |
| 37  | h     | 521 | 0IE  | C6-C7   | -2.19 | 1.41        | 1.46     |
| 31  | 2     | 303 | CLA  | CMD-C2D | -2.19 | 1.46        | 1.50     |
| 31  | c     | 612 | CLA  | CHC-C1C | 2.19  | 1.42        | 1.38     |
| 31  | 2     | 314 | CLA  | MG-NB   | -2.19 | 2.01        | 2.05     |
| 31  | 8     | 311 | CLA  | CMD-C2D | -2.19 | 1.46        | 1.50     |
| 31  | B     | 806 | CLA  | CMD-C2D | -2.19 | 1.46        | 1.50     |
| 31  | 1     | 314 | CLA  | C3B-C4B | 2.19  | 1.49        | 1.42     |
| 31  | 8     | 314 | CLA  | C3B-C4B | 2.19  | 1.49        | 1.42     |
| 31  | L     | 204 | CLA  | C3B-C4B | 2.19  | 1.49        | 1.42     |
| 31  | A     | 813 | CLA  | CHC-C1C | 2.19  | 1.42        | 1.38     |
| 31  | 5     | 314 | CLA  | MG-NB   | -2.19 | 2.01        | 2.05     |
| 31  | f     | 611 | CLA  | CHC-C1C | 2.19  | 1.42        | 1.38     |
| 31  | B     | 803 | CLA  | C3B-C4B | 2.19  | 1.49        | 1.42     |
| 31  | A     | 853 | CLA  | MG-NB   | -2.19 | 2.01        | 2.05     |
| 31  | A     | 833 | CLA  | CMD-C2D | -2.19 | 1.46        | 1.50     |
| 31  | c     | 611 | CLA  | MG-NB   | -2.19 | 2.01        | 2.05     |
| 31  | f     | 611 | CLA  | MG-NB   | -2.19 | 2.01        | 2.05     |
| 31  | A     | 833 | CLA  | C3B-C4B | 2.19  | 1.49        | 1.42     |
| 31  | L     | 203 | CLA  | C3B-C4B | 2.19  | 1.49        | 1.42     |
| 31  | H     | 202 | CLA  | CHC-C1C | 2.19  | 1.42        | 1.38     |
| 31  | 8     | 314 | CLA  | MG-NB   | -2.19 | 2.01        | 2.05     |
| 31  | 3     | 320 | CLA  | CMB-C2B | -2.19 | 1.46        | 1.50     |
| 31  | 1     | 311 | CLA  | CMD-C2D | -2.19 | 1.46        | 1.50     |
| 31  | A     | 822 | CLA  | CMD-C2D | -2.19 | 1.46        | 1.50     |
| 31  | A     | 836 | CLA  | CMD-C2D | -2.19 | 1.46        | 1.50     |
| 31  | B     | 822 | CLA  | CMB-C2B | -2.19 | 1.46        | 1.50     |
| 31  | e     | 603 | CLA  | CHC-C1C | 2.19  | 1.42        | 1.38     |
| 31  | B     | 822 | CLA  | MG-NB   | -2.19 | 2.01        | 2.05     |
| 31  | B     | 816 | CLA  | C3B-C4B | 2.19  | 1.49        | 1.42     |
| 37  | g     | 522 | 0IE  | C6-C7   | -2.19 | 1.41        | 1.46     |
| 31  | 6     | 314 | CLA  | CMD-C2D | -2.19 | 1.46        | 1.50     |
| 31  | 9     | 300 | CLA  | CMB-C2B | -2.19 | 1.46        | 1.50     |
| 31  | 9     | 310 | CLA  | CHC-C1C | 2.19  | 1.42        | 1.38     |
| 31  | A     | 835 | CLA  | CMD-C2D | -2.19 | 1.46        | 1.50     |
| 31  | L     | 202 | CLA  | CMB-C2B | -2.19 | 1.46        | 1.50     |
| 31  | M     | 101 | CLA  | CMD-C2D | -2.19 | 1.46        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 9     | 308 | CLA  | MG-NB   | -2.19 | 2.01        | 2.05     |
| 31  | 5     | 308 | CLA  | CMD-C2D | -2.19 | 1.46        | 1.50     |
| 31  | A     | 815 | CLA  | CMC-C2C | -2.19 | 1.46        | 1.50     |
| 31  | B     | 850 | CLA  | CMB-C2B | -2.19 | 1.46        | 1.50     |
| 31  | 9     | 309 | CLA  | MG-NB   | -2.19 | 2.01        | 2.05     |
| 30  | 8     | 313 | CHL  | CBD-CGD | -2.19 | 1.49        | 1.52     |
| 31  | J     | 103 | CLA  | MG-NB   | -2.19 | 2.01        | 2.05     |
| 31  | A     | 814 | CLA  | CMD-C2D | -2.19 | 1.46        | 1.50     |
| 31  | A     | 830 | CLA  | CMD-C2D | -2.19 | 1.46        | 1.50     |
| 31  | 4     | 314 | CLA  | CMD-C2D | -2.19 | 1.46        | 1.50     |
| 31  | B     | 814 | CLA  | CHC-C1C | 2.18  | 1.42        | 1.38     |
| 31  | A     | 818 | CLA  | CMB-C2B | -2.18 | 1.46        | 1.50     |
| 31  | f     | 604 | CLA  | CMB-C2B | -2.18 | 1.46        | 1.50     |
| 31  | b     | 603 | CLA  | MG-NB   | -2.18 | 2.01        | 2.05     |
| 31  | B     | 808 | CLA  | C3B-C4B | 2.18  | 1.49        | 1.42     |
| 31  | 3     | 309 | CLA  | C1B-C2B | 2.18  | 1.48        | 1.43     |
| 31  | 1     | 311 | CLA  | CHC-C1C | 2.18  | 1.42        | 1.38     |
| 37  | a     | 522 | 0IE  | C13-C12 | -2.18 | 1.41        | 1.46     |
| 31  | B     | 816 | CLA  | CMD-C2D | -2.18 | 1.46        | 1.50     |
| 32  | 1     | 402 | 8CT  | C33-C32 | -2.18 | 1.44        | 1.50     |
| 31  | 2     | 310 | CLA  | CHC-C1C | 2.18  | 1.42        | 1.38     |
| 31  | B     | 850 | CLA  | MG-NB   | -2.18 | 2.01        | 2.05     |
| 30  | 1     | 306 | CHL  | CBD-CGD | -2.18 | 1.49        | 1.52     |
| 31  | 9     | 304 | CLA  | C3B-C4B | 2.18  | 1.49        | 1.42     |
| 31  | A     | 822 | CLA  | C3B-C4B | 2.18  | 1.49        | 1.42     |
| 31  | b     | 603 | CLA  | C3B-C4B | 2.18  | 1.49        | 1.42     |
| 31  | A     | 803 | CLA  | CHC-C1C | 2.18  | 1.42        | 1.38     |
| 31  | H     | 201 | CLA  | CMD-C2D | -2.18 | 1.46        | 1.50     |
| 31  | B     | 827 | CLA  | CMB-C2B | -2.18 | 1.46        | 1.50     |
| 31  | A     | 825 | CLA  | C3B-C4B | 2.18  | 1.49        | 1.42     |
| 31  | b     | 612 | CLA  | MG-NB   | -2.18 | 2.01        | 2.05     |
| 31  | A     | 828 | CLA  | CHC-C1C | 2.18  | 1.42        | 1.38     |
| 31  | b     | 604 | CLA  | CHC-C1C | 2.18  | 1.42        | 1.38     |
| 31  | d     | 612 | CLA  | CHC-C1C | 2.18  | 1.42        | 1.38     |
| 31  | e     | 604 | CLA  | CMB-C2B | -2.18 | 1.46        | 1.50     |
| 31  | 3     | 306 | CLA  | MG-NB   | -2.18 | 2.01        | 2.05     |
| 31  | e     | 604 | CLA  | MG-NB   | -2.18 | 2.01        | 2.05     |
| 31  | 3     | 318 | CLA  | CHC-C1C | 2.18  | 1.42        | 1.38     |
| 31  | 0     | 311 | CLA  | CMC-C2C | -2.18 | 1.46        | 1.50     |
| 31  | B     | 827 | CLA  | CMD-C2D | -2.18 | 1.46        | 1.50     |
| 31  | G     | 103 | CLA  | CMB-C2B | -2.18 | 1.46        | 1.50     |
| 31  | i     | 604 | CLA  | CHC-C1C | 2.18  | 1.42        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | B     | 837 | CLA  | CMB-C2B | -2.18 | 1.46        | 1.50     |
| 31  | B     | 817 | CLA  | C3B-C4B | 2.18  | 1.49        | 1.42     |
| 31  | 8     | 312 | CLA  | CMC-C2C | -2.18 | 1.46        | 1.50     |
| 31  | 9     | 311 | CLA  | CMD-C2D | -2.18 | 1.46        | 1.50     |
| 31  | A     | 838 | CLA  | MG-NB   | -2.18 | 2.01        | 2.05     |
| 30  | 3     | 307 | CHL  | CBD-CGD | -2.18 | 1.49        | 1.52     |
| 31  | A     | 853 | CLA  | CHC-C1C | 2.18  | 1.42        | 1.38     |
| 31  | g     | 613 | CLA  | CHC-C1C | 2.18  | 1.42        | 1.38     |
| 31  | 4     | 303 | CLA  | C3B-C4B | 2.18  | 1.49        | 1.42     |
| 31  | 1     | 312 | CLA  | CMC-C2C | -2.18 | 1.46        | 1.50     |
| 31  | 8     | 304 | CLA  | CHC-C1C | 2.18  | 1.42        | 1.38     |
| 31  | B     | 825 | CLA  | CHC-C1C | 2.18  | 1.42        | 1.38     |
| 31  | A     | 817 | CLA  | C3B-C4B | 2.18  | 1.49        | 1.42     |
| 31  | 8     | 304 | CLA  | MG-NB   | -2.18 | 2.01        | 2.05     |
| 31  | 1     | 310 | CLA  | MG-NB   | -2.18 | 2.01        | 2.05     |
| 31  | b     | 604 | CLA  | MG-NB   | -2.18 | 2.01        | 2.05     |
| 31  | B     | 807 | CLA  | CMD-C2D | -2.18 | 1.46        | 1.50     |
| 31  | A     | 829 | CLA  | CHC-C1C | 2.18  | 1.42        | 1.38     |
| 30  | 7     | 313 | CHL  | CBD-CGD | -2.18 | 1.49        | 1.52     |
| 31  | A     | 820 | CLA  | C3B-C4B | 2.18  | 1.49        | 1.42     |
| 31  | 3     | 306 | CLA  | CMD-C2D | -2.18 | 1.46        | 1.50     |
| 31  | 3     | 310 | CLA  | CHC-C1C | 2.18  | 1.42        | 1.38     |
| 31  | A     | 832 | CLA  | C3B-C4B | 2.18  | 1.49        | 1.42     |
| 31  | L     | 201 | CLA  | C3B-C4B | 2.18  | 1.49        | 1.42     |
| 31  | B     | 817 | CLA  | CMD-C2D | -2.18 | 1.46        | 1.50     |
| 31  | 6     | 311 | CLA  | CHC-C1C | 2.18  | 1.42        | 1.38     |
| 31  | 2     | 312 | CLA  | CMD-C2D | -2.18 | 1.46        | 1.50     |
| 31  | B     | 821 | CLA  | CMD-C2D | -2.18 | 1.46        | 1.50     |
| 31  | B     | 850 | CLA  | CMD-C2D | -2.18 | 1.46        | 1.50     |
| 30  | 1     | 302 | CHL  | CBD-CGD | -2.18 | 1.49        | 1.52     |
| 31  | A     | 824 | CLA  | CMD-C2D | -2.17 | 1.46        | 1.50     |
| 31  | e     | 610 | CLA  | CMB-C2B | -2.17 | 1.46        | 1.50     |
| 31  | f     | 604 | CLA  | CHC-C1C | 2.17  | 1.42        | 1.38     |
| 31  | L     | 202 | CLA  | C3B-C4B | 2.17  | 1.49        | 1.42     |
| 31  | 7     | 318 | CLA  | CMD-C2D | -2.17 | 1.46        | 1.50     |
| 31  | B     | 805 | CLA  | CMC-C2C | -2.17 | 1.46        | 1.50     |
| 31  | 0     | 312 | CLA  | CMD-C2D | -2.17 | 1.46        | 1.50     |
| 31  | A     | 828 | CLA  | CMD-C2D | -2.17 | 1.46        | 1.50     |
| 31  | B     | 812 | CLA  | CMD-C2D | -2.17 | 1.46        | 1.50     |
| 31  | 3     | 312 | CLA  | CMD-C2D | -2.17 | 1.46        | 1.50     |
| 31  | 7     | 311 | CLA  | CMD-C2D | -2.17 | 1.46        | 1.50     |
| 31  | 7     | 318 | CLA  | CMC-C2C | -2.17 | 1.46        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | B     | 805 | CLA  | CMB-C2B | -2.17 | 1.46        | 1.50     |
| 31  | L     | 201 | CLA  | CHC-C1C | 2.17  | 1.42        | 1.38     |
| 31  | A     | 825 | CLA  | CMB-C2B | -2.17 | 1.46        | 1.50     |
| 31  | e     | 610 | CLA  | MG-NB   | -2.17 | 2.01        | 2.05     |
| 30  | 6     | 301 | CHL  | CBD-CGD | -2.17 | 1.49        | 1.52     |
| 31  | B     | 813 | CLA  | CMD-C2D | -2.17 | 1.46        | 1.50     |
| 31  | F     | 301 | CLA  | CMD-C2D | -2.17 | 1.46        | 1.50     |
| 37  | b     | 522 | 0IE  | C17-C16 | -2.17 | 1.41        | 1.46     |
| 31  | 1     | 309 | CLA  | CMB-C2B | -2.17 | 1.46        | 1.50     |
| 31  | 3     | 313 | CLA  | CMB-C2B | -2.17 | 1.46        | 1.50     |
| 31  | A     | 814 | CLA  | CMC-C2C | -2.17 | 1.46        | 1.50     |
| 30  | 5     | 307 | CHL  | CBD-CGD | -2.17 | 1.49        | 1.52     |
| 31  | 9     | 302 | CLA  | CMD-C2D | -2.17 | 1.46        | 1.50     |
| 31  | B     | 850 | CLA  | CMC-C2C | -2.17 | 1.46        | 1.50     |
| 31  | 8     | 312 | CLA  | CHC-C1C | 2.17  | 1.42        | 1.38     |
| 31  | f     | 612 | CLA  | CHC-C1C | 2.17  | 1.42        | 1.38     |
| 31  | A     | 831 | CLA  | C3B-C4B | 2.17  | 1.49        | 1.42     |
| 31  | b     | 610 | CLA  | CMB-C2B | -2.17 | 1.46        | 1.50     |
| 31  | 9     | 312 | CLA  | C3B-C4B | 2.17  | 1.49        | 1.42     |
| 31  | b     | 603 | CLA  | CHC-C1C | 2.17  | 1.42        | 1.38     |
| 36  | O     | 207 | LMG  | O7-C8   | -2.17 | 1.41        | 1.46     |
| 31  | 0     | 311 | CLA  | CMD-C2D | -2.17 | 1.46        | 1.50     |
| 31  | A     | 833 | CLA  | CMB-C2B | -2.17 | 1.46        | 1.50     |
| 31  | A     | 810 | CLA  | MG-NB   | -2.17 | 2.01        | 2.05     |
| 31  | A     | 831 | CLA  | CHC-C1C | 2.17  | 1.42        | 1.38     |
| 31  | 7     | 316 | CLA  | CMB-C2B | -2.17 | 1.46        | 1.50     |
| 31  | e     | 612 | CLA  | CMD-C2D | -2.17 | 1.46        | 1.50     |
| 31  | L     | 203 | CLA  | CHC-C1C | 2.17  | 1.42        | 1.38     |
| 31  | B     | 810 | CLA  | CMB-C2B | -2.17 | 1.46        | 1.50     |
| 31  | H     | 205 | CLA  | CMB-C2B | -2.17 | 1.46        | 1.50     |
| 31  | 4     | 303 | CLA  | CMB-C2B | -2.17 | 1.46        | 1.50     |
| 31  | L     | 207 | CLA  | MG-NB   | -2.17 | 2.01        | 2.05     |
| 31  | B     | 836 | CLA  | C3B-C4B | 2.17  | 1.49        | 1.42     |
| 31  | B     | 817 | CLA  | CHC-C1C | 2.17  | 1.42        | 1.38     |
| 31  | 3     | 303 | CLA  | CMB-C2B | -2.17 | 1.46        | 1.50     |
| 31  | A     | 826 | CLA  | CMB-C2B | -2.17 | 1.46        | 1.50     |
| 31  | O     | 206 | CLA  | CMD-C2D | -2.17 | 1.46        | 1.50     |
| 31  | 4     | 304 | CLA  | CMB-C2B | -2.17 | 1.46        | 1.50     |
| 32  | J     | 101 | 8CT  | C33-C32 | -2.17 | 1.44        | 1.50     |
| 31  | 0     | 312 | CLA  | MG-NB   | -2.17 | 2.01        | 2.05     |
| 30  | 0     | 302 | CHL  | CBD-CGD | -2.17 | 1.49        | 1.52     |
| 30  | 2     | 319 | CHL  | CBD-CGD | -2.17 | 1.49        | 1.52     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 30  | 4     | 305 | CHL  | CBD-CGD | -2.17 | 1.49        | 1.52     |
| 33  | c     | 520 | 0UR  | C19-C18 | 2.17  | 1.53        | 1.50     |
| 31  | B     | 828 | CLA  | CHC-C1C | 2.17  | 1.42        | 1.38     |
| 31  | h     | 603 | CLA  | CHC-C1C | 2.17  | 1.42        | 1.38     |
| 31  | 1     | 303 | CLA  | CMB-C2B | -2.17 | 1.46        | 1.50     |
| 31  | 8     | 310 | CLA  | CMD-C2D | -2.17 | 1.46        | 1.50     |
| 31  | A     | 809 | CLA  | CMB-C2B | -2.17 | 1.46        | 1.50     |
| 31  | B     | 808 | CLA  | CHC-C1C | 2.17  | 1.42        | 1.38     |
| 31  | 2     | 310 | CLA  | CMB-C2B | -2.17 | 1.46        | 1.50     |
| 31  | 9     | 300 | CLA  | C3B-C4B | 2.17  | 1.49        | 1.42     |
| 31  | 6     | 318 | CLA  | CHC-C1C | 2.17  | 1.42        | 1.38     |
| 31  | c     | 604 | CLA  | CHC-C1C | 2.17  | 1.42        | 1.38     |
| 31  | B     | 823 | CLA  | C3B-C4B | 2.17  | 1.49        | 1.42     |
| 31  | 1     | 311 | CLA  | CMC-C2C | -2.17 | 1.46        | 1.50     |
| 31  | B     | 818 | CLA  | CHC-C1C | 2.16  | 1.42        | 1.38     |
| 31  | B     | 837 | CLA  | CHC-C1C | 2.16  | 1.42        | 1.38     |
| 31  | 8     | 309 | CLA  | CMB-C2B | -2.16 | 1.46        | 1.50     |
| 31  | B     | 818 | CLA  | CMD-C2D | -2.16 | 1.46        | 1.50     |
| 34  | G     | 105 | LHG  | P-O6    | 2.16  | 1.67        | 1.59     |
| 37  | h     | 522 | 0IE  | C6-C7   | -2.16 | 1.41        | 1.46     |
| 31  | c     | 613 | CLA  | CHC-C1C | 2.16  | 1.42        | 1.38     |
| 31  | 7     | 310 | CLA  | CMB-C2B | -2.16 | 1.46        | 1.50     |
| 31  | c     | 604 | CLA  | MG-NB   | -2.16 | 2.01        | 2.05     |
| 31  | 0     | 308 | CLA  | CMD-C2D | -2.16 | 1.46        | 1.50     |
| 31  | B     | 801 | CLA  | CMC-C2C | -2.16 | 1.46        | 1.50     |
| 31  | A     | 837 | CLA  | CMB-C2B | -2.16 | 1.46        | 1.50     |
| 31  | f     | 610 | CLA  | MG-NB   | -2.16 | 2.01        | 2.05     |
| 34  | 1     | 601 | LHG  | O8-C23  | 2.16  | 1.39        | 1.33     |
| 31  | 1     | 310 | CLA  | CMB-C2B | -2.16 | 1.46        | 1.50     |
| 31  | A     | 804 | CLA  | CMB-C2B | -2.16 | 1.46        | 1.50     |
| 37  | c     | 521 | 0IE  | C8-C7   | 2.16  | 1.40        | 1.35     |
| 31  | 0     | 312 | CLA  | CHC-C1C | 2.16  | 1.42        | 1.38     |
| 31  | 8     | 310 | CLA  | CHC-C1C | 2.16  | 1.42        | 1.38     |
| 31  | 7     | 317 | CLA  | CMB-C2B | -2.16 | 1.46        | 1.50     |
| 34  | 3     | 601 | LHG  | P-O6    | 2.16  | 1.67        | 1.59     |
| 31  | 0     | 308 | CLA  | CHC-C1C | 2.16  | 1.42        | 1.38     |
| 31  | 0     | 304 | CLA  | CMD-C2D | -2.16 | 1.46        | 1.50     |
| 31  | 7     | 309 | CLA  | CMC-C2C | -2.16 | 1.46        | 1.50     |
| 31  | 5     | 311 | CLA  | C3B-C4B | 2.16  | 1.49        | 1.42     |
| 31  | 3     | 304 | CLA  | C3B-C4B | 2.16  | 1.49        | 1.42     |
| 31  | 9     | 309 | CLA  | CMD-C2D | -2.16 | 1.46        | 1.50     |
| 31  | f     | 603 | CLA  | CHC-C1C | 2.16  | 1.42        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | B     | 820 | CLA  | C3B-C4B | 2.16  | 1.49        | 1.42     |
| 30  | 1     | 307 | CHL  | CBD-CGD | -2.16 | 1.49        | 1.52     |
| 31  | 4     | 303 | CLA  | CHC-C1C | 2.16  | 1.42        | 1.38     |
| 31  | 0     | 313 | CLA  | CMB-C2B | -2.16 | 1.46        | 1.50     |
| 31  | 1     | 304 | CLA  | CMB-C2B | -2.16 | 1.46        | 1.50     |
| 31  | 6     | 312 | CLA  | CMB-C2B | -2.16 | 1.46        | 1.50     |
| 31  | B     | 837 | CLA  | CMD-C2D | -2.16 | 1.46        | 1.50     |
| 31  | B     | 838 | CLA  | CMB-C2B | -2.16 | 1.46        | 1.50     |
| 31  | G     | 101 | CLA  | CMD-C2D | -2.16 | 1.46        | 1.50     |
| 31  | 3     | 303 | CLA  | C3B-C4B | 2.16  | 1.49        | 1.42     |
| 34  | 2     | 601 | LHG  | O8-C23  | 2.16  | 1.39        | 1.33     |
| 31  | A     | 852 | CLA  | CHC-C1C | 2.16  | 1.42        | 1.38     |
| 31  | 3     | 311 | CLA  | CMB-C2B | -2.16 | 1.46        | 1.50     |
| 31  | K     | 104 | CLA  | CMB-C2B | -2.16 | 1.46        | 1.50     |
| 31  | A     | 811 | CLA  | CMC-C2C | -2.16 | 1.46        | 1.50     |
| 31  | 7     | 310 | CLA  | CHC-C1C | 2.16  | 1.42        | 1.38     |
| 31  | B     | 809 | CLA  | CHC-C1C | 2.16  | 1.42        | 1.38     |
| 31  | 6     | 312 | CLA  | C3B-C4B | 2.16  | 1.49        | 1.42     |
| 31  | A     | 803 | CLA  | CMB-C2B | -2.16 | 1.46        | 1.50     |
| 31  | 1     | 312 | CLA  | C3B-C4B | 2.16  | 1.49        | 1.42     |
| 31  | 0     | 313 | CLA  | CMD-C2D | -2.16 | 1.46        | 1.50     |
| 31  | B     | 835 | CLA  | CMB-C2B | -2.16 | 1.46        | 1.50     |
| 31  | A     | 805 | CLA  | MG-NB   | -2.16 | 2.01        | 2.05     |
| 31  | B     | 821 | CLA  | MG-NB   | -2.16 | 2.01        | 2.05     |
| 31  | 1     | 308 | CLA  | CMB-C2B | -2.16 | 1.46        | 1.50     |
| 31  | 6     | 320 | CLA  | CMB-C2B | -2.16 | 1.46        | 1.50     |
| 31  | A     | 839 | CLA  | CMD-C2D | -2.16 | 1.46        | 1.50     |
| 31  | A     | 821 | CLA  | CHC-C1C | 2.16  | 1.42        | 1.38     |
| 31  | O     | 201 | CLA  | CHC-C1C | 2.16  | 1.42        | 1.38     |
| 34  | A     | 844 | LHG  | O8-C23  | 2.16  | 1.39        | 1.33     |
| 30  | 4     | 302 | CHL  | CBD-CGD | -2.16 | 1.49        | 1.52     |
| 31  | B     | 807 | CLA  | CMB-C2B | -2.16 | 1.46        | 1.50     |
| 34  | f     | 630 | LHG  | O7-C7   | 2.16  | 1.40        | 1.34     |
| 31  | 6     | 310 | CLA  | CMB-C2B | -2.16 | 1.46        | 1.50     |
| 31  | L     | 207 | CLA  | CMB-C2B | -2.16 | 1.46        | 1.50     |
| 31  | 7     | 308 | CLA  | CMB-C2B | -2.15 | 1.46        | 1.50     |
| 31  | B     | 806 | CLA  | CMB-C2B | -2.15 | 1.46        | 1.50     |
| 31  | f     | 610 | CLA  | CMD-C2D | -2.15 | 1.46        | 1.50     |
| 31  | f     | 603 | CLA  | MG-NB   | -2.15 | 2.01        | 2.05     |
| 31  | A     | 807 | CLA  | CMD-C2D | -2.15 | 1.46        | 1.50     |
| 31  | B     | 808 | CLA  | CMC-C2C | -2.15 | 1.46        | 1.50     |
| 31  | L     | 203 | CLA  | CMD-C2D | -2.15 | 1.46        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 6     | 320 | CLA  | CHC-C1C | 2.15  | 1.42        | 1.38     |
| 31  | 8     | 309 | CLA  | CHC-C1C | 2.15  | 1.42        | 1.38     |
| 31  | A     | 807 | CLA  | CHC-C1C | 2.15  | 1.42        | 1.38     |
| 31  | 2     | 310 | CLA  | CMD-C2D | -2.15 | 1.46        | 1.50     |
| 31  | B     | 809 | CLA  | CMC-C2C | -2.15 | 1.46        | 1.50     |
| 31  | f     | 611 | CLA  | CMD-C2D | -2.15 | 1.46        | 1.50     |
| 31  | 3     | 306 | CLA  | CMB-C2B | -2.15 | 1.46        | 1.50     |
| 31  | A     | 820 | CLA  | CHC-C1C | 2.15  | 1.42        | 1.38     |
| 31  | 0     | 311 | CLA  | C3B-C4B | 2.15  | 1.49        | 1.42     |
| 31  | 1     | 311 | CLA  | CMB-C2B | -2.15 | 1.46        | 1.50     |
| 31  | a     | 604 | CLA  | CMB-C2B | -2.15 | 1.46        | 1.50     |
| 31  | 9     | 300 | CLA  | CHC-C1C | 2.15  | 1.42        | 1.38     |
| 31  | 4     | 311 | CLA  | C3B-C4B | 2.15  | 1.49        | 1.42     |
| 31  | L     | 207 | CLA  | CMD-C2D | -2.15 | 1.46        | 1.50     |
| 31  | A     | 811 | CLA  | MG-NB   | -2.15 | 2.01        | 2.05     |
| 31  | B     | 835 | CLA  | C3B-C4B | 2.15  | 1.49        | 1.42     |
| 37  | d     | 521 | 0IE  | C15-C16 | 2.15  | 1.40        | 1.35     |
| 31  | B     | 813 | CLA  | MG-NB   | -2.15 | 2.01        | 2.05     |
| 31  | L     | 207 | CLA  | CHC-C1C | 2.15  | 1.42        | 1.38     |
| 31  | 6     | 304 | CLA  | CMD-C2D | -2.15 | 1.46        | 1.50     |
| 37  | c     | 521 | 0IE  | C11-C12 | 2.15  | 1.40        | 1.35     |
| 31  | 2     | 312 | CLA  | CMB-C2B | -2.15 | 1.46        | 1.50     |
| 31  | A     | 824 | CLA  | CMC-C2C | -2.15 | 1.46        | 1.50     |
| 31  | B     | 826 | CLA  | CMB-C2B | -2.15 | 1.46        | 1.50     |
| 31  | 4     | 312 | CLA  | CMC-C2C | -2.15 | 1.46        | 1.50     |
| 31  | O     | 206 | CLA  | MG-NB   | -2.15 | 2.01        | 2.05     |
| 31  | 5     | 304 | CLA  | CHC-C1C | 2.15  | 1.42        | 1.38     |
| 31  | B     | 820 | CLA  | CHC-C1C | 2.15  | 1.42        | 1.38     |
| 31  | e     | 604 | CLA  | CHC-C1C | 2.15  | 1.42        | 1.38     |
| 31  | 9     | 302 | CLA  | CMB-C2B | -2.15 | 1.46        | 1.50     |
| 31  | 4     | 310 | CLA  | CMD-C2D | -2.15 | 1.46        | 1.50     |
| 31  | 0     | 304 | CLA  | C3B-C4B | 2.15  | 1.49        | 1.42     |
| 31  | A     | 822 | CLA  | CMB-C2B | -2.15 | 1.46        | 1.50     |
| 31  | c     | 611 | CLA  | CMD-C2D | -2.15 | 1.46        | 1.50     |
| 32  | 3     | 402 | 8CT  | C33-C32 | -2.15 | 1.44        | 1.50     |
| 31  | A     | 828 | CLA  | CMC-C2C | -2.15 | 1.46        | 1.50     |
| 31  | B     | 836 | CLA  | CMB-C2B | -2.15 | 1.46        | 1.50     |
| 31  | 5     | 309 | CLA  | CMD-C2D | -2.15 | 1.46        | 1.50     |
| 31  | 5     | 310 | CLA  | CHC-C1C | 2.15  | 1.42        | 1.38     |
| 31  | B     | 840 | CLA  | C3B-C4B | 2.15  | 1.49        | 1.42     |
| 31  | 6     | 310 | CLA  | CMD-C2D | -2.15 | 1.46        | 1.50     |
| 31  | 4     | 304 | CLA  | CMC-C2C | -2.15 | 1.46        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | A     | 824 | CLA  | CHC-C1C | 2.15  | 1.42        | 1.38     |
| 31  | B     | 834 | CLA  | CHC-C1C | 2.15  | 1.42        | 1.38     |
| 31  | 0     | 303 | CLA  | CMB-C2B | -2.15 | 1.46        | 1.50     |
| 31  | 6     | 318 | CLA  | CMD-C2D | -2.15 | 1.46        | 1.50     |
| 31  | 7     | 312 | CLA  | CMD-C2D | -2.15 | 1.46        | 1.50     |
| 31  | B     | 825 | CLA  | CMB-C2B | -2.15 | 1.46        | 1.50     |
| 31  | B     | 841 | CLA  | CMD-C2D | -2.15 | 1.46        | 1.50     |
| 31  | B     | 823 | CLA  | CHC-C1C | 2.15  | 1.42        | 1.38     |
| 31  | 1     | 314 | CLA  | CMB-C2B | -2.15 | 1.46        | 1.50     |
| 31  | A     | 816 | CLA  | MG-NB   | -2.15 | 2.01        | 2.05     |
| 31  | 8     | 303 | CLA  | CMD-C2D | -2.15 | 1.46        | 1.50     |
| 31  | B     | 814 | CLA  | CMB-C2B | -2.15 | 1.46        | 1.50     |
| 31  | B     | 822 | CLA  | CMD-C2D | -2.15 | 1.46        | 1.50     |
| 31  | B     | 824 | CLA  | CMC-C2C | -2.15 | 1.46        | 1.50     |
| 31  | B     | 820 | CLA  | CMD-C2D | -2.15 | 1.46        | 1.50     |
| 34  | A     | 845 | LHG  | O8-C23  | 2.14  | 1.39        | 1.33     |
| 31  | A     | 813 | CLA  | CMD-C2D | -2.14 | 1.46        | 1.50     |
| 30  | 4     | 308 | CHL  | CBD-CGD | -2.14 | 1.49        | 1.52     |
| 33  | 9     | 502 | 0UR  | C23-C1  | -2.14 | 1.50        | 1.53     |
| 31  | a     | 603 | CLA  | MG-NB   | -2.14 | 2.01        | 2.05     |
| 31  | f     | 604 | CLA  | MG-NB   | -2.14 | 2.01        | 2.05     |
| 31  | 9     | 308 | CLA  | CMC-C2C | -2.14 | 1.46        | 1.50     |
| 31  | 2     | 312 | CLA  | C3B-C4B | 2.14  | 1.49        | 1.42     |
| 31  | M     | 101 | CLA  | CMC-C2C | -2.14 | 1.46        | 1.50     |
| 31  | 4     | 309 | CLA  | CMB-C2B | -2.14 | 1.46        | 1.50     |
| 30  | 9     | 305 | CHL  | CBD-CGD | -2.14 | 1.49        | 1.52     |
| 31  | 6     | 317 | CLA  | CHC-C1C | 2.14  | 1.42        | 1.38     |
| 31  | f     | 613 | CLA  | MG-NB   | -2.14 | 2.01        | 2.05     |
| 31  | 5     | 310 | CLA  | CMB-C2B | -2.14 | 1.46        | 1.50     |
| 31  | B     | 813 | CLA  | CHC-C1C | 2.14  | 1.42        | 1.38     |
| 31  | B     | 835 | CLA  | CMD-C2D | -2.14 | 1.46        | 1.50     |
| 31  | 9     | 304 | CLA  | CMD-C2D | -2.14 | 1.46        | 1.50     |
| 31  | B     | 810 | CLA  | CMC-C2C | -2.14 | 1.46        | 1.50     |
| 31  | 3     | 303 | CLA  | CHC-C1C | 2.14  | 1.42        | 1.38     |
| 31  | B     | 810 | CLA  | CHC-C1C | 2.14  | 1.42        | 1.38     |
| 31  | B     | 831 | CLA  | CHC-C1C | 2.14  | 1.42        | 1.38     |
| 31  | b     | 610 | CLA  | MG-NB   | -2.14 | 2.01        | 2.05     |
| 31  | H     | 204 | CLA  | CMD-C2D | -2.14 | 1.46        | 1.50     |
| 31  | 7     | 308 | CLA  | CHC-C1C | 2.14  | 1.42        | 1.38     |
| 31  | 2     | 309 | CLA  | CMB-C2B | -2.14 | 1.46        | 1.50     |
| 31  | 6     | 317 | CLA  | CMB-C2B | -2.14 | 1.46        | 1.50     |
| 30  | 4     | 306 | CHL  | CBD-CGD | -2.14 | 1.49        | 1.52     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 8     | 314 | CLA  | CHC-C1C | 2.14  | 1.42        | 1.38     |
| 31  | A     | 843 | CLA  | CMB-C2B | -2.14 | 1.46        | 1.50     |
| 31  | 1     | 310 | CLA  | C3B-C4B | 2.14  | 1.49        | 1.42     |
| 31  | K     | 101 | CLA  | CMB-C2B | -2.14 | 1.46        | 1.50     |
| 31  | H     | 204 | CLA  | MG-NB   | -2.14 | 2.01        | 2.05     |
| 31  | 7     | 308 | CLA  | C3B-C4B | 2.14  | 1.49        | 1.42     |
| 31  | 2     | 311 | CLA  | CMD-C2D | -2.14 | 1.46        | 1.50     |
| 31  | O     | 201 | CLA  | CMD-C2D | -2.14 | 1.46        | 1.50     |
| 31  | 3     | 313 | CLA  | CHC-C1C | 2.14  | 1.42        | 1.38     |
| 31  | 4     | 310 | CLA  | CHC-C1C | 2.14  | 1.42        | 1.38     |
| 31  | 3     | 312 | CLA  | CMC-C2C | -2.14 | 1.46        | 1.50     |
| 31  | f     | 612 | CLA  | CMD-C2D | -2.14 | 1.46        | 1.50     |
| 31  | 1     | 303 | CLA  | CMC-C2C | -2.14 | 1.46        | 1.50     |
| 31  | O     | 202 | CLA  | CMB-C2B | -2.14 | 1.46        | 1.50     |
| 31  | 8     | 311 | CLA  | CMC-C2C | -2.14 | 1.46        | 1.50     |
| 31  | A     | 843 | CLA  | CMD-C2D | -2.14 | 1.46        | 1.50     |
| 31  | A     | 836 | CLA  | C3B-C4B | 2.14  | 1.49        | 1.42     |
| 31  | a     | 612 | CLA  | CHC-C1C | 2.14  | 1.42        | 1.38     |
| 31  | 1     | 309 | CLA  | CMD-C2D | -2.14 | 1.46        | 1.50     |
| 31  | G     | 102 | CLA  | CHC-C1C | 2.14  | 1.42        | 1.38     |
| 34  | 6     | 603 | LHG  | P-O6    | 2.14  | 1.67        | 1.59     |
| 31  | c     | 603 | CLA  | MG-NB   | -2.14 | 2.01        | 2.05     |
| 31  | 9     | 308 | CLA  | C3B-C4B | 2.14  | 1.49        | 1.42     |
| 31  | 5     | 304 | CLA  | MG-NB   | -2.14 | 2.01        | 2.05     |
| 31  | 9     | 311 | CLA  | MG-NB   | -2.14 | 2.01        | 2.05     |
| 31  | f     | 612 | CLA  | MG-NB   | -2.14 | 2.01        | 2.05     |
| 31  | 0     | 321 | CLA  | CHC-C1C | 2.13  | 1.42        | 1.38     |
| 31  | b     | 612 | CLA  | CHC-C1C | 2.13  | 1.42        | 1.38     |
| 34  | h     | 630 | LHG  | P-O6    | 2.13  | 1.67        | 1.59     |
| 31  | 8     | 303 | CLA  | CMC-C2C | -2.13 | 1.46        | 1.50     |
| 31  | 8     | 311 | CLA  | CMB-C2B | -2.13 | 1.46        | 1.50     |
| 31  | 3     | 306 | CLA  | CHC-C1C | 2.13  | 1.42        | 1.38     |
| 31  | 9     | 311 | CLA  | CMC-C2C | -2.13 | 1.46        | 1.50     |
| 31  | 9     | 312 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 31  | a     | 603 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 31  | H     | 204 | CLA  | C3B-C4B | 2.13  | 1.49        | 1.42     |
| 31  | c     | 613 | CLA  | MG-NB   | -2.13 | 2.01        | 2.05     |
| 31  | d     | 603 | CLA  | MG-NB   | -2.13 | 2.01        | 2.05     |
| 31  | h     | 604 | CLA  | MG-NB   | -2.13 | 2.01        | 2.05     |
| 31  | e     | 611 | CLA  | MG-NB   | -2.13 | 2.01        | 2.05     |
| 31  | B     | 827 | CLA  | C3B-C4B | 2.13  | 1.49        | 1.42     |
| 31  | 7     | 317 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 9     | 310 | CLA  | CMB-C2B | -2.13 | 1.46        | 1.50     |
| 31  | J     | 103 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 31  | K     | 105 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 34  | 1     | 601 | LHG  | O7-C7   | 2.13  | 1.40        | 1.34     |
| 30  | 2     | 313 | CHL  | CBD-CGD | -2.13 | 1.49        | 1.52     |
| 31  | 5     | 312 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 31  | c     | 604 | CLA  | CMB-C2B | -2.13 | 1.46        | 1.50     |
| 34  | B     | 852 | LHG  | O7-C5   | -2.13 | 1.41        | 1.46     |
| 31  | 2     | 314 | CLA  | CMB-C2B | -2.13 | 1.46        | 1.50     |
| 31  | 1     | 308 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 31  | 6     | 317 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 31  | 3     | 320 | CLA  | C3B-C4B | 2.13  | 1.48        | 1.42     |
| 31  | 4     | 314 | CLA  | CHC-C1C | 2.13  | 1.42        | 1.38     |
| 31  | L     | 201 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 31  | A     | 838 | CLA  | CHC-C1C | 2.13  | 1.42        | 1.38     |
| 31  | K     | 102 | CLA  | CHC-C1C | 2.13  | 1.42        | 1.38     |
| 31  | A     | 819 | CLA  | CMC-C2C | -2.13 | 1.46        | 1.50     |
| 31  | B     | 818 | CLA  | C3B-C4B | 2.13  | 1.48        | 1.42     |
| 31  | 1     | 303 | CLA  | CHC-C1C | 2.13  | 1.42        | 1.38     |
| 31  | B     | 835 | CLA  | CHC-C1C | 2.13  | 1.42        | 1.38     |
| 31  | c     | 610 | CLA  | MG-NB   | -2.13 | 2.01        | 2.05     |
| 31  | i     | 612 | CLA  | MG-NB   | -2.13 | 2.01        | 2.05     |
| 31  | 0     | 310 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 31  | A     | 804 | CLA  | MG-NB   | -2.13 | 2.01        | 2.05     |
| 37  | b     | 522 | 0IE  | C13-C12 | -2.13 | 1.41        | 1.46     |
| 31  | 7     | 315 | CLA  | CMB-C2B | -2.13 | 1.46        | 1.50     |
| 31  | A     | 812 | CLA  | CMC-C2C | -2.13 | 1.46        | 1.50     |
| 31  | J     | 103 | CLA  | CMB-C2B | -2.13 | 1.46        | 1.50     |
| 31  | A     | 817 | CLA  | CHC-C1C | 2.13  | 1.42        | 1.38     |
| 31  | A     | 825 | CLA  | CHC-C1C | 2.13  | 1.42        | 1.38     |
| 31  | B     | 821 | CLA  | C3B-C4B | 2.13  | 1.48        | 1.42     |
| 31  | 1     | 312 | CLA  | CMB-C2B | -2.13 | 1.46        | 1.50     |
| 31  | 8     | 312 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 31  | A     | 806 | CLA  | CMC-C2C | -2.13 | 1.46        | 1.50     |
| 31  | 3     | 318 | CLA  | CMB-C2B | -2.13 | 1.46        | 1.50     |
| 31  | 7     | 315 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 31  | 8     | 309 | CLA  | CMC-C2C | -2.13 | 1.46        | 1.50     |
| 31  | 0     | 313 | CLA  | C3B-C4B | 2.13  | 1.48        | 1.42     |
| 31  | L     | 204 | CLA  | CMB-C2B | -2.13 | 1.46        | 1.50     |
| 31  | 0     | 309 | CLA  | CMD-C2D | -2.12 | 1.46        | 1.50     |
| 31  | 3     | 320 | CLA  | CMD-C2D | -2.12 | 1.46        | 1.50     |
| 31  | d     | 604 | CLA  | MG-NB   | -2.12 | 2.01        | 2.05     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 7     | 317 | CLA  | C3B-C4B | 2.12  | 1.48        | 1.42     |
| 31  | H     | 202 | CLA  | MG-NB   | -2.12 | 2.01        | 2.05     |
| 31  | B     | 832 | CLA  | CMC-C2C | -2.12 | 1.46        | 1.50     |
| 31  | 4     | 303 | CLA  | CMC-C2C | -2.12 | 1.46        | 1.50     |
| 31  | 8     | 310 | CLA  | CMB-C2B | -2.12 | 1.46        | 1.50     |
| 31  | B     | 833 | CLA  | CMD-C2D | -2.12 | 1.46        | 1.50     |
| 31  | B     | 822 | CLA  | CHC-C1C | 2.12  | 1.42        | 1.38     |
| 36  | 9     | 602 | LMG  | O8-C9   | -2.12 | 1.40        | 1.45     |
| 31  | 7     | 310 | CLA  | CMD-C2D | -2.12 | 1.46        | 1.50     |
| 31  | K     | 104 | CLA  | CMC-C2C | -2.12 | 1.46        | 1.50     |
| 31  | e     | 603 | CLA  | MG-NB   | -2.12 | 2.01        | 2.05     |
| 37  | g     | 522 | 0IE  | C13-C12 | -2.12 | 1.41        | 1.46     |
| 31  | H     | 202 | CLA  | CMD-C2D | -2.12 | 1.46        | 1.50     |
| 31  | 9     | 310 | CLA  | CMD-C2D | -2.12 | 1.46        | 1.50     |
| 31  | A     | 843 | CLA  | CMC-C2C | -2.12 | 1.46        | 1.50     |
| 34  | K     | 106 | LHG  | P-O6    | 2.12  | 1.67        | 1.59     |
| 31  | H     | 205 | CLA  | CMD-C2D | -2.12 | 1.46        | 1.50     |
| 31  | e     | 604 | CLA  | CMD-C2D | -2.12 | 1.46        | 1.50     |
| 31  | M     | 101 | CLA  | CMB-C2B | -2.12 | 1.46        | 1.50     |
| 31  | e     | 612 | CLA  | MG-NB   | -2.12 | 2.01        | 2.05     |
| 31  | 7     | 303 | CLA  | CHC-C1C | 2.12  | 1.42        | 1.38     |
| 31  | B     | 807 | CLA  | CMC-C2C | -2.12 | 1.46        | 1.50     |
| 31  | B     | 830 | CLA  | CMC-C2C | -2.12 | 1.46        | 1.50     |
| 31  | H     | 201 | CLA  | C3B-C4B | 2.12  | 1.48        | 1.42     |
| 31  | 4     | 311 | CLA  | CHC-C1C | 2.12  | 1.42        | 1.38     |
| 31  | 3     | 303 | CLA  | CMC-C2C | -2.12 | 1.46        | 1.50     |
| 31  | A     | 802 | CLA  | CMC-C2C | -2.12 | 1.46        | 1.50     |
| 31  | A     | 827 | CLA  | CMB-C2B | -2.12 | 1.46        | 1.50     |
| 31  | 2     | 304 | CLA  | C3B-C4B | 2.12  | 1.48        | 1.42     |
| 31  | 6     | 311 | CLA  | MG-NB   | -2.12 | 2.01        | 2.05     |
| 31  | 9     | 312 | CLA  | CMB-C2B | -2.12 | 1.46        | 1.50     |
| 31  | 6     | 314 | CLA  | CMB-C2B | -2.12 | 1.46        | 1.50     |
| 31  | A     | 830 | CLA  | C1B-C2B | 2.12  | 1.48        | 1.43     |
| 31  | b     | 612 | CLA  | CMC-C2C | -2.12 | 1.46        | 1.50     |
| 31  | A     | 852 | CLA  | CMD-C2D | -2.12 | 1.46        | 1.50     |
| 31  | 5     | 303 | CLA  | C3B-C4B | 2.12  | 1.48        | 1.42     |
| 31  | i     | 604 | CLA  | MG-NB   | -2.12 | 2.01        | 2.05     |
| 37  | d     | 522 | 0IE  | C6-C7   | -2.12 | 1.41        | 1.46     |
| 31  | 7     | 317 | CLA  | MG-NB   | -2.11 | 2.01        | 2.05     |
| 31  | A     | 817 | CLA  | CMC-C2C | -2.11 | 1.46        | 1.50     |
| 31  | B     | 828 | CLA  | CMB-C2B | -2.11 | 1.46        | 1.50     |
| 31  | B     | 828 | CLA  | CMC-C2C | -2.11 | 1.46        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | d     | 612 | CLA  | CMB-C2B | -2.11 | 1.46        | 1.50     |
| 34  | A     | 844 | LHG  | O7-C7   | 2.11  | 1.40        | 1.34     |
| 31  | F     | 301 | CLA  | CMC-C2C | -2.11 | 1.46        | 1.50     |
| 31  | A     | 804 | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 31  | A     | 830 | CLA  | C1B-NB  | -2.11 | 1.35        | 1.37     |
| 31  | 7     | 308 | CLA  | CMC-C2C | -2.11 | 1.46        | 1.50     |
| 31  | 9     | 303 | CLA  | CMC-C2C | -2.11 | 1.46        | 1.50     |
| 31  | c     | 612 | CLA  | MG-NB   | -2.11 | 2.01        | 2.05     |
| 31  | 9     | 304 | CLA  | CHC-C1C | 2.11  | 1.42        | 1.38     |
| 30  | 9     | 306 | CHL  | CBD-CGD | -2.11 | 1.49        | 1.52     |
| 31  | i     | 603 | CLA  | MG-NB   | -2.11 | 2.01        | 2.05     |
| 34  | e     | 630 | LHG  | P-O6    | 2.11  | 1.67        | 1.59     |
| 31  | f     | 613 | CLA  | CMB-C2B | -2.11 | 1.46        | 1.50     |
| 31  | d     | 612 | CLA  | MG-NB   | -2.11 | 2.01        | 2.05     |
| 31  | 6     | 309 | CLA  | CMB-C2B | -2.11 | 1.46        | 1.50     |
| 31  | i     | 611 | CLA  | MG-NB   | -2.11 | 2.01        | 2.05     |
| 31  | 3     | 309 | CLA  | CMC-C2C | -2.11 | 1.46        | 1.50     |
| 31  | B     | 830 | CLA  | MG-ND   | -2.11 | 2.01        | 2.05     |
| 31  | 3     | 311 | CLA  | CHC-C1C | 2.11  | 1.42        | 1.38     |
| 32  | 7     | 402 | 8CT  | C33-C32 | -2.11 | 1.44        | 1.50     |
| 31  | A     | 839 | CLA  | C3B-C4B | 2.11  | 1.48        | 1.42     |
| 31  | 6     | 310 | CLA  | CHC-C1C | 2.11  | 1.42        | 1.38     |
| 31  | A     | 840 | CLA  | CHC-C1C | 2.11  | 1.42        | 1.38     |
| 31  | L     | 203 | CLA  | CMB-C2B | -2.11 | 1.46        | 1.50     |
| 31  | A     | 822 | CLA  | CHC-C1C | 2.11  | 1.42        | 1.38     |
| 31  | A     | 835 | CLA  | CHC-C1C | 2.11  | 1.42        | 1.38     |
| 32  | O     | 205 | 8CT  | C33-C32 | -2.11 | 1.44        | 1.50     |
| 31  | 1     | 309 | CLA  | CMC-C2C | -2.11 | 1.46        | 1.50     |
| 31  | B     | 825 | CLA  | CMC-C2C | -2.11 | 1.46        | 1.50     |
| 31  | 1     | 314 | CLA  | CHC-C1C | 2.11  | 1.42        | 1.38     |
| 31  | 6     | 312 | CLA  | CHC-C1C | 2.11  | 1.42        | 1.38     |
| 31  | A     | 837 | CLA  | C3B-C4B | 2.11  | 1.48        | 1.42     |
| 31  | a     | 611 | CLA  | MG-NB   | -2.11 | 2.01        | 2.05     |
| 30  | 8     | 305 | CHL  | CBD-CGD | -2.11 | 1.49        | 1.52     |
| 31  | 7     | 316 | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 31  | 8     | 304 | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 31  | i     | 613 | CLA  | MG-NB   | -2.11 | 2.01        | 2.05     |
| 31  | 7     | 311 | CLA  | CHC-C1C | 2.11  | 1.42        | 1.38     |
| 31  | A     | 840 | CLA  | CMC-C2C | -2.11 | 1.46        | 1.50     |
| 31  | H     | 204 | CLA  | CMC-C2C | -2.11 | 1.46        | 1.50     |
| 31  | 7     | 318 | CLA  | C3B-C4B | 2.11  | 1.48        | 1.42     |
| 31  | 5     | 310 | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 8     | 304 | CLA  | CMB-C2B | -2.11 | 1.46        | 1.50     |
| 31  | b     | 603 | CLA  | CMB-C2B | -2.11 | 1.46        | 1.50     |
| 31  | e     | 611 | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 31  | 4     | 312 | CLA  | C3B-C4B | 2.11  | 1.48        | 1.42     |
| 30  | 7     | 301 | CHL  | CBD-CGD | -2.11 | 1.49        | 1.52     |
| 31  | a     | 603 | CLA  | CHC-C1C | 2.10  | 1.42        | 1.38     |
| 31  | 6     | 309 | CLA  | CMC-C2C | -2.10 | 1.46        | 1.50     |
| 31  | c     | 612 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 31  | B     | 832 | CLA  | CHC-C1C | 2.10  | 1.42        | 1.38     |
| 31  | B     | 808 | CLA  | CMB-C2B | -2.10 | 1.46        | 1.50     |
| 31  | B     | 841 | CLA  | CMB-C2B | -2.10 | 1.46        | 1.50     |
| 31  | K     | 102 | CLA  | CMB-C2B | -2.10 | 1.46        | 1.50     |
| 31  | 1     | 310 | CLA  | CHC-C1C | 2.10  | 1.42        | 1.38     |
| 31  | 7     | 316 | CLA  | C3B-C4B | 2.10  | 1.48        | 1.42     |
| 34  | H     | 203 | LHG  | P-O6    | 2.10  | 1.67        | 1.59     |
| 31  | 2     | 311 | CLA  | C3B-C4B | 2.10  | 1.48        | 1.42     |
| 31  | 5     | 311 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 31  | 6     | 318 | CLA  | CMB-C2B | -2.10 | 1.46        | 1.50     |
| 31  | A     | 809 | CLA  | CMC-C2C | -2.10 | 1.46        | 1.50     |
| 31  | B     | 815 | CLA  | CMC-C2C | -2.10 | 1.46        | 1.50     |
| 31  | i     | 603 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 31  | 0     | 304 | CLA  | CHC-C1C | 2.10  | 1.42        | 1.38     |
| 31  | F     | 301 | CLA  | CHC-C1C | 2.10  | 1.42        | 1.38     |
| 31  | 2     | 314 | CLA  | CHC-C1C | 2.10  | 1.42        | 1.38     |
| 31  | A     | 818 | CLA  | CMC-C2C | -2.10 | 1.46        | 1.50     |
| 31  | O     | 201 | CLA  | CMB-C2B | -2.10 | 1.46        | 1.50     |
| 31  | A     | 815 | CLA  | C3B-C4B | 2.10  | 1.48        | 1.42     |
| 31  | c     | 613 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 31  | B     | 819 | CLA  | C3B-C4B | 2.10  | 1.48        | 1.42     |
| 31  | H     | 201 | CLA  | CMB-C2B | -2.10 | 1.46        | 1.50     |
| 31  | B     | 812 | CLA  | C3B-C4B | 2.10  | 1.48        | 1.42     |
| 37  | b     | 522 | 0IE  | C6-C7   | -2.10 | 1.41        | 1.46     |
| 31  | a     | 604 | CLA  | MG-NB   | -2.10 | 2.01        | 2.05     |
| 31  | 1     | 312 | CLA  | CHC-C1C | 2.10  | 1.42        | 1.38     |
| 31  | A     | 819 | CLA  | CHC-C1C | 2.10  | 1.42        | 1.38     |
| 31  | c     | 610 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 34  | 7     | 602 | LHG  | P-O6    | 2.10  | 1.67        | 1.59     |
| 31  | 0     | 310 | CLA  | CMB-C2B | -2.10 | 1.46        | 1.50     |
| 31  | B     | 813 | CLA  | CMC-C2C | -2.10 | 1.46        | 1.50     |
| 31  | A     | 808 | CLA  | C3B-C4B | 2.10  | 1.48        | 1.42     |
| 34  | d     | 630 | LHG  | P-O6    | 2.10  | 1.67        | 1.59     |
| 31  | K     | 104 | CLA  | CHC-C1C | 2.10  | 1.42        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | A     | 817 | CLA  | CMB-C2B | -2.10 | 1.46        | 1.50     |
| 31  | c     | 610 | CLA  | CMB-C2B | -2.10 | 1.46        | 1.50     |
| 37  | c     | 521 | 0IE  | C15-C16 | 2.10  | 1.40        | 1.35     |
| 34  | g     | 630 | LHG  | P-O6    | 2.10  | 1.67        | 1.59     |
| 31  | 2     | 312 | CLA  | CMC-C2C | -2.10 | 1.46        | 1.50     |
| 31  | A     | 832 | CLA  | CMC-C2C | -2.10 | 1.46        | 1.50     |
| 31  | b     | 604 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 31  | 3     | 308 | CLA  | C3B-C4B | 2.10  | 1.48        | 1.42     |
| 31  | A     | 821 | CLA  | CMC-C2C | -2.10 | 1.46        | 1.50     |
| 31  | e     | 610 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 31  | b     | 611 | CLA  | MG-NB   | -2.10 | 2.01        | 2.05     |
| 31  | i     | 610 | CLA  | MG-NB   | -2.10 | 2.01        | 2.05     |
| 31  | A     | 837 | CLA  | CHC-C1C | 2.10  | 1.42        | 1.38     |
| 31  | B     | 817 | CLA  | CMB-C2B | -2.09 | 1.46        | 1.50     |
| 31  | A     | 834 | CLA  | C3B-C4B | 2.09  | 1.48        | 1.42     |
| 31  | A     | 837 | CLA  | CMC-C2C | -2.09 | 1.46        | 1.50     |
| 31  | g     | 604 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 31  | B     | 816 | CLA  | CHC-C1C | 2.09  | 1.42        | 1.38     |
| 31  | A     | 809 | CLA  | C3B-C4B | 2.09  | 1.48        | 1.42     |
| 31  | 5     | 303 | CLA  | CHC-C1C | 2.09  | 1.42        | 1.38     |
| 31  | 5     | 312 | CLA  | CHC-C1C | 2.09  | 1.42        | 1.38     |
| 34  | 7     | 602 | LHG  | O7-C7   | 2.09  | 1.40        | 1.34     |
| 31  | A     | 838 | CLA  | CMC-C2C | -2.09 | 1.46        | 1.50     |
| 31  | B     | 834 | CLA  | CMC-C2C | -2.09 | 1.46        | 1.50     |
| 31  | B     | 836 | CLA  | CMC-C2C | -2.09 | 1.46        | 1.50     |
| 31  | H     | 202 | CLA  | CMC-C2C | -2.09 | 1.46        | 1.50     |
| 31  | 4     | 304 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 31  | G     | 103 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 30  | 6     | 305 | CHL  | CBD-CGD | -2.09 | 1.49        | 1.52     |
| 31  | A     | 816 | CLA  | CMC-C2C | -2.09 | 1.46        | 1.50     |
| 34  | 3     | 603 | LHG  | P-O6    | 2.09  | 1.67        | 1.59     |
| 34  | a     | 630 | LHG  | P-O6    | 2.09  | 1.67        | 1.59     |
| 37  | d     | 522 | 0IE  | C13-C12 | -2.09 | 1.41        | 1.46     |
| 31  | 3     | 318 | CLA  | CMC-C2C | -2.09 | 1.46        | 1.50     |
| 31  | c     | 603 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 31  | a     | 612 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 31  | 3     | 312 | CLA  | CHC-C1C | 2.09  | 1.42        | 1.38     |
| 31  | 7     | 312 | CLA  | CHC-C1C | 2.09  | 1.42        | 1.38     |
| 31  | 0     | 311 | CLA  | CHC-C1C | 2.09  | 1.42        | 1.38     |
| 31  | A     | 808 | CLA  | CHC-C1C | 2.09  | 1.42        | 1.38     |
| 31  | B     | 839 | CLA  | CHC-C1C | 2.09  | 1.42        | 1.38     |
| 31  | L     | 202 | CLA  | CHC-C1C | 2.09  | 1.42        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | K     | 105 | CLA  | CHC-C1C | 2.09  | 1.42        | 1.38     |
| 31  | g     | 603 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 31  | A     | 809 | CLA  | CHC-C1C | 2.09  | 1.42        | 1.38     |
| 34  | A     | 855 | LHG  | P-O6    | 2.09  | 1.67        | 1.59     |
| 31  | 6     | 314 | CLA  | C3B-C4B | 2.09  | 1.48        | 1.42     |
| 31  | B     | 803 | CLA  | CMB-C2B | -2.09 | 1.46        | 1.50     |
| 31  | d     | 604 | CLA  | CMB-C2B | -2.09 | 1.46        | 1.50     |
| 31  | a     | 610 | CLA  | MG-NB   | -2.09 | 2.01        | 2.05     |
| 34  | 7     | 603 | LHG  | P-O6    | 2.09  | 1.67        | 1.59     |
| 31  | 2     | 314 | CLA  | CMC-C2C | -2.09 | 1.46        | 1.50     |
| 31  | 7     | 315 | CLA  | CHC-C1C | 2.09  | 1.42        | 1.38     |
| 31  | O     | 206 | CLA  | CMB-C2B | -2.09 | 1.46        | 1.50     |
| 31  | b     | 610 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 31  | A     | 841 | CLA  | C3B-C4B | 2.09  | 1.48        | 1.42     |
| 31  | A     | 804 | CLA  | CMC-C2C | -2.09 | 1.46        | 1.50     |
| 31  | i     | 612 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 31  | 4     | 311 | CLA  | CMB-C2B | -2.09 | 1.46        | 1.50     |
| 31  | g     | 613 | CLA  | MG-NB   | -2.09 | 2.01        | 2.05     |
| 31  | B     | 826 | CLA  | CMC-C2C | -2.09 | 1.46        | 1.50     |
| 31  | A     | 839 | CLA  | CHC-C1C | 2.09  | 1.42        | 1.38     |
| 31  | O     | 203 | CLA  | MG-NB   | -2.09 | 2.01        | 2.05     |
| 31  | A     | 807 | CLA  | CMC-C2C | -2.09 | 1.46        | 1.50     |
| 31  | d     | 610 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 31  | d     | 613 | CLA  | MG-NB   | -2.09 | 2.01        | 2.05     |
| 31  | B     | 835 | CLA  | CMC-C2C | -2.09 | 1.46        | 1.50     |
| 31  | H     | 201 | CLA  | CHC-C1C | 2.08  | 1.42        | 1.38     |
| 37  | 7     | 502 | 0IE  | C8-C7   | 2.08  | 1.40        | 1.35     |
| 31  | 0     | 321 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 31  | 2     | 311 | CLA  | CMB-C2B | -2.08 | 1.46        | 1.50     |
| 31  | c     | 604 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 31  | A     | 833 | CLA  | CHC-C1C | 2.08  | 1.42        | 1.38     |
| 31  | 0     | 321 | CLA  | MG-NB   | -2.08 | 2.01        | 2.05     |
| 31  | f     | 603 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 31  | h     | 603 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 31  | h     | 613 | CLA  | MG-NB   | -2.08 | 2.01        | 2.05     |
| 31  | H     | 204 | CLA  | CHC-C1C | 2.08  | 1.42        | 1.38     |
| 31  | 6     | 312 | CLA  | CMC-C2C | -2.08 | 1.46        | 1.50     |
| 31  | 1     | 304 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 31  | A     | 825 | CLA  | CMC-C2C | -2.08 | 1.46        | 1.50     |
| 31  | b     | 612 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 31  | 4     | 309 | CLA  | MG-NB   | -2.08 | 2.01        | 2.05     |
| 31  | H     | 202 | CLA  | CMB-C2B | -2.08 | 1.46        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | d     | 611 | CLA  | MG-NB   | -2.08 | 2.01        | 2.05     |
| 31  | 5     | 308 | CLA  | CHC-C1C | 2.08  | 1.42        | 1.38     |
| 31  | 9     | 309 | CLA  | CMB-C2B | -2.08 | 1.46        | 1.50     |
| 31  | A     | 811 | CLA  | C3B-C4B | 2.08  | 1.48        | 1.42     |
| 31  | h     | 604 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 31  | i     | 603 | CLA  | CMB-C2B | -2.08 | 1.46        | 1.50     |
| 34  | i     | 630 | LHG  | P-O6    | 2.08  | 1.67        | 1.59     |
| 31  | 2     | 310 | CLA  | CMC-C2C | -2.08 | 1.46        | 1.50     |
| 31  | A     | 831 | CLA  | CMC-C2C | -2.08 | 1.46        | 1.50     |
| 31  | A     | 810 | CLA  | CMC-C2C | -2.08 | 1.46        | 1.50     |
| 31  | A     | 829 | CLA  | CMC-C2C | -2.08 | 1.46        | 1.50     |
| 31  | A     | 836 | CLA  | CHC-C1C | 2.08  | 1.42        | 1.38     |
| 31  | B     | 811 | CLA  | CHC-C1C | 2.08  | 1.42        | 1.38     |
| 31  | B     | 810 | CLA  | C3B-C4B | 2.08  | 1.48        | 1.42     |
| 31  | A     | 839 | CLA  | CMC-C2C | -2.08 | 1.46        | 1.50     |
| 31  | b     | 611 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 31  | f     | 603 | CLA  | CMB-C2B | -2.08 | 1.46        | 1.50     |
| 31  | 7     | 316 | CLA  | CHC-C1C | 2.08  | 1.42        | 1.38     |
| 31  | 5     | 312 | CLA  | CMB-C2B | -2.08 | 1.46        | 1.50     |
| 31  | B     | 812 | CLA  | CMC-C2C | -2.08 | 1.46        | 1.50     |
| 31  | f     | 611 | CLA  | CMB-C2B | -2.08 | 1.46        | 1.50     |
| 30  | g     | 609 | CHL  | CMC-C2C | 2.08  | 1.49        | 1.44     |
| 31  | 4     | 312 | CLA  | CHC-C1C | 2.08  | 1.42        | 1.38     |
| 31  | L     | 201 | CLA  | CMC-C2C | -2.08 | 1.46        | 1.50     |
| 31  | c     | 603 | CLA  | CMB-C2B | -2.08 | 1.46        | 1.50     |
| 31  | d     | 613 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 31  | 5     | 304 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 31  | A     | 820 | CLA  | CMC-C2C | -2.07 | 1.46        | 1.50     |
| 31  | 1     | 308 | CLA  | CHC-C1C | 2.07  | 1.42        | 1.38     |
| 31  | A     | 828 | CLA  | CMB-C2B | -2.07 | 1.46        | 1.50     |
| 31  | 5     | 311 | CLA  | CMB-C2B | -2.07 | 1.46        | 1.50     |
| 31  | 5     | 308 | CLA  | CMB-C2B | -2.07 | 1.46        | 1.50     |
| 31  | A     | 852 | CLA  | CMC-C2C | -2.07 | 1.46        | 1.50     |
| 31  | B     | 838 | CLA  | CMC-C2C | -2.07 | 1.46        | 1.50     |
| 31  | B     | 819 | CLA  | CMC-C2C | -2.07 | 1.46        | 1.50     |
| 31  | A     | 843 | CLA  | CHC-C1C | 2.07  | 1.42        | 1.38     |
| 31  | 6     | 304 | CLA  | CMC-C2C | -2.07 | 1.46        | 1.50     |
| 31  | h     | 603 | CLA  | MG-NB   | -2.07 | 2.01        | 2.05     |
| 31  | e     | 613 | CLA  | MG-NB   | -2.07 | 2.01        | 2.05     |
| 31  | B     | 823 | CLA  | CMC-C2C | -2.07 | 1.46        | 1.50     |
| 31  | A     | 841 | CLA  | CHC-C1C | 2.07  | 1.42        | 1.38     |
| 31  | d     | 610 | CLA  | MG-NB   | -2.07 | 2.01        | 2.05     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | A     | 823 | CLA  | CMC-C2C | -2.07 | 1.46        | 1.50     |
| 31  | c     | 612 | CLA  | CMB-C2B | -2.07 | 1.46        | 1.50     |
| 31  | 7     | 316 | CLA  | CMC-C2C | -2.07 | 1.46        | 1.50     |
| 31  | A     | 834 | CLA  | CMC-C2C | -2.07 | 1.46        | 1.50     |
| 31  | 0     | 303 | CLA  | CHC-C1C | 2.07  | 1.42        | 1.38     |
| 31  | A     | 814 | CLA  | C3B-C4B | 2.07  | 1.48        | 1.42     |
| 31  | B     | 829 | CLA  | CMC-C2C | -2.07 | 1.46        | 1.50     |
| 31  | L     | 203 | CLA  | CMC-C2C | -2.07 | 1.46        | 1.50     |
| 31  | f     | 612 | CLA  | CMC-C2C | -2.07 | 1.46        | 1.50     |
| 31  | d     | 603 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 33  | 4     | 501 | 0UR  | C29-C28 | -2.07 | 1.52        | 1.54     |
| 31  | i     | 611 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 31  | 9     | 310 | CLA  | CMC-C2C | -2.07 | 1.46        | 1.50     |
| 31  | e     | 603 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 31  | g     | 612 | CLA  | MG-NB   | -2.07 | 2.01        | 2.05     |
| 31  | h     | 612 | CLA  | MG-NB   | -2.07 | 2.01        | 2.05     |
| 31  | a     | 611 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 31  | f     | 612 | CLA  | CMB-C2B | -2.07 | 1.46        | 1.50     |
| 33  | 6     | 501 | 0UR  | C29-C28 | -2.07 | 1.52        | 1.54     |
| 31  | B     | 831 | CLA  | C3B-C4B | 2.07  | 1.48        | 1.42     |
| 31  | K     | 102 | CLA  | CMC-C2C | -2.07 | 1.46        | 1.50     |
| 31  | A     | 823 | CLA  | CHC-C1C | 2.07  | 1.42        | 1.38     |
| 37  | 3     | 502 | 0IE  | C11-C12 | 2.07  | 1.40        | 1.35     |
| 31  | 5     | 308 | CLA  | MG-NB   | -2.07 | 2.01        | 2.05     |
| 31  | 0     | 312 | CLA  | CMC-C2C | -2.07 | 1.46        | 1.50     |
| 31  | 9     | 302 | CLA  | CMC-C2C | -2.07 | 1.46        | 1.50     |
| 31  | f     | 610 | CLA  | CMB-C2B | -2.07 | 1.46        | 1.50     |
| 31  | 8     | 314 | CLA  | CMB-C2B | -2.07 | 1.46        | 1.50     |
| 31  | 1     | 308 | CLA  | MG-NB   | -2.07 | 2.01        | 2.05     |
| 31  | B     | 805 | CLA  | C3B-C4B | 2.07  | 1.48        | 1.42     |
| 37  | c     | 522 | 0IE  | C13-C12 | -2.07 | 1.41        | 1.46     |
| 31  | f     | 604 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 34  | B     | 854 | LHG  | P-O6    | 2.06  | 1.67        | 1.59     |
| 31  | L     | 204 | CLA  | CMC-C2C | -2.06 | 1.46        | 1.50     |
| 30  | 8     | 301 | CHL  | CBD-CGD | -2.06 | 1.49        | 1.52     |
| 31  | A     | 836 | CLA  | CMC-C2C | -2.06 | 1.46        | 1.50     |
| 31  | L     | 204 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 31  | d     | 612 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 31  | G     | 101 | CLA  | CMB-C2B | -2.06 | 1.46        | 1.50     |
| 31  | L     | 202 | CLA  | CMC-C2C | -2.06 | 1.46        | 1.50     |
| 31  | 3     | 320 | CLA  | CMC-C2C | -2.06 | 1.46        | 1.50     |
| 31  | A     | 833 | CLA  | CMC-C2C | -2.06 | 1.46        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 2     | 304 | CLA  | CMC-C2C | -2.06 | 1.46        | 1.50     |
| 31  | 3     | 308 | CLA  | CHC-C1C | 2.06  | 1.42        | 1.38     |
| 31  | O     | 203 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 31  | c     | 613 | CLA  | CMB-C2B | -2.06 | 1.46        | 1.50     |
| 31  | 8     | 310 | CLA  | CMC-C2C | -2.06 | 1.46        | 1.50     |
| 31  | a     | 610 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 32  | 9     | 401 | 8CT  | C33-C32 | -2.06 | 1.44        | 1.50     |
| 37  | 3     | 502 | 0IE  | C8-C7   | 2.06  | 1.40        | 1.35     |
| 31  | 5     | 314 | CLA  | CMB-C2B | -2.06 | 1.46        | 1.50     |
| 31  | A     | 802 | CLA  | C3B-C4B | 2.06  | 1.48        | 1.42     |
| 31  | B     | 815 | CLA  | CMB-C2B | -2.06 | 1.46        | 1.50     |
| 31  | g     | 604 | CLA  | CMB-C2B | -2.06 | 1.46        | 1.50     |
| 31  | 7     | 303 | CLA  | CMC-C2C | -2.06 | 1.46        | 1.50     |
| 31  | a     | 613 | CLA  | MG-NB   | -2.06 | 2.01        | 2.05     |
| 31  | 8     | 303 | CLA  | CHC-C1C | 2.06  | 1.42        | 1.38     |
| 31  | i     | 604 | CLA  | CMB-C2B | -2.06 | 1.46        | 1.50     |
| 31  | i     | 610 | CLA  | CMC-C2C | -2.06 | 1.46        | 1.50     |
| 31  | B     | 830 | CLA  | C1B-NB  | -2.06 | 1.35        | 1.37     |
| 31  | 9     | 312 | CLA  | CMC-C2C | -2.06 | 1.46        | 1.50     |
| 36  | J     | 105 | LMG  | O6-C5   | -2.06 | 1.39        | 1.44     |
| 33  | 6     | 502 | 0UR  | C19-C18 | 2.06  | 1.53        | 1.50     |
| 31  | g     | 611 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 31  | 4     | 314 | CLA  | CMB-C2B | -2.06 | 1.46        | 1.50     |
| 31  | 7     | 315 | CLA  | MG-NB   | -2.06 | 2.01        | 2.05     |
| 30  | 1     | 305 | CHL  | CBD-CGD | -2.06 | 1.49        | 1.52     |
| 31  | a     | 613 | CLA  | CMC-C2C | -2.06 | 1.46        | 1.50     |
| 31  | B     | 819 | CLA  | CHC-C1C | 2.05  | 1.42        | 1.38     |
| 31  | B     | 817 | CLA  | CMC-C2C | -2.05 | 1.46        | 1.50     |
| 31  | g     | 613 | CLA  | CMB-C2B | -2.05 | 1.46        | 1.50     |
| 31  | h     | 613 | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 31  | g     | 610 | CLA  | MG-NB   | -2.05 | 2.01        | 2.05     |
| 31  | 0     | 309 | CLA  | CMC-C2C | -2.05 | 1.46        | 1.50     |
| 31  | B     | 805 | CLA  | CHC-C1C | 2.05  | 1.42        | 1.38     |
| 30  | 2     | 302 | CHL  | CBD-CGD | -2.05 | 1.49        | 1.52     |
| 31  | B     | 831 | CLA  | CMC-C2C | -2.05 | 1.46        | 1.50     |
| 31  | B     | 801 | CLA  | C1B-C2B | 2.05  | 1.47        | 1.43     |
| 31  | A     | 822 | CLA  | CMC-C2C | -2.05 | 1.46        | 1.50     |
| 31  | K     | 101 | CLA  | CMC-C2C | -2.05 | 1.46        | 1.50     |
| 31  | d     | 603 | CLA  | CMB-C2B | -2.05 | 1.46        | 1.50     |
| 31  | g     | 603 | CLA  | MG-NB   | -2.05 | 2.01        | 2.05     |
| 31  | B     | 838 | CLA  | CHC-C1C | 2.05  | 1.42        | 1.38     |
| 31  | B     | 820 | CLA  | CMC-C2C | -2.05 | 1.46        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | h     | 612 | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 30  | 3     | 305 | CHL  | CBD-CGD | -2.05 | 1.49        | 1.52     |
| 31  | 0     | 310 | CLA  | CMC-C2C | -2.05 | 1.46        | 1.50     |
| 31  | a     | 603 | CLA  | CMB-C2B | -2.05 | 1.46        | 1.50     |
| 31  | h     | 610 | CLA  | MG-NB   | -2.05 | 2.01        | 2.05     |
| 31  | B     | 837 | CLA  | CMC-C2C | -2.05 | 1.46        | 1.50     |
| 31  | a     | 604 | CLA  | CMC-C2C | -2.05 | 1.46        | 1.50     |
| 31  | 7     | 304 | CLA  | CHC-C1C | 2.05  | 1.42        | 1.38     |
| 31  | 2     | 303 | CLA  | CHC-C1C | 2.05  | 1.42        | 1.38     |
| 37  | 7     | 502 | 0IE  | C11-C12 | 2.05  | 1.40        | 1.35     |
| 34  | 9     | 601 | LHG  | P-O6    | 2.05  | 1.67        | 1.59     |
| 30  | g     | 605 | CHL  | CMC-C2C | 2.05  | 1.49        | 1.44     |
| 31  | 3     | 313 | CLA  | CMC-C2C | -2.05 | 1.46        | 1.50     |
| 31  | 9     | 309 | CLA  | CMC-C2C | -2.05 | 1.46        | 1.50     |
| 31  | d     | 604 | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 31  | a     | 612 | CLA  | MG-NB   | -2.05 | 2.01        | 2.05     |
| 31  | g     | 604 | CLA  | MG-NB   | -2.05 | 2.01        | 2.05     |
| 31  | A     | 826 | CLA  | CMC-C2C | -2.05 | 1.46        | 1.50     |
| 31  | G     | 102 | CLA  | CMB-C2B | -2.05 | 1.46        | 1.50     |
| 31  | B     | 839 | CLA  | CMC-C2C | -2.05 | 1.46        | 1.50     |
| 31  | 0     | 304 | CLA  | CMC-C2C | -2.05 | 1.46        | 1.50     |
| 31  | B     | 830 | CLA  | C3B-C4B | 2.05  | 1.48        | 1.42     |
| 30  | a     | 607 | CHL  | CMC-C2C | 2.05  | 1.49        | 1.44     |
| 31  | 6     | 314 | CLA  | CHC-C1C | 2.05  | 1.42        | 1.38     |
| 31  | 7     | 304 | CLA  | CMC-C2C | -2.04 | 1.46        | 1.50     |
| 31  | f     | 604 | CLA  | CMC-C2C | -2.04 | 1.46        | 1.50     |
| 31  | f     | 610 | CLA  | CMC-C2C | -2.04 | 1.46        | 1.50     |
| 31  | B     | 821 | CLA  | CHC-C1C | 2.04  | 1.42        | 1.38     |
| 30  | h     | 609 | CHL  | CMC-C2C | 2.04  | 1.49        | 1.44     |
| 31  | a     | 613 | CLA  | CMB-C2B | -2.04 | 1.46        | 1.50     |
| 31  | 1     | 310 | CLA  | CMC-C2C | -2.04 | 1.46        | 1.50     |
| 31  | b     | 613 | CLA  | CMB-C2B | -2.04 | 1.46        | 1.50     |
| 31  | 6     | 304 | CLA  | CHC-C1C | 2.04  | 1.42        | 1.38     |
| 31  | O     | 206 | CLA  | CMC-C2C | -2.04 | 1.46        | 1.50     |
| 31  | i     | 604 | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 31  | e     | 604 | CLA  | CMC-C2C | -2.04 | 1.46        | 1.50     |
| 31  | O     | 203 | CLA  | CMB-C2B | -2.04 | 1.46        | 1.50     |
| 30  | g     | 614 | CHL  | CMC-C2C | 2.04  | 1.49        | 1.44     |
| 31  | h     | 604 | CLA  | CMB-C2B | -2.04 | 1.46        | 1.50     |
| 31  | 5     | 311 | CLA  | CHC-C1C | 2.04  | 1.42        | 1.38     |
| 31  | 9     | 308 | CLA  | CHC-C1C | 2.04  | 1.42        | 1.38     |
| 31  | 6     | 317 | CLA  | CMC-C2C | -2.04 | 1.46        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 0     | 313 | CLA  | CHC-C1C | 2.04  | 1.42        | 1.38     |
| 31  | i     | 610 | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 31  | e     | 610 | CLA  | CMC-C2C | -2.04 | 1.46        | 1.50     |
| 36  | J     | 102 | LMG  | O4-C4   | -2.04 | 1.37        | 1.43     |
| 31  | B     | 806 | CLA  | MG-ND   | -2.04 | 2.01        | 2.05     |
| 31  | O     | 202 | CLA  | CMC-C2C | -2.04 | 1.46        | 1.50     |
| 31  | d     | 613 | CLA  | CMB-C2B | -2.04 | 1.46        | 1.50     |
| 33  | 2     | 501 | 0UR  | C29-C28 | -2.04 | 1.52        | 1.54     |
| 31  | 0     | 303 | CLA  | CMC-C2C | -2.04 | 1.46        | 1.50     |
| 31  | g     | 612 | CLA  | CMB-C2B | -2.04 | 1.46        | 1.50     |
| 33  | O     | 204 | 0UR  | C29-C28 | -2.04 | 1.52        | 1.54     |
| 31  | 4     | 304 | CLA  | CHC-C1C | 2.04  | 1.42        | 1.38     |
| 31  | 1     | 314 | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 31  | a     | 613 | CLA  | CMD-C2D | -2.03 | 1.46        | 1.50     |
| 31  | g     | 611 | CLA  | MG-NB   | -2.03 | 2.01        | 2.05     |
| 31  | A     | 830 | CLA  | C3B-C4B | 2.03  | 1.48        | 1.42     |
| 31  | d     | 610 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 31  | h     | 610 | CLA  | CMD-C2D | -2.03 | 1.46        | 1.50     |
| 31  | e     | 603 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 30  | h     | 605 | CHL  | CMC-C2C | 2.03  | 1.49        | 1.44     |
| 31  | 1     | 304 | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 31  | 3     | 320 | CLA  | CHC-C1C | 2.03  | 1.42        | 1.38     |
| 30  | g     | 601 | CHL  | CMC-C2C | 2.03  | 1.49        | 1.44     |
| 34  | b     | 630 | LHG  | P-O6    | 2.03  | 1.67        | 1.59     |
| 31  | 7     | 312 | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 31  | L     | 207 | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 30  | h     | 614 | CHL  | CMC-C2C | 2.03  | 1.49        | 1.44     |
| 31  | 0     | 313 | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 31  | 6     | 320 | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 31  | d     | 613 | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 31  | 4     | 309 | CLA  | CMD-C2D | -2.03 | 1.46        | 1.50     |
| 31  | b     | 610 | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 30  | f     | 605 | CHL  | CMC-C2C | 2.03  | 1.49        | 1.44     |
| 31  | 3     | 308 | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 31  | d     | 612 | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 30  | d     | 614 | CHL  | CMC-C2C | 2.03  | 1.49        | 1.44     |
| 31  | 6     | 314 | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 31  | A     | 830 | CLA  | MG-ND   | -2.03 | 2.01        | 2.05     |
| 31  | 1     | 308 | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 31  | h     | 603 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 31  | c     | 610 | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 31  | 6     | 303 | CLA  | C3B-C4B | 2.03  | 1.48        | 1.42     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | c     | 612 | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 31  | b     | 612 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 31  | f     | 611 | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 31  | g     | 613 | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 31  | B     | 827 | CLA  | CHC-C1C | 2.02  | 1.42        | 1.38     |
| 31  | B     | 803 | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 31  | i     | 611 | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 31  | 4     | 314 | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 34  | 0     | 601 | LHG  | P-O6    | 2.02  | 1.67        | 1.59     |
| 31  | g     | 613 | CLA  | CMD-C2D | -2.02 | 1.46        | 1.50     |
| 31  | 2     | 312 | CLA  | CHC-C1C | 2.02  | 1.42        | 1.38     |
| 31  | 5     | 310 | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 31  | A     | 816 | CLA  | CHC-C1C | 2.02  | 1.42        | 1.38     |
| 31  | 3     | 310 | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 31  | J     | 103 | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 31  | 3     | 306 | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 31  | B     | 821 | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 31  | 5     | 308 | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 34  | 5     | 601 | LHG  | P-O6    | 2.02  | 1.67        | 1.59     |
| 31  | 6     | 318 | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 31  | A     | 808 | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 31  | e     | 612 | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 31  | B     | 841 | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 31  | G     | 102 | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 31  | O     | 201 | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 31  | h     | 611 | CLA  | CMD-C2D | -2.02 | 1.46        | 1.50     |
| 31  | B     | 821 | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 31  | h     | 611 | CLA  | MG-NB   | -2.02 | 2.01        | 2.05     |
| 35  | 0     | 603 | SQD  | O3-C3   | -2.02 | 1.38        | 1.43     |
| 31  | d     | 610 | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 31  | e     | 611 | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 31  | 3     | 304 | CLA  | CHC-C1C | 2.02  | 1.42        | 1.38     |
| 31  | e     | 611 | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 31  | 7     | 318 | CLA  | CHC-C1C | 2.02  | 1.42        | 1.38     |
| 31  | 6     | 310 | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 31  | a     | 604 | CLA  | CMD-C2D | -2.02 | 1.46        | 1.50     |
| 31  | b     | 611 | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 30  | h     | 607 | CHL  | CMC-C2C | 2.02  | 1.49        | 1.44     |
| 31  | h     | 612 | CLA  | CMB-C2B | -2.01 | 1.46        | 1.50     |
| 30  | 1     | 313 | CHL  | CBD-CGD | -2.01 | 1.50        | 1.52     |
| 31  | A     | 815 | CLA  | CHC-C1C | 2.01  | 1.42        | 1.38     |
| 31  | A     | 832 | CLA  | CHC-C1C | 2.01  | 1.42        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | g     | 610 | CLA  | CMD-C2D | -2.01 | 1.46        | 1.50     |
| 31  | H     | 205 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 31  | b     | 613 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 31  | e     | 613 | CLA  | CMD-C2D | -2.01 | 1.46        | 1.50     |
| 30  | 5     | 313 | CHL  | CBD-CGD | -2.01 | 1.50        | 1.52     |
| 31  | 9     | 304 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 30  | i     | 614 | CHL  | CMC-C2C | 2.01  | 1.49        | 1.44     |
| 31  | A     | 802 | CLA  | CHC-C1C | 2.01  | 1.42        | 1.38     |
| 31  | 5     | 309 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 31  | A     | 853 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 31  | c     | 604 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 30  | d     | 609 | CHL  | CMC-C2C | 2.01  | 1.49        | 1.44     |
| 31  | 7     | 310 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 31  | a     | 611 | CLA  | CMB-C2B | -2.01 | 1.46        | 1.50     |
| 31  | H     | 201 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 31  | B     | 840 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 31  | e     | 612 | CLA  | CMB-C2B | -2.01 | 1.46        | 1.50     |
| 31  | B     | 830 | CLA  | C1B-C2B | 2.01  | 1.47        | 1.43     |
| 34  | 7     | 601 | LHG  | P-O6    | 2.01  | 1.67        | 1.59     |
| 30  | 6     | 302 | CHL  | CBD-CGD | -2.01 | 1.50        | 1.52     |
| 31  | h     | 610 | CLA  | CMB-C2B | -2.01 | 1.46        | 1.50     |
| 34  | 8     | 601 | LHG  | P-O6    | 2.01  | 1.67        | 1.59     |
| 35  | 0     | 603 | SQD  | O2-C2   | -2.01 | 1.38        | 1.43     |
| 30  | a     | 605 | CHL  | CMC-C2C | 2.01  | 1.49        | 1.44     |
| 31  | d     | 611 | CLA  | CMB-C2B | -2.00 | 1.46        | 1.50     |
| 34  | M     | 104 | LHG  | P-O6    | 2.00  | 1.67        | 1.59     |
| 31  | 0     | 308 | CLA  | CMC-C2C | -2.00 | 1.46        | 1.50     |
| 33  | 3     | 501 | 0UR  | C29-C28 | -2.00 | 1.52        | 1.54     |
| 31  | 8     | 314 | CLA  | CMC-C2C | -2.00 | 1.46        | 1.50     |
| 31  | b     | 603 | CLA  | CMC-C2C | -2.00 | 1.46        | 1.50     |
| 31  | i     | 613 | CLA  | CMD-C2D | -2.00 | 1.46        | 1.50     |
| 30  | c     | 609 | CHL  | CMC-C2C | 2.00  | 1.49        | 1.44     |
| 34  | 6     | 601 | LHG  | P-O6    | 2.00  | 1.67        | 1.59     |
| 36  | A     | 856 | LMG  | O7-C8   | -2.00 | 1.41        | 1.46     |
| 31  | K     | 105 | CLA  | CMC-C2C | -2.00 | 1.46        | 1.50     |
| 31  | d     | 611 | CLA  | CMD-C2D | -2.00 | 1.46        | 1.50     |
| 31  | c     | 613 | CLA  | CMC-C2C | -2.00 | 1.46        | 1.50     |
| 31  | A     | 834 | CLA  | CHC-C1C | 2.00  | 1.42        | 1.38     |

All (5235) bond angle outliers are listed below:

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| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 31  | B     | 823 | CLA  | O2A-CGA-O1A | -19.95 | 73.72       | 123.63   |
| 42  | a     | 523 | NEX  | O24-C25-C24 | 15.72  | 128.22      | 113.49   |
| 42  | i     | 523 | NEX  | O24-C25-C24 | 15.69  | 128.19      | 113.49   |
| 42  | c     | 523 | NEX  | O24-C25-C24 | 15.68  | 128.18      | 113.49   |
| 42  | f     | 523 | NEX  | O24-C25-C24 | 15.68  | 128.18      | 113.49   |
| 42  | d     | 523 | NEX  | O24-C25-C24 | 15.67  | 128.18      | 113.49   |
| 42  | g     | 523 | NEX  | O24-C25-C24 | 15.67  | 128.18      | 113.49   |
| 42  | b     | 523 | NEX  | O24-C25-C24 | 15.67  | 128.17      | 113.49   |
| 42  | h     | 523 | NEX  | O24-C25-C24 | 15.65  | 128.16      | 113.49   |
| 31  | B     | 823 | CLA  | O2A-CGA-CBA | 15.02  | 157.64      | 111.83   |
| 42  | d     | 523 | NEX  | C20-C13-C12 | 13.91  | 139.34      | 118.09   |
| 42  | h     | 523 | NEX  | C20-C13-C12 | 13.90  | 139.33      | 118.09   |
| 42  | f     | 523 | NEX  | C20-C13-C12 | 13.89  | 139.30      | 118.09   |
| 42  | b     | 523 | NEX  | C20-C13-C12 | 13.88  | 139.29      | 118.09   |
| 42  | a     | 523 | NEX  | C20-C13-C12 | 13.87  | 139.28      | 118.09   |
| 42  | c     | 523 | NEX  | C20-C13-C12 | 13.87  | 139.28      | 118.09   |
| 42  | i     | 523 | NEX  | C20-C13-C12 | 13.87  | 139.28      | 118.09   |
| 42  | g     | 523 | NEX  | C20-C13-C12 | 13.86  | 139.25      | 118.09   |
| 42  | c     | 523 | NEX  | C12-C13-C14 | -11.92 | 100.26      | 119.01   |
| 42  | h     | 523 | NEX  | C12-C13-C14 | -11.90 | 100.29      | 119.01   |
| 42  | d     | 523 | NEX  | C12-C13-C14 | -11.90 | 100.29      | 119.01   |
| 42  | g     | 523 | NEX  | C12-C13-C14 | -11.90 | 100.29      | 119.01   |
| 42  | i     | 523 | NEX  | C12-C13-C14 | -11.90 | 100.30      | 119.01   |
| 42  | f     | 523 | NEX  | C12-C13-C14 | -11.89 | 100.31      | 119.01   |
| 42  | b     | 523 | NEX  | C12-C13-C14 | -11.88 | 100.32      | 119.01   |
| 32  | K     | 107 | 8CT  | C33-C32-C31 | -11.86 | 113.51      | 124.83   |
| 42  | a     | 523 | NEX  | C12-C13-C14 | -11.86 | 100.35      | 119.01   |
| 32  | G     | 104 | 8CT  | C33-C32-C31 | -11.78 | 113.59      | 124.83   |
| 31  | B     | 826 | CLA  | CHA-C4D-ND  | 11.48  | 135.04      | 125.22   |
| 30  | 0     | 306 | CHL  | O2D-CGD-CBD | 11.23  | 123.28      | 110.95   |
| 32  | A     | 849 | 8CT  | C33-C32-C31 | -11.19 | 114.15      | 124.83   |
| 32  | M     | 102 | 8CT  | C33-C32-C31 | -11.05 | 114.28      | 124.83   |
| 32  | A     | 847 | 8CT  | C33-C32-C31 | -10.83 | 114.49      | 124.83   |
| 32  | 7     | 404 | 8CT  | C33-C32-C31 | -10.74 | 114.58      | 124.83   |
| 32  | J     | 104 | 8CT  | C33-C32-C31 | -10.74 | 114.58      | 124.83   |
| 30  | 8     | 301 | CHL  | O2D-CGD-CBD | 10.69  | 122.69      | 110.95   |
| 32  | B     | 844 | 8CT  | C33-C32-C31 | -10.69 | 114.63      | 124.83   |
| 32  | J     | 101 | 8CT  | C33-C32-C31 | -10.67 | 114.65      | 124.83   |
| 32  | B     | 845 | 8CT  | C33-C32-C31 | -10.66 | 114.66      | 124.83   |
| 32  | 3     | 402 | 8CT  | C33-C32-C31 | -10.36 | 114.94      | 124.83   |
| 32  | A     | 846 | 8CT  | C33-C32-C31 | -10.34 | 114.96      | 124.83   |

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| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 32  | 6     | 402 | 8CT  | C14-C13-C12 | -10.28 | 112.87      | 127.28   |
| 32  | J     | 104 | 8CT  | C18-C17-C16 | -10.20 | 112.97      | 127.28   |
| 32  | 2     | 402 | 8CT  | C33-C32-C31 | -10.20 | 115.09      | 124.83   |
| 31  | B     | 823 | CLA  | O1A-CGA-CBA | -10.18 | 83.98       | 123.78   |
| 30  | 6     | 302 | CHL  | O2D-CGD-CBD | 10.08  | 122.02      | 110.95   |
| 32  | B     | 847 | 8CT  | C33-C32-C31 | -10.07 | 115.22      | 124.83   |
| 32  | 0     | 401 | 8CT  | C33-C32-C31 | -9.99  | 115.30      | 124.83   |
| 42  | c     | 523 | NEX  | C30-C31-C32 | -9.95  | 94.38       | 123.20   |
| 42  | i     | 523 | NEX  | C30-C31-C32 | -9.94  | 94.39       | 123.20   |
| 42  | d     | 523 | NEX  | C30-C31-C32 | -9.94  | 94.40       | 123.20   |
| 42  | f     | 523 | NEX  | C30-C31-C32 | -9.94  | 94.40       | 123.20   |
| 42  | g     | 523 | NEX  | C30-C31-C32 | -9.93  | 94.42       | 123.20   |
| 42  | h     | 523 | NEX  | C30-C31-C32 | -9.93  | 94.43       | 123.20   |
| 42  | b     | 523 | NEX  | C30-C31-C32 | -9.92  | 94.46       | 123.20   |
| 42  | a     | 523 | NEX  | C30-C31-C32 | -9.92  | 94.46       | 123.20   |
| 32  | L     | 205 | 8CT  | C33-C32-C31 | -9.87  | 115.41      | 124.83   |
| 32  | A     | 850 | 8CT  | C33-C32-C31 | -9.86  | 115.42      | 124.83   |
| 32  | 8     | 402 | 8CT  | C33-C32-C31 | -9.85  | 115.43      | 124.83   |
| 32  | 4     | 402 | 8CT  | C33-C32-C31 | -9.82  | 115.46      | 124.83   |
| 32  | A     | 854 | 8CT  | C33-C32-C31 | -9.78  | 115.49      | 124.83   |
| 32  | I     | 101 | 8CT  | C33-C32-C31 | -9.78  | 115.50      | 124.83   |
| 32  | 7     | 404 | 8CT  | C14-C13-C12 | -9.76  | 113.60      | 127.28   |
| 30  | 6     | 306 | CHL  | C1B-CHB-C4A | 9.75   | 127.60      | 121.32   |
| 30  | 9     | 306 | CHL  | O2D-CGD-CBD | 9.75   | 121.66      | 110.95   |
| 30  | 2     | 307 | CHL  | C1B-CHB-C4A | 9.64   | 127.53      | 121.32   |
| 32  | 3     | 402 | 8CT  | C14-C13-C12 | -9.64  | 113.76      | 127.28   |
| 30  | 2     | 305 | CHL  | C1B-CHB-C4A | 9.48   | 127.42      | 121.32   |
| 32  | 7     | 404 | 8CT  | C10-C11-C12 | -9.47  | 112.22      | 126.23   |
| 30  | 4     | 313 | CHL  | O2D-CGD-CBD | 9.43   | 121.31      | 110.95   |
| 30  | 6     | 301 | CHL  | O2D-CGD-CBD | 9.39   | 121.27      | 110.95   |
| 30  | 9     | 305 | CHL  | C1B-CHB-C4A | 9.35   | 127.34      | 121.32   |
| 30  | 2     | 319 | CHL  | O2D-CGD-CBD | 9.35   | 121.22      | 110.95   |
| 30  | 3     | 307 | CHL  | C1B-CHB-C4A | 9.33   | 127.32      | 121.32   |
| 30  | 1     | 302 | CHL  | C1B-CHB-C4A | 9.26   | 127.28      | 121.32   |
| 30  | 3     | 302 | CHL  | C1B-CHB-C4A | 9.25   | 127.27      | 121.32   |
| 32  | F     | 302 | 8CT  | C33-C32-C31 | -9.22  | 116.03      | 124.83   |
| 30  | 5     | 302 | CHL  | C1B-CHB-C4A | 9.22   | 127.25      | 121.32   |
| 30  | 5     | 313 | CHL  | O2D-CGD-CBD | 9.21   | 121.06      | 110.95   |
| 30  | 7     | 301 | CHL  | O2D-CGD-CBD | 9.17   | 121.02      | 110.95   |
| 32  | J     | 104 | 8CT  | C10-C11-C12 | -9.17  | 112.68      | 126.23   |
| 32  | 7     | 405 | 8CT  | C33-C32-C31 | -9.15  | 116.10      | 124.83   |
| 30  | 2     | 306 | CHL  | O2D-CGD-CBD | 9.14   | 120.99      | 110.95   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | 7     | 306 | CHL  | O2D-CGD-CBD | 9.11  | 120.95      | 110.95   |
| 30  | 1     | 305 | CHL  | C1B-CHB-C4A | 9.11  | 127.18      | 121.32   |
| 30  | 9     | 313 | CHL  | O2D-CGD-CBD | 9.07  | 120.92      | 110.95   |
| 30  | 7     | 302 | CHL  | C1B-CHB-C4A | 9.07  | 127.16      | 121.32   |
| 30  | 8     | 302 | CHL  | C1B-CHB-C4A | 9.02  | 127.12      | 121.32   |
| 30  | h     | 609 | CHL  | O2D-CGD-CBD | 9.01  | 120.84      | 110.95   |
| 30  | 0     | 305 | CHL  | O2D-CGD-CBD | 8.99  | 120.83      | 110.95   |
| 32  | B     | 848 | 8CT  | C33-C32-C31 | -8.98 | 116.25      | 124.83   |
| 30  | 6     | 302 | CHL  | C1B-CHB-C4A | 8.98  | 127.10      | 121.32   |
| 30  | g     | 606 | CHL  | O2D-CGD-CBD | 8.98  | 120.81      | 110.95   |
| 30  | f     | 606 | CHL  | O2D-CGD-CBD | 8.95  | 120.78      | 110.95   |
| 30  | 4     | 305 | CHL  | C1B-CHB-C4A | 8.92  | 127.06      | 121.32   |
| 30  | 4     | 305 | CHL  | O2D-CGD-CBD | 8.91  | 120.73      | 110.95   |
| 30  | d     | 601 | CHL  | O2D-CGD-CBD | 8.89  | 120.72      | 110.95   |
| 30  | 4     | 308 | CHL  | O2D-CGD-CBD | 8.89  | 120.72      | 110.95   |
| 30  | c     | 614 | CHL  | O2D-CGD-CBD | 8.88  | 120.71      | 110.95   |
| 30  | b     | 602 | CHL  | O2D-CGD-CBD | 8.86  | 120.68      | 110.95   |
| 30  | 2     | 301 | CHL  | O2D-CGD-CBD | 8.84  | 120.66      | 110.95   |
| 32  | 6     | 402 | 8CT  | C18-C17-C16 | -8.83 | 114.89      | 127.28   |
| 42  | e     | 523 | NEX  | O24-C25-C24 | 8.83  | 121.77      | 113.49   |
| 30  | 5     | 305 | CHL  | O2D-CGD-CBD | 8.83  | 120.65      | 110.95   |
| 42  | e     | 523 | NEX  | C38-C25-C26 | -8.83 | 107.77      | 122.30   |
| 30  | 3     | 305 | CHL  | O2D-CGD-CBD | 8.82  | 120.64      | 110.95   |
| 30  | 9     | 301 | CHL  | O2D-CGD-CBD | 8.82  | 120.64      | 110.95   |
| 30  | 8     | 306 | CHL  | O2D-CGD-CBD | 8.81  | 120.62      | 110.95   |
| 31  | B     | 826 | CLA  | CBD-CHA-C1A | 8.80  | 130.50      | 118.85   |
| 32  | L     | 209 | 8CT  | C33-C32-C31 | -8.80 | 116.43      | 124.83   |
| 32  | 6     | 402 | 8CT  | C10-C11-C12 | -8.78 | 113.25      | 126.23   |
| 30  | 7     | 302 | CHL  | O2D-CGD-CBD | 8.76  | 120.58      | 110.95   |
| 30  | i     | 602 | CHL  | O2D-CGD-CBD | 8.75  | 120.56      | 110.95   |
| 30  | 7     | 313 | CHL  | O2D-CGD-CBD | 8.75  | 120.56      | 110.95   |
| 30  | 2     | 302 | CHL  | O2D-CGD-CBD | 8.75  | 120.56      | 110.95   |
| 30  | e     | 607 | CHL  | O2D-CGD-CBD | 8.73  | 120.54      | 110.95   |
| 30  | a     | 602 | CHL  | O2D-CGD-CBD | 8.73  | 120.54      | 110.95   |
| 30  | 2     | 302 | CHL  | C1B-CHB-C4A | 8.71  | 126.92      | 121.32   |
| 30  | 2     | 319 | CHL  | C1B-CHB-C4A | 8.70  | 126.92      | 121.32   |
| 30  | a     | 606 | CHL  | O2D-CGD-CBD | 8.68  | 120.49      | 110.95   |
| 30  | c     | 607 | CHL  | O2D-CGD-CBD | 8.68  | 120.49      | 110.95   |
| 30  | c     | 602 | CHL  | O2D-CGD-CBD | 8.68  | 120.49      | 110.95   |
| 30  | 6     | 305 | CHL  | C1B-CHB-C4A | 8.68  | 126.91      | 121.32   |
| 30  | h     | 601 | CHL  | O2D-CGD-CBD | 8.68  | 120.48      | 110.95   |
| 30  | 4     | 306 | CHL  | O2D-CGD-CBD | 8.65  | 120.45      | 110.95   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | 9     | 401 | 8CT  | C33-C32-C31 | -8.64 | 116.59      | 124.83   |
| 32  | L     | 206 | 8CT  | C33-C32-C31 | -8.63 | 116.59      | 124.83   |
| 30  | f     | 608 | CHL  | C1B-CHB-C4A | 8.62  | 126.87      | 121.32   |
| 30  | g     | 601 | CHL  | O2D-CGD-CBD | 8.62  | 120.42      | 110.95   |
| 30  | 7     | 305 | CHL  | C1B-CHB-C4A | 8.62  | 126.87      | 121.32   |
| 30  | 4     | 319 | CHL  | C1B-CHB-C4A | 8.62  | 126.87      | 121.32   |
| 30  | i     | 601 | CHL  | O2D-CGD-CBD | 8.61  | 120.41      | 110.95   |
| 30  | 1     | 313 | CHL  | O2D-CGD-CBD | 8.61  | 120.40      | 110.95   |
| 30  | 8     | 315 | CHL  | O2D-CGD-CBD | 8.59  | 120.38      | 110.95   |
| 30  | e     | 602 | CHL  | O2D-CGD-CBD | 8.59  | 120.38      | 110.95   |
| 30  | g     | 614 | CHL  | O2D-CGD-CBD | 8.57  | 120.36      | 110.95   |
| 30  | b     | 614 | CHL  | O2D-CGD-CBD | 8.55  | 120.34      | 110.95   |
| 30  | c     | 602 | CHL  | C1B-CHB-C4A | 8.54  | 126.82      | 121.32   |
| 30  | c     | 601 | CHL  | O2D-CGD-CBD | 8.54  | 120.33      | 110.95   |
| 32  | A     | 848 | 8CT  | C33-C32-C31 | -8.54 | 116.68      | 124.83   |
| 30  | 0     | 302 | CHL  | O2D-CGD-CBD | 8.53  | 120.32      | 110.95   |
| 32  | 6     | 402 | 8CT  | C33-C32-C31 | -8.52 | 116.70      | 124.83   |
| 30  | 4     | 319 | CHL  | O2D-CGD-CBD | 8.51  | 120.30      | 110.95   |
| 30  | 8     | 313 | CHL  | O2D-CGD-CBD | 8.50  | 120.29      | 110.95   |
| 30  | e     | 601 | CHL  | O2D-CGD-CBD | 8.49  | 120.28      | 110.95   |
| 30  | e     | 606 | CHL  | O2D-CGD-CBD | 8.49  | 120.28      | 110.95   |
| 32  | B     | 846 | 8CT  | C33-C32-C31 | -8.49 | 116.73      | 124.83   |
| 30  | h     | 602 | CHL  | O2D-CGD-CBD | 8.47  | 120.26      | 110.95   |
| 30  | a     | 601 | CHL  | O2D-CGD-CBD | 8.46  | 120.25      | 110.95   |
| 30  | f     | 601 | CHL  | O2D-CGD-CBD | 8.46  | 120.24      | 110.95   |
| 30  | a     | 607 | CHL  | O2D-CGD-CBD | 8.45  | 120.23      | 110.95   |
| 32  | B     | 846 | 8CT  | C24-C25-C26 | -8.44 | 115.44      | 127.28   |
| 30  | f     | 602 | CHL  | O2D-CGD-CBD | 8.42  | 120.20      | 110.95   |
| 30  | g     | 602 | CHL  | O2D-CGD-CBD | 8.42  | 120.20      | 110.95   |
| 30  | 5     | 301 | CHL  | O2D-CGD-CBD | 8.42  | 120.19      | 110.95   |
| 30  | 2     | 305 | CHL  | O2D-CGD-CBD | 8.41  | 120.19      | 110.95   |
| 30  | g     | 609 | CHL  | O2D-CGD-CBD | 8.39  | 120.16      | 110.95   |
| 30  | c     | 609 | CHL  | O2D-CGD-CBD | 8.37  | 120.15      | 110.95   |
| 30  | 6     | 305 | CHL  | O2D-CGD-CBD | 8.37  | 120.14      | 110.95   |
| 30  | h     | 605 | CHL  | O2D-CGD-CBD | 8.37  | 120.14      | 110.95   |
| 30  | 6     | 315 | CHL  | O2D-CGD-CBD | 8.37  | 120.14      | 110.95   |
| 30  | 4     | 302 | CHL  | C1B-CHB-C4A | 8.36  | 126.70      | 121.32   |
| 30  | 3     | 302 | CHL  | O2D-CGD-CBD | 8.35  | 120.12      | 110.95   |
| 32  | 7     | 402 | 8CT  | C33-C32-C31 | -8.34 | 116.86      | 124.83   |
| 30  | 8     | 308 | CHL  | O2D-CGD-CBD | 8.34  | 120.11      | 110.95   |
| 30  | d     | 609 | CHL  | O2D-CGD-CBD | 8.34  | 120.11      | 110.95   |
| 30  | 5     | 302 | CHL  | O2D-CGD-CBD | 8.32  | 120.09      | 110.95   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | 1     | 306 | CHL  | O2D-CGD-CBD | 8.31  | 120.08      | 110.95   |
| 30  | 4     | 313 | CHL  | C1B-CHB-C4A | 8.31  | 126.67      | 121.32   |
| 30  | d     | 605 | CHL  | O2D-CGD-CBD | 8.31  | 120.08      | 110.95   |
| 30  | 7     | 305 | CHL  | O2D-CGD-CBD | 8.31  | 120.07      | 110.95   |
| 30  | i     | 606 | CHL  | O2D-CGD-CBD | 8.31  | 120.07      | 110.95   |
| 30  | 2     | 301 | CHL  | C1B-CHB-C4A | 8.30  | 126.67      | 121.32   |
| 30  | d     | 614 | CHL  | O2D-CGD-CBD | 8.30  | 120.07      | 110.95   |
| 30  | 6     | 313 | CHL  | O2D-CGD-CBD | 8.30  | 120.07      | 110.95   |
| 30  | d     | 602 | CHL  | O2D-CGD-CBD | 8.29  | 120.06      | 110.95   |
| 30  | 1     | 305 | CHL  | O2D-CGD-CBD | 8.29  | 120.06      | 110.95   |
| 30  | f     | 607 | CHL  | O2D-CGD-CBD | 8.28  | 120.04      | 110.95   |
| 30  | i     | 605 | CHL  | O2D-CGD-CBD | 8.27  | 120.03      | 110.95   |
| 30  | a     | 614 | CHL  | O2D-CGD-CBD | 8.26  | 120.03      | 110.95   |
| 32  | B     | 846 | 8CT  | C10-C11-C12 | -8.26 | 114.01      | 126.23   |
| 30  | h     | 606 | CHL  | O2D-CGD-CBD | 8.26  | 120.02      | 110.95   |
| 30  | d     | 607 | CHL  | O2D-CGD-CBD | 8.25  | 120.02      | 110.95   |
| 30  | 2     | 307 | CHL  | CHA-C1A-C2A | -8.25 | 113.94      | 133.31   |
| 30  | d     | 606 | CHL  | O2D-CGD-CBD | 8.25  | 120.01      | 110.95   |
| 30  | 6     | 313 | CHL  | C1B-CHB-C4A | 8.23  | 126.61      | 121.32   |
| 30  | i     | 607 | CHL  | O2D-CGD-CBD | 8.23  | 119.99      | 110.95   |
| 30  | c     | 605 | CHL  | O2D-CGD-CBD | 8.23  | 119.98      | 110.95   |
| 30  | b     | 606 | CHL  | O2D-CGD-CBD | 8.18  | 119.94      | 110.95   |
| 32  | O     | 205 | 8CT  | C33-C32-C31 | -8.17 | 117.03      | 124.83   |
| 30  | 7     | 302 | CHL  | CHA-C1A-C2A | -8.16 | 114.15      | 133.31   |
| 30  | 3     | 302 | CHL  | CHA-C1A-C2A | -8.14 | 114.20      | 133.31   |
| 30  | 8     | 305 | CHL  | O2D-CGD-CBD | 8.14  | 119.89      | 110.95   |
| 30  | 2     | 305 | CHL  | CHA-C1A-C2A | -8.14 | 114.21      | 133.31   |
| 30  | c     | 606 | CHL  | O2D-CGD-CBD | 8.13  | 119.88      | 110.95   |
| 30  | f     | 614 | CHL  | O2D-CGD-CBD | 8.13  | 119.88      | 110.95   |
| 30  | i     | 614 | CHL  | O2D-CGD-CBD | 8.13  | 119.88      | 110.95   |
| 30  | a     | 605 | CHL  | O2D-CGD-CBD | 8.12  | 119.87      | 110.95   |
| 32  | B     | 851 | 8CT  | C33-C32-C31 | -8.11 | 117.09      | 124.83   |
| 30  | 3     | 307 | CHL  | CHA-C1A-C2A | -8.10 | 114.29      | 133.31   |
| 30  | 9     | 305 | CHL  | CHA-C1A-C2A | -8.08 | 114.33      | 133.31   |
| 30  | 1     | 305 | CHL  | CHA-C1A-C2A | -8.08 | 114.34      | 133.31   |
| 30  | 8     | 302 | CHL  | CHA-C1A-C2A | -8.07 | 114.35      | 133.31   |
| 32  | K     | 107 | 8CT  | C14-C13-C12 | -8.06 | 115.98      | 127.28   |
| 30  | 6     | 308 | CHL  | O2D-CGD-CBD | 8.05  | 119.79      | 110.95   |
| 30  | 3     | 307 | CHL  | O2D-CGD-CBD | 8.05  | 119.79      | 110.95   |
| 30  | d     | 602 | CHL  | CHA-C1A-C2A | -8.03 | 114.45      | 133.31   |
| 30  | 1     | 302 | CHL  | CHA-C1A-C2A | -8.03 | 114.46      | 133.31   |
| 30  | g     | 605 | CHL  | O2D-CGD-CBD | 8.03  | 119.77      | 110.95   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | 5     | 302 | CHL  | CHA-C1A-C2A | -8.02 | 114.47      | 133.31   |
| 30  | a     | 609 | CHL  | O2D-CGD-CBD | 8.01  | 119.75      | 110.95   |
| 30  | b     | 607 | CHL  | O2D-CGD-CBD | 8.01  | 119.75      | 110.95   |
| 30  | 6     | 306 | CHL  | CHA-C1A-C2A | -8.00 | 114.52      | 133.31   |
| 30  | 4     | 302 | CHL  | O2D-CGD-CBD | 8.00  | 119.74      | 110.95   |
| 30  | f     | 602 | CHL  | CHA-C1A-C2A | -8.00 | 114.53      | 133.31   |
| 30  | d     | 602 | CHL  | C1B-CHB-C4A | 7.99  | 126.47      | 121.32   |
| 30  | 4     | 313 | CHL  | CHA-C1A-C2A | -7.99 | 114.56      | 133.31   |
| 30  | 6     | 305 | CHL  | CHA-C1A-C2A | -7.98 | 114.57      | 133.31   |
| 30  | 2     | 302 | CHL  | CHA-C1A-C2A | -7.97 | 114.58      | 133.31   |
| 30  | f     | 608 | CHL  | CHA-C1A-C2A | -7.96 | 114.62      | 133.31   |
| 30  | h     | 607 | CHL  | O2D-CGD-CBD | 7.95  | 119.69      | 110.95   |
| 30  | 1     | 302 | CHL  | O2D-CGD-CBD | 7.95  | 119.68      | 110.95   |
| 30  | 8     | 305 | CHL  | CHA-C1A-C2A | -7.94 | 114.66      | 133.31   |
| 32  | A     | 850 | 8CT  | C19-C18-C17 | -7.94 | 107.27      | 123.52   |
| 30  | 6     | 302 | CHL  | CHA-C1A-C2A | -7.94 | 114.66      | 133.31   |
| 32  | G     | 104 | 8CT  | C18-C17-C16 | -7.94 | 116.15      | 127.28   |
| 30  | i     | 609 | CHL  | O2D-CGD-CBD | 7.92  | 119.64      | 110.95   |
| 32  | L     | 206 | 8CT  | C14-C13-C12 | -7.91 | 116.19      | 127.28   |
| 30  | f     | 605 | CHL  | O2D-CGD-CBD | 7.90  | 119.63      | 110.95   |
| 30  | 9     | 305 | CHL  | O2D-CGD-CBD | 7.90  | 119.62      | 110.95   |
| 30  | c     | 602 | CHL  | CHA-C1A-C2A | -7.90 | 114.77      | 133.31   |
| 30  | 8     | 313 | CHL  | CHA-C1A-C2A | -7.89 | 114.78      | 133.31   |
| 32  | B     | 845 | 8CT  | C19-C18-C17 | -7.89 | 107.38      | 123.52   |
| 30  | 4     | 302 | CHL  | CHA-C1A-C2A | -7.86 | 114.85      | 133.31   |
| 30  | 6     | 313 | CHL  | CHA-C1A-C2A | -7.85 | 114.88      | 133.31   |
| 30  | 4     | 319 | CHL  | CHA-C1A-C2A | -7.85 | 114.88      | 133.31   |
| 30  | b     | 601 | CHL  | O2D-CGD-CBD | 7.85  | 119.57      | 110.95   |
| 30  | 4     | 305 | CHL  | CHA-C1A-C2A | -7.84 | 114.90      | 133.31   |
| 30  | 4     | 306 | CHL  | CHA-C1A-C2A | -7.84 | 114.91      | 133.31   |
| 30  | 7     | 305 | CHL  | CHA-C1A-C2A | -7.83 | 114.93      | 133.31   |
| 30  | 9     | 313 | CHL  | CHA-C1A-C2A | -7.82 | 114.94      | 133.31   |
| 30  | 4     | 307 | CHL  | C1B-CHB-C4A | 7.82  | 126.35      | 121.32   |
| 30  | 4     | 307 | CHL  | CHA-C1A-C2A | -7.81 | 114.96      | 133.31   |
| 30  | 0     | 302 | CHL  | C1B-CHB-C4A | 7.81  | 126.35      | 121.32   |
| 30  | e     | 605 | CHL  | O2D-CGD-CBD | 7.80  | 119.52      | 110.95   |
| 30  | 2     | 301 | CHL  | CHA-C1A-C2A | -7.79 | 115.01      | 133.31   |
| 30  | 2     | 308 | CHL  | C1B-CHB-C4A | 7.78  | 126.33      | 121.32   |
| 30  | 2     | 306 | CHL  | CHA-C1A-C2A | -7.78 | 115.04      | 133.31   |
| 30  | 0     | 302 | CHL  | CHA-C1A-C2A | -7.77 | 115.06      | 133.31   |
| 30  | b     | 602 | CHL  | CHA-C1A-C2A | -7.77 | 115.07      | 133.31   |
| 30  | 8     | 302 | CHL  | O2D-CGD-CBD | 7.77  | 119.48      | 110.95   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | 2     | 308 | CHL  | CHA-C1A-C2A | -7.76 | 115.08      | 133.31   |
| 30  | 5     | 307 | CHL  | O2D-CGD-CBD | 7.76  | 119.47      | 110.95   |
| 30  | 2     | 319 | CHL  | CHA-C1A-C2A | -7.75 | 115.11      | 133.31   |
| 30  | 6     | 306 | CHL  | O2D-CGD-CBD | 7.75  | 119.46      | 110.95   |
| 32  | K     | 107 | 8CT  | C18-C17-C16 | -7.75 | 116.42      | 127.28   |
| 30  | 6     | 301 | CHL  | CHA-C1A-C2A | -7.74 | 115.12      | 133.31   |
| 32  | B     | 846 | 8CT  | C04-C03-C02 | -7.74 | 112.06      | 122.64   |
| 30  | 6     | 307 | CHL  | O2D-CGD-CBD | 7.74  | 119.45      | 110.95   |
| 30  | 5     | 306 | CHL  | O2D-CGD-CBD | 7.72  | 119.43      | 110.95   |
| 30  | 8     | 307 | CHL  | CHA-C1A-C2A | -7.71 | 115.20      | 133.31   |
| 30  | e     | 601 | CHL  | CHA-C1A-C2A | -7.71 | 115.21      | 133.31   |
| 30  | 0     | 301 | CHL  | CHA-C1A-C2A | -7.71 | 115.21      | 133.31   |
| 32  | 1     | 402 | 8CT  | C33-C32-C31 | -7.71 | 117.47      | 124.83   |
| 30  | 1     | 307 | CHL  | O2D-CGD-CBD | 7.70  | 119.41      | 110.95   |
| 30  | g     | 607 | CHL  | O2D-CGD-CBD | 7.70  | 119.40      | 110.95   |
| 30  | b     | 606 | CHL  | CHA-C1A-C2A | -7.69 | 115.25      | 133.31   |
| 30  | 4     | 307 | CHL  | O2D-CGD-CBD | 7.66  | 119.37      | 110.95   |
| 30  | 6     | 307 | CHL  | CHA-C1A-C2A | -7.65 | 115.34      | 133.31   |
| 30  | 4     | 306 | CHL  | C1B-CHB-C4A | 7.65  | 126.24      | 121.32   |
| 30  | b     | 608 | CHL  | CHA-C1A-C2A | -7.65 | 115.36      | 133.31   |
| 30  | c     | 601 | CHL  | CHA-C1A-C2A | -7.64 | 115.38      | 133.31   |
| 30  | 2     | 313 | CHL  | O2D-CGD-CBD | 7.63  | 119.33      | 110.95   |
| 32  | A     | 854 | 8CT  | C24-C25-C26 | -7.63 | 116.58      | 127.28   |
| 30  | f     | 606 | CHL  | CHA-C1A-C2A | -7.62 | 115.41      | 133.31   |
| 30  | 9     | 306 | CHL  | CHA-C1A-C2A | -7.62 | 115.42      | 133.31   |
| 30  | e     | 614 | CHL  | O2D-CGD-CBD | 7.61  | 119.31      | 110.95   |
| 30  | 8     | 308 | CHL  | CHA-C1A-C2A | -7.59 | 115.49      | 133.31   |
| 30  | b     | 609 | CHL  | O2D-CGD-CBD | 7.58  | 119.27      | 110.95   |
| 32  | B     | 843 | 8CT  | C18-C17-C16 | -7.57 | 116.66      | 127.28   |
| 30  | e     | 606 | CHL  | CHA-C1A-C2A | -7.57 | 115.54      | 133.31   |
| 30  | a     | 608 | CHL  | O2D-CGD-CBD | 7.56  | 119.25      | 110.95   |
| 30  | e     | 609 | CHL  | O2D-CGD-CBD | 7.55  | 119.25      | 110.95   |
| 30  | 3     | 305 | CHL  | CHA-C1A-C2A | -7.54 | 115.61      | 133.31   |
| 32  | 8     | 406 | 8CT  | C33-C32-C31 | -7.53 | 117.64      | 124.83   |
| 32  | A     | 849 | 8CT  | C10-C11-C12 | -7.53 | 115.10      | 126.23   |
| 30  | 2     | 313 | CHL  | CHA-C1A-C2A | -7.52 | 115.64      | 133.31   |
| 30  | 1     | 313 | CHL  | CHA-C1A-C2A | -7.52 | 115.64      | 133.31   |
| 30  | 9     | 313 | CHL  | C1B-CHB-C4A | 7.52  | 126.16      | 121.32   |
| 30  | f     | 601 | CHL  | CHA-C1A-C2A | -7.52 | 115.65      | 133.31   |
| 30  | 8     | 307 | CHL  | O2D-CGD-CBD | 7.51  | 119.20      | 110.95   |
| 30  | h     | 614 | CHL  | O2D-CGD-CBD | 7.51  | 119.20      | 110.95   |
| 32  | 7     | 404 | 8CT  | C29-C28-C26 | -7.50 | 110.19      | 126.32   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | 6     | 308 | CHL  | CHA-C1A-C2A | -7.50 | 115.70      | 133.31   |
| 30  | e     | 602 | CHL  | CHA-C1A-C2A | -7.50 | 115.70      | 133.31   |
| 32  | 6     | 402 | 8CT  | C24-C25-C26 | -7.50 | 116.76      | 127.28   |
| 32  | A     | 847 | 8CT  | C30-C29-C28 | -7.49 | 112.92      | 124.58   |
| 30  | f     | 609 | CHL  | O2D-CGD-CBD | 7.49  | 119.18      | 110.95   |
| 30  | f     | 602 | CHL  | C1B-CHB-C4A | 7.48  | 126.13      | 121.32   |
| 30  | 7     | 306 | CHL  | CHA-C1A-C2A | -7.47 | 115.77      | 133.31   |
| 30  | 0     | 305 | CHL  | CHA-C1A-C2A | -7.46 | 115.80      | 133.31   |
| 30  | 5     | 305 | CHL  | CHA-C1A-C2A | -7.45 | 115.81      | 133.31   |
| 30  | 0     | 306 | CHL  | CHA-C1A-C2A | -7.45 | 115.82      | 133.31   |
| 30  | 8     | 313 | CHL  | C1B-CHB-C4A | 7.45  | 126.11      | 121.32   |
| 32  | 4     | 402 | 8CT  | C30-C31-C32 | -7.44 | 112.31      | 121.47   |
| 32  | 7     | 404 | 8CT  | C18-C17-C16 | -7.40 | 116.89      | 127.28   |
| 32  | 3     | 403 | 8CT  | C33-C32-C31 | -7.40 | 117.76      | 124.83   |
| 30  | 7     | 301 | CHL  | CHA-C1A-C2A | -7.40 | 115.93      | 133.31   |
| 30  | 9     | 301 | CHL  | CHA-C1A-C2A | -7.39 | 115.96      | 133.31   |
| 30  | a     | 602 | CHL  | CHA-C1A-C2A | -7.39 | 115.97      | 133.31   |
| 30  | f     | 608 | CHL  | O2D-CGD-CBD | 7.38  | 119.06      | 110.95   |
| 30  | e     | 609 | CHL  | CHA-C1A-C2A | -7.38 | 115.99      | 133.31   |
| 30  | 8     | 306 | CHL  | CHA-C1A-C2A | -7.38 | 115.99      | 133.31   |
| 30  | 4     | 308 | CHL  | CHA-C1A-C2A | -7.37 | 116.00      | 133.31   |
| 32  | B     | 804 | 8CT  | C33-C32-C31 | -7.37 | 117.80      | 124.83   |
| 30  | 2     | 307 | CHL  | O2D-CGD-CBD | 7.37  | 119.04      | 110.95   |
| 30  | 8     | 307 | CHL  | C1B-CHB-C4A | 7.37  | 126.06      | 121.32   |
| 30  | b     | 608 | CHL  | O2D-CGD-CBD | 7.36  | 119.03      | 110.95   |
| 32  | B     | 847 | 8CT  | C30-C31-C32 | -7.31 | 112.47      | 121.47   |
| 30  | 6     | 315 | CHL  | CHA-C1A-C2A | -7.30 | 116.17      | 133.31   |
| 32  | 3     | 402 | 8CT  | C30-C31-C32 | -7.27 | 112.52      | 121.47   |
| 30  | g     | 606 | CHL  | CHA-C1A-C2A | -7.26 | 116.25      | 133.31   |
| 30  | 0     | 301 | CHL  | C1B-CHB-C4A | 7.26  | 126.00      | 121.32   |
| 30  | e     | 608 | CHL  | CHA-C1A-C2A | -7.26 | 116.27      | 133.31   |
| 30  | c     | 609 | CHL  | CHA-C1A-C2A | -7.24 | 116.31      | 133.31   |
| 30  | 8     | 301 | CHL  | CHA-C1A-C2A | -7.23 | 116.33      | 133.31   |
| 30  | b     | 609 | CHL  | CHA-C1A-C2A | -7.23 | 116.34      | 133.31   |
| 32  | B     | 847 | 8CT  | C14-C13-C12 | -7.22 | 117.16      | 127.28   |
| 30  | i     | 602 | CHL  | CHA-C1A-C2A | -7.20 | 116.40      | 133.31   |
| 30  | 9     | 306 | CHL  | C1B-CHB-C4A | 7.19  | 125.95      | 121.32   |
| 30  | 2     | 308 | CHL  | O2D-CGD-CBD | 7.19  | 118.85      | 110.95   |
| 30  | e     | 607 | CHL  | CHA-C1A-C2A | -7.19 | 116.43      | 133.31   |
| 30  | 5     | 307 | CHL  | CHA-C1A-C2A | -7.18 | 116.45      | 133.31   |
| 30  | d     | 614 | CHL  | C4D-ND-C1D  | 7.14  | 110.64      | 105.22   |
| 30  | d     | 605 | CHL  | C4D-ND-C1D  | 7.14  | 110.64      | 105.22   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | d     | 606 | CHL  | CHA-C1A-C2A | -7.14 | 116.54      | 133.31   |
| 30  | l     | 307 | CHL  | CHA-C1A-C2A | -7.13 | 116.56      | 133.31   |
| 42  | c     | 523 | NEX  | C27-C28-C29 | 7.12  | 136.58      | 125.53   |
| 32  | J     | 101 | 8CT  | C30-C31-C32 | -7.12 | 112.71      | 121.47   |
| 30  | e     | 608 | CHL  | O2D-CGD-CBD | 7.11  | 118.76      | 110.95   |
| 42  | b     | 523 | NEX  | C27-C28-C29 | 7.11  | 136.56      | 125.53   |
| 42  | g     | 523 | NEX  | C27-C28-C29 | 7.10  | 136.55      | 125.53   |
| 30  | a     | 606 | CHL  | CHA-C1A-C2A | -7.10 | 116.64      | 133.31   |
| 30  | i     | 605 | CHL  | C4D-ND-C1D  | 7.10  | 110.61      | 105.22   |
| 30  | i     | 608 | CHL  | O2D-CGD-CBD | 7.10  | 118.75      | 110.95   |
| 42  | h     | 523 | NEX  | C27-C28-C29 | 7.09  | 136.53      | 125.53   |
| 30  | 7     | 307 | CHL  | O2D-CGD-CBD | 7.09  | 118.73      | 110.95   |
| 42  | d     | 523 | NEX  | C27-C28-C29 | 7.08  | 136.52      | 125.53   |
| 30  | g     | 614 | CHL  | C4D-ND-C1D  | 7.08  | 110.59      | 105.22   |
| 30  | c     | 608 | CHL  | O2D-CGD-CBD | 7.08  | 118.72      | 110.95   |
| 42  | i     | 523 | NEX  | C27-C28-C29 | 7.08  | 136.51      | 125.53   |
| 30  | l     | 306 | CHL  | CHA-C1A-C2A | -7.08 | 116.69      | 133.31   |
| 30  | c     | 605 | CHL  | C4D-ND-C1D  | 7.08  | 110.59      | 105.22   |
| 30  | d     | 608 | CHL  | O2D-CGD-CBD | 7.08  | 118.72      | 110.95   |
| 42  | f     | 523 | NEX  | C27-C28-C29 | 7.07  | 136.51      | 125.53   |
| 42  | a     | 523 | NEX  | C27-C28-C29 | 7.07  | 136.50      | 125.53   |
| 30  | d     | 609 | CHL  | CHA-C1A-C2A | -7.07 | 116.72      | 133.31   |
| 30  | 7     | 307 | CHL  | CHA-C1A-C2A | -7.06 | 116.73      | 133.31   |
| 31  | 3     | 304 | CLA  | C4A-NA-C1A  | 7.06  | 109.90      | 106.68   |
| 30  | c     | 601 | CHL  | C1B-CHB-C4A | 7.05  | 125.86      | 121.32   |
| 42  | i     | 523 | NEX  | C35-C34-C33 | -7.04 | 117.41      | 127.28   |
| 30  | 5     | 301 | CHL  | CHA-C1A-C2A | -7.03 | 116.79      | 133.31   |
| 31  | g     | 613 | CLA  | C4A-NA-C1A  | 7.03  | 109.89      | 106.68   |
| 42  | g     | 523 | NEX  | C35-C34-C33 | -7.03 | 117.42      | 127.28   |
| 42  | b     | 523 | NEX  | C35-C34-C33 | -7.02 | 117.43      | 127.28   |
| 30  | 3     | 307 | CHL  | OBD-CAD-CBD | 7.02  | 136.13      | 125.82   |
| 42  | f     | 523 | NEX  | C35-C34-C33 | -7.02 | 117.43      | 127.28   |
| 42  | a     | 523 | NEX  | C35-C34-C33 | -7.02 | 117.43      | 127.28   |
| 42  | d     | 523 | NEX  | C35-C34-C33 | -7.01 | 117.44      | 127.28   |
| 42  | c     | 523 | NEX  | C35-C34-C33 | -7.01 | 117.45      | 127.28   |
| 30  | c     | 608 | CHL  | CHA-C1A-C2A | -7.00 | 116.86      | 133.31   |
| 30  | b     | 607 | CHL  | CHA-C1A-C2A | -7.00 | 116.86      | 133.31   |
| 42  | h     | 523 | NEX  | C35-C34-C33 | -7.00 | 117.46      | 127.28   |
| 31  | H     | 204 | CLA  | C4A-NA-C1A  | 7.00  | 109.87      | 106.68   |
| 30  | g     | 602 | CHL  | CHA-C1A-C2A | -7.00 | 116.88      | 133.31   |
| 31  | f     | 612 | CLA  | C4A-NA-C1A  | 6.98  | 109.86      | 106.68   |
| 30  | h     | 608 | CHL  | O2D-CGD-CBD | 6.98  | 118.61      | 110.95   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | b     | 602 | CHL  | C1B-CHB-C4A | 6.97  | 125.81      | 121.32   |
| 30  | 8     | 305 | CHL  | C1B-CHB-C4A | 6.97  | 125.81      | 121.32   |
| 31  | 7     | 317 | CLA  | C4A-NA-C1A  | 6.96  | 109.85      | 106.68   |
| 30  | 8     | 315 | CHL  | CHA-C1A-C2A | -6.95 | 116.98      | 133.31   |
| 30  | g     | 601 | CHL  | C4D-ND-C1D  | 6.95  | 110.50      | 105.22   |
| 32  | O     | 205 | 8CT  | C14-C13-C12 | -6.95 | 117.54      | 127.28   |
| 31  | A     | 817 | CLA  | C4A-NA-C1A  | 6.94  | 109.85      | 106.68   |
| 30  | 7     | 313 | CHL  | CHA-C1A-C2A | -6.94 | 117.01      | 133.31   |
| 30  | f     | 609 | CHL  | CHA-C1A-C2A | -6.94 | 117.01      | 133.31   |
| 31  | A     | 816 | CLA  | C4A-NA-C1A  | 6.94  | 109.85      | 106.68   |
| 31  | B     | 835 | CLA  | C4A-NA-C1A  | 6.94  | 109.84      | 106.68   |
| 30  | a     | 614 | CHL  | C4D-ND-C1D  | 6.94  | 110.48      | 105.22   |
| 31  | B     | 821 | CLA  | C4A-NA-C1A  | 6.93  | 109.84      | 106.68   |
| 30  | 5     | 306 | CHL  | CHA-C1A-C2A | -6.93 | 117.03      | 133.31   |
| 30  | 2     | 307 | CHL  | OBD-CAD-CBD | 6.92  | 135.99      | 125.82   |
| 30  | i     | 606 | CHL  | CHA-C1A-C2A | -6.92 | 117.06      | 133.31   |
| 30  | h     | 606 | CHL  | CHA-C1A-C2A | -6.91 | 117.08      | 133.31   |
| 32  | L     | 209 | 8CT  | C10-C11-C12 | -6.91 | 116.01      | 126.23   |
| 32  | B     | 843 | 8CT  | C19-C20-C21 | -6.90 | 117.60      | 127.28   |
| 30  | c     | 606 | CHL  | CHA-C1A-C2A | -6.89 | 117.12      | 133.31   |
| 32  | A     | 854 | 8CT  | C14-C13-C12 | -6.89 | 117.61      | 127.28   |
| 30  | g     | 608 | CHL  | O2D-CGD-CBD | 6.89  | 118.52      | 110.95   |
| 30  | c     | 607 | CHL  | CHA-C1A-C2A | -6.89 | 117.13      | 133.31   |
| 30  | 0     | 301 | CHL  | O2D-CGD-CBD | 6.88  | 118.51      | 110.95   |
| 30  | g     | 605 | CHL  | C4D-ND-C1D  | 6.88  | 110.44      | 105.22   |
| 31  | 5     | 312 | CLA  | C4A-NA-C1A  | 6.88  | 109.82      | 106.68   |
| 31  | 9     | 308 | CLA  | C4A-NA-C1A  | 6.87  | 109.81      | 106.68   |
| 32  | A     | 846 | 8CT  | C14-C13-C12 | -6.87 | 117.64      | 127.28   |
| 31  | 5     | 303 | CLA  | C4A-NA-C1A  | 6.87  | 109.81      | 106.68   |
| 32  | B     | 843 | 8CT  | C33-C32-C31 | -6.87 | 118.28      | 124.83   |
| 32  | A     | 850 | 8CT  | C04-C03-C02 | -6.86 | 113.26      | 122.64   |
| 33  | 2     | 502 | 0UR  | C14-C15-C16 | -6.86 | 117.66      | 127.28   |
| 31  | 0     | 311 | CLA  | C4A-NA-C1A  | 6.86  | 109.81      | 106.68   |
| 31  | a     | 612 | CLA  | C4A-NA-C1A  | 6.86  | 109.81      | 106.68   |
| 31  | A     | 837 | CLA  | C4A-NA-C1A  | 6.85  | 109.81      | 106.68   |
| 31  | B     | 832 | CLA  | C4A-NA-C1A  | 6.85  | 109.80      | 106.68   |
| 31  | e     | 612 | CLA  | C4A-NA-C1A  | 6.85  | 109.80      | 106.68   |
| 31  | 3     | 311 | CLA  | C4A-NA-C1A  | 6.83  | 109.80      | 106.68   |
| 32  | L     | 205 | 8CT  | C30-C31-C32 | -6.83 | 113.06      | 121.47   |
| 31  | 2     | 311 | CLA  | C4A-NA-C1A  | 6.83  | 109.80      | 106.68   |
| 30  | a     | 608 | CHL  | CHA-C1A-C2A | -6.83 | 117.28      | 133.31   |
| 30  | 8     | 308 | CHL  | C1B-CHB-C4A | 6.82  | 125.71      | 121.32   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | G     | 104 | 8CT  | C10-C11-C12 | -6.82 | 116.14      | 126.23   |
| 31  | 1     | 311 | CLA  | C4A-NA-C1A  | 6.82  | 109.79      | 106.68   |
| 42  | d     | 523 | NEX  | C35-C15-C14 | 6.81  | 137.46      | 123.52   |
| 31  | B     | 808 | CLA  | C4A-NA-C1A  | 6.81  | 109.79      | 106.68   |
| 30  | a     | 605 | CHL  | C4D-ND-C1D  | 6.81  | 110.39      | 105.22   |
| 31  | B     | 837 | CLA  | C4A-NA-C1A  | 6.81  | 109.78      | 106.68   |
| 42  | i     | 523 | NEX  | C35-C15-C14 | 6.81  | 137.45      | 123.52   |
| 42  | a     | 523 | NEX  | C35-C15-C14 | 6.80  | 137.44      | 123.52   |
| 42  | g     | 523 | NEX  | C35-C15-C14 | 6.79  | 137.42      | 123.52   |
| 30  | h     | 609 | CHL  | CHA-C1A-C2A | -6.79 | 117.36      | 133.31   |
| 42  | b     | 523 | NEX  | C35-C15-C14 | 6.79  | 137.41      | 123.52   |
| 31  | 1     | 303 | CLA  | C4A-NA-C1A  | 6.79  | 109.78      | 106.68   |
| 31  | 9     | 303 | CLA  | C4A-NA-C1A  | 6.78  | 109.77      | 106.68   |
| 30  | f     | 605 | CHL  | C4D-ND-C1D  | 6.78  | 110.37      | 105.22   |
| 31  | A     | 809 | CLA  | C4A-NA-C1A  | 6.78  | 109.77      | 106.68   |
| 31  | c     | 612 | CLA  | C4A-NA-C1A  | 6.78  | 109.77      | 106.68   |
| 42  | f     | 523 | NEX  | C35-C15-C14 | 6.78  | 137.40      | 123.52   |
| 30  | i     | 608 | CHL  | CHA-C1A-C2A | -6.78 | 117.39      | 133.31   |
| 30  | 3     | 305 | CHL  | C1B-CHB-C4A | 6.78  | 125.69      | 121.32   |
| 42  | c     | 523 | NEX  | C35-C15-C14 | 6.78  | 137.38      | 123.52   |
| 32  | 2     | 402 | 8CT  | C30-C31-C32 | -6.77 | 113.13      | 121.47   |
| 31  | 1     | 310 | CLA  | C4A-NA-C1A  | 6.77  | 109.77      | 106.68   |
| 31  | L     | 203 | CLA  | C4A-NA-C1A  | 6.77  | 109.77      | 106.68   |
| 30  | d     | 608 | CHL  | CHA-C1A-C2A | -6.76 | 117.43      | 133.31   |
| 42  | h     | 523 | NEX  | C35-C15-C14 | 6.76  | 137.35      | 123.52   |
| 30  | h     | 608 | CHL  | CHA-C1A-C2A | -6.76 | 117.44      | 133.31   |
| 31  | M     | 101 | CLA  | C4A-NA-C1A  | 6.76  | 109.76      | 106.68   |
| 30  | i     | 614 | CHL  | C4D-ND-C1D  | 6.75  | 110.34      | 105.22   |
| 31  | 6     | 303 | CLA  | C4A-NA-C1A  | 6.75  | 109.76      | 106.68   |
| 31  | A     | 820 | CLA  | C4A-NA-C1A  | 6.75  | 109.76      | 106.68   |
| 31  | i     | 611 | CLA  | C4A-NA-C1A  | 6.75  | 109.76      | 106.68   |
| 30  | h     | 614 | CHL  | C4D-ND-C1D  | 6.74  | 110.34      | 105.22   |
| 31  | 7     | 311 | CLA  | C4A-NA-C1A  | 6.74  | 109.75      | 106.68   |
| 31  | B     | 840 | CLA  | C4A-NA-C1A  | 6.74  | 109.75      | 106.68   |
| 31  | A     | 804 | CLA  | C4A-NA-C1A  | 6.74  | 109.75      | 106.68   |
| 31  | B     | 827 | CLA  | C4A-NA-C1A  | 6.74  | 109.75      | 106.68   |
| 31  | A     | 808 | CLA  | C4A-NA-C1A  | 6.74  | 109.75      | 106.68   |
| 31  | A     | 830 | CLA  | C4A-NA-C1A  | 6.73  | 109.75      | 106.68   |
| 30  | a     | 607 | CHL  | CHA-C1A-C2A | -6.73 | 117.50      | 133.31   |
| 30  | h     | 602 | CHL  | CHA-C1A-C2A | -6.73 | 117.51      | 133.31   |
| 31  | 3     | 320 | CLA  | C4A-NA-C1A  | 6.73  | 109.75      | 106.68   |
| 31  | b     | 611 | CLA  | C4A-NA-C1A  | 6.72  | 109.75      | 106.68   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | B     | 807 | CLA  | C4A-NA-C1A  | 6.72  | 109.74      | 106.68   |
| 31  | A     | 834 | CLA  | C4A-NA-C1A  | 6.72  | 109.74      | 106.68   |
| 30  | i     | 601 | CHL  | CHA-C1A-C2A | -6.71 | 117.54      | 133.31   |
| 31  | h     | 603 | CLA  | C4A-NA-C1A  | 6.71  | 109.74      | 106.68   |
| 30  | g     | 607 | CHL  | C4D-ND-C1D  | 6.71  | 110.31      | 105.22   |
| 31  | b     | 612 | CLA  | C4A-NA-C1A  | 6.70  | 109.74      | 106.68   |
| 31  | A     | 843 | CLA  | C4A-NA-C1A  | 6.70  | 109.74      | 106.68   |
| 30  | h     | 605 | CHL  | C4D-ND-C1D  | 6.70  | 110.30      | 105.22   |
| 32  | A     | 847 | 8CT  | C30-C31-C32 | -6.70 | 113.22      | 121.47   |
| 31  | 7     | 309 | CLA  | C4A-NA-C1A  | 6.70  | 109.73      | 106.68   |
| 31  | B     | 838 | CLA  | C4A-NA-C1A  | 6.70  | 109.73      | 106.68   |
| 31  | 3     | 308 | CLA  | C4A-NA-C1A  | 6.70  | 109.73      | 106.68   |
| 30  | d     | 607 | CHL  | C4D-ND-C1D  | 6.69  | 110.30      | 105.22   |
| 32  | A     | 847 | 8CT  | C18-C17-C16 | -6.69 | 117.89      | 127.28   |
| 31  | B     | 818 | CLA  | C4A-NA-C1A  | 6.69  | 109.73      | 106.68   |
| 33  | 2     | 501 | 0UR  | C4-C3-C2    | -6.69 | 114.34      | 120.16   |
| 31  | B     | 811 | CLA  | C4A-NA-C1A  | 6.69  | 109.73      | 106.68   |
| 31  | c     | 604 | CLA  | C4A-NA-C1A  | 6.68  | 109.73      | 106.68   |
| 31  | B     | 817 | CLA  | C4A-NA-C1A  | 6.67  | 109.72      | 106.68   |
| 32  | 2     | 402 | 8CT  | C18-C17-C16 | -6.66 | 117.93      | 127.28   |
| 31  | B     | 816 | CLA  | C4A-NA-C1A  | 6.66  | 109.72      | 106.68   |
| 31  | K     | 104 | CLA  | C4A-NA-C1A  | 6.66  | 109.72      | 106.68   |
| 30  | a     | 601 | CHL  | C4D-ND-C1D  | 6.66  | 110.27      | 105.22   |
| 31  | B     | 812 | CLA  | C4A-NA-C1A  | 6.66  | 109.72      | 106.68   |
| 31  | 1     | 312 | CLA  | C4A-NA-C1A  | 6.65  | 109.72      | 106.68   |
| 31  | 2     | 303 | CLA  | C4A-NA-C1A  | 6.65  | 109.72      | 106.68   |
| 31  | 4     | 310 | CLA  | C4A-NA-C1A  | 6.65  | 109.72      | 106.68   |
| 30  | f     | 607 | CHL  | C4D-ND-C1D  | 6.65  | 110.27      | 105.22   |
| 31  | 7     | 304 | CLA  | C4A-NA-C1A  | 6.65  | 109.71      | 106.68   |
| 31  | a     | 603 | CLA  | C4A-NA-C1A  | 6.64  | 109.71      | 106.68   |
| 31  | A     | 818 | CLA  | C4A-NA-C1A  | 6.63  | 109.71      | 106.68   |
| 32  | 4     | 402 | 8CT  | C18-C17-C16 | -6.63 | 117.97      | 127.28   |
| 30  | h     | 601 | CHL  | C4D-ND-C1D  | 6.63  | 110.25      | 105.22   |
| 31  | A     | 833 | CLA  | C4A-NA-C1A  | 6.63  | 109.70      | 106.68   |
| 31  | 7     | 315 | CLA  | C4A-NA-C1A  | 6.62  | 109.70      | 106.68   |
| 31  | B     | 810 | CLA  | C4A-NA-C1A  | 6.62  | 109.70      | 106.68   |
| 31  | h     | 610 | CLA  | C4A-NA-C1A  | 6.62  | 109.70      | 106.68   |
| 31  | 8     | 312 | CLA  | C4A-NA-C1A  | 6.62  | 109.70      | 106.68   |
| 30  | 2     | 306 | CHL  | C1B-CHB-C4A | 6.61  | 125.58      | 121.32   |
| 30  | f     | 607 | CHL  | CHA-C1A-C2A | -6.61 | 117.78      | 133.31   |
| 31  | e     | 604 | CLA  | C4A-NA-C1A  | 6.61  | 109.69      | 106.68   |
| 31  | B     | 822 | CLA  | C4A-NA-C1A  | 6.61  | 109.69      | 106.68   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | c     | 603 | CLA  | C4A-NA-C1A  | 6.61  | 109.69      | 106.68   |
| 31  | d     | 603 | CLA  | C4A-NA-C1A  | 6.61  | 109.69      | 106.68   |
| 30  | a     | 609 | CHL  | C4D-ND-C1D  | 6.61  | 110.23      | 105.22   |
| 30  | a     | 609 | CHL  | CHA-C1A-C2A | -6.61 | 117.80      | 133.31   |
| 31  | 5     | 311 | CLA  | C4A-NA-C1A  | 6.60  | 109.69      | 106.68   |
| 30  | g     | 608 | CHL  | C4D-ND-C1D  | 6.60  | 110.23      | 105.22   |
| 31  | L     | 202 | CLA  | C4A-NA-C1A  | 6.60  | 109.69      | 106.68   |
| 30  | e     | 614 | CHL  | C4D-ND-C1D  | 6.60  | 110.22      | 105.22   |
| 31  | 2     | 312 | CLA  | C4A-NA-C1A  | 6.58  | 109.68      | 106.68   |
| 31  | 7     | 316 | CLA  | C4A-NA-C1A  | 6.58  | 109.68      | 106.68   |
| 31  | A     | 827 | CLA  | C4A-NA-C1A  | 6.58  | 109.68      | 106.68   |
| 30  | i     | 609 | CHL  | CHA-C1A-C2A | -6.58 | 117.86      | 133.31   |
| 31  | 0     | 312 | CLA  | C4A-NA-C1A  | 6.57  | 109.68      | 106.68   |
| 31  | 1     | 308 | CLA  | C4A-NA-C1A  | 6.57  | 109.67      | 106.68   |
| 31  | 6     | 320 | CLA  | C4A-NA-C1A  | 6.57  | 109.67      | 106.68   |
| 32  | A     | 847 | 8CT  | C14-C13-C12 | -6.56 | 118.08      | 127.28   |
| 31  | h     | 613 | CLA  | C4A-NA-C1A  | 6.56  | 109.67      | 106.68   |
| 31  | e     | 603 | CLA  | C4A-NA-C1A  | 6.56  | 109.67      | 106.68   |
| 31  | 0     | 309 | CLA  | C4A-NA-C1A  | 6.55  | 109.67      | 106.68   |
| 31  | A     | 840 | CLA  | C4A-NA-C1A  | 6.55  | 109.67      | 106.68   |
| 31  | A     | 831 | CLA  | C4A-NA-C1A  | 6.55  | 109.67      | 106.68   |
| 30  | i     | 609 | CHL  | C4D-ND-C1D  | 6.54  | 110.19      | 105.22   |
| 31  | G     | 102 | CLA  | C4A-NA-C1A  | 6.54  | 109.66      | 106.68   |
| 31  | a     | 613 | CLA  | C4A-NA-C1A  | 6.54  | 109.66      | 106.68   |
| 31  | 6     | 304 | CLA  | C4A-NA-C1A  | 6.54  | 109.66      | 106.68   |
| 31  | 6     | 314 | CLA  | C4A-NA-C1A  | 6.54  | 109.66      | 106.68   |
| 31  | B     | 823 | CLA  | C4A-NA-C1A  | 6.54  | 109.66      | 106.68   |
| 31  | H     | 202 | CLA  | C4A-NA-C1A  | 6.54  | 109.66      | 106.68   |
| 31  | B     | 806 | CLA  | C4A-NA-C1A  | 6.54  | 109.66      | 106.68   |
| 31  | A     | 815 | CLA  | C4A-NA-C1A  | 6.53  | 109.66      | 106.68   |
| 31  | i     | 604 | CLA  | C4A-NA-C1A  | 6.53  | 109.66      | 106.68   |
| 31  | a     | 610 | CLA  | C4A-NA-C1A  | 6.53  | 109.66      | 106.68   |
| 31  | d     | 612 | CLA  | C4A-NA-C1A  | 6.52  | 109.65      | 106.68   |
| 31  | H     | 205 | CLA  | C4A-NA-C1A  | 6.52  | 109.65      | 106.68   |
| 31  | g     | 612 | CLA  | C4A-NA-C1A  | 6.51  | 109.65      | 106.68   |
| 31  | 4     | 311 | CLA  | C4A-NA-C1A  | 6.51  | 109.65      | 106.68   |
| 30  | h     | 607 | CHL  | CHA-C1A-C2A | -6.51 | 118.02      | 133.31   |
| 31  | B     | 805 | CLA  | C4A-NA-C1A  | 6.51  | 109.65      | 106.68   |
| 31  | A     | 814 | CLA  | C4A-NA-C1A  | 6.50  | 109.65      | 106.68   |
| 31  | G     | 101 | CLA  | C4A-NA-C1A  | 6.50  | 109.65      | 106.68   |
| 30  | b     | 601 | CHL  | C4D-ND-C1D  | 6.50  | 110.15      | 105.22   |
| 31  | f     | 604 | CLA  | C4A-NA-C1A  | 6.50  | 109.64      | 106.68   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | e     | 611 | CLA  | C4A-NA-C1A  | 6.50  | 109.64      | 106.68   |
| 31  | A     | 839 | CLA  | C4A-NA-C1A  | 6.50  | 109.64      | 106.68   |
| 31  | f     | 611 | CLA  | C4A-NA-C1A  | 6.50  | 109.64      | 106.68   |
| 31  | A     | 811 | CLA  | C4A-NA-C1A  | 6.49  | 109.64      | 106.68   |
| 31  | 0     | 321 | CLA  | C4A-NA-C1A  | 6.49  | 109.64      | 106.68   |
| 30  | 9     | 301 | CHL  | C1B-CHB-C4A | 6.49  | 125.50      | 121.32   |
| 30  | 6     | 301 | CHL  | C1B-CHB-C4A | 6.49  | 125.50      | 121.32   |
| 31  | 8     | 314 | CLA  | C4A-NA-C1A  | 6.49  | 109.64      | 106.68   |
| 31  | b     | 613 | CLA  | C4A-NA-C1A  | 6.49  | 109.64      | 106.68   |
| 30  | d     | 601 | CHL  | CHA-C1A-C2A | -6.49 | 118.07      | 133.31   |
| 30  | 5     | 313 | CHL  | C4D-ND-C1D  | 6.49  | 110.14      | 105.22   |
| 30  | b     | 614 | CHL  | C4D-ND-C1D  | 6.49  | 110.14      | 105.22   |
| 30  | e     | 605 | CHL  | C4D-ND-C1D  | 6.49  | 110.14      | 105.22   |
| 31  | c     | 613 | CLA  | C4A-NA-C1A  | 6.48  | 109.64      | 106.68   |
| 42  | i     | 523 | NEX  | C11-C12-C13 | -6.48 | 108.59      | 126.36   |
| 31  | d     | 613 | CLA  | C4A-NA-C1A  | 6.48  | 109.64      | 106.68   |
| 31  | 6     | 311 | CLA  | C4A-NA-C1A  | 6.48  | 109.64      | 106.68   |
| 31  | g     | 604 | CLA  | C4A-NA-C1A  | 6.48  | 109.64      | 106.68   |
| 42  | c     | 523 | NEX  | C11-C12-C13 | -6.47 | 108.62      | 126.36   |
| 42  | b     | 523 | NEX  | C11-C12-C13 | -6.47 | 108.63      | 126.36   |
| 31  | A     | 841 | CLA  | C4A-NA-C1A  | 6.47  | 109.63      | 106.68   |
| 31  | 4     | 312 | CLA  | C4A-NA-C1A  | 6.47  | 109.63      | 106.68   |
| 31  | A     | 822 | CLA  | C4A-NA-C1A  | 6.46  | 109.63      | 106.68   |
| 42  | d     | 523 | NEX  | C11-C12-C13 | -6.46 | 108.64      | 126.36   |
| 42  | h     | 523 | NEX  | C11-C12-C13 | -6.46 | 108.64      | 126.36   |
| 31  | 9     | 311 | CLA  | C4A-NA-C1A  | 6.46  | 109.62      | 106.68   |
| 31  | d     | 611 | CLA  | C4A-NA-C1A  | 6.46  | 109.62      | 106.68   |
| 42  | f     | 523 | NEX  | C11-C12-C13 | -6.45 | 108.66      | 126.36   |
| 42  | a     | 523 | NEX  | C11-C12-C13 | -6.45 | 108.67      | 126.36   |
| 42  | g     | 523 | NEX  | C11-C12-C13 | -6.45 | 108.68      | 126.36   |
| 31  | A     | 823 | CLA  | C4A-NA-C1A  | 6.45  | 109.62      | 106.68   |
| 31  | b     | 604 | CLA  | C4A-NA-C1A  | 6.45  | 109.62      | 106.68   |
| 31  | i     | 603 | CLA  | C4A-NA-C1A  | 6.45  | 109.62      | 106.68   |
| 31  | i     | 612 | CLA  | C4A-NA-C1A  | 6.44  | 109.62      | 106.68   |
| 31  | 9     | 309 | CLA  | C4A-NA-C1A  | 6.44  | 109.61      | 106.68   |
| 31  | A     | 829 | CLA  | C4A-NA-C1A  | 6.44  | 109.61      | 106.68   |
| 30  | i     | 607 | CHL  | C4D-ND-C1D  | 6.43  | 110.10      | 105.22   |
| 31  | J     | 103 | CLA  | C4A-NA-C1A  | 6.43  | 109.61      | 106.68   |
| 31  | 7     | 308 | CLA  | C4A-NA-C1A  | 6.43  | 109.61      | 106.68   |
| 30  | h     | 609 | CHL  | C4D-ND-C1D  | 6.43  | 110.09      | 105.22   |
| 31  | 2     | 304 | CLA  | C4A-NA-C1A  | 6.42  | 109.61      | 106.68   |
| 32  | M     | 102 | 8CT  | C10-C11-C12 | -6.42 | 116.73      | 126.23   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 3     | 306 | CLA  | C4A-NA-C1A  | 6.42  | 109.61      | 106.68   |
| 31  | g     | 603 | CLA  | C4A-NA-C1A  | 6.42  | 109.61      | 106.68   |
| 31  | 6     | 310 | CLA  | C4A-NA-C1A  | 6.42  | 109.61      | 106.68   |
| 31  | 7     | 318 | CLA  | C4A-NA-C1A  | 6.42  | 109.61      | 106.68   |
| 31  | g     | 611 | CLA  | C4A-NA-C1A  | 6.42  | 109.61      | 106.68   |
| 31  | i     | 613 | CLA  | C4A-NA-C1A  | 6.42  | 109.61      | 106.68   |
| 31  | h     | 604 | CLA  | C4A-NA-C1A  | 6.41  | 109.60      | 106.68   |
| 31  | b     | 603 | CLA  | C4A-NA-C1A  | 6.41  | 109.60      | 106.68   |
| 31  | 6     | 318 | CLA  | C4A-NA-C1A  | 6.40  | 109.60      | 106.68   |
| 31  | A     | 805 | CLA  | C4A-NA-C1A  | 6.40  | 109.60      | 106.68   |
| 31  | 1     | 314 | CLA  | C4A-NA-C1A  | 6.40  | 109.60      | 106.68   |
| 31  | O     | 201 | CLA  | C4A-NA-C1A  | 6.40  | 109.60      | 106.68   |
| 32  | B     | 846 | 8CT  | C19-C20-C21 | -6.39 | 118.31      | 127.28   |
| 32  | F     | 302 | 8CT  | C14-C13-C12 | -6.39 | 118.31      | 127.28   |
| 31  | A     | 835 | CLA  | C4A-NA-C1A  | 6.39  | 109.59      | 106.68   |
| 31  | f     | 613 | CLA  | C4A-NA-C1A  | 6.39  | 109.59      | 106.68   |
| 31  | 8     | 303 | CLA  | C4A-NA-C1A  | 6.39  | 109.59      | 106.68   |
| 31  | B     | 825 | CLA  | C4A-NA-C1A  | 6.38  | 109.59      | 106.68   |
| 32  | A     | 846 | 8CT  | C30-C29-C28 | -6.38 | 114.65      | 124.58   |
| 30  | h     | 607 | CHL  | C4D-ND-C1D  | 6.38  | 110.06      | 105.22   |
| 31  | h     | 612 | CLA  | C4A-NA-C1A  | 6.38  | 109.59      | 106.68   |
| 30  | 3     | 307 | CHL  | OBD-CAD-C3D | -6.37 | 117.95      | 127.89   |
| 33  | 5     | 502 | 0UR  | C14-C15-C16 | -6.37 | 118.35      | 127.28   |
| 31  | 5     | 310 | CLA  | C4A-NA-C1A  | 6.37  | 109.58      | 106.68   |
| 31  | h     | 611 | CLA  | C4A-NA-C1A  | 6.37  | 109.58      | 106.68   |
| 31  | B     | 850 | CLA  | C4A-NA-C1A  | 6.36  | 109.58      | 106.68   |
| 31  | g     | 610 | CLA  | C4A-NA-C1A  | 6.36  | 109.58      | 106.68   |
| 31  | 5     | 304 | CLA  | C4A-NA-C1A  | 6.36  | 109.58      | 106.68   |
| 31  | A     | 852 | CLA  | C4A-NA-C1A  | 6.36  | 109.58      | 106.68   |
| 31  | B     | 809 | CLA  | C4A-NA-C1A  | 6.36  | 109.58      | 106.68   |
| 32  | B     | 804 | 8CT  | C18-C17-C16 | -6.36 | 118.36      | 127.28   |
| 31  | 0     | 304 | CLA  | C4A-NA-C1A  | 6.36  | 109.58      | 106.68   |
| 30  | d     | 601 | CHL  | C4D-ND-C1D  | 6.36  | 110.04      | 105.22   |
| 31  | e     | 613 | CLA  | C4A-NA-C1A  | 6.35  | 109.58      | 106.68   |
| 32  | 1     | 402 | 8CT  | C24-C25-C26 | -6.35 | 118.37      | 127.28   |
| 30  | d     | 607 | CHL  | CHA-C1A-C2A | -6.35 | 118.40      | 133.31   |
| 31  | B     | 815 | CLA  | C4A-NA-C1A  | 6.35  | 109.58      | 106.68   |
| 30  | b     | 608 | CHL  | C1B-CHB-C4A | 6.35  | 125.41      | 121.32   |
| 31  | 0     | 303 | CLA  | C4A-NA-C1A  | 6.35  | 109.58      | 106.68   |
| 31  | 6     | 312 | CLA  | C4A-NA-C1A  | 6.35  | 109.58      | 106.68   |
| 31  | B     | 814 | CLA  | C4A-NA-C1A  | 6.35  | 109.57      | 106.68   |
| 32  | B     | 804 | 8CT  | C14-C13-C12 | -6.34 | 118.39      | 127.28   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | h     | 605 | CHL  | CHA-C1A-C2A | -6.34 | 118.42      | 133.31   |
| 31  | 9     | 312 | CLA  | C4A-NA-C1A  | 6.34  | 109.57      | 106.68   |
| 32  | A     | 848 | 8CT  | C30-C29-C28 | -6.34 | 114.72      | 124.58   |
| 31  | A     | 803 | CLA  | C4A-NA-C1A  | 6.34  | 109.57      | 106.68   |
| 31  | c     | 610 | CLA  | C4A-NA-C1A  | 6.34  | 109.57      | 106.68   |
| 31  | c     | 611 | CLA  | C4A-NA-C1A  | 6.34  | 109.57      | 106.68   |
| 32  | 1     | 402 | 8CT  | C18-C17-C16 | -6.34 | 118.39      | 127.28   |
| 31  | A     | 832 | CLA  | C4A-NA-C1A  | 6.33  | 109.57      | 106.68   |
| 31  | 7     | 312 | CLA  | C4A-NA-C1A  | 6.33  | 109.57      | 106.68   |
| 31  | O     | 203 | CLA  | C4A-NA-C1A  | 6.33  | 109.57      | 106.68   |
| 31  | f     | 603 | CLA  | C4A-NA-C1A  | 6.33  | 109.57      | 106.68   |
| 31  | B     | 834 | CLA  | C4A-NA-C1A  | 6.33  | 109.57      | 106.68   |
| 32  | O     | 205 | 8CT  | C10-C11-C12 | -6.33 | 116.88      | 126.23   |
| 31  | B     | 820 | CLA  | C4A-NA-C1A  | 6.32  | 109.56      | 106.68   |
| 31  | 3     | 312 | CLA  | C4A-NA-C1A  | 6.32  | 109.56      | 106.68   |
| 31  | B     | 833 | CLA  | C4A-NA-C1A  | 6.32  | 109.56      | 106.68   |
| 31  | 9     | 302 | CLA  | C4A-NA-C1A  | 6.32  | 109.56      | 106.68   |
| 31  | a     | 611 | CLA  | C4A-NA-C1A  | 6.32  | 109.56      | 106.68   |
| 30  | g     | 609 | CHL  | C4D-ND-C1D  | 6.32  | 110.01      | 105.22   |
| 31  | 8     | 311 | CLA  | C4A-NA-C1A  | 6.31  | 109.56      | 106.68   |
| 31  | 4     | 314 | CLA  | C4A-NA-C1A  | 6.31  | 109.56      | 106.68   |
| 31  | 0     | 308 | CLA  | C4A-NA-C1A  | 6.31  | 109.56      | 106.68   |
| 31  | 3     | 310 | CLA  | C4A-NA-C1A  | 6.31  | 109.56      | 106.68   |
| 31  | B     | 828 | CLA  | C4A-NA-C1A  | 6.31  | 109.56      | 106.68   |
| 31  | B     | 839 | CLA  | C4A-NA-C1A  | 6.31  | 109.56      | 106.68   |
| 30  | 5     | 313 | CHL  | CHA-C1A-C2A | -6.30 | 118.50      | 133.31   |
| 31  | 9     | 304 | CLA  | C4A-NA-C1A  | 6.30  | 109.56      | 106.68   |
| 32  | 6     | 402 | 8CT  | C01-C02-C03 | -6.30 | 117.61      | 124.48   |
| 30  | f     | 609 | CHL  | C4D-ND-C1D  | 6.30  | 110.00      | 105.22   |
| 30  | f     | 601 | CHL  | C1B-CHB-C4A | 6.30  | 125.37      | 121.32   |
| 31  | 7     | 303 | CLA  | C4A-NA-C1A  | 6.30  | 109.55      | 106.68   |
| 31  | K     | 105 | CLA  | C4A-NA-C1A  | 6.30  | 109.55      | 106.68   |
| 31  | A     | 828 | CLA  | C4A-NA-C1A  | 6.29  | 109.55      | 106.68   |
| 31  | A     | 810 | CLA  | C4A-NA-C1A  | 6.29  | 109.55      | 106.68   |
| 31  | d     | 604 | CLA  | C4A-NA-C1A  | 6.29  | 109.55      | 106.68   |
| 31  | L     | 207 | CLA  | C4A-NA-C1A  | 6.29  | 109.55      | 106.68   |
| 31  | 2     | 310 | CLA  | C4A-NA-C1A  | 6.28  | 109.55      | 106.68   |
| 30  | i     | 607 | CHL  | CHA-C1A-C2A | -6.28 | 118.57      | 133.31   |
| 31  | 5     | 314 | CLA  | C4A-NA-C1A  | 6.28  | 109.54      | 106.68   |
| 33  | 3     | 501 | 0UR  | C4-C3-C2    | -6.28 | 114.70      | 120.16   |
| 30  | 6     | 307 | CHL  | OBD-CAD-CBD | 6.27  | 135.03      | 125.82   |
| 42  | c     | 523 | NEX  | C38-C25-C26 | -6.27 | 111.98      | 122.30   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 8     | 309 | CLA  | C4A-NA-C1A  | 6.27  | 109.54      | 106.68   |
| 31  | 6     | 309 | CLA  | C4A-NA-C1A  | 6.26  | 109.54      | 106.68   |
| 31  | B     | 831 | CLA  | C4A-NA-C1A  | 6.26  | 109.54      | 106.68   |
| 31  | 0     | 310 | CLA  | C4A-NA-C1A  | 6.26  | 109.54      | 106.68   |
| 31  | 2     | 314 | CLA  | C4A-NA-C1A  | 6.26  | 109.53      | 106.68   |
| 31  | K     | 102 | CLA  | C4A-NA-C1A  | 6.26  | 109.53      | 106.68   |
| 31  | a     | 604 | CLA  | C4A-NA-C1A  | 6.26  | 109.53      | 106.68   |
| 32  | 8     | 406 | 8CT  | C30-C29-C28 | -6.26 | 114.84      | 124.58   |
| 30  | i     | 601 | CHL  | C4D-ND-C1D  | 6.26  | 109.97      | 105.22   |
| 31  | K     | 101 | CLA  | C4A-NA-C1A  | 6.26  | 109.53      | 106.68   |
| 33  | 7     | 501 | 0UR  | C4-C3-C2    | -6.24 | 114.72      | 120.16   |
| 31  | 3     | 303 | CLA  | C4A-NA-C1A  | 6.24  | 109.53      | 106.68   |
| 31  | 1     | 309 | CLA  | C4A-NA-C1A  | 6.24  | 109.53      | 106.68   |
| 31  | A     | 806 | CLA  | C4A-NA-C1A  | 6.24  | 109.53      | 106.68   |
| 31  | L     | 201 | CLA  | C4A-NA-C1A  | 6.24  | 109.52      | 106.68   |
| 31  | 5     | 308 | CLA  | C4A-NA-C1A  | 6.23  | 109.52      | 106.68   |
| 31  | 1     | 304 | CLA  | C4A-NA-C1A  | 6.23  | 109.52      | 106.68   |
| 42  | i     | 523 | NEX  | C38-C25-C26 | -6.23 | 112.05      | 122.30   |
| 42  | d     | 523 | NEX  | C38-C25-C26 | -6.23 | 112.05      | 122.30   |
| 42  | h     | 523 | NEX  | C38-C25-C26 | -6.23 | 112.06      | 122.30   |
| 42  | f     | 523 | NEX  | C38-C25-C26 | -6.22 | 112.06      | 122.30   |
| 30  | b     | 601 | CHL  | CHA-C1A-C2A | -6.22 | 118.69      | 133.31   |
| 31  | 9     | 300 | CLA  | C4A-NA-C1A  | 6.22  | 109.52      | 106.68   |
| 31  | B     | 813 | CLA  | C4A-NA-C1A  | 6.22  | 109.52      | 106.68   |
| 32  | B     | 848 | 8CT  | C10-C11-C12 | -6.22 | 117.03      | 126.23   |
| 42  | b     | 523 | NEX  | C38-C25-C26 | -6.22 | 112.07      | 122.30   |
| 42  | g     | 523 | NEX  | C38-C25-C26 | -6.22 | 112.07      | 122.30   |
| 31  | 9     | 310 | CLA  | C4A-NA-C1A  | 6.22  | 109.52      | 106.68   |
| 31  | B     | 819 | CLA  | C4A-NA-C1A  | 6.22  | 109.52      | 106.68   |
| 42  | a     | 523 | NEX  | C38-C25-C26 | -6.21 | 112.08      | 122.30   |
| 31  | G     | 103 | CLA  | C4A-NA-C1A  | 6.21  | 109.51      | 106.68   |
| 30  | i     | 606 | CHL  | C4D-ND-C1D  | 6.21  | 109.93      | 105.22   |
| 31  | A     | 807 | CLA  | C4A-NA-C1A  | 6.21  | 109.51      | 106.68   |
| 31  | A     | 836 | CLA  | C4A-NA-C1A  | 6.21  | 109.51      | 106.68   |
| 31  | L     | 204 | CLA  | C4A-NA-C1A  | 6.21  | 109.51      | 106.68   |
| 32  | A     | 846 | 8CT  | C18-C17-C16 | -6.20 | 118.58      | 127.28   |
| 30  | f     | 614 | CHL  | C4D-ND-C1D  | 6.20  | 109.92      | 105.22   |
| 32  | A     | 849 | 8CT  | C18-C17-C16 | -6.19 | 118.59      | 127.28   |
| 31  | 7     | 310 | CLA  | C4A-NA-C1A  | 6.19  | 109.50      | 106.68   |
| 30  | a     | 607 | CHL  | C4D-ND-C1D  | 6.19  | 109.91      | 105.22   |
| 31  | A     | 813 | CLA  | C4A-NA-C1A  | 6.18  | 109.50      | 106.68   |
| 31  | 2     | 309 | CLA  | C4A-NA-C1A  | 6.18  | 109.50      | 106.68   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | H     | 201 | CLA  | C4A-NA-C1A  | 6.18  | 109.50      | 106.68   |
| 30  | 2     | 307 | CHL  | OBD-CAD-C3D | -6.17 | 118.27      | 127.89   |
| 32  | B     | 843 | 8CT  | C14-C13-C12 | -6.17 | 118.63      | 127.28   |
| 31  | A     | 826 | CLA  | C4A-NA-C1A  | 6.16  | 109.49      | 106.68   |
| 32  | A     | 848 | 8CT  | C04-C03-C02 | -6.15 | 114.23      | 122.64   |
| 31  | B     | 836 | CLA  | C4A-NA-C1A  | 6.15  | 109.48      | 106.68   |
| 31  | A     | 838 | CLA  | C4A-NA-C1A  | 6.14  | 109.48      | 106.68   |
| 32  | 2     | 402 | 8CT  | C07-C02-C03 | -6.14 | 114.41      | 122.70   |
| 30  | 5     | 306 | CHL  | C4D-ND-C1D  | 6.14  | 109.88      | 105.22   |
| 30  | e     | 601 | CHL  | C1B-CHB-C4A | 6.14  | 125.27      | 121.32   |
| 31  | A     | 853 | CLA  | C4A-NA-C1A  | 6.14  | 109.48      | 106.68   |
| 30  | h     | 602 | CHL  | C4D-ND-C1D  | 6.13  | 109.87      | 105.22   |
| 32  | B     | 804 | 8CT  | C10-C11-C12 | -6.13 | 117.17      | 126.23   |
| 30  | 2     | 313 | CHL  | C1B-CHB-C4A | 6.13  | 125.26      | 121.32   |
| 30  | 6     | 308 | CHL  | C1B-CHB-C4A | 6.13  | 125.26      | 121.32   |
| 30  | a     | 601 | CHL  | CHA-C1A-C2A | -6.12 | 118.93      | 133.31   |
| 32  | 9     | 401 | 8CT  | C19-C20-C21 | -6.12 | 118.69      | 127.28   |
| 31  | 4     | 303 | CLA  | C4A-NA-C1A  | 6.12  | 109.47      | 106.68   |
| 31  | F     | 301 | CLA  | C4A-NA-C1A  | 6.12  | 109.47      | 106.68   |
| 32  | B     | 847 | 8CT  | C35-C30-C29 | -6.11 | 105.81      | 112.83   |
| 30  | 4     | 307 | CHL  | OBD-CAD-CBD | 6.10  | 134.78      | 125.82   |
| 30  | e     | 609 | CHL  | OBD-CAD-CBD | 6.10  | 134.78      | 125.82   |
| 31  | A     | 821 | CLA  | C4A-NA-C1A  | 6.10  | 109.46      | 106.68   |
| 31  | A     | 825 | CLA  | C4A-NA-C1A  | 6.10  | 109.46      | 106.68   |
| 30  | 8     | 315 | CHL  | C4D-ND-C1D  | 6.09  | 109.84      | 105.22   |
| 32  | 7     | 402 | 8CT  | C35-C30-C29 | -6.07 | 105.84      | 112.83   |
| 30  | e     | 605 | CHL  | CHA-C1A-C2A | -6.07 | 119.05      | 133.31   |
| 31  | 4     | 304 | CLA  | C4A-NA-C1A  | 6.07  | 109.45      | 106.68   |
| 32  | 9     | 401 | 8CT  | C10-C11-C12 | -6.07 | 117.25      | 126.23   |
| 31  | f     | 610 | CLA  | C4A-NA-C1A  | 6.07  | 109.45      | 106.68   |
| 31  | 0     | 313 | CLA  | C4A-NA-C1A  | 6.06  | 109.44      | 106.68   |
| 30  | 5     | 307 | CHL  | C4D-ND-C1D  | 6.05  | 109.81      | 105.22   |
| 31  | i     | 610 | CLA  | C4A-NA-C1A  | 6.05  | 109.44      | 106.68   |
| 31  | 3     | 318 | CLA  | C4A-NA-C1A  | 6.05  | 109.44      | 106.68   |
| 31  | O     | 206 | CLA  | C4A-NA-C1A  | 6.03  | 109.43      | 106.68   |
| 31  | 6     | 317 | CLA  | C4A-NA-C1A  | 6.03  | 109.43      | 106.68   |
| 31  | B     | 824 | CLA  | C4A-NA-C1A  | 6.03  | 109.43      | 106.68   |
| 31  | 8     | 310 | CLA  | C4A-NA-C1A  | 6.02  | 109.42      | 106.68   |
| 30  | b     | 609 | CHL  | C4D-ND-C1D  | 6.02  | 109.78      | 105.22   |
| 33  | 0     | 502 | 0UR  | C4-C3-C2    | -6.01 | 114.93      | 120.16   |
| 30  | h     | 601 | CHL  | CHA-C1A-C2A | -6.00 | 119.21      | 133.31   |
| 31  | 3     | 309 | CLA  | C4A-NA-C1A  | 6.00  | 109.42      | 106.68   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | F     | 302 | 8CT  | C18-C17-C16 | -6.00 | 118.86      | 127.28   |
| 30  | g     | 608 | CHL  | CHA-C1A-C2A | -6.00 | 119.23      | 133.31   |
| 30  | c     | 614 | CHL  | C4D-ND-C1D  | 6.00  | 109.77      | 105.22   |
| 31  | A     | 824 | CLA  | C4A-NA-C1A  | 5.99  | 109.41      | 106.68   |
| 31  | e     | 610 | CLA  | C4A-NA-C1A  | 5.99  | 109.41      | 106.68   |
| 30  | 8     | 306 | CHL  | C1B-CHB-C4A | 5.98  | 125.17      | 121.32   |
| 30  | f     | 608 | CHL  | OBD-CAD-CBD | 5.98  | 134.60      | 125.82   |
| 32  | L     | 205 | 8CT  | C24-C25-C26 | -5.98 | 118.90      | 127.28   |
| 31  | 3     | 313 | CLA  | C4A-NA-C1A  | 5.97  | 109.40      | 106.68   |
| 32  | 7     | 404 | 8CT  | C19-C20-C21 | -5.96 | 118.91      | 127.28   |
| 31  | d     | 610 | CLA  | C4A-NA-C1A  | 5.96  | 109.40      | 106.68   |
| 30  | d     | 609 | CHL  | C4D-ND-C1D  | 5.96  | 109.74      | 105.22   |
| 30  | c     | 609 | CHL  | C4D-ND-C1D  | 5.95  | 109.74      | 105.22   |
| 32  | 1     | 402 | 8CT  | C14-C13-C12 | -5.95 | 118.93      | 127.28   |
| 31  | A     | 819 | CLA  | C4A-NA-C1A  | 5.95  | 109.39      | 106.68   |
| 32  | J     | 101 | 8CT  | C19-C20-C21 | -5.95 | 118.93      | 127.28   |
| 32  | A     | 849 | 8CT  | C30-C31-C32 | -5.95 | 114.15      | 121.47   |
| 32  | A     | 850 | 8CT  | C29-C28-C26 | -5.94 | 113.54      | 126.32   |
| 31  | 8     | 304 | CLA  | C4A-NA-C1A  | 5.94  | 109.39      | 106.68   |
| 30  | 8     | 301 | CHL  | C1A-CHA-C4D | -5.94 | 109.07      | 118.98   |
| 30  | a     | 608 | CHL  | C1A-CHA-C4D | -5.94 | 109.08      | 118.98   |
| 30  | b     | 606 | CHL  | C1B-CHB-C4A | 5.93  | 125.14      | 121.32   |
| 30  | f     | 605 | CHL  | CHA-C1A-C2A | -5.92 | 119.40      | 133.31   |
| 31  | B     | 801 | CLA  | C4A-NA-C1A  | 5.92  | 109.38      | 106.68   |
| 33  | g     | 520 | 0UR  | C10-C11-C12 | -5.91 | 118.98      | 127.28   |
| 33  | 4     | 501 | 0UR  | C43-C3-C4   | -5.91 | 118.05      | 125.03   |
| 32  | M     | 102 | 8CT  | C14-C13-C12 | -5.91 | 118.99      | 127.28   |
| 32  | A     | 850 | 8CT  | C07-C02-C03 | -5.90 | 114.73      | 122.70   |
| 31  | B     | 841 | CLA  | C4A-NA-C1A  | 5.90  | 109.37      | 106.68   |
| 33  | g     | 520 | 0UR  | C14-C15-C16 | -5.89 | 119.02      | 127.28   |
| 30  | g     | 607 | CHL  | CHA-C1A-C2A | -5.89 | 119.49      | 133.31   |
| 30  | 0     | 306 | CHL  | C1A-CHA-C4D | -5.89 | 109.16      | 118.98   |
| 30  | 0     | 305 | CHL  | C1B-CHB-C4A | 5.89  | 125.11      | 121.32   |
| 30  | c     | 607 | CHL  | C4D-ND-C1D  | 5.88  | 109.68      | 105.22   |
| 31  | O     | 202 | CLA  | C4A-NA-C1A  | 5.88  | 109.36      | 106.68   |
| 30  | g     | 608 | CHL  | C1A-CHA-C4D | -5.88 | 109.17      | 118.98   |
| 32  | B     | 847 | 8CT  | C24-C25-C26 | -5.88 | 119.04      | 127.28   |
| 30  | 6     | 307 | CHL  | C1A-CHA-C4D | -5.88 | 109.18      | 118.98   |
| 30  | a     | 614 | CHL  | C1A-CHA-C4D | -5.87 | 109.18      | 118.98   |
| 32  | F     | 302 | 8CT  | C24-C25-C26 | -5.87 | 119.05      | 127.28   |
| 30  | h     | 614 | CHL  | C1A-CHA-C4D | -5.87 | 109.19      | 118.98   |
| 30  | f     | 605 | CHL  | C1A-CHA-C4D | -5.86 | 109.20      | 118.98   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | 0     | 401 | 8CT  | C19-C20-C21 | -5.86 | 119.07      | 127.28   |
| 32  | F     | 302 | 8CT  | C19-C20-C21 | -5.85 | 119.07      | 127.28   |
| 31  | A     | 812 | CLA  | C4A-NA-C1A  | 5.85  | 109.35      | 106.68   |
| 32  | 1     | 402 | 8CT  | C19-C20-C21 | -5.85 | 119.08      | 127.28   |
| 30  | g     | 602 | CHL  | C4D-ND-C1D  | 5.85  | 109.66      | 105.22   |
| 31  | B     | 829 | CLA  | C4A-NA-C1A  | 5.83  | 109.34      | 106.68   |
| 33  | c     | 520 | 0UR  | C14-C15-C16 | -5.83 | 119.09      | 127.28   |
| 30  | h     | 606 | CHL  | C4D-ND-C1D  | 5.83  | 109.64      | 105.22   |
| 30  | 8     | 315 | CHL  | C1A-CHA-C4D | -5.83 | 109.26      | 118.98   |
| 30  | e     | 601 | CHL  | C1A-CHA-C4D | -5.82 | 109.27      | 118.98   |
| 30  | 1     | 307 | CHL  | C1A-CHA-C4D | -5.82 | 109.27      | 118.98   |
| 30  | d     | 614 | CHL  | C1A-CHA-C4D | -5.82 | 109.27      | 118.98   |
| 30  | e     | 609 | CHL  | C4D-ND-C1D  | 5.82  | 109.63      | 105.22   |
| 30  | d     | 605 | CHL  | C1A-CHA-C4D | -5.82 | 109.28      | 118.98   |
| 30  | 2     | 305 | CHL  | C1A-CHA-C4D | -5.81 | 109.28      | 118.98   |
| 30  | 2     | 313 | CHL  | C1A-CHA-C4D | -5.81 | 109.29      | 118.98   |
| 30  | a     | 608 | CHL  | C4D-ND-C1D  | 5.80  | 109.62      | 105.22   |
| 30  | a     | 609 | CHL  | C1A-CHA-C4D | -5.80 | 109.31      | 118.98   |
| 32  | L     | 206 | 8CT  | C18-C17-C16 | -5.80 | 119.15      | 127.28   |
| 30  | i     | 605 | CHL  | C1A-CHA-C4D | -5.80 | 109.31      | 118.98   |
| 30  | e     | 605 | CHL  | C1A-CHA-C4D | -5.79 | 109.31      | 118.98   |
| 33  | 4     | 501 | 0UR  | C4-C3-C2    | -5.79 | 115.12      | 120.16   |
| 33  | 8     | 502 | 0UR  | C14-C15-C16 | -5.79 | 119.16      | 127.28   |
| 30  | a     | 606 | CHL  | C4D-ND-C1D  | 5.79  | 109.61      | 105.22   |
| 30  | d     | 606 | CHL  | C4D-ND-C1D  | 5.79  | 109.61      | 105.22   |
| 30  | b     | 607 | CHL  | C4D-ND-C1D  | 5.78  | 109.60      | 105.22   |
| 32  | B     | 847 | 8CT  | C18-C17-C16 | -5.77 | 119.18      | 127.28   |
| 30  | d     | 608 | CHL  | C4D-ND-C1D  | 5.77  | 109.60      | 105.22   |
| 30  | f     | 606 | CHL  | C1A-CHA-C4D | -5.76 | 109.36      | 118.98   |
| 30  | 6     | 313 | CHL  | C1A-CHA-C4D | -5.76 | 109.36      | 118.98   |
| 30  | d     | 608 | CHL  | C1A-CHA-C4D | -5.76 | 109.37      | 118.98   |
| 30  | a     | 605 | CHL  | CHA-C1A-C2A | -5.76 | 119.78      | 133.31   |
| 30  | d     | 608 | CHL  | OBD-CAD-CBD | 5.76  | 134.28      | 125.82   |
| 32  | 2     | 402 | 8CT  | C01-C02-C03 | -5.76 | 118.20      | 124.48   |
| 30  | c     | 605 | CHL  | CHA-C1A-C2A | -5.76 | 119.79      | 133.31   |
| 30  | g     | 601 | CHL  | C1A-CHA-C4D | -5.76 | 109.38      | 118.98   |
| 30  | f     | 614 | CHL  | C1A-CHA-C4D | -5.76 | 109.38      | 118.98   |
| 30  | 2     | 307 | CHL  | C1A-CHA-C4D | -5.75 | 109.38      | 118.98   |
| 30  | b     | 601 | CHL  | C1A-CHA-C4D | -5.75 | 109.38      | 118.98   |
| 30  | e     | 614 | CHL  | C1A-CHA-C4D | -5.75 | 109.38      | 118.98   |
| 30  | c     | 606 | CHL  | C4D-ND-C1D  | 5.75  | 109.58      | 105.22   |
| 31  | A     | 802 | CLA  | C4A-NA-C1A  | 5.74  | 109.30      | 106.68   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | g     | 605 | CHL  | C1A-CHA-C4D | -5.74 | 109.40      | 118.98   |
| 30  | i     | 614 | CHL  | C1A-CHA-C4D | -5.74 | 109.40      | 118.98   |
| 30  | 6     | 307 | CHL  | C1B-CHB-C4A | 5.74  | 125.02      | 121.32   |
| 30  | b     | 608 | CHL  | C1A-CHA-C4D | -5.74 | 109.40      | 118.98   |
| 30  | i     | 605 | CHL  | CHA-C1A-C2A | -5.74 | 119.83      | 133.31   |
| 30  | i     | 607 | CHL  | C1A-CHA-C4D | -5.74 | 109.41      | 118.98   |
| 30  | e     | 608 | CHL  | C1A-CHA-C4D | -5.74 | 109.41      | 118.98   |
| 30  | g     | 614 | CHL  | C1A-CHA-C4D | -5.74 | 109.41      | 118.98   |
| 31  | 4     | 309 | CLA  | C4A-NA-C1A  | 5.73  | 109.29      | 106.68   |
| 30  | 1     | 305 | CHL  | C1A-CHA-C4D | -5.73 | 109.42      | 118.98   |
| 30  | c     | 605 | CHL  | C1A-CHA-C4D | -5.73 | 109.42      | 118.98   |
| 30  | 4     | 308 | CHL  | C4D-ND-C1D  | 5.73  | 109.57      | 105.22   |
| 30  | d     | 607 | CHL  | C1A-CHA-C4D | -5.73 | 109.43      | 118.98   |
| 30  | h     | 608 | CHL  | C4D-ND-C1D  | 5.72  | 109.56      | 105.22   |
| 30  | g     | 601 | CHL  | CHA-C1A-C2A | -5.72 | 119.88      | 133.31   |
| 30  | 9     | 313 | CHL  | C1A-CHA-C4D | -5.72 | 109.44      | 118.98   |
| 30  | g     | 607 | CHL  | C1A-CHA-C4D | -5.72 | 109.44      | 118.98   |
| 30  | e     | 606 | CHL  | C1A-CHA-C4D | -5.72 | 109.44      | 118.98   |
| 30  | 8     | 313 | CHL  | C1A-CHA-C4D | -5.72 | 109.44      | 118.98   |
| 30  | i     | 608 | CHL  | C4D-ND-C1D  | 5.71  | 109.56      | 105.22   |
| 31  | B     | 826 | CLA  | C4A-NA-C1A  | 5.71  | 109.28      | 106.68   |
| 31  | B     | 830 | CLA  | C4A-NA-C1A  | 5.71  | 109.28      | 106.68   |
| 30  | f     | 608 | CHL  | C1A-CHA-C4D | -5.71 | 109.45      | 118.98   |
| 30  | 1     | 306 | CHL  | C4D-ND-C1D  | 5.71  | 109.55      | 105.22   |
| 30  | 7     | 307 | CHL  | C1A-CHA-C4D | -5.71 | 109.46      | 118.98   |
| 30  | 1     | 307 | CHL  | C4D-ND-C1D  | 5.70  | 109.55      | 105.22   |
| 30  | g     | 602 | CHL  | C1A-CHA-C4D | -5.70 | 109.48      | 118.98   |
| 30  | d     | 601 | CHL  | C1A-CHA-C4D | -5.69 | 109.48      | 118.98   |
| 30  | 0     | 305 | CHL  | C1A-CHA-C4D | -5.69 | 109.49      | 118.98   |
| 30  | 3     | 307 | CHL  | C1A-CHA-C4D | -5.69 | 109.49      | 118.98   |
| 30  | i     | 601 | CHL  | C1A-CHA-C4D | -5.68 | 109.50      | 118.98   |
| 30  | a     | 601 | CHL  | C1A-CHA-C4D | -5.68 | 109.50      | 118.98   |
| 30  | a     | 606 | CHL  | C1A-CHA-C4D | -5.68 | 109.50      | 118.98   |
| 32  | 3     | 403 | 8CT  | C24-C25-C26 | -5.68 | 119.31      | 127.28   |
| 30  | a     | 607 | CHL  | C1A-CHA-C4D | -5.68 | 109.51      | 118.98   |
| 32  | L     | 205 | 8CT  | C18-C17-C16 | -5.68 | 119.32      | 127.28   |
| 30  | i     | 606 | CHL  | C1A-CHA-C4D | -5.67 | 109.51      | 118.98   |
| 30  | a     | 605 | CHL  | C1A-CHA-C4D | -5.67 | 109.52      | 118.98   |
| 30  | i     | 609 | CHL  | C1A-CHA-C4D | -5.67 | 109.52      | 118.98   |
| 30  | i     | 608 | CHL  | C1A-CHA-C4D | -5.66 | 109.53      | 118.98   |
| 32  | B     | 845 | 8CT  | C04-C03-C02 | -5.66 | 114.90      | 122.64   |
| 30  | 6     | 307 | CHL  | OBD-CAD-C3D | -5.66 | 119.06      | 127.89   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | 4     | 308 | CHL  | C1B-CHB-C4A | 5.66  | 124.97      | 121.32   |
| 30  | h     | 608 | CHL  | C1A-CHA-C4D | -5.66 | 109.54      | 118.98   |
| 30  | 6     | 308 | CHL  | C1A-CHA-C4D | -5.66 | 109.54      | 118.98   |
| 30  | 7     | 313 | CHL  | C1A-CHA-C4D | -5.66 | 109.54      | 118.98   |
| 30  | 8     | 305 | CHL  | C1A-CHA-C4D | -5.66 | 109.54      | 118.98   |
| 30  | g     | 605 | CHL  | CHA-C1A-C2A | -5.66 | 120.03      | 133.31   |
| 30  | 2     | 319 | CHL  | C1A-CHA-C4D | -5.66 | 109.55      | 118.98   |
| 30  | e     | 609 | CHL  | OBD-CAD-C3D | -5.65 | 119.07      | 127.89   |
| 30  | g     | 606 | CHL  | C1A-CHA-C4D | -5.65 | 109.55      | 118.98   |
| 30  | i     | 602 | CHL  | C1A-CHA-C4D | -5.65 | 109.55      | 118.98   |
| 31  | 5     | 309 | CLA  | C4A-NA-C1A  | 5.65  | 109.26      | 106.68   |
| 30  | 3     | 305 | CHL  | C1A-CHA-C4D | -5.65 | 109.56      | 118.98   |
| 32  | 7     | 405 | 8CT  | C01-C02-C03 | -5.65 | 118.32      | 124.48   |
| 30  | c     | 606 | CHL  | C1A-CHA-C4D | -5.65 | 109.56      | 118.98   |
| 30  | b     | 601 | CHL  | OBD-CAD-CBD | 5.65  | 134.11      | 125.82   |
| 30  | c     | 608 | CHL  | C1A-CHA-C4D | -5.65 | 109.56      | 118.98   |
| 30  | 7     | 302 | CHL  | C1A-CHA-C4D | -5.64 | 109.56      | 118.98   |
| 30  | h     | 605 | CHL  | C1A-CHA-C4D | -5.64 | 109.56      | 118.98   |
| 30  | i     | 602 | CHL  | C4D-ND-C1D  | 5.64  | 109.50      | 105.22   |
| 30  | 9     | 305 | CHL  | C1A-CHA-C4D | -5.64 | 109.58      | 118.98   |
| 30  | g     | 606 | CHL  | C4D-ND-C1D  | 5.63  | 109.50      | 105.22   |
| 30  | b     | 606 | CHL  | C1A-CHA-C4D | -5.63 | 109.58      | 118.98   |
| 30  | f     | 609 | CHL  | C1A-CHA-C4D | -5.63 | 109.59      | 118.98   |
| 30  | 4     | 319 | CHL  | C1A-CHA-C4D | -5.63 | 109.59      | 118.98   |
| 33  | 8     | 502 | OUR  | C19-C18-C17 | -5.63 | 115.82      | 124.58   |
| 30  | h     | 607 | CHL  | C1A-CHA-C4D | -5.63 | 109.60      | 118.98   |
| 30  | h     | 601 | CHL  | C1A-CHA-C4D | -5.62 | 109.60      | 118.98   |
| 30  | d     | 606 | CHL  | C1A-CHA-C4D | -5.62 | 109.61      | 118.98   |
| 30  | h     | 609 | CHL  | C1A-CHA-C4D | -5.61 | 109.62      | 118.98   |
| 30  | 8     | 308 | CHL  | C1A-CHA-C4D | -5.61 | 109.62      | 118.98   |
| 30  | 5     | 306 | CHL  | C1A-CHA-C4D | -5.61 | 109.63      | 118.98   |
| 30  | b     | 614 | CHL  | C1A-CHA-C4D | -5.61 | 109.63      | 118.98   |
| 30  | h     | 606 | CHL  | C1A-CHA-C4D | -5.60 | 109.63      | 118.98   |
| 31  | B     | 803 | CLA  | C4A-NA-C1A  | 5.60  | 109.24      | 106.68   |
| 30  | e     | 607 | CHL  | C4D-ND-C1D  | 5.60  | 109.47      | 105.22   |
| 30  | 7     | 313 | CHL  | C4D-ND-C1D  | 5.60  | 109.47      | 105.22   |
| 30  | b     | 609 | CHL  | C1A-CHA-C4D | -5.60 | 109.64      | 118.98   |
| 30  | 1     | 313 | CHL  | C1A-CHA-C4D | -5.60 | 109.64      | 118.98   |
| 30  | c     | 607 | CHL  | C1A-CHA-C4D | -5.59 | 109.66      | 118.98   |
| 32  | B     | 846 | 8CT  | C29-C28-C26 | -5.59 | 114.31      | 126.32   |
| 32  | 8     | 402 | 8CT  | C30-C31-C32 | -5.58 | 114.60      | 121.47   |
| 30  | 5     | 305 | CHL  | C1A-CHA-C4D | -5.58 | 109.67      | 118.98   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | 5     | 301 | CHL  | C1A-CHA-C4D | -5.58 | 109.67      | 118.98   |
| 32  | 8     | 402 | 8CT  | C18-C17-C16 | -5.58 | 119.45      | 127.28   |
| 30  | c     | 614 | CHL  | C1A-CHA-C4D | -5.58 | 109.67      | 118.98   |
| 32  | 7     | 405 | 8CT  | C14-C13-C12 | -5.58 | 119.45      | 127.28   |
| 33  | f     | 520 | 0UR  | C14-C15-C16 | -5.57 | 119.46      | 127.28   |
| 30  | 5     | 301 | CHL  | C4D-ND-C1D  | 5.57  | 109.45      | 105.22   |
| 30  | d     | 605 | CHL  | CHA-C1A-C2A | -5.57 | 120.22      | 133.31   |
| 42  | d     | 523 | NEX  | O24-C26-C27 | -5.57 | 100.92      | 116.88   |
| 30  | f     | 607 | CHL  | C1A-CHA-C4D | -5.57 | 109.69      | 118.98   |
| 32  | 1     | 402 | 8CT  | C01-C02-C03 | -5.57 | 118.41      | 124.48   |
| 30  | e     | 608 | CHL  | OBD-CAD-CBD | 5.57  | 134.00      | 125.82   |
| 42  | i     | 523 | NEX  | O24-C26-C27 | -5.57 | 100.93      | 116.88   |
| 42  | g     | 523 | NEX  | O24-C26-C27 | -5.57 | 100.93      | 116.88   |
| 30  | c     | 602 | CHL  | C1A-CHA-C4D | -5.57 | 109.69      | 118.98   |
| 42  | a     | 523 | NEX  | O24-C26-C27 | -5.56 | 100.94      | 116.88   |
| 30  | h     | 602 | CHL  | C1A-CHA-C4D | -5.56 | 109.70      | 118.98   |
| 42  | f     | 523 | NEX  | O24-C26-C27 | -5.56 | 100.95      | 116.88   |
| 30  | c     | 609 | CHL  | C1A-CHA-C4D | -5.56 | 109.70      | 118.98   |
| 32  | 2     | 402 | 8CT  | C14-C13-C12 | -5.56 | 119.48      | 127.28   |
| 30  | 6     | 315 | CHL  | C4D-ND-C1D  | 5.56  | 109.44      | 105.22   |
| 30  | 8     | 301 | CHL  | C4D-ND-C1D  | 5.56  | 109.44      | 105.22   |
| 42  | h     | 523 | NEX  | O24-C26-C27 | -5.56 | 100.96      | 116.88   |
| 30  | 0     | 306 | CHL  | C4D-ND-C1D  | 5.55  | 109.43      | 105.22   |
| 30  | 6     | 315 | CHL  | C1A-CHA-C4D | -5.55 | 109.72      | 118.98   |
| 30  | 7     | 306 | CHL  | C4D-ND-C1D  | 5.55  | 109.43      | 105.22   |
| 42  | b     | 523 | NEX  | O24-C26-C27 | -5.55 | 100.99      | 116.88   |
| 32  | I     | 101 | 8CT  | C14-C13-C12 | -5.54 | 119.50      | 127.28   |
| 30  | g     | 609 | CHL  | C1A-CHA-C4D | -5.54 | 109.73      | 118.98   |
| 32  | 0     | 401 | 8CT  | C04-C03-C02 | -5.54 | 115.06      | 122.64   |
| 30  | 6     | 305 | CHL  | C1A-CHA-C4D | -5.54 | 109.74      | 118.98   |
| 30  | f     | 606 | CHL  | C4D-ND-C1D  | 5.54  | 109.42      | 105.22   |
| 30  | 4     | 307 | CHL  | C1A-CHA-C4D | -5.54 | 109.74      | 118.98   |
| 31  | B     | 826 | CLA  | CBD-CHA-C4D | -5.54 | 107.52      | 117.29   |
| 42  | c     | 523 | NEX  | O24-C26-C27 | -5.54 | 101.02      | 116.88   |
| 30  | e     | 607 | CHL  | C1A-CHA-C4D | -5.53 | 109.75      | 118.98   |
| 30  | d     | 609 | CHL  | C1A-CHA-C4D | -5.53 | 109.75      | 118.98   |
| 32  | 7     | 405 | 8CT  | C10-C11-C12 | -5.53 | 118.06      | 126.23   |
| 30  | 4     | 305 | CHL  | C1A-CHA-C4D | -5.53 | 109.76      | 118.98   |
| 32  | M     | 102 | 8CT  | C19-C20-C21 | -5.53 | 119.53      | 127.28   |
| 30  | b     | 607 | CHL  | C1A-CHA-C4D | -5.52 | 109.77      | 118.98   |
| 30  | f     | 602 | CHL  | C1A-CHA-C4D | -5.52 | 109.77      | 118.98   |
| 30  | 8     | 306 | CHL  | C1A-CHA-C4D | -5.52 | 109.77      | 118.98   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | A     | 850 | 8CT  | C01-C02-C03 | -5.52 | 118.47      | 124.48   |
| 32  | B     | 845 | 8CT  | C14-C13-C12 | -5.51 | 119.55      | 127.28   |
| 32  | L     | 205 | 8CT  | C14-C13-C12 | -5.51 | 119.55      | 127.28   |
| 30  | 5     | 307 | CHL  | C1A-CHA-C4D | -5.51 | 109.80      | 118.98   |
| 30  | 3     | 302 | CHL  | C1A-CHA-C4D | -5.50 | 109.80      | 118.98   |
| 30  | 6     | 306 | CHL  | C1A-CHA-C4D | -5.50 | 109.80      | 118.98   |
| 30  | e     | 609 | CHL  | C1A-CHA-C4D | -5.50 | 109.80      | 118.98   |
| 30  | e     | 602 | CHL  | C1A-CHA-C4D | -5.50 | 109.80      | 118.98   |
| 30  | f     | 601 | CHL  | C1A-CHA-C4D | -5.50 | 109.81      | 118.98   |
| 30  | 1     | 306 | CHL  | C1A-CHA-C4D | -5.49 | 109.83      | 118.98   |
| 33  | 3     | 501 | 0UR  | C43-C3-C4   | -5.48 | 118.56      | 125.03   |
| 32  | B     | 851 | 8CT  | C10-C11-C12 | -5.48 | 118.13      | 126.23   |
| 30  | 6     | 301 | CHL  | C1A-CHA-C4D | -5.48 | 109.84      | 118.98   |
| 32  | J     | 104 | 8CT  | C11-C12-C13 | 5.47  | 127.61      | 119.01   |
| 31  | b     | 610 | CLA  | C4A-NA-C1A  | 5.47  | 109.17      | 106.68   |
| 32  | 8     | 406 | 8CT  | C10-C11-C12 | -5.47 | 118.15      | 126.23   |
| 30  | 1     | 307 | CHL  | OBD-CAD-CBD | 5.47  | 133.84      | 125.82   |
| 30  | a     | 602 | CHL  | C1A-CHA-C4D | -5.46 | 109.86      | 118.98   |
| 30  | 8     | 307 | CHL  | C1A-CHA-C4D | -5.46 | 109.87      | 118.98   |
| 30  | 7     | 305 | CHL  | C1A-CHA-C4D | -5.46 | 109.87      | 118.98   |
| 30  | 0     | 301 | CHL  | C1A-CHA-C4D | -5.46 | 109.88      | 118.98   |
| 30  | 2     | 306 | CHL  | C1A-CHA-C4D | -5.46 | 109.88      | 118.98   |
| 32  | A     | 849 | 8CT  | C14-C13-C12 | -5.45 | 119.64      | 127.28   |
| 32  | A     | 854 | 8CT  | C19-C20-C21 | -5.45 | 119.64      | 127.28   |
| 30  | b     | 602 | CHL  | C1A-CHA-C4D | -5.45 | 109.89      | 118.98   |
| 32  | K     | 107 | 8CT  | C07-C02-C03 | -5.45 | 115.34      | 122.70   |
| 30  | 4     | 306 | CHL  | C1A-CHA-C4D | -5.45 | 109.90      | 118.98   |
| 30  | a     | 602 | CHL  | C4D-ND-C1D  | 5.42  | 109.33      | 105.22   |
| 32  | 7     | 405 | 8CT  | C24-C25-C26 | -5.42 | 119.68      | 127.28   |
| 32  | 3     | 402 | 8CT  | C01-C02-C03 | -5.42 | 118.57      | 124.48   |
| 30  | 7     | 301 | CHL  | C1A-CHA-C4D | -5.42 | 109.94      | 118.98   |
| 30  | 4     | 307 | CHL  | OBD-CAD-C3D | -5.42 | 119.44      | 127.89   |
| 32  | 8     | 402 | 8CT  | C30-C29-C28 | -5.42 | 116.15      | 124.58   |
| 32  | 7     | 402 | 8CT  | C18-C17-C16 | -5.41 | 119.69      | 127.28   |
| 30  | 6     | 302 | CHL  | OBD-CAD-CBD | 5.40  | 133.75      | 125.82   |
| 33  | 6     | 501 | 0UR  | C10-C11-C12 | -5.40 | 119.70      | 127.28   |
| 30  | 4     | 308 | CHL  | C1A-CHA-C4D | -5.40 | 109.97      | 118.98   |
| 30  | 7     | 306 | CHL  | C1A-CHA-C4D | -5.40 | 109.97      | 118.98   |
| 32  | 9     | 401 | 8CT  | C01-C02-C03 | -5.39 | 118.60      | 124.48   |
| 33  | f     | 520 | 0UR  | C10-C11-C12 | -5.39 | 119.71      | 127.28   |
| 32  | L     | 209 | 8CT  | C01-C02-C03 | -5.39 | 118.60      | 124.48   |
| 30  | f     | 601 | CHL  | C4D-ND-C1D  | 5.39  | 109.31      | 105.22   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | 2     | 302 | CHL  | C1A-CHA-C4D | -5.39 | 109.99      | 118.98   |
| 30  | 5     | 305 | CHL  | C4D-ND-C1D  | 5.39  | 109.31      | 105.22   |
| 30  | c     | 608 | CHL  | C4D-ND-C1D  | 5.39  | 109.31      | 105.22   |
| 30  | e     | 606 | CHL  | C4D-ND-C1D  | 5.39  | 109.31      | 105.22   |
| 30  | 1     | 302 | CHL  | C1A-CHA-C4D | -5.38 | 110.00      | 118.98   |
| 30  | g     | 608 | CHL  | OBD-CAD-CBD | 5.38  | 133.72      | 125.82   |
| 30  | c     | 601 | CHL  | C1A-CHA-C4D | -5.38 | 110.01      | 118.98   |
| 32  | 7     | 404 | 8CT  | C28-C26-C25 | 5.38  | 127.47      | 119.01   |
| 32  | B     | 843 | 8CT  | C24-C25-C26 | -5.37 | 119.74      | 127.28   |
| 30  | 9     | 301 | CHL  | C1A-CHA-C4D | -5.37 | 110.03      | 118.98   |
| 32  | 4     | 402 | 8CT  | C07-C02-C03 | -5.37 | 115.45      | 122.70   |
| 30  | 8     | 308 | CHL  | C4D-ND-C1D  | 5.37  | 109.29      | 105.22   |
| 30  | e     | 608 | CHL  | C4D-ND-C1D  | 5.36  | 109.29      | 105.22   |
| 30  | 6     | 308 | CHL  | C4D-ND-C1D  | 5.36  | 109.28      | 105.22   |
| 30  | 4     | 302 | CHL  | C1A-CHA-C4D | -5.36 | 110.05      | 118.98   |
| 32  | A     | 848 | 8CT  | C07-C02-C03 | -5.35 | 115.47      | 122.70   |
| 32  | 8     | 402 | 8CT  | C01-C02-C03 | -5.35 | 118.64      | 124.48   |
| 33  | O     | 204 | 0UR  | C9-C8-C7    | -5.35 | 119.77      | 127.28   |
| 30  | 8     | 302 | CHL  | C1A-CHA-C4D | -5.35 | 110.06      | 118.98   |
| 32  | 0     | 401 | 8CT  | C30-C31-C32 | -5.35 | 114.89      | 121.47   |
| 30  | 2     | 301 | CHL  | C1A-CHA-C4D | -5.34 | 110.07      | 118.98   |
| 30  | d     | 602 | CHL  | C1A-CHA-C4D | -5.34 | 110.08      | 118.98   |
| 30  | 7     | 301 | CHL  | C4D-ND-C1D  | 5.33  | 109.27      | 105.22   |
| 30  | 9     | 306 | CHL  | C4D-ND-C1D  | 5.33  | 109.26      | 105.22   |
| 30  | 0     | 302 | CHL  | C1A-CHA-C4D | -5.33 | 110.09      | 118.98   |
| 30  | 7     | 306 | CHL  | C1B-CHB-C4A | 5.33  | 124.75      | 121.32   |
| 33  | 7     | 501 | 0UR  | C43-C3-C4   | -5.33 | 118.74      | 125.03   |
| 32  | 7     | 402 | 8CT  | C19-C20-C21 | -5.32 | 119.81      | 127.28   |
| 32  | J     | 104 | 8CT  | C13-C14-C15 | -5.31 | 107.81      | 123.20   |
| 30  | 2     | 308 | CHL  | C1A-CHA-C4D | -5.30 | 110.13      | 118.98   |
| 33  | e     | 520 | 0UR  | C43-C3-C4   | -5.30 | 118.78      | 125.03   |
| 30  | 1     | 313 | CHL  | C4D-ND-C1D  | 5.29  | 109.23      | 105.22   |
| 30  | i     | 602 | CHL  | OBD-CAD-CBD | 5.28  | 133.57      | 125.82   |
| 30  | c     | 608 | CHL  | OBD-CAD-CBD | 5.28  | 133.57      | 125.82   |
| 30  | c     | 601 | CHL  | OBD-CAD-CBD | 5.28  | 133.57      | 125.82   |
| 30  | 4     | 313 | CHL  | C1A-CHA-C4D | -5.27 | 110.18      | 118.98   |
| 30  | 5     | 305 | CHL  | C1B-CHB-C4A | 5.27  | 124.71      | 121.32   |
| 32  | G     | 104 | 8CT  | C30-C31-C32 | -5.27 | 114.99      | 121.47   |
| 30  | a     | 602 | CHL  | C1B-CHB-C4A | 5.25  | 124.70      | 121.32   |
| 30  | a     | 608 | CHL  | OBD-CAD-CBD | 5.25  | 133.53      | 125.82   |
| 32  | 0     | 401 | 8CT  | C01-C02-C03 | -5.25 | 118.76      | 124.48   |
| 30  | 5     | 302 | CHL  | C1A-CHA-C4D | -5.25 | 110.22      | 118.98   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | 6     | 302 | CHL  | C1A-CHA-C4D | -5.25 | 110.23      | 118.98   |
| 33  | i     | 520 | 0UR  | C48-C47-C46 | -5.24 | 119.89      | 125.84   |
| 32  | I     | 101 | 8CT  | C10-C11-C12 | -5.24 | 118.48      | 126.23   |
| 30  | f     | 608 | CHL  | OBD-CAD-C3D | -5.24 | 119.72      | 127.89   |
| 32  | K     | 107 | 8CT  | C30-C31-C32 | -5.24 | 115.02      | 121.47   |
| 32  | A     | 854 | 8CT  | C30-C31-C32 | -5.24 | 115.02      | 121.47   |
| 30  | 9     | 306 | CHL  | C1A-CHA-C4D | -5.23 | 110.25      | 118.98   |
| 30  | 1     | 313 | CHL  | C1B-CHB-C4A | 5.23  | 124.69      | 121.32   |
| 30  | 7     | 307 | CHL  | C4D-ND-C1D  | 5.23  | 109.19      | 105.22   |
| 30  | 7     | 307 | CHL  | OBD-CAD-CBD | 5.23  | 133.50      | 125.82   |
| 32  | 3     | 403 | 8CT  | C14-C13-C12 | -5.23 | 119.95      | 127.28   |
| 33  | 5     | 502 | 0UR  | C9-C8-C7    | -5.22 | 119.95      | 127.28   |
| 32  | 4     | 402 | 8CT  | C01-C02-C03 | -5.22 | 118.78      | 124.48   |
| 32  | 9     | 401 | 8CT  | C18-C17-C16 | -5.22 | 119.96      | 127.28   |
| 30  | 2     | 313 | CHL  | C4D-ND-C1D  | 5.22  | 109.18      | 105.22   |
| 30  | 0     | 305 | CHL  | C4D-ND-C1D  | 5.21  | 109.18      | 105.22   |
| 30  | 5     | 307 | CHL  | OBD-CAD-CBD | 5.21  | 133.47      | 125.82   |
| 32  | B     | 845 | 8CT  | C18-C19-C20 | 5.20  | 134.16      | 123.52   |
| 32  | 3     | 403 | 8CT  | C04-C03-C02 | -5.19 | 115.54      | 122.64   |
| 33  | 2     | 502 | 0UR  | C19-C18-C17 | -5.19 | 116.50      | 124.58   |
| 30  | 2     | 319 | CHL  | OBD-CAD-CBD | 5.19  | 133.43      | 125.82   |
| 32  | B     | 848 | 8CT  | C29-C28-C26 | -5.19 | 115.17      | 126.32   |
| 30  | 8     | 307 | CHL  | OBD-CAD-CBD | 5.18  | 133.43      | 125.82   |
| 30  | 5     | 313 | CHL  | C1A-CHA-C4D | -5.17 | 110.35      | 118.98   |
| 33  | 2     | 501 | 0UR  | C43-C3-C4   | -5.17 | 118.93      | 125.03   |
| 30  | 9     | 306 | CHL  | OBD-CAD-CBD | 5.17  | 133.41      | 125.82   |
| 33  | 4     | 502 | 0UR  | C19-C18-C17 | -5.17 | 116.54      | 124.58   |
| 32  | K     | 107 | 8CT  | C01-C02-C03 | -5.16 | 118.85      | 124.48   |
| 32  | 3     | 402 | 8CT  | C19-C20-C21 | -5.16 | 120.04      | 127.28   |
| 33  | 5     | 501 | 0UR  | C10-C11-C12 | -5.14 | 120.06      | 127.28   |
| 30  | b     | 608 | CHL  | OBD-CAD-CBD | 5.14  | 133.37      | 125.82   |
| 32  | 0     | 401 | 8CT  | C24-C25-C26 | -5.14 | 120.07      | 127.28   |
| 30  | 2     | 306 | CHL  | C4D-ND-C1D  | 5.14  | 109.12      | 105.22   |
| 30  | 9     | 301 | CHL  | C4D-ND-C1D  | 5.13  | 109.11      | 105.22   |
| 32  | B     | 804 | 8CT  | C01-C02-C03 | -5.13 | 118.89      | 124.48   |
| 32  | 4     | 402 | 8CT  | C04-C03-C02 | -5.13 | 115.63      | 122.64   |
| 30  | 2     | 305 | CHL  | OBD-CAD-CBD | 5.13  | 133.35      | 125.82   |
| 32  | A     | 850 | 8CT  | C13-C14-C15 | -5.11 | 108.39      | 123.20   |
| 30  | 8     | 301 | CHL  | OBD-CAD-CBD | 5.11  | 133.32      | 125.82   |
| 32  | 8     | 406 | 8CT  | C28-C26-C25 | 5.11  | 127.04      | 119.01   |
| 33  | e     | 520 | 0UR  | C4-C3-C2    | -5.10 | 115.72      | 120.16   |
| 42  | e     | 523 | NEX  | O24-C25-C38 | 5.09  | 120.74      | 115.05   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | 6     | 313 | CHL  | C4D-ND-C1D  | 5.09  | 109.08      | 105.22   |
| 42  | d     | 523 | NEX  | C15-C35-C34 | 5.09  | 133.93      | 123.52   |
| 42  | a     | 523 | NEX  | C15-C35-C34 | 5.08  | 133.92      | 123.52   |
| 30  | b     | 606 | CHL  | C4D-ND-C1D  | 5.08  | 109.07      | 105.22   |
| 33  | 9     | 502 | OUR  | C19-C18-C17 | -5.07 | 116.69      | 124.58   |
| 42  | i     | 523 | NEX  | C15-C35-C34 | 5.07  | 133.90      | 123.52   |
| 30  | b     | 601 | CHL  | OBD-CAD-C3D | -5.07 | 119.99      | 127.89   |
| 33  | 0     | 502 | OUR  | C9-C8-C7    | -5.06 | 120.17      | 127.28   |
| 32  | G     | 104 | 8CT  | C35-C30-C29 | -5.06 | 107.00      | 112.83   |
| 30  | e     | 602 | CHL  | C4D-ND-C1D  | 5.06  | 109.06      | 105.22   |
| 42  | h     | 523 | NEX  | C15-C35-C34 | 5.06  | 133.87      | 123.52   |
| 30  | c     | 606 | CHL  | OBD-CAD-CBD | 5.06  | 133.25      | 125.82   |
| 42  | c     | 523 | NEX  | C15-C35-C34 | 5.06  | 133.87      | 123.52   |
| 42  | b     | 523 | NEX  | C15-C35-C34 | 5.06  | 133.86      | 123.52   |
| 42  | g     | 523 | NEX  | C15-C35-C34 | 5.06  | 133.86      | 123.52   |
| 32  | L     | 206 | 8CT  | C24-C25-C26 | -5.05 | 120.19      | 127.28   |
| 42  | f     | 523 | NEX  | C15-C35-C34 | 5.05  | 133.86      | 123.52   |
| 32  | A     | 847 | 8CT  | C04-C03-C02 | -5.05 | 115.74      | 122.64   |
| 30  | e     | 601 | CHL  | OBD-CAD-CBD | 5.04  | 133.22      | 125.82   |
| 30  | a     | 601 | CHL  | OBD-CAD-CBD | 5.04  | 133.22      | 125.82   |
| 30  | i     | 608 | CHL  | OBD-CAD-CBD | 5.04  | 133.22      | 125.82   |
| 30  | 8     | 306 | CHL  | C4D-ND-C1D  | 5.04  | 109.04      | 105.22   |
| 30  | 2     | 301 | CHL  | C4D-ND-C1D  | 5.03  | 109.04      | 105.22   |
| 30  | f     | 601 | CHL  | OBD-CAD-CBD | 5.03  | 133.21      | 125.82   |
| 32  | 2     | 402 | 8CT  | C04-C03-C02 | -5.03 | 115.77      | 122.64   |
| 30  | 7     | 301 | CHL  | OBD-CAD-CBD | 5.02  | 133.19      | 125.82   |
| 32  | 3     | 403 | 8CT  | C19-C20-C21 | -5.01 | 120.25      | 127.28   |
| 30  | 3     | 305 | CHL  | OBD-CAD-CBD | 5.00  | 133.16      | 125.82   |
| 42  | e     | 523 | NEX  | C35-C34-C33 | -5.00 | 120.26      | 127.28   |
| 30  | d     | 608 | CHL  | OBD-CAD-C3D | -5.00 | 120.10      | 127.89   |
| 42  | e     | 523 | NEX  | C27-C28-C29 | -4.99 | 117.78      | 125.53   |
| 30  | 0     | 301 | CHL  | C4D-ND-C1D  | 4.99  | 109.00      | 105.22   |
| 32  | 7     | 404 | 8CT  | C01-C02-C03 | -4.98 | 119.05      | 124.48   |
| 30  | 8     | 305 | CHL  | C4D-ND-C1D  | 4.98  | 109.00      | 105.22   |
| 30  | 2     | 313 | CHL  | OBD-CAD-CBD | 4.97  | 133.12      | 125.82   |
| 32  | A     | 846 | 8CT  | C30-C31-C32 | -4.97 | 115.35      | 121.47   |
| 41  | B     | 849 | DGD  | O2G-C1B-C2B | 4.97  | 122.23      | 111.48   |
| 30  | h     | 601 | CHL  | OBD-CAD-CBD | 4.97  | 133.12      | 125.82   |
| 33  | 6     | 501 | OUR  | C14-C15-C16 | -4.96 | 120.32      | 127.28   |
| 30  | 4     | 305 | CHL  | OBD-CAD-CBD | 4.96  | 133.11      | 125.82   |
| 32  | M     | 102 | 8CT  | C24-C25-C26 | -4.96 | 120.32      | 127.28   |
| 30  | 3     | 305 | CHL  | C4D-ND-C1D  | 4.96  | 108.98      | 105.22   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | i     | 602 | CHL  | OBD-CAD-C3D | -4.96 | 120.15      | 127.89   |
| 32  | A     | 850 | 8CT  | C15-C16-C17 | -4.96 | 111.21      | 119.01   |
| 30  | 1     | 313 | CHL  | OBD-CAD-CBD | 4.96  | 133.10      | 125.82   |
| 30  | 9     | 313 | CHL  | C4D-ND-C1D  | 4.95  | 108.97      | 105.22   |
| 30  | f     | 607 | CHL  | OBD-CAD-CBD | 4.95  | 133.08      | 125.82   |
| 30  | 4     | 319 | CHL  | OBD-CAD-CBD | 4.95  | 133.08      | 125.82   |
| 32  | 9     | 401 | 8CT  | C04-C03-C02 | -4.94 | 115.88      | 122.64   |
| 30  | b     | 608 | CHL  | C4D-ND-C1D  | 4.94  | 108.97      | 105.22   |
| 42  | a     | 523 | NEX  | O24-C25-C38 | 4.94  | 120.57      | 115.05   |
| 33  | O     | 204 | 0UR  | C5-C4-C3    | -4.94 | 121.01      | 126.92   |
| 30  | e     | 601 | CHL  | C4D-ND-C1D  | 4.94  | 108.97      | 105.22   |
| 30  | 7     | 302 | CHL  | OBD-CAD-CBD | 4.94  | 133.07      | 125.82   |
| 32  | L     | 206 | 8CT  | C01-C02-C03 | -4.94 | 119.10      | 124.48   |
| 42  | c     | 523 | NEX  | O24-C25-C38 | 4.93  | 120.56      | 115.05   |
| 42  | f     | 523 | NEX  | O24-C25-C38 | 4.93  | 120.56      | 115.05   |
| 42  | g     | 523 | NEX  | O24-C25-C38 | 4.93  | 120.56      | 115.05   |
| 42  | c     | 523 | NEX  | C15-C14-C13 | -4.93 | 120.37      | 127.28   |
| 42  | h     | 523 | NEX  | O24-C25-C38 | 4.92  | 120.55      | 115.05   |
| 32  | L     | 209 | 8CT  | C30-C29-C28 | -4.92 | 116.92      | 124.58   |
| 30  | 5     | 301 | CHL  | OBD-CAD-CBD | 4.92  | 133.04      | 125.82   |
| 42  | b     | 523 | NEX  | O24-C25-C38 | 4.92  | 120.55      | 115.05   |
| 30  | c     | 601 | CHL  | C4D-ND-C1D  | 4.91  | 108.95      | 105.22   |
| 42  | h     | 523 | NEX  | C15-C14-C13 | -4.91 | 120.39      | 127.28   |
| 32  | 6     | 402 | 8CT  | C14-C15-C16 | -4.91 | 112.89      | 126.36   |
| 32  | 7     | 402 | 8CT  | C01-C02-C03 | -4.91 | 119.12      | 124.48   |
| 42  | d     | 523 | NEX  | O24-C25-C38 | 4.91  | 120.53      | 115.05   |
| 30  | 2     | 308 | CHL  | C4D-ND-C1D  | 4.90  | 108.94      | 105.22   |
| 32  | B     | 846 | 8CT  | C07-C02-C03 | -4.90 | 116.09      | 122.70   |
| 33  | c     | 520 | 0UR  | C10-C11-C12 | -4.90 | 120.41      | 127.28   |
| 42  | g     | 523 | NEX  | C15-C14-C13 | -4.89 | 120.42      | 127.28   |
| 42  | i     | 523 | NEX  | C15-C14-C13 | -4.89 | 120.42      | 127.28   |
| 42  | i     | 523 | NEX  | O24-C25-C38 | 4.89  | 120.51      | 115.05   |
| 42  | f     | 523 | NEX  | C15-C14-C13 | -4.88 | 120.43      | 127.28   |
| 30  | 4     | 302 | CHL  | OBD-CAD-CBD | 4.88  | 132.98      | 125.82   |
| 32  | B     | 844 | 8CT  | C30-C31-C32 | -4.88 | 115.47      | 121.47   |
| 42  | d     | 523 | NEX  | C15-C14-C13 | -4.87 | 120.44      | 127.28   |
| 33  | 4     | 501 | 0UR  | C19-C18-C17 | -4.87 | 117.00      | 124.58   |
| 30  | 9     | 306 | CHL  | OBD-CAD-C3D | -4.87 | 120.29      | 127.89   |
| 30  | 2     | 301 | CHL  | OBD-CAD-CBD | 4.87  | 132.97      | 125.82   |
| 32  | B     | 848 | 8CT  | C19-C18-C17 | -4.87 | 113.55      | 123.52   |
| 30  | 0     | 306 | CHL  | OBD-CAD-CBD | 4.87  | 132.97      | 125.82   |
| 32  | J     | 104 | 8CT  | C30-C31-C32 | -4.87 | 115.48      | 121.47   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | b     | 602 | CHL  | C4D-ND-C1D  | 4.87  | 108.91      | 105.22   |
| 42  | b     | 523 | NEX  | C15-C14-C13 | -4.86 | 120.46      | 127.28   |
| 32  | 8     | 406 | 8CT  | C14-C13-C12 | -4.86 | 120.46      | 127.28   |
| 30  | e     | 605 | CHL  | OBD-CAD-CBD | 4.86  | 132.96      | 125.82   |
| 30  | 6     | 307 | CHL  | C4D-ND-C1D  | 4.86  | 108.91      | 105.22   |
| 37  | g     | 522 | 0IE  | C10-C9-C8   | 4.86  | 133.46      | 123.52   |
| 42  | a     | 523 | NEX  | C15-C14-C13 | -4.86 | 120.46      | 127.28   |
| 30  | 0     | 301 | CHL  | OBD-CAD-CBD | 4.86  | 132.95      | 125.82   |
| 30  | 2     | 305 | CHL  | C4D-ND-C1D  | 4.85  | 108.90      | 105.22   |
| 32  | A     | 848 | 8CT  | C10-C11-C12 | -4.84 | 119.08      | 126.23   |
| 32  | L     | 205 | 8CT  | C19-C20-C21 | -4.84 | 120.50      | 127.28   |
| 30  | 9     | 313 | CHL  | OBD-CAD-CBD | 4.83  | 132.91      | 125.82   |
| 32  | B     | 847 | 8CT  | C07-C02-C03 | -4.82 | 116.19      | 122.70   |
| 32  | 7     | 405 | 8CT  | C18-C17-C16 | -4.82 | 120.51      | 127.28   |
| 32  | J     | 104 | 8CT  | C01-C02-C03 | -4.82 | 119.22      | 124.48   |
| 30  | d     | 605 | CHL  | C1B-CHB-C4A | -4.82 | 118.22      | 121.32   |
| 30  | e     | 608 | CHL  | OBD-CAD-C3D | -4.82 | 120.37      | 127.89   |
| 33  | h     | 520 | 0UR  | C10-C11-C12 | -4.82 | 120.52      | 127.28   |
| 33  | 5     | 501 | 0UR  | C19-C18-C17 | -4.82 | 117.08      | 124.58   |
| 32  | B     | 851 | 8CT  | C19-C20-C21 | -4.82 | 120.52      | 127.28   |
| 32  | J     | 101 | 8CT  | C07-C02-C03 | -4.82 | 116.19      | 122.70   |
| 30  | 0     | 302 | CHL  | OBD-CAD-CBD | 4.82  | 132.90      | 125.82   |
| 32  | 8     | 402 | 8CT  | C19-C20-C21 | -4.81 | 120.53      | 127.28   |
| 32  | A     | 854 | 8CT  | C18-C17-C16 | -4.81 | 120.53      | 127.28   |
| 33  | 9     | 502 | 0UR  | C9-C8-C7    | -4.81 | 120.53      | 127.28   |
| 30  | 5     | 307 | CHL  | OBD-CAD-C3D | -4.81 | 120.39      | 127.89   |
| 32  | 7     | 404 | 8CT  | C14-C15-C16 | -4.80 | 113.19      | 126.36   |
| 32  | A     | 848 | 8CT  | C19-C20-C21 | -4.80 | 120.54      | 127.28   |
| 32  | L     | 205 | 8CT  | C29-C28-C26 | -4.80 | 116.00      | 126.32   |
| 30  | h     | 608 | CHL  | OBD-CAD-CBD | 4.80  | 132.87      | 125.82   |
| 30  | 6     | 305 | CHL  | C4D-ND-C1D  | 4.80  | 108.86      | 105.22   |
| 32  | B     | 843 | 8CT  | C10-C11-C12 | -4.79 | 119.15      | 126.23   |
| 30  | 6     | 315 | CHL  | OBD-CAD-CBD | 4.79  | 132.85      | 125.82   |
| 30  | 8     | 301 | CHL  | OBD-CAD-C3D | -4.79 | 120.43      | 127.89   |
| 30  | 4     | 306 | CHL  | OBD-CAD-CBD | 4.78  | 132.84      | 125.82   |
| 30  | 6     | 302 | CHL  | OBD-CAD-C3D | -4.78 | 120.44      | 127.89   |
| 30  | a     | 608 | CHL  | OBD-CAD-C3D | -4.78 | 120.44      | 127.89   |
| 30  | 7     | 305 | CHL  | C4D-ND-C1D  | 4.77  | 108.84      | 105.22   |
| 30  | f     | 606 | CHL  | OBD-CAD-CBD | 4.76  | 132.81      | 125.82   |
| 32  | J     | 104 | 8CT  | C24-C25-C26 | -4.76 | 120.60      | 127.28   |
| 30  | 2     | 319 | CHL  | C4D-ND-C1D  | 4.76  | 108.83      | 105.22   |
| 30  | 3     | 307 | CHL  | C4D-ND-C1D  | 4.76  | 108.83      | 105.22   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | L     | 205 | 8CT  | C10-C11-C12 | -4.75 | 119.21      | 126.23   |
| 32  | F     | 302 | 8CT  | C01-C02-C03 | -4.74 | 119.31      | 124.48   |
| 30  | d     | 614 | CHL  | OBD-CAD-CBD | 4.74  | 132.78      | 125.82   |
| 30  | 2     | 306 | CHL  | OBD-CAD-CBD | 4.74  | 132.78      | 125.82   |
| 30  | 4     | 306 | CHL  | C4D-ND-C1D  | 4.73  | 108.81      | 105.22   |
| 32  | B     | 845 | 8CT  | C30-C31-C32 | -4.73 | 115.64      | 121.47   |
| 32  | 4     | 402 | 8CT  | C24-C25-C26 | -4.73 | 120.64      | 127.28   |
| 32  | A     | 854 | 8CT  | C01-C02-C03 | -4.73 | 119.32      | 124.48   |
| 42  | c     | 523 | NEX  | C31-C30-C29 | -4.73 | 120.65      | 127.28   |
| 30  | a     | 614 | CHL  | OBD-CAD-CBD | 4.73  | 132.76      | 125.82   |
| 30  | h     | 606 | CHL  | OBD-CAD-CBD | 4.73  | 132.76      | 125.82   |
| 32  | 4     | 402 | 8CT  | C14-C13-C12 | -4.73 | 120.65      | 127.28   |
| 30  | 1     | 307 | CHL  | OBD-CAD-C3D | -4.72 | 120.52      | 127.89   |
| 42  | d     | 523 | NEX  | C31-C30-C29 | -4.72 | 120.66      | 127.28   |
| 32  | B     | 846 | 8CT  | C39-C16-C17 | -4.72 | 115.17      | 122.82   |
| 30  | e     | 606 | CHL  | C1B-CHB-C4A | 4.72  | 124.36      | 121.32   |
| 30  | g     | 608 | CHL  | OBD-CAD-C3D | -4.72 | 120.53      | 127.89   |
| 30  | d     | 601 | CHL  | OBD-CAD-CBD | 4.72  | 132.75      | 125.82   |
| 32  | I     | 101 | 8CT  | C19-C20-C21 | -4.71 | 120.67      | 127.28   |
| 30  | c     | 601 | CHL  | OBD-CAD-C3D | -4.71 | 120.54      | 127.89   |
| 30  | g     | 614 | CHL  | OBD-CAD-CBD | 4.71  | 132.74      | 125.82   |
| 32  | 8     | 406 | 8CT  | C01-C02-C03 | -4.70 | 119.35      | 124.48   |
| 32  | B     | 847 | 8CT  | C01-C02-C03 | -4.70 | 119.35      | 124.48   |
| 30  | 6     | 306 | CHL  | C4D-ND-C1D  | 4.70  | 108.79      | 105.22   |
| 42  | a     | 523 | NEX  | C31-C30-C29 | -4.70 | 120.69      | 127.28   |
| 30  | 1     | 305 | CHL  | OBD-CAD-CBD | 4.70  | 132.72      | 125.82   |
| 30  | 7     | 301 | CHL  | OBD-CAD-C3D | -4.70 | 120.57      | 127.89   |
| 32  | 7     | 405 | 8CT  | C19-C20-C21 | -4.70 | 120.69      | 127.28   |
| 33  | 0     | 501 | 0UR  | C19-C18-C17 | -4.69 | 117.27      | 124.58   |
| 33  | 1     | 502 | 0UR  | C9-C8-C7    | -4.69 | 120.69      | 127.28   |
| 42  | f     | 523 | NEX  | C31-C30-C29 | -4.69 | 120.70      | 127.28   |
| 42  | i     | 523 | NEX  | C31-C30-C29 | -4.69 | 120.70      | 127.28   |
| 30  | 8     | 313 | CHL  | C4D-ND-C1D  | 4.69  | 108.78      | 105.22   |
| 32  | K     | 107 | 8CT  | C10-C11-C12 | -4.69 | 119.30      | 126.23   |
| 30  | 3     | 302 | CHL  | OBD-CAD-CBD | 4.68  | 132.69      | 125.82   |
| 32  | B     | 845 | 8CT  | C39-C16-C17 | -4.68 | 115.23      | 122.82   |
| 42  | g     | 523 | NEX  | C31-C30-C29 | -4.68 | 120.71      | 127.28   |
| 30  | 1     | 305 | CHL  | C4D-ND-C1D  | 4.68  | 108.77      | 105.22   |
| 42  | h     | 523 | NEX  | C31-C30-C29 | -4.68 | 120.72      | 127.28   |
| 42  | b     | 523 | NEX  | C31-C30-C29 | -4.67 | 120.73      | 127.28   |
| 32  | 3     | 403 | 8CT  | C07-C02-C03 | -4.67 | 116.40      | 122.70   |
| 30  | 6     | 305 | CHL  | OBD-CAD-CBD | 4.67  | 132.67      | 125.82   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | 8     | 305 | CHL  | OBD-CAD-CBD | 4.66  | 132.66      | 125.82   |
| 32  | A     | 848 | 8CT  | C18-C17-C16 | -4.66 | 120.75      | 127.28   |
| 32  | B     | 847 | 8CT  | C29-C28-C26 | -4.65 | 116.31      | 126.32   |
| 30  | 2     | 319 | CHL  | OBD-CAD-C3D | -4.65 | 120.63      | 127.89   |
| 30  | e     | 602 | CHL  | OBD-CAD-CBD | 4.65  | 132.65      | 125.82   |
| 30  | 6     | 301 | CHL  | C4D-ND-C1D  | 4.65  | 108.75      | 105.22   |
| 30  | f     | 608 | CHL  | C4D-ND-C1D  | 4.65  | 108.75      | 105.22   |
| 30  | 9     | 305 | CHL  | C4D-ND-C1D  | 4.65  | 108.75      | 105.22   |
| 30  | f     | 614 | CHL  | OBD-CAD-CBD | 4.65  | 132.64      | 125.82   |
| 30  | g     | 608 | CHL  | C1A-CHA-CBD | 4.65  | 144.26      | 132.36   |
| 30  | 4     | 305 | CHL  | C4D-ND-C1D  | 4.64  | 108.74      | 105.22   |
| 30  | g     | 605 | CHL  | OBD-CAD-CBD | 4.64  | 132.64      | 125.82   |
| 30  | 5     | 302 | CHL  | OBD-CAD-CBD | 4.64  | 132.64      | 125.82   |
| 30  | f     | 607 | CHL  | OBD-CAD-C3D | -4.64 | 120.65      | 127.89   |
| 30  | 0     | 305 | CHL  | OBD-CAD-CBD | 4.64  | 132.63      | 125.82   |
| 33  | 0     | 501 | 0UR  | C4-C3-C2    | -4.64 | 116.12      | 120.16   |
| 30  | d     | 614 | CHL  | C1A-CHA-CBD | 4.64  | 144.24      | 132.36   |
| 30  | 6     | 302 | CHL  | C4D-ND-C1D  | 4.64  | 108.74      | 105.22   |
| 30  | d     | 602 | CHL  | C4D-ND-C1D  | 4.63  | 108.73      | 105.22   |
| 30  | a     | 606 | CHL  | OBD-CAD-CBD | 4.63  | 132.62      | 125.82   |
| 30  | d     | 606 | CHL  | OBD-CAD-CBD | 4.63  | 132.62      | 125.82   |
| 30  | e     | 614 | CHL  | C1A-CHA-CBD | 4.63  | 144.21      | 132.36   |
| 30  | i     | 601 | CHL  | OBD-CAD-CBD | 4.62  | 132.60      | 125.82   |
| 30  | 8     | 307 | CHL  | C4D-ND-C1D  | 4.62  | 108.72      | 105.22   |
| 30  | d     | 605 | CHL  | C1A-CHA-CBD | 4.62  | 144.18      | 132.36   |
| 32  | B     | 844 | 8CT  | C10-C11-C12 | -4.61 | 119.41      | 126.23   |
| 30  | c     | 608 | CHL  | OBD-CAD-C3D | -4.61 | 120.70      | 127.89   |
| 30  | 8     | 315 | CHL  | OBD-CAD-CBD | 4.61  | 132.59      | 125.82   |
| 32  | I     | 101 | 8CT  | C35-C30-C29 | -4.61 | 107.52      | 112.83   |
| 33  | 1     | 502 | 0UR  | C5-C4-C3    | -4.61 | 121.41      | 126.92   |
| 30  | 0     | 302 | CHL  | C4D-ND-C1D  | 4.61  | 108.72      | 105.22   |
| 42  | a     | 523 | NEX  | C38-C25-C24 | -4.60 | 109.07      | 114.24   |
| 32  | K     | 107 | 8CT  | C35-C30-C29 | -4.60 | 107.54      | 112.83   |
| 30  | i     | 605 | CHL  | C1A-CHA-CBD | 4.60  | 144.14      | 132.36   |
| 32  | J     | 104 | 8CT  | C40-C12-C13 | -4.60 | 115.37      | 122.82   |
| 30  | d     | 605 | CHL  | OBD-CAD-CBD | 4.60  | 132.57      | 125.82   |
| 30  | i     | 602 | CHL  | C1B-CHB-C4A | 4.60  | 124.28      | 121.32   |
| 30  | a     | 614 | CHL  | C1A-CHA-CBD | 4.60  | 144.13      | 132.36   |
| 30  | g     | 614 | CHL  | C1A-CHA-CBD | 4.59  | 144.13      | 132.36   |
| 32  | B     | 845 | 8CT  | C23-C21-C20 | -4.59 | 111.78      | 119.01   |
| 30  | 4     | 302 | CHL  | C4D-ND-C1D  | 4.59  | 108.70      | 105.22   |
| 30  | 7     | 305 | CHL  | OBD-CAD-CBD | 4.59  | 132.56      | 125.82   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | f     | 601 | CHL  | OBD-CAD-C3D | -4.59 | 120.73      | 127.89   |
| 30  | g     | 606 | CHL  | OBD-CAD-CBD | 4.59  | 132.56      | 125.82   |
| 30  | 4     | 319 | CHL  | OBD-CAD-C3D | -4.59 | 120.74      | 127.89   |
| 30  | 6     | 313 | CHL  | OBD-CAD-CBD | 4.58  | 132.54      | 125.82   |
| 30  | 7     | 307 | CHL  | OBD-CAD-C3D | -4.58 | 120.75      | 127.89   |
| 32  | B     | 846 | 8CT  | C19-C18-C17 | -4.58 | 114.15      | 123.52   |
| 32  | 4     | 402 | 8CT  | C35-C30-C29 | -4.58 | 107.56      | 112.83   |
| 42  | f     | 523 | NEX  | C38-C25-C24 | -4.57 | 109.11      | 114.24   |
| 33  | 6     | 502 | 0UR  | C5-C4-C3    | -4.57 | 121.45      | 126.92   |
| 30  | 8     | 302 | CHL  | OBD-CAD-CBD | 4.57  | 132.53      | 125.82   |
| 30  | h     | 607 | CHL  | OBD-CAD-CBD | 4.56  | 132.52      | 125.82   |
| 32  | O     | 205 | 8CT  | C30-C29-C28 | -4.56 | 117.48      | 124.58   |
| 42  | b     | 523 | NEX  | C38-C25-C24 | -4.56 | 109.12      | 114.24   |
| 30  | h     | 609 | CHL  | OBD-CAD-CBD | 4.56  | 132.52      | 125.82   |
| 30  | e     | 605 | CHL  | C1A-CHA-CBD | 4.56  | 144.03      | 132.36   |
| 30  | 7     | 302 | CHL  | OBD-CAD-C3D | -4.55 | 120.79      | 127.89   |
| 32  | I     | 101 | 8CT  | C18-C17-C16 | -4.55 | 120.89      | 127.28   |
| 33  | 8     | 501 | 0UR  | C19-C18-C17 | -4.55 | 117.50      | 124.58   |
| 30  | 1     | 302 | CHL  | OBD-CAD-CBD | 4.55  | 132.50      | 125.82   |
| 30  | c     | 602 | CHL  | C4D-ND-C1D  | 4.55  | 108.67      | 105.22   |
| 30  | 4     | 313 | CHL  | C4D-ND-C1D  | 4.55  | 108.67      | 105.22   |
| 30  | g     | 607 | CHL  | C1A-CHA-CBD | 4.55  | 144.00      | 132.36   |
| 42  | c     | 523 | NEX  | C38-C25-C24 | -4.55 | 109.13      | 114.24   |
| 42  | g     | 523 | NEX  | C38-C25-C24 | -4.54 | 109.14      | 114.24   |
| 30  | f     | 606 | CHL  | C1B-CHB-C4A | 4.54  | 124.25      | 121.32   |
| 30  | c     | 605 | CHL  | C1A-CHA-CBD | 4.54  | 143.99      | 132.36   |
| 42  | h     | 523 | NEX  | C38-C25-C24 | -4.54 | 109.14      | 114.24   |
| 30  | b     | 607 | CHL  | OBD-CAD-CBD | 4.54  | 132.49      | 125.82   |
| 30  | d     | 607 | CHL  | OBD-CAD-CBD | 4.54  | 132.49      | 125.82   |
| 30  | f     | 605 | CHL  | C1A-CHA-CBD | 4.54  | 143.99      | 132.36   |
| 30  | e     | 606 | CHL  | OBD-CAD-CBD | 4.54  | 132.48      | 125.82   |
| 42  | d     | 523 | NEX  | C38-C25-C24 | -4.54 | 109.14      | 114.24   |
| 42  | i     | 523 | NEX  | C38-C25-C24 | -4.54 | 109.14      | 114.24   |
| 30  | 9     | 301 | CHL  | OBD-CAD-CBD | 4.53  | 132.48      | 125.82   |
| 30  | h     | 614 | CHL  | OBD-CAD-CBD | 4.53  | 132.47      | 125.82   |
| 30  | 2     | 302 | CHL  | C4D-ND-C1D  | 4.53  | 108.66      | 105.22   |
| 30  | i     | 607 | CHL  | OBD-CAD-CBD | 4.53  | 132.47      | 125.82   |
| 33  | g     | 520 | 0UR  | C5-C4-C3    | -4.52 | 121.52      | 126.92   |
| 30  | e     | 607 | CHL  | OBD-CAD-CBD | 4.52  | 132.45      | 125.82   |
| 30  | a     | 605 | CHL  | C1A-CHA-CBD | 4.51  | 143.92      | 132.36   |
| 30  | g     | 605 | CHL  | C1A-CHA-CBD | 4.51  | 143.92      | 132.36   |
| 30  | e     | 602 | CHL  | C1B-CHB-C4A | 4.51  | 124.23      | 121.32   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 33  | i     | 520 | 0UR  | C19-C18-C17 | -4.51 | 117.56      | 124.58   |
| 30  | 6     | 301 | CHL  | OBD-CAD-CBD | 4.51  | 132.44      | 125.82   |
| 32  | 7     | 404 | 8CT  | C35-C30-C29 | -4.51 | 107.64      | 112.83   |
| 32  | 3     | 402 | 8CT  | C07-C02-C03 | -4.50 | 116.62      | 122.70   |
| 30  | g     | 601 | CHL  | C1A-CHA-CBD | 4.50  | 143.90      | 132.36   |
| 30  | 5     | 301 | CHL  | OBD-CAD-C3D | -4.50 | 120.87      | 127.89   |
| 30  | 4     | 307 | CHL  | C4D-ND-C1D  | 4.50  | 108.63      | 105.22   |
| 32  | B     | 848 | 8CT  | C01-C02-C03 | -4.50 | 119.58      | 124.48   |
| 30  | i     | 614 | CHL  | C1A-CHA-CBD | 4.49  | 143.87      | 132.36   |
| 32  | 1     | 402 | 8CT  | C10-C11-C12 | -4.49 | 119.59      | 126.23   |
| 30  | a     | 601 | CHL  | C1A-CHA-CBD | 4.49  | 143.85      | 132.36   |
| 30  | g     | 607 | CHL  | OBD-CAD-CBD | 4.49  | 132.41      | 125.82   |
| 30  | i     | 606 | CHL  | OBD-CAD-CBD | 4.48  | 132.40      | 125.82   |
| 30  | a     | 607 | CHL  | OBD-CAD-CBD | 4.48  | 132.40      | 125.82   |
| 30  | 4     | 302 | CHL  | OBD-CAD-C3D | -4.48 | 120.91      | 127.89   |
| 30  | e     | 614 | CHL  | OBD-CAD-CBD | 4.48  | 132.40      | 125.82   |
| 30  | h     | 601 | CHL  | OBD-CAD-C3D | -4.48 | 120.91      | 127.89   |
| 33  | 6     | 501 | 0UR  | C4-C3-C2    | -4.47 | 116.27      | 120.16   |
| 32  | J     | 101 | 8CT  | C29-C28-C26 | -4.46 | 116.72      | 126.32   |
| 30  | 2     | 313 | CHL  | OBD-CAD-C3D | -4.46 | 120.93      | 127.89   |
| 32  | B     | 845 | 8CT  | C19-C20-C21 | 4.46  | 133.54      | 127.28   |
| 32  | B     | 851 | 8CT  | C14-C13-C12 | -4.46 | 121.02      | 127.28   |
| 32  | 3     | 403 | 8CT  | C01-C02-C03 | -4.46 | 119.62      | 124.48   |
| 30  | c     | 614 | CHL  | OBD-CAD-CBD | 4.46  | 132.36      | 125.82   |
| 30  | f     | 614 | CHL  | C1A-CHA-CBD | 4.46  | 143.77      | 132.36   |
| 30  | 7     | 302 | CHL  | C4D-ND-C1D  | 4.45  | 108.60      | 105.22   |
| 30  | 4     | 319 | CHL  | C4D-ND-C1D  | 4.45  | 108.60      | 105.22   |
| 32  | A     | 847 | 8CT  | C10-C11-C12 | -4.45 | 119.65      | 126.23   |
| 30  | b     | 614 | CHL  | OBD-CAD-CBD | 4.45  | 132.35      | 125.82   |
| 30  | e     | 601 | CHL  | OBD-CAD-C3D | -4.45 | 120.96      | 127.89   |
| 30  | 5     | 302 | CHL  | C4D-ND-C1D  | 4.44  | 108.59      | 105.22   |
| 30  | 0     | 306 | CHL  | C1A-CHA-CBD | 4.44  | 143.74      | 132.36   |
| 32  | G     | 104 | 8CT  | C24-C25-C26 | -4.44 | 121.05      | 127.28   |
| 32  | B     | 851 | 8CT  | C24-C25-C26 | -4.44 | 121.05      | 127.28   |
| 32  | J     | 104 | 8CT  | C15-C16-C17 | 4.44  | 125.99      | 119.01   |
| 32  | L     | 206 | 8CT  | C07-C02-C03 | -4.44 | 116.71      | 122.70   |
| 33  | b     | 520 | 0UR  | C10-C11-C12 | -4.43 | 121.06      | 127.28   |
| 30  | d     | 609 | CHL  | OBD-CAD-CBD | 4.43  | 132.32      | 125.82   |
| 30  | 8     | 306 | CHL  | OBD-CAD-CBD | 4.43  | 132.32      | 125.82   |
| 30  | f     | 602 | CHL  | C4D-ND-C1D  | 4.43  | 108.58      | 105.22   |
| 30  | 2     | 301 | CHL  | OBD-CAD-C3D | -4.43 | 120.99      | 127.89   |
| 30  | c     | 607 | CHL  | OBD-CAD-CBD | 4.43  | 132.32      | 125.82   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | h     | 614 | CHL  | C1A-CHA-CBD | 4.42  | 143.69      | 132.36   |
| 30  | h     | 602 | CHL  | OBD-CAD-CBD | 4.42  | 132.31      | 125.82   |
| 30  | d     | 601 | CHL  | OBD-CAD-C3D | -4.42 | 121.00      | 127.89   |
| 30  | a     | 608 | CHL  | C1A-CHA-CBD | 4.42  | 143.67      | 132.36   |
| 32  | A     | 846 | 8CT  | C04-C03-C02 | -4.42 | 116.60      | 122.64   |
| 32  | I     | 101 | 8CT  | C18-C19-C20 | -4.42 | 114.48      | 123.52   |
| 30  | 8     | 307 | CHL  | OBD-CAD-C3D | -4.42 | 121.00      | 127.89   |
| 33  | h     | 520 | 0UR  | C9-C8-C7    | -4.42 | 121.09      | 127.28   |
| 32  | K     | 107 | 8CT  | C04-C03-C02 | -4.42 | 116.60      | 122.64   |
| 33  | 4     | 501 | 0UR  | C43-C3-C2   | 4.41  | 126.83      | 116.56   |
| 33  | 2     | 501 | 0UR  | C19-C18-C17 | -4.41 | 117.71      | 124.58   |
| 30  | 1     | 302 | CHL  | C4D-ND-C1D  | 4.41  | 108.57      | 105.22   |
| 30  | g     | 601 | CHL  | OBD-CAD-CBD | 4.41  | 132.30      | 125.82   |
| 30  | 1     | 313 | CHL  | OBD-CAD-C3D | -4.41 | 121.02      | 127.89   |
| 30  | b     | 609 | CHL  | C1B-CHB-C4A | 4.41  | 124.16      | 121.32   |
| 30  | a     | 605 | CHL  | OBD-CAD-CBD | 4.41  | 132.29      | 125.82   |
| 30  | 1     | 307 | CHL  | C1A-CHA-CBD | 4.41  | 143.65      | 132.36   |
| 32  | B     | 845 | 8CT  | C10-C11-C12 | -4.40 | 119.72      | 126.23   |
| 33  | b     | 520 | 0UR  | C19-C18-C17 | -4.40 | 117.73      | 124.58   |
| 30  | 8     | 308 | CHL  | OBD-CAD-CBD | 4.40  | 132.28      | 125.82   |
| 32  | 3     | 403 | 8CT  | C10-C11-C12 | -4.40 | 119.73      | 126.23   |
| 30  | d     | 608 | CHL  | C1A-CHA-CBD | 4.40  | 143.62      | 132.36   |
| 30  | i     | 607 | CHL  | C1A-CHA-CBD | 4.40  | 143.62      | 132.36   |
| 30  | b     | 601 | CHL  | C1A-CHA-CBD | 4.40  | 143.62      | 132.36   |
| 33  | h     | 520 | 0UR  | C14-C15-C16 | -4.39 | 121.12      | 127.28   |
| 32  | J     | 101 | 8CT  | C01-C02-C03 | -4.39 | 119.70      | 124.48   |
| 30  | 3     | 302 | CHL  | OBD-CAD-C3D | -4.39 | 121.05      | 127.89   |
| 30  | h     | 608 | CHL  | C1A-CHA-CBD | 4.38  | 143.59      | 132.36   |
| 30  | 6     | 306 | CHL  | OBD-CAD-CBD | 4.38  | 132.26      | 125.82   |
| 30  | 8     | 302 | CHL  | C4D-ND-C1D  | 4.38  | 108.55      | 105.22   |
| 33  | 3     | 501 | 0UR  | C43-C3-C2   | 4.38  | 126.75      | 116.56   |
| 30  | 5     | 305 | CHL  | OBD-CAD-CBD | 4.38  | 132.25      | 125.82   |
| 30  | 6     | 308 | CHL  | OBD-CAD-CBD | 4.38  | 132.25      | 125.82   |
| 32  | I     | 101 | 8CT  | C24-C25-C26 | -4.38 | 121.14      | 127.28   |
| 30  | 2     | 305 | CHL  | OBD-CAD-C3D | -4.38 | 121.07      | 127.89   |
| 30  | 6     | 315 | CHL  | OBD-CAD-C3D | -4.38 | 121.07      | 127.89   |
| 30  | a     | 601 | CHL  | OBD-CAD-C3D | -4.37 | 121.07      | 127.89   |
| 30  | h     | 605 | CHL  | OBD-CAD-CBD | 4.37  | 132.24      | 125.82   |
| 34  | A     | 855 | LHG  | O7-C7-C8    | 4.37  | 120.93      | 111.48   |
| 32  | B     | 845 | 8CT  | C01-C02-C03 | -4.37 | 119.72      | 124.48   |
| 30  | b     | 608 | CHL  | OBD-CAD-C3D | -4.37 | 121.08      | 127.89   |
| 30  | c     | 609 | CHL  | OBD-CAD-CBD | 4.36  | 132.23      | 125.82   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | B     | 844 | 8CT  | C01-C02-C03 | -4.36 | 119.72      | 124.48   |
| 30  | 7     | 313 | CHL  | OBD-CAD-CBD | 4.36  | 132.22      | 125.82   |
| 30  | 9     | 313 | CHL  | OBD-CAD-C3D | -4.36 | 121.09      | 127.89   |
| 33  | 2     | 501 | 0UR  | C43-C3-C2   | 4.36  | 126.70      | 116.56   |
| 30  | b     | 614 | CHL  | C1A-CHA-CBD | 4.36  | 143.52      | 132.36   |
| 34  | G     | 105 | LHG  | O7-C7-C8    | 4.36  | 120.91      | 111.48   |
| 32  | J     | 104 | 8CT  | C29-C28-C26 | -4.35 | 116.96      | 126.32   |
| 32  | M     | 102 | 8CT  | C07-C02-C03 | -4.35 | 116.82      | 122.70   |
| 33  | 9     | 501 | 0UR  | C19-C18-C17 | -4.35 | 117.81      | 124.58   |
| 30  | h     | 609 | CHL  | OBD-CAD-C3D | -4.35 | 121.11      | 127.89   |
| 30  | i     | 605 | CHL  | C1B-CHB-C4A | -4.35 | 118.53      | 121.32   |
| 30  | f     | 605 | CHL  | OBD-CAD-CBD | 4.35  | 132.21      | 125.82   |
| 33  | 4     | 502 | 0UR  | C10-C11-C12 | -4.35 | 121.18      | 127.28   |
| 30  | 7     | 307 | CHL  | C1A-CHA-CBD | 4.35  | 143.49      | 132.36   |
| 32  | A     | 847 | 8CT  | C07-C02-C03 | -4.34 | 116.84      | 122.70   |
| 32  | B     | 851 | 8CT  | C01-C02-C03 | -4.34 | 119.75      | 124.48   |
| 30  | i     | 605 | CHL  | OBD-CAD-CBD | 4.34  | 132.19      | 125.82   |
| 30  | c     | 606 | CHL  | OBD-CAD-C3D | -4.33 | 121.13      | 127.89   |
| 33  | 1     | 502 | 0UR  | C14-C15-C16 | -4.33 | 121.20      | 127.28   |
| 32  | 7     | 402 | 8CT  | C04-C03-C02 | -4.33 | 116.72      | 122.64   |
| 30  | 8     | 302 | CHL  | OBD-CAD-C3D | -4.33 | 121.14      | 127.89   |
| 32  | L     | 205 | 8CT  | C07-C02-C03 | -4.33 | 116.86      | 122.70   |
| 33  | a     | 520 | 0UR  | C10-C11-C12 | -4.32 | 121.21      | 127.28   |
| 37  | e     | 522 | 0IE  | C10-C9-C8   | 4.32  | 132.36      | 123.52   |
| 30  | d     | 614 | CHL  | C1B-CHB-C4A | -4.32 | 118.54      | 121.32   |
| 32  | G     | 104 | 8CT  | C01-C02-C03 | -4.32 | 119.77      | 124.48   |
| 30  | g     | 605 | CHL  | C1B-CHB-C4A | -4.32 | 118.54      | 121.32   |
| 37  | f     | 522 | 0IE  | C10-C9-C8   | 4.32  | 132.36      | 123.52   |
| 30  | i     | 601 | CHL  | OBD-CAD-C3D | -4.32 | 121.15      | 127.89   |
| 30  | h     | 601 | CHL  | C1A-CHA-CBD | 4.32  | 143.41      | 132.36   |
| 30  | 2     | 306 | CHL  | OBD-CAD-C3D | -4.32 | 121.16      | 127.89   |
| 30  | i     | 608 | CHL  | OBD-CAD-C3D | -4.31 | 121.16      | 127.89   |
| 33  | 6     | 502 | 0UR  | C9-C8-C7    | -4.31 | 121.23      | 127.28   |
| 30  | c     | 605 | CHL  | C1B-CHB-C4A | -4.31 | 118.55      | 121.32   |
| 30  | 8     | 315 | CHL  | OBD-CAD-C3D | -4.31 | 121.17      | 127.89   |
| 30  | 8     | 301 | CHL  | C1A-CHA-CBD | 4.31  | 143.40      | 132.36   |
| 32  | L     | 205 | 8CT  | C01-C02-C03 | -4.31 | 119.78      | 124.48   |
| 32  | 2     | 402 | 8CT  | C24-C25-C26 | -4.31 | 121.24      | 127.28   |
| 30  | 2     | 313 | CHL  | C1A-CHA-CBD | 4.31  | 143.39      | 132.36   |
| 30  | 4     | 305 | CHL  | OBD-CAD-C3D | -4.30 | 121.18      | 127.89   |
| 30  | 0     | 301 | CHL  | OBD-CAD-C3D | -4.30 | 121.18      | 127.89   |
| 30  | i     | 608 | CHL  | C1A-CHA-CBD | 4.30  | 143.37      | 132.36   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | c     | 606 | CHL  | C1A-CHA-CBD | 4.30  | 143.36      | 132.36   |
| 32  | B     | 845 | 8CT  | C07-C02-C03 | -4.29 | 116.90      | 122.70   |
| 30  | a     | 602 | CHL  | OBD-CAD-CBD | 4.29  | 132.12      | 125.82   |
| 32  | 7     | 402 | 8CT  | C07-C02-C03 | -4.29 | 116.91      | 122.70   |
| 32  | J     | 101 | 8CT  | C18-C19-C20 | -4.29 | 114.75      | 123.52   |
| 32  | 2     | 402 | 8CT  | C35-C30-C29 | -4.29 | 107.90      | 112.83   |
| 33  | 7     | 501 | 0UR  | C43-C3-C2   | 4.29  | 126.53      | 116.56   |
| 30  | e     | 608 | CHL  | C1A-CHA-CBD | 4.28  | 143.33      | 132.36   |
| 30  | c     | 602 | CHL  | OBD-CAD-CBD | 4.28  | 132.11      | 125.82   |
| 30  | a     | 609 | CHL  | C1A-CHA-CBD | 4.28  | 143.33      | 132.36   |
| 30  | 3     | 305 | CHL  | OBD-CAD-C3D | -4.28 | 121.22      | 127.89   |
| 30  | d     | 607 | CHL  | C1A-CHA-CBD | 4.28  | 143.32      | 132.36   |
| 32  | A     | 849 | 8CT  | C24-C25-C26 | -4.28 | 121.28      | 127.28   |
| 30  | 6     | 302 | CHL  | C1-C2-C3    | -4.28 | 119.19      | 126.20   |
| 30  | 4     | 306 | CHL  | OBD-CAD-C3D | -4.28 | 121.22      | 127.89   |
| 30  | f     | 609 | CHL  | OBD-CAD-CBD | 4.27  | 132.10      | 125.82   |
| 32  | J     | 101 | 8CT  | C04-C03-C02 | -4.27 | 116.80      | 122.64   |
| 37  | i     | 522 | 0IE  | C10-C9-C8   | 4.27  | 132.26      | 123.52   |
| 33  | i     | 520 | 0UR  | C10-C11-C12 | -4.27 | 121.29      | 127.28   |
| 32  | 3     | 402 | 8CT  | C24-C25-C26 | -4.27 | 121.29      | 127.28   |
| 37  | h     | 521 | 0IE  | C10-C9-C8   | 4.27  | 132.26      | 123.52   |
| 32  | B     | 845 | 8CT  | C35-C30-C29 | -4.26 | 107.92      | 112.83   |
| 33  | g     | 520 | 0UR  | C9-C8-C7    | -4.26 | 121.30      | 127.28   |
| 30  | h     | 607 | CHL  | OBD-CAD-C3D | -4.26 | 121.25      | 127.89   |
| 37  | h     | 522 | 0IE  | C10-C9-C8   | 4.26  | 132.23      | 123.52   |
| 30  | 3     | 302 | CHL  | C4D-ND-C1D  | 4.26  | 108.45      | 105.22   |
| 30  | a     | 614 | CHL  | OBD-CAD-C3D | -4.25 | 121.25      | 127.89   |
| 30  | d     | 606 | CHL  | OBD-CAD-C3D | -4.25 | 121.26      | 127.89   |
| 30  | h     | 602 | CHL  | OBD-CAD-C3D | -4.25 | 121.26      | 127.89   |
| 33  | 1     | 501 | 0UR  | C10-C11-C12 | -4.25 | 121.32      | 127.28   |
| 33  | 2     | 502 | 0UR  | C9-C8-C7    | -4.25 | 121.32      | 127.28   |
| 30  | a     | 606 | CHL  | OBD-CAD-C3D | -4.25 | 121.27      | 127.89   |
| 32  | F     | 302 | 8CT  | C29-C28-C26 | -4.25 | 117.19      | 126.32   |
| 30  | c     | 605 | CHL  | OBD-CAD-CBD | 4.24  | 132.05      | 125.82   |
| 34  | f     | 630 | LHG  | O7-C7-C8    | 4.24  | 120.66      | 111.48   |
| 30  | d     | 609 | CHL  | OBD-CAD-C3D | -4.24 | 121.27      | 127.89   |
| 30  | e     | 605 | CHL  | OBD-CAD-C3D | -4.24 | 121.27      | 127.89   |
| 30  | g     | 602 | CHL  | OBD-CAD-CBD | 4.24  | 132.05      | 125.82   |
| 30  | 8     | 308 | CHL  | OBD-CAD-C3D | -4.24 | 121.28      | 127.89   |
| 32  | 8     | 402 | 8CT  | C14-C13-C12 | -4.24 | 121.33      | 127.28   |
| 30  | 1     | 302 | CHL  | OBD-CAD-C3D | -4.23 | 121.29      | 127.89   |
| 30  | d     | 607 | CHL  | OBD-CAD-C3D | -4.23 | 121.30      | 127.89   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | 7     | 405 | 8CT  | C30-C29-C28 | -4.23 | 118.00      | 124.58   |
| 32  | B     | 804 | 8CT  | C35-C30-C29 | -4.23 | 107.97      | 112.83   |
| 30  | d     | 614 | CHL  | OBD-CAD-C3D | -4.23 | 121.30      | 127.89   |
| 33  | 5     | 501 | 0UR  | C9-C8-C7    | -4.22 | 121.35      | 127.28   |
| 32  | 3     | 403 | 8CT  | C18-C17-C16 | -4.22 | 121.36      | 127.28   |
| 32  | B     | 847 | 8CT  | C10-C11-C12 | -4.22 | 119.99      | 126.23   |
| 30  | g     | 614 | CHL  | OBD-CAD-C3D | -4.22 | 121.31      | 127.89   |
| 30  | f     | 602 | CHL  | OBD-CAD-CBD | 4.22  | 132.02      | 125.82   |
| 32  | A     | 849 | 8CT  | C19-C20-C21 | -4.22 | 121.36      | 127.28   |
| 32  | M     | 102 | 8CT  | C01-C02-C03 | -4.22 | 119.88      | 124.48   |
| 30  | h     | 606 | CHL  | OBD-CAD-C3D | -4.22 | 121.31      | 127.89   |
| 30  | 7     | 313 | CHL  | C1A-CHA-CBD | 4.22  | 143.16      | 132.36   |
| 30  | d     | 601 | CHL  | C1A-CHA-CBD | 4.22  | 143.16      | 132.36   |
| 30  | 0     | 306 | CHL  | OBD-CAD-C3D | -4.22 | 121.32      | 127.89   |
| 33  | d     | 520 | 0UR  | C10-C11-C12 | -4.21 | 121.38      | 127.28   |
| 30  | e     | 602 | CHL  | OBD-CAD-C3D | -4.20 | 121.34      | 127.89   |
| 37  | a     | 522 | 0IE  | C10-C9-C8   | 4.20  | 132.11      | 123.52   |
| 32  | F     | 302 | 8CT  | C10-C11-C12 | -4.20 | 120.02      | 126.23   |
| 32  | B     | 844 | 8CT  | C19-C20-C21 | -4.20 | 121.39      | 127.28   |
| 30  | c     | 608 | CHL  | C1A-CHA-CBD | 4.20  | 143.11      | 132.36   |
| 30  | g     | 614 | CHL  | C1B-CHB-C4A | -4.20 | 118.62      | 121.32   |
| 30  | 4     | 308 | CHL  | OBD-CAD-CBD | 4.19  | 131.98      | 125.82   |
| 32  | 8     | 406 | 8CT  | C18-C17-C16 | -4.19 | 121.40      | 127.28   |
| 32  | B     | 843 | 8CT  | C07-C02-C03 | -4.19 | 117.04      | 122.70   |
| 32  | I     | 101 | 8CT  | C01-C02-C03 | -4.19 | 119.91      | 124.48   |
| 30  | 6     | 307 | CHL  | C1A-CHA-CBD | 4.19  | 143.09      | 132.36   |
| 32  | A     | 849 | 8CT  | C01-C02-C03 | -4.19 | 119.91      | 124.48   |
| 30  | a     | 607 | CHL  | C1A-CHA-CBD | 4.19  | 143.09      | 132.36   |
| 30  | b     | 608 | CHL  | C1A-CHA-CBD | 4.19  | 143.09      | 132.36   |
| 30  | 0     | 302 | CHL  | OBD-CAD-C3D | -4.19 | 121.36      | 127.89   |
| 32  | M     | 102 | 8CT  | C18-C17-C16 | -4.18 | 121.41      | 127.28   |
| 30  | a     | 609 | CHL  | OBD-CAD-CBD | 4.18  | 131.96      | 125.82   |
| 32  | 6     | 402 | 8CT  | C30-C29-C28 | -4.18 | 118.07      | 124.58   |
| 30  | i     | 609 | CHL  | C1A-CHA-CBD | 4.18  | 143.07      | 132.36   |
| 30  | c     | 614 | CHL  | C1A-CHA-CBD | 4.18  | 143.07      | 132.36   |
| 30  | 4     | 307 | CHL  | C1-C2-C3    | -4.18 | 120.00      | 126.76   |
| 30  | h     | 606 | CHL  | C1A-CHA-CBD | 4.18  | 143.06      | 132.36   |
| 32  | L     | 206 | 8CT  | C35-C30-C29 | -4.18 | 108.02      | 112.83   |
| 30  | 8     | 313 | CHL  | OBD-CAD-CBD | 4.18  | 131.95      | 125.82   |
| 30  | 2     | 302 | CHL  | OBD-CAD-CBD | 4.17  | 131.94      | 125.82   |
| 30  | 8     | 315 | CHL  | C1A-CHA-CBD | 4.17  | 143.04      | 132.36   |
| 30  | b     | 602 | CHL  | OBD-CAD-CBD | 4.17  | 131.94      | 125.82   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | i     | 614 | CHL  | OBD-CAD-CBD | 4.16  | 131.94      | 125.82   |
| 30  | f     | 606 | CHL  | OBD-CAD-C3D | -4.16 | 121.40      | 127.89   |
| 32  | K     | 107 | 8CT  | C24-C25-C26 | -4.16 | 121.44      | 127.28   |
| 33  | 2     | 502 | 0UR  | C10-C11-C12 | -4.16 | 121.44      | 127.28   |
| 32  | 9     | 401 | 8CT  | C07-C02-C03 | -4.16 | 117.08      | 122.70   |
| 33  | O     | 204 | 0UR  | C43-C3-C4   | -4.16 | 120.12      | 125.03   |
| 34  | 5     | 601 | LHG  | O7-C7-C8    | 4.16  | 120.47      | 111.48   |
| 30  | 6     | 313 | CHL  | C1A-CHA-CBD | 4.15  | 143.00      | 132.36   |
| 30  | c     | 609 | CHL  | OBD-CAD-C3D | -4.15 | 121.42      | 127.89   |
| 30  | i     | 601 | CHL  | C1A-CHA-CBD | 4.15  | 142.99      | 132.36   |
| 32  | B     | 851 | 8CT  | C07-C02-C03 | -4.15 | 117.10      | 122.70   |
| 30  | h     | 605 | CHL  | C1A-CHA-CBD | 4.14  | 142.97      | 132.36   |
| 30  | g     | 606 | CHL  | OBD-CAD-C3D | -4.14 | 121.43      | 127.89   |
| 30  | 0     | 305 | CHL  | OBD-CAD-C3D | -4.14 | 121.43      | 127.89   |
| 30  | 1     | 306 | CHL  | OBD-CAD-CBD | 4.14  | 131.90      | 125.82   |
| 34  | 1     | 601 | LHG  | O7-C7-C8    | 4.14  | 120.44      | 111.48   |
| 32  | I     | 101 | 8CT  | C30-C31-C32 | -4.14 | 116.37      | 121.47   |
| 30  | 5     | 302 | CHL  | OBD-CAD-C3D | -4.14 | 121.44      | 127.89   |
| 30  | 3     | 305 | CHL  | C1A-CHA-CBD | 4.14  | 142.95      | 132.36   |
| 30  | e     | 608 | CHL  | C1B-CHB-C4A | 4.14  | 123.98      | 121.32   |
| 32  | I     | 101 | 8CT  | C04-C03-C02 | -4.13 | 116.99      | 122.64   |
| 34  | K     | 106 | LHG  | O7-C7-C8    | 4.13  | 120.42      | 111.48   |
| 33  | 8     | 501 | 0UR  | C4-C3-C2    | -4.13 | 116.56      | 120.16   |
| 32  | A     | 847 | 8CT  | C01-C02-C03 | -4.13 | 119.98      | 124.48   |
| 30  | 6     | 305 | CHL  | OBD-CAD-C3D | -4.13 | 121.45      | 127.89   |
| 30  | h     | 614 | CHL  | OBD-CAD-C3D | -4.13 | 121.45      | 127.89   |
| 33  | 8     | 501 | 0UR  | C10-C11-C12 | -4.13 | 121.49      | 127.28   |
| 30  | h     | 607 | CHL  | C1A-CHA-CBD | 4.13  | 142.93      | 132.36   |
| 32  | 3     | 402 | 8CT  | C39-C16-C15 | 4.12  | 124.39      | 118.09   |
| 30  | g     | 609 | CHL  | OBD-CAD-CBD | 4.12  | 131.88      | 125.82   |
| 30  | 6     | 315 | CHL  | C1B-CHB-C4A | 4.12  | 123.97      | 121.32   |
| 30  | e     | 607 | CHL  | OBD-CAD-C3D | -4.12 | 121.46      | 127.89   |
| 30  | f     | 608 | CHL  | C1A-CHA-CBD | 4.12  | 142.91      | 132.36   |
| 32  | B     | 851 | 8CT  | C18-C17-C16 | -4.12 | 121.50      | 127.28   |
| 32  | L     | 209 | 8CT  | C18-C17-C16 | -4.12 | 121.50      | 127.28   |
| 32  | O     | 205 | 8CT  | C18-C17-C16 | -4.12 | 121.50      | 127.28   |
| 37  | e     | 522 | 0IE  | C20-C3-C4   | -4.12 | 119.03      | 124.72   |
| 30  | h     | 605 | CHL  | OBD-CAD-C3D | -4.12 | 121.47      | 127.89   |
| 30  | g     | 605 | CHL  | OBD-CAD-C3D | -4.11 | 121.48      | 127.89   |
| 30  | f     | 614 | CHL  | OBD-CAD-C3D | -4.11 | 121.48      | 127.89   |
| 33  | d     | 520 | 0UR  | C9-C8-C7    | -4.11 | 121.51      | 127.28   |
| 30  | a     | 607 | CHL  | OBD-CAD-C3D | -4.11 | 121.48      | 127.89   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | b     | 607 | CHL  | OBD-CAD-C3D | -4.11 | 121.48      | 127.89   |
| 32  | 7     | 404 | 8CT  | C04-C03-C02 | -4.11 | 117.02      | 122.64   |
| 34  | A     | 844 | LHG  | O7-C7-C8    | 4.11  | 120.37      | 111.48   |
| 34  | 9     | 601 | LHG  | O7-C7-C8    | 4.11  | 120.37      | 111.48   |
| 33  | 7     | 501 | 0UR  | C19-C18-C17 | -4.11 | 118.19      | 124.58   |
| 34  | 7     | 602 | LHG  | O7-C7-C8    | 4.11  | 120.36      | 111.48   |
| 30  | e     | 609 | CHL  | C1B-CHB-C4A | 4.10  | 123.96      | 121.32   |
| 32  | A     | 848 | 8CT  | C01-C02-C03 | -4.10 | 120.01      | 124.48   |
| 30  | i     | 606 | CHL  | C1A-CHA-CBD | 4.10  | 142.86      | 132.36   |
| 34  | 3     | 603 | LHG  | O7-C7-C8    | 4.10  | 120.35      | 111.48   |
| 34  | A     | 845 | LHG  | O7-C7-C8    | 4.10  | 120.35      | 111.48   |
| 33  | c     | 520 | 0UR  | C34-C27-C1  | -4.10 | 119.34      | 124.45   |
| 30  | 6     | 308 | CHL  | C1A-CHA-CBD | 4.09  | 142.85      | 132.36   |
| 30  | b     | 607 | CHL  | C1A-CHA-CBD | 4.09  | 142.85      | 132.36   |
| 32  | A     | 846 | 8CT  | C07-C02-C03 | -4.09 | 117.17      | 122.70   |
| 30  | 8     | 313 | CHL  | C1A-CHA-CBD | 4.09  | 142.83      | 132.36   |
| 30  | d     | 605 | CHL  | OBD-CAD-C3D | -4.09 | 121.52      | 127.89   |
| 30  | 1     | 305 | CHL  | OBD-CAD-C3D | -4.08 | 121.52      | 127.89   |
| 34  | H     | 203 | LHG  | O7-C7-C8    | 4.08  | 120.31      | 111.48   |
| 32  | J     | 101 | 8CT  | C24-C25-C26 | -4.08 | 121.56      | 127.28   |
| 30  | c     | 607 | CHL  | OBD-CAD-C3D | -4.08 | 121.53      | 127.89   |
| 30  | f     | 609 | CHL  | C1A-CHA-CBD | 4.08  | 142.80      | 132.36   |
| 30  | b     | 606 | CHL  | OBD-CAD-CBD | 4.07  | 131.80      | 125.82   |
| 30  | 2     | 307 | CHL  | C1A-CHA-CBD | 4.06  | 142.77      | 132.36   |
| 30  | e     | 601 | CHL  | C1A-CHA-CBD | 4.06  | 142.77      | 132.36   |
| 33  | 6     | 501 | 0UR  | C34-C27-C1  | -4.06 | 119.39      | 124.45   |
| 30  | f     | 607 | CHL  | C1A-CHA-CBD | 4.06  | 142.76      | 132.36   |
| 33  | 9     | 501 | 0UR  | C10-C11-C12 | -4.06 | 121.58      | 127.28   |
| 30  | h     | 609 | CHL  | C1A-CHA-CBD | 4.06  | 142.75      | 132.36   |
| 32  | 3     | 403 | 8CT  | C29-C28-C26 | -4.06 | 117.60      | 126.32   |
| 32  | O     | 205 | 8CT  | C07-C02-C03 | -4.06 | 117.22      | 122.70   |
| 30  | a     | 606 | CHL  | C1A-CHA-CBD | 4.05  | 142.74      | 132.36   |
| 34  | 3     | 601 | LHG  | O7-C7-C8    | 4.05  | 120.25      | 111.48   |
| 30  | i     | 602 | CHL  | C1A-CHA-CBD | 4.05  | 142.74      | 132.36   |
| 34  | 6     | 601 | LHG  | O7-C7-C8    | 4.05  | 120.25      | 111.48   |
| 32  | O     | 205 | 8CT  | C19-C20-C21 | -4.05 | 121.59      | 127.28   |
| 30  | 7     | 301 | CHL  | C1B-CHB-C4A | 4.05  | 123.93      | 121.32   |
| 32  | A     | 850 | 8CT  | C18-C19-C20 | 4.05  | 131.81      | 123.52   |
| 30  | h     | 608 | CHL  | OBD-CAD-C3D | -4.05 | 121.57      | 127.89   |
| 30  | f     | 609 | CHL  | OBD-CAD-C3D | -4.05 | 121.58      | 127.89   |
| 30  | 6     | 313 | CHL  | OBD-CAD-C3D | -4.05 | 121.58      | 127.89   |
| 30  | a     | 602 | CHL  | OBD-CAD-C3D | -4.05 | 121.58      | 127.89   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | i     | 607 | CHL  | OBD-CAD-C3D | -4.04 | 121.58      | 127.89   |
| 33  | 1     | 501 | 0UR  | C19-C18-C17 | -4.04 | 118.28      | 124.58   |
| 30  | b     | 609 | CHL  | C1A-CHA-CBD | 4.04  | 142.72      | 132.36   |
| 30  | a     | 605 | CHL  | C1B-CHB-C4A | -4.04 | 118.72      | 121.32   |
| 30  | 8     | 307 | CHL  | C1A-CHA-CBD | 4.04  | 142.71      | 132.36   |
| 30  | g     | 602 | CHL  | C1A-CHA-CBD | 4.04  | 142.71      | 132.36   |
| 30  | i     | 606 | CHL  | OBD-CAD-C3D | -4.04 | 121.59      | 127.89   |
| 32  | L     | 209 | 8CT  | C07-C02-C03 | -4.04 | 117.25      | 122.70   |
| 30  | 0     | 305 | CHL  | C1A-CHA-CBD | 4.03  | 142.69      | 132.36   |
| 30  | 1     | 306 | CHL  | C1A-CHA-CBD | 4.03  | 142.69      | 132.36   |
| 30  | 4     | 308 | CHL  | OBD-CAD-C3D | -4.03 | 121.61      | 127.89   |
| 30  | 2     | 305 | CHL  | C1A-CHA-CBD | 4.03  | 142.68      | 132.36   |
| 30  | c     | 607 | CHL  | C1A-CHA-CBD | 4.03  | 142.68      | 132.36   |
| 42  | g     | 523 | NEX  | C11-C10-C9  | -4.03 | 121.63      | 127.28   |
| 30  | 0     | 301 | CHL  | C1A-CHA-CBD | 4.03  | 142.67      | 132.36   |
| 32  | 3     | 402 | 8CT  | C10-C11-C12 | -4.03 | 120.28      | 126.23   |
| 30  | e     | 606 | CHL  | C1A-CHA-CBD | 4.02  | 142.66      | 132.36   |
| 30  | 6     | 308 | CHL  | OBD-CAD-C3D | -4.02 | 121.62      | 127.89   |
| 30  | f     | 605 | CHL  | C1B-CHB-C4A | -4.02 | 118.74      | 121.32   |
| 30  | b     | 606 | CHL  | C1A-CHA-CBD | 4.02  | 142.66      | 132.36   |
| 33  | i     | 520 | 0UR  | C9-C8-C7    | -4.02 | 121.64      | 127.28   |
| 32  | 7     | 404 | 8CT  | C11-C12-C13 | 4.02  | 125.33      | 119.01   |
| 30  | 7     | 305 | CHL  | OBD-CAD-C3D | -4.02 | 121.62      | 127.89   |
| 32  | 0     | 401 | 8CT  | C18-C17-C16 | -4.02 | 121.64      | 127.28   |
| 32  | 4     | 402 | 8CT  | C10-C11-C12 | -4.02 | 120.29      | 126.23   |
| 30  | e     | 606 | CHL  | OBD-CAD-C3D | -4.01 | 121.63      | 127.89   |
| 30  | 1     | 313 | CHL  | C1A-CHA-CBD | 4.01  | 142.64      | 132.36   |
| 42  | f     | 523 | NEX  | C11-C10-C9  | -4.01 | 121.65      | 127.28   |
| 30  | 2     | 307 | CHL  | C1-C2-C3    | -4.01 | 120.27      | 126.76   |
| 34  | g     | 630 | LHG  | O7-C7-C8    | 4.01  | 120.16      | 111.48   |
| 30  | g     | 601 | CHL  | OBD-CAD-C3D | -4.01 | 121.64      | 127.89   |
| 30  | 1     | 302 | CHL  | C1-C2-C3    | -4.01 | 119.63      | 126.20   |
| 42  | a     | 523 | NEX  | C11-C10-C9  | -4.01 | 121.66      | 127.28   |
| 32  | B     | 844 | 8CT  | C39-C16-C17 | -4.01 | 116.32      | 122.82   |
| 32  | 8     | 406 | 8CT  | C19-C20-C21 | -4.00 | 121.66      | 127.28   |
| 30  | 5     | 306 | CHL  | C1A-CHA-CBD | 4.00  | 142.61      | 132.36   |
| 30  | 6     | 301 | CHL  | OBD-CAD-C3D | -4.00 | 121.65      | 127.89   |
| 30  | 4     | 307 | CHL  | C1A-CHA-CBD | 4.00  | 142.61      | 132.36   |
| 34  | 2     | 601 | LHG  | O7-C7-C8    | 4.00  | 120.14      | 111.48   |
| 30  | 5     | 301 | CHL  | C1A-CHA-CBD | 4.00  | 142.61      | 132.36   |
| 30  | i     | 609 | CHL  | OBD-CAD-CBD | 4.00  | 131.69      | 125.82   |
| 42  | b     | 523 | NEX  | C11-C10-C9  | -4.00 | 121.67      | 127.28   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 34  | i     | 630 | LHG  | O7-C7-C8    | 4.00  | 120.12      | 111.48   |
| 30  | 8     | 302 | CHL  | C1-C2-C3    | -3.99 | 119.65      | 126.20   |
| 42  | d     | 523 | NEX  | C11-C10-C9  | -3.99 | 121.68      | 127.28   |
| 30  | 4     | 305 | CHL  | C1A-CHA-CBD | 3.99  | 142.58      | 132.36   |
| 30  | g     | 602 | CHL  | OBD-CAD-C3D | -3.99 | 121.67      | 127.89   |
| 30  | 8     | 305 | CHL  | OBD-CAD-C3D | -3.99 | 121.67      | 127.89   |
| 32  | B     | 843 | 8CT  | C01-C02-C03 | -3.99 | 120.14      | 124.48   |
| 30  | 2     | 307 | CHL  | C4D-ND-C1D  | 3.98  | 108.24      | 105.22   |
| 30  | 5     | 307 | CHL  | C1A-CHA-CBD | 3.98  | 142.56      | 132.36   |
| 42  | e     | 523 | NEX  | C11-C10-C9  | -3.98 | 121.69      | 127.28   |
| 33  | 8     | 501 | 0UR  | C34-C27-C1  | -3.98 | 119.48      | 124.45   |
| 33  | e     | 520 | 0UR  | C9-C8-C7    | -3.98 | 121.69      | 127.28   |
| 42  | i     | 523 | NEX  | C11-C10-C9  | -3.98 | 121.69      | 127.28   |
| 30  | 9     | 301 | CHL  | C1A-CHA-CBD | 3.98  | 142.55      | 132.36   |
| 42  | h     | 523 | NEX  | C11-C10-C9  | -3.98 | 121.70      | 127.28   |
| 30  | 5     | 305 | CHL  | C1A-CHA-CBD | 3.98  | 142.55      | 132.36   |
| 33  | g     | 520 | 0UR  | C43-C3-C4   | -3.98 | 120.34      | 125.03   |
| 30  | 9     | 305 | CHL  | C1A-CHA-CBD | 3.97  | 142.54      | 132.36   |
| 37  | d     | 522 | 0IE  | C10-C9-C8   | 3.97  | 131.65      | 123.52   |
| 30  | e     | 607 | CHL  | C1A-CHA-CBD | 3.97  | 142.53      | 132.36   |
| 32  | 9     | 401 | 8CT  | C14-C13-C12 | -3.97 | 121.71      | 127.28   |
| 30  | 2     | 319 | CHL  | C1A-CHA-CBD | 3.97  | 142.52      | 132.36   |
| 30  | g     | 606 | CHL  | C1A-CHA-CBD | 3.97  | 142.52      | 132.36   |
| 37  | d     | 522 | 0IE  | C9-C10-C11  | 3.97  | 131.63      | 123.52   |
| 30  | 1     | 305 | CHL  | C1A-CHA-CBD | 3.97  | 142.52      | 132.36   |
| 30  | c     | 614 | CHL  | OBD-CAD-C3D | -3.97 | 121.71      | 127.89   |
| 30  | d     | 606 | CHL  | C1A-CHA-CBD | 3.97  | 142.51      | 132.36   |
| 33  | 2     | 501 | 0UR  | C10-C11-C12 | -3.96 | 121.72      | 127.28   |
| 33  | 7     | 501 | 0UR  | C10-C11-C12 | -3.96 | 121.72      | 127.28   |
| 30  | e     | 609 | CHL  | C1A-CHA-CBD | 3.96  | 142.51      | 132.36   |
| 42  | c     | 523 | NEX  | C11-C10-C9  | -3.96 | 121.72      | 127.28   |
| 32  | A     | 848 | 8CT  | C14-C13-C12 | -3.96 | 121.73      | 127.28   |
| 32  | B     | 848 | 8CT  | C14-C13-C12 | -3.96 | 121.73      | 127.28   |
| 30  | f     | 601 | CHL  | C1A-CHA-CBD | 3.96  | 142.50      | 132.36   |
| 30  | 5     | 313 | CHL  | OBD-CAD-CBD | 3.96  | 131.63      | 125.82   |
| 33  | 8     | 502 | 0UR  | O44-C45-C46 | 3.96  | 121.31      | 111.55   |
| 30  | 8     | 305 | CHL  | C1A-CHA-CBD | 3.96  | 142.49      | 132.36   |
| 34  | B     | 854 | LHG  | O7-C7-C8    | 3.96  | 120.04      | 111.48   |
| 30  | 6     | 315 | CHL  | C1A-CHA-CBD | 3.95  | 142.49      | 132.36   |
| 30  | f     | 606 | CHL  | C1A-CHA-CBD | 3.95  | 142.48      | 132.36   |
| 34  | a     | 630 | LHG  | O7-C7-C8    | 3.95  | 120.03      | 111.48   |
| 30  | h     | 602 | CHL  | C1A-CHA-CBD | 3.95  | 142.48      | 132.36   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | 9     | 313 | CHL  | C1A-CHA-CBD | 3.95  | 142.47      | 132.36   |
| 32  | B     | 846 | 8CT  | C30-C31-C32 | -3.95 | 116.61      | 121.47   |
| 32  | I     | 101 | 8CT  | C07-C02-C03 | -3.95 | 117.37      | 122.70   |
| 30  | g     | 609 | CHL  | C1A-CHA-CBD | 3.95  | 142.47      | 132.36   |
| 34  | e     | 630 | LHG  | O7-C7-C8    | 3.94  | 120.01      | 111.48   |
| 30  | a     | 609 | CHL  | OBD-CAD-C3D | -3.94 | 121.74      | 127.89   |
| 30  | f     | 606 | CHL  | CMD-C2D-C3D | -3.94 | 116.81      | 124.68   |
| 30  | g     | 609 | CHL  | OBD-CAD-C3D | -3.94 | 121.75      | 127.89   |
| 30  | 8     | 308 | CHL  | C1A-CHA-CBD | 3.94  | 142.45      | 132.36   |
| 34  | 0     | 601 | LHG  | O7-C7-C8    | 3.94  | 120.00      | 111.48   |
| 30  | 3     | 307 | CHL  | C1A-CHA-CBD | 3.94  | 142.45      | 132.36   |
| 33  | 5     | 502 | 0UR  | C5-C4-C3    | -3.94 | 122.21      | 126.92   |
| 32  | 0     | 401 | 8CT  | C10-C11-C12 | -3.94 | 120.41      | 126.23   |
| 30  | 5     | 305 | CHL  | OBD-CAD-C3D | -3.94 | 121.75      | 127.89   |
| 30  | 6     | 306 | CHL  | C1A-CHA-CBD | 3.94  | 142.44      | 132.36   |
| 30  | b     | 614 | CHL  | OBD-CAD-C3D | -3.93 | 121.76      | 127.89   |
| 30  | 1     | 307 | CHL  | C1B-CHB-C4A | 3.92  | 123.85      | 121.32   |
| 30  | 4     | 313 | CHL  | OBD-CAD-CBD | 3.92  | 131.58      | 125.82   |
| 30  | b     | 602 | CHL  | OBD-CAD-C3D | -3.92 | 121.77      | 127.89   |
| 30  | 7     | 305 | CHL  | C1A-CHA-CBD | 3.92  | 142.40      | 132.36   |
| 32  | 8     | 402 | 8CT  | C10-C11-C12 | -3.92 | 120.44      | 126.23   |
| 30  | 2     | 308 | CHL  | C1A-CHA-CBD | 3.92  | 142.40      | 132.36   |
| 34  | h     | 630 | LHG  | O7-C7-C8    | 3.92  | 119.95      | 111.48   |
| 30  | 6     | 305 | CHL  | C1A-CHA-CBD | 3.92  | 142.39      | 132.36   |
| 30  | 7     | 313 | CHL  | OBD-CAD-C3D | -3.91 | 121.79      | 127.89   |
| 37  | g     | 521 | 0IE  | C10-C9-C8   | 3.91  | 131.52      | 123.52   |
| 32  | L     | 209 | 8CT  | C14-C15-C16 | -3.91 | 115.65      | 126.36   |
| 30  | 9     | 301 | CHL  | OBD-CAD-C3D | -3.91 | 121.80      | 127.89   |
| 32  | J     | 101 | 8CT  | C13-C14-C15 | -3.90 | 111.89      | 123.20   |
| 33  | 5     | 502 | 0UR  | C34-C27-C1  | -3.90 | 119.58      | 124.45   |
| 34  | 7     | 601 | LHG  | O7-C7-C8    | 3.90  | 119.92      | 111.48   |
| 30  | 2     | 301 | CHL  | C1-C2-C3    | -3.89 | 119.82      | 126.20   |
| 34  | d     | 630 | LHG  | O7-C7-C8    | 3.89  | 119.90      | 111.48   |
| 30  | c     | 601 | CHL  | C1A-CHA-CBD | 3.89  | 142.32      | 132.36   |
| 30  | a     | 614 | CHL  | C1B-CHB-C4A | -3.89 | 118.82      | 121.32   |
| 30  | 8     | 306 | CHL  | C1A-CHA-CBD | 3.89  | 142.32      | 132.36   |
| 30  | d     | 602 | CHL  | OBD-CAD-CBD | 3.89  | 131.53      | 125.82   |
| 33  | a     | 520 | 0UR  | C19-C18-C17 | -3.88 | 118.54      | 124.58   |
| 32  | L     | 206 | 8CT  | C29-C28-C26 | -3.88 | 117.97      | 126.32   |
| 30  | 8     | 307 | CHL  | C1-C2-C3    | -3.88 | 120.48      | 126.76   |
| 39  | A     | 857 | CL0  | C1B-CHB-C4A | 3.88  | 123.82      | 121.32   |
| 37  | c     | 522 | 0IE  | C10-C9-C8   | 3.88  | 131.46      | 123.52   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | 7     | 402 | 8CT  | C24-C25-C26 | -3.88 | 121.84      | 127.28   |
| 30  | 4     | 319 | CHL  | C1A-CHA-CBD | 3.87  | 142.28      | 132.36   |
| 34  | B     | 852 | LHG  | O7-C7-C8    | 3.87  | 119.86      | 111.48   |
| 30  | c     | 602 | CHL  | C1A-CHA-CBD | 3.87  | 142.28      | 132.36   |
| 30  | d     | 609 | CHL  | C1A-CHA-CBD | 3.87  | 142.28      | 132.36   |
| 30  | 5     | 313 | CHL  | C1A-CHA-CBD | 3.87  | 142.28      | 132.36   |
| 30  | 8     | 306 | CHL  | OBD-CAD-C3D | -3.86 | 121.86      | 127.89   |
| 30  | b     | 609 | CHL  | OBD-CAD-CBD | 3.86  | 131.49      | 125.82   |
| 37  | b     | 522 | 0IE  | C10-C9-C8   | 3.86  | 131.42      | 123.52   |
| 30  | 4     | 308 | CHL  | C1A-CHA-CBD | 3.86  | 142.24      | 132.36   |
| 30  | a     | 605 | CHL  | OBD-CAD-C3D | -3.86 | 121.88      | 127.89   |
| 33  | 1     | 501 | 0UR  | C34-C27-C1  | -3.85 | 119.65      | 124.45   |
| 30  | 6     | 306 | CHL  | OBD-CAD-C3D | -3.85 | 121.88      | 127.89   |
| 33  | e     | 520 | 0UR  | C10-C11-C12 | -3.85 | 121.88      | 127.28   |
| 34  | b     | 630 | LHG  | O7-C7-C8    | 3.85  | 119.81      | 111.48   |
| 32  | 8     | 406 | 8CT  | C27-C26-C25 | -3.85 | 116.58      | 122.82   |
| 30  | f     | 605 | CHL  | OBD-CAD-C3D | -3.85 | 121.89      | 127.89   |
| 33  | 2     | 502 | 0UR  | C34-C27-C1  | -3.84 | 119.66      | 124.45   |
| 30  | 7     | 301 | CHL  | C1A-CHA-CBD | 3.84  | 142.20      | 132.36   |
| 30  | 1     | 306 | CHL  | OBD-CAD-C3D | -3.84 | 121.90      | 127.89   |
| 30  | i     | 605 | CHL  | OBD-CAD-C3D | -3.84 | 121.90      | 127.89   |
| 33  | 8     | 502 | 0UR  | C34-C27-C1  | -3.84 | 119.66      | 124.45   |
| 30  | d     | 602 | CHL  | C1-C2-C3    | -3.84 | 119.91      | 126.20   |
| 30  | g     | 607 | CHL  | OBD-CAD-C3D | -3.84 | 121.91      | 127.89   |
| 30  | 5     | 306 | CHL  | OBD-CAD-CBD | 3.84  | 131.46      | 125.82   |
| 32  | L     | 206 | 8CT  | C19-C20-C21 | -3.84 | 121.90      | 127.28   |
| 30  | e     | 614 | CHL  | OBD-CAD-C3D | -3.84 | 121.91      | 127.89   |
| 32  | 9     | 401 | 8CT  | C30-C31-C32 | -3.84 | 116.75      | 121.47   |
| 30  | 4     | 306 | CHL  | C1A-CHA-CBD | 3.84  | 142.18      | 132.36   |
| 30  | c     | 609 | CHL  | C1A-CHA-CBD | 3.83  | 142.17      | 132.36   |
| 30  | 8     | 301 | CHL  | C1-C2-C3    | -3.83 | 119.92      | 126.20   |
| 33  | 3     | 501 | 0UR  | O44-C45-C46 | 3.82  | 120.99      | 111.55   |
| 32  | I     | 101 | 8CT  | C29-C28-C26 | -3.82 | 118.10      | 126.32   |
| 34  | 8     | 601 | LHG  | O7-C7-C8    | 3.82  | 119.75      | 111.48   |
| 33  | e     | 520 | 0UR  | C43-C3-C2   | 3.82  | 125.44      | 116.56   |
| 30  | 0     | 302 | CHL  | C1A-CHA-CBD | 3.82  | 142.14      | 132.36   |
| 32  | A     | 847 | 8CT  | C19-C20-C21 | -3.81 | 121.93      | 127.28   |
| 30  | 2     | 306 | CHL  | C1A-CHA-CBD | 3.81  | 142.13      | 132.36   |
| 30  | b     | 602 | CHL  | C1A-CHA-CBD | 3.81  | 142.11      | 132.36   |
| 32  | 6     | 402 | 8CT  | C19-C20-C21 | -3.81 | 121.94      | 127.28   |
| 30  | f     | 602 | CHL  | OBD-CAD-C3D | -3.80 | 121.96      | 127.89   |
| 37  | e     | 521 | 0IE  | C10-C9-C8   | 3.80  | 131.30      | 123.52   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | 6     | 301 | CHL  | C1A-CHA-CBD | 3.80  | 142.10      | 132.36   |
| 30  | c     | 602 | CHL  | OBD-CAD-C3D | -3.80 | 121.96      | 127.89   |
| 32  | B     | 845 | 8CT  | C30-C29-C28 | -3.80 | 118.67      | 124.58   |
| 33  | 1     | 502 | 0UR  | C43-C3-C4   | -3.80 | 120.55      | 125.03   |
| 32  | B     | 845 | 8CT  | C25-C24-C23 | -3.80 | 112.19      | 123.20   |
| 30  | 2     | 302 | CHL  | OBD-CAD-C3D | -3.80 | 121.97      | 127.89   |
| 30  | 7     | 302 | CHL  | C1A-CHA-CBD | 3.79  | 142.07      | 132.36   |
| 32  | B     | 848 | 8CT  | C05-C04-C03 | 3.79  | 115.94      | 110.44   |
| 32  | A     | 850 | 8CT  | C39-C16-C15 | 3.79  | 123.88      | 118.09   |
| 30  | a     | 602 | CHL  | C1A-CHA-CBD | 3.79  | 142.06      | 132.36   |
| 30  | f     | 602 | CHL  | C1A-CHA-CBD | 3.79  | 142.06      | 132.36   |
| 33  | 1     | 502 | 0UR  | C34-C27-C1  | -3.79 | 119.73      | 124.45   |
| 30  | 2     | 301 | CHL  | C1A-CHA-CBD | 3.78  | 142.05      | 132.36   |
| 32  | O     | 205 | 8CT  | C30-C31-C32 | -3.78 | 116.81      | 121.47   |
| 30  | c     | 605 | CHL  | OBD-CAD-C3D | -3.78 | 122.00      | 127.89   |
| 34  | 6     | 603 | LHG  | O7-C7-C8    | 3.78  | 119.65      | 111.48   |
| 34  | 7     | 603 | LHG  | O7-C7-C8    | 3.78  | 119.65      | 111.48   |
| 32  | 1     | 402 | 8CT  | C29-C28-C26 | -3.77 | 118.21      | 126.32   |
| 32  | L     | 205 | 8CT  | C04-C03-C02 | -3.77 | 117.48      | 122.64   |
| 37  | c     | 522 | 0IE  | C9-C10-C11  | 3.77  | 131.23      | 123.52   |
| 33  | 8     | 502 | 0UR  | C5-C4-C3    | -3.77 | 122.41      | 126.92   |
| 30  | e     | 602 | CHL  | C1A-CHA-CBD | 3.77  | 142.00      | 132.36   |
| 37  | a     | 521 | 0IE  | C10-C9-C8   | 3.76  | 131.22      | 123.52   |
| 34  | 4     | 601 | LHG  | O7-C7-C8    | 3.76  | 119.62      | 111.48   |
| 32  | 6     | 402 | 8CT  | C11-C12-C13 | 3.76  | 124.92      | 119.01   |
| 32  | A     | 846 | 8CT  | C19-C20-C21 | -3.76 | 122.00      | 127.28   |
| 30  | 5     | 302 | CHL  | C1A-CHA-CBD | 3.76  | 141.98      | 132.36   |
| 32  | A     | 846 | 8CT  | C01-C02-C03 | -3.76 | 120.39      | 124.48   |
| 34  | c     | 630 | LHG  | O7-C7-C8    | 3.75  | 119.60      | 111.48   |
| 30  | 0     | 301 | CHL  | C1-C2-C3    | -3.75 | 120.05      | 126.20   |
| 32  | B     | 846 | 8CT  | C11-C12-C13 | 3.75  | 124.91      | 119.01   |
| 33  | 7     | 501 | 0UR  | C9-C8-C7    | -3.75 | 122.02      | 127.28   |
| 30  | b     | 606 | CHL  | OBD-CAD-C3D | -3.75 | 122.05      | 127.89   |
| 32  | B     | 847 | 8CT  | C18-C19-C20 | -3.75 | 115.85      | 123.52   |
| 33  | b     | 520 | 0UR  | C34-C27-C1  | -3.75 | 119.78      | 124.45   |
| 30  | i     | 609 | CHL  | OBD-CAD-C3D | -3.74 | 122.05      | 127.89   |
| 30  | 2     | 302 | CHL  | C1A-CHA-CBD | 3.74  | 141.94      | 132.36   |
| 32  | A     | 850 | 8CT  | C18-C17-C16 | 3.74  | 132.52      | 127.28   |
| 30  | 5     | 313 | CHL  | OBD-CAD-C3D | -3.74 | 122.06      | 127.89   |
| 30  | 6     | 302 | CHL  | C1A-CHA-CBD | 3.73  | 141.92      | 132.36   |
| 30  | 7     | 306 | CHL  | OBD-CAD-C3D | -3.73 | 122.07      | 127.89   |
| 34  | M     | 104 | LHG  | O7-C7-C8    | 3.73  | 119.55      | 111.48   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | B     | 844 | 8CT  | C07-C02-C03 | -3.73 | 117.67      | 122.70   |
| 33  | O     | 204 | 0UR  | C28-C19-C18 | -3.73 | 108.54      | 112.83   |
| 32  | B     | 844 | 8CT  | C14-C13-C12 | -3.72 | 122.07      | 127.28   |
| 37  | i     | 521 | 0IE  | C10-C9-C8   | 3.72  | 131.12      | 123.52   |
| 30  | i     | 614 | CHL  | OBD-CAD-C3D | -3.71 | 122.10      | 127.89   |
| 33  | 8     | 502 | 0UR  | C10-C11-C12 | -3.71 | 122.08      | 127.28   |
| 33  | 6     | 502 | 0UR  | C34-C27-C1  | -3.71 | 119.83      | 124.45   |
| 30  | 5     | 302 | CHL  | C1-C2-C3    | -3.71 | 120.12      | 126.20   |
| 30  | 2     | 308 | CHL  | OBD-CAD-CBD | 3.71  | 131.26      | 125.82   |
| 37  | d     | 522 | 0IE  | C15-C14-C13 | 3.71  | 133.94      | 123.20   |
| 33  | 1     | 502 | 0UR  | O44-C45-C46 | 3.70  | 120.69      | 111.55   |
| 33  | 2     | 501 | 0UR  | C9-C8-C7    | -3.70 | 122.09      | 127.28   |
| 37  | f     | 521 | 0IE  | C10-C9-C8   | 3.70  | 131.09      | 123.52   |
| 30  | 4     | 313 | CHL  | C1A-CHA-CBD | 3.70  | 141.83      | 132.36   |
| 33  | h     | 520 | 0UR  | C43-C3-C4   | -3.70 | 120.67      | 125.03   |
| 37  | g     | 522 | 0IE  | C20-C3-C4   | -3.69 | 119.61      | 124.72   |
| 32  | G     | 104 | 8CT  | C19-C20-C21 | -3.69 | 122.10      | 127.28   |
| 33  | 3     | 501 | 0UR  | C9-C8-C7    | -3.69 | 122.10      | 127.28   |
| 30  | 1     | 302 | CHL  | C1A-CHA-CBD | 3.69  | 141.81      | 132.36   |
| 30  | 0     | 306 | CHL  | O1D-CGD-CBD | -3.69 | 119.13      | 124.72   |
| 33  | 8     | 502 | 0UR  | C9-C8-C7    | -3.69 | 122.11      | 127.28   |
| 37  | d     | 521 | 0IE  | C10-C9-C8   | 3.69  | 131.06      | 123.52   |
| 30  | 4     | 302 | CHL  | C1A-CHA-CBD | 3.68  | 141.80      | 132.36   |
| 32  | B     | 843 | 8CT  | C04-C03-C02 | -3.68 | 117.60      | 122.64   |
| 30  | 7     | 306 | CHL  | C1A-CHA-CBD | 3.68  | 141.79      | 132.36   |
| 30  | e     | 601 | CHL  | C1-C2-C3    | -3.68 | 120.81      | 126.76   |
| 30  | 2     | 302 | CHL  | C1-C2-C3    | -3.68 | 120.17      | 126.20   |
| 32  | A     | 849 | 8CT  | C18-C19-C20 | -3.68 | 116.00      | 123.52   |
| 37  | f     | 522 | 0IE  | C23-C16-C15 | -3.68 | 116.86      | 122.82   |
| 30  | 9     | 306 | CHL  | C1A-CHA-CBD | 3.68  | 141.77      | 132.36   |
| 32  | 9     | 401 | 8CT  | C35-C30-C29 | -3.67 | 108.60      | 112.83   |
| 33  | O     | 204 | 0UR  | C14-C15-C16 | -3.67 | 122.13      | 127.28   |
| 33  | 4     | 502 | 0UR  | C34-C27-C1  | -3.67 | 119.87      | 124.45   |
| 32  | A     | 850 | 8CT  | C11-C10-C03 | -3.67 | 117.19      | 127.00   |
| 30  | 8     | 313 | CHL  | OBD-CAD-C3D | -3.67 | 122.17      | 127.89   |
| 33  | h     | 520 | 0UR  | O44-C45-C46 | 3.67  | 120.61      | 111.55   |
| 33  | b     | 520 | 0UR  | C9-C8-C7    | -3.67 | 122.13      | 127.28   |
| 32  | B     | 844 | 8CT  | C29-C28-C26 | -3.67 | 118.43      | 126.32   |
| 30  | g     | 602 | CHL  | C1B-CHB-C4A | 3.66  | 123.68      | 121.32   |
| 37  | f     | 521 | 0IE  | C20-C3-C4   | -3.66 | 119.66      | 124.72   |
| 30  | 0     | 306 | CHL  | C1B-CHB-C4A | 3.66  | 123.68      | 121.32   |
| 33  | 0     | 502 | 0UR  | O44-C45-C46 | 3.66  | 120.58      | 111.55   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | 2     | 402 | 8CT  | C10-C11-C12 | -3.66 | 120.83      | 126.23   |
| 33  | 8     | 502 | 0UR  | C43-C3-C4   | -3.65 | 120.72      | 125.03   |
| 30  | d     | 602 | CHL  | OBD-CAD-C3D | -3.65 | 122.19      | 127.89   |
| 30  | 6     | 308 | CHL  | CBC-CAC-C3C | -3.65 | 107.64      | 112.87   |
| 33  | 0     | 501 | 0UR  | C9-C8-C7    | -3.65 | 122.16      | 127.28   |
| 33  | 5     | 502 | 0UR  | O44-C45-C46 | 3.65  | 120.55      | 111.55   |
| 32  | 8     | 406 | 8CT  | C25-C24-C23 | -3.64 | 112.64      | 123.20   |
| 30  | b     | 609 | CHL  | OBD-CAD-C3D | -3.64 | 122.21      | 127.89   |
| 32  | G     | 104 | 8CT  | C14-C13-C12 | -3.64 | 122.17      | 127.28   |
| 32  | J     | 104 | 8CT  | C14-C13-C12 | 3.64  | 132.38      | 127.28   |
| 33  | h     | 520 | 0UR  | C5-C4-C3    | -3.64 | 122.57      | 126.92   |
| 33  | 7     | 501 | 0UR  | O44-C45-C46 | 3.64  | 120.52      | 111.55   |
| 33  | 7     | 501 | 0UR  | C28-C19-C18 | -3.64 | 108.65      | 112.83   |
| 33  | a     | 520 | 0UR  | C9-C8-C7    | -3.64 | 122.18      | 127.28   |
| 33  | g     | 520 | 0UR  | C34-C27-C1  | -3.63 | 119.92      | 124.45   |
| 30  | d     | 602 | CHL  | C1A-CHA-CBD | 3.63  | 141.67      | 132.36   |
| 30  | 3     | 302 | CHL  | C1A-CHA-CBD | 3.63  | 141.67      | 132.36   |
| 33  | e     | 520 | 0UR  | C19-C18-C17 | -3.63 | 118.93      | 124.58   |
| 37  | c     | 521 | 0IE  | C10-C9-C8   | 3.63  | 130.94      | 123.52   |
| 30  | 8     | 313 | CHL  | CBC-CAC-C3C | -3.63 | 107.68      | 112.87   |
| 30  | 2     | 305 | CHL  | CMD-C2D-C3D | -3.62 | 117.45      | 124.68   |
| 37  | i     | 521 | 0IE  | C9-C10-C11  | 3.62  | 130.92      | 123.52   |
| 32  | A     | 849 | 8CT  | C04-C03-C02 | -3.61 | 117.70      | 122.64   |
| 30  | 8     | 302 | CHL  | C1A-CHA-CBD | 3.61  | 141.60      | 132.36   |
| 32  | 7     | 405 | 8CT  | C07-C02-C03 | -3.61 | 117.83      | 122.70   |
| 42  | e     | 523 | NEX  | C15-C14-C13 | -3.60 | 122.22      | 127.28   |
| 30  | 7     | 306 | CHL  | OBD-CAD-CBD | 3.60  | 131.11      | 125.82   |
| 32  | 6     | 402 | 8CT  | C18-C19-C20 | -3.60 | 116.15      | 123.52   |
| 32  | M     | 102 | 8CT  | C30-C31-C32 | -3.60 | 117.04      | 121.47   |
| 33  | b     | 520 | 0UR  | C5-C4-C3    | -3.60 | 122.61      | 126.92   |
| 30  | 0     | 302 | CHL  | C1-C2-C3    | -3.59 | 120.31      | 126.20   |
| 33  | d     | 520 | 0UR  | C19-C18-C17 | -3.59 | 118.99      | 124.58   |
| 30  | 3     | 305 | CHL  | C1-C2-C3    | -3.59 | 120.95      | 126.76   |
| 30  | 7     | 306 | CHL  | C1-C2-C3    | -3.59 | 120.31      | 126.20   |
| 32  | A     | 846 | 8CT  | C10-C11-C12 | -3.59 | 120.92      | 126.23   |
| 37  | b     | 521 | 0IE  | C9-C10-C11  | 3.58  | 130.85      | 123.52   |
| 30  | 4     | 302 | CHL  | C1-C2-C3    | -3.58 | 120.33      | 126.20   |
| 30  | b     | 602 | CHL  | C1-C2-C3    | -3.58 | 120.33      | 126.20   |
| 30  | a     | 602 | CHL  | C1-C2-C3    | -3.58 | 120.33      | 126.20   |
| 30  | 6     | 302 | CHL  | CBC-CAC-C3C | -3.57 | 107.76      | 112.87   |
| 32  | A     | 847 | 8CT  | C24-C25-C26 | -3.57 | 122.27      | 127.28   |
| 33  | 4     | 501 | 0UR  | C9-C8-C7    | -3.57 | 122.27      | 127.28   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 33  | 4     | 501 | 0UR  | O44-C45-C46 | 3.57  | 120.37      | 111.55   |
| 30  | g     | 601 | CHL  | C1B-CHB-C4A | -3.57 | 119.03      | 121.32   |
| 33  | 9     | 502 | 0UR  | O44-C45-C46 | 3.57  | 120.36      | 111.55   |
| 30  | 2     | 313 | CHL  | C1-C2-C3    | -3.57 | 120.99      | 126.76   |
| 30  | d     | 606 | CHL  | C1-C2-C3    | -3.56 | 120.99      | 126.76   |
| 32  | K     | 107 | 8CT  | C29-C28-C26 | -3.56 | 118.67      | 126.32   |
| 32  | 7     | 405 | 8CT  | C35-C30-C29 | -3.56 | 108.73      | 112.83   |
| 37  | f     | 522 | 0IE  | C20-C3-C4   | -3.56 | 119.80      | 124.72   |
| 32  | B     | 848 | 8CT  | C25-C24-C23 | -3.56 | 112.89      | 123.20   |
| 33  | e     | 520 | 0UR  | O44-C45-C46 | 3.56  | 120.33      | 111.55   |
| 30  | 6     | 306 | CHL  | C1-C2-C3    | -3.56 | 121.01      | 126.76   |
| 33  | c     | 520 | 0UR  | C9-C8-C7    | -3.55 | 122.30      | 127.28   |
| 32  | B     | 845 | 8CT  | C22-C21-C23 | 3.55  | 123.52      | 118.09   |
| 32  | 7     | 404 | 8CT  | C30-C31-C32 | -3.55 | 117.10      | 121.47   |
| 30  | 3     | 302 | CHL  | C1-C2-C3    | -3.55 | 120.38      | 126.20   |
| 33  | 2     | 501 | 0UR  | O44-C45-C46 | 3.55  | 120.30      | 111.55   |
| 32  | A     | 848 | 8CT  | C35-C30-C29 | -3.54 | 108.75      | 112.83   |
| 32  | 8     | 402 | 8CT  | C04-C03-C02 | -3.54 | 117.80      | 122.64   |
| 33  | 9     | 502 | 0UR  | C24-C23-C1  | -3.54 | 105.92      | 110.61   |
| 30  | 4     | 313 | CHL  | OBD-CAD-C3D | -3.54 | 122.38      | 127.89   |
| 37  | i     | 522 | 0IE  | C23-C16-C15 | -3.54 | 117.09      | 122.82   |
| 33  | 2     | 502 | 0UR  | C5-C4-C3    | -3.53 | 122.70      | 126.92   |
| 31  | A     | 835 | CLA  | O2D-CGD-O1D | -3.53 | 116.98      | 123.85   |
| 31  | B     | 803 | CLA  | C1-C2-C3    | -3.53 | 120.42      | 126.20   |
| 32  | 7     | 402 | 8CT  | C11-C10-C03 | -3.53 | 117.58      | 127.00   |
| 32  | J     | 104 | 8CT  | C05-C04-C03 | 3.53  | 115.56      | 110.44   |
| 30  | c     | 602 | CHL  | C1-C2-C3    | -3.53 | 120.42      | 126.20   |
| 30  | 5     | 301 | CHL  | C1-C2-C3    | -3.52 | 120.42      | 126.20   |
| 33  | 0     | 501 | 0UR  | C10-C11-C12 | -3.52 | 122.34      | 127.28   |
| 32  | B     | 845 | 8CT  | C39-C16-C15 | 3.52  | 123.47      | 118.09   |
| 31  | B     | 811 | CLA  | O2D-CGD-O1D | -3.52 | 116.99      | 123.85   |
| 30  | d     | 601 | CHL  | C1-C2-C3    | -3.52 | 121.06      | 126.76   |
| 30  | 5     | 306 | CHL  | OBD-CAD-C3D | -3.52 | 122.41      | 127.89   |
| 37  | g     | 522 | 0IE  | C6-C7-C8    | 3.52  | 124.54      | 119.01   |
| 33  | 6     | 502 | 0UR  | C43-C3-C4   | -3.52 | 120.88      | 125.03   |
| 37  | d     | 522 | 0IE  | C13-C12-C11 | 3.51  | 124.53      | 119.01   |
| 32  | 0     | 401 | 8CT  | C19-C18-C17 | -3.50 | 116.35      | 123.52   |
| 32  | B     | 846 | 8CT  | C01-C02-C03 | -3.50 | 120.67      | 124.48   |
| 37  | b     | 522 | 0IE  | C9-C10-C11  | 3.50  | 130.68      | 123.52   |
| 33  | 9     | 501 | 0UR  | O44-C45-C46 | 3.50  | 120.18      | 111.55   |
| 30  | 6     | 308 | CHL  | C1-C2-C3    | -3.49 | 120.47      | 126.20   |
| 30  | 6     | 306 | CHL  | CBC-CAC-C3C | -3.49 | 107.88      | 112.87   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 33  | 5     | 502 | 0UR  | C10-C11-C12 | -3.49 | 122.38      | 127.28   |
| 32  | 4     | 402 | 8CT  | C19-C20-C21 | -3.49 | 122.39      | 127.28   |
| 32  | B     | 844 | 8CT  | C22-C21-C23 | 3.48  | 123.41      | 118.09   |
| 30  | i     | 606 | CHL  | C1-C2-C3    | -3.47 | 121.14      | 126.76   |
| 38  | B     | 842 | PQN  | C14-C13-C15 | 3.47  | 121.26      | 115.23   |
| 30  | 1     | 307 | CHL  | CMD-C2D-C3D | -3.47 | 117.75      | 124.68   |
| 32  | O     | 205 | 8CT  | C04-C03-C02 | -3.47 | 117.90      | 122.64   |
| 42  | e     | 523 | NEX  | C24-C23-C22 | -3.46 | 104.31      | 110.79   |
| 33  | h     | 520 | 0UR  | C34-C27-C1  | -3.46 | 120.14      | 124.45   |
| 33  | 4     | 501 | 0UR  | C28-C19-C18 | -3.45 | 108.86      | 112.83   |
| 30  | h     | 602 | CHL  | C1-C2-C3    | -3.45 | 120.54      | 126.20   |
| 32  | B     | 848 | 8CT  | C28-C26-C25 | 3.45  | 124.44      | 119.01   |
| 33  | 1     | 501 | 0UR  | O44-C45-C46 | 3.45  | 120.06      | 111.55   |
| 31  | B     | 801 | CLA  | C3B-C4B-NB  | -3.45 | 107.45      | 110.53   |
| 37  | c     | 521 | 0IE  | C23-C16-C15 | -3.45 | 117.23      | 122.82   |
| 33  | 6     | 502 | 0UR  | O44-C45-C46 | 3.45  | 120.06      | 111.55   |
| 30  | c     | 609 | CHL  | CMD-C2D-C3D | -3.44 | 117.80      | 124.68   |
| 30  | 9     | 305 | CHL  | OBD-CAD-CBD | 3.44  | 130.87      | 125.82   |
| 30  | 2     | 308 | CHL  | OBD-CAD-C3D | -3.44 | 122.53      | 127.89   |
| 32  | J     | 101 | 8CT  | C24-C23-C21 | -3.44 | 116.94      | 126.36   |
| 32  | B     | 846 | 8CT  | C28-C26-C25 | 3.44  | 124.42      | 119.01   |
| 31  | A     | 830 | CLA  | O2D-CGD-O1D | -3.43 | 117.16      | 123.85   |
| 30  | d     | 608 | CHL  | C1-C2-C3    | -3.43 | 121.21      | 126.76   |
| 30  | b     | 606 | CHL  | C1-C2-C3    | -3.43 | 121.21      | 126.76   |
| 33  | O     | 204 | 0UR  | C19-C18-C17 | -3.43 | 119.24      | 124.58   |
| 30  | 4     | 313 | CHL  | C1-C2-C3    | -3.43 | 121.21      | 126.76   |
| 33  | O     | 204 | 0UR  | C34-C27-C1  | -3.43 | 120.17      | 124.45   |
| 31  | A     | 812 | CLA  | C3B-C4B-NB  | -3.43 | 107.47      | 110.53   |
| 33  | 9     | 502 | 0UR  | C34-C27-C26 | 3.43  | 120.72      | 114.42   |
| 32  | A     | 846 | 8CT  | C35-C30-C29 | -3.43 | 108.89      | 112.83   |
| 32  | M     | 102 | 8CT  | C30-C29-C28 | -3.43 | 119.25      | 124.58   |
| 32  | 0     | 401 | 8CT  | C14-C13-C12 | -3.43 | 122.47      | 127.28   |
| 30  | e     | 601 | CHL  | CMD-C2D-C3D | -3.42 | 117.84      | 124.68   |
| 32  | 6     | 402 | 8CT  | C07-C02-C03 | -3.42 | 118.08      | 122.70   |
| 30  | f     | 602 | CHL  | C1-C2-C3    | -3.42 | 120.59      | 126.20   |
| 30  | 5     | 307 | CHL  | CMD-C2D-C3D | -3.42 | 117.85      | 124.68   |
| 37  | c     | 522 | 0IE  | C23-C16-C15 | -3.42 | 117.28      | 122.82   |
| 32  | B     | 845 | 8CT  | C29-C28-C26 | -3.42 | 118.97      | 126.32   |
| 32  | L     | 205 | 8CT  | C11-C10-C03 | -3.42 | 117.87      | 127.00   |
| 32  | A     | 854 | 8CT  | C10-C11-C12 | -3.42 | 121.18      | 126.23   |
| 30  | f     | 606 | CHL  | C1-C2-C3    | -3.42 | 121.23      | 126.76   |
| 30  | 6     | 313 | CHL  | C4-C3-C5    | 3.41  | 120.15      | 116.13   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | B     | 844 | 8CT  | C24-C25-C26 | -3.41 | 122.50      | 127.28   |
| 37  | 3     | 502 | 0IE  | C10-C9-C8   | 3.41  | 130.50      | 123.52   |
| 35  | 0     | 603 | SQD  | O47-C7-C8   | 3.41  | 118.86      | 111.48   |
| 35  | 0     | 603 | SQD  | C44-O6-C1   | 3.41  | 121.10      | 113.80   |
| 30  | 1     | 313 | CHL  | C1-C2-C3    | -3.40 | 120.62      | 126.20   |
| 33  | i     | 520 | 0UR  | C34-C27-C1  | -3.40 | 120.21      | 124.45   |
| 32  | K     | 107 | 8CT  | C19-C20-C21 | -3.40 | 122.51      | 127.28   |
| 30  | i     | 606 | CHL  | CMD-C2D-C3D | -3.40 | 117.89      | 124.68   |
| 31  | B     | 806 | CLA  | C3B-C4B-NB  | -3.40 | 107.50      | 110.53   |
| 30  | 6     | 313 | CHL  | CBC-CAC-C3C | -3.40 | 108.01      | 112.87   |
| 32  | 2     | 402 | 8CT  | C14-C15-C16 | -3.40 | 117.05      | 126.36   |
| 32  | M     | 102 | 8CT  | C29-C28-C26 | -3.39 | 119.02      | 126.32   |
| 30  | 1     | 306 | CHL  | C1B-CHB-C4A | 3.39  | 123.51      | 121.32   |
| 32  | B     | 848 | 8CT  | C30-C31-C32 | -3.39 | 117.30      | 121.47   |
| 30  | 4     | 319 | CHL  | O2A-CGA-CBA | 3.39  | 122.17      | 111.83   |
| 33  | b     | 520 | 0UR  | C43-C3-C4   | -3.39 | 121.03      | 125.03   |
| 33  | 9     | 501 | 0UR  | C34-C27-C1  | -3.39 | 120.22      | 124.45   |
| 32  | B     | 843 | 8CT  | C39-C16-C15 | 3.39  | 123.26      | 118.09   |
| 41  | B     | 849 | DGD  | O1G-C1A-C2A | 3.39  | 122.16      | 111.83   |
| 33  | d     | 520 | 0UR  | O44-C45-C46 | 3.39  | 119.91      | 111.55   |
| 37  | e     | 522 | 0IE  | C23-C16-C15 | -3.38 | 117.33      | 122.82   |
| 37  | c     | 522 | 0IE  | C6-C7-C8    | 3.38  | 124.33      | 119.01   |
| 32  | B     | 844 | 8CT  | C22-C21-C20 | -3.38 | 117.34      | 122.82   |
| 32  | L     | 206 | 8CT  | C10-C11-C12 | -3.38 | 121.23      | 126.23   |
| 32  | G     | 104 | 8CT  | C05-C04-C03 | 3.38  | 115.35      | 110.44   |
| 33  | O     | 204 | 0UR  | O44-C45-C46 | 3.38  | 119.89      | 111.55   |
| 37  | h     | 521 | 0IE  | C23-C16-C15 | -3.38 | 117.34      | 122.82   |
| 30  | 8     | 301 | CHL  | C1B-CHB-C4A | 3.38  | 123.50      | 121.32   |
| 30  | e     | 606 | CHL  | C1-C2-C3    | -3.38 | 121.30      | 126.76   |
| 37  | g     | 522 | 0IE  | C23-C16-C15 | -3.38 | 117.35      | 122.82   |
| 33  | 5     | 501 | 0UR  | C34-C27-C1  | -3.38 | 120.24      | 124.45   |
| 30  | h     | 614 | CHL  | CMD-C2D-C3D | -3.37 | 117.94      | 124.68   |
| 32  | 2     | 402 | 8CT  | C19-C20-C21 | -3.37 | 122.55      | 127.28   |
| 33  | f     | 520 | 0UR  | O44-C45-C46 | 3.37  | 119.87      | 111.55   |
| 31  | B     | 829 | CLA  | C3B-C4B-NB  | -3.37 | 107.52      | 110.53   |
| 30  | g     | 606 | CHL  | C1-C2-C3    | -3.37 | 121.31      | 126.76   |
| 30  | 8     | 301 | CHL  | O1D-CGD-CBD | -3.37 | 119.62      | 124.72   |
| 30  | 1     | 305 | CHL  | CMD-C2D-C3D | -3.37 | 117.95      | 124.68   |
| 30  | 6     | 313 | CHL  | C1-C2-C3    | -3.36 | 120.69      | 126.20   |
| 33  | 4     | 502 | 0UR  | C9-C8-C7    | -3.36 | 122.56      | 127.28   |
| 33  | a     | 520 | 0UR  | C34-C27-C1  | -3.36 | 120.26      | 124.45   |
| 33  | 0     | 502 | 0UR  | C28-C19-C18 | -3.36 | 108.97      | 112.83   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | 7     | 402 | 8CT  | C14-C13-C12 | -3.36 | 122.57      | 127.28   |
| 33  | 0     | 501 | 0UR  | C34-C27-C1  | -3.35 | 120.27      | 124.45   |
| 31  | B     | 818 | CLA  | C3B-C4B-NB  | -3.35 | 107.54      | 110.53   |
| 30  | 6     | 313 | CHL  | CMD-C2D-C3D | -3.35 | 117.99      | 124.68   |
| 32  | O     | 205 | 8CT  | C01-C02-C03 | -3.35 | 120.83      | 124.48   |
| 30  | h     | 606 | CHL  | C1-C2-C3    | -3.35 | 121.34      | 126.76   |
| 32  | A     | 848 | 8CT  | C25-C24-C23 | -3.35 | 113.50      | 123.20   |
| 37  | b     | 522 | 0IE  | C23-C16-C15 | -3.35 | 117.39      | 122.82   |
| 37  | 7     | 502 | 0IE  | C10-C9-C8   | 3.35  | 130.37      | 123.52   |
| 33  | 3     | 501 | 0UR  | C10-C11-C12 | -3.35 | 122.58      | 127.28   |
| 37  | g     | 521 | 0IE  | C23-C16-C15 | -3.35 | 117.39      | 122.82   |
| 30  | b     | 609 | CHL  | C1-C2-C3    | -3.35 | 120.72      | 126.20   |
| 32  | 7     | 404 | 8CT  | C07-C02-C03 | -3.35 | 118.18      | 122.70   |
| 37  | f     | 521 | 0IE  | C23-C16-C15 | -3.34 | 117.40      | 122.82   |
| 32  | B     | 844 | 8CT  | C39-C16-C15 | 3.34  | 123.19      | 118.09   |
| 33  | 2     | 501 | 0UR  | C28-C19-C18 | -3.34 | 108.98      | 112.83   |
| 33  | 9     | 502 | 0UR  | C4-C3-C2    | -3.34 | 117.25      | 120.16   |
| 37  | h     | 522 | 0IE  | C23-C16-C15 | -3.34 | 117.41      | 122.82   |
| 33  | f     | 520 | 0UR  | C34-C27-C1  | -3.34 | 120.28      | 124.45   |
| 30  | g     | 607 | CHL  | C1-C2-C3    | -3.34 | 121.36      | 126.76   |
| 37  | a     | 522 | 0IE  | C23-C16-C15 | -3.34 | 117.41      | 122.82   |
| 30  | 8     | 305 | CHL  | CMD-C2D-C3D | -3.34 | 118.02      | 124.68   |
| 33  | 0     | 502 | 0UR  | C9-C10-C11  | -3.33 | 116.70      | 123.52   |
| 31  | A     | 817 | CLA  | O2D-CGD-O1D | -3.33 | 117.36      | 123.85   |
| 37  | a     | 521 | 0IE  | C23-C16-C15 | -3.33 | 117.42      | 122.82   |
| 32  | K     | 107 | 8CT  | C14-C15-C16 | -3.33 | 117.23      | 126.36   |
| 32  | L     | 205 | 8CT  | C01-C02-C07 | 3.33  | 120.70      | 113.60   |
| 32  | A     | 854 | 8CT  | C04-C03-C02 | -3.33 | 118.08      | 122.64   |
| 30  | 0     | 301 | CHL  | O2A-CGA-CBA | 3.33  | 121.99      | 111.83   |
| 31  | B     | 809 | CLA  | C3B-C4B-NB  | -3.33 | 107.56      | 110.53   |
| 33  | d     | 520 | 0UR  | C34-C27-C1  | -3.33 | 120.30      | 124.45   |
| 30  | 8     | 315 | CHL  | CBC-CAC-C3C | -3.33 | 108.11      | 112.87   |
| 30  | h     | 609 | CHL  | CMD-C2D-C3D | -3.33 | 118.03      | 124.68   |
| 33  | d     | 520 | 0UR  | C14-C15-C16 | -3.32 | 122.61      | 127.28   |
| 31  | A     | 803 | CLA  | O2D-CGD-O1D | -3.32 | 117.38      | 123.85   |
| 33  | 1     | 501 | 0UR  | C9-C8-C7    | -3.32 | 122.62      | 127.28   |
| 33  | 7     | 501 | 0UR  | C34-C27-C1  | -3.32 | 120.31      | 124.45   |
| 30  | f     | 609 | CHL  | C1-C2-C3    | -3.32 | 120.76      | 126.20   |
| 32  | B     | 847 | 8CT  | C11-C10-C03 | -3.32 | 118.13      | 127.00   |
| 31  | L     | 202 | CLA  | O2D-CGD-O1D | -3.32 | 117.39      | 123.85   |
| 33  | i     | 520 | 0UR  | O44-C45-C46 | 3.31  | 119.73      | 111.55   |
| 31  | A     | 808 | CLA  | O2D-CGD-O1D | -3.31 | 117.40      | 123.85   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | B     | 851 | 8CT  | C04-C03-C02 | -3.31 | 118.11      | 122.64   |
| 31  | A     | 804 | CLA  | O2D-CGD-O1D | -3.31 | 117.40      | 123.85   |
| 31  | B     | 808 | CLA  | O2D-CGD-O1D | -3.31 | 117.41      | 123.85   |
| 37  | c     | 522 | 0IE  | C20-C3-C4   | -3.31 | 120.15      | 124.72   |
| 31  | A     | 853 | CLA  | C3B-C4B-NB  | -3.30 | 107.58      | 110.53   |
| 30  | i     | 614 | CHL  | C1B-CHB-C4A | -3.30 | 119.20      | 121.32   |
| 31  | A     | 805 | CLA  | C3B-C4B-NB  | -3.30 | 107.58      | 110.53   |
| 32  | 7     | 402 | 8CT  | C29-C28-C26 | -3.30 | 119.23      | 126.32   |
| 33  | 8     | 501 | 0UR  | C9-C8-C7    | -3.30 | 122.66      | 127.28   |
| 31  | L     | 203 | CLA  | O2D-CGD-O1D | -3.29 | 117.44      | 123.85   |
| 31  | 9     | 300 | CLA  | CAA-C2A-C3A | -3.29 | 104.10      | 113.00   |
| 30  | c     | 609 | CHL  | C1-C2-C3    | -3.29 | 120.80      | 126.20   |
| 37  | e     | 521 | 0IE  | C23-C16-C15 | -3.29 | 117.48      | 122.82   |
| 30  | 3     | 307 | CHL  | C1-C2-C3    | -3.29 | 120.81      | 126.20   |
| 32  | 2     | 402 | 8CT  | C22-C21-C20 | -3.29 | 117.49      | 122.82   |
| 31  | B     | 810 | CLA  | O2D-CGD-O1D | -3.29 | 117.45      | 123.85   |
| 30  | 5     | 305 | CHL  | CBC-CAC-C3C | -3.29 | 108.17      | 112.87   |
| 32  | B     | 804 | 8CT  | C30-C29-C28 | -3.28 | 119.47      | 124.58   |
| 32  | 0     | 401 | 8CT  | C07-C02-C03 | -3.28 | 118.27      | 122.70   |
| 30  | c     | 606 | CHL  | C1B-CHB-C4A | 3.28  | 123.43      | 121.32   |
| 30  | 2     | 307 | CHL  | CBC-CAC-C3C | -3.28 | 108.18      | 112.87   |
| 37  | f     | 521 | 0IE  | C9-C10-C11  | 3.28  | 130.23      | 123.52   |
| 30  | 9     | 313 | CHL  | CMD-C2D-C3D | -3.28 | 118.13      | 124.68   |
| 32  | B     | 847 | 8CT  | C14-C15-C16 | -3.28 | 117.38      | 126.36   |
| 33  | 9     | 501 | 0UR  | C9-C8-C7    | -3.28 | 122.68      | 127.28   |
| 32  | B     | 804 | 8CT  | C14-C15-C16 | -3.28 | 117.38      | 126.36   |
| 32  | B     | 843 | 8CT  | C35-C30-C29 | -3.27 | 109.06      | 112.83   |
| 33  | 5     | 502 | 0UR  | C43-C3-C4   | -3.27 | 121.17      | 125.03   |
| 30  | 2     | 308 | CHL  | CBC-CAC-C3C | -3.27 | 108.19      | 112.87   |
| 32  | J     | 101 | 8CT  | C11-C10-C03 | -3.27 | 118.26      | 127.00   |
| 30  | a     | 609 | CHL  | CMD-C2D-C3D | -3.27 | 118.15      | 124.68   |
| 32  | B     | 846 | 8CT  | C39-C16-C15 | 3.27  | 123.08      | 118.09   |
| 32  | A     | 850 | 8CT  | C10-C11-C12 | -3.27 | 121.40      | 126.23   |
| 30  | 7     | 302 | CHL  | C1-C2-C3    | -3.27 | 120.84      | 126.20   |
| 32  | L     | 209 | 8CT  | C35-C30-C29 | -3.26 | 109.07      | 112.83   |
| 30  | 2     | 319 | CHL  | O2A-CGA-CBA | 3.26  | 121.78      | 111.83   |
| 32  | B     | 844 | 8CT  | C04-C03-C02 | -3.26 | 118.18      | 122.64   |
| 31  | A     | 833 | CLA  | O2D-CGD-O1D | -3.26 | 117.50      | 123.85   |
| 32  | A     | 854 | 8CT  | C07-C02-C03 | -3.26 | 118.30      | 122.70   |
| 31  | 0     | 321 | CLA  | O2D-CGD-O1D | -3.26 | 117.50      | 123.85   |
| 33  | 0     | 502 | 0UR  | C19-C18-C17 | -3.26 | 119.50      | 124.58   |
| 32  | B     | 848 | 8CT  | C14-C15-C16 | -3.26 | 117.42      | 126.36   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 33  | O     | 204 | 0UR  | C9-C10-C11  | -3.26 | 116.85      | 123.52   |
| 32  | L     | 209 | 8CT  | C14-C13-C12 | -3.26 | 122.71      | 127.28   |
| 37  | b     | 521 | 0IE  | C23-C16-C15 | -3.26 | 117.54      | 122.82   |
| 37  | 3     | 502 | 0IE  | C20-C3-C4   | -3.25 | 120.22      | 124.72   |
| 30  | e     | 609 | CHL  | C1-C2-C3    | -3.25 | 120.86      | 126.20   |
| 32  | B     | 846 | 8CT  | C40-C12-C13 | -3.25 | 117.55      | 122.82   |
| 39  | A     | 857 | CL0  | C4D-CHA-CBD | -3.25 | 105.69      | 108.97   |
| 32  | A     | 849 | 8CT  | C07-C02-C03 | -3.25 | 118.31      | 122.70   |
| 31  | A     | 810 | CLA  | C3B-C4B-NB  | -3.25 | 107.63      | 110.53   |
| 32  | L     | 209 | 8CT  | C25-C24-C23 | -3.25 | 113.79      | 123.20   |
| 32  | 9     | 401 | 8CT  | C24-C25-C26 | -3.25 | 122.72      | 127.28   |
| 37  | d     | 521 | 0IE  | C23-C16-C15 | -3.25 | 117.56      | 122.82   |
| 31  | B     | 827 | CLA  | O2D-CGD-O1D | -3.25 | 117.53      | 123.85   |
| 32  | 0     | 401 | 8CT  | C30-C29-C28 | -3.24 | 119.53      | 124.58   |
| 32  | A     | 846 | 8CT  | C11-C10-C03 | -3.24 | 118.33      | 127.00   |
| 30  | 6     | 301 | CHL  | C1-C2-C3    | -3.24 | 120.88      | 126.20   |
| 33  | 6     | 501 | 0UR  | C43-C3-C4   | -3.24 | 121.20      | 125.03   |
| 37  | e     | 522 | 0IE  | C6-C7-C8    | 3.24  | 124.11      | 119.01   |
| 37  | e     | 521 | 0IE  | C20-C3-C4   | -3.24 | 120.24      | 124.72   |
| 33  | 3     | 501 | 0UR  | C19-C18-C17 | -3.24 | 119.53      | 124.58   |
| 31  | B     | 841 | CLA  | C3B-C4B-NB  | -3.24 | 107.64      | 110.53   |
| 30  | 3     | 307 | CHL  | O2A-CGA-CBA | 3.24  | 121.71      | 111.83   |
| 30  | f     | 601 | CHL  | C1-C2-C3    | -3.24 | 120.89      | 126.20   |
| 30  | f     | 609 | CHL  | CMD-C2D-C3D | -3.24 | 118.21      | 124.68   |
| 30  | i     | 609 | CHL  | CMD-C2D-C3D | -3.24 | 118.22      | 124.68   |
| 30  | 6     | 302 | CHL  | O2D-CGD-O1D | -3.24 | 117.55      | 123.85   |
| 37  | i     | 521 | 0IE  | C23-C16-C15 | -3.23 | 117.58      | 122.82   |
| 30  | d     | 609 | CHL  | CMD-C2D-C3D | -3.23 | 118.22      | 124.68   |
| 32  | 8     | 406 | 8CT  | C05-C04-C03 | 3.23  | 115.13      | 110.44   |
| 33  | 1     | 502 | 0UR  | C48-C47-C46 | -3.23 | 119.20      | 125.92   |
| 31  | B     | 841 | CLA  | O2D-CGD-O1D | -3.23 | 117.56      | 123.85   |
| 30  | d     | 614 | CHL  | CMD-C2D-C3D | -3.23 | 118.23      | 124.68   |
| 30  | 0     | 306 | CHL  | O2D-CGD-O1D | -3.23 | 117.57      | 123.85   |
| 31  | A     | 818 | CLA  | O2D-CGD-O1D | -3.23 | 117.57      | 123.85   |
| 30  | f     | 605 | CHL  | CMD-C2D-C3D | -3.22 | 118.24      | 124.68   |
| 30  | 2     | 302 | CHL  | OMC-CMC-C2C | -3.22 | 119.52      | 125.12   |
| 31  | B     | 824 | CLA  | C3B-C4B-NB  | -3.22 | 107.65      | 110.53   |
| 32  | L     | 206 | 8CT  | C11-C10-C03 | -3.22 | 118.39      | 127.00   |
| 31  | 6     | 314 | CLA  | O2D-CGD-O1D | -3.22 | 117.58      | 123.85   |
| 31  | F     | 301 | CLA  | C3B-C4B-NB  | -3.22 | 107.65      | 110.53   |
| 31  | A     | 825 | CLA  | O2D-CGD-O1D | -3.22 | 117.58      | 123.85   |
| 30  | i     | 602 | CHL  | C1-C2-C3    | -3.22 | 120.92      | 126.20   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 33  | g     | 520 | 0UR  | C18-C17-C16 | -3.22 | 119.40      | 126.32   |
| 31  | B     | 826 | CLA  | C3D-C4D-ND  | 3.22  | 111.81      | 109.68   |
| 37  | c     | 521 | 0IE  | C20-C3-C4   | -3.22 | 120.27      | 124.72   |
| 32  | 3     | 402 | 8CT  | C29-C28-C26 | -3.22 | 119.41      | 126.32   |
| 32  | A     | 854 | 8CT  | C11-C10-C03 | -3.22 | 118.41      | 127.00   |
| 30  | a     | 609 | CHL  | C1-C2-C3    | -3.21 | 120.93      | 126.20   |
| 37  | b     | 521 | 0IE  | C20-C3-C4   | -3.21 | 120.28      | 124.72   |
| 31  | B     | 819 | CLA  | O2D-CGD-O1D | -3.21 | 117.59      | 123.85   |
| 30  | h     | 605 | CHL  | CMD-C2D-C3D | -3.21 | 118.26      | 124.68   |
| 31  | B     | 838 | CLA  | O2D-CGD-O1D | -3.21 | 117.59      | 123.85   |
| 33  | c     | 520 | 0UR  | C36-C28-C19 | 3.21  | 114.41      | 109.55   |
| 30  | 3     | 307 | CHL  | CBC-CAC-C3C | -3.21 | 108.28      | 112.87   |
| 30  | e     | 609 | CHL  | CMD-C2D-C3D | -3.21 | 118.27      | 124.68   |
| 31  | B     | 818 | CLA  | O2D-CGD-O1D | -3.21 | 117.60      | 123.85   |
| 30  | g     | 614 | CHL  | CMD-C2D-C3D | -3.21 | 118.27      | 124.68   |
| 30  | 6     | 313 | CHL  | O2A-CGA-CBA | 3.21  | 121.62      | 111.83   |
| 30  | 4     | 302 | CHL  | OMC-CMC-C2C | -3.21 | 119.55      | 125.12   |
| 30  | d     | 609 | CHL  | C1-C2-C3    | -3.21 | 120.94      | 126.20   |
| 31  | B     | 803 | CLA  | O2D-CGD-O1D | -3.21 | 117.61      | 123.85   |
| 31  | O     | 201 | CLA  | O2D-CGD-O1D | -3.21 | 117.61      | 123.85   |
| 31  | A     | 806 | CLA  | C3B-C4B-NB  | -3.21 | 107.67      | 110.53   |
| 32  | 9     | 401 | 8CT  | C30-C29-C28 | -3.21 | 119.59      | 124.58   |
| 31  | B     | 833 | CLA  | O2D-CGD-O1D | -3.20 | 117.61      | 123.85   |
| 37  | 7     | 502 | 0IE  | C23-C16-C15 | -3.20 | 117.62      | 122.82   |
| 30  | 8     | 301 | CHL  | O2A-CGA-CBA | 3.20  | 121.61      | 111.83   |
| 37  | a     | 521 | 0IE  | C9-C10-C11  | 3.20  | 130.08      | 123.52   |
| 30  | e     | 606 | CHL  | CMD-C2D-C3D | -3.20 | 118.28      | 124.68   |
| 32  | 9     | 401 | 8CT  | C18-C19-C20 | -3.20 | 116.97      | 123.52   |
| 30  | 5     | 301 | CHL  | O2A-CGA-CBA | 3.20  | 121.59      | 111.83   |
| 32  | 2     | 402 | 8CT  | C23-C21-C20 | 3.20  | 124.04      | 119.01   |
| 31  | A     | 827 | CLA  | C3B-C4B-NB  | -3.20 | 107.67      | 110.53   |
| 31  | A     | 839 | CLA  | C3B-C4B-NB  | -3.20 | 107.67      | 110.53   |
| 33  | 4     | 501 | 0UR  | C48-C47-C46 | -3.20 | 119.26      | 125.92   |
| 37  | d     | 522 | 0IE  | C6-C7-C8    | 3.20  | 124.04      | 119.01   |
| 32  | L     | 209 | 8CT  | C19-C18-C17 | -3.20 | 116.98      | 123.52   |
| 30  | e     | 602 | CHL  | C1-C2-C3    | -3.20 | 120.96      | 126.20   |
| 33  | 4     | 501 | 0UR  | C10-C11-C12 | -3.20 | 122.80      | 127.28   |
| 31  | a     | 603 | CLA  | O2D-CGD-O1D | -3.20 | 117.63      | 123.85   |
| 31  | A     | 827 | CLA  | O2D-CGD-O1D | -3.19 | 117.63      | 123.85   |
| 31  | 3     | 320 | CLA  | CAC-C3C-C4C | 3.19  | 128.94      | 124.79   |
| 32  | 4     | 402 | 8CT  | C23-C21-C20 | 3.19  | 124.03      | 119.01   |
| 32  | B     | 846 | 8CT  | C01-C02-C07 | 3.19  | 120.40      | 113.60   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | B     | 830 | CLA  | CMB-C2B-C1B | -3.19 | 120.56      | 125.42   |
| 33  | e     | 520 | 0UR  | C14-C15-C16 | -3.19 | 122.80      | 127.28   |
| 31  | B     | 833 | CLA  | C3B-C4B-NB  | -3.19 | 107.68      | 110.53   |
| 32  | A     | 848 | 8CT  | C11-C10-C03 | -3.19 | 118.48      | 127.00   |
| 30  | e     | 608 | CHL  | CMD-C2D-C3D | -3.19 | 118.31      | 124.68   |
| 30  | 2     | 307 | CHL  | O2A-CGA-CBA | 3.19  | 121.55      | 111.83   |
| 32  | 1     | 402 | 8CT  | C07-C02-C03 | -3.18 | 118.40      | 122.70   |
| 37  | d     | 521 | 0IE  | C4-C3-C2    | -3.18 | 117.39      | 120.16   |
| 33  | 0     | 501 | 0UR  | O44-C45-C46 | 3.18  | 119.40      | 111.55   |
| 31  | 8     | 311 | CLA  | C3B-C4B-NB  | -3.18 | 107.69      | 110.53   |
| 30  | c     | 608 | CHL  | C1-C2-C3    | -3.17 | 121.00      | 126.20   |
| 30  | c     | 601 | CHL  | C1-C2-C3    | -3.17 | 121.00      | 126.20   |
| 30  | 9     | 306 | CHL  | O1D-CGD-CBD | -3.17 | 119.91      | 124.72   |
| 30  | c     | 609 | CHL  | C1B-CHB-C4A | 3.17  | 123.36      | 121.32   |
| 30  | d     | 605 | CHL  | CMD-C2D-C3D | -3.17 | 118.35      | 124.68   |
| 31  | 9     | 300 | CLA  | O2D-CGD-O1D | -3.17 | 117.68      | 123.85   |
| 31  | A     | 819 | CLA  | O2D-CGD-O1D | -3.17 | 117.68      | 123.85   |
| 31  | 3     | 318 | CLA  | C3B-C4B-NB  | -3.17 | 107.70      | 110.53   |
| 30  | d     | 607 | CHL  | CMD-C2D-C3D | -3.17 | 118.35      | 124.68   |
| 32  | 0     | 401 | 8CT  | C01-C02-C07 | 3.17  | 120.35      | 113.60   |
| 31  | A     | 826 | CLA  | C3B-C4B-NB  | -3.17 | 107.70      | 110.53   |
| 37  | 3     | 502 | 0IE  | C23-C16-C15 | -3.17 | 117.68      | 122.82   |
| 30  | 6     | 301 | CHL  | O2A-CGA-CBA | 3.17  | 121.49      | 111.83   |
| 32  | A     | 850 | 8CT  | C40-C12-C11 | 3.17  | 122.93      | 118.09   |
| 37  | b     | 522 | 0IE  | C20-C3-C4   | -3.17 | 120.34      | 124.72   |
| 31  | B     | 813 | CLA  | C3B-C4B-NB  | -3.17 | 107.70      | 110.53   |
| 31  | 3     | 313 | CLA  | O2D-CGD-O1D | -3.17 | 117.69      | 123.85   |
| 30  | 8     | 301 | CHL  | O2D-CGD-O1D | -3.16 | 117.69      | 123.85   |
| 30  | d     | 606 | CHL  | CMD-C2D-C3D | -3.16 | 118.36      | 124.68   |
| 31  | A     | 838 | CLA  | O2D-CGD-O1D | -3.16 | 117.69      | 123.85   |
| 31  | L     | 201 | CLA  | O2D-CGD-O1D | -3.16 | 117.69      | 123.85   |
| 31  | K     | 101 | CLA  | O2D-CGD-O1D | -3.16 | 117.70      | 123.85   |
| 32  | I     | 101 | 8CT  | C01-C02-C07 | 3.16  | 120.33      | 113.60   |
| 37  | h     | 522 | 0IE  | C20-C3-C4   | -3.16 | 120.35      | 124.72   |
| 30  | a     | 601 | CHL  | CMD-C2D-C3D | -3.16 | 118.37      | 124.68   |
| 30  | b     | 609 | CHL  | CMD-C2D-C3D | -3.16 | 118.37      | 124.68   |
| 32  | A     | 847 | 8CT  | C18-C19-C20 | -3.16 | 117.06      | 123.52   |
| 30  | 3     | 307 | CHL  | CMD-C2D-C3D | -3.16 | 118.37      | 124.68   |
| 30  | f     | 614 | CHL  | CAA-C2A-C3A | -3.16 | 108.99      | 116.23   |
| 37  | b     | 521 | 0IE  | C20-C3-C2   | 3.16  | 122.26      | 115.01   |
| 38  | A     | 842 | PQN  | C14-C13-C15 | 3.16  | 120.71      | 115.23   |
| 33  | 5     | 501 | 0UR  | O44-C45-C46 | 3.16  | 119.34      | 111.55   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | e     | 601 | CHL  | CBC-CAC-C3C | -3.16 | 108.36      | 112.87   |
| 33  | f     | 520 | 0UR  | C18-C17-C16 | -3.16 | 119.54      | 126.32   |
| 33  | 1     | 502 | 0UR  | C36-C28-C19 | 3.15  | 114.32      | 109.55   |
| 37  | a     | 522 | 0IE  | C9-C10-C11  | 3.15  | 129.97      | 123.52   |
| 30  | h     | 608 | CHL  | CMD-C2D-C3D | -3.15 | 118.38      | 124.68   |
| 30  | a     | 608 | CHL  | CBC-CAC-C3C | -3.15 | 108.36      | 112.87   |
| 31  | B     | 820 | CLA  | C3B-C4B-NB  | -3.15 | 107.72      | 110.53   |
| 32  | 3     | 402 | 8CT  | C04-C03-C02 | -3.15 | 118.33      | 122.64   |
| 30  | 6     | 301 | CHL  | O1D-CGD-CBD | -3.15 | 119.94      | 124.72   |
| 33  | f     | 520 | 0UR  | C43-C3-C4   | -3.15 | 121.31      | 125.03   |
| 31  | B     | 814 | CLA  | C3B-C4B-NB  | -3.15 | 107.72      | 110.53   |
| 30  | g     | 605 | CHL  | CMD-C2D-C3D | -3.15 | 118.39      | 124.68   |
| 31  | A     | 840 | CLA  | O2D-CGD-O1D | -3.15 | 117.72      | 123.85   |
| 37  | 3     | 502 | 0IE  | C20-C3-C2   | 3.15  | 122.24      | 115.01   |
| 37  | f     | 522 | 0IE  | C6-C7-C8    | 3.15  | 123.96      | 119.01   |
| 30  | b     | 614 | CHL  | CMD-C2D-C3D | -3.15 | 118.40      | 124.68   |
| 31  | B     | 825 | CLA  | O2D-CGD-O1D | -3.14 | 117.73      | 123.85   |
| 31  | 2     | 310 | CLA  | C3B-C4B-NB  | -3.14 | 107.72      | 110.53   |
| 30  | 7     | 302 | CHL  | C4-C3-C5    | 3.14  | 120.68      | 115.23   |
| 32  | A     | 849 | 8CT  | C14-C15-C16 | -3.14 | 117.75      | 126.36   |
| 37  | d     | 522 | 0IE  | C22-C12-C11 | -3.14 | 117.73      | 122.82   |
| 30  | 0     | 305 | CHL  | C1-C2-C3    | -3.14 | 121.68      | 126.76   |
| 30  | g     | 601 | CHL  | C4-C3-C5    | 3.14  | 119.82      | 116.13   |
| 32  | A     | 848 | 8CT  | C01-C02-C07 | 3.14  | 120.28      | 113.60   |
| 37  | g     | 521 | 0IE  | C4-C3-C2    | -3.14 | 117.43      | 120.16   |
| 31  | 6     | 317 | CLA  | O2D-CGD-O1D | -3.14 | 117.75      | 123.85   |
| 33  | 2     | 501 | 0UR  | C48-C47-C46 | -3.14 | 119.39      | 125.92   |
| 30  | b     | 601 | CHL  | CMD-C2D-C3D | -3.14 | 118.42      | 124.68   |
| 31  | B     | 837 | CLA  | O2D-CGD-O1D | -3.13 | 117.75      | 123.85   |
| 33  | 5     | 502 | 0UR  | C48-C47-C46 | -3.13 | 119.39      | 125.92   |
| 31  | O     | 202 | CLA  | C3B-C4B-NB  | -3.13 | 107.73      | 110.53   |
| 30  | i     | 601 | CHL  | CMD-C2D-C3D | -3.13 | 118.43      | 124.68   |
| 31  | 3     | 309 | CLA  | C3B-C4B-NB  | -3.13 | 107.73      | 110.53   |
| 37  | g     | 522 | 0IE  | C21-C7-C8   | -3.13 | 117.74      | 122.82   |
| 30  | 9     | 305 | CHL  | OBD-CAD-C3D | -3.13 | 123.01      | 127.89   |
| 37  | b     | 521 | 0IE  | C10-C9-C8   | 3.13  | 129.92      | 123.52   |
| 31  | 6     | 311 | CLA  | C3B-C4B-NB  | -3.13 | 107.74      | 110.53   |
| 30  | h     | 601 | CHL  | CMD-C2D-C3D | -3.13 | 118.43      | 124.68   |
| 37  | c     | 522 | 0IE  | C21-C7-C8   | -3.13 | 117.75      | 122.82   |
| 30  | i     | 614 | CHL  | CMD-C2D-C3D | -3.13 | 118.44      | 124.68   |
| 37  | a     | 521 | 0IE  | C20-C3-C4   | -3.12 | 120.40      | 124.72   |
| 31  | B     | 834 | CLA  | C3B-C4B-NB  | -3.12 | 107.74      | 110.53   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 7     | 303 | CLA  | C3B-C4B-NB  | -3.12 | 107.74      | 110.53   |
| 31  | B     | 807 | CLA  | O2D-CGD-O1D | -3.12 | 117.77      | 123.85   |
| 33  | e     | 520 | 0UR  | C5-C4-C3    | -3.12 | 123.18      | 126.92   |
| 30  | a     | 606 | CHL  | CMD-C2D-C3D | -3.12 | 118.45      | 124.68   |
| 30  | b     | 608 | CHL  | C1-C2-C3    | -3.12 | 121.09      | 126.20   |
| 30  | 8     | 313 | CHL  | C4-C3-C5    | 3.12  | 120.64      | 115.23   |
| 30  | a     | 614 | CHL  | CMD-C2D-C3D | -3.12 | 118.45      | 124.68   |
| 31  | B     | 831 | CLA  | C3B-C4B-NB  | -3.12 | 107.75      | 110.53   |
| 32  | J     | 104 | 8CT  | C07-C02-C03 | -3.12 | 118.49      | 122.70   |
| 30  | c     | 605 | CHL  | CMD-C2D-C3D | -3.12 | 118.46      | 124.68   |
| 31  | A     | 824 | CLA  | O2D-CGD-O1D | -3.11 | 117.78      | 123.85   |
| 30  | b     | 608 | CHL  | CMD-C2D-C3D | -3.11 | 118.46      | 124.68   |
| 34  | G     | 105 | LHG  | O8-C23-C24  | 3.11  | 121.33      | 111.83   |
| 32  | 8     | 402 | 8CT  | C07-C02-C03 | -3.11 | 118.50      | 122.70   |
| 30  | g     | 609 | CHL  | CMD-C2D-C3D | -3.11 | 118.46      | 124.68   |
| 31  | A     | 831 | CLA  | O2D-CGD-O1D | -3.11 | 117.79      | 123.85   |
| 30  | 1     | 305 | CHL  | CBC-CAC-C3C | -3.11 | 108.42      | 112.87   |
| 31  | 1     | 314 | CLA  | O2D-CGD-O1D | -3.11 | 117.79      | 123.85   |
| 30  | c     | 608 | CHL  | CMD-C2D-C3D | -3.11 | 118.47      | 124.68   |
| 30  | f     | 601 | CHL  | CMD-C2D-C3D | -3.11 | 118.47      | 124.68   |
| 32  | 7     | 404 | 8CT  | C40-C12-C13 | -3.11 | 117.78      | 122.82   |
| 31  | 6     | 312 | CLA  | O2D-CGD-O1D | -3.11 | 117.80      | 123.85   |
| 30  | 0     | 305 | CHL  | CMD-C2D-C3D | -3.11 | 118.47      | 124.68   |
| 30  | 2     | 301 | CHL  | O2A-CGA-CBA | 3.11  | 121.31      | 111.83   |
| 31  | 9     | 310 | CLA  | C3B-C4B-NB  | -3.11 | 107.76      | 110.53   |
| 33  | c     | 520 | 0UR  | C43-C3-C4   | -3.11 | 121.37      | 125.03   |
| 31  | 3     | 320 | CLA  | O2D-CGD-O1D | -3.10 | 117.81      | 123.85   |
| 30  | 5     | 313 | CHL  | O1D-CGD-CBD | -3.10 | 120.02      | 124.72   |
| 33  | 1     | 502 | 0UR  | C10-C11-C12 | -3.10 | 122.93      | 127.28   |
| 31  | A     | 836 | CLA  | O2D-CGD-O1D | -3.10 | 117.81      | 123.85   |
| 33  | 2     | 501 | 0UR  | C34-C27-C1  | -3.10 | 120.58      | 124.45   |
| 30  | 8     | 313 | CHL  | CMD-C2D-C3D | -3.10 | 118.49      | 124.68   |
| 30  | a     | 605 | CHL  | CMD-C2D-C3D | -3.10 | 118.49      | 124.68   |
| 33  | 5     | 501 | 0UR  | C43-C3-C4   | -3.10 | 121.37      | 125.03   |
| 30  | c     | 607 | CHL  | CBC-CAC-C3C | -3.10 | 108.44      | 112.87   |
| 30  | g     | 606 | CHL  | CMD-C2D-C3D | -3.10 | 118.49      | 124.68   |
| 31  | A     | 812 | CLA  | O2D-CGD-O1D | -3.10 | 117.82      | 123.85   |
| 37  | b     | 521 | 0IE  | C4-C3-C2    | -3.10 | 117.46      | 120.16   |
| 30  | 5     | 305 | CHL  | CMD-C2D-C3D | -3.10 | 118.50      | 124.68   |
| 33  | g     | 520 | 0UR  | C48-C47-C46 | -3.10 | 119.47      | 125.92   |
| 31  | 6     | 318 | CLA  | C3B-C4B-NB  | -3.10 | 107.77      | 110.53   |
| 31  | A     | 840 | CLA  | C3B-C4B-NB  | -3.10 | 107.77      | 110.53   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | 7     | 306 | CHL  | CMA-C3A-C4A | -3.10 | 107.94      | 114.61   |
| 31  | 2     | 314 | CLA  | O2D-CGD-O1D | -3.10 | 117.82      | 123.85   |
| 30  | g     | 601 | CHL  | CMD-C2D-C3D | -3.09 | 118.50      | 124.68   |
| 31  | A     | 814 | CLA  | O2D-CGD-O1D | -3.09 | 117.83      | 123.85   |
| 31  | g     | 610 | CLA  | O2D-CGD-O1D | -3.09 | 117.83      | 123.85   |
| 30  | a     | 607 | CHL  | CMD-C2D-C3D | -3.09 | 118.50      | 124.68   |
| 30  | g     | 608 | CHL  | CMD-C2D-C3D | -3.09 | 118.50      | 124.68   |
| 30  | f     | 614 | CHL  | CMD-C2D-C3D | -3.09 | 118.50      | 124.68   |
| 30  | i     | 602 | CHL  | CMD-C2D-C3D | -3.09 | 118.50      | 124.68   |
| 31  | 9     | 302 | CLA  | O2D-CGD-O1D | -3.09 | 117.83      | 123.85   |
| 31  | h     | 604 | CLA  | O2D-CGD-O1D | -3.09 | 117.83      | 123.85   |
| 33  | i     | 520 | 0UR  | C43-C3-C4   | -3.09 | 121.38      | 125.03   |
| 32  | A     | 850 | 8CT  | C10-C03-C02 | -3.09 | 114.44      | 121.56   |
| 31  | A     | 815 | CLA  | O2D-CGD-O1D | -3.09 | 117.83      | 123.85   |
| 33  | e     | 520 | 0UR  | C28-C19-C18 | -3.09 | 109.28      | 112.83   |
| 30  | g     | 607 | CHL  | CMD-C2D-C3D | -3.09 | 118.51      | 124.68   |
| 37  | d     | 521 | 0IE  | C9-C10-C11  | 3.09  | 129.84      | 123.52   |
| 31  | K     | 101 | CLA  | C3B-C4B-NB  | -3.09 | 107.78      | 110.53   |
| 37  | h     | 522 | 0IE  | C6-C7-C8    | 3.09  | 123.86      | 119.01   |
| 32  | B     | 851 | 8CT  | C29-C28-C26 | -3.08 | 119.69      | 126.32   |
| 31  | 3     | 306 | CLA  | O2D-CGD-O1D | -3.08 | 117.84      | 123.85   |
| 31  | B     | 821 | CLA  | O2D-CGD-O1D | -3.08 | 117.84      | 123.85   |
| 30  | e     | 602 | CHL  | CMD-C2D-C3D | -3.08 | 118.52      | 124.68   |
| 32  | 3     | 402 | 8CT  | C19-C18-C17 | -3.08 | 117.21      | 123.52   |
| 32  | 7     | 402 | 8CT  | C30-C29-C28 | -3.08 | 119.78      | 124.58   |
| 31  | B     | 830 | CLA  | O2D-CGD-O1D | -3.08 | 117.85      | 123.85   |
| 30  | d     | 614 | CHL  | CAA-C2A-C3A | -3.08 | 109.16      | 116.23   |
| 30  | f     | 608 | CHL  | C1-C2-C3    | -3.08 | 121.78      | 126.76   |
| 31  | A     | 830 | CLA  | CMB-C2B-C1B | -3.08 | 120.73      | 125.42   |
| 37  | i     | 522 | 0IE  | C6-C7-C8    | 3.08  | 123.85      | 119.01   |
| 32  | 1     | 402 | 8CT  | C24-C23-C21 | -3.08 | 117.92      | 126.36   |
| 30  | 8     | 315 | CHL  | CMD-C2D-C3D | -3.08 | 118.53      | 124.68   |
| 30  | d     | 608 | CHL  | CMD-C2D-C3D | -3.08 | 118.53      | 124.68   |
| 30  | 5     | 301 | CHL  | C4-C3-C5    | 3.08  | 119.75      | 116.13   |
| 31  | 4     | 303 | CLA  | O2D-CGD-O1D | -3.08 | 117.86      | 123.85   |
| 31  | B     | 807 | CLA  | C3B-C4B-NB  | -3.08 | 107.78      | 110.53   |
| 31  | K     | 105 | CLA  | C3B-C4B-NB  | -3.08 | 107.78      | 110.53   |
| 30  | 2     | 313 | CHL  | O2A-CGA-CBA | 3.07  | 121.21      | 111.83   |
| 33  | b     | 520 | 0UR  | C28-C19-C18 | -3.07 | 109.29      | 112.83   |
| 31  | B     | 801 | CLA  | O2D-CGD-O1D | -3.07 | 117.87      | 123.85   |
| 31  | 4     | 303 | CLA  | C3B-C4B-NB  | -3.07 | 107.79      | 110.53   |
| 30  | 1     | 302 | CHL  | CBC-CAC-C3C | -3.07 | 108.47      | 112.87   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | 7     | 307 | CHL  | C1B-CHB-C4A | 3.07  | 123.30      | 121.32   |
| 37  | h     | 522 | 0IE  | C9-C10-C11  | 3.07  | 129.80      | 123.52   |
| 30  | 3     | 302 | CHL  | O2A-CGA-CBA | 3.07  | 121.20      | 111.83   |
| 30  | i     | 605 | CHL  | CMD-C2D-C3D | -3.07 | 118.55      | 124.68   |
| 31  | 3     | 306 | CLA  | C3B-C4B-NB  | -3.07 | 107.79      | 110.53   |
| 31  | 5     | 309 | CLA  | O2D-CGD-O1D | -3.07 | 117.87      | 123.85   |
| 31  | A     | 820 | CLA  | C3B-C4B-NB  | -3.07 | 107.79      | 110.53   |
| 31  | A     | 831 | CLA  | C3B-C4B-NB  | -3.07 | 107.79      | 110.53   |
| 31  | 7     | 312 | CLA  | O2D-CGD-O1D | -3.07 | 117.87      | 123.85   |
| 30  | 7     | 306 | CHL  | O1D-CGD-CBD | -3.07 | 120.07      | 124.72   |
| 33  | 6     | 501 | 0UR  | C36-C28-C19 | 3.07  | 114.19      | 109.55   |
| 31  | A     | 823 | CLA  | O2D-CGD-O1D | -3.07 | 117.88      | 123.85   |
| 31  | 3     | 313 | CLA  | C3B-C4B-NB  | -3.06 | 107.79      | 110.53   |
| 30  | 5     | 306 | CHL  | CMD-C2D-C3D | -3.06 | 118.56      | 124.68   |
| 30  | 6     | 302 | CHL  | OMC-CMC-C2C | -3.06 | 119.80      | 125.12   |
| 31  | A     | 809 | CLA  | C3B-C4B-NB  | -3.06 | 107.80      | 110.53   |
| 30  | 2     | 306 | CHL  | O1D-CGD-CBD | -3.06 | 120.08      | 124.72   |
| 31  | B     | 813 | CLA  | O2D-CGD-O1D | -3.06 | 117.89      | 123.85   |
| 30  | 8     | 306 | CHL  | CMD-C2D-C3D | -3.06 | 118.57      | 124.68   |
| 31  | g     | 612 | CLA  | O2D-CGD-O1D | -3.06 | 117.90      | 123.85   |
| 30  | a     | 614 | CHL  | CAA-C2A-C3A | -3.06 | 109.22      | 116.23   |
| 31  | 7     | 308 | CLA  | C3B-C4B-NB  | -3.06 | 107.80      | 110.53   |
| 31  | A     | 837 | CLA  | O2D-CGD-O1D | -3.06 | 117.90      | 123.85   |
| 31  | B     | 815 | CLA  | O2D-CGD-O1D | -3.06 | 117.90      | 123.85   |
| 30  | 6     | 313 | CHL  | O1D-CGD-CBD | -3.06 | 120.09      | 124.72   |
| 30  | h     | 607 | CHL  | CMD-C2D-C3D | -3.06 | 118.58      | 124.68   |
| 30  | 2     | 319 | CHL  | CMD-C2D-C3D | -3.05 | 118.58      | 124.68   |
| 31  | 3     | 310 | CLA  | C3B-C4B-NB  | -3.05 | 107.81      | 110.53   |
| 31  | A     | 824 | CLA  | C3B-C4B-NB  | -3.05 | 107.81      | 110.53   |
| 31  | A     | 841 | CLA  | C3B-C4B-NB  | -3.05 | 107.81      | 110.53   |
| 31  | 3     | 312 | CLA  | O2D-CGD-O1D | -3.05 | 117.91      | 123.85   |
| 32  | 1     | 402 | 8CT  | C04-C03-C02 | -3.05 | 118.47      | 122.64   |
| 30  | 6     | 315 | CHL  | CBC-CAC-C3C | -3.05 | 108.50      | 112.87   |
| 31  | B     | 816 | CLA  | O2D-CGD-O1D | -3.05 | 117.91      | 123.85   |
| 31  | A     | 816 | CLA  | O2D-CGD-O1D | -3.05 | 117.91      | 123.85   |
| 30  | i     | 614 | CHL  | CAA-C2A-C3A | -3.05 | 109.24      | 116.23   |
| 32  | G     | 104 | 8CT  | C29-C28-C26 | -3.05 | 119.76      | 126.32   |
| 30  | 8     | 313 | CHL  | C1-C2-C3    | -3.05 | 121.20      | 126.20   |
| 30  | f     | 608 | CHL  | CMD-C2D-C3D | -3.05 | 118.59      | 124.68   |
| 33  | 9     | 502 | 0UR  | C15-C14-C13 | -3.05 | 114.37      | 123.20   |
| 31  | A     | 829 | CLA  | C1-C2-C3    | -3.05 | 121.20      | 126.20   |
| 30  | e     | 607 | CHL  | CMD-C2D-C3D | -3.05 | 118.59      | 124.68   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | B     | 851 | 8CT  | C18-C19-C20 | -3.05 | 117.29      | 123.52   |
| 33  | 9     | 502 | 0UR  | C9-C10-C11  | -3.05 | 117.29      | 123.52   |
| 37  | g     | 521 | 0IE  | C9-C10-C11  | 3.04  | 129.75      | 123.52   |
| 33  | 5     | 501 | 0UR  | C5-C4-C3    | -3.04 | 123.28      | 126.92   |
| 32  | J     | 104 | 8CT  | C35-C30-C29 | -3.04 | 109.33      | 112.83   |
| 31  | A     | 828 | CLA  | C1-C2-C3    | -3.04 | 121.21      | 126.20   |
| 37  | e     | 521 | 0IE  | C9-C10-C11  | 3.04  | 129.74      | 123.52   |
| 33  | 0     | 502 | 0UR  | C10-C11-C12 | -3.04 | 123.01      | 127.28   |
| 31  | B     | 832 | CLA  | O2D-CGD-O1D | -3.04 | 117.93      | 123.85   |
| 31  | 3     | 312 | CLA  | C3B-C4B-NB  | -3.04 | 107.82      | 110.53   |
| 30  | 2     | 306 | CHL  | CMD-C2D-C3D | -3.04 | 118.61      | 124.68   |
| 30  | a     | 602 | CHL  | CMD-C2D-C3D | -3.04 | 118.61      | 124.68   |
| 33  | 4     | 502 | 0UR  | C14-C15-C16 | -3.04 | 123.02      | 127.28   |
| 31  | 4     | 310 | CLA  | C3B-C4B-NB  | -3.04 | 107.82      | 110.53   |
| 33  | 4     | 501 | 0UR  | C34-C27-C1  | -3.04 | 120.66      | 124.45   |
| 31  | B     | 840 | CLA  | O2D-CGD-O1D | -3.04 | 117.93      | 123.85   |
| 37  | e     | 522 | 0IE  | C9-C10-C11  | 3.04  | 129.74      | 123.52   |
| 37  | c     | 521 | 0IE  | C20-C3-C2   | 3.04  | 121.98      | 115.01   |
| 30  | 5     | 313 | CHL  | CMD-C2D-C3D | -3.04 | 118.61      | 124.68   |
| 33  | g     | 520 | 0UR  | O44-C45-C46 | 3.04  | 119.05      | 111.55   |
| 30  | f     | 607 | CHL  | CMD-C2D-C3D | -3.04 | 118.62      | 124.68   |
| 32  | B     | 845 | 8CT  | C01-C02-C07 | 3.04  | 120.07      | 113.60   |
| 32  | 7     | 402 | 8CT  | C25-C24-C23 | -3.04 | 114.41      | 123.20   |
| 31  | F     | 301 | CLA  | O2D-CGD-O1D | -3.04 | 117.94      | 123.85   |
| 31  | g     | 613 | CLA  | O2D-CGD-O1D | -3.04 | 117.94      | 123.85   |
| 31  | 1     | 309 | CLA  | C3B-C4B-NB  | -3.03 | 107.82      | 110.53   |
| 31  | 6     | 318 | CLA  | O2D-CGD-O1D | -3.03 | 117.94      | 123.85   |
| 31  | B     | 828 | CLA  | O2D-CGD-O1D | -3.03 | 117.94      | 123.85   |
| 33  | f     | 520 | 0UR  | C36-C28-C19 | 3.03  | 114.14      | 109.55   |
| 31  | 2     | 309 | CLA  | C3B-C4B-NB  | -3.03 | 107.82      | 110.53   |
| 31  | 7     | 312 | CLA  | C3B-C4B-NB  | -3.03 | 107.82      | 110.53   |
| 31  | 2     | 312 | CLA  | O2D-CGD-O1D | -3.03 | 117.95      | 123.85   |
| 37  | a     | 522 | 0IE  | C6-C7-C8    | 3.03  | 123.78      | 119.01   |
| 31  | A     | 823 | CLA  | C3B-C4B-NB  | -3.03 | 107.83      | 110.53   |
| 31  | M     | 101 | CLA  | O2D-CGD-O1D | -3.03 | 117.95      | 123.85   |
| 33  | 8     | 501 | 0UR  | C28-C19-C18 | -3.03 | 109.34      | 112.83   |
| 30  | 1     | 306 | CHL  | O2A-CGA-CBA | 3.03  | 121.07      | 111.83   |
| 30  | 1     | 313 | CHL  | O2A-CGA-CBA | 3.03  | 121.07      | 111.83   |
| 30  | 6     | 307 | CHL  | CMD-C2D-C3D | -3.03 | 118.63      | 124.68   |
| 31  | 9     | 311 | CLA  | C3B-C4B-NB  | -3.03 | 107.83      | 110.53   |
| 33  | c     | 520 | 0UR  | C48-C47-C46 | -3.03 | 119.61      | 125.92   |
| 31  | 3     | 318 | CLA  | O2D-CGD-O1D | -3.03 | 117.95      | 123.85   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | a     | 608 | CHL  | CMD-C2D-C3D | -3.03 | 118.63      | 124.68   |
| 31  | A     | 832 | CLA  | O2D-CGD-O1D | -3.03 | 117.96      | 123.85   |
| 30  | e     | 605 | CHL  | CMD-C2D-C3D | -3.02 | 118.64      | 124.68   |
| 31  | B     | 817 | CLA  | O2D-CGD-O1D | -3.02 | 117.96      | 123.85   |
| 37  | 3     | 502 | 0IE  | C4-C3-C2    | -3.02 | 117.53      | 120.16   |
| 31  | G     | 103 | CLA  | C3B-C4B-NB  | -3.02 | 107.83      | 110.53   |
| 31  | H     | 205 | CLA  | O2D-CGD-O1D | -3.02 | 117.97      | 123.85   |
| 33  | 8     | 501 | 0UR  | O44-C45-C46 | 3.02  | 119.01      | 111.55   |
| 32  | B     | 848 | 8CT  | C04-C03-C02 | -3.02 | 118.51      | 122.64   |
| 31  | 0     | 312 | CLA  | C3B-C4B-NB  | -3.02 | 107.83      | 110.53   |
| 33  | 2     | 502 | 0UR  | O44-C45-C46 | 3.02  | 119.00      | 111.55   |
| 31  | L     | 204 | CLA  | O2D-CGD-O1D | -3.02 | 117.97      | 123.85   |
| 32  | B     | 844 | 8CT  | C18-C17-C16 | -3.02 | 123.05      | 127.28   |
| 33  | 5     | 501 | 0UR  | C14-C15-C16 | -3.02 | 123.05      | 127.28   |
| 37  | 7     | 502 | 0IE  | C9-C10-C11  | 3.02  | 129.69      | 123.52   |
| 30  | 0     | 305 | CHL  | O1D-CGD-CBD | -3.02 | 120.15      | 124.72   |
| 32  | 3     | 403 | 8CT  | C11-C10-C03 | -3.02 | 118.94      | 127.00   |
| 30  | 6     | 315 | CHL  | CMD-C2D-C3D | -3.02 | 118.66      | 124.68   |
| 30  | h     | 606 | CHL  | CMD-C2D-C3D | -3.02 | 118.66      | 124.68   |
| 30  | g     | 614 | CHL  | CAA-C2A-C3A | -3.02 | 109.31      | 116.23   |
| 30  | a     | 601 | CHL  | CBC-CAC-C3C | -3.01 | 108.56      | 112.87   |
| 31  | 0     | 308 | CLA  | C3B-C4B-NB  | -3.01 | 107.84      | 110.53   |
| 31  | A     | 835 | CLA  | C3B-C4B-NB  | -3.01 | 107.84      | 110.53   |
| 30  | 4     | 313 | CHL  | O1D-CGD-CBD | -3.01 | 120.16      | 124.72   |
| 31  | A     | 853 | CLA  | C1-C2-C3    | -3.01 | 121.26      | 126.20   |
| 31  | 0     | 309 | CLA  | O2D-CGD-O1D | -3.01 | 117.99      | 123.85   |
| 30  | 1     | 302 | CHL  | OMC-CMC-C2C | -3.01 | 119.89      | 125.12   |
| 33  | h     | 520 | 0UR  | C19-C18-C17 | -3.01 | 119.89      | 124.58   |
| 33  | 3     | 501 | 0UR  | C34-C27-C1  | -3.01 | 120.69      | 124.45   |
| 31  | 8     | 312 | CLA  | C3B-C4B-NB  | -3.01 | 107.84      | 110.53   |
| 37  | d     | 522 | 0IE  | C21-C7-C8   | -3.01 | 117.94      | 122.82   |
| 37  | h     | 521 | 0IE  | C6-C7-C8    | 3.01  | 123.74      | 119.01   |
| 31  | 6     | 310 | CLA  | O2D-CGD-O1D | -3.01 | 117.99      | 123.85   |
| 37  | i     | 522 | 0IE  | C9-C10-C11  | 3.01  | 129.67      | 123.52   |
| 32  | 9     | 401 | 8CT  | C01-C02-C07 | 3.00  | 120.00      | 113.60   |
| 31  | B     | 820 | CLA  | O2D-CGD-O1D | -3.00 | 118.00      | 123.85   |
| 30  | g     | 602 | CHL  | CMD-C2D-C3D | -3.00 | 118.68      | 124.68   |
| 31  | H     | 202 | CLA  | C3B-C4B-NB  | -3.00 | 107.85      | 110.53   |
| 30  | 5     | 302 | CHL  | OMC-CMC-C2C | -3.00 | 119.90      | 125.12   |
| 30  | d     | 601 | CHL  | CMD-C2D-C3D | -3.00 | 118.68      | 124.68   |
| 31  | G     | 101 | CLA  | O2D-CGD-O1D | -3.00 | 118.00      | 123.85   |
| 30  | g     | 602 | CHL  | C4-C3-C5    | 3.00  | 119.66      | 116.13   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 37  | b     | 522 | 0IE  | C6-C7-C8    | 3.00  | 123.73      | 119.01   |
| 31  | 7     | 318 | CLA  | O2D-CGD-O1D | -3.00 | 118.01      | 123.85   |
| 30  | 7     | 307 | CHL  | CBC-CAC-C3C | -3.00 | 108.58      | 112.87   |
| 32  | 7     | 405 | 8CT  | C29-C28-C26 | -3.00 | 119.87      | 126.32   |
| 31  | 2     | 303 | CLA  | O2D-CGD-O1D | -3.00 | 118.01      | 123.85   |
| 30  | 6     | 302 | CHL  | O2A-CGA-CBA | 3.00  | 120.98      | 111.83   |
| 37  | e     | 522 | 0IE  | C21-C7-C8   | -3.00 | 117.95      | 122.82   |
| 32  | L     | 206 | 8CT  | C14-C15-C16 | -3.00 | 118.14      | 126.36   |
| 31  | A     | 803 | CLA  | C3B-C4B-NB  | -3.00 | 107.85      | 110.53   |
| 30  | 7     | 301 | CHL  | CMD-C2D-C3D | -3.00 | 118.69      | 124.68   |
| 31  | A     | 813 | CLA  | C3B-C4B-NB  | -3.00 | 107.85      | 110.53   |
| 31  | G     | 102 | CLA  | O2D-CGD-O1D | -3.00 | 118.01      | 123.85   |
| 30  | c     | 607 | CHL  | CMD-C2D-C3D | -3.00 | 118.69      | 124.68   |
| 31  | 4     | 311 | CLA  | O2D-CGD-O1D | -3.00 | 118.01      | 123.85   |
| 31  | 3     | 304 | CLA  | O2D-CGD-O1D | -3.00 | 118.01      | 123.85   |
| 30  | h     | 602 | CHL  | CMD-C2D-C3D | -3.00 | 118.69      | 124.68   |
| 30  | e     | 614 | CHL  | CAA-C2A-C3A | -3.00 | 109.36      | 116.23   |
| 32  | B     | 851 | 8CT  | C11-C10-C03 | -3.00 | 119.00      | 127.00   |
| 37  | d     | 521 | 0IE  | C20-C3-C2   | 3.00  | 121.89      | 115.01   |
| 31  | 3     | 310 | CLA  | O2D-CGD-O1D | -3.00 | 118.02      | 123.85   |
| 31  | A     | 805 | CLA  | O2D-CGD-O1D | -3.00 | 118.02      | 123.85   |
| 31  | B     | 836 | CLA  | O2D-CGD-O1D | -3.00 | 118.02      | 123.85   |
| 32  | A     | 846 | 8CT  | C25-C24-C23 | -3.00 | 114.52      | 123.20   |
| 31  | 8     | 304 | CLA  | O2D-CGD-O1D | -3.00 | 118.02      | 123.85   |
| 32  | B     | 851 | 8CT  | C01-C02-C07 | 2.99  | 119.98      | 113.60   |
| 31  | A     | 820 | CLA  | O2D-CGD-O1D | -2.99 | 118.02      | 123.85   |
| 30  | i     | 608 | CHL  | CMD-C2D-C3D | -2.99 | 118.70      | 124.68   |
| 31  | A     | 843 | CLA  | O2D-CGD-O1D | -2.99 | 118.02      | 123.85   |
| 34  | 3     | 601 | LHG  | O8-C23-C24  | 2.99  | 120.96      | 111.83   |
| 30  | 0     | 301 | CHL  | C4-C3-C5    | 2.99  | 119.65      | 116.13   |
| 32  | B     | 846 | 8CT  | C22-C21-C23 | 2.99  | 122.66      | 118.09   |
| 37  | f     | 522 | 0IE  | C9-C10-C11  | 2.99  | 129.64      | 123.52   |
| 32  | B     | 843 | 8CT  | C22-C21-C20 | -2.99 | 117.97      | 122.82   |
| 32  | O     | 205 | 8CT  | C35-C30-C29 | -2.99 | 109.39      | 112.83   |
| 31  | B     | 801 | CLA  | CMB-C2B-C1B | -2.99 | 120.86      | 125.42   |
| 31  | J     | 103 | CLA  | C3B-C4B-NB  | -2.99 | 107.86      | 110.53   |
| 33  | 6     | 501 | 0UR  | C18-C17-C16 | -2.99 | 119.89      | 126.32   |
| 30  | 6     | 308 | CHL  | O2A-CGA-CBA | 2.99  | 120.95      | 111.83   |
| 32  | 6     | 402 | 8CT  | C40-C12-C13 | -2.99 | 117.97      | 122.82   |
| 31  | G     | 101 | CLA  | C3B-C4B-NB  | -2.99 | 107.86      | 110.53   |
| 31  | A     | 819 | CLA  | C3B-C4B-NB  | -2.99 | 107.86      | 110.53   |
| 32  | A     | 849 | 8CT  | C35-C30-C29 | -2.98 | 109.39      | 112.83   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | i     | 607 | CHL  | CMD-C2D-C3D | -2.98 | 118.72      | 124.68   |
| 30  | g     | 601 | CHL  | C1-C2-C3    | -2.98 | 121.31      | 126.20   |
| 32  | A     | 850 | 8CT  | C25-C24-C23 | -2.98 | 114.56      | 123.20   |
| 32  | A     | 850 | 8CT  | C11-C12-C13 | -2.98 | 114.32      | 119.01   |
| 32  | J     | 101 | 8CT  | C01-C02-C07 | 2.98  | 119.95      | 113.60   |
| 31  | 9     | 312 | CLA  | O2D-CGD-O1D | -2.98 | 118.05      | 123.85   |
| 31  | 6     | 310 | CLA  | C3B-C4B-NB  | -2.98 | 107.87      | 110.53   |
| 32  | G     | 104 | 8CT  | C14-C15-C16 | -2.98 | 118.20      | 126.36   |
| 33  | a     | 520 | 0UR  | C14-C15-C16 | -2.98 | 123.10      | 127.28   |
| 32  | G     | 104 | 8CT  | C39-C16-C17 | -2.98 | 117.99      | 122.82   |
| 32  | J     | 104 | 8CT  | C39-C16-C17 | -2.98 | 117.99      | 122.82   |
| 31  | 2     | 310 | CLA  | O2D-CGD-O1D | -2.98 | 118.05      | 123.85   |
| 31  | A     | 841 | CLA  | O2D-CGD-O1D | -2.98 | 118.05      | 123.85   |
| 31  | A     | 802 | CLA  | O2D-CGD-O1D | -2.98 | 118.05      | 123.85   |
| 30  | 8     | 301 | CHL  | CMD-C2D-C3D | -2.98 | 118.73      | 124.68   |
| 30  | b     | 614 | CHL  | CAA-C2A-C3A | -2.98 | 109.41      | 116.23   |
| 32  | B     | 804 | 8CT  | C19-C20-C21 | -2.98 | 123.10      | 127.28   |
| 37  | d     | 522 | 0IE  | C20-C3-C4   | -2.98 | 120.61      | 124.72   |
| 32  | B     | 848 | 8CT  | C27-C26-C25 | -2.98 | 118.00      | 122.82   |
| 30  | e     | 602 | CHL  | CBC-CAC-C3C | -2.98 | 108.61      | 112.87   |
| 30  | c     | 601 | CHL  | CMD-C2D-C3D | -2.98 | 118.74      | 124.68   |
| 31  | c     | 611 | CLA  | C3B-C4B-NB  | -2.97 | 107.88      | 110.53   |
| 37  | 7     | 502 | 0IE  | C4-C3-C2    | -2.97 | 117.57      | 120.16   |
| 31  | A     | 852 | CLA  | O2D-CGD-O1D | -2.97 | 118.06      | 123.85   |
| 31  | a     | 613 | CLA  | C3B-C4B-NB  | -2.97 | 107.88      | 110.53   |
| 31  | B     | 814 | CLA  | O2D-CGD-O1D | -2.97 | 118.06      | 123.85   |
| 31  | B     | 829 | CLA  | O2D-CGD-O1D | -2.97 | 118.06      | 123.85   |
| 31  | a     | 613 | CLA  | O2D-CGD-O1D | -2.97 | 118.06      | 123.85   |
| 30  | 9     | 301 | CHL  | O1D-CGD-CBD | -2.97 | 120.22      | 124.72   |
| 31  | d     | 611 | CLA  | O2D-CGD-O1D | -2.97 | 118.06      | 123.85   |
| 33  | 4     | 501 | 0UR  | C5-C4-C3    | -2.97 | 123.36      | 126.92   |
| 31  | 9     | 312 | CLA  | C3B-C4B-NB  | -2.97 | 107.88      | 110.53   |
| 31  | O     | 201 | CLA  | C3B-C4B-NB  | -2.97 | 107.88      | 110.53   |
| 30  | 9     | 305 | CHL  | O2A-CGA-CBA | 2.97  | 120.89      | 111.83   |
| 33  | 3     | 501 | 0UR  | O44-C43-C3  | 2.97  | 116.82      | 109.09   |
| 30  | 5     | 301 | CHL  | CMD-C2D-C3D | -2.97 | 118.75      | 124.68   |
| 32  | O     | 205 | 8CT  | C24-C25-C26 | -2.97 | 123.11      | 127.28   |
| 30  | 4     | 313 | CHL  | CBC-CAC-C3C | -2.97 | 108.62      | 112.87   |
| 31  | A     | 829 | CLA  | O2D-CGD-O1D | -2.97 | 118.07      | 123.85   |
| 30  | e     | 614 | CHL  | CMD-C2D-C3D | -2.97 | 118.75      | 124.68   |
| 31  | B     | 811 | CLA  | C3B-C4B-NB  | -2.97 | 107.88      | 110.53   |
| 31  | c     | 613 | CLA  | O2D-CGD-O1D | -2.97 | 118.07      | 123.85   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | 6     | 402 | 8CT  | C15-C16-C17 | 2.97  | 123.68      | 119.01   |
| 31  | O     | 202 | CLA  | C3A-C2A-C1A | -2.97 | 103.27      | 106.30   |
| 32  | G     | 104 | 8CT  | C01-C02-C07 | 2.97  | 119.92      | 113.60   |
| 39  | A     | 857 | CL0  | CHA-C1A-C2A | -2.97 | 126.34      | 133.31   |
| 37  | d     | 522 | 0IE  | C14-C15-C16 | 2.97  | 131.44      | 127.28   |
| 31  | c     | 610 | CLA  | C3B-C4B-NB  | -2.97 | 107.88      | 110.53   |
| 30  | c     | 614 | CHL  | CAA-C2A-C3A | -2.96 | 109.43      | 116.23   |
| 31  | 8     | 310 | CLA  | O2D-CGD-O1D | -2.96 | 118.08      | 123.85   |
| 31  | 7     | 310 | CLA  | C3B-C4B-NB  | -2.96 | 107.89      | 110.53   |
| 31  | L     | 207 | CLA  | C3B-C4B-NB  | -2.96 | 107.89      | 110.53   |
| 31  | g     | 610 | CLA  | C3B-C4B-NB  | -2.96 | 107.89      | 110.53   |
| 33  | 4     | 502 | 0UR  | O44-C45-C46 | 2.96  | 118.86      | 111.55   |
| 31  | 5     | 304 | CLA  | O2D-CGD-O1D | -2.96 | 118.08      | 123.85   |
| 31  | 8     | 312 | CLA  | O2D-CGD-O1D | -2.96 | 118.08      | 123.85   |
| 30  | 7     | 305 | CHL  | CMD-C2D-C3D | -2.96 | 118.77      | 124.68   |
| 33  | 1     | 502 | 0UR  | C9-C10-C11  | -2.96 | 117.47      | 123.52   |
| 31  | B     | 850 | CLA  | C3B-C4B-NB  | -2.96 | 107.89      | 110.53   |
| 38  | A     | 842 | PQN  | C11-C12-C13 | -2.96 | 121.74      | 126.83   |
| 35  | 0     | 603 | SQD  | O6-C1-C2    | 2.96  | 112.76      | 108.27   |
| 32  | J     | 104 | 8CT  | C22-C21-C23 | 2.96  | 122.60      | 118.09   |
| 31  | 5     | 314 | CLA  | C3B-C4B-NB  | -2.96 | 107.89      | 110.53   |
| 31  | 1     | 303 | CLA  | O2D-CGD-O1D | -2.96 | 118.09      | 123.85   |
| 31  | 9     | 303 | CLA  | O2D-CGD-O1D | -2.96 | 118.09      | 123.85   |
| 33  | 3     | 501 | 0UR  | C28-C19-C18 | -2.95 | 109.43      | 112.83   |
| 31  | B     | 817 | CLA  | CHB-C4A-NA  | 2.95  | 128.66      | 124.40   |
| 33  | 4     | 502 | 0UR  | C5-C4-C3    | -2.95 | 123.39      | 126.92   |
| 30  | 2     | 301 | CHL  | CMD-C2D-C3D | -2.95 | 118.78      | 124.68   |
| 34  | 6     | 603 | LHG  | O8-C23-C24  | 2.95  | 120.84      | 111.83   |
| 30  | e     | 614 | CHL  | OMC-CMC-C2C | -2.95 | 119.99      | 125.12   |
| 31  | b     | 613 | CLA  | O2D-CGD-O1D | -2.95 | 118.10      | 123.85   |
| 33  | 6     | 502 | 0UR  | C10-C11-C12 | -2.95 | 123.14      | 127.28   |
| 30  | 0     | 306 | CHL  | CMD-C2D-C3D | -2.95 | 118.78      | 124.68   |
| 30  | 4     | 319 | CHL  | O2D-CGD-O1D | -2.95 | 118.10      | 123.85   |
| 33  | e     | 520 | 0UR  | C34-C27-C1  | -2.95 | 120.77      | 124.45   |
| 31  | a     | 611 | CLA  | C3B-C4B-NB  | -2.95 | 107.90      | 110.53   |
| 30  | 1     | 306 | CHL  | CMD-C2D-C3D | -2.95 | 118.79      | 124.68   |
| 37  | f     | 522 | 0IE  | C21-C7-C8   | -2.95 | 118.04      | 122.82   |
| 37  | h     | 522 | 0IE  | C21-C7-C8   | -2.95 | 118.04      | 122.82   |
| 31  | A     | 810 | CLA  | O2D-CGD-O1D | -2.95 | 118.11      | 123.85   |
| 32  | F     | 302 | 8CT  | C05-C04-C03 | 2.95  | 114.72      | 110.44   |
| 31  | A     | 815 | CLA  | C3B-C4B-NB  | -2.95 | 107.90      | 110.53   |
| 31  | A     | 810 | CLA  | C1-C2-C3    | -2.95 | 121.37      | 126.20   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 9     | 304 | CLA  | O2D-CGD-O1D | -2.95 | 118.11      | 123.85   |
| 30  | 9     | 313 | CHL  | CBC-CAC-C3C | -2.95 | 108.66      | 112.87   |
| 31  | 0     | 310 | CLA  | O2D-CGD-O1D | -2.95 | 118.11      | 123.85   |
| 30  | h     | 607 | CHL  | CBC-CAC-C3C | -2.94 | 108.66      | 112.87   |
| 31  | A     | 826 | CLA  | O2D-CGD-O1D | -2.94 | 118.12      | 123.85   |
| 32  | A     | 849 | 8CT  | C29-C28-C26 | -2.94 | 119.99      | 126.32   |
| 30  | 8     | 306 | CHL  | C1-C2-C3    | -2.94 | 122.00      | 126.76   |
| 31  | f     | 611 | CLA  | O2D-CGD-O1D | -2.94 | 118.12      | 123.85   |
| 31  | B     | 823 | CLA  | O2D-CGD-O1D | -2.94 | 118.12      | 123.85   |
| 30  | 7     | 313 | CHL  | CMD-C2D-C3D | -2.94 | 118.81      | 124.68   |
| 30  | f     | 606 | CHL  | O1D-CGD-CBD | -2.94 | 120.26      | 124.72   |
| 30  | h     | 609 | CHL  | O1D-CGD-CBD | -2.94 | 120.26      | 124.72   |
| 31  | b     | 610 | CLA  | C3B-C4B-NB  | -2.94 | 107.91      | 110.53   |
| 31  | A     | 832 | CLA  | C3B-C4B-NB  | -2.94 | 107.91      | 110.53   |
| 31  | 7     | 309 | CLA  | C3B-C4B-NB  | -2.94 | 107.91      | 110.53   |
| 30  | b     | 602 | CHL  | C4-C3-C5    | 2.94  | 120.33      | 115.23   |
| 31  | A     | 821 | CLA  | O2D-CGD-O1D | -2.94 | 118.13      | 123.85   |
| 30  | 9     | 306 | CHL  | CBC-CAC-C3C | -2.94 | 108.67      | 112.87   |
| 31  | B     | 822 | CLA  | O2D-CGD-O1D | -2.94 | 118.13      | 123.85   |
| 30  | c     | 606 | CHL  | CMD-C2D-C3D | -2.94 | 118.82      | 124.68   |
| 33  | 6     | 501 | 0UR  | C9-C8-C7    | -2.93 | 123.16      | 127.28   |
| 33  | i     | 520 | 0UR  | C4-C3-C2    | -2.93 | 117.60      | 120.16   |
| 30  | 9     | 301 | CHL  | CMD-C2D-C3D | -2.93 | 118.82      | 124.68   |
| 31  | f     | 612 | CLA  | O2D-CGD-O1D | -2.93 | 118.14      | 123.85   |
| 33  | 6     | 502 | 0UR  | C14-C15-C16 | -2.93 | 123.17      | 127.28   |
| 31  | 0     | 310 | CLA  | C3B-C4B-NB  | -2.93 | 107.91      | 110.53   |
| 31  | A     | 852 | CLA  | C3B-C4B-NB  | -2.93 | 107.91      | 110.53   |
| 30  | 4     | 307 | CHL  | O2A-CGA-CBA | 2.93  | 120.78      | 111.83   |
| 30  | e     | 602 | CHL  | O2A-CGA-CBA | 2.93  | 120.78      | 111.83   |
| 30  | 1     | 313 | CHL  | CMD-C2D-C3D | -2.93 | 118.82      | 124.68   |
| 30  | 6     | 306 | CHL  | O2A-CGA-CBA | 2.93  | 120.77      | 111.83   |
| 37  | i     | 522 | 0IE  | C21-C7-C8   | -2.93 | 118.07      | 122.82   |
| 31  | A     | 807 | CLA  | O2D-CGD-O1D | -2.93 | 118.14      | 123.85   |
| 30  | 8     | 308 | CHL  | CMD-C2D-C3D | -2.93 | 118.83      | 124.68   |
| 30  | 7     | 307 | CHL  | CMD-C2D-C3D | -2.93 | 118.83      | 124.68   |
| 31  | 5     | 310 | CLA  | C3B-C4B-NB  | -2.93 | 107.92      | 110.53   |
| 31  | 6     | 312 | CLA  | C3B-C4B-NB  | -2.93 | 107.92      | 110.53   |
| 31  | L     | 203 | CLA  | C3B-C4B-NB  | -2.93 | 107.92      | 110.53   |
| 34  | A     | 845 | LHG  | O8-C23-C24  | 2.93  | 120.04      | 111.15   |
| 30  | 8     | 308 | CHL  | CBC-CAC-C3C | -2.93 | 108.68      | 112.87   |
| 30  | d     | 601 | CHL  | O1D-CGD-CBD | -2.93 | 120.28      | 124.72   |
| 37  | h     | 521 | 0IE  | C21-C7-C8   | -2.93 | 118.07      | 122.82   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 4     | 312 | CLA  | O2D-CGD-O1D | -2.93 | 118.15      | 123.85   |
| 33  | d     | 520 | 0UR  | C28-C19-C18 | -2.93 | 109.46      | 112.83   |
| 30  | 7     | 301 | CHL  | O2A-CGA-CBA | 2.93  | 120.76      | 111.83   |
| 31  | 6     | 304 | CLA  | O2D-CGD-O1D | -2.93 | 118.15      | 123.85   |
| 30  | 7     | 302 | CHL  | O2A-CGA-CBA | 2.93  | 120.75      | 111.83   |
| 32  | 7     | 404 | 8CT  | C27-C26-C25 | -2.93 | 118.08      | 122.82   |
| 30  | 4     | 308 | CHL  | CMD-C2D-C3D | -2.92 | 118.84      | 124.68   |
| 31  | A     | 804 | CLA  | CHB-C4A-NA  | 2.92  | 128.62      | 124.40   |
| 31  | 7     | 316 | CLA  | O2D-CGD-O1D | -2.92 | 118.16      | 123.85   |
| 33  | 7     | 501 | 0UR  | C48-C47-C46 | -2.92 | 119.83      | 125.92   |
| 31  | 7     | 308 | CLA  | O2D-CGD-O1D | -2.92 | 118.16      | 123.85   |
| 37  | d     | 522 | 0IE  | C23-C16-C15 | -2.92 | 118.08      | 122.82   |
| 30  | 7     | 302 | CHL  | CMD-C2D-C3D | -2.92 | 118.84      | 124.68   |
| 33  | 9     | 502 | 0UR  | C10-C11-C12 | -2.92 | 123.18      | 127.28   |
| 30  | 7     | 306 | CHL  | O2A-CGA-CBA | 2.92  | 120.74      | 111.83   |
| 31  | a     | 610 | CLA  | O2D-CGD-O1D | -2.92 | 118.16      | 123.85   |
| 31  | B     | 831 | CLA  | O2D-CGD-O1D | -2.92 | 118.17      | 123.85   |
| 39  | A     | 857 | CL0  | CBC-CAC-C3C | -2.92 | 108.69      | 112.87   |
| 31  | 1     | 312 | CLA  | O2D-CGD-O1D | -2.92 | 118.17      | 123.85   |
| 30  | f     | 601 | CHL  | C4-C3-C5    | 2.92  | 120.29      | 115.23   |
| 32  | A     | 846 | 8CT  | C14-C15-C16 | -2.92 | 118.36      | 126.36   |
| 32  | L     | 209 | 8CT  | C04-C03-C02 | -2.92 | 118.65      | 122.64   |
| 31  | 8     | 309 | CLA  | C3B-C4B-NB  | -2.92 | 107.92      | 110.53   |
| 33  | 9     | 501 | 0UR  | C48-C47-C46 | -2.92 | 119.84      | 125.92   |
| 30  | 5     | 302 | CHL  | O2A-CGA-CBA | 2.92  | 120.73      | 111.83   |
| 32  | 4     | 402 | 8CT  | C14-C15-C16 | -2.92 | 118.36      | 126.36   |
| 30  | 6     | 302 | CHL  | CMB-C2B-C3B | 2.92  | 130.51      | 124.68   |
| 37  | 7     | 502 | 0IE  | C20-C3-C2   | 2.92  | 121.71      | 115.01   |
| 32  | L     | 206 | 8CT  | C18-C19-C20 | -2.92 | 117.55      | 123.52   |
| 33  | b     | 520 | 0UR  | O44-C45-C46 | 2.92  | 118.75      | 111.55   |
| 30  | c     | 614 | CHL  | CMD-C2D-C3D | -2.92 | 118.86      | 124.68   |
| 31  | 0     | 304 | CLA  | O2D-CGD-O1D | -2.91 | 118.18      | 123.85   |
| 30  | 6     | 307 | CHL  | CBC-CAC-C3C | -2.91 | 108.70      | 112.87   |
| 31  | h     | 612 | CLA  | C3B-C4B-NB  | -2.91 | 107.93      | 110.53   |
| 36  | J     | 102 | LMG  | O6-C1-O1    | -2.91 | 103.16      | 110.04   |
| 33  | f     | 520 | 0UR  | C10-C9-C8   | -2.91 | 117.56      | 123.52   |
| 30  | a     | 602 | CHL  | O1D-CGD-CBD | -2.91 | 120.31      | 124.72   |
| 34  | f     | 630 | LHG  | O8-C23-C24  | 2.91  | 120.71      | 111.83   |
| 32  | A     | 849 | 8CT  | C01-C02-C07 | 2.91  | 119.80      | 113.60   |
| 30  | 4     | 305 | CHL  | O1D-CGD-CBD | -2.91 | 120.31      | 124.72   |
| 30  | b     | 606 | CHL  | CMD-C2D-C3D | -2.91 | 118.87      | 124.68   |
| 37  | c     | 521 | 0IE  | C9-C10-C11  | 2.91  | 129.47      | 123.52   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | f     | 609 | CHL  | O2A-CGA-CBA | 2.91  | 120.71      | 111.83   |
| 31  | f     | 610 | CLA  | C3B-C4B-NB  | -2.91 | 107.93      | 110.53   |
| 30  | i     | 607 | CHL  | CBC-CAC-C3C | -2.91 | 108.71      | 112.87   |
| 31  | B     | 839 | CLA  | O2D-CGD-O1D | -2.91 | 118.19      | 123.85   |
| 38  | A     | 842 | PQN  | C11-C3-C2   | -2.91 | 119.90      | 124.89   |
| 30  | h     | 608 | CHL  | CBC-CAC-C3C | -2.91 | 108.71      | 112.87   |
| 31  | B     | 839 | CLA  | C3B-C4B-NB  | -2.91 | 107.93      | 110.53   |
| 30  | 2     | 302 | CHL  | O2A-CGA-CBA | 2.91  | 120.70      | 111.83   |
| 30  | i     | 606 | CHL  | O1D-CGD-CBD | -2.91 | 120.31      | 124.72   |
| 31  | O     | 201 | CLA  | CAA-C2A-C3A | -2.91 | 109.56      | 116.23   |
| 37  | h     | 521 | 0IE  | C9-C10-C11  | 2.91  | 129.47      | 123.52   |
| 30  | g     | 606 | CHL  | O1D-CGD-CBD | -2.91 | 120.32      | 124.72   |
| 31  | e     | 604 | CLA  | O2D-CGD-O1D | -2.90 | 118.19      | 123.85   |
| 31  | 5     | 309 | CLA  | C3B-C4B-NB  | -2.90 | 107.94      | 110.53   |
| 32  | 6     | 402 | 8CT  | C29-C28-C26 | -2.90 | 120.08      | 126.32   |
| 30  | g     | 602 | CHL  | C1-C2-C3    | -2.90 | 121.44      | 126.20   |
| 30  | 7     | 305 | CHL  | CBC-CAC-C3C | -2.90 | 108.72      | 112.87   |
| 32  | B     | 847 | 8CT  | C01-C02-C07 | 2.90  | 119.78      | 113.60   |
| 37  | g     | 521 | 0IE  | C20-C3-C2   | 2.90  | 121.67      | 115.01   |
| 31  | A     | 817 | CLA  | C3B-C4B-NB  | -2.90 | 107.94      | 110.53   |
| 31  | 5     | 310 | CLA  | O2D-CGD-O1D | -2.90 | 118.20      | 123.85   |
| 30  | 4     | 305 | CHL  | CMD-C2D-C3D | -2.90 | 118.89      | 124.68   |
| 31  | 7     | 315 | CLA  | C3B-C4B-NB  | -2.90 | 107.94      | 110.53   |
| 32  | F     | 302 | 8CT  | C01-C02-C07 | 2.90  | 119.78      | 113.60   |
| 30  | e     | 609 | CHL  | CBC-CAC-C3C | -2.90 | 108.72      | 112.87   |
| 32  | A     | 848 | 8CT  | C19-C18-C17 | -2.90 | 117.58      | 123.52   |
| 30  | 7     | 302 | CHL  | CBC-CAC-C3C | -2.90 | 108.72      | 112.87   |
| 30  | c     | 607 | CHL  | O1D-CGD-CBD | -2.90 | 120.33      | 124.72   |
| 33  | 1     | 501 | 0UR  | C48-C47-C46 | -2.90 | 119.88      | 125.92   |
| 31  | 0     | 312 | CLA  | O2D-CGD-O1D | -2.90 | 118.21      | 123.85   |
| 30  | 6     | 305 | CHL  | CMD-C2D-C3D | -2.90 | 118.89      | 124.68   |
| 31  | 1     | 310 | CLA  | O2D-CGD-O1D | -2.90 | 118.21      | 123.85   |
| 31  | A     | 836 | CLA  | C3B-C4B-NB  | -2.90 | 107.94      | 110.53   |
| 31  | 7     | 303 | CLA  | O2D-CGD-O1D | -2.90 | 118.21      | 123.85   |
| 31  | 9     | 309 | CLA  | O2D-CGD-O1D | -2.90 | 118.21      | 123.85   |
| 31  | e     | 603 | CLA  | O2D-CGD-O1D | -2.90 | 118.21      | 123.85   |
| 37  | a     | 522 | 0IE  | C21-C7-C8   | -2.90 | 118.12      | 122.82   |
| 30  | 8     | 302 | CHL  | CBC-CAC-C3C | -2.90 | 108.72      | 112.87   |
| 31  | h     | 610 | CLA  | C3B-C4B-NB  | -2.90 | 107.94      | 110.53   |
| 32  | G     | 104 | 8CT  | C15-C16-C17 | 2.90  | 123.56      | 119.01   |
| 31  | O     | 203 | CLA  | CAA-C2A-C3A | -2.90 | 109.59      | 116.23   |
| 30  | 1     | 306 | CHL  | CBC-CAC-C3C | -2.90 | 108.73      | 112.87   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 33  | 0     | 501 | 0UR  | C14-C15-C16 | -2.90 | 123.22      | 127.28   |
| 30  | 5     | 305 | CHL  | O1D-CGD-CBD | -2.90 | 120.33      | 124.72   |
| 31  | 1     | 304 | CLA  | O2D-CGD-O1D | -2.90 | 118.21      | 123.85   |
| 31  | c     | 604 | CLA  | O2D-CGD-O1D | -2.90 | 118.21      | 123.85   |
| 31  | g     | 604 | CLA  | O2D-CGD-O1D | -2.89 | 118.21      | 123.85   |
| 30  | 7     | 306 | CHL  | CMD-C2D-C3D | -2.89 | 118.90      | 124.68   |
| 31  | i     | 610 | CLA  | C3B-C4B-NB  | -2.89 | 107.95      | 110.53   |
| 31  | e     | 612 | CLA  | O2D-CGD-O1D | -2.89 | 118.22      | 123.85   |
| 37  | d     | 521 | 0IE  | C20-C3-C4   | -2.89 | 120.72      | 124.72   |
| 30  | 8     | 313 | CHL  | O1D-CGD-CBD | -2.89 | 120.33      | 124.72   |
| 31  | B     | 812 | CLA  | O2D-CGD-O1D | -2.89 | 118.22      | 123.85   |
| 32  | B     | 848 | 8CT  | C07-C02-C03 | -2.89 | 118.80      | 122.70   |
| 32  | B     | 804 | 8CT  | C04-C03-C02 | -2.89 | 118.68      | 122.64   |
| 30  | 8     | 307 | CHL  | O2A-CGA-CBA | 2.89  | 120.65      | 111.83   |
| 30  | 5     | 302 | CHL  | CBC-CAC-C3C | -2.89 | 108.73      | 112.87   |
| 30  | 4     | 313 | CHL  | O2A-CGA-CBA | 2.89  | 120.65      | 111.83   |
| 33  | 5     | 502 | 0UR  | C29-C30-C31 | -2.89 | 106.89      | 111.18   |
| 30  | 8     | 307 | CHL  | CMD-C2D-C3D | -2.89 | 118.91      | 124.68   |
| 33  | 1     | 501 | 0UR  | C28-C19-C18 | -2.89 | 109.50      | 112.83   |
| 37  | 7     | 502 | 0IE  | C20-C3-C4   | -2.89 | 120.72      | 124.72   |
| 31  | h     | 611 | CLA  | O2D-CGD-O1D | -2.89 | 118.22      | 123.85   |
| 31  | B     | 815 | CLA  | C3B-C4B-NB  | -2.89 | 107.95      | 110.53   |
| 31  | e     | 610 | CLA  | C3B-C4B-NB  | -2.89 | 107.95      | 110.53   |
| 30  | b     | 601 | CHL  | C1-C2-C3    | -2.89 | 121.46      | 126.20   |
| 30  | 6     | 306 | CHL  | CMD-C2D-C3D | -2.89 | 118.91      | 124.68   |
| 31  | M     | 101 | CLA  | C3B-C4B-NB  | -2.89 | 107.95      | 110.53   |
| 31  | 2     | 314 | CLA  | C3B-C4B-NB  | -2.89 | 107.95      | 110.53   |
| 30  | 4     | 306 | CHL  | O1D-CGD-CBD | -2.89 | 120.34      | 124.72   |
| 37  | a     | 521 | 0IE  | C20-C3-C2   | 2.89  | 121.64      | 115.01   |
| 31  | B     | 809 | CLA  | O2D-CGD-O1D | -2.89 | 118.23      | 123.85   |
| 37  | b     | 522 | 0IE  | C21-C7-C8   | -2.89 | 118.14      | 122.82   |
| 31  | 2     | 309 | CLA  | O2D-CGD-O1D | -2.88 | 118.23      | 123.85   |
| 32  | B     | 844 | 8CT  | C35-C30-C29 | -2.88 | 109.51      | 112.83   |
| 30  | 4     | 306 | CHL  | CMD-C2D-C3D | -2.88 | 118.92      | 124.68   |
| 37  | 3     | 502 | 0IE  | C9-C10-C11  | 2.88  | 129.42      | 123.52   |
| 30  | 2     | 319 | CHL  | C4-C3-C5    | 2.88  | 120.23      | 115.23   |
| 33  | 4     | 502 | 0UR  | C43-C3-C4   | -2.88 | 121.63      | 125.03   |
| 31  | 1     | 310 | CLA  | C3B-C4B-NB  | -2.88 | 107.96      | 110.53   |
| 31  | A     | 837 | CLA  | C3B-C4B-NB  | -2.88 | 107.96      | 110.53   |
| 32  | B     | 843 | 8CT  | C22-C21-C23 | 2.88  | 122.49      | 118.09   |
| 30  | c     | 608 | CHL  | O2A-CGA-CBA | 2.88  | 120.62      | 111.83   |
| 31  | J     | 103 | CLA  | O2D-CGD-O1D | -2.88 | 118.24      | 123.85   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | i     | 607 | CHL  | OMC-CMC-C2C | -2.88 | 120.12      | 125.12   |
| 32  | I     | 101 | 8CT  | C11-C10-C03 | -2.88 | 119.31      | 127.00   |
| 31  | A     | 834 | CLA  | O2D-CGD-O1D | -2.88 | 118.25      | 123.85   |
| 32  | B     | 846 | 8CT  | C30-C29-C28 | 2.88  | 129.06      | 124.58   |
| 33  | b     | 520 | 0UR  | C48-C47-C46 | -2.88 | 119.93      | 125.92   |
| 30  | d     | 608 | CHL  | O2A-CGA-CBA | 2.88  | 120.61      | 111.83   |
| 33  | 0     | 501 | 0UR  | C4-C5-C6    | -2.88 | 114.86      | 123.20   |
| 30  | 9     | 313 | CHL  | O1D-CGD-CBD | -2.88 | 120.36      | 124.72   |
| 31  | K     | 105 | CLA  | O2D-CGD-O1D | -2.88 | 118.25      | 123.85   |
| 37  | e     | 522 | 0IE  | C22-C12-C11 | -2.88 | 118.16      | 122.82   |
| 30  | 0     | 301 | CHL  | CMD-C2D-C3D | -2.87 | 118.94      | 124.68   |
| 30  | 8     | 302 | CHL  | OMC-CMC-C2C | -2.87 | 120.14      | 125.12   |
| 31  | B     | 805 | CLA  | O2D-CGD-O1D | -2.87 | 118.26      | 123.85   |
| 30  | 2     | 319 | CHL  | O1D-CGD-CBD | -2.87 | 120.37      | 124.72   |
| 30  | c     | 614 | CHL  | O2D-CGD-O1D | -2.87 | 118.27      | 123.85   |
| 31  | O     | 206 | CLA  | O2D-CGD-O1D | -2.87 | 118.27      | 123.85   |
| 31  | 0     | 303 | CLA  | O2D-CGD-O1D | -2.87 | 118.27      | 123.85   |
| 31  | A     | 821 | CLA  | C3B-C4B-NB  | -2.87 | 107.97      | 110.53   |
| 31  | f     | 613 | CLA  | C3B-C4B-NB  | -2.87 | 107.97      | 110.53   |
| 32  | 7     | 404 | 8CT  | C01-C02-C07 | 2.87  | 119.71      | 113.60   |
| 37  | a     | 522 | 0IE  | C20-C3-C4   | -2.87 | 120.76      | 124.72   |
| 32  | A     | 847 | 8CT  | C11-C10-C03 | -2.86 | 119.35      | 127.00   |
| 31  | c     | 611 | CLA  | O2D-CGD-O1D | -2.86 | 118.27      | 123.85   |
| 31  | 7     | 304 | CLA  | O2D-CGD-O1D | -2.86 | 118.28      | 123.85   |
| 31  | B     | 850 | CLA  | O2D-CGD-O1D | -2.86 | 118.28      | 123.85   |
| 31  | A     | 811 | CLA  | O2D-CGD-O1D | -2.86 | 118.28      | 123.85   |
| 31  | 8     | 310 | CLA  | C3B-C4B-NB  | -2.86 | 107.98      | 110.53   |
| 31  | 2     | 311 | CLA  | O2D-CGD-O1D | -2.86 | 118.28      | 123.85   |
| 31  | 6     | 311 | CLA  | O2D-CGD-O1D | -2.86 | 118.28      | 123.85   |
| 30  | 9     | 306 | CHL  | O2A-CGA-CBA | 2.86  | 120.55      | 111.83   |
| 30  | 3     | 305 | CHL  | CMD-C2D-C3D | -2.86 | 118.97      | 124.68   |
| 30  | b     | 607 | CHL  | CMD-C2D-C3D | -2.86 | 118.97      | 124.68   |
| 30  | 5     | 301 | CHL  | O1D-CGD-CBD | -2.86 | 120.39      | 124.72   |
| 30  | 6     | 302 | CHL  | O1D-CGD-CBD | -2.86 | 120.39      | 124.72   |
| 31  | 8     | 303 | CLA  | C3B-C4B-NB  | -2.86 | 107.98      | 110.53   |
| 31  | d     | 612 | CLA  | C3B-C4B-NB  | -2.86 | 107.98      | 110.53   |
| 30  | c     | 609 | CHL  | O2A-CGA-CBA | 2.86  | 120.54      | 111.83   |
| 31  | b     | 604 | CLA  | O2D-CGD-O1D | -2.86 | 118.29      | 123.85   |
| 31  | B     | 835 | CLA  | O2D-CGD-O1D | -2.85 | 118.29      | 123.85   |
| 33  | c     | 520 | 0UR  | C5-C4-C3    | -2.85 | 123.50      | 126.92   |
| 33  | 2     | 502 | 0UR  | C43-C3-C4   | -2.85 | 121.66      | 125.03   |
| 31  | A     | 829 | CLA  | C3B-C4B-NB  | -2.85 | 107.98      | 110.53   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 33  | 8     | 502 | 0UR  | C9-C10-C11  | -2.85 | 117.68      | 123.52   |
| 33  | g     | 520 | 0UR  | C14-C13-C12 | -2.85 | 118.54      | 126.36   |
| 34  | 4     | 601 | LHG  | O8-C23-C24  | 2.85  | 120.53      | 111.83   |
| 31  | A     | 839 | CLA  | O2D-CGD-O1D | -2.85 | 118.30      | 123.85   |
| 31  | L     | 207 | CLA  | O2D-CGD-O1D | -2.85 | 118.30      | 123.85   |
| 31  | a     | 612 | CLA  | O2D-CGD-O1D | -2.85 | 118.30      | 123.85   |
| 31  | 2     | 303 | CLA  | C3B-C4B-NB  | -2.85 | 107.98      | 110.53   |
| 31  | a     | 604 | CLA  | O2D-CGD-O1D | -2.85 | 118.30      | 123.85   |
| 32  | B     | 848 | 8CT  | C18-C19-C20 | 2.85  | 129.35      | 123.52   |
| 31  | 7     | 311 | CLA  | O2D-CGD-O1D | -2.85 | 118.30      | 123.85   |
| 31  | 7     | 316 | CLA  | C3B-C4B-NB  | -2.85 | 107.99      | 110.53   |
| 31  | K     | 102 | CLA  | C3B-C4B-NB  | -2.85 | 107.99      | 110.53   |
| 30  | b     | 609 | CHL  | O2A-CGA-CBA | 2.85  | 120.52      | 111.83   |
| 32  | 7     | 404 | 8CT  | C15-C16-C17 | 2.85  | 123.49      | 119.01   |
| 33  | 7     | 501 | 0UR  | O44-C43-C3  | 2.85  | 116.50      | 109.09   |
| 30  | f     | 602 | CHL  | O2A-CGA-CBA | 2.85  | 120.52      | 111.83   |
| 31  | 2     | 304 | CLA  | O2D-CGD-O1D | -2.85 | 118.31      | 123.85   |
| 31  | B     | 805 | CLA  | C3B-C4B-NB  | -2.85 | 107.99      | 110.53   |
| 31  | f     | 603 | CLA  | C3B-C4B-NB  | -2.85 | 107.99      | 110.53   |
| 33  | 2     | 501 | 0UR  | O44-C43-C3  | 2.85  | 116.50      | 109.09   |
| 31  | e     | 613 | CLA  | O2D-CGD-O1D | -2.85 | 118.31      | 123.85   |
| 30  | 7     | 307 | CHL  | C1-C2-C3    | -2.85 | 122.16      | 126.76   |
| 30  | 3     | 305 | CHL  | O2A-CGA-CBA | 2.85  | 120.51      | 111.83   |
| 31  | A     | 806 | CLA  | O2D-CGD-O1D | -2.85 | 118.31      | 123.85   |
| 31  | 3     | 308 | CLA  | C3B-C4B-NB  | -2.85 | 107.99      | 110.53   |
| 32  | B     | 804 | 8CT  | C07-C02-C03 | -2.84 | 118.86      | 122.70   |
| 42  | h     | 523 | NEX  | C26-C27-C28 | 2.84  | 132.01      | 125.99   |
| 31  | c     | 603 | CLA  | O2D-CGD-O1D | -2.84 | 118.31      | 123.85   |
| 32  | F     | 302 | 8CT  | C11-C10-C03 | -2.84 | 119.40      | 127.00   |
| 37  | f     | 521 | 0IE  | C21-C7-C8   | -2.84 | 118.21      | 122.82   |
| 31  | A     | 809 | CLA  | O2D-CGD-O1D | -2.84 | 118.31      | 123.85   |
| 30  | f     | 602 | CHL  | C4-C3-C5    | 2.84  | 120.16      | 115.23   |
| 31  | A     | 813 | CLA  | O2D-CGD-O1D | -2.84 | 118.32      | 123.85   |
| 31  | 6     | 304 | CLA  | C3B-C4B-NB  | -2.84 | 107.99      | 110.53   |
| 31  | 8     | 314 | CLA  | C3B-C4B-NB  | -2.84 | 107.99      | 110.53   |
| 31  | 3     | 308 | CLA  | C1-C2-C3    | -2.84 | 121.54      | 126.20   |
| 31  | h     | 610 | CLA  | O2D-CGD-O1D | -2.84 | 118.32      | 123.85   |
| 34  | d     | 630 | LHG  | O8-C23-C24  | 2.84  | 120.50      | 111.83   |
| 31  | i     | 613 | CLA  | C3B-C4B-NB  | -2.84 | 107.99      | 110.53   |
| 31  | e     | 613 | CLA  | C3B-C4B-NB  | -2.84 | 107.99      | 110.53   |
| 32  | 8     | 406 | 8CT  | C01-C02-C07 | 2.84  | 119.65      | 113.60   |
| 31  | 5     | 312 | CLA  | O2D-CGD-O1D | -2.84 | 118.32      | 123.85   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | 4     | 319 | CHL  | CMD-C2D-C3D | -2.84 | 119.01      | 124.68   |
| 31  | b     | 610 | CLA  | O2D-CGD-O1D | -2.84 | 118.32      | 123.85   |
| 31  | B     | 827 | CLA  | C1-C2-C3    | -2.84 | 121.54      | 126.20   |
| 31  | h     | 612 | CLA  | O2D-CGD-O1D | -2.84 | 118.32      | 123.85   |
| 30  | 5     | 302 | CHL  | CMD-C2D-C3D | -2.84 | 119.01      | 124.68   |
| 30  | 7     | 313 | CHL  | O1D-CGD-CBD | -2.84 | 120.42      | 124.72   |
| 30  | g     | 608 | CHL  | C1B-CHB-C4A | -2.84 | 119.50      | 121.32   |
| 31  | A     | 828 | CLA  | O2D-CGD-O1D | -2.84 | 118.32      | 123.85   |
| 32  | L     | 209 | 8CT  | C01-C02-C07 | 2.84  | 119.64      | 113.60   |
| 30  | 2     | 313 | CHL  | CMD-C2D-C3D | -2.84 | 119.02      | 124.68   |
| 31  | c     | 610 | CLA  | O2D-CGD-O1D | -2.84 | 118.33      | 123.85   |
| 30  | 0     | 302 | CHL  | O1D-CGD-CBD | -2.84 | 120.42      | 124.72   |
| 31  | A     | 804 | CLA  | C3B-C4B-NB  | -2.84 | 108.00      | 110.53   |
| 42  | g     | 523 | NEX  | C26-C27-C28 | 2.83  | 131.99      | 125.99   |
| 31  | i     | 603 | CLA  | C3B-C4B-NB  | -2.83 | 108.00      | 110.53   |
| 42  | b     | 523 | NEX  | C26-C27-C28 | 2.83  | 131.98      | 125.99   |
| 37  | e     | 522 | 0IE  | C13-C12-C11 | 2.83  | 123.47      | 119.01   |
| 31  | H     | 201 | CLA  | O2D-CGD-O1D | -2.83 | 118.33      | 123.85   |
| 30  | d     | 602 | CHL  | CMD-C2D-C3D | -2.83 | 119.02      | 124.68   |
| 33  | 9     | 501 | 0UR  | C15-C14-C13 | -2.83 | 114.99      | 123.20   |
| 37  | g     | 522 | 0IE  | C9-C10-C11  | 2.83  | 129.31      | 123.52   |
| 32  | J     | 101 | 8CT  | C10-C11-C12 | -2.83 | 122.05      | 126.23   |
| 34  | K     | 106 | LHG  | O8-C23-C24  | 2.83  | 120.47      | 111.83   |
| 33  | i     | 520 | 0UR  | C5-C4-C3    | -2.83 | 123.53      | 126.92   |
| 33  | 9     | 501 | 0UR  | C4-C3-C2    | -2.83 | 117.69      | 120.16   |
| 32  | B     | 846 | 8CT  | C27-C26-C25 | -2.83 | 118.23      | 122.82   |
| 31  | L     | 201 | CLA  | CMB-C2B-C1B | -2.83 | 121.11      | 125.42   |
| 31  | f     | 604 | CLA  | O2D-CGD-O1D | -2.83 | 118.34      | 123.85   |
| 31  | L     | 201 | CLA  | C3B-C4B-NB  | -2.83 | 108.00      | 110.53   |
| 31  | i     | 611 | CLA  | C3B-C4B-NB  | -2.83 | 108.00      | 110.53   |
| 32  | 7     | 402 | 8CT  | C01-C02-C07 | 2.83  | 119.63      | 113.60   |
| 30  | e     | 602 | CHL  | CMB-C2B-C3B | 2.83  | 130.34      | 124.68   |
| 31  | 4     | 310 | CLA  | O2D-CGD-O1D | -2.83 | 118.34      | 123.85   |
| 42  | d     | 523 | NEX  | C26-C27-C28 | 2.83  | 131.97      | 125.99   |
| 31  | 9     | 302 | CLA  | C3B-C4B-NB  | -2.83 | 108.00      | 110.53   |
| 31  | A     | 838 | CLA  | C3B-C4B-NB  | -2.83 | 108.00      | 110.53   |
| 32  | O     | 205 | 8CT  | C01-C02-C07 | 2.83  | 119.63      | 113.60   |
| 32  | 7     | 404 | 8CT  | C05-C04-C03 | 2.83  | 114.55      | 110.44   |
| 33  | c     | 520 | 0UR  | O44-C45-C46 | 2.83  | 118.53      | 111.55   |
| 37  | f     | 521 | 0IE  | C6-C7-C8    | 2.83  | 123.46      | 119.01   |
| 31  | 3     | 303 | CLA  | O2D-CGD-O1D | -2.83 | 118.34      | 123.85   |
| 31  | A     | 816 | CLA  | C3B-C4B-NB  | -2.83 | 108.01      | 110.53   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | B     | 817 | CLA  | C3B-C4B-NB  | -2.83 | 108.01      | 110.53   |
| 31  | 4     | 312 | CLA  | C3B-C4B-NB  | -2.83 | 108.01      | 110.53   |
| 42  | c     | 523 | NEX  | C26-C27-C28 | 2.83  | 131.97      | 125.99   |
| 37  | e     | 521 | 0IE  | C20-C3-C2   | 2.83  | 121.50      | 115.01   |
| 30  | 1     | 307 | CHL  | C4-C3-C5    | 2.83  | 120.13      | 115.23   |
| 37  | 7     | 502 | 0IE  | C23-C16-C17 | 2.83  | 122.40      | 118.09   |
| 32  | 2     | 402 | 8CT  | C11-C10-C03 | -2.83 | 119.45      | 127.00   |
| 30  | 1     | 307 | CHL  | O2A-CGA-CBA | 2.82  | 120.45      | 111.83   |
| 31  | d     | 603 | CLA  | O2D-CGD-O1D | -2.82 | 118.35      | 123.85   |
| 31  | H     | 204 | CLA  | O2D-CGD-O1D | -2.82 | 118.35      | 123.85   |
| 30  | 1     | 305 | CHL  | O2A-CGA-CBA | 2.82  | 120.45      | 111.83   |
| 31  | H     | 202 | CLA  | O2D-CGD-O1D | -2.82 | 118.35      | 123.85   |
| 42  | f     | 523 | NEX  | C26-C27-C28 | 2.82  | 131.96      | 125.99   |
| 30  | 4     | 319 | CHL  | C4-C3-C5    | 2.82  | 120.13      | 115.23   |
| 30  | 7     | 301 | CHL  | O1D-CGD-CBD | -2.82 | 120.44      | 124.72   |
| 42  | i     | 523 | NEX  | C26-C27-C28 | 2.82  | 131.96      | 125.99   |
| 31  | 1     | 308 | CLA  | O2D-CGD-O1D | -2.82 | 118.35      | 123.85   |
| 30  | a     | 606 | CHL  | O1D-CGD-CBD | -2.82 | 120.44      | 124.72   |
| 31  | 3     | 309 | CLA  | O2D-CGD-O1D | -2.82 | 118.36      | 123.85   |
| 31  | 8     | 311 | CLA  | O2D-CGD-O1D | -2.82 | 118.36      | 123.85   |
| 31  | 1     | 303 | CLA  | C3B-C4B-NB  | -2.82 | 108.01      | 110.53   |
| 33  | 1     | 501 | 0UR  | C43-C3-C4   | -2.82 | 121.70      | 125.03   |
| 30  | e     | 609 | CHL  | O2A-CGA-CBA | 2.82  | 120.44      | 111.83   |
| 32  | L     | 206 | 8CT  | C05-C04-C03 | 2.82  | 114.54      | 110.44   |
| 30  | 1     | 307 | CHL  | C1-C2-C3    | -2.82 | 121.58      | 126.20   |
| 30  | d     | 607 | CHL  | O1D-CGD-CBD | -2.82 | 120.44      | 124.72   |
| 31  | 1     | 308 | CLA  | C3B-C4B-NB  | -2.82 | 108.01      | 110.53   |
| 31  | i     | 612 | CLA  | O2D-CGD-O1D | -2.82 | 118.36      | 123.85   |
| 30  | 6     | 301 | CHL  | CMD-C2D-C3D | -2.82 | 119.05      | 124.68   |
| 31  | 7     | 311 | CLA  | C3B-C4B-NB  | -2.82 | 108.01      | 110.53   |
| 31  | B     | 822 | CLA  | C3B-C4B-NB  | -2.82 | 108.01      | 110.53   |
| 30  | 9     | 305 | CHL  | CMD-C2D-C3D | -2.82 | 119.05      | 124.68   |
| 30  | c     | 602 | CHL  | CMD-C2D-C3D | -2.82 | 119.05      | 124.68   |
| 42  | a     | 523 | NEX  | C26-C27-C28 | 2.82  | 131.95      | 125.99   |
| 37  | e     | 521 | 0IE  | C6-C7-C8    | 2.82  | 123.44      | 119.01   |
| 31  | d     | 604 | CLA  | O2D-CGD-O1D | -2.82 | 118.36      | 123.85   |
| 31  | g     | 611 | CLA  | O2D-CGD-O1D | -2.82 | 118.36      | 123.85   |
| 30  | c     | 601 | CHL  | O2A-CGA-CBA | 2.82  | 120.42      | 111.83   |
| 30  | 4     | 302 | CHL  | CMD-C2D-C3D | -2.82 | 119.06      | 124.68   |
| 31  | h     | 603 | CLA  | O2D-CGD-O1D | -2.82 | 118.37      | 123.85   |
| 31  | d     | 613 | CLA  | C3B-C4B-NB  | -2.82 | 108.02      | 110.53   |
| 31  | i     | 611 | CLA  | O2D-CGD-O1D | -2.82 | 118.37      | 123.85   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | b     | 614 | CHL  | O1D-CGD-CBD | -2.82 | 120.45      | 124.72   |
| 30  | 4     | 307 | CHL  | CMD-C2D-C3D | -2.82 | 119.06      | 124.68   |
| 30  | 0     | 302 | CHL  | C4-C3-C5    | 2.81  | 120.11      | 115.23   |
| 31  | A     | 822 | CLA  | O2D-CGD-O1D | -2.81 | 118.37      | 123.85   |
| 37  | i     | 522 | 0IE  | C17-C16-C15 | 2.81  | 123.43      | 119.01   |
| 31  | A     | 825 | CLA  | C3B-C4B-NB  | -2.81 | 108.02      | 110.53   |
| 31  | 5     | 314 | CLA  | O2D-CGD-O1D | -2.81 | 118.37      | 123.85   |
| 30  | 2     | 306 | CHL  | O2A-CGA-CBA | 2.81  | 120.41      | 111.83   |
| 34  | M     | 104 | LHG  | O8-C23-C24  | 2.81  | 120.41      | 111.83   |
| 33  | g     | 520 | 0UR  | C19-C18-C17 | -2.81 | 120.20      | 124.58   |
| 30  | c     | 602 | CHL  | O2A-CGA-CBA | 2.81  | 120.41      | 111.83   |
| 31  | g     | 603 | CLA  | O2D-CGD-O1D | -2.81 | 118.38      | 123.85   |
| 30  | 4     | 308 | CHL  | O1D-CGD-CBD | -2.81 | 120.46      | 124.72   |
| 31  | 4     | 304 | CLA  | O2D-CGD-O1D | -2.81 | 118.38      | 123.85   |
| 31  | B     | 824 | CLA  | O2D-CGD-O1D | -2.81 | 118.38      | 123.85   |
| 37  | i     | 522 | 0IE  | C20-C3-C4   | -2.81 | 120.84      | 124.72   |
| 32  | I     | 101 | 8CT  | C30-C29-C28 | -2.81 | 120.21      | 124.58   |
| 31  | B     | 832 | CLA  | C3B-C4B-NB  | -2.81 | 108.02      | 110.53   |
| 37  | e     | 521 | 0IE  | C21-C7-C8   | -2.81 | 118.27      | 122.82   |
| 30  | 0     | 305 | CHL  | O2A-CGA-CBA | 2.81  | 120.39      | 111.83   |
| 30  | 1     | 302 | CHL  | C4-C3-C5    | 2.81  | 120.10      | 115.23   |
| 31  | K     | 102 | CLA  | O2D-CGD-O1D | -2.81 | 118.39      | 123.85   |
| 30  | 9     | 306 | CHL  | CMD-C2D-C3D | -2.81 | 119.08      | 124.68   |
| 31  | 1     | 311 | CLA  | C3B-C4B-NB  | -2.81 | 108.03      | 110.53   |
| 31  | 6     | 320 | CLA  | C3B-C4B-NB  | -2.81 | 108.03      | 110.53   |
| 31  | e     | 610 | CLA  | O2D-CGD-O1D | -2.81 | 118.39      | 123.85   |
| 33  | 9     | 501 | 0UR  | C10-C9-C8   | -2.81 | 117.78      | 123.52   |
| 32  | A     | 847 | 8CT  | C01-C02-C07 | 2.81  | 119.58      | 113.60   |
| 30  | 0     | 302 | CHL  | CBC-CAC-C3C | -2.81 | 108.86      | 112.87   |
| 30  | 9     | 301 | CHL  | CBC-CAC-C3C | -2.81 | 108.86      | 112.87   |
| 32  | L     | 206 | 8CT  | C01-C02-C07 | 2.81  | 119.58      | 113.60   |
| 31  | e     | 603 | CLA  | C3B-C4B-NB  | -2.80 | 108.03      | 110.53   |
| 37  | h     | 521 | 0IE  | C20-C3-C4   | -2.80 | 120.84      | 124.72   |
| 31  | f     | 603 | CLA  | O2D-CGD-O1D | -2.80 | 118.39      | 123.85   |
| 30  | h     | 606 | CHL  | O2A-CGA-CBA | 2.80  | 120.39      | 111.83   |
| 31  | A     | 807 | CLA  | CMB-C2B-C1B | -2.80 | 121.15      | 125.42   |
| 30  | d     | 606 | CHL  | O2A-CGA-CBA | 2.80  | 120.39      | 111.83   |
| 30  | e     | 601 | CHL  | O2A-CGA-CBA | 2.80  | 120.38      | 111.83   |
| 31  | K     | 104 | CLA  | C3B-C4B-NB  | -2.80 | 108.03      | 110.53   |
| 30  | 2     | 305 | CHL  | O1D-CGD-CBD | -2.80 | 120.47      | 124.72   |
| 33  | f     | 520 | 0UR  | C9-C8-C7    | -2.80 | 123.35      | 127.28   |
| 30  | 4     | 305 | CHL  | CBC-CAC-C3C | -2.80 | 108.86      | 112.87   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | e     | 602 | CHL  | O1D-CGD-CBD | -2.80 | 120.48      | 124.72   |
| 31  | 0     | 311 | CLA  | C3B-C4B-NB  | -2.80 | 108.03      | 110.53   |
| 31  | c     | 612 | CLA  | C3B-C4B-NB  | -2.80 | 108.03      | 110.53   |
| 30  | c     | 614 | CHL  | CMB-C2B-C3B | 2.80  | 130.28      | 124.68   |
| 31  | 6     | 317 | CLA  | C3B-C4B-NB  | -2.80 | 108.03      | 110.53   |
| 31  | b     | 613 | CLA  | C3B-C4B-NB  | -2.80 | 108.03      | 110.53   |
| 30  | b     | 602 | CHL  | O2A-CGA-CBA | 2.80  | 120.37      | 111.83   |
| 30  | e     | 602 | CHL  | C4-C3-C5    | 2.80  | 120.08      | 115.23   |
| 30  | 2     | 301 | CHL  | O1D-CGD-CBD | -2.80 | 120.48      | 124.72   |
| 31  | H     | 205 | CLA  | C3B-C4B-NB  | -2.80 | 108.03      | 110.53   |
| 31  | 1     | 311 | CLA  | O2D-CGD-O1D | -2.80 | 118.40      | 123.85   |
| 30  | i     | 606 | CHL  | O2A-CGA-CBA | 2.80  | 120.36      | 111.83   |
| 34  | A     | 855 | LHG  | O8-C23-C24  | 2.80  | 120.36      | 111.83   |
| 30  | i     | 609 | CHL  | O2A-CGA-CBA | 2.80  | 120.36      | 111.83   |
| 30  | b     | 606 | CHL  | O2A-CGA-CBA | 2.79  | 120.36      | 111.83   |
| 31  | 9     | 309 | CLA  | C3B-C4B-NB  | -2.79 | 108.03      | 110.53   |
| 30  | h     | 601 | CHL  | O1D-CGD-CBD | -2.79 | 120.49      | 124.72   |
| 31  | B     | 808 | CLA  | C3B-C4B-NB  | -2.79 | 108.04      | 110.53   |
| 31  | h     | 604 | CLA  | C3B-C4B-NB  | -2.79 | 108.04      | 110.53   |
| 32  | B     | 804 | 8CT  | C25-C24-C23 | -2.79 | 115.11      | 123.20   |
| 30  | 2     | 319 | CHL  | O2D-CGD-O1D | -2.79 | 118.41      | 123.85   |
| 33  | h     | 520 | 0UR  | C18-C17-C16 | -2.79 | 120.31      | 126.32   |
| 31  | 8     | 304 | CLA  | C3B-C4B-NB  | -2.79 | 108.04      | 110.53   |
| 33  | 3     | 501 | 0UR  | C5-C4-C3    | -2.79 | 123.58      | 126.92   |
| 30  | e     | 607 | CHL  | O1D-CGD-CBD | -2.79 | 120.49      | 124.72   |
| 33  | 6     | 501 | 0UR  | C48-C47-C46 | -2.79 | 120.11      | 125.92   |
| 31  | 9     | 311 | CLA  | O2D-CGD-O1D | -2.79 | 118.41      | 123.85   |
| 30  | b     | 608 | CHL  | O2A-CGA-CBA | 2.79  | 120.35      | 111.83   |
| 30  | 8     | 302 | CHL  | C4-C3-C5    | 2.79  | 120.07      | 115.23   |
| 32  | 7     | 404 | 8CT  | C25-C24-C23 | -2.79 | 115.11      | 123.20   |
| 32  | B     | 843 | 8CT  | C30-C29-C28 | -2.79 | 120.24      | 124.58   |
| 30  | i     | 608 | CHL  | O2A-CGA-CBA | 2.79  | 120.34      | 111.83   |
| 32  | O     | 205 | 8CT  | C25-C24-C23 | -2.79 | 115.12      | 123.20   |
| 31  | 7     | 304 | CLA  | C3B-C4B-NB  | -2.79 | 108.04      | 110.53   |
| 31  | a     | 611 | CLA  | O2D-CGD-O1D | -2.79 | 118.42      | 123.85   |
| 31  | f     | 610 | CLA  | O2D-CGD-O1D | -2.79 | 118.42      | 123.85   |
| 30  | 5     | 307 | CHL  | C1B-CHB-C4A | 2.79  | 123.12      | 121.32   |
| 30  | 7     | 305 | CHL  | O2A-CGA-CBA | 2.79  | 120.34      | 111.83   |
| 31  | 3     | 308 | CLA  | O2D-CGD-O1D | -2.79 | 118.42      | 123.85   |
| 32  | 4     | 402 | 8CT  | C22-C21-C20 | -2.79 | 118.30      | 122.82   |
| 30  | f     | 608 | CHL  | O2A-CGA-CBA | 2.79  | 120.34      | 111.83   |
| 31  | 0     | 308 | CLA  | O2D-CGD-O1D | -2.79 | 118.42      | 123.85   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 9     | 310 | CLA  | CAA-C2A-C3A | -2.79 | 109.84      | 116.23   |
| 31  | d     | 611 | CLA  | C3B-C4B-NB  | -2.79 | 108.04      | 110.53   |
| 37  | g     | 521 | 0IE  | C21-C7-C8   | -2.79 | 118.30      | 122.82   |
| 33  | 0     | 502 | 0UR  | C15-C14-C13 | -2.79 | 115.13      | 123.20   |
| 30  | b     | 601 | CHL  | O2A-CGA-CBA | 2.79  | 120.33      | 111.83   |
| 36  | L     | 211 | LMG  | O6-C1-O1    | -2.79 | 103.46      | 110.04   |
| 30  | 6     | 308 | CHL  | CMD-C2D-C3D | -2.78 | 119.12      | 124.68   |
| 32  | 1     | 402 | 8CT  | C35-C30-C29 | -2.78 | 109.63      | 112.83   |
| 30  | 9     | 306 | CHL  | O2D-CGD-O1D | -2.78 | 118.43      | 123.85   |
| 31  | 5     | 303 | CLA  | O2D-CGD-O1D | -2.78 | 118.43      | 123.85   |
| 33  | 0     | 502 | 0UR  | C34-C27-C1  | -2.78 | 120.98      | 124.45   |
| 31  | 0     | 313 | CLA  | O2D-CGD-O1D | -2.78 | 118.44      | 123.85   |
| 31  | B     | 811 | CLA  | O2A-CGA-O1A | -2.78 | 116.67      | 123.63   |
| 37  | g     | 521 | 0IE  | C6-C7-C8    | 2.78  | 123.38      | 119.01   |
| 37  | i     | 522 | 0IE  | C22-C12-C11 | -2.78 | 118.31      | 122.82   |
| 31  | 3     | 311 | CLA  | O2D-CGD-O1D | -2.78 | 118.44      | 123.85   |
| 31  | i     | 610 | CLA  | O2D-CGD-O1D | -2.78 | 118.44      | 123.85   |
| 33  | O     | 204 | 0UR  | C18-C17-C16 | -2.78 | 120.35      | 126.32   |
| 30  | i     | 602 | CHL  | C4-C3-C5    | 2.78  | 120.05      | 115.23   |
| 37  | c     | 521 | 0IE  | C4-C3-C2    | -2.78 | 117.74      | 120.16   |
| 30  | a     | 608 | CHL  | O2A-CGA-CBA | 2.78  | 120.31      | 111.83   |
| 37  | i     | 521 | 0IE  | C13-C12-C11 | 2.78  | 123.38      | 119.01   |
| 30  | a     | 609 | CHL  | O2A-CGA-CBA | 2.78  | 120.30      | 111.83   |
| 32  | B     | 843 | 8CT  | C29-C28-C26 | -2.78 | 120.35      | 126.32   |
| 30  | 7     | 313 | CHL  | CBC-CAC-C3C | -2.78 | 108.90      | 112.87   |
| 32  | 7     | 404 | 8CT  | C39-C16-C17 | -2.78 | 118.32      | 122.82   |
| 39  | A     | 857 | CL0  | C1C-CHC-C4B | 2.78  | 126.00      | 116.07   |
| 31  | L     | 204 | CLA  | C3B-C4B-NB  | -2.78 | 108.05      | 110.53   |
| 32  | A     | 854 | 8CT  | C01-C02-C07 | 2.78  | 119.51      | 113.60   |
| 30  | 3     | 305 | CHL  | O1D-CGD-CBD | -2.78 | 120.51      | 124.72   |
| 31  | B     | 836 | CLA  | C3B-C4B-NB  | -2.77 | 108.05      | 110.53   |
| 37  | i     | 521 | 0IE  | C21-C7-C8   | -2.77 | 118.32      | 122.82   |
| 31  | 8     | 314 | CLA  | O2D-CGD-O1D | -2.77 | 118.45      | 123.85   |
| 31  | 7     | 315 | CLA  | O2D-CGD-O1D | -2.77 | 118.45      | 123.85   |
| 31  | f     | 612 | CLA  | C3B-C4B-NB  | -2.77 | 108.06      | 110.53   |
| 30  | 0     | 302 | CHL  | O2A-CGA-CBA | 2.77  | 120.29      | 111.83   |
| 33  | 8     | 501 | 0UR  | C4-C5-C6    | -2.77 | 115.17      | 123.20   |
| 30  | c     | 608 | CHL  | CBC-CAC-C3C | -2.77 | 108.91      | 112.87   |
| 32  | L     | 206 | 8CT  | C40-C12-C13 | -2.77 | 118.33      | 122.82   |
| 30  | 0     | 302 | CHL  | CMD-C2D-C3D | -2.77 | 119.15      | 124.68   |
| 32  | A     | 848 | 8CT  | C27-C26-C28 | 2.77  | 122.32      | 118.09   |
| 31  | 6     | 303 | CLA  | O2D-CGD-O1D | -2.77 | 118.46      | 123.85   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | b     | 602 | CHL  | CMD-C2D-C3D | -2.77 | 119.15      | 124.68   |
| 33  | O     | 204 | 0UR  | C15-C14-C13 | -2.77 | 115.18      | 123.20   |
| 31  | 1     | 314 | CLA  | C3B-C4B-NB  | -2.77 | 108.06      | 110.53   |
| 31  | 4     | 311 | CLA  | C3B-C4B-NB  | -2.77 | 108.06      | 110.53   |
| 30  | e     | 607 | CHL  | C1B-CHB-C4A | 2.77  | 123.10      | 121.32   |
| 30  | h     | 605 | CHL  | O1D-CGD-CBD | -2.77 | 120.53      | 124.72   |
| 37  | i     | 522 | 0IE  | C13-C12-C11 | 2.77  | 123.36      | 119.01   |
| 31  | b     | 603 | CLA  | O2D-CGD-O1D | -2.77 | 118.46      | 123.85   |
| 37  | g     | 521 | 0IE  | C20-C3-C4   | -2.77 | 120.89      | 124.72   |
| 37  | a     | 521 | 0IE  | C21-C7-C8   | -2.77 | 118.33      | 122.82   |
| 30  | e     | 601 | CHL  | O1D-CGD-CBD | -2.76 | 120.53      | 124.72   |
| 30  | a     | 607 | CHL  | O1D-CGD-CBD | -2.76 | 120.53      | 124.72   |
| 31  | 6     | 309 | CLA  | C3B-C4B-NB  | -2.76 | 108.06      | 110.53   |
| 31  | h     | 613 | CLA  | C3B-C4B-NB  | -2.76 | 108.06      | 110.53   |
| 32  | 8     | 402 | 8CT  | C24-C25-C26 | -2.76 | 123.40      | 127.28   |
| 30  | a     | 601 | CHL  | O1D-CGD-CBD | -2.76 | 120.53      | 124.72   |
| 31  | e     | 611 | CLA  | O2D-CGD-O1D | -2.76 | 118.47      | 123.85   |
| 31  | G     | 103 | CLA  | O2D-CGD-O1D | -2.76 | 118.47      | 123.85   |
| 30  | b     | 602 | CHL  | O1D-CGD-CBD | -2.76 | 120.53      | 124.72   |
| 32  | A     | 854 | 8CT  | C14-C15-C16 | -2.76 | 118.79      | 126.36   |
| 30  | 2     | 307 | CHL  | CMD-C2D-C3D | -2.76 | 119.17      | 124.68   |
| 32  | 1     | 402 | 8CT  | C05-C04-C03 | 2.76  | 114.45      | 110.44   |
| 30  | 8     | 302 | CHL  | O2A-CGA-CBA | 2.76  | 120.25      | 111.83   |
| 37  | c     | 522 | 0IE  | C22-C12-C11 | -2.76 | 118.34      | 122.82   |
| 31  | A     | 808 | CLA  | C3B-C4B-NB  | -2.76 | 108.07      | 110.53   |
| 30  | g     | 607 | CHL  | O2A-CGA-CBA | 2.76  | 120.25      | 111.83   |
| 30  | c     | 602 | CHL  | O1D-CGD-CBD | -2.76 | 120.54      | 124.72   |
| 30  | i     | 602 | CHL  | O1D-CGD-CBD | -2.76 | 120.54      | 124.72   |
| 31  | 9     | 308 | CLA  | O2D-CGD-O1D | -2.76 | 118.48      | 123.85   |
| 37  | f     | 521 | 0IE  | C20-C3-C2   | 2.76  | 121.34      | 115.01   |
| 31  | h     | 613 | CLA  | O2D-CGD-O1D | -2.76 | 118.48      | 123.85   |
| 30  | d     | 601 | CHL  | O2A-CGA-CBA | 2.76  | 120.24      | 111.83   |
| 30  | f     | 614 | CHL  | CBC-CAC-C3C | -2.76 | 108.92      | 112.87   |
| 30  | 2     | 302 | CHL  | CMD-C2D-C3D | -2.76 | 119.17      | 124.68   |
| 32  | J     | 104 | 8CT  | C23-C21-C20 | -2.76 | 114.67      | 119.01   |
| 34  | b     | 630 | LHG  | O8-C23-C24  | 2.76  | 120.24      | 111.83   |
| 32  | A     | 848 | 8CT  | C13-C14-C15 | -2.76 | 115.21      | 123.20   |
| 36  | J     | 105 | LMG  | O6-C1-O1    | -2.75 | 103.53      | 110.04   |
| 30  | g     | 601 | CHL  | O2A-CGA-CBA | 2.75  | 120.23      | 111.83   |
| 39  | A     | 857 | CL0  | C4D-ND-C1D  | 2.75  | 107.31      | 105.22   |
| 31  | d     | 603 | CLA  | C3B-C4B-NB  | -2.75 | 108.07      | 110.53   |
| 31  | 7     | 309 | CLA  | O2D-CGD-O1D | -2.75 | 118.49      | 123.85   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 34  | a     | 630 | LHG  | O8-C23-C24  | 2.75  | 120.23      | 111.83   |
| 33  | O     | 204 | 0UR  | C10-C11-C12 | -2.75 | 123.42      | 127.28   |
| 31  | d     | 610 | CLA  | C3B-C4B-NB  | -2.75 | 108.07      | 110.53   |
| 30  | 8     | 306 | CHL  | CBC-CAC-C3C | -2.75 | 108.94      | 112.87   |
| 34  | 7     | 602 | LHG  | O8-C23-C24  | 2.75  | 120.22      | 111.83   |
| 31  | O     | 206 | CLA  | C3B-C4B-NB  | -2.75 | 108.08      | 110.53   |
| 32  | 8     | 402 | 8CT  | C05-C04-C03 | 2.75  | 114.43      | 110.44   |
| 30  | 3     | 302 | CHL  | CMD-C2D-C3D | -2.75 | 119.19      | 124.68   |
| 37  | c     | 521 | 0IE  | C21-C7-C8   | -2.75 | 118.36      | 122.82   |
| 31  | i     | 604 | CLA  | C3B-C4B-NB  | -2.75 | 108.08      | 110.53   |
| 30  | g     | 614 | CHL  | O1D-CGD-CBD | -2.75 | 120.56      | 124.72   |
| 32  | 7     | 405 | 8CT  | C04-C03-C02 | -2.75 | 118.88      | 122.64   |
| 31  | d     | 610 | CLA  | O2D-CGD-O1D | -2.75 | 118.50      | 123.85   |
| 34  | 5     | 601 | LHG  | O8-C23-C24  | 2.75  | 120.21      | 111.83   |
| 30  | 1     | 313 | CHL  | CBC-CAC-C3C | -2.75 | 108.94      | 112.87   |
| 30  | 4     | 308 | CHL  | CBC-CAC-C3C | -2.75 | 108.94      | 112.87   |
| 30  | f     | 606 | CHL  | O2A-CGA-CBA | 2.75  | 120.20      | 111.83   |
| 32  | M     | 102 | 8CT  | C04-C03-C02 | -2.74 | 118.89      | 122.64   |
| 32  | G     | 104 | 8CT  | C18-C19-C20 | -2.74 | 117.90      | 123.52   |
| 33  | 3     | 501 | 0UR  | C15-C14-C13 | -2.74 | 115.25      | 123.20   |
| 31  | 6     | 320 | CLA  | O2D-CGD-O1D | -2.74 | 118.51      | 123.85   |
| 30  | a     | 605 | CHL  | CBC-CAC-C3C | -2.74 | 108.95      | 112.87   |
| 37  | a     | 521 | 0IE  | C6-C7-C8    | 2.74  | 123.32      | 119.01   |
| 30  | 6     | 307 | CHL  | C1-C2-C3    | -2.74 | 122.33      | 126.76   |
| 37  | b     | 522 | 0IE  | C22-C12-C11 | -2.74 | 118.37      | 122.82   |
| 31  | 8     | 309 | CLA  | O2D-CGD-O1D | -2.74 | 118.51      | 123.85   |
| 31  | i     | 603 | CLA  | O2D-CGD-O1D | -2.74 | 118.51      | 123.85   |
| 34  | 7     | 603 | LHG  | O8-C23-C24  | 2.74  | 120.19      | 111.83   |
| 30  | g     | 606 | CHL  | O2A-CGA-CBA | 2.74  | 120.19      | 111.83   |
| 32  | 7     | 405 | 8CT  | C01-C02-C07 | 2.74  | 119.44      | 113.60   |
| 34  | 2     | 601 | LHG  | O8-C23-C24  | 2.74  | 120.19      | 111.83   |
| 37  | i     | 521 | 0IE  | C6-C7-C8    | 2.74  | 123.32      | 119.01   |
| 37  | d     | 521 | 0IE  | C21-C7-C8   | -2.74 | 118.38      | 122.82   |
| 30  | f     | 602 | CHL  | CMD-C2D-C3D | -2.74 | 119.21      | 124.68   |
| 31  | A     | 833 | CLA  | C3B-C4B-NB  | -2.74 | 108.08      | 110.53   |
| 31  | B     | 825 | CLA  | C3B-C4B-NB  | -2.74 | 108.08      | 110.53   |
| 30  | e     | 606 | CHL  | O1D-CGD-CBD | -2.74 | 120.57      | 124.72   |
| 30  | 1     | 302 | CHL  | O2A-CGA-CBA | 2.74  | 120.18      | 111.83   |
| 33  | b     | 520 | 0UR  | C14-C15-C16 | -2.74 | 123.44      | 127.28   |
| 33  | i     | 520 | 0UR  | C14-C15-C16 | -2.74 | 123.44      | 127.28   |
| 30  | e     | 606 | CHL  | O2A-CGA-CBA | 2.74  | 120.18      | 111.83   |
| 32  | 6     | 402 | 8CT  | C05-C04-C03 | 2.74  | 114.41      | 110.44   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | e     | 608 | CHL  | O2A-CGA-CBA | 2.74  | 120.18      | 111.83   |
| 31  | A     | 834 | CLA  | C3B-C4B-NB  | -2.74 | 108.09      | 110.53   |
| 32  | 7     | 402 | 8CT  | C30-C31-C32 | -2.74 | 118.10      | 121.47   |
| 30  | 1     | 313 | CHL  | O1D-CGD-CBD | -2.74 | 120.58      | 124.72   |
| 30  | d     | 602 | CHL  | C4-C3-C5    | 2.73  | 119.97      | 115.23   |
| 30  | a     | 606 | CHL  | O2A-CGA-CBA | 2.73  | 120.17      | 111.83   |
| 31  | 7     | 318 | CLA  | C3B-C4B-NB  | -2.73 | 108.09      | 110.53   |
| 31  | 4     | 309 | CLA  | C3B-C4B-NB  | -2.73 | 108.09      | 110.53   |
| 31  | c     | 612 | CLA  | O2D-CGD-O1D | -2.73 | 118.53      | 123.85   |
| 32  | 3     | 403 | 8CT  | C01-C02-C07 | 2.73  | 119.42      | 113.60   |
| 32  | L     | 209 | 8CT  | C19-C20-C21 | -2.73 | 123.45      | 127.28   |
| 30  | 4     | 302 | CHL  | O2A-CGA-CBA | 2.73  | 120.17      | 111.83   |
| 30  | f     | 601 | CHL  | O2A-CGA-CBA | 2.73  | 120.16      | 111.83   |
| 30  | 8     | 302 | CHL  | CMD-C2D-C3D | -2.73 | 119.22      | 124.68   |
| 37  | h     | 522 | 0IE  | C22-C12-C11 | -2.73 | 118.39      | 122.82   |
| 36  | L     | 210 | LMG  | O6-C1-O1    | -2.73 | 103.59      | 110.04   |
| 30  | 7     | 301 | CHL  | O2D-CGD-O1D | -2.73 | 118.53      | 123.85   |
| 30  | 4     | 313 | CHL  | O2D-CGD-O1D | -2.73 | 118.54      | 123.85   |
| 31  | B     | 826 | CLA  | C3B-C4B-NB  | -2.73 | 108.09      | 110.53   |
| 31  | G     | 102 | CLA  | C3B-C4B-NB  | -2.73 | 108.09      | 110.53   |
| 34  | H     | 203 | LHG  | O8-C23-C24  | 2.73  | 120.16      | 111.83   |
| 30  | g     | 601 | CHL  | O1D-CGD-CBD | -2.73 | 120.58      | 124.72   |
| 31  | 8     | 303 | CLA  | O2D-CGD-O1D | -2.73 | 118.54      | 123.85   |
| 37  | a     | 522 | 0IE  | C22-C12-C11 | -2.73 | 118.40      | 122.82   |
| 31  | i     | 604 | CLA  | O2D-CGD-O1D | -2.73 | 118.54      | 123.85   |
| 33  | 0     | 502 | 0UR  | C14-C15-C16 | -2.73 | 123.45      | 127.28   |
| 31  | 4     | 314 | CLA  | C3B-C4B-NB  | -2.73 | 108.10      | 110.53   |
| 30  | 4     | 306 | CHL  | CBC-CAC-C3C | -2.73 | 108.97      | 112.87   |
| 30  | 2     | 308 | CHL  | CMD-C2D-C3D | -2.73 | 119.24      | 124.68   |
| 31  | B     | 827 | CLA  | C3B-C4B-NB  | -2.73 | 108.10      | 110.53   |
| 31  | B     | 834 | CLA  | O2D-CGD-O1D | -2.72 | 118.55      | 123.85   |
| 30  | d     | 605 | CHL  | O1D-CGD-CBD | -2.72 | 120.59      | 124.72   |
| 30  | 9     | 305 | CHL  | CBC-CAC-C3C | -2.72 | 108.97      | 112.87   |
| 30  | d     | 602 | CHL  | O1D-CGD-CBD | -2.72 | 120.59      | 124.72   |
| 31  | 0     | 311 | CLA  | O2D-CGD-O1D | -2.72 | 118.55      | 123.85   |
| 30  | 6     | 307 | CHL  | O2A-CGA-CBA | 2.72  | 120.14      | 111.83   |
| 30  | 8     | 308 | CHL  | CMA-C3A-C4A | -2.72 | 108.74      | 114.61   |
| 34  | 6     | 601 | LHG  | O8-C23-C24  | 2.72  | 120.14      | 111.83   |
| 32  | K     | 107 | 8CT  | C01-C02-C07 | 2.72  | 119.40      | 113.60   |
| 31  | 3     | 311 | CLA  | C3B-C4B-NB  | -2.72 | 108.10      | 110.53   |
| 30  | 8     | 315 | CHL  | O1D-CGD-CBD | -2.72 | 120.60      | 124.72   |
| 31  | 5     | 311 | CLA  | C3B-C4B-NB  | -2.72 | 108.10      | 110.53   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | 8     | 301 | CHL  | C4-C3-C5    | 2.72  | 119.95      | 115.23   |
| 30  | g     | 609 | CHL  | O1D-CGD-CBD | -2.72 | 120.60      | 124.72   |
| 33  | 2     | 502 | OUR  | C17-C16-C15 | 2.72  | 123.29      | 119.01   |
| 30  | c     | 601 | CHL  | O1D-CGD-CBD | -2.72 | 120.60      | 124.72   |
| 38  | A     | 842 | PQN  | C2M-C2-C3   | -2.72 | 119.98      | 124.45   |
| 31  | B     | 806 | CLA  | O2D-CGD-O1D | -2.72 | 118.56      | 123.85   |
| 31  | c     | 613 | CLA  | C3B-C4B-NB  | -2.72 | 108.10      | 110.53   |
| 37  | i     | 521 | OIE  | C22-C12-C11 | -2.72 | 118.41      | 122.82   |
| 31  | d     | 612 | CLA  | O2D-CGD-O1D | -2.72 | 118.56      | 123.85   |
| 30  | 8     | 305 | CHL  | O1D-CGD-CBD | -2.72 | 120.60      | 124.72   |
| 31  | 2     | 304 | CLA  | C3B-C4B-NB  | -2.72 | 108.11      | 110.53   |
| 30  | 4     | 302 | CHL  | C4-C3-C5    | 2.72  | 119.94      | 115.23   |
| 30  | 7     | 305 | CHL  | O1D-CGD-CBD | -2.72 | 120.61      | 124.72   |
| 30  | f     | 602 | CHL  | O1D-CGD-CBD | -2.72 | 120.61      | 124.72   |
| 30  | 2     | 319 | CHL  | C1-C2-C3    | -2.72 | 121.75      | 126.20   |
| 31  | A     | 841 | CLA  | C1-C2-C3    | -2.72 | 121.75      | 126.20   |
| 30  | 2     | 305 | CHL  | CBC-CAC-C3C | -2.71 | 108.99      | 112.87   |
| 32  | 4     | 402 | 8CT  | C24-C23-C21 | -2.71 | 118.92      | 126.36   |
| 32  | A     | 850 | 8CT  | C27-C26-C28 | 2.71  | 122.23      | 118.09   |
| 30  | 7     | 306 | CHL  | CBC-CAC-C3C | -2.71 | 108.99      | 112.87   |
| 30  | 6     | 315 | CHL  | O1D-CGD-CBD | -2.71 | 120.61      | 124.72   |
| 30  | 4     | 313 | CHL  | CMD-C2D-C3D | -2.71 | 119.26      | 124.68   |
| 31  | 5     | 308 | CLA  | O2D-CGD-O1D | -2.71 | 118.57      | 123.85   |
| 30  | c     | 606 | CHL  | CBC-CAC-C3C | -2.71 | 108.99      | 112.87   |
| 30  | b     | 602 | CHL  | CBC-CAC-C3C | -2.71 | 108.99      | 112.87   |
| 30  | e     | 609 | CHL  | C4-C3-C5    | 2.71  | 119.93      | 115.23   |
| 31  | 7     | 317 | CLA  | O2D-CGD-O1D | -2.71 | 118.57      | 123.85   |
| 37  | c     | 521 | OIE  | C6-C7-C8    | 2.71  | 123.27      | 119.01   |
| 32  | F     | 302 | 8CT  | C30-C31-C32 | -2.71 | 118.13      | 121.47   |
| 32  | 7     | 402 | 8CT  | C13-C14-C15 | -2.71 | 115.35      | 123.20   |
| 32  | A     | 847 | 8CT  | C25-C24-C23 | -2.71 | 115.35      | 123.20   |
| 30  | 8     | 313 | CHL  | O2A-CGA-CBA | 2.71  | 120.10      | 111.83   |
| 37  | 3     | 502 | OIE  | C23-C16-C17 | 2.71  | 122.22      | 118.09   |
| 31  | d     | 613 | CLA  | O2D-CGD-O1D | -2.71 | 118.58      | 123.85   |
| 38  | A     | 842 | PQN  | C12-C11-C3  | -2.71 | 105.42      | 112.08   |
| 32  | A     | 850 | 8CT  | C28-C26-C25 | -2.71 | 114.75      | 119.01   |
| 30  | b     | 609 | CHL  | C4-C3-C5    | 2.71  | 119.92      | 115.23   |
| 33  | 5     | 501 | OUR  | C48-C47-C46 | -2.71 | 120.29      | 125.92   |
| 32  | B     | 847 | 8CT  | C05-C04-C03 | 2.70  | 114.37      | 110.44   |
| 34  | A     | 844 | LHG  | O8-C23-C24  | 2.70  | 120.08      | 111.83   |
| 32  | O     | 205 | 8CT  | C14-C15-C16 | -2.70 | 118.95      | 126.36   |
| 31  | 6     | 317 | CLA  | CAA-CBA-CGA | -2.70 | 105.53      | 113.21   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 9     | 310 | CLA  | O2D-CGD-O1D | -2.70 | 118.59      | 123.85   |
| 36  | 3     | 602 | LMG  | O6-C1-O1    | -2.70 | 103.66      | 110.04   |
| 33  | 6     | 501 | 0UR  | O44-C45-C46 | 2.70  | 118.22      | 111.55   |
| 31  | 1     | 309 | CLA  | O2D-CGD-O1D | -2.70 | 118.59      | 123.85   |
| 33  | 1     | 502 | 0UR  | C18-C17-C16 | -2.70 | 120.51      | 126.32   |
| 31  | 5     | 308 | CLA  | C3B-C4B-NB  | -2.70 | 108.12      | 110.53   |
| 31  | c     | 603 | CLA  | C3B-C4B-NB  | -2.70 | 108.12      | 110.53   |
| 31  | g     | 612 | CLA  | C3B-C4B-NB  | -2.70 | 108.12      | 110.53   |
| 30  | 1     | 305 | CHL  | CMB-C2B-C3B | 2.70  | 130.08      | 124.68   |
| 30  | f     | 607 | CHL  | O1D-CGD-CBD | -2.70 | 120.63      | 124.72   |
| 30  | 1     | 305 | CHL  | O1D-CGD-CBD | -2.70 | 120.63      | 124.72   |
| 32  | 7     | 402 | 8CT  | C18-C19-C20 | -2.70 | 117.99      | 123.52   |
| 37  | b     | 522 | 0IE  | C13-C12-C11 | 2.70  | 123.26      | 119.01   |
| 31  | K     | 104 | CLA  | O2D-CGD-O1D | -2.70 | 118.59      | 123.85   |
| 30  | h     | 602 | CHL  | C4-C3-C5    | 2.70  | 119.91      | 115.23   |
| 32  | G     | 104 | 8CT  | C04-C03-C02 | -2.70 | 118.95      | 122.64   |
| 31  | B     | 819 | CLA  | C3B-C4B-NB  | -2.70 | 108.12      | 110.53   |
| 31  | A     | 836 | CLA  | C1-C2-C3    | -2.70 | 121.78      | 126.20   |
| 32  | 6     | 402 | 8CT  | C39-C16-C17 | -2.70 | 118.45      | 122.82   |
| 30  | 8     | 305 | CHL  | CBC-CAC-C3C | -2.70 | 109.01      | 112.87   |
| 30  | 6     | 305 | CHL  | O1D-CGD-CBD | -2.70 | 120.63      | 124.72   |
| 31  | 4     | 309 | CLA  | O2D-CGD-O1D | -2.69 | 118.60      | 123.85   |
| 30  | d     | 608 | CHL  | CBC-CAC-C3C | -2.69 | 109.02      | 112.87   |
| 30  | f     | 601 | CHL  | O1D-CGD-CBD | -2.69 | 120.64      | 124.72   |
| 33  | 8     | 501 | 0UR  | C48-C47-C46 | -2.69 | 120.31      | 125.92   |
| 33  | 4     | 501 | 0UR  | C15-C14-C13 | -2.69 | 115.40      | 123.20   |
| 33  | 6     | 502 | 0UR  | C48-C47-C46 | -2.69 | 120.31      | 125.92   |
| 31  | a     | 610 | CLA  | C3B-C4B-NB  | -2.69 | 108.13      | 110.53   |
| 30  | c     | 608 | CHL  | C1B-CHB-C4A | 2.69  | 123.05      | 121.32   |
| 34  | e     | 630 | LHG  | O8-C23-C24  | 2.69  | 120.03      | 111.83   |
| 31  | 3     | 304 | CLA  | CHB-C4A-NA  | 2.69  | 128.28      | 124.40   |
| 30  | d     | 609 | CHL  | O1D-CGD-CBD | -2.69 | 120.64      | 124.72   |
| 31  | 0     | 311 | CLA  | CHB-C4A-NA  | 2.69  | 128.28      | 124.40   |
| 31  | B     | 840 | CLA  | C3B-C4B-NB  | -2.69 | 108.13      | 110.53   |
| 30  | 5     | 306 | CHL  | O2A-CGA-CBA | 2.69  | 120.03      | 111.83   |
| 30  | g     | 602 | CHL  | O2A-CGA-CBA | 2.69  | 120.03      | 111.83   |
| 30  | 3     | 305 | CHL  | CBC-CAC-C3C | -2.69 | 109.03      | 112.87   |
| 31  | B     | 816 | CLA  | C3B-C4B-NB  | -2.69 | 108.13      | 110.53   |
| 32  | B     | 804 | 8CT  | C24-C25-C26 | -2.69 | 123.51      | 127.28   |
| 30  | g     | 602 | CHL  | O1D-CGD-CBD | -2.69 | 120.65      | 124.72   |
| 33  | 8     | 502 | 0UR  | C48-C47-C46 | -2.69 | 120.33      | 125.92   |
| 31  | 6     | 317 | CLA  | CMB-C2B-C1B | -2.68 | 121.33      | 125.42   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | 1     | 302 | CHL  | CMA-C3A-C4A | -2.68 | 108.83      | 114.61   |
| 30  | a     | 602 | CHL  | C4-C3-C5    | 2.68  | 119.89      | 115.23   |
| 30  | a     | 605 | CHL  | O1D-CGD-CBD | -2.68 | 120.65      | 124.72   |
| 30  | e     | 608 | CHL  | C4-C3-C5    | 2.68  | 119.88      | 115.23   |
| 32  | B     | 804 | 8CT  | C05-C04-C03 | 2.68  | 114.33      | 110.44   |
| 34  | g     | 630 | LHG  | O8-C23-C24  | 2.68  | 120.01      | 111.83   |
| 31  | A     | 853 | CLA  | O2D-CGD-O1D | -2.68 | 118.63      | 123.85   |
| 30  | h     | 602 | CHL  | O2A-CGA-CBA | 2.68  | 120.01      | 111.83   |
| 34  | 3     | 603 | LHG  | O8-C23-C24  | 2.68  | 120.01      | 111.83   |
| 30  | 8     | 308 | CHL  | O1D-CGD-CBD | -2.68 | 120.66      | 124.72   |
| 34  | c     | 630 | LHG  | O8-C23-C24  | 2.68  | 120.00      | 111.83   |
| 38  | B     | 842 | PQN  | C11-C12-C13 | -2.68 | 122.22      | 126.83   |
| 37  | g     | 522 | OIE  | C22-C12-C11 | -2.68 | 118.48      | 122.82   |
| 33  | d     | 520 | OUR  | C4-C3-C2    | -2.68 | 117.83      | 120.16   |
| 30  | a     | 602 | CHL  | O2A-CGA-CBA | 2.68  | 120.00      | 111.83   |
| 32  | 4     | 402 | 8CT  | C11-C10-C03 | -2.68 | 119.85      | 127.00   |
| 30  | g     | 607 | CHL  | CBC-CAC-C3C | -2.68 | 109.04      | 112.87   |
| 31  | A     | 822 | CLA  | C3B-C4B-NB  | -2.67 | 108.14      | 110.53   |
| 31  | 7     | 317 | CLA  | CHB-C4A-NA  | 2.67  | 128.26      | 124.40   |
| 30  | d     | 614 | CHL  | O1D-CGD-CBD | -2.67 | 120.67      | 124.72   |
| 31  | d     | 604 | CLA  | C1-C2-C3    | -2.67 | 122.44      | 126.76   |
| 34  | B     | 854 | LHG  | O8-C23-C24  | 2.67  | 119.98      | 111.83   |
| 32  | A     | 849 | 8CT  | C25-C24-C23 | -2.67 | 115.46      | 123.20   |
| 32  | B     | 845 | 8CT  | C24-C25-C26 | -2.67 | 123.53      | 127.28   |
| 30  | 0     | 301 | CHL  | OMC-CMC-C2C | -2.67 | 120.48      | 125.12   |
| 32  | A     | 847 | 8CT  | C27-C26-C28 | 2.67  | 122.17      | 118.09   |
| 30  | 7     | 302 | CHL  | O2D-CGD-O1D | -2.67 | 118.65      | 123.85   |
| 37  | a     | 522 | OIE  | C13-C12-C11 | 2.67  | 123.21      | 119.01   |
| 31  | A     | 807 | CLA  | C3B-C4B-NB  | -2.67 | 108.15      | 110.53   |
| 30  | 7     | 301 | CHL  | C1-C2-C3    | -2.67 | 121.83      | 126.20   |
| 37  | f     | 522 | OIE  | C22-C12-C11 | -2.67 | 118.50      | 122.82   |
| 30  | b     | 608 | CHL  | CBC-CAC-C3C | -2.67 | 109.06      | 112.87   |
| 37  | i     | 521 | OIE  | C20-C3-C4   | -2.67 | 121.03      | 124.72   |
| 37  | 3     | 502 | OIE  | C21-C7-C8   | -2.66 | 118.50      | 122.82   |
| 30  | f     | 609 | CHL  | CBC-CAC-C3C | -2.66 | 109.06      | 112.87   |
| 34  | 0     | 601 | LHG  | O8-C23-C24  | 2.66  | 119.96      | 111.83   |
| 33  | 6     | 501 | OUR  | C10-C9-C8   | -2.66 | 118.07      | 123.52   |
| 31  | a     | 604 | CLA  | C3B-C4B-NB  | -2.66 | 108.15      | 110.53   |
| 31  | H     | 201 | CLA  | C3B-C4B-NB  | -2.66 | 108.15      | 110.53   |
| 30  | d     | 607 | CHL  | CBC-CAC-C3C | -2.66 | 109.06      | 112.87   |
| 30  | 9     | 305 | CHL  | CMB-C2B-C3B | 2.66  | 130.00      | 124.68   |
| 30  | d     | 609 | CHL  | O2A-CGA-CBA | 2.66  | 119.95      | 111.83   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | A     | 839 | CLA  | C1-C2-C3    | -2.66 | 121.83      | 126.20   |
| 31  | B     | 807 | CLA  | CHB-C4A-NA  | 2.66  | 128.24      | 124.40   |
| 37  | 7     | 502 | 0IE  | C21-C7-C8   | -2.66 | 118.50      | 122.82   |
| 34  | 7     | 601 | LHG  | O8-C23-C24  | 2.66  | 119.95      | 111.83   |
| 30  | 8     | 306 | CHL  | O2D-CGD-O1D | -2.66 | 118.67      | 123.85   |
| 31  | b     | 611 | CLA  | O2D-CGD-O1D | -2.66 | 118.67      | 123.85   |
| 30  | d     | 606 | CHL  | O1D-CGD-CBD | -2.66 | 120.69      | 124.72   |
| 30  | c     | 614 | CHL  | CBC-CAC-C3C | -2.66 | 109.06      | 112.87   |
| 31  | 9     | 308 | CLA  | C3B-C4B-NB  | -2.66 | 108.16      | 110.53   |
| 31  | g     | 603 | CLA  | C3B-C4B-NB  | -2.66 | 108.16      | 110.53   |
| 31  | b     | 612 | CLA  | O2D-CGD-O1D | -2.66 | 118.67      | 123.85   |
| 30  | 4     | 319 | CHL  | C1-C2-C3    | -2.66 | 121.84      | 126.20   |
| 32  | B     | 843 | 8CT  | C01-C02-C07 | 2.66  | 119.27      | 113.60   |
| 30  | f     | 607 | CHL  | CBC-CAC-C3C | -2.66 | 109.07      | 112.87   |
| 30  | i     | 602 | CHL  | O2A-CGA-CBA | 2.66  | 119.94      | 111.83   |
| 37  | g     | 522 | 0IE  | C13-C12-C11 | 2.66  | 123.19      | 119.01   |
| 30  | c     | 606 | CHL  | O1D-CGD-CBD | -2.66 | 120.69      | 124.72   |
| 34  | i     | 630 | LHG  | O8-C23-C24  | 2.66  | 119.94      | 111.83   |
| 30  | b     | 606 | CHL  | O1D-CGD-CBD | -2.66 | 120.69      | 124.72   |
| 36  | 9     | 602 | LMG  | O1-C1-C2    | -2.66 | 104.24      | 108.27   |
| 30  | a     | 602 | CHL  | CBC-CAC-C3C | -2.66 | 109.07      | 112.87   |
| 30  | g     | 607 | CHL  | OMC-CMC-C2C | -2.66 | 120.51      | 125.12   |
| 32  | 9     | 401 | 8CT  | C29-C28-C26 | -2.65 | 120.61      | 126.32   |
| 42  | e     | 523 | NEX  | C31-C30-C29 | -2.65 | 123.56      | 127.28   |
| 31  | A     | 806 | CLA  | CHB-C4A-NA  | 2.65  | 128.23      | 124.40   |
| 34  | 1     | 601 | LHG  | O8-C23-C24  | 2.65  | 119.92      | 111.83   |
| 31  | f     | 613 | CLA  | O2D-CGD-O1D | -2.65 | 118.69      | 123.85   |
| 30  | a     | 609 | CHL  | C4-C3-C5    | 2.65  | 119.83      | 115.23   |
| 32  | 0     | 401 | 8CT  | C11-C10-C03 | -2.65 | 119.91      | 127.00   |
| 31  | b     | 604 | CLA  | C3B-C4B-NB  | -2.65 | 108.16      | 110.53   |
| 30  | 2     | 302 | CHL  | O2D-CGD-O1D | -2.65 | 118.69      | 123.85   |
| 31  | 6     | 309 | CLA  | O2D-CGD-O1D | -2.65 | 118.69      | 123.85   |
| 30  | c     | 602 | CHL  | C4-C3-C5    | 2.65  | 119.83      | 115.23   |
| 31  | 0     | 309 | CLA  | C3B-C4B-NB  | -2.65 | 108.17      | 110.53   |
| 31  | i     | 613 | CLA  | O2D-CGD-O1D | -2.65 | 118.69      | 123.85   |
| 30  | 8     | 306 | CHL  | O1D-CGD-CBD | -2.65 | 120.71      | 124.72   |
| 31  | 5     | 303 | CLA  | C3B-C4B-NB  | -2.65 | 108.17      | 110.53   |
| 37  | h     | 522 | 0IE  | C13-C12-C11 | 2.65  | 123.17      | 119.01   |
| 31  | 1     | 308 | CLA  | CHB-C4A-NA  | 2.65  | 128.22      | 124.40   |
| 30  | h     | 614 | CHL  | CBC-CAC-C3C | -2.65 | 109.08      | 112.87   |
| 30  | a     | 614 | CHL  | O1D-CGD-CBD | -2.65 | 120.71      | 124.72   |
| 30  | f     | 609 | CHL  | C4-C3-C5    | 2.65  | 119.82      | 115.23   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 4     | 314 | CLA  | O2D-CGD-O1D | -2.65 | 118.70      | 123.85   |
| 30  | d     | 609 | CHL  | C4-C3-C5    | 2.64  | 119.82      | 115.23   |
| 33  | 0     | 502 | 0UR  | C48-C47-C46 | -2.64 | 120.41      | 125.92   |
| 30  | c     | 609 | CHL  | C4-C3-C5    | 2.64  | 119.82      | 115.23   |
| 31  | B     | 830 | CLA  | C3B-C4B-NB  | -2.64 | 108.17      | 110.53   |
| 32  | M     | 102 | 8CT  | C01-C02-C07 | 2.64  | 119.23      | 113.60   |
| 31  | 5     | 311 | CLA  | CHB-C4A-NA  | 2.64  | 128.21      | 124.40   |
| 32  | 4     | 402 | 8CT  | C04-C03-C10 | 2.64  | 122.81      | 115.65   |
| 30  | c     | 609 | CHL  | CMB-C2B-C3B | 2.64  | 129.96      | 124.68   |
| 31  | a     | 610 | CLA  | C1-C2-C3    | -2.64 | 121.87      | 126.20   |
| 30  | c     | 605 | CHL  | O1D-CGD-CBD | -2.64 | 120.72      | 124.72   |
| 31  | L     | 202 | CLA  | C3B-C4B-NB  | -2.64 | 108.17      | 110.53   |
| 31  | a     | 603 | CLA  | C3B-C4B-NB  | -2.64 | 108.17      | 110.53   |
| 30  | 2     | 301 | CHL  | CMB-C2B-C3B | 2.64  | 129.96      | 124.68   |
| 31  | g     | 613 | CLA  | CHB-C4A-NA  | 2.64  | 128.21      | 124.40   |
| 34  | 9     | 601 | LHG  | O8-C23-C24  | 2.64  | 119.88      | 111.83   |
| 31  | 5     | 311 | CLA  | O2D-CGD-O1D | -2.64 | 118.71      | 123.85   |
| 30  | h     | 609 | CHL  | CBC-CAC-C3C | -2.64 | 109.10      | 112.87   |
| 34  | h     | 630 | LHG  | O8-C23-C24  | 2.64  | 119.87      | 111.83   |
| 31  | b     | 603 | CLA  | C3B-C4B-NB  | -2.64 | 108.18      | 110.53   |
| 32  | K     | 107 | 8CT  | C11-C10-C03 | -2.64 | 119.96      | 127.00   |
| 30  | i     | 608 | CHL  | CBC-CAC-C3C | -2.64 | 109.10      | 112.87   |
| 31  | A     | 806 | CLA  | C1-C2-C3    | -2.63 | 121.88      | 126.20   |
| 31  | g     | 604 | CLA  | C3B-C4B-NB  | -2.63 | 108.18      | 110.53   |
| 31  | A     | 843 | CLA  | C3B-C4B-NB  | -2.63 | 108.18      | 110.53   |
| 30  | 9     | 313 | CHL  | O2D-CGD-O1D | -2.63 | 118.72      | 123.85   |
| 30  | b     | 609 | CHL  | CBC-CAC-C3C | -2.63 | 109.10      | 112.87   |
| 32  | G     | 104 | 8CT  | C07-C02-C03 | -2.63 | 119.15      | 122.70   |
| 33  | 0     | 502 | 0UR  | C43-C3-C2   | 2.63  | 122.68      | 116.56   |
| 31  | 3     | 311 | CLA  | CHB-C4A-NA  | 2.63  | 128.20      | 124.40   |
| 30  | 1     | 302 | CHL  | C6-C5-C3    | -2.63 | 107.06      | 113.47   |
| 31  | 0     | 303 | CLA  | C3B-C4B-NB  | -2.63 | 108.18      | 110.53   |
| 30  | 9     | 305 | CHL  | CMA-C3A-C4A | -2.63 | 108.94      | 114.61   |
| 34  | 4     | 601 | LHG  | C26-C25-C24 | 2.63  | 122.79      | 113.13   |
| 31  | B     | 825 | CLA  | CHB-C4A-NA  | 2.63  | 128.19      | 124.40   |
| 30  | 2     | 305 | CHL  | CMA-C3A-C4A | -2.63 | 108.95      | 114.61   |
| 32  | 6     | 402 | 8CT  | C35-C30-C29 | -2.63 | 109.80      | 112.83   |
| 30  | b     | 607 | CHL  | O1D-CGD-CBD | -2.63 | 120.74      | 124.72   |
| 32  | A     | 854 | 8CT  | C27-C26-C25 | -2.63 | 118.56      | 122.82   |
| 37  | a     | 521 | 0IE  | C22-C12-C11 | -2.63 | 118.56      | 122.82   |
| 31  | 9     | 300 | CLA  | C3B-C4B-NB  | -2.63 | 108.18      | 110.53   |
| 37  | g     | 521 | 0IE  | C22-C12-C11 | -2.63 | 118.56      | 122.82   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | B     | 812 | CLA  | C3B-C4B-NB  | -2.63 | 108.19      | 110.53   |
| 30  | 4     | 307 | CHL  | OMC-CMC-C2C | -2.63 | 120.56      | 125.12   |
| 30  | d     | 602 | CHL  | O2A-CGA-CBA | 2.63  | 119.84      | 111.83   |
| 30  | i     | 607 | CHL  | O1D-CGD-CBD | -2.63 | 120.74      | 124.72   |
| 36  | O     | 207 | LMG  | O6-C1-O1    | -2.62 | 103.84      | 110.04   |
| 37  | h     | 521 | 0IE  | C22-C12-C11 | -2.62 | 118.56      | 122.82   |
| 32  | J     | 101 | 8CT  | C39-C16-C15 | 2.62  | 122.10      | 118.09   |
| 30  | 5     | 302 | CHL  | C4-C3-C5    | 2.62  | 119.78      | 115.23   |
| 30  | 6     | 306 | CHL  | O1D-CGD-CBD | -2.62 | 120.75      | 124.72   |
| 34  | 8     | 601 | LHG  | O8-C23-C24  | 2.62  | 119.83      | 111.83   |
| 37  | c     | 522 | 0IE  | C20-C3-C2   | 2.62  | 121.03      | 115.01   |
| 30  | i     | 601 | CHL  | O2D-CGD-O1D | -2.62 | 118.75      | 123.85   |
| 30  | 6     | 308 | CHL  | CMA-C3A-C4A | -2.62 | 108.97      | 114.61   |
| 37  | d     | 521 | 0IE  | C6-C7-C8    | 2.62  | 123.13      | 119.01   |
| 30  | 2     | 302 | CHL  | O1D-CGD-CBD | -2.62 | 120.75      | 124.72   |
| 32  | L     | 206 | 8CT  | C11-C12-C13 | 2.62  | 123.13      | 119.01   |
| 30  | c     | 609 | CHL  | O1D-CGD-CBD | -2.62 | 120.75      | 124.72   |
| 30  | g     | 602 | CHL  | CBC-CAC-C3C | -2.62 | 109.12      | 112.87   |
| 31  | 0     | 321 | CLA  | C3B-C4B-NB  | -2.62 | 108.19      | 110.53   |
| 32  | 7     | 402 | 8CT  | C10-C11-C12 | -2.62 | 122.36      | 126.23   |
| 32  | A     | 846 | 8CT  | C24-C25-C26 | -2.62 | 123.61      | 127.28   |
| 32  | A     | 846 | 8CT  | C01-C02-C07 | 2.62  | 119.17      | 113.60   |
| 31  | A     | 808 | CLA  | CHB-C4A-NA  | 2.61  | 128.17      | 124.40   |
| 30  | h     | 606 | CHL  | O1D-CGD-CBD | -2.61 | 120.76      | 124.72   |
| 31  | B     | 808 | CLA  | CHB-C4A-NA  | 2.61  | 128.17      | 124.40   |
| 37  | f     | 522 | 0IE  | C13-C12-C11 | 2.61  | 123.12      | 119.01   |
| 32  | A     | 854 | 8CT  | C30-C29-C28 | -2.61 | 120.51      | 124.58   |
| 32  | M     | 102 | 8CT  | C14-C15-C16 | -2.61 | 119.20      | 126.36   |
| 37  | f     | 522 | 0IE  | C17-C16-C15 | 2.61  | 123.12      | 119.01   |
| 30  | 0     | 306 | CHL  | O2A-CGA-CBA | 2.61  | 119.80      | 111.83   |
| 31  | 9     | 300 | CLA  | CHB-C4A-NA  | 2.61  | 128.17      | 124.40   |
| 30  | g     | 609 | CHL  | CBC-CAC-C3C | -2.61 | 109.14      | 112.87   |
| 31  | A     | 819 | CLA  | CMB-C2B-C1B | -2.61 | 121.44      | 125.42   |
| 30  | d     | 614 | CHL  | CBC-CAC-C3C | -2.61 | 109.14      | 112.87   |
| 32  | 8     | 402 | 8CT  | C11-C10-C03 | -2.61 | 120.03      | 127.00   |
| 31  | e     | 611 | CLA  | C3B-C4B-NB  | -2.61 | 108.20      | 110.53   |
| 30  | h     | 602 | CHL  | O1D-CGD-CBD | -2.61 | 120.77      | 124.72   |
| 31  | i     | 611 | CLA  | CHB-C4A-NA  | 2.61  | 128.16      | 124.40   |
| 31  | 3     | 304 | CLA  | C3B-C4B-NB  | -2.61 | 108.20      | 110.53   |
| 31  | B     | 823 | CLA  | C3B-C4B-NB  | -2.61 | 108.20      | 110.53   |
| 30  | 7     | 306 | CHL  | C4-C3-C5    | 2.61  | 119.75      | 115.23   |
| 32  | A     | 854 | 8CT  | C24-C23-C21 | -2.61 | 119.22      | 126.36   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 8     | 309 | CLA  | C1-C2-C3    | -2.61 | 121.93      | 126.20   |
| 30  | 7     | 302 | CHL  | O1D-CGD-CBD | -2.61 | 120.77      | 124.72   |
| 30  | h     | 607 | CHL  | O1D-CGD-CBD | -2.61 | 120.77      | 124.72   |
| 33  | a     | 520 | 0UR  | C4-C5-C6    | -2.61 | 115.65      | 123.20   |
| 30  | 5     | 306 | CHL  | O1D-CGD-CBD | -2.61 | 120.77      | 124.72   |
| 30  | g     | 605 | CHL  | O1D-CGD-CBD | -2.61 | 120.77      | 124.72   |
| 31  | b     | 611 | CLA  | C3B-C4B-NB  | -2.61 | 108.20      | 110.53   |
| 30  | i     | 605 | CHL  | O1D-CGD-CBD | -2.61 | 120.77      | 124.72   |
| 33  | 3     | 501 | 0UR  | C18-C17-C16 | -2.61 | 120.72      | 126.32   |
| 32  | 9     | 401 | 8CT  | C25-C24-C23 | -2.60 | 115.65      | 123.20   |
| 33  | d     | 520 | 0UR  | C43-C3-C4   | -2.60 | 121.96      | 125.03   |
| 30  | i     | 608 | CHL  | OMC-CMC-C2C | -2.60 | 120.60      | 125.12   |
| 30  | b     | 608 | CHL  | C4-C3-C5    | 2.60  | 119.75      | 115.23   |
| 31  | f     | 604 | CLA  | C3B-C4B-NB  | -2.60 | 108.20      | 110.53   |
| 33  | 7     | 501 | 0UR  | C10-C9-C8   | -2.60 | 118.19      | 123.52   |
| 36  | 9     | 602 | LMG  | O6-C1-O1    | -2.60 | 103.89      | 110.04   |
| 31  | A     | 820 | CLA  | CHB-C4A-NA  | 2.60  | 128.16      | 124.40   |
| 30  | b     | 602 | CHL  | O2D-CGD-O1D | -2.60 | 118.78      | 123.85   |
| 31  | 2     | 312 | CLA  | C3B-C4B-NB  | -2.60 | 108.21      | 110.53   |
| 33  | 3     | 501 | 0UR  | C48-C47-C46 | -2.60 | 120.50      | 125.92   |
| 32  | 3     | 402 | 8CT  | C15-C16-C17 | -2.60 | 114.92      | 119.01   |
| 30  | 6     | 301 | CHL  | O2D-CGD-O1D | -2.60 | 118.78      | 123.85   |
| 31  | A     | 840 | CLA  | O2A-CGA-O1A | -2.60 | 117.12      | 123.63   |
| 30  | 4     | 306 | CHL  | O2A-CGA-CBA | 2.60  | 119.76      | 111.83   |
| 31  | 7     | 310 | CLA  | CAA-C2A-C3A | -2.60 | 110.27      | 116.23   |
| 32  | B     | 804 | 8CT  | C18-C19-C20 | -2.60 | 118.20      | 123.52   |
| 31  | O     | 202 | CLA  | O2D-CGD-O1D | -2.60 | 118.18      | 124.08   |
| 33  | e     | 520 | 0UR  | C48-C47-C46 | -2.60 | 120.51      | 125.92   |
| 32  | B     | 846 | 8CT  | C25-C24-C23 | 2.60  | 130.73      | 123.20   |
| 33  | 2     | 501 | 0UR  | C15-C14-C13 | -2.60 | 115.67      | 123.20   |
| 33  | f     | 520 | 0UR  | C4-C3-C2    | -2.60 | 117.90      | 120.16   |
| 33  | 0     | 502 | 0UR  | C34-C27-C26 | 2.60  | 119.20      | 114.42   |
| 31  | 5     | 309 | CLA  | CMB-C2B-C1B | -2.60 | 121.46      | 125.42   |
| 33  | 4     | 502 | 0UR  | C15-C14-C13 | -2.60 | 115.68      | 123.20   |
| 31  | A     | 811 | CLA  | C3B-C4B-NB  | -2.60 | 108.21      | 110.53   |
| 30  | i     | 609 | CHL  | O1D-CGD-CBD | -2.60 | 120.79      | 124.72   |
| 31  | i     | 610 | CLA  | C1-C2-C3    | -2.59 | 121.95      | 126.20   |
| 33  | b     | 520 | 0UR  | C4-C5-C6    | -2.59 | 115.68      | 123.20   |
| 33  | f     | 520 | 0UR  | C14-C13-C12 | -2.59 | 119.25      | 126.36   |
| 31  | B     | 837 | CLA  | C3B-C4B-NB  | -2.59 | 108.22      | 110.53   |
| 31  | 0     | 312 | CLA  | CHB-C4A-NA  | 2.59  | 128.14      | 124.40   |
| 30  | 8     | 302 | CHL  | CMB-C2B-C3B | 2.59  | 129.86      | 124.68   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | f     | 611 | CLA  | C3B-C4B-NB  | -2.59 | 108.22      | 110.53   |
| 30  | 2     | 302 | CHL  | CBC-CAC-C3C | -2.59 | 109.16      | 112.87   |
| 30  | 7     | 301 | CHL  | CBC-CAC-C3C | -2.59 | 109.16      | 112.87   |
| 30  | 9     | 305 | CHL  | O1D-CGD-CBD | -2.59 | 120.79      | 124.72   |
| 30  | 4     | 308 | CHL  | O2D-CGD-O1D | -2.59 | 118.81      | 123.85   |
| 30  | c     | 602 | CHL  | CBC-CAC-C3C | -2.59 | 109.16      | 112.87   |
| 30  | 3     | 307 | CHL  | C4-C3-C5    | 2.59  | 119.72      | 115.23   |
| 31  | 9     | 308 | CLA  | CHB-C4A-NA  | 2.59  | 128.14      | 124.40   |
| 31  | 3     | 303 | CLA  | C3B-C4B-NB  | -2.59 | 108.22      | 110.53   |
| 32  | B     | 844 | 8CT  | C30-C29-C28 | -2.59 | 120.55      | 124.58   |
| 31  | b     | 612 | CLA  | C3B-C4B-NB  | -2.59 | 108.22      | 110.53   |
| 32  | A     | 848 | 8CT  | C10-C03-C02 | -2.59 | 115.59      | 121.56   |
| 32  | 1     | 402 | 8CT  | C14-C15-C16 | -2.59 | 119.27      | 126.36   |
| 31  | 1     | 311 | CLA  | CHB-C4A-NA  | 2.59  | 128.13      | 124.40   |
| 37  | c     | 521 | 0IE  | C22-C12-C11 | -2.59 | 118.63      | 122.82   |
| 30  | 3     | 302 | CHL  | O1D-CGD-CBD | -2.59 | 120.80      | 124.72   |
| 31  | 6     | 314 | CLA  | C3B-C4B-NB  | -2.59 | 108.22      | 110.53   |
| 32  | 8     | 402 | 8CT  | C25-C24-C23 | -2.59 | 115.71      | 123.20   |
| 30  | 6     | 305 | CHL  | CBC-CAC-C3C | -2.58 | 109.17      | 112.87   |
| 32  | K     | 107 | 8CT  | C11-C12-C13 | 2.58  | 123.07      | 119.01   |
| 33  | 5     | 502 | 0UR  | C9-C10-C11  | -2.58 | 118.23      | 123.52   |
| 31  | c     | 612 | CLA  | CHB-C4A-NA  | 2.58  | 128.13      | 124.40   |
| 31  | e     | 604 | CLA  | C3B-C4B-NB  | -2.58 | 108.22      | 110.53   |
| 37  | b     | 521 | 0IE  | C21-C7-C8   | -2.58 | 118.63      | 122.82   |
| 30  | 8     | 306 | CHL  | O2A-CGA-CBA | 2.58  | 119.71      | 111.83   |
| 31  | 1     | 304 | CLA  | C3B-C4B-NB  | -2.58 | 108.23      | 110.53   |
| 30  | g     | 609 | CHL  | CMB-C2B-C3B | 2.58  | 129.84      | 124.68   |
| 31  | A     | 831 | CLA  | CHB-C4A-NA  | 2.58  | 128.12      | 124.40   |
| 33  | 8     | 501 | 0UR  | C43-C3-C4   | -2.58 | 121.99      | 125.03   |
| 31  | A     | 818 | CLA  | C3B-C4B-NB  | -2.58 | 108.23      | 110.53   |
| 32  | 7     | 405 | 8CT  | C11-C10-C03 | -2.58 | 120.11      | 127.00   |
| 37  | 7     | 502 | 0IE  | C6-C7-C8    | 2.58  | 123.06      | 119.01   |
| 31  | 7     | 317 | CLA  | C3B-C4B-NB  | -2.58 | 108.23      | 110.53   |
| 33  | a     | 520 | 0UR  | C28-C19-C18 | -2.58 | 109.86      | 112.83   |
| 31  | 5     | 312 | CLA  | C3B-C4B-NB  | -2.58 | 108.23      | 110.53   |
| 30  | 3     | 307 | CHL  | O1D-CGD-CBD | -2.58 | 120.82      | 124.72   |
| 37  | f     | 521 | 0IE  | C22-C12-C11 | -2.58 | 118.64      | 122.82   |
| 30  | 5     | 302 | CHL  | O1D-CGD-CBD | -2.58 | 120.82      | 124.72   |
| 33  | a     | 520 | 0UR  | C43-C3-C4   | -2.57 | 121.99      | 125.03   |
| 31  | 4     | 304 | CLA  | C3B-C4B-NB  | -2.57 | 108.23      | 110.53   |
| 30  | f     | 614 | CHL  | OMC-CMC-C2C | -2.57 | 120.65      | 125.12   |
| 31  | B     | 813 | CLA  | CHB-C4A-NA  | 2.57  | 128.11      | 124.40   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | b     | 601 | CHL  | C4-C3-C5    | 2.57  | 119.69      | 115.23   |
| 30  | g     | 606 | CHL  | C1B-CHB-C4A | 2.57  | 122.98      | 121.32   |
| 30  | 3     | 305 | CHL  | O2D-CGD-O1D | -2.57 | 118.84      | 123.85   |
| 30  | 5     | 313 | CHL  | CMB-C2B-C3B | 2.57  | 129.82      | 124.68   |
| 30  | c     | 608 | CHL  | C4-C3-C5    | 2.57  | 119.69      | 115.23   |
| 31  | d     | 604 | CLA  | C3B-C4B-NB  | -2.57 | 108.24      | 110.53   |
| 31  | 1     | 303 | CLA  | CHB-C4A-NA  | 2.57  | 128.11      | 124.40   |
| 33  | i     | 520 | 0UR  | C15-C14-C13 | -2.57 | 115.76      | 123.20   |
| 30  | i     | 614 | CHL  | CBC-CAC-C3C | -2.57 | 109.20      | 112.87   |
| 30  | a     | 609 | CHL  | O1D-CGD-CBD | -2.57 | 120.83      | 124.72   |
| 33  | 6     | 501 | 0UR  | C43-C3-C2   | 2.57  | 122.53      | 116.56   |
| 37  | b     | 521 | 0IE  | C22-C12-C11 | -2.57 | 118.66      | 122.82   |
| 31  | 6     | 310 | CLA  | C1-C2-C3    | -2.57 | 121.99      | 126.20   |
| 37  | b     | 521 | 0IE  | C23-C16-C17 | 2.57  | 122.01      | 118.09   |
| 31  | B     | 816 | CLA  | CHB-C4A-NA  | 2.57  | 128.10      | 124.40   |
| 31  | 9     | 303 | CLA  | C3B-C4B-NB  | -2.56 | 108.24      | 110.53   |
| 31  | B     | 835 | CLA  | C3B-C4B-NB  | -2.56 | 108.24      | 110.53   |
| 30  | 2     | 301 | CHL  | O2D-CGD-O1D | -2.56 | 118.86      | 123.85   |
| 30  | g     | 608 | CHL  | CBC-CAC-C3C | -2.56 | 109.20      | 112.87   |
| 33  | 4     | 501 | 0UR  | C4-C5-C6    | -2.56 | 115.78      | 123.20   |
| 31  | 5     | 303 | CLA  | CHB-C4A-NA  | 2.56  | 128.10      | 124.40   |
| 37  | g     | 522 | 0IE  | C4-C5-C6    | 2.56  | 130.62      | 123.20   |
| 31  | B     | 818 | CLA  | CHB-C4A-NA  | 2.56  | 128.10      | 124.40   |
| 30  | i     | 601 | CHL  | O1D-CGD-CBD | -2.56 | 120.84      | 124.72   |
| 30  | 8     | 301 | CHL  | CBC-CAC-C3C | -2.56 | 109.21      | 112.87   |
| 31  | B     | 832 | CLA  | CAA-CBA-CGA | -2.56 | 105.94      | 113.21   |
| 30  | e     | 609 | CHL  | CMB-C2B-C3B | 2.56  | 129.80      | 124.68   |
| 31  | h     | 611 | CLA  | CAA-C2A-C3A | -2.56 | 110.36      | 116.23   |
| 31  | 0     | 321 | CLA  | CHB-C4A-NA  | 2.56  | 128.09      | 124.40   |
| 31  | a     | 612 | CLA  | CHB-C4A-NA  | 2.56  | 128.09      | 124.40   |
| 33  | 7     | 501 | 0UR  | C15-C14-C13 | -2.56 | 115.79      | 123.20   |
| 31  | 9     | 309 | CLA  | C1-C2-C3    | -2.56 | 122.01      | 126.20   |
| 31  | 3     | 309 | CLA  | CHB-C4A-NA  | 2.56  | 128.09      | 124.40   |
| 31  | c     | 604 | CLA  | C3B-C4B-NB  | -2.56 | 108.25      | 110.53   |
| 30  | g     | 606 | CHL  | O2D-CGD-O1D | -2.56 | 118.87      | 123.85   |
| 37  | c     | 522 | 0IE  | C15-C14-C13 | 2.56  | 130.60      | 123.20   |
| 32  | 0     | 401 | 8CT  | C29-C28-C26 | -2.55 | 120.83      | 126.32   |
| 30  | 3     | 302 | CHL  | C4-C3-C5    | 2.55  | 119.66      | 115.23   |
| 32  | L     | 209 | 8CT  | C22-C21-C23 | 2.55  | 121.99      | 118.09   |
| 30  | 4     | 319 | CHL  | CMB-C2B-C3B | 2.55  | 129.79      | 124.68   |
| 31  | B     | 808 | CLA  | CMB-C2B-C1B | -2.55 | 121.53      | 125.42   |
| 32  | B     | 845 | 8CT  | C11-C10-C03 | -2.55 | 120.18      | 127.00   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | g     | 608 | CHL  | CMB-C2B-C3B | 2.55  | 129.78      | 124.68   |
| 30  | 4     | 308 | CHL  | CMB-C2B-C3B | 2.55  | 129.78      | 124.68   |
| 31  | A     | 831 | CLA  | C1-C2-C3    | -2.55 | 122.63      | 126.76   |
| 37  | e     | 521 | 0IE  | C22-C12-C11 | -2.55 | 118.68      | 122.82   |
| 31  | 9     | 304 | CLA  | C3B-C4B-NB  | -2.55 | 108.25      | 110.53   |
| 31  | 6     | 303 | CLA  | C3B-C4B-NB  | -2.55 | 108.25      | 110.53   |
| 31  | B     | 806 | CLA  | CHB-C4A-NA  | 2.55  | 128.08      | 124.40   |
| 36  | A     | 856 | LMG  | O6-C5-C4    | 2.55  | 114.29      | 109.70   |
| 30  | h     | 608 | CHL  | CMB-C2B-C3B | 2.55  | 129.78      | 124.68   |
| 33  | 4     | 501 | 0UR  | O44-C43-C3  | 2.55  | 115.72      | 109.09   |
| 31  | 2     | 311 | CLA  | CHB-C4A-NA  | 2.55  | 128.08      | 124.40   |
| 30  | h     | 609 | CHL  | O2D-CGD-O1D | -2.55 | 118.89      | 123.85   |
| 31  | 9     | 303 | CLA  | CHB-C4A-NA  | 2.55  | 128.07      | 124.40   |
| 32  | M     | 102 | 8CT  | C18-C19-C20 | -2.55 | 118.31      | 123.52   |
| 30  | 9     | 301 | CHL  | OMC-CMC-C2C | -2.55 | 120.70      | 125.12   |
| 31  | B     | 821 | CLA  | CHB-C4A-NA  | 2.55  | 128.07      | 124.40   |
| 30  | i     | 602 | CHL  | O2D-CGD-O1D | -2.55 | 118.89      | 123.85   |
| 32  | B     | 846 | 8CT  | C22-C21-C20 | -2.55 | 118.69      | 122.82   |
| 42  | e     | 523 | NEX  | C26-C27-C28 | -2.54 | 120.61      | 125.99   |
| 31  | h     | 603 | CLA  | C3B-C4B-NB  | -2.54 | 108.26      | 110.53   |
| 30  | d     | 608 | CHL  | OMC-CMC-C2C | -2.54 | 120.70      | 125.12   |
| 30  | 4     | 308 | CHL  | CMA-C3A-C4A | -2.54 | 109.13      | 114.61   |
| 33  | 6     | 502 | 0UR  | C28-C19-C18 | 2.54  | 115.75      | 112.83   |
| 31  | 0     | 309 | CLA  | CHB-C4A-NA  | 2.54  | 128.07      | 124.40   |
| 31  | A     | 827 | CLA  | CHB-C4A-NA  | 2.54  | 128.07      | 124.40   |
| 30  | 4     | 302 | CHL  | O1D-CGD-CBD | -2.54 | 120.87      | 124.72   |
| 30  | e     | 614 | CHL  | C4D-CHA-CBD | -2.54 | 106.41      | 108.97   |
| 30  | b     | 601 | CHL  | CMB-C2B-C3B | 2.54  | 129.76      | 124.68   |
| 30  | 6     | 301 | CHL  | C4-C3-C5    | 2.54  | 119.64      | 115.23   |
| 32  | K     | 107 | 8CT  | C40-C12-C13 | -2.54 | 118.70      | 122.82   |
| 31  | 3     | 318 | CLA  | CHB-C4A-NA  | 2.54  | 128.06      | 124.40   |
| 39  | A     | 857 | CL0  | C4C-CHD-C1D | 2.54  | 125.16      | 116.07   |
| 30  | c     | 606 | CHL  | CMB-C2B-C3B | 2.54  | 129.76      | 124.68   |
| 36  | 2     | 602 | LMG  | O6-C1-O1    | -2.54 | 104.05      | 110.04   |
| 31  | A     | 817 | CLA  | CHB-C4A-NA  | 2.54  | 128.06      | 124.40   |
| 32  | 4     | 402 | 8CT  | C01-C02-C07 | 2.54  | 119.01      | 113.60   |
| 30  | i     | 608 | CHL  | CMB-C2B-C3B | 2.54  | 129.75      | 124.68   |
| 33  | f     | 520 | 0UR  | C5-C4-C3    | -2.54 | 123.88      | 126.92   |
| 33  | 4     | 501 | 0UR  | C14-C15-C16 | -2.54 | 123.72      | 127.28   |
| 31  | i     | 612 | CLA  | C3B-C4B-NB  | -2.54 | 108.27      | 110.53   |
| 31  | H     | 204 | CLA  | CHB-C4A-NA  | 2.53  | 128.06      | 124.40   |
| 31  | b     | 612 | CLA  | CHB-C4A-NA  | 2.53  | 128.06      | 124.40   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | 1     | 313 | CHL  | CMB-C2B-C3B | 2.53  | 129.75      | 124.68   |
| 30  | 1     | 307 | CHL  | O1D-CGD-CBD | -2.53 | 120.88      | 124.72   |
| 30  | 5     | 313 | CHL  | O2D-CGD-O1D | -2.53 | 118.92      | 123.85   |
| 32  | 2     | 402 | 8CT  | C24-C23-C21 | -2.53 | 119.42      | 126.36   |
| 33  | 9     | 501 | 0UR  | C28-C19-C18 | -2.53 | 109.91      | 112.83   |
| 30  | 5     | 305 | CHL  | CMB-C2B-C3B | 2.53  | 129.74      | 124.68   |
| 30  | b     | 606 | CHL  | CMB-C2B-C3B | 2.53  | 129.74      | 124.68   |
| 31  | a     | 603 | CLA  | CHB-C4A-NA  | 2.53  | 128.05      | 124.40   |
| 31  | h     | 610 | CLA  | CHB-C4A-NA  | 2.53  | 128.05      | 124.40   |
| 30  | e     | 608 | CHL  | C1-C2-C3    | -2.53 | 122.05      | 126.20   |
| 31  | B     | 828 | CLA  | C3B-C4B-NB  | -2.53 | 108.27      | 110.53   |
| 31  | h     | 611 | CLA  | C3B-C4B-NB  | -2.53 | 108.27      | 110.53   |
| 30  | d     | 606 | CHL  | CBC-CAC-C3C | -2.53 | 109.25      | 112.87   |
| 30  | 2     | 306 | CHL  | O2D-CGD-O1D | -2.53 | 118.92      | 123.85   |
| 30  | e     | 614 | CHL  | O1D-CGD-CBD | -2.53 | 120.89      | 124.72   |
| 30  | c     | 605 | CHL  | CBC-CAC-C3C | -2.53 | 109.25      | 112.87   |
| 31  | B     | 806 | CLA  | CAC-C3C-C4C | 2.53  | 128.08      | 124.79   |
| 30  | 5     | 313 | CHL  | CBC-CAC-C3C | -2.53 | 109.25      | 112.87   |
| 30  | i     | 606 | CHL  | CBC-CAC-C3C | -2.53 | 109.25      | 112.87   |
| 31  | 0     | 310 | CLA  | CAA-C2A-C3A | -2.53 | 110.43      | 116.23   |
| 32  | L     | 205 | 8CT  | C05-C04-C03 | 2.53  | 114.11      | 110.44   |
| 30  | 6     | 308 | CHL  | O1D-CGD-CBD | -2.53 | 120.89      | 124.72   |
| 32  | 1     | 402 | 8CT  | C11-C10-C03 | -2.53 | 120.25      | 127.00   |
| 31  | 1     | 312 | CLA  | C3B-C4B-NB  | -2.52 | 108.28      | 110.53   |
| 32  | L     | 206 | 8CT  | C30-C31-C32 | -2.52 | 118.36      | 121.47   |
| 31  | A     | 809 | CLA  | O2A-CGA-O1A | -2.52 | 117.31      | 123.63   |
| 30  | 8     | 305 | CHL  | CMA-C3A-C4A | -2.52 | 109.17      | 114.61   |
| 31  | e     | 612 | CLA  | C3B-C4B-NB  | -2.52 | 108.28      | 110.53   |
| 30  | e     | 605 | CHL  | O1D-CGD-CBD | -2.52 | 120.90      | 124.72   |
| 31  | 8     | 314 | CLA  | CHB-C4A-NA  | 2.52  | 128.04      | 124.40   |
| 32  | M     | 102 | 8CT  | C11-C10-C03 | -2.52 | 120.26      | 127.00   |
| 31  | 4     | 311 | CLA  | CHB-C4A-NA  | 2.52  | 128.04      | 124.40   |
| 30  | a     | 614 | CHL  | CMB-C2B-C3B | 2.52  | 129.72      | 124.68   |
| 37  | a     | 521 | 0IE  | C4-C3-C2    | -2.52 | 117.96      | 120.16   |
| 31  | 7     | 309 | CLA  | CHB-C4A-NA  | 2.52  | 128.04      | 124.40   |
| 30  | h     | 606 | CHL  | CBC-CAC-C3C | -2.52 | 109.26      | 112.87   |
| 31  | i     | 604 | CLA  | CHB-C4A-NA  | 2.52  | 128.04      | 124.40   |
| 31  | 3     | 309 | CLA  | CMB-C2B-C1B | -2.52 | 121.58      | 125.42   |
| 31  | 9     | 309 | CLA  | CHB-C4A-NA  | 2.52  | 128.04      | 124.40   |
| 31  | B     | 831 | CLA  | C1-C2-C3    | -2.52 | 122.69      | 126.76   |
| 30  | f     | 606 | CHL  | O2D-CGD-O1D | -2.52 | 118.95      | 123.85   |
| 31  | h     | 603 | CLA  | CHB-C4A-NA  | 2.52  | 128.03      | 124.40   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | e     | 605 | CHL  | CBC-CAC-C3C | -2.52 | 109.27      | 112.87   |
| 30  | h     | 614 | CHL  | CMB-C2B-C3B | 2.52  | 129.71      | 124.68   |
| 30  | 2     | 313 | CHL  | CMB-C2B-C3B | 2.52  | 129.71      | 124.68   |
| 30  | 4     | 305 | CHL  | O2D-CGD-O1D | -2.52 | 118.95      | 123.85   |
| 30  | a     | 607 | CHL  | CBC-CAC-C3C | -2.52 | 109.27      | 112.87   |
| 30  | f     | 605 | CHL  | O1D-CGD-CBD | -2.52 | 120.91      | 124.72   |
| 32  | O     | 205 | 8CT  | C18-C19-C20 | -2.51 | 118.37      | 123.52   |
| 30  | b     | 614 | CHL  | CBC-CAC-C3C | -2.51 | 109.27      | 112.87   |
| 30  | 1     | 306 | CHL  | O1D-CGD-CBD | -2.51 | 120.91      | 124.72   |
| 30  | 6     | 307 | CHL  | O1D-CGD-CBD | -2.51 | 120.91      | 124.72   |
| 31  | A     | 825 | CLA  | C1-C2-C3    | -2.51 | 122.08      | 126.20   |
| 30  | d     | 602 | CHL  | CMB-C2B-C3B | 2.51  | 129.71      | 124.68   |
| 30  | f     | 608 | CHL  | CMB-C2B-C3B | 2.51  | 129.70      | 124.68   |
| 31  | f     | 612 | CLA  | CHB-C4A-NA  | 2.51  | 128.03      | 124.40   |
| 31  | A     | 815 | CLA  | CHB-C4A-NA  | 2.51  | 128.03      | 124.40   |
| 31  | e     | 612 | CLA  | CHB-C4A-NA  | 2.51  | 128.02      | 124.40   |
| 30  | 2     | 319 | CHL  | CMB-C2B-C3B | 2.51  | 129.70      | 124.68   |
| 33  | 1     | 501 | 0UR  | C4-C3-C2    | -2.51 | 117.97      | 120.16   |
| 31  | 0     | 311 | CLA  | O2A-CGA-O1A | -2.51 | 117.35      | 123.63   |
| 30  | d     | 614 | CHL  | CMB-C2B-C3B | 2.51  | 129.70      | 124.68   |
| 30  | e     | 605 | CHL  | CMB-C2B-C3B | 2.51  | 129.70      | 124.68   |
| 32  | 1     | 402 | 8CT  | C01-C02-C07 | 2.51  | 118.95      | 113.60   |
| 31  | 7     | 315 | CLA  | CHB-C4A-NA  | 2.51  | 128.02      | 124.40   |
| 30  | i     | 614 | CHL  | CMB-C2B-C3B | 2.51  | 129.70      | 124.68   |
| 30  | e     | 607 | CHL  | O2D-CGD-O1D | -2.51 | 118.97      | 123.85   |
| 31  | a     | 613 | CLA  | CHB-C4A-NA  | 2.51  | 128.02      | 124.40   |
| 30  | 5     | 307 | CHL  | O1D-CGD-CBD | -2.51 | 120.92      | 124.72   |
| 30  | c     | 602 | CHL  | O2D-CGD-O1D | -2.51 | 118.97      | 123.85   |
| 31  | g     | 613 | CLA  | C3B-C4B-NB  | -2.51 | 108.29      | 110.53   |
| 30  | e     | 614 | CHL  | CBC-CAC-C3C | -2.51 | 109.28      | 112.87   |
| 30  | d     | 608 | CHL  | CMB-C2B-C3B | 2.51  | 129.69      | 124.68   |
| 33  | f     | 520 | 0UR  | C4-C5-C6    | -2.51 | 115.94      | 123.20   |
| 30  | i     | 609 | CHL  | CMA-C3A-C4A | -2.51 | 109.21      | 114.61   |
| 30  | 7     | 313 | CHL  | CMB-C2B-C3B | 2.51  | 129.69      | 124.68   |
| 31  | B     | 815 | CLA  | CHB-C4A-NA  | 2.50  | 128.01      | 124.40   |
| 31  | B     | 827 | CLA  | CHB-C4A-NA  | 2.50  | 128.01      | 124.40   |
| 32  | J     | 104 | 8CT  | C04-C03-C02 | -2.50 | 119.21      | 122.64   |
| 33  | 9     | 501 | 0UR  | C4-C5-C6    | -2.50 | 115.94      | 123.20   |
| 30  | 7     | 307 | CHL  | O2A-CGA-CBA | 2.50  | 119.47      | 111.83   |
| 30  | 7     | 306 | CHL  | O2D-CGD-O1D | -2.50 | 118.98      | 123.85   |
| 30  | h     | 602 | CHL  | O2D-CGD-O1D | -2.50 | 118.98      | 123.85   |
| 32  | 3     | 402 | 8CT  | C04-C03-C10 | 2.50  | 122.44      | 115.65   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | 1     | 302 | CHL  | CMD-C2D-C3D | -2.50 | 119.68      | 124.68   |
| 30  | 9     | 301 | CHL  | CMB-C2B-C3B | 2.50  | 129.68      | 124.68   |
| 30  | h     | 609 | CHL  | CMB-C2B-C3B | 2.50  | 129.68      | 124.68   |
| 30  | 9     | 306 | CHL  | CMB-C2B-C3B | 2.50  | 129.68      | 124.68   |
| 30  | e     | 601 | CHL  | CMB-C2B-C3B | 2.50  | 129.68      | 124.68   |
| 36  | J     | 105 | LMG  | C40-C39-C38 | -2.50 | 101.73      | 114.37   |
| 42  | e     | 523 | NEX  | O24-C25-C26 | -2.50 | 56.95       | 58.93    |
| 30  | b     | 602 | CHL  | CMA-C3A-C4A | -2.50 | 109.22      | 114.61   |
| 31  | A     | 839 | CLA  | CHB-C4A-NA  | 2.50  | 128.01      | 124.40   |
| 30  | i     | 605 | CHL  | CMB-C2B-C3B | 2.50  | 129.68      | 124.68   |
| 30  | 2     | 313 | CHL  | CBC-CAC-C3C | -2.50 | 109.30      | 112.87   |
| 31  | J     | 103 | CLA  | CHB-C4A-NA  | 2.50  | 128.00      | 124.40   |
| 33  | 2     | 501 | 0UR  | C10-C9-C8   | -2.50 | 118.41      | 123.52   |
| 31  | 6     | 311 | CLA  | CHB-C4A-NA  | 2.50  | 128.00      | 124.40   |
| 31  | K     | 102 | CLA  | CHB-C4A-NA  | 2.50  | 128.00      | 124.40   |
| 30  | c     | 602 | CHL  | CMB-C2B-C3B | 2.50  | 129.67      | 124.68   |
| 31  | B     | 836 | CLA  | CMB-C2B-C1B | -2.50 | 121.62      | 125.42   |
| 31  | 4     | 310 | CLA  | CHB-C4A-NA  | 2.50  | 128.00      | 124.40   |
| 30  | 6     | 302 | CHL  | C4-C3-C5    | 2.50  | 119.56      | 115.23   |
| 30  | a     | 608 | CHL  | CMB-C2B-C3B | 2.50  | 129.67      | 124.68   |
| 31  | B     | 810 | CLA  | C3B-C4B-NB  | -2.49 | 108.30      | 110.53   |
| 32  | 8     | 402 | 8CT  | C01-C02-C07 | 2.49  | 118.92      | 113.60   |
| 31  | 5     | 312 | CLA  | CHB-C4A-NA  | 2.49  | 128.00      | 124.40   |
| 31  | g     | 610 | CLA  | CHB-C4A-NA  | 2.49  | 128.00      | 124.40   |
| 31  | B     | 830 | CLA  | CHB-C1B-NB  | 2.49  | 127.79      | 124.05   |
| 30  | e     | 608 | CHL  | CMB-C2B-C3B | 2.49  | 129.67      | 124.68   |
| 36  | 9     | 602 | LMG  | O1-C7-C8    | -2.49 | 104.75      | 110.82   |
| 30  | g     | 601 | CHL  | O2D-CGD-O1D | -2.49 | 119.00      | 123.85   |
| 30  | 6     | 315 | CHL  | CMB-C2B-C3B | 2.49  | 129.66      | 124.68   |
| 33  | b     | 520 | 0UR  | C15-C14-C13 | -2.49 | 115.98      | 123.20   |
| 31  | H     | 204 | CLA  | C3B-C4B-NB  | -2.49 | 108.31      | 110.53   |
| 30  | d     | 601 | CHL  | O2D-CGD-O1D | -2.49 | 119.00      | 123.85   |
| 31  | A     | 809 | CLA  | CHB-C4A-NA  | 2.49  | 128.00      | 124.40   |
| 31  | B     | 820 | CLA  | CHB-C4A-NA  | 2.49  | 128.00      | 124.40   |
| 31  | K     | 104 | CLA  | CHB-C4A-NA  | 2.49  | 128.00      | 124.40   |
| 30  | g     | 605 | CHL  | CMB-C2B-C3B | 2.49  | 129.66      | 124.68   |
| 31  | c     | 604 | CLA  | CHB-C4A-NA  | 2.49  | 127.99      | 124.40   |
| 30  | 1     | 306 | CHL  | O2D-CGD-O1D | -2.49 | 119.00      | 123.85   |
| 30  | 4     | 313 | CHL  | CMB-C2B-C3B | 2.49  | 129.66      | 124.68   |
| 30  | 2     | 302 | CHL  | C4-C3-C5    | 2.49  | 119.55      | 115.23   |
| 30  | d     | 605 | CHL  | CMB-C2B-C3B | 2.49  | 129.66      | 124.68   |
| 31  | B     | 837 | CLA  | CHB-C4A-NA  | 2.49  | 127.99      | 124.40   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | H     | 201 | CLA  | C1-C2-C3    | -2.49 | 122.12      | 126.20   |
| 37  | d     | 521 | 0IE  | C23-C16-C17 | 2.49  | 121.89      | 118.09   |
| 31  | O     | 203 | CLA  | CMB-C2B-C3B | 2.49  | 130.14      | 123.53   |
| 30  | c     | 605 | CHL  | CMB-C2B-C3B | 2.49  | 129.65      | 124.68   |
| 31  | A     | 837 | CLA  | CHB-C4A-NA  | 2.48  | 127.98      | 124.40   |
| 31  | L     | 201 | CLA  | CHB-C4A-NA  | 2.48  | 127.98      | 124.40   |
| 30  | g     | 614 | CHL  | C4D-CHA-CBD | -2.48 | 106.46      | 108.97   |
| 31  | A     | 818 | CLA  | CHB-C4A-NA  | 2.48  | 127.98      | 124.40   |
| 30  | 0     | 305 | CHL  | O2D-CGD-O1D | -2.48 | 119.02      | 123.85   |
| 31  | 0     | 304 | CLA  | C3B-C4B-NB  | -2.48 | 108.31      | 110.53   |
| 30  | g     | 614 | CHL  | CBC-CAC-C3C | -2.48 | 109.32      | 112.87   |
| 30  | 8     | 302 | CHL  | CMA-C3A-C4A | -2.48 | 109.26      | 114.61   |
| 30  | h     | 605 | CHL  | CBC-CAC-C3C | -2.48 | 109.32      | 112.87   |
| 30  | 8     | 315 | CHL  | O2D-CGD-O1D | -2.48 | 119.02      | 123.85   |
| 32  | B     | 847 | 8CT  | C04-C03-C02 | -2.48 | 119.25      | 122.64   |
| 30  | 5     | 313 | CHL  | C1B-CHB-C4A | -2.48 | 119.73      | 121.32   |
| 30  | 9     | 306 | CHL  | CMA-C3A-C4A | -2.48 | 109.27      | 114.61   |
| 31  | G     | 101 | CLA  | CHB-C4A-NA  | 2.48  | 127.98      | 124.40   |
| 37  | g     | 521 | 0IE  | C13-C12-C11 | 2.48  | 122.91      | 119.01   |
| 32  | B     | 848 | 8CT  | C01-C02-C07 | 2.48  | 118.88      | 113.60   |
| 31  | 5     | 304 | CLA  | C3B-C4B-NB  | -2.48 | 108.32      | 110.53   |
| 31  | 6     | 310 | CLA  | CHB-C4A-NA  | 2.48  | 127.98      | 124.40   |
| 30  | 7     | 313 | CHL  | O2D-CGD-O1D | -2.48 | 119.02      | 123.85   |
| 31  | 1     | 309 | CLA  | CHB-C4A-NA  | 2.48  | 127.98      | 124.40   |
| 31  | b     | 611 | CLA  | CHB-C4A-NA  | 2.48  | 127.98      | 124.40   |
| 31  | g     | 603 | CLA  | CHB-C4A-NA  | 2.48  | 127.98      | 124.40   |
| 30  | 5     | 305 | CHL  | O2D-CGD-O1D | -2.48 | 119.02      | 123.85   |
| 30  | 4     | 302 | CHL  | CMB-C2B-C3B | 2.48  | 129.64      | 124.68   |
| 30  | 1     | 313 | CHL  | O2D-CGD-O1D | -2.48 | 119.02      | 123.85   |
| 30  | 2     | 308 | CHL  | CMA-C3A-C4A | -2.48 | 109.27      | 114.61   |
| 30  | 2     | 308 | CHL  | CMB-C2B-C3B | 2.48  | 129.64      | 124.68   |
| 37  | d     | 521 | 0IE  | C22-C12-C11 | -2.48 | 118.80      | 122.82   |
| 31  | 7     | 311 | CLA  | CHB-C4A-NA  | 2.48  | 127.98      | 124.40   |
| 31  | B     | 840 | CLA  | CHB-C4A-NA  | 2.48  | 127.98      | 124.40   |
| 31  | B     | 841 | CLA  | CHB-C4A-NA  | 2.48  | 127.98      | 124.40   |
| 31  | G     | 102 | CLA  | CHB-C4A-NA  | 2.48  | 127.98      | 124.40   |
| 30  | b     | 609 | CHL  | CMA-C3A-C4A | -2.48 | 109.27      | 114.61   |
| 31  | B     | 821 | CLA  | C3B-C4B-NB  | -2.48 | 108.32      | 110.53   |
| 35  | 0     | 603 | SQD  | O48-C23-C24 | 2.48  | 119.39      | 111.83   |
| 30  | 8     | 306 | CHL  | CMB-C2B-C3B | 2.48  | 129.63      | 124.68   |
| 30  | 7     | 306 | CHL  | OMC-CMC-C2C | -2.48 | 120.82      | 125.12   |
| 30  | g     | 607 | CHL  | O1D-CGD-CBD | -2.48 | 120.97      | 124.72   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 2     | 312 | CLA  | CMB-C2B-C1B | -2.48 | 121.65      | 125.42   |
| 30  | f     | 602 | CHL  | CMB-C2B-C3B | 2.48  | 129.63      | 124.68   |
| 33  | 1     | 501 | 0UR  | C5-C4-C3    | -2.48 | 123.96      | 126.92   |
| 30  | b     | 601 | CHL  | CBC-CAC-C3C | -2.48 | 109.33      | 112.87   |
| 37  | f     | 521 | 0IE  | C13-C12-C11 | 2.48  | 122.90      | 119.01   |
| 31  | O     | 203 | CLA  | CAB-C3B-C2B | 2.48  | 130.11      | 123.53   |
| 32  | L     | 205 | 8CT  | C14-C15-C16 | -2.48 | 119.58      | 126.36   |
| 31  | g     | 611 | CLA  | CHB-C4A-NA  | 2.48  | 127.97      | 124.40   |
| 30  | f     | 605 | CHL  | CMB-C2B-C3B | 2.48  | 129.63      | 124.68   |
| 30  | h     | 601 | CHL  | O2D-CGD-O1D | -2.47 | 119.03      | 123.85   |
| 31  | L     | 203 | CLA  | CHB-C4A-NA  | 2.47  | 127.97      | 124.40   |
| 37  | a     | 522 | 0IE  | C20-C3-C2   | 2.47  | 120.69      | 115.01   |
| 31  | 7     | 304 | CLA  | CHB-C4A-NA  | 2.47  | 127.97      | 124.40   |
| 31  | F     | 301 | CLA  | CHB-C4A-NA  | 2.47  | 127.97      | 124.40   |
| 31  | h     | 604 | CLA  | CHB-C4A-NA  | 2.47  | 127.97      | 124.40   |
| 30  | b     | 601 | CHL  | O1D-CGD-CBD | -2.47 | 120.97      | 124.72   |
| 30  | f     | 614 | CHL  | O1D-CGD-CBD | -2.47 | 120.97      | 124.72   |
| 30  | i     | 601 | CHL  | CMB-C2B-C3B | 2.47  | 129.62      | 124.68   |
| 31  | B     | 809 | CLA  | CHB-C4A-NA  | 2.47  | 127.97      | 124.40   |
| 31  | g     | 604 | CLA  | CHB-C4A-NA  | 2.47  | 127.97      | 124.40   |
| 37  | a     | 521 | 0IE  | C13-C12-C11 | 2.47  | 122.90      | 119.01   |
| 30  | f     | 614 | CHL  | CMB-C2B-C3B | 2.47  | 129.62      | 124.68   |
| 31  | 6     | 318 | CLA  | CHB-C4A-NA  | 2.47  | 127.97      | 124.40   |
| 31  | 8     | 312 | CLA  | CHB-C4A-NA  | 2.47  | 127.97      | 124.40   |
| 31  | a     | 610 | CLA  | CHB-C4A-NA  | 2.47  | 127.97      | 124.40   |
| 30  | c     | 602 | CHL  | OMC-CMC-C2C | -2.47 | 120.83      | 125.12   |
| 30  | 5     | 307 | CHL  | CMB-C2B-C3B | 2.47  | 129.62      | 124.68   |
| 32  | J     | 104 | 8CT  | C25-C24-C23 | -2.47 | 116.04      | 123.20   |
| 30  | 6     | 307 | CHL  | CMB-C2B-C3B | 2.47  | 129.62      | 124.68   |
| 31  | A     | 840 | CLA  | CHB-C4A-NA  | 2.47  | 127.96      | 124.40   |
| 32  | M     | 102 | 8CT  | C05-C04-C03 | 2.47  | 114.03      | 110.44   |
| 31  | 7     | 316 | CLA  | CHB-C4A-NA  | 2.47  | 127.96      | 124.40   |
| 31  | d     | 603 | CLA  | CHB-C4A-NA  | 2.47  | 127.96      | 124.40   |
| 31  | e     | 613 | CLA  | CHB-C4A-NA  | 2.47  | 127.96      | 124.40   |
| 33  | 9     | 501 | 0UR  | C43-C3-C4   | -2.47 | 122.12      | 125.03   |
| 33  | 8     | 501 | 0UR  | C14-C15-C16 | -2.47 | 123.82      | 127.28   |
| 32  | B     | 804 | 8CT  | C27-C26-C28 | 2.47  | 121.86      | 118.09   |
| 31  | g     | 612 | CLA  | CHB-C4A-NA  | 2.47  | 127.96      | 124.40   |
| 37  | h     | 521 | 0IE  | C20-C3-C2   | 2.47  | 120.68      | 115.01   |
| 30  | 3     | 302 | CHL  | OMC-CMC-C2C | -2.47 | 120.84      | 125.12   |
| 33  | 0     | 502 | 0UR  | C4-C5-C6    | -2.47 | 116.05      | 123.20   |
| 31  | A     | 814 | CLA  | C3B-C4B-NB  | -2.47 | 108.33      | 110.53   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | d     | 609 | CHL  | CMB-C2B-C3B | 2.47  | 129.61      | 124.68   |
| 30  | g     | 607 | CHL  | CMB-C2B-C3B | 2.47  | 129.61      | 124.68   |
| 31  | 6     | 309 | CLA  | C1-C2-C3    | -2.47 | 122.16      | 126.20   |
| 31  | A     | 834 | CLA  | CHB-C4A-NA  | 2.47  | 127.96      | 124.40   |
| 30  | 6     | 307 | CHL  | OMC-CMC-C2C | -2.47 | 120.84      | 125.12   |
| 31  | c     | 603 | CLA  | CHB-C4A-NA  | 2.47  | 127.96      | 124.40   |
| 31  | d     | 612 | CLA  | CHB-C4A-NA  | 2.47  | 127.96      | 124.40   |
| 37  | h     | 521 | 0IE  | C13-C12-C11 | 2.47  | 122.89      | 119.01   |
| 30  | c     | 608 | CHL  | CMB-C2B-C3B | 2.47  | 129.61      | 124.68   |
| 30  | 4     | 306 | CHL  | OMC-CMC-C2C | -2.46 | 120.84      | 125.12   |
| 30  | e     | 609 | CHL  | O1D-CGD-CBD | -2.46 | 120.98      | 124.72   |
| 31  | O     | 203 | CLA  | O2D-CGD-O1D | -2.46 | 118.49      | 124.08   |
| 31  | B     | 815 | CLA  | CMB-C2B-C1B | -2.46 | 121.67      | 125.42   |
| 31  | d     | 613 | CLA  | CHB-C4A-NA  | 2.46  | 127.95      | 124.40   |
| 30  | f     | 609 | CHL  | CMB-C2B-C3B | 2.46  | 129.60      | 124.68   |
| 30  | f     | 609 | CHL  | CMA-C3A-C4A | -2.46 | 109.30      | 114.61   |
| 30  | i     | 614 | CHL  | O2D-CGD-O1D | -2.46 | 119.05      | 123.85   |
| 31  | B     | 835 | CLA  | CHB-C4A-NA  | 2.46  | 127.95      | 124.40   |
| 31  | H     | 201 | CLA  | CHB-C4A-NA  | 2.46  | 127.95      | 124.40   |
| 31  | i     | 612 | CLA  | CHB-C4A-NA  | 2.46  | 127.95      | 124.40   |
| 33  | d     | 520 | 0UR  | C5-C4-C3    | -2.46 | 123.97      | 126.92   |
| 32  | 3     | 403 | 8CT  | C30-C31-C32 | -2.46 | 118.44      | 121.47   |
| 30  | b     | 607 | CHL  | CMB-C2B-C3B | 2.46  | 129.60      | 124.68   |
| 31  | 6     | 317 | CLA  | CHB-C4A-NA  | 2.46  | 127.95      | 124.40   |
| 31  | 8     | 311 | CLA  | CHB-C4A-NA  | 2.46  | 127.95      | 124.40   |
| 31  | 3     | 320 | CLA  | CHB-C4A-NA  | 2.46  | 127.95      | 124.40   |
| 30  | e     | 607 | CHL  | CMB-C2B-C3B | 2.46  | 129.60      | 124.68   |
| 31  | A     | 837 | CLA  | O2A-CGA-O1A | -2.46 | 117.47      | 123.63   |
| 31  | B     | 826 | CLA  | CAA-C2A-C1A | -2.46 | 103.91      | 111.97   |
| 30  | h     | 602 | CHL  | CMA-C3A-C4A | -2.46 | 109.31      | 114.61   |
| 30  | 5     | 305 | CHL  | OMC-CMC-C2C | -2.46 | 120.85      | 125.12   |
| 31  | 0     | 308 | CLA  | CHB-C4A-NA  | 2.46  | 127.95      | 124.40   |
| 30  | c     | 601 | CHL  | O2D-CGD-O1D | -2.46 | 119.06      | 123.85   |
| 30  | 6     | 306 | CHL  | CMB-C2B-C3B | 2.46  | 129.60      | 124.68   |
| 31  | f     | 611 | CLA  | CHB-C4A-NA  | 2.46  | 127.95      | 124.40   |
| 30  | b     | 614 | CHL  | C1B-CHB-C4A | -2.46 | 119.74      | 121.32   |
| 31  | 2     | 311 | CLA  | C3B-C4B-NB  | -2.46 | 108.34      | 110.53   |
| 30  | a     | 606 | CHL  | O2D-CGD-O1D | -2.46 | 119.06      | 123.85   |
| 31  | B     | 817 | CLA  | CAA-C2A-C3A | -2.46 | 106.36      | 113.00   |
| 31  | h     | 613 | CLA  | CHB-C4A-NA  | 2.46  | 127.94      | 124.40   |
| 32  | 8     | 406 | 8CT  | C04-C03-C02 | -2.46 | 119.28      | 122.64   |
| 31  | e     | 613 | CLA  | O2A-CGA-O1A | -2.46 | 117.49      | 123.63   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | 2     | 307 | CHL  | CMA-C3A-C4A | -2.46 | 109.32      | 114.61   |
| 30  | d     | 614 | CHL  | C4D-CHA-CBD | -2.45 | 106.49      | 108.97   |
| 31  | A     | 813 | CLA  | CHB-C4A-NA  | 2.45  | 127.94      | 124.40   |
| 31  | d     | 611 | CLA  | CHB-C4A-NA  | 2.45  | 127.94      | 124.40   |
| 30  | d     | 605 | CHL  | CBC-CAC-C3C | -2.45 | 109.36      | 112.87   |
| 32  | K     | 107 | 8CT  | C39-C16-C17 | -2.45 | 118.84      | 122.82   |
| 37  | 3     | 502 | 0IE  | C6-C7-C8    | 2.45  | 122.87      | 119.01   |
| 30  | d     | 602 | CHL  | CMA-C3A-C4A | -2.45 | 109.33      | 114.61   |
| 30  | 6     | 301 | CHL  | CBC-CAC-C3C | -2.45 | 109.36      | 112.87   |
| 31  | A     | 828 | CLA  | C3B-C4B-NB  | -2.45 | 108.34      | 110.53   |
| 31  | 3     | 313 | CLA  | CHB-C4A-NA  | 2.45  | 127.94      | 124.40   |
| 33  | 8     | 501 | 0UR  | C15-C14-C13 | -2.45 | 116.10      | 123.20   |
| 30  | c     | 601 | CHL  | C4-C3-C5    | 2.45  | 119.48      | 115.23   |
| 30  | 2     | 302 | CHL  | CMB-C2B-C3B | 2.45  | 129.58      | 124.68   |
| 30  | h     | 601 | CHL  | CMB-C2B-C3B | 2.45  | 129.58      | 124.68   |
| 31  | O     | 201 | CLA  | CHB-C4A-NA  | 2.45  | 127.94      | 124.40   |
| 30  | 3     | 302 | CHL  | O2D-CGD-O1D | -2.45 | 119.08      | 123.85   |
| 31  | A     | 803 | CLA  | C1-C2-C3    | -2.45 | 122.18      | 126.20   |
| 32  | 6     | 402 | 8CT  | C04-C03-C02 | -2.45 | 119.29      | 122.64   |
| 30  | 1     | 302 | CHL  | O2D-CGD-O1D | -2.45 | 119.08      | 123.85   |
| 31  | e     | 610 | CLA  | C1-C2-C3    | -2.45 | 122.18      | 126.20   |
| 30  | a     | 609 | CHL  | CMB-C2B-C3B | 2.45  | 129.58      | 124.68   |
| 30  | e     | 606 | CHL  | CMB-C2B-C3B | 2.45  | 129.58      | 124.68   |
| 33  | 3     | 501 | 0UR  | C29-C30-C31 | -2.45 | 107.55      | 111.18   |
| 31  | 3     | 308 | CLA  | CHB-C4A-NA  | 2.45  | 127.93      | 124.40   |
| 30  | b     | 614 | CHL  | CMB-C2B-C3B | 2.45  | 129.57      | 124.68   |
| 30  | g     | 614 | CHL  | O2D-CGD-O1D | -2.45 | 119.08      | 123.85   |
| 31  | 3     | 306 | CLA  | CHB-C4A-NA  | 2.45  | 127.93      | 124.40   |
| 31  | g     | 611 | CLA  | C3B-C4B-NB  | -2.45 | 108.35      | 110.53   |
| 30  | 6     | 302 | CHL  | CMD-C2D-C3D | -2.45 | 119.80      | 124.68   |
| 30  | 1     | 307 | CHL  | CMB-C2B-C3B | 2.45  | 129.57      | 124.68   |
| 30  | 5     | 302 | CHL  | O2D-CGD-O1D | -2.44 | 119.09      | 123.85   |
| 30  | i     | 601 | CHL  | CBC-CAC-C3C | -2.44 | 109.37      | 112.87   |
| 30  | e     | 608 | CHL  | CBC-CAC-C3C | -2.44 | 109.37      | 112.87   |
| 31  | 9     | 311 | CLA  | CHB-C4A-NA  | 2.44  | 127.93      | 124.40   |
| 30  | i     | 602 | CHL  | OMC-CMC-C2C | -2.44 | 120.88      | 125.12   |
| 31  | A     | 805 | CLA  | CHB-C4A-NA  | 2.44  | 127.92      | 124.40   |
| 31  | M     | 101 | CLA  | CHB-C4A-NA  | 2.44  | 127.92      | 124.40   |
| 32  | 3     | 402 | 8CT  | C11-C10-C03 | -2.44 | 120.47      | 127.00   |
| 30  | 0     | 301 | CHL  | CMB-C2B-C3B | 2.44  | 129.56      | 124.68   |
| 30  | g     | 614 | CHL  | CMB-C2B-C3B | 2.44  | 129.56      | 124.68   |
| 31  | A     | 803 | CLA  | CHB-C4A-NA  | 2.44  | 127.92      | 124.40   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 2     | 310 | CLA  | CHB-C4A-NA  | 2.44  | 127.92      | 124.40   |
| 31  | 9     | 304 | CLA  | CHB-C4A-NA  | 2.44  | 127.92      | 124.40   |
| 30  | c     | 609 | CHL  | O2D-CGD-O1D | -2.44 | 119.10      | 123.85   |
| 33  | e     | 520 | 0UR  | C18-C17-C16 | -2.44 | 121.08      | 126.32   |
| 31  | H     | 202 | CLA  | CHB-C4A-NA  | 2.44  | 127.92      | 124.40   |
| 30  | 6     | 307 | CHL  | CMA-C3A-C4A | -2.44 | 109.35      | 114.61   |
| 30  | 7     | 302 | CHL  | CMB-C2B-C3B | 2.44  | 129.56      | 124.68   |
| 30  | e     | 614 | CHL  | CMB-C2B-C3B | 2.44  | 129.56      | 124.68   |
| 33  | 9     | 502 | 0UR  | C22-C16-C17 | 2.44  | 121.81      | 118.09   |
| 30  | c     | 614 | CHL  | O1D-CGD-CBD | -2.44 | 121.03      | 124.72   |
| 30  | b     | 609 | CHL  | CMB-C2B-C3B | 2.44  | 129.55      | 124.68   |
| 33  | 1     | 501 | 0UR  | C10-C9-C8   | -2.44 | 118.53      | 123.52   |
| 30  | a     | 605 | CHL  | CMB-C2B-C3B | 2.44  | 129.55      | 124.68   |
| 37  | c     | 522 | 0IE  | C13-C12-C11 | 2.44  | 122.84      | 119.01   |
| 31  | 2     | 309 | CLA  | CHB-C4A-NA  | 2.44  | 127.92      | 124.40   |
| 31  | 3     | 303 | CLA  | CHB-C4A-NA  | 2.44  | 127.92      | 124.40   |
| 31  | a     | 604 | CLA  | CHB-C4A-NA  | 2.44  | 127.92      | 124.40   |
| 33  | 9     | 502 | 0UR  | C4-C5-C6    | -2.44 | 116.14      | 123.20   |
| 30  | i     | 609 | CHL  | CMB-C2B-C3B | 2.44  | 129.55      | 124.68   |
| 31  | 7     | 308 | CLA  | CHB-C4A-NA  | 2.44  | 127.91      | 124.40   |
| 31  | c     | 613 | CLA  | CHB-C4A-NA  | 2.44  | 127.91      | 124.40   |
| 30  | i     | 607 | CHL  | CMB-C2B-C3B | 2.43  | 129.55      | 124.68   |
| 31  | H     | 205 | CLA  | CHB-C4A-NA  | 2.43  | 127.91      | 124.40   |
| 30  | 5     | 301 | CHL  | CMB-C2B-C3B | 2.43  | 129.54      | 124.68   |
| 33  | h     | 520 | 0UR  | C28-C19-C18 | -2.43 | 110.03      | 112.83   |
| 31  | e     | 610 | CLA  | CMB-C2B-C1B | -2.43 | 121.72      | 125.42   |
| 31  | A     | 827 | CLA  | C1-C2-C3    | -2.43 | 122.21      | 126.20   |
| 33  | i     | 520 | 0UR  | C4-C5-C6    | -2.43 | 116.15      | 123.20   |
| 31  | a     | 612 | CLA  | C3B-C4B-NB  | -2.43 | 108.36      | 110.53   |
| 31  | B     | 811 | CLA  | CHB-C4A-NA  | 2.43  | 127.91      | 124.40   |
| 31  | h     | 611 | CLA  | CHB-C4A-NA  | 2.43  | 127.91      | 124.40   |
| 30  | 5     | 306 | CHL  | CMB-C2B-C3B | 2.43  | 129.54      | 124.68   |
| 31  | h     | 612 | CLA  | CHB-C4A-NA  | 2.43  | 127.91      | 124.40   |
| 30  | g     | 601 | CHL  | CBC-CAC-C3C | -2.43 | 109.39      | 112.87   |
| 32  | 0     | 401 | 8CT  | C35-C30-C29 | -2.43 | 110.03      | 112.83   |
| 30  | d     | 607 | CHL  | CMB-C2B-C3B | 2.43  | 129.54      | 124.68   |
| 30  | f     | 607 | CHL  | CMB-C2B-C3B | 2.43  | 129.54      | 124.68   |
| 31  | 6     | 309 | CLA  | CHB-C4A-NA  | 2.43  | 127.91      | 124.40   |
| 30  | 4     | 307 | CHL  | CMB-C2B-C3B | 2.43  | 129.54      | 124.68   |
| 33  | a     | 520 | 0UR  | C4-C3-C2    | -2.43 | 118.04      | 120.16   |
| 31  | c     | 610 | CLA  | CHB-C4A-NA  | 2.43  | 127.91      | 124.40   |
| 30  | f     | 601 | CHL  | O2D-CGD-O1D | -2.43 | 119.12      | 123.85   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 2     | 304 | CLA  | CHB-C4A-NA  | 2.43  | 127.90      | 124.40   |
| 31  | B     | 822 | CLA  | CHB-C4A-NA  | 2.43  | 127.90      | 124.40   |
| 30  | a     | 614 | CHL  | CBC-CAC-C3C | -2.43 | 109.40      | 112.87   |
| 30  | f     | 601 | CHL  | CMB-C2B-C3B | 2.43  | 129.53      | 124.68   |
| 30  | 0     | 305 | CHL  | CBC-CAC-C3C | -2.43 | 109.40      | 112.87   |
| 30  | 4     | 313 | CHL  | OMC-CMC-C2C | -2.43 | 120.91      | 125.12   |
| 31  | B     | 814 | CLA  | CHB-C4A-NA  | 2.43  | 127.90      | 124.40   |
| 31  | A     | 807 | CLA  | CHB-C4A-NA  | 2.43  | 127.90      | 124.40   |
| 30  | i     | 605 | CHL  | CBC-CAC-C3C | -2.43 | 109.40      | 112.87   |
| 31  | e     | 603 | CLA  | CHB-C4A-NA  | 2.43  | 127.90      | 124.40   |
| 30  | 8     | 307 | CHL  | C5-C3-C4    | 2.42  | 120.17      | 114.59   |
| 31  | B     | 850 | CLA  | CHB-C4A-NA  | 2.42  | 127.90      | 124.40   |
| 31  | i     | 610 | CLA  | O2A-CGA-O1A | -2.42 | 117.57      | 123.63   |
| 30  | c     | 607 | CHL  | CMB-C2B-C3B | 2.42  | 129.52      | 124.68   |
| 31  | 9     | 310 | CLA  | CHB-C4A-NA  | 2.42  | 127.89      | 124.40   |
| 31  | B     | 839 | CLA  | CHB-C4A-NA  | 2.42  | 127.89      | 124.40   |
| 30  | f     | 608 | CHL  | CBC-CAC-C3C | -2.42 | 109.41      | 112.87   |
| 31  | A     | 837 | CLA  | C1-C2-C3    | -2.42 | 122.23      | 126.20   |
| 31  | 4     | 314 | CLA  | CHB-C4A-NA  | 2.42  | 127.89      | 124.40   |
| 30  | e     | 602 | CHL  | O2D-CGD-O1D | -2.42 | 119.14      | 123.85   |
| 31  | 1     | 310 | CLA  | CHB-C4A-NA  | 2.42  | 127.89      | 124.40   |
| 37  | c     | 522 | 0IE  | C19-C18-C17 | 2.42  | 128.34      | 124.58   |
| 37  | b     | 521 | 0IE  | C6-C7-C8    | 2.42  | 122.81      | 119.01   |
| 31  | f     | 604 | CLA  | C1-C2-C3    | -2.42 | 122.85      | 126.76   |
| 30  | f     | 614 | CHL  | O2D-CGD-O1D | -2.42 | 119.14      | 123.85   |
| 30  | e     | 605 | CHL  | C1B-CHB-C4A | -2.42 | 119.77      | 121.32   |
| 31  | A     | 817 | CLA  | O2D-CGD-CBD | 2.42  | 115.46      | 111.23   |
| 31  | A     | 853 | CLA  | O2A-CGA-O1A | -2.42 | 117.58      | 123.63   |
| 32  | 3     | 402 | 8CT  | C01-C02-C07 | 2.42  | 118.75      | 113.60   |
| 31  | b     | 613 | CLA  | CHB-C4A-NA  | 2.42  | 127.89      | 124.40   |
| 30  | 1     | 313 | CHL  | OMC-CMC-C2C | -2.42 | 120.92      | 125.12   |
| 30  | 9     | 301 | CHL  | O2D-CGD-O1D | -2.42 | 119.15      | 123.85   |
| 30  | 8     | 307 | CHL  | O1D-CGD-CBD | -2.42 | 121.06      | 124.72   |
| 32  | 0     | 401 | 8CT  | C10-C03-C02 | -2.42 | 115.99      | 121.56   |
| 30  | 8     | 307 | CHL  | CBC-CAC-C3C | -2.41 | 109.42      | 112.87   |
| 30  | d     | 602 | CHL  | OMC-CMC-C2C | -2.41 | 120.93      | 125.12   |
| 30  | g     | 602 | CHL  | O2D-CGD-O1D | -2.41 | 119.15      | 123.85   |
| 31  | 3     | 304 | CLA  | C1-C2-C3    | -2.41 | 122.24      | 126.20   |
| 31  | 2     | 312 | CLA  | CHB-C4A-NA  | 2.41  | 127.88      | 124.40   |
| 31  | 9     | 302 | CLA  | CHB-C4A-NA  | 2.41  | 127.88      | 124.40   |
| 30  | e     | 601 | CHL  | C5-C3-C4    | 2.41  | 120.14      | 114.59   |
| 30  | i     | 614 | CHL  | O1D-CGD-CBD | -2.41 | 121.06      | 124.72   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | e     | 606 | CHL  | O2D-CGD-O1D | -2.41 | 119.15      | 123.85   |
| 31  | B     | 801 | CLA  | CHB-C4A-NA  | 2.41  | 127.88      | 124.40   |
| 30  | a     | 602 | CHL  | O2D-CGD-O1D | -2.41 | 119.15      | 123.85   |
| 30  | 7     | 301 | CHL  | C6-C5-C3    | -2.41 | 107.59      | 113.47   |
| 31  | B     | 833 | CLA  | C1-C2-C3    | -2.41 | 122.25      | 126.20   |
| 30  | 2     | 307 | CHL  | O1D-CGD-CBD | -2.41 | 121.07      | 124.72   |
| 31  | B     | 810 | CLA  | CHB-C4A-NA  | 2.41  | 127.88      | 124.40   |
| 31  | K     | 105 | CLA  | CHB-C4A-NA  | 2.41  | 127.88      | 124.40   |
| 31  | c     | 611 | CLA  | CHB-C4A-NA  | 2.41  | 127.88      | 124.40   |
| 30  | 2     | 301 | CHL  | CMA-C3A-C4A | -2.41 | 109.42      | 114.61   |
| 30  | 6     | 315 | CHL  | CMA-C3A-C4A | -2.41 | 109.42      | 114.61   |
| 30  | 2     | 306 | CHL  | CMB-C2B-C3B | 2.41  | 129.50      | 124.68   |
| 30  | 6     | 308 | CHL  | CMB-C2B-C3B | 2.41  | 129.50      | 124.68   |
| 30  | g     | 607 | CHL  | C1B-CHB-C4A | -2.41 | 119.77      | 121.32   |
| 31  | 2     | 303 | CLA  | CHB-C4A-NA  | 2.41  | 127.88      | 124.40   |
| 31  | A     | 816 | CLA  | CHB-C4A-NA  | 2.41  | 127.88      | 124.40   |
| 31  | A     | 833 | CLA  | CHB-C4A-NA  | 2.41  | 127.87      | 124.40   |
| 30  | 7     | 301 | CHL  | CMB-C2B-C3B | 2.41  | 129.49      | 124.68   |
| 30  | d     | 605 | CHL  | C4D-CHA-CBD | -2.41 | 106.54      | 108.97   |
| 31  | A     | 821 | CLA  | CHB-C4A-NA  | 2.41  | 127.87      | 124.40   |
| 31  | B     | 836 | CLA  | CHB-C4A-NA  | 2.41  | 127.87      | 124.40   |
| 41  | B     | 849 | DGD  | O1G-C1A-O1A | -2.41 | 117.61      | 123.63   |
| 30  | f     | 609 | CHL  | O1D-CGD-CBD | -2.41 | 121.08      | 124.72   |
| 32  | 8     | 402 | 8CT  | C27-C26-C28 | 2.41  | 121.76      | 118.09   |
| 31  | A     | 830 | CLA  | O2D-CGD-CBD | 2.40  | 115.43      | 111.23   |
| 33  | 5     | 501 | 0UR  | C10-C9-C8   | -2.40 | 118.60      | 123.52   |
| 33  | b     | 520 | 0UR  | C10-C9-C8   | -2.40 | 118.60      | 123.52   |
| 30  | b     | 609 | CHL  | O1D-CGD-CBD | -2.40 | 121.08      | 124.72   |
| 36  | 9     | 602 | LMG  | O2-C2-C1    | -2.40 | 104.35      | 110.08   |
| 30  | 6     | 301 | CHL  | CMA-C3A-C4A | -2.40 | 109.43      | 114.61   |
| 31  | A     | 825 | CLA  | CHB-C4A-NA  | 2.40  | 127.87      | 124.40   |
| 31  | B     | 838 | CLA  | CHB-C4A-NA  | 2.40  | 127.87      | 124.40   |
| 31  | A     | 811 | CLA  | CHB-C4A-NA  | 2.40  | 127.87      | 124.40   |
| 31  | B     | 832 | CLA  | CMB-C2B-C1B | -2.40 | 121.76      | 125.42   |
| 36  | A     | 856 | LMG  | O3-C3-C2    | -2.40 | 104.72      | 110.38   |
| 37  | 7     | 502 | 0IE  | C22-C12-C11 | -2.40 | 118.93      | 122.82   |
| 33  | 6     | 501 | 0UR  | C4-C5-C6    | -2.40 | 116.24      | 123.20   |
| 32  | B     | 804 | 8CT  | C01-C02-C07 | 2.40  | 118.71      | 113.60   |
| 31  | 6     | 309 | CLA  | CMB-C2B-C1B | -2.40 | 121.76      | 125.42   |
| 31  | d     | 610 | CLA  | CMB-C2B-C1B | -2.40 | 121.76      | 125.42   |
| 31  | 3     | 310 | CLA  | CHB-C4A-NA  | 2.40  | 127.86      | 124.40   |
| 30  | 8     | 307 | CHL  | CMB-C2B-C3B | 2.40  | 129.48      | 124.68   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | f     | 606 | CHL  | OMC-CMC-C2C | -2.40 | 120.95      | 125.12   |
| 31  | f     | 613 | CLA  | CHB-C4A-NA  | 2.40  | 127.86      | 124.40   |
| 30  | i     | 605 | CHL  | C4D-CHA-CBD | -2.40 | 106.55      | 108.97   |
| 30  | a     | 607 | CHL  | CMB-C2B-C3B | 2.40  | 129.47      | 124.68   |
| 32  | M     | 102 | 8CT  | C35-C30-C29 | -2.40 | 110.07      | 112.83   |
| 37  | 3     | 502 | 0IE  | C22-C12-C11 | -2.40 | 118.93      | 122.82   |
| 31  | 6     | 303 | CLA  | CHB-C4A-NA  | 2.40  | 127.86      | 124.40   |
| 30  | c     | 607 | CHL  | O2D-CGD-O1D | -2.40 | 119.18      | 123.85   |
| 32  | A     | 849 | 8CT  | C10-C03-C02 | -2.40 | 116.04      | 121.56   |
| 31  | a     | 611 | CLA  | CHB-C4A-NA  | 2.40  | 127.86      | 124.40   |
| 30  | 7     | 301 | CHL  | C4-C3-C5    | 2.40  | 119.39      | 115.23   |
| 33  | a     | 520 | 0UR  | C15-C14-C13 | -2.39 | 116.26      | 123.20   |
| 32  | B     | 847 | 8CT  | C19-C20-C21 | -2.39 | 123.92      | 127.28   |
| 30  | g     | 607 | CHL  | C4D-CHA-CBD | -2.39 | 106.55      | 108.97   |
| 36  | B     | 853 | LMG  | O1-C7-C8    | -2.39 | 105.00      | 110.82   |
| 30  | i     | 606 | CHL  | OMC-CMC-C2C | -2.39 | 120.96      | 125.12   |
| 31  | G     | 103 | CLA  | CHB-C4A-NA  | 2.39  | 127.85      | 124.40   |
| 37  | b     | 521 | 0IE  | C13-C12-C11 | 2.39  | 122.77      | 119.01   |
| 30  | g     | 606 | CHL  | CBC-CAC-C3C | -2.39 | 109.45      | 112.87   |
| 30  | e     | 601 | CHL  | O2D-CGD-O1D | -2.39 | 119.19      | 123.85   |
| 30  | h     | 607 | CHL  | CMB-C2B-C3B | 2.39  | 129.46      | 124.68   |
| 30  | i     | 605 | CHL  | O2D-CGD-O1D | -2.39 | 119.19      | 123.85   |
| 30  | f     | 602 | CHL  | O2D-CGD-O1D | -2.39 | 119.19      | 123.85   |
| 31  | b     | 604 | CLA  | CHB-C4A-NA  | 2.39  | 127.85      | 124.40   |
| 32  | B     | 851 | 8CT  | C30-C29-C28 | -2.39 | 120.86      | 124.58   |
| 31  | G     | 101 | CLA  | C1-C2-C3    | -2.39 | 122.89      | 126.76   |
| 31  | A     | 819 | CLA  | CHB-C4A-NA  | 2.39  | 127.85      | 124.40   |
| 31  | A     | 830 | CLA  | CHB-C4A-NA  | 2.39  | 127.85      | 124.40   |
| 32  | 9     | 401 | 8CT  | C11-C10-C03 | -2.39 | 120.61      | 127.00   |
| 30  | h     | 602 | CHL  | CMB-C2B-C3B | 2.39  | 129.46      | 124.68   |
| 30  | d     | 601 | CHL  | CMB-C2B-C3B | 2.39  | 129.46      | 124.68   |
| 31  | e     | 604 | CLA  | CHB-C4A-NA  | 2.39  | 127.85      | 124.40   |
| 30  | 7     | 305 | CHL  | CMA-C3A-C4A | -2.39 | 109.47      | 114.61   |
| 30  | 9     | 313 | CHL  | CMA-C3A-C4A | -2.39 | 109.47      | 114.61   |
| 30  | 4     | 306 | CHL  | CMA-C3A-C4A | -2.39 | 109.47      | 114.61   |
| 30  | 3     | 302 | CHL  | CBC-CAC-C3C | -2.39 | 109.45      | 112.87   |
| 30  | a     | 609 | CHL  | CBC-CAC-C3C | -2.39 | 109.45      | 112.87   |
| 30  | 0     | 302 | CHL  | CMB-C2B-C3B | 2.39  | 129.45      | 124.68   |
| 31  | i     | 613 | CLA  | CHB-C4A-NA  | 2.39  | 127.84      | 124.40   |
| 33  | 9     | 501 | 0UR  | C5-C4-C3    | -2.39 | 124.06      | 126.92   |
| 36  | 9     | 602 | LMG  | C38-C37-C36 | -2.39 | 102.31      | 114.37   |
| 31  | 7     | 312 | CLA  | CHB-C4A-NA  | 2.39  | 127.84      | 124.40   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | A     | 832 | CLA  | CHB-C4A-NA  | 2.39  | 127.84      | 124.40   |
| 30  | b     | 608 | CHL  | O1D-CGD-CBD | -2.39 | 121.11      | 124.72   |
| 30  | a     | 605 | CHL  | C4D-CHA-CBD | -2.39 | 106.56      | 108.97   |
| 30  | g     | 605 | CHL  | CBC-CAC-C3C | -2.39 | 109.46      | 112.87   |
| 31  | 0     | 313 | CLA  | C3B-C4B-NB  | -2.38 | 108.40      | 110.53   |
| 31  | 3     | 312 | CLA  | CHB-C4A-NA  | 2.38  | 127.84      | 124.40   |
| 30  | 4     | 306 | CHL  | O2D-CGD-O1D | -2.38 | 119.21      | 123.85   |
| 32  | A     | 854 | 8CT  | C28-C26-C25 | 2.38  | 122.76      | 119.01   |
| 31  | 8     | 309 | CLA  | O2A-CGA-O1A | -2.38 | 117.67      | 123.63   |
| 30  | 2     | 305 | CHL  | CMB-C2B-C3B | 2.38  | 129.45      | 124.68   |
| 31  | B     | 836 | CLA  | C1-C2-C3    | -2.38 | 122.29      | 126.20   |
| 31  | A     | 825 | CLA  | CMB-C2B-C1B | -2.38 | 121.79      | 125.42   |
| 30  | 8     | 302 | CHL  | O1D-CGD-CBD | -2.38 | 121.11      | 124.72   |
| 30  | b     | 614 | CHL  | O2D-CGD-O1D | -2.38 | 119.21      | 123.85   |
| 32  | G     | 104 | 8CT  | C10-C03-C02 | -2.38 | 116.07      | 121.56   |
| 32  | 7     | 404 | 8CT  | C27-C26-C28 | -2.38 | 114.45      | 118.09   |
| 36  | 9     | 602 | LMG  | C40-C39-C38 | -2.38 | 102.33      | 114.37   |
| 30  | g     | 608 | CHL  | C4D-CHA-CBD | -2.38 | 106.57      | 108.97   |
| 32  | K     | 107 | 8CT  | C18-C19-C20 | -2.38 | 118.65      | 123.52   |
| 31  | A     | 808 | CLA  | O2D-CGD-CBD | 2.38  | 115.39      | 111.23   |
| 32  | B     | 844 | 8CT  | C01-C02-C07 | 2.38  | 118.67      | 113.60   |
| 30  | 6     | 305 | CHL  | O2D-CGD-O1D | -2.38 | 119.22      | 123.85   |
| 32  | L     | 205 | 8CT  | C18-C19-C20 | -2.38 | 118.65      | 123.52   |
| 31  | B     | 831 | CLA  | CHB-C4A-NA  | 2.38  | 127.83      | 124.40   |
| 30  | 6     | 306 | CHL  | CMA-C3A-C4A | -2.38 | 109.49      | 114.61   |
| 31  | 0     | 310 | CLA  | CHB-C4A-NA  | 2.38  | 127.83      | 124.40   |
| 31  | i     | 610 | CLA  | CHB-C4A-NA  | 2.38  | 127.83      | 124.40   |
| 30  | 8     | 308 | CHL  | O2D-CGD-O1D | -2.38 | 119.22      | 123.85   |
| 31  | A     | 836 | CLA  | CHB-C4A-NA  | 2.38  | 127.83      | 124.40   |
| 31  | L     | 207 | CLA  | CHB-C4A-NA  | 2.38  | 127.83      | 124.40   |
| 30  | a     | 601 | CHL  | O2D-CGD-O1D | -2.38 | 119.22      | 123.85   |
| 30  | h     | 606 | CHL  | O2D-CGD-O1D | -2.38 | 119.22      | 123.85   |
| 33  | 0     | 502 | 0UR  | C18-C17-C16 | -2.38 | 121.21      | 126.32   |
| 37  | e     | 521 | 0IE  | C23-C16-C17 | 2.38  | 121.72      | 118.09   |
| 31  | A     | 809 | CLA  | C1-C2-C3    | -2.38 | 122.31      | 126.20   |
| 31  | e     | 611 | CLA  | CHB-C4A-NA  | 2.38  | 127.83      | 124.40   |
| 32  | J     | 104 | 8CT  | C19-C18-C17 | -2.38 | 118.66      | 123.52   |
| 37  | i     | 521 | 0IE  | C20-C3-C2   | 2.38  | 120.46      | 115.01   |
| 30  | g     | 609 | CHL  | O2D-CGD-O1D | -2.38 | 119.22      | 123.85   |
| 31  | A     | 843 | CLA  | CMB-C2B-C1B | -2.37 | 121.80      | 125.42   |
| 31  | 7     | 310 | CLA  | CHB-C4A-NA  | 2.37  | 127.83      | 124.40   |
| 31  | B     | 801 | CLA  | C1-C2-C3    | -2.37 | 122.31      | 126.20   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | f     | 604 | CLA  | CHB-C4A-NA  | 2.37  | 127.82      | 124.40   |
| 30  | h     | 614 | CHL  | O1D-CGD-CBD | -2.37 | 121.12      | 124.72   |
| 31  | B     | 801 | CLA  | CMB-C2B-C3B | 2.37  | 132.13      | 126.55   |
| 33  | 9     | 502 | 0UR  | C21-C12-C13 | 2.37  | 121.71      | 118.09   |
| 33  | e     | 520 | 0UR  | C15-C14-C13 | -2.37 | 116.33      | 123.20   |
| 31  | A     | 814 | CLA  | CHB-C4A-NA  | 2.37  | 127.82      | 124.40   |
| 31  | A     | 838 | CLA  | CHB-C4A-NA  | 2.37  | 127.82      | 124.40   |
| 31  | B     | 805 | CLA  | C1-C2-C3    | -2.37 | 122.31      | 126.20   |
| 33  | 2     | 501 | 0UR  | C22-C16-C17 | 2.37  | 121.71      | 118.09   |
| 30  | g     | 606 | CHL  | CMB-C2B-C3B | 2.37  | 129.42      | 124.68   |
| 31  | A     | 841 | CLA  | CHB-C4A-NA  | 2.37  | 127.82      | 124.40   |
| 30  | h     | 605 | CHL  | CMB-C2B-C3B | 2.37  | 129.42      | 124.68   |
| 31  | B     | 812 | CLA  | C1-C2-C3    | -2.37 | 122.31      | 126.20   |
| 30  | 5     | 307 | CHL  | CBC-CAC-C3C | -2.37 | 109.48      | 112.87   |
| 30  | d     | 602 | CHL  | CBC-CAC-C3C | -2.37 | 109.48      | 112.87   |
| 30  | 3     | 302 | CHL  | CMB-C2B-C3B | 2.37  | 129.42      | 124.68   |
| 31  | e     | 604 | CLA  | C1-C2-C3    | -2.37 | 122.93      | 126.76   |
| 30  | 4     | 306 | CHL  | CMB-C2B-C3B | 2.37  | 129.42      | 124.68   |
| 31  | f     | 603 | CLA  | CHB-C4A-NA  | 2.37  | 127.82      | 124.40   |
| 31  | 4     | 304 | CLA  | CHB-C4A-NA  | 2.37  | 127.82      | 124.40   |
| 32  | 8     | 406 | 8CT  | C10-C03-C02 | -2.37 | 116.10      | 121.56   |
| 31  | H     | 205 | CLA  | O2A-CGA-O1A | -2.37 | 117.70      | 123.63   |
| 31  | 2     | 314 | CLA  | CHB-C4A-NA  | 2.37  | 127.82      | 124.40   |
| 31  | A     | 852 | CLA  | CHB-C4A-NA  | 2.37  | 127.82      | 124.40   |
| 30  | d     | 609 | CHL  | CBC-CAC-C3C | -2.37 | 109.48      | 112.87   |
| 30  | 7     | 307 | CHL  | CMB-C2B-C3B | 2.37  | 129.41      | 124.68   |
| 30  | a     | 607 | CHL  | O2D-CGD-O1D | -2.37 | 119.24      | 123.85   |
| 30  | d     | 609 | CHL  | O2D-CGD-O1D | -2.37 | 119.24      | 123.85   |
| 36  | J     | 105 | LMG  | C38-C37-C36 | -2.37 | 102.41      | 114.37   |
| 30  | c     | 609 | CHL  | CBC-CAC-C3C | -2.37 | 109.48      | 112.87   |
| 30  | f     | 602 | CHL  | CBC-CAC-C3C | -2.37 | 109.48      | 112.87   |
| 30  | g     | 601 | CHL  | CMB-C2B-C3B | 2.37  | 129.41      | 124.68   |
| 31  | B     | 834 | CLA  | CHB-C4A-NA  | 2.37  | 127.81      | 124.40   |
| 30  | d     | 614 | CHL  | O2D-CGD-O1D | -2.37 | 119.24      | 123.85   |
| 37  | i     | 521 | 0IE  | C23-C16-C17 | 2.37  | 121.70      | 118.09   |
| 31  | A     | 835 | CLA  | CHB-C4A-NA  | 2.37  | 127.81      | 124.40   |
| 31  | A     | 853 | CLA  | CHB-C4A-NA  | 2.37  | 127.81      | 124.40   |
| 31  | B     | 809 | CLA  | C1-C2-C3    | -2.36 | 122.32      | 126.20   |
| 31  | 4     | 303 | CLA  | CHB-C4A-NA  | 2.36  | 127.81      | 124.40   |
| 30  | a     | 608 | CHL  | CMA-C3A-C4A | -2.36 | 109.52      | 114.61   |
| 31  | b     | 610 | CLA  | C1-C2-C3    | -2.36 | 122.32      | 126.20   |
| 30  | 6     | 315 | CHL  | O2D-CGD-O1D | -2.36 | 119.25      | 123.85   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | b     | 602 | CHL  | CMB-C2B-C3B | 2.36  | 129.40      | 124.68   |
| 30  | c     | 605 | CHL  | C4D-CHA-CBD | -2.36 | 106.59      | 108.97   |
| 32  | A     | 847 | 8CT  | C13-C14-C15 | -2.36 | 116.36      | 123.20   |
| 33  | 1     | 501 | 0UR  | C15-C14-C13 | -2.36 | 116.36      | 123.20   |
| 31  | B     | 811 | CLA  | C1-C2-C3    | -2.36 | 122.33      | 126.20   |
| 31  | 3     | 303 | CLA  | O2A-CGA-O1A | -2.36 | 117.72      | 123.63   |
| 30  | 0     | 302 | CHL  | O2D-CGD-O1D | -2.36 | 119.25      | 123.85   |
| 31  | A     | 835 | CLA  | O2D-CGD-CBD | 2.36  | 115.36      | 111.23   |
| 30  | a     | 614 | CHL  | O2D-CGD-O1D | -2.36 | 119.26      | 123.85   |
| 33  | 0     | 501 | 0UR  | C10-C9-C8   | -2.36 | 118.69      | 123.52   |
| 30  | 7     | 313 | CHL  | OMC-CMC-C2C | -2.36 | 121.02      | 125.12   |
| 32  | B     | 851 | 8CT  | C13-C14-C15 | -2.36 | 116.36      | 123.20   |
| 30  | i     | 609 | CHL  | CBC-CAC-C3C | -2.36 | 109.50      | 112.87   |
| 31  | B     | 807 | CLA  | CMB-C2B-C1B | -2.36 | 121.83      | 125.42   |
| 31  | 5     | 308 | CLA  | CHB-C4A-NA  | 2.36  | 127.80      | 124.40   |
| 30  | 2     | 301 | CHL  | C6-C5-C3    | -2.36 | 107.73      | 113.47   |
| 31  | A     | 810 | CLA  | CHB-C4A-NA  | 2.36  | 127.80      | 124.40   |
| 32  | B     | 804 | 8CT  | C29-C28-C26 | -2.36 | 121.26      | 126.32   |
| 32  | A     | 848 | 8CT  | C24-C25-C26 | -2.36 | 123.97      | 127.28   |
| 30  | 6     | 305 | CHL  | CMB-C2B-C3B | 2.36  | 129.39      | 124.68   |
| 30  | h     | 606 | CHL  | CMB-C2B-C3B | 2.36  | 129.39      | 124.68   |
| 42  | e     | 523 | NEX  | C39-C29-C30 | -2.36 | 119.00      | 122.82   |
| 31  | 8     | 310 | CLA  | CHB-C4A-NA  | 2.36  | 127.80      | 124.40   |
| 31  | 5     | 304 | CLA  | CHB-C4A-NA  | 2.35  | 127.80      | 124.40   |
| 31  | A     | 826 | CLA  | CHB-C4A-NA  | 2.35  | 127.80      | 124.40   |
| 31  | 3     | 303 | CLA  | CMB-C2B-C1B | -2.35 | 121.83      | 125.42   |
| 30  | e     | 608 | CHL  | OMC-CMC-C2C | -2.35 | 121.03      | 125.12   |
| 31  | 8     | 309 | CLA  | CHB-C4A-NA  | 2.35  | 127.80      | 124.40   |
| 32  | L     | 206 | 8CT  | C04-C03-C02 | -2.35 | 119.42      | 122.64   |
| 30  | f     | 601 | CHL  | CMA-C3A-C4A | -2.35 | 109.54      | 114.61   |
| 31  | 1     | 312 | CLA  | CHB-C4A-NA  | 2.35  | 127.80      | 124.40   |
| 31  | 6     | 314 | CLA  | CHB-C4A-NA  | 2.35  | 127.80      | 124.40   |
| 30  | a     | 606 | CHL  | CMB-C2B-C3B | 2.35  | 129.38      | 124.68   |
| 31  | B     | 816 | CLA  | C1-C2-C3    | -2.35 | 122.34      | 126.20   |
| 37  | e     | 522 | 0IE  | C4-C5-C6    | 2.35  | 130.01      | 123.20   |
| 30  | 7     | 305 | CHL  | CMB-C2B-C3B | 2.35  | 129.38      | 124.68   |
| 30  | i     | 607 | CHL  | O2D-CGD-O1D | -2.35 | 119.27      | 123.85   |
| 30  | 2     | 313 | CHL  | C5-C3-C4    | 2.35  | 120.00      | 114.59   |
| 31  | 4     | 312 | CLA  | CHB-C4A-NA  | 2.35  | 127.79      | 124.40   |
| 33  | 0     | 501 | 0UR  | C15-C14-C13 | -2.35 | 116.39      | 123.20   |
| 36  | L     | 210 | LMG  | O1-C1-C2    | -2.35 | 104.70      | 108.27   |
| 32  | A     | 854 | 8CT  | C29-C28-C26 | -2.35 | 121.27      | 126.32   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | L     | 209 | 8CT  | C04-C03-C10 | 2.35  | 122.02      | 115.65   |
| 31  | A     | 822 | CLA  | CHB-C4A-NA  | 2.35  | 127.79      | 124.40   |
| 31  | 5     | 309 | CLA  | CHB-C4A-NA  | 2.35  | 127.79      | 124.40   |
| 31  | 6     | 320 | CLA  | CHB-C4A-NA  | 2.35  | 127.79      | 124.40   |
| 31  | 7     | 318 | CLA  | CHB-C4A-NA  | 2.35  | 127.79      | 124.40   |
| 31  | A     | 824 | CLA  | CHB-C4A-NA  | 2.35  | 127.79      | 124.40   |
| 31  | A     | 843 | CLA  | CHB-C4A-NA  | 2.35  | 127.79      | 124.40   |
| 31  | e     | 610 | CLA  | CHB-C4A-NA  | 2.35  | 127.79      | 124.40   |
| 30  | g     | 608 | CHL  | OMC-CMC-C2C | -2.35 | 121.05      | 125.12   |
| 31  | A     | 815 | CLA  | C1-C2-C3    | -2.35 | 122.35      | 126.20   |
| 30  | 4     | 302 | CHL  | CBC-CAC-C3C | -2.35 | 109.51      | 112.87   |
| 36  | J     | 102 | LMG  | O3-C3-C2    | -2.35 | 104.85      | 110.38   |
| 30  | f     | 609 | CHL  | C1B-CHB-C4A | 2.34  | 122.83      | 121.32   |
| 31  | c     | 610 | CLA  | O2A-CGA-O1A | -2.34 | 117.76      | 123.63   |
| 31  | B     | 824 | CLA  | CHB-C4A-NA  | 2.34  | 127.78      | 124.40   |
| 31  | K     | 101 | CLA  | CHB-C4A-NA  | 2.34  | 127.78      | 124.40   |
| 30  | 1     | 302 | CHL  | CMB-C2B-C3B | 2.34  | 129.37      | 124.68   |
| 36  | J     | 105 | LMG  | O3-C3-C2    | -2.34 | 104.85      | 110.38   |
| 36  | 3     | 602 | LMG  | O3-C3-C2    | -2.34 | 104.85      | 110.38   |
| 33  | 2     | 501 | 0UR  | C5-C4-C3    | -2.34 | 124.12      | 126.92   |
| 30  | f     | 605 | CHL  | CBC-CAC-C3C | -2.34 | 109.52      | 112.87   |
| 30  | 8     | 315 | CHL  | CMB-C2B-C3B | 2.34  | 129.36      | 124.68   |
| 30  | 2     | 313 | CHL  | O1D-CGD-CBD | -2.34 | 121.17      | 124.72   |
| 31  | 4     | 309 | CLA  | CHB-C4A-NA  | 2.34  | 127.78      | 124.40   |
| 34  | G     | 105 | LHG  | C26-C25-C24 | 2.34  | 121.73      | 113.13   |
| 31  | 1     | 314 | CLA  | CHB-C4A-NA  | 2.34  | 127.78      | 124.40   |
| 30  | g     | 602 | CHL  | CMA-C3A-C4A | -2.34 | 109.57      | 114.61   |
| 31  | 6     | 312 | CLA  | CHB-C4A-NA  | 2.34  | 127.78      | 124.40   |
| 30  | c     | 605 | CHL  | O2D-CGD-O1D | -2.34 | 119.30      | 123.85   |
| 32  | A     | 850 | 8CT  | C01-C02-C07 | 2.34  | 118.58      | 113.60   |
| 31  | 8     | 303 | CLA  | CHB-C4A-NA  | 2.34  | 127.77      | 124.40   |
| 31  | d     | 604 | CLA  | CHB-C4A-NA  | 2.34  | 127.77      | 124.40   |
| 32  | J     | 101 | 8CT  | C15-C16-C17 | -2.34 | 115.33      | 119.01   |
| 31  | B     | 833 | CLA  | CHB-C4A-NA  | 2.34  | 127.77      | 124.40   |
| 31  | A     | 826 | CLA  | CAA-C2A-C1A | -2.34 | 104.32      | 111.97   |
| 31  | L     | 201 | CLA  | CMB-C2B-C3B | 2.34  | 132.05      | 126.55   |
| 30  | b     | 602 | CHL  | CAC-C3C-C4C | 2.34  | 130.04      | 124.03   |
| 30  | 8     | 308 | CHL  | CMB-C2B-C3B | 2.34  | 129.35      | 124.68   |
| 30  | e     | 608 | CHL  | O1D-CGD-CBD | -2.34 | 121.18      | 124.72   |
| 31  | f     | 610 | CLA  | CHB-C4A-NA  | 2.34  | 127.77      | 124.40   |
| 33  | a     | 520 | 0UR  | C10-C9-C8   | -2.34 | 118.74      | 123.52   |
| 31  | 7     | 309 | CLA  | CMB-C2B-C1B | -2.34 | 121.86      | 125.42   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | A     | 813 | CLA  | CMB-C2B-C1B | -2.34 | 121.86      | 125.42   |
| 31  | 5     | 309 | CLA  | O2A-CGA-O1A | -2.34 | 117.79      | 123.63   |
| 30  | d     | 606 | CHL  | O2D-CGD-O1D | -2.33 | 119.30      | 123.85   |
| 31  | A     | 821 | CLA  | CMB-C2B-C1B | -2.33 | 121.86      | 125.42   |
| 30  | 4     | 307 | CHL  | O1D-CGD-CBD | -2.33 | 121.18      | 124.72   |
| 33  | 8     | 501 | 0UR  | C10-C9-C8   | -2.33 | 118.74      | 123.52   |
| 30  | 8     | 301 | CHL  | CMB-C2B-C3B | 2.33  | 129.35      | 124.68   |
| 33  | 6     | 502 | 0UR  | C18-C17-C16 | -2.33 | 121.30      | 126.32   |
| 31  | 3     | 320 | CLA  | C3B-C4B-NB  | -2.33 | 108.45      | 110.53   |
| 31  | c     | 604 | CLA  | C1-C2-C3    | -2.33 | 122.99      | 126.76   |
| 32  | A     | 848 | 8CT  | C18-C19-C20 | -2.33 | 118.75      | 123.52   |
| 30  | 6     | 308 | CHL  | O2D-CGD-O1D | -2.33 | 119.31      | 123.85   |
| 32  | B     | 845 | 8CT  | C04-C03-C10 | 2.33  | 121.98      | 115.65   |
| 31  | d     | 610 | CLA  | CHB-C4A-NA  | 2.33  | 127.77      | 124.40   |
| 31  | A     | 839 | CLA  | O2A-CGA-O1A | -2.33 | 117.79      | 123.63   |
| 32  | J     | 101 | 8CT  | C40-C12-C11 | 2.33  | 121.65      | 118.09   |
| 30  | 1     | 305 | CHL  | O2D-CGD-O1D | -2.33 | 119.31      | 123.85   |
| 31  | A     | 829 | CLA  | CHB-C4A-NA  | 2.33  | 127.76      | 124.40   |
| 37  | e     | 521 | 0IE  | C13-C12-C11 | 2.33  | 122.67      | 119.01   |
| 31  | 0     | 303 | CLA  | CHB-C4A-NA  | 2.33  | 127.76      | 124.40   |
| 32  | A     | 850 | 8CT  | C24-C23-C21 | -2.33 | 119.98      | 126.36   |
| 31  | B     | 812 | CLA  | CHB-C4A-NA  | 2.33  | 127.76      | 124.40   |
| 31  | O     | 203 | CLA  | CHB-C4A-NA  | 2.33  | 127.76      | 124.40   |
| 30  | 0     | 306 | CHL  | CMA-C3A-C4A | -2.33 | 109.59      | 114.61   |
| 31  | 5     | 310 | CLA  | CHB-C4A-NA  | 2.33  | 127.76      | 124.40   |
| 31  | 9     | 312 | CLA  | CHB-C4A-NA  | 2.33  | 127.76      | 124.40   |
| 30  | 2     | 307 | CHL  | CMB-C2B-C3B | 2.33  | 129.33      | 124.68   |
| 31  | 7     | 303 | CLA  | CHB-C4A-NA  | 2.33  | 127.76      | 124.40   |
| 30  | 7     | 305 | CHL  | O2D-CGD-O1D | -2.33 | 119.32      | 123.85   |
| 30  | a     | 602 | CHL  | OMC-CMC-C2C | -2.33 | 121.08      | 125.12   |
| 33  | 4     | 501 | 0UR  | C22-C16-C17 | 2.33  | 121.64      | 118.09   |
| 30  | i     | 602 | CHL  | CBC-CAC-C3C | -2.33 | 109.54      | 112.87   |
| 31  | i     | 603 | CLA  | CHB-C4A-NA  | 2.32  | 127.75      | 124.40   |
| 30  | c     | 601 | CHL  | CMB-C2B-C3B | 2.32  | 129.33      | 124.68   |
| 30  | c     | 608 | CHL  | OMC-CMC-C2C | -2.32 | 121.08      | 125.12   |
| 31  | 2     | 309 | CLA  | O2A-CGA-O1A | -2.32 | 117.81      | 123.63   |
| 31  | c     | 603 | CLA  | C1-C2-C3    | -2.32 | 122.39      | 126.20   |
| 33  | c     | 520 | 0UR  | C14-C13-C12 | -2.32 | 119.99      | 126.36   |
| 31  | d     | 610 | CLA  | C1-C2-C3    | -2.32 | 122.39      | 126.20   |
| 32  | K     | 107 | 8CT  | C10-C03-C02 | -2.32 | 116.20      | 121.56   |
| 31  | K     | 105 | CLA  | C1-C2-C3    | -2.32 | 123.00      | 126.76   |
| 31  | B     | 838 | CLA  | C3B-C4B-NB  | -2.32 | 108.46      | 110.53   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | f     | 607 | CHL  | O2D-CGD-O1D | -2.32 | 119.33      | 123.85   |
| 30  | 2     | 305 | CHL  | O2D-CGD-O1D | -2.32 | 119.33      | 123.85   |
| 31  | 0     | 304 | CLA  | CHB-C4A-NA  | 2.32  | 127.75      | 124.40   |
| 31  | 5     | 314 | CLA  | CHB-C4A-NA  | 2.32  | 127.75      | 124.40   |
| 30  | d     | 605 | CHL  | O2D-CGD-O1D | -2.32 | 119.33      | 123.85   |
| 32  | A     | 848 | 8CT  | C40-C12-C11 | 2.32  | 121.63      | 118.09   |
| 30  | 1     | 306 | CHL  | CMB-C2B-C3B | 2.32  | 129.32      | 124.68   |
| 30  | h     | 605 | CHL  | O2D-CGD-O1D | -2.32 | 119.33      | 123.85   |
| 30  | f     | 607 | CHL  | O2A-CGA-CBA | 2.32  | 120.90      | 112.14   |
| 31  | B     | 826 | CLA  | CMB-C2B-C1B | -2.32 | 121.89      | 125.42   |
| 31  | 6     | 317 | CLA  | CMB-C2B-C3B | 2.32  | 132.00      | 126.55   |
| 33  | 2     | 502 | 0UR  | C22-C16-C15 | -2.32 | 119.06      | 122.82   |
| 31  | A     | 805 | CLA  | O2A-CGA-O1A | -2.32 | 117.84      | 123.63   |
| 32  | 8     | 402 | 8CT  | C39-C16-C15 | 2.32  | 121.62      | 118.09   |
| 31  | 9     | 309 | CLA  | CMB-C2B-C1B | -2.31 | 121.89      | 125.42   |
| 31  | 6     | 304 | CLA  | CHB-C4A-NA  | 2.31  | 127.74      | 124.40   |
| 30  | d     | 602 | CHL  | O2D-CGD-O1D | -2.31 | 119.35      | 123.85   |
| 31  | 1     | 312 | CLA  | C1-C2-C3    | -2.31 | 122.41      | 126.20   |
| 31  | B     | 823 | CLA  | CHB-C4A-NA  | 2.31  | 127.73      | 124.40   |
| 32  | 7     | 404 | 8CT  | C10-C03-C02 | -2.31 | 116.23      | 121.56   |
| 30  | 6     | 313 | CHL  | CMB-C2B-C3B | 2.31  | 129.30      | 124.68   |
| 30  | 2     | 302 | CHL  | C6-C5-C3    | -2.31 | 107.84      | 113.47   |
| 37  | e     | 522 | 0IE  | C20-C3-C2   | 2.31  | 120.31      | 115.01   |
| 30  | 2     | 306 | CHL  | CMA-C3A-C4A | -2.31 | 109.64      | 114.61   |
| 31  | B     | 826 | CLA  | CHB-C4A-NA  | 2.31  | 127.73      | 124.40   |
| 37  | c     | 521 | 0IE  | C13-C12-C11 | 2.31  | 122.64      | 119.01   |
| 30  | 8     | 313 | CHL  | O2D-CGD-O1D | -2.31 | 119.36      | 123.85   |
| 31  | 3     | 309 | CLA  | O2A-CGA-O1A | -2.31 | 117.86      | 123.63   |
| 33  | 9     | 502 | 0UR  | C28-C19-C18 | -2.31 | 110.17      | 112.83   |
| 42  | e     | 523 | NEX  | C35-C15-C14 | -2.31 | 118.80      | 123.52   |
| 31  | b     | 610 | CLA  | O2A-CGA-O1A | -2.31 | 117.86      | 123.63   |
| 33  | 6     | 502 | 0UR  | C15-C14-C13 | -2.31 | 116.52      | 123.20   |
| 31  | 7     | 309 | CLA  | O2A-CGA-O1A | -2.31 | 117.86      | 123.63   |
| 30  | b     | 606 | CHL  | O2D-CGD-O1D | -2.31 | 119.36      | 123.85   |
| 30  | a     | 601 | CHL  | C4D-CHA-CBD | -2.30 | 106.64      | 108.97   |
| 30  | f     | 606 | CHL  | CMB-C2B-C3B | 2.30  | 129.29      | 124.68   |
| 30  | a     | 608 | CHL  | O2D-CGD-O1D | -2.30 | 119.36      | 123.85   |
| 36  | 3     | 602 | LMG  | O1-C7-C8    | -2.30 | 105.22      | 110.82   |
| 33  | 1     | 502 | 0UR  | C5-C6-C7    | -2.30 | 120.05      | 126.36   |
| 31  | B     | 819 | CLA  | CHB-C4A-NA  | 2.30  | 127.72      | 124.40   |
| 31  | d     | 610 | CLA  | O2A-CGA-O1A | -2.30 | 117.87      | 123.63   |
| 32  | K     | 107 | 8CT  | C05-C04-C03 | 2.30  | 113.78      | 110.44   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 33  | i     | 520 | 0UR  | C10-C9-C8   | -2.30 | 118.81      | 123.52   |
| 31  | c     | 610 | CLA  | C1-C2-C3    | -2.30 | 122.43      | 126.20   |
| 31  | 7     | 318 | CLA  | O2A-CGA-O1A | -2.30 | 117.88      | 123.63   |
| 33  | e     | 520 | 0UR  | C4-C5-C6    | -2.30 | 116.54      | 123.20   |
| 32  | B     | 804 | 8CT  | C11-C10-C03 | -2.30 | 120.86      | 127.00   |
| 32  | I     | 101 | 8CT  | C24-C23-C21 | -2.30 | 120.06      | 126.36   |
| 36  | 9     | 602 | LMG  | O3-C3-C2    | -2.30 | 104.96      | 110.38   |
| 32  | 8     | 406 | 8CT  | C18-C19-C20 | -2.30 | 118.82      | 123.52   |
| 30  | b     | 608 | CHL  | CMB-C2B-C3B | 2.30  | 129.27      | 124.68   |
| 31  | b     | 603 | CLA  | CHB-C4A-NA  | 2.30  | 127.71      | 124.40   |
| 30  | 1     | 302 | CHL  | O1D-CGD-CBD | -2.30 | 121.24      | 124.72   |
| 41  | B     | 849 | DGD  | O2G-C1B-O1B | -2.30 | 118.34      | 123.70   |
| 30  | c     | 609 | CHL  | CMA-C3A-C4A | -2.30 | 109.67      | 114.61   |
| 30  | a     | 602 | CHL  | CMB-C2B-C3B | 2.29  | 129.27      | 124.68   |
| 30  | 8     | 306 | CHL  | OMC-CMC-C2C | -2.29 | 121.14      | 125.12   |
| 31  | B     | 819 | CLA  | C1-C2-C3    | -2.29 | 122.44      | 126.20   |
| 31  | 4     | 309 | CLA  | C1-C2-C3    | -2.29 | 122.44      | 126.20   |
| 30  | 6     | 305 | CHL  | CMA-C3A-C4A | -2.29 | 109.67      | 114.61   |
| 30  | f     | 608 | CHL  | O1D-CGD-CBD | -2.29 | 121.25      | 124.72   |
| 32  | K     | 107 | 8CT  | C25-C24-C23 | -2.29 | 116.56      | 123.20   |
| 33  | 5     | 502 | 0UR  | C22-C16-C15 | -2.29 | 119.10      | 122.82   |
| 31  | B     | 806 | CLA  | C1-C2-C3    | -2.29 | 122.44      | 126.20   |
| 31  | A     | 814 | CLA  | O2A-CGA-O1A | -2.29 | 117.90      | 123.63   |
| 31  | e     | 611 | CLA  | C1-C2-C3    | -2.29 | 122.44      | 126.20   |
| 30  | c     | 601 | CHL  | OMC-CMC-C2C | -2.29 | 121.14      | 125.12   |
| 31  | O     | 203 | CLA  | C3B-C4B-NB  | -2.29 | 107.95      | 110.33   |
| 30  | 8     | 313 | CHL  | CMB-C2B-C3B | 2.29  | 129.26      | 124.68   |
| 31  | B     | 803 | CLA  | C3B-C4B-NB  | -2.29 | 108.49      | 110.53   |
| 30  | 3     | 307 | CHL  | O2D-CGD-O1D | -2.29 | 119.39      | 123.85   |
| 30  | 4     | 302 | CHL  | O2D-CGD-O1D | -2.29 | 119.39      | 123.85   |
| 30  | e     | 605 | CHL  | C4D-CHA-CBD | -2.29 | 106.66      | 108.97   |
| 31  | B     | 810 | CLA  | O2D-CGD-CBD | 2.29  | 115.23      | 111.23   |
| 31  | A     | 807 | CLA  | C1-C2-C3    | -2.29 | 122.45      | 126.20   |
| 30  | h     | 601 | CHL  | CBC-CAC-C3C | -2.29 | 109.60      | 112.87   |
| 32  | 7     | 405 | 8CT  | C14-C15-C16 | -2.29 | 120.09      | 126.36   |
| 30  | 9     | 313 | CHL  | CMB-C2B-C3B | 2.29  | 129.25      | 124.68   |
| 30  | 5     | 307 | CHL  | OMC-CMC-C2C | -2.29 | 121.15      | 125.12   |
| 30  | 9     | 313 | CHL  | O2A-CGA-CBA | 2.29  | 120.78      | 112.14   |
| 31  | B     | 825 | CLA  | O2A-CGA-O1A | -2.29 | 117.91      | 123.63   |
| 31  | A     | 807 | CLA  | O2A-CGA-O1A | -2.28 | 117.91      | 123.63   |
| 35  | 0     | 603 | SQD  | C1-O5-C5    | 2.28  | 118.18      | 113.72   |
| 30  | 8     | 306 | CHL  | C5-C3-C4    | 2.28  | 119.84      | 114.59   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | d     | 603 | CLA  | C1-C2-C3    | -2.28 | 122.45      | 126.20   |
| 30  | 3     | 305 | CHL  | CMB-C2B-C3B | 2.28  | 129.25      | 124.68   |
| 30  | 2     | 313 | CHL  | OMC-CMC-C2C | -2.28 | 121.16      | 125.12   |
| 32  | A     | 849 | 8CT  | C11-C10-C03 | -2.28 | 120.90      | 127.00   |
| 30  | a     | 602 | CHL  | CMA-C3A-C4A | -2.28 | 109.69      | 114.61   |
| 32  | A     | 846 | 8CT  | C27-C26-C28 | 2.28  | 121.57      | 118.09   |
| 30  | 5     | 313 | CHL  | O2A-CGA-CBA | 2.28  | 120.75      | 112.14   |
| 30  | 5     | 301 | CHL  | O2D-CGD-O1D | -2.28 | 119.41      | 123.85   |
| 33  | 5     | 501 | 0UR  | C28-C19-C18 | -2.28 | 110.20      | 112.83   |
| 31  | G     | 101 | CLA  | O2A-CGA-O1A | -2.28 | 117.93      | 123.63   |
| 30  | 8     | 302 | CHL  | O2D-CGD-O1D | -2.28 | 119.41      | 123.85   |
| 31  | 0     | 309 | CLA  | CMB-C2B-C1B | -2.28 | 121.95      | 125.42   |
| 30  | a     | 606 | CHL  | OMC-CMC-C2C | -2.28 | 121.16      | 125.12   |
| 30  | d     | 601 | CHL  | CBC-CAC-C3C | -2.28 | 109.61      | 112.87   |
| 31  | B     | 832 | CLA  | CHB-C4A-NA  | 2.28  | 127.69      | 124.40   |
| 32  | 3     | 403 | 8CT  | C19-C18-C17 | -2.28 | 118.86      | 123.52   |
| 32  | 8     | 406 | 8CT  | C07-C02-C03 | -2.28 | 119.63      | 122.70   |
| 41  | B     | 849 | DGD  | C1E-O6E-C5E | -2.28 | 109.28      | 113.72   |
| 32  | B     | 844 | 8CT  | C11-C10-C03 | -2.28 | 120.92      | 127.00   |
| 30  | e     | 609 | CHL  | CMA-C3A-C4A | -2.28 | 109.71      | 114.61   |
| 30  | a     | 609 | CHL  | O2D-CGD-O1D | -2.28 | 119.42      | 123.85   |
| 36  | O     | 207 | LMG  | O2-C2-C1    | -2.28 | 104.65      | 110.08   |
| 30  | 2     | 308 | CHL  | O1D-CGD-CBD | -2.28 | 121.27      | 124.72   |
| 31  | K     | 101 | CLA  | O2A-CGA-O1A | -2.28 | 117.94      | 123.63   |
| 36  | 9     | 602 | LMG  | O7-C10-O9   | -2.28 | 118.39      | 123.70   |
| 30  | f     | 601 | CHL  | CBC-CAC-C3C | -2.27 | 109.62      | 112.87   |
| 31  | A     | 823 | CLA  | CHB-C4A-NA  | 2.27  | 127.68      | 124.40   |
| 31  | b     | 610 | CLA  | CHB-C4A-NA  | 2.27  | 127.68      | 124.40   |
| 32  | F     | 302 | 8CT  | C07-C02-C03 | -2.27 | 119.63      | 122.70   |
| 30  | 1     | 313 | CHL  | C4-C3-C5    | 2.27  | 119.17      | 115.23   |
| 36  | L     | 210 | LMG  | O1-C7-C8    | -2.27 | 105.29      | 110.82   |
| 31  | A     | 818 | CLA  | C1-C2-C3    | -2.27 | 122.47      | 126.20   |
| 31  | 7     | 310 | CLA  | CMA-C3A-C2A | -2.27 | 111.02      | 116.23   |
| 30  | 1     | 307 | CHL  | OMC-CMC-C2C | -2.27 | 121.18      | 125.12   |
| 32  | B     | 804 | 8CT  | C30-C31-C32 | -2.27 | 118.67      | 121.47   |
| 30  | c     | 606 | CHL  | O2D-CGD-O1D | -2.27 | 119.43      | 123.85   |
| 32  | 6     | 402 | 8CT  | C01-C02-C07 | 2.27  | 118.44      | 113.60   |
| 31  | A     | 819 | CLA  | C1-C2-C3    | -2.27 | 122.48      | 126.20   |
| 36  | 2     | 602 | LMG  | O1-C1-C2    | -2.27 | 104.83      | 108.27   |
| 31  | 2     | 309 | CLA  | C1-C2-C3    | -2.27 | 122.48      | 126.20   |
| 31  | B     | 830 | CLA  | O2A-CGA-O1A | -2.27 | 117.95      | 123.63   |
| 31  | 8     | 304 | CLA  | C1-C2-C3    | -2.27 | 122.48      | 126.20   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | 2     | 307 | CHL  | OMC-CMC-C2C | -2.27 | 121.18      | 125.12   |
| 33  | c     | 520 | 0UR  | C4-C3-C2    | -2.27 | 118.18      | 120.16   |
| 30  | g     | 605 | CHL  | C4D-CHA-CBD | -2.27 | 106.68      | 108.97   |
| 30  | a     | 606 | CHL  | CBC-CAC-C3C | -2.27 | 109.63      | 112.87   |
| 30  | f     | 606 | CHL  | CBC-CAC-C3C | -2.27 | 109.63      | 112.87   |
| 36  | 3     | 602 | LMG  | O2-C2-C1    | -2.27 | 104.67      | 110.08   |
| 33  | 9     | 502 | 0UR  | O44-C45-O57 | -2.27 | 118.19      | 122.96   |
| 30  | 4     | 319 | CHL  | O2A-CGA-O1A | -2.27 | 117.96      | 123.63   |
| 30  | 4     | 307 | CHL  | O2D-CGD-O1D | -2.27 | 119.44      | 123.85   |
| 31  | 9     | 309 | CLA  | O2A-CGA-O1A | -2.27 | 117.96      | 123.63   |
| 31  | O     | 206 | CLA  | CHB-C4A-NA  | 2.27  | 127.67      | 124.40   |
| 30  | h     | 606 | CHL  | C5-C3-C4    | 2.27  | 119.80      | 114.59   |
| 30  | h     | 614 | CHL  | C1B-CHB-C4A | -2.27 | 119.87      | 121.32   |
| 32  | B     | 847 | 8CT  | C38-C31-C32 | -2.26 | 114.76      | 122.37   |
| 30  | e     | 602 | CHL  | OMC-CMC-C2C | -2.26 | 121.19      | 125.12   |
| 31  | B     | 821 | CLA  | CMB-C2B-C1B | -2.26 | 121.97      | 125.42   |
| 30  | 7     | 307 | CHL  | O1D-CGD-CBD | -2.26 | 121.29      | 124.72   |
| 31  | B     | 833 | CLA  | O2A-CGA-O1A | -2.26 | 117.97      | 123.63   |
| 31  | A     | 812 | CLA  | CHB-C4A-NA  | 2.26  | 127.66      | 124.40   |
| 42  | i     | 523 | NEX  | C31-C32-C33 | -2.26 | 120.16      | 126.36   |
| 30  | a     | 614 | CHL  | C4D-CHA-CBD | -2.26 | 106.69      | 108.97   |
| 31  | B     | 821 | CLA  | C1-C2-C3    | -2.26 | 123.11      | 126.76   |
| 30  | b     | 606 | CHL  | C5-C3-C4    | 2.26  | 119.79      | 114.59   |
| 31  | H     | 201 | CLA  | CMB-C2B-C1B | -2.26 | 121.98      | 125.42   |
| 31  | B     | 817 | CLA  | CBA-CAA-C2A | 2.26  | 120.51      | 113.79   |
| 33  | 7     | 501 | 0UR  | C5-C4-C3    | -2.26 | 124.22      | 126.92   |
| 30  | 9     | 306 | CHL  | OMC-CMC-C2C | -2.26 | 121.20      | 125.12   |
| 30  | b     | 601 | CHL  | O2D-CGD-O1D | -2.26 | 119.45      | 123.85   |
| 30  | g     | 605 | CHL  | O2D-CGD-O1D | -2.26 | 119.45      | 123.85   |
| 31  | A     | 832 | CLA  | C1-C2-C3    | -2.26 | 122.50      | 126.20   |
| 37  | i     | 522 | 0IE  | C20-C3-C2   | 2.26  | 120.19      | 115.01   |
| 32  | 7     | 405 | 8CT  | C30-C31-C32 | -2.26 | 118.69      | 121.47   |
| 31  | 0     | 313 | CLA  | CHB-C4A-NA  | 2.26  | 127.66      | 124.40   |
| 36  | B     | 853 | LMG  | O6-C1-O1    | -2.26 | 104.71      | 110.04   |
| 32  | F     | 302 | 8CT  | C10-C03-C02 | -2.26 | 116.36      | 121.56   |
| 30  | g     | 606 | CHL  | C5-C3-C4    | 2.25  | 119.78      | 114.59   |
| 31  | B     | 813 | CLA  | O2A-CGA-O1A | -2.25 | 117.99      | 123.63   |
| 30  | f     | 605 | CHL  | O2D-CGD-O1D | -2.25 | 119.46      | 123.85   |
| 37  | d     | 521 | 0IE  | C13-C12-C11 | 2.25  | 122.55      | 119.01   |
| 36  | B     | 853 | LMG  | O3-C3-C2    | -2.25 | 105.06      | 110.38   |
| 31  | 7     | 317 | CLA  | C2A-C1A-CHA | 2.25  | 127.78      | 123.87   |
| 30  | 1     | 306 | CHL  | CMA-C3A-C4A | -2.25 | 109.76      | 114.61   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | d     | 601 | CHL  | C5-C3-C4    | 2.25  | 119.77      | 114.59   |
| 31  | L     | 202 | CLA  | CHB-C4A-NA  | 2.25  | 127.65      | 124.40   |
| 30  | 2     | 313 | CHL  | O2D-CGD-O1D | -2.25 | 119.47      | 123.85   |
| 42  | f     | 523 | NEX  | C31-C32-C33 | -2.25 | 120.19      | 126.36   |
| 31  | f     | 610 | CLA  | C1-C2-C3    | -2.25 | 122.51      | 126.20   |
| 30  | d     | 608 | CHL  | C5-C3-C4    | 2.25  | 119.77      | 114.59   |
| 33  | g     | 520 | 0UR  | C10-C9-C8   | -2.25 | 118.92      | 123.52   |
| 33  | 8     | 502 | 0UR  | C22-C16-C15 | -2.25 | 119.17      | 122.82   |
| 34  | K     | 106 | LHG  | C26-C25-C24 | 2.25  | 121.39      | 113.13   |
| 37  | h     | 522 | 0IE  | C20-C3-C2   | 2.25  | 120.17      | 115.01   |
| 42  | d     | 523 | NEX  | C31-C32-C33 | -2.25 | 120.20      | 126.36   |
| 30  | g     | 602 | CHL  | CMB-C2B-C3B | 2.25  | 129.18      | 124.68   |
| 31  | B     | 828 | CLA  | CHB-C4A-NA  | 2.25  | 127.64      | 124.40   |
| 31  | L     | 204 | CLA  | CHB-C4A-NA  | 2.25  | 127.64      | 124.40   |
| 39  | A     | 857 | CL0  | O2A-CGA-O1A | -2.25 | 118.01      | 123.63   |
| 31  | 9     | 311 | CLA  | C1-C2-C3    | -2.25 | 122.52      | 126.20   |
| 36  | A     | 856 | LMG  | O2-C2-C1    | -2.25 | 104.72      | 110.08   |
| 30  | a     | 605 | CHL  | O2D-CGD-O1D | -2.25 | 119.48      | 123.85   |
| 31  | 1     | 312 | CLA  | O2A-CGA-O1A | -2.25 | 118.01      | 123.63   |
| 31  | A     | 826 | CLA  | O2A-CGA-O1A | -2.25 | 118.01      | 123.63   |
| 30  | i     | 606 | CHL  | C5-C3-C4    | 2.25  | 119.76      | 114.59   |
| 42  | e     | 523 | NEX  | C30-C31-C32 | -2.25 | 116.69      | 123.20   |
| 42  | c     | 523 | NEX  | C31-C32-C33 | -2.24 | 120.21      | 126.36   |
| 33  | 7     | 501 | 0UR  | C22-C16-C17 | 2.24  | 121.52      | 118.09   |
| 30  | 1     | 302 | CHL  | CAC-C3C-C4C | 2.24  | 129.80      | 124.03   |
| 31  | A     | 807 | CLA  | CMB-C2B-C3B | 2.24  | 131.83      | 126.55   |
| 30  | 0     | 305 | CHL  | C5-C3-C4    | 2.24  | 119.75      | 114.59   |
| 30  | c     | 608 | CHL  | O1D-CGD-CBD | -2.24 | 121.32      | 124.72   |
| 31  | 1     | 304 | CLA  | CHB-C4A-NA  | 2.24  | 127.64      | 124.40   |
| 30  | c     | 601 | CHL  | C6-C5-C3    | -2.24 | 108.01      | 113.47   |
| 42  | g     | 523 | NEX  | C31-C32-C33 | -2.24 | 120.22      | 126.36   |
| 31  | B     | 830 | CLA  | CHB-C4A-NA  | 2.24  | 127.63      | 124.40   |
| 36  | L     | 211 | LMG  | O2-C2-C1    | -2.24 | 104.73      | 110.08   |
| 33  | 1     | 501 | 0UR  | C4-C5-C6    | -2.24 | 116.71      | 123.20   |
| 42  | h     | 523 | NEX  | C31-C32-C33 | -2.24 | 120.22      | 126.36   |
| 33  | 0     | 502 | 0UR  | C43-C3-C4   | -2.24 | 122.39      | 125.03   |
| 30  | 1     | 305 | CHL  | CMA-C3A-C4A | -2.24 | 109.79      | 114.61   |
| 30  | 8     | 315 | CHL  | CMA-C3A-C4A | -2.24 | 109.79      | 114.61   |
| 30  | 8     | 302 | CHL  | CAC-C3C-C4C | 2.24  | 129.79      | 124.03   |
| 33  | c     | 520 | 0UR  | C33-C32-C31 | -2.24 | 118.06      | 123.36   |
| 30  | 1     | 307 | CHL  | CBC-CAC-C3C | -2.24 | 109.67      | 112.87   |
| 31  | B     | 838 | CLA  | O2A-CGA-O1A | -2.24 | 118.03      | 123.63   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | B     | 808 | CLA  | O2A-CGA-O1A | -2.24 | 118.03      | 123.63   |
| 30  | 4     | 313 | CHL  | C5-C3-C4    | 2.24  | 119.74      | 114.59   |
| 32  | B     | 843 | 8CT  | C39-C16-C17 | -2.24 | 119.19      | 122.82   |
| 30  | 0     | 302 | CHL  | OMC-CMC-C2C | -2.24 | 121.24      | 125.12   |
| 36  | L     | 210 | LMG  | O2-C2-C1    | -2.24 | 104.75      | 110.08   |
| 30  | 6     | 313 | CHL  | CMA-C3A-C4A | -2.24 | 109.79      | 114.61   |
| 31  | A     | 825 | CLA  | O2A-CGA-O1A | -2.24 | 118.04      | 123.63   |
| 30  | d     | 606 | CHL  | C5-C3-C4    | 2.23  | 119.73      | 114.59   |
| 30  | 8     | 313 | CHL  | OMC-CMC-C2C | -2.23 | 121.24      | 125.12   |
| 31  | K     | 102 | CLA  | O2A-CGA-O1A | -2.23 | 118.04      | 123.63   |
| 42  | b     | 523 | NEX  | C31-C32-C33 | -2.23 | 120.24      | 126.36   |
| 32  | O     | 205 | 8CT  | C05-C04-C03 | 2.23  | 113.68      | 110.44   |
| 31  | f     | 610 | CLA  | O2A-CGA-O1A | -2.23 | 118.04      | 123.63   |
| 30  | 6     | 307 | CHL  | C5-C3-C4    | 2.23  | 119.73      | 114.59   |
| 30  | f     | 606 | CHL  | C5-C3-C4    | 2.23  | 119.73      | 114.59   |
| 30  | g     | 607 | CHL  | C5-C3-C4    | 2.23  | 119.73      | 114.59   |
| 42  | a     | 523 | NEX  | C31-C32-C33 | -2.23 | 120.24      | 126.36   |
| 33  | 6     | 502 | 0UR  | C9-C10-C11  | -2.23 | 118.95      | 123.52   |
| 33  | c     | 520 | 0UR  | C10-C9-C8   | -2.23 | 118.95      | 123.52   |
| 30  | a     | 608 | CHL  | O1D-CGD-CBD | -2.23 | 121.34      | 124.72   |
| 30  | 2     | 306 | CHL  | CBC-CAC-C3C | -2.23 | 109.68      | 112.87   |
| 30  | d     | 606 | CHL  | OMC-CMC-C2C | -2.23 | 121.25      | 125.12   |
| 31  | B     | 828 | CLA  | O2A-CGA-O1A | -2.23 | 118.05      | 123.63   |
| 30  | 2     | 302 | CHL  | CAC-C3C-C4C | 2.23  | 129.76      | 124.03   |
| 31  | A     | 818 | CLA  | O2A-CGA-O1A | -2.23 | 118.05      | 123.63   |
| 30  | 8     | 305 | CHL  | O2D-CGD-O1D | -2.23 | 119.51      | 123.85   |
| 32  | M     | 102 | 8CT  | C24-C23-C21 | -2.23 | 120.25      | 126.36   |
| 30  | a     | 609 | CHL  | CMA-C3A-C4A | -2.23 | 109.81      | 114.61   |
| 33  | d     | 520 | 0UR  | C4-C5-C6    | -2.23 | 116.75      | 123.20   |
| 39  | A     | 857 | CL0  | CMA-C3A-C4A | -2.23 | 109.81      | 114.61   |
| 32  | 7     | 405 | 8CT  | C18-C19-C20 | -2.23 | 118.96      | 123.52   |
| 30  | b     | 607 | CHL  | O2D-CGD-O1D | -2.23 | 119.51      | 123.85   |
| 36  | J     | 102 | LMG  | C6-C5-C4    | -2.23 | 107.55      | 113.02   |
| 30  | i     | 602 | CHL  | CMA-C3A-C4A | -2.23 | 109.81      | 114.61   |
| 36  | L     | 211 | LMG  | O3-C3-C2    | -2.23 | 105.13      | 110.38   |
| 30  | d     | 609 | CHL  | CMA-C3A-C4A | -2.23 | 109.81      | 114.61   |
| 31  | B     | 803 | CLA  | O2A-CGA-O1A | -2.22 | 118.07      | 123.63   |
| 31  | L     | 207 | CLA  | O2A-CGA-O1A | -2.22 | 118.07      | 123.63   |
| 31  | 2     | 311 | CLA  | O2A-CGA-O1A | -2.22 | 118.07      | 123.63   |
| 30  | g     | 601 | CHL  | C4D-CHA-CBD | -2.22 | 106.73      | 108.97   |
| 36  | L     | 210 | LMG  | O3-C3-C2    | -2.22 | 105.14      | 110.38   |
| 32  | 8     | 402 | 8CT  | C39-C16-C17 | -2.22 | 119.22      | 122.82   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | e     | 606 | CHL  | OMC-CMC-C2C | -2.22 | 121.26      | 125.12   |
| 30  | e     | 606 | CHL  | CMA-C3A-C4A | -2.22 | 109.83      | 114.61   |
| 31  | A     | 808 | CLA  | O2A-CGA-O1A | -2.22 | 118.08      | 123.63   |
| 30  | e     | 606 | CHL  | C5-C3-C4    | 2.22  | 119.69      | 114.59   |
| 32  | A     | 846 | 8CT  | C19-C18-C17 | -2.22 | 118.98      | 123.52   |
| 30  | 3     | 305 | CHL  | CMA-C3A-C4A | -2.22 | 109.83      | 114.61   |
| 31  | 3     | 308 | CLA  | O2A-CGA-O1A | -2.22 | 118.08      | 123.63   |
| 30  | 1     | 306 | CHL  | OMC-CMC-C2C | -2.22 | 121.27      | 125.12   |
| 30  | 2     | 319 | CHL  | CMA-C3A-C4A | -2.22 | 109.83      | 114.61   |
| 30  | i     | 614 | CHL  | C4D-CHA-CBD | -2.22 | 106.73      | 108.97   |
| 31  | A     | 830 | CLA  | C3B-C4B-NB  | -2.22 | 108.55      | 110.53   |
| 33  | O     | 204 | 0UR  | C5-C6-C7    | -2.22 | 120.29      | 126.36   |
| 32  | 3     | 402 | 8CT  | C18-C17-C16 | -2.22 | 124.17      | 127.28   |
| 31  | 8     | 304 | CLA  | CHB-C4A-NA  | 2.22  | 127.60      | 124.40   |
| 30  | 7     | 302 | CHL  | OMC-CMC-C2C | -2.22 | 121.27      | 125.12   |
| 31  | B     | 832 | CLA  | O2A-CGA-O1A | -2.21 | 118.09      | 123.63   |
| 30  | d     | 607 | CHL  | O2D-CGD-O1D | -2.21 | 119.54      | 123.85   |
| 30  | c     | 602 | CHL  | CAC-C3C-C4C | 2.21  | 129.72      | 124.03   |
| 30  | h     | 607 | CHL  | O2D-CGD-O1D | -2.21 | 119.54      | 123.85   |
| 32  | A     | 849 | 8CT  | C22-C21-C23 | 2.21  | 121.47      | 118.09   |
| 33  | 4     | 502 | 0UR  | C4-C5-C6    | -2.21 | 116.79      | 123.20   |
| 31  | B     | 841 | CLA  | C1-C2-C3    | -2.21 | 122.57      | 126.20   |
| 31  | B     | 833 | CLA  | O2D-CGD-CBD | 2.21  | 115.09      | 111.23   |
| 31  | 6     | 309 | CLA  | O2A-CGA-O1A | -2.21 | 118.10      | 123.63   |
| 31  | L     | 203 | CLA  | O2A-CGA-O1A | -2.21 | 118.10      | 123.63   |
| 33  | 4     | 502 | 0UR  | C25-C26-C27 | -2.21 | 106.67      | 112.18   |
| 32  | 0     | 401 | 8CT  | C24-C23-C21 | -2.21 | 120.30      | 126.36   |
| 31  | A     | 827 | CLA  | CMB-C2B-C1B | -2.21 | 122.05      | 125.42   |
| 30  | d     | 608 | CHL  | O1D-CGD-CBD | -2.21 | 121.37      | 124.72   |
| 31  | A     | 830 | CLA  | O2A-CGA-O1A | -2.21 | 118.10      | 123.63   |
| 31  | e     | 610 | CLA  | O2A-CGA-O1A | -2.21 | 118.10      | 123.63   |
| 33  | d     | 520 | 0UR  | C18-C17-C16 | -2.21 | 121.57      | 126.32   |
| 36  | 2     | 602 | LMG  | O3-C3-C2    | -2.21 | 105.17      | 110.38   |
| 30  | 6     | 306 | CHL  | OMC-CMC-C2C | -2.21 | 121.29      | 125.12   |
| 30  | f     | 602 | CHL  | CAC-C3C-C4C | 2.21  | 129.71      | 124.03   |
| 33  | 2     | 501 | 0UR  | C29-C30-C31 | -2.21 | 107.91      | 111.18   |
| 30  | i     | 608 | CHL  | O1D-CGD-CBD | -2.21 | 121.38      | 124.72   |
| 30  | 5     | 302 | CHL  | CMB-C2B-C3B | 2.21  | 129.09      | 124.68   |
| 30  | e     | 609 | CHL  | OMC-CMC-C2C | -2.21 | 121.29      | 125.12   |
| 30  | 2     | 319 | CHL  | O2A-CGA-O1A | -2.21 | 118.11      | 123.63   |
| 32  | 2     | 402 | 8CT  | C18-C19-C20 | -2.21 | 119.00      | 123.52   |
| 30  | 0     | 306 | CHL  | CMB-C2B-C3B | 2.21  | 129.09      | 124.68   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | F     | 302 | 8CT  | C14-C15-C16 | -2.21 | 120.31      | 126.36   |
| 32  | 7     | 405 | 8CT  | C19-C18-C17 | -2.21 | 119.01      | 123.52   |
| 31  | A     | 813 | CLA  | O2A-CGA-O1A | -2.20 | 118.11      | 123.63   |
| 33  | 1     | 501 | 0UR  | C14-C15-C16 | -2.20 | 124.19      | 127.28   |
| 31  | B     | 825 | CLA  | C1-C2-C3    | -2.20 | 122.58      | 126.20   |
| 30  | 8     | 306 | CHL  | CMA-C3A-C4A | -2.20 | 109.86      | 114.61   |
| 30  | b     | 607 | CHL  | CMA-C3A-C4A | -2.20 | 109.86      | 114.61   |
| 33  | 3     | 501 | 0UR  | C14-C15-C16 | -2.20 | 124.19      | 127.28   |
| 33  | d     | 520 | 0UR  | C48-C47-C46 | -2.20 | 120.85      | 125.28   |
| 31  | A     | 817 | CLA  | O2A-CGA-O1A | -2.20 | 118.12      | 123.63   |
| 30  | 6     | 301 | CHL  | CMB-C2B-C3B | 2.20  | 129.08      | 124.68   |
| 32  | A     | 854 | 8CT  | C05-C04-C03 | 2.20  | 113.64      | 110.44   |
| 33  | 9     | 501 | 0UR  | C22-C16-C17 | 2.20  | 121.45      | 118.09   |
| 31  | B     | 817 | CLA  | CMB-C2B-C1B | -2.20 | 122.07      | 125.42   |
| 31  | B     | 808 | CLA  | CMB-C2B-C3B | 2.20  | 131.73      | 126.55   |
| 30  | 2     | 306 | CHL  | OMC-CMC-C2C | -2.20 | 121.30      | 125.12   |
| 30  | g     | 609 | CHL  | CMA-C3A-C4A | -2.20 | 109.87      | 114.61   |
| 30  | 4     | 305 | CHL  | CMA-C3A-C4A | -2.20 | 109.87      | 114.61   |
| 31  | 2     | 311 | CLA  | CMB-C2B-C1B | -2.20 | 122.07      | 125.42   |
| 36  | 2     | 602 | LMG  | O1-C7-C8    | -2.20 | 105.46      | 110.82   |
| 33  | 0     | 501 | 0UR  | C48-C47-C46 | -2.20 | 121.34      | 125.92   |
| 33  | a     | 520 | 0UR  | C5-C4-C3    | -2.20 | 124.29      | 126.92   |
| 32  | F     | 302 | 8CT  | C24-C23-C21 | -2.20 | 120.33      | 126.36   |
| 31  | 6     | 303 | CLA  | O2A-CGA-O1A | -2.20 | 118.12      | 123.63   |
| 30  | d     | 606 | CHL  | C1B-CHB-C4A | 2.20  | 122.74      | 121.32   |
| 30  | i     | 609 | CHL  | O2D-CGD-O1D | -2.20 | 119.57      | 123.85   |
| 31  | 7     | 304 | CLA  | CMB-C2B-C1B | -2.20 | 122.07      | 125.42   |
| 30  | g     | 602 | CHL  | OMC-CMC-C2C | -2.20 | 121.31      | 125.12   |
| 30  | c     | 607 | CHL  | O2A-CGA-CBA | 2.20  | 120.43      | 112.14   |
| 31  | B     | 811 | CLA  | O2D-CGD-CBD | 2.20  | 115.07      | 111.23   |
| 31  | A     | 836 | CLA  | CMB-C2B-C1B | -2.19 | 122.08      | 125.42   |
| 30  | 9     | 305 | CHL  | O2D-CGD-O1D | -2.19 | 119.58      | 123.85   |
| 33  | 4     | 502 | 0UR  | C9-C10-C11  | -2.19 | 119.03      | 123.52   |
| 31  | B     | 810 | CLA  | O2A-CGA-O1A | -2.19 | 118.14      | 123.63   |
| 30  | 6     | 308 | CHL  | C4-C3-C5    | 2.19  | 119.03      | 115.23   |
| 32  | 8     | 406 | 8CT  | C22-C21-C23 | 2.19  | 121.44      | 118.09   |
| 30  | e     | 605 | CHL  | O2D-CGD-O1D | -2.19 | 119.58      | 123.85   |
| 32  | F     | 302 | 8CT  | C04-C03-C02 | -2.19 | 119.64      | 122.64   |
| 32  | A     | 849 | 8CT  | C30-C29-C28 | -2.19 | 121.17      | 124.58   |
| 31  | 1     | 303 | CLA  | O2A-CGA-O1A | -2.19 | 118.15      | 123.63   |
| 31  | A     | 804 | CLA  | O2A-CGA-O1A | -2.19 | 118.15      | 123.63   |
| 32  | 6     | 402 | 8CT  | C22-C21-C23 | 2.19  | 121.43      | 118.09   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | e     | 607 | CHL  | O2A-CGA-CBA | 2.19  | 120.41      | 112.14   |
| 31  | B     | 827 | CLA  | CMB-C2B-C1B | -2.19 | 122.09      | 125.42   |
| 31  | B     | 826 | CLA  | O2A-CGA-O1A | -2.19 | 118.16      | 123.63   |
| 33  | 8     | 502 | 0UR  | O44-C45-O57 | -2.19 | 118.36      | 122.96   |
| 32  | 7     | 405 | 8CT  | C05-C04-C03 | 2.19  | 113.61      | 110.44   |
| 31  | 7     | 308 | CLA  | O2A-CGA-O1A | -2.19 | 118.16      | 123.63   |
| 31  | B     | 840 | CLA  | O2A-CGA-O1A | -2.19 | 118.16      | 123.63   |
| 31  | B     | 836 | CLA  | CMB-C2B-C3B | 2.18  | 131.69      | 126.55   |
| 30  | 7     | 305 | CHL  | OMC-CMC-C2C | -2.18 | 121.33      | 125.12   |
| 33  | 3     | 501 | 0UR  | C9-C10-C11  | -2.18 | 119.05      | 123.52   |
| 32  | 8     | 402 | 8CT  | C13-C14-C15 | -2.18 | 116.88      | 123.20   |
| 30  | b     | 614 | CHL  | OMC-CMC-C2C | -2.18 | 121.33      | 125.12   |
| 31  | B     | 829 | CLA  | CHB-C4A-NA  | 2.18  | 127.55      | 124.40   |
| 31  | 7     | 318 | CLA  | C1-C2-C3    | -2.18 | 122.62      | 126.20   |
| 34  | A     | 844 | LHG  | C5-O7-C7    | -2.18 | 112.57      | 117.80   |
| 37  | g     | 521 | 0IE  | C23-C16-C17 | 2.18  | 121.42      | 118.09   |
| 30  | 5     | 307 | CHL  | O2D-CGD-O1D | -2.18 | 119.60      | 123.85   |
| 31  | b     | 610 | CLA  | CMB-C2B-C1B | -2.18 | 122.10      | 125.42   |
| 37  | e     | 521 | 0IE  | C4-C3-C2    | -2.18 | 118.26      | 120.16   |
| 30  | 4     | 305 | CHL  | CMB-C2B-C3B | 2.18  | 129.04      | 124.68   |
| 33  | 4     | 501 | 0UR  | C41-C2-C3   | 2.18  | 125.06      | 119.12   |
| 31  | A     | 843 | CLA  | O1D-CGD-CBD | 2.18  | 128.81      | 124.52   |
| 37  | b     | 522 | 0IE  | C33-C32-C31 | 2.18  | 113.49      | 110.61   |
| 30  | f     | 608 | CHL  | C5-C3-C4    | 2.18  | 119.60      | 114.59   |
| 30  | i     | 606 | CHL  | O2D-CGD-O1D | -2.18 | 119.61      | 123.85   |
| 33  | 4     | 501 | 0UR  | C10-C9-C8   | -2.18 | 119.07      | 123.52   |
| 31  | A     | 818 | CLA  | CMB-C2B-C1B | -2.18 | 122.11      | 125.42   |
| 31  | B     | 819 | CLA  | CMB-C2B-C1B | -2.17 | 122.11      | 125.42   |
| 36  | J     | 105 | LMG  | C42-C41-C40 | -2.17 | 103.38      | 114.37   |
| 36  | J     | 102 | LMG  | O7-C10-O9   | -2.17 | 118.62      | 123.70   |
| 30  | g     | 608 | CHL  | O1D-CGD-CBD | -2.17 | 121.43      | 124.72   |
| 31  | 3     | 312 | CLA  | O2A-CGA-O1A | -2.17 | 118.19      | 123.63   |
| 33  | 1     | 501 | 0UR  | C22-C16-C17 | 2.17  | 121.41      | 118.09   |
| 30  | b     | 606 | CHL  | OMC-CMC-C2C | -2.17 | 121.35      | 125.12   |
| 36  | O     | 207 | LMG  | O3-C3-C2    | -2.17 | 105.26      | 110.38   |
| 30  | 5     | 305 | CHL  | CMA-C3A-C4A | -2.17 | 109.93      | 114.61   |
| 31  | 3     | 306 | CLA  | O2A-CGA-O1A | -2.17 | 118.20      | 123.63   |
| 31  | B     | 812 | CLA  | CMB-C2B-C1B | -2.17 | 122.11      | 125.42   |
| 30  | i     | 606 | CHL  | CMB-C2B-C3B | 2.17  | 129.02      | 124.68   |
| 31  | B     | 818 | CLA  | O2D-CGD-CBD | 2.17  | 115.02      | 111.23   |
| 33  | 0     | 502 | 0UR  | C21-C12-C13 | 2.17  | 121.40      | 118.09   |
| 30  | 6     | 301 | CHL  | O2A-CGA-O1A | -2.17 | 118.20      | 123.63   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 4     | 310 | CLA  | O2A-CGA-O1A | -2.17 | 118.20      | 123.63   |
| 30  | e     | 607 | CHL  | CMA-C3A-C4A | -2.17 | 109.94      | 114.61   |
| 31  | A     | 827 | CLA  | O2A-CGA-O1A | -2.17 | 118.20      | 123.63   |
| 30  | g     | 607 | CHL  | O2D-CGD-O1D | -2.17 | 119.63      | 123.85   |
| 30  | b     | 602 | CHL  | OMC-CMC-C2C | -2.17 | 121.36      | 125.12   |
| 31  | 1     | 309 | CLA  | O2A-CGA-O1A | -2.17 | 118.21      | 123.63   |
| 31  | 4     | 309 | CLA  | O2A-CGA-O1A | -2.17 | 118.21      | 123.63   |
| 30  | 7     | 307 | CHL  | C5-C3-C4    | 2.16  | 119.57      | 114.59   |
| 31  | O     | 202 | CLA  | CHB-C4A-NA  | 2.16  | 127.52      | 124.40   |
| 30  | d     | 605 | CHL  | OMC-CMC-C2C | -2.16 | 121.36      | 125.12   |
| 30  | h     | 602 | CHL  | OMC-CMC-C2C | -2.16 | 121.36      | 125.12   |
| 31  | B     | 809 | CLA  | O2A-CGA-O1A | -2.16 | 118.21      | 123.63   |
| 36  | 2     | 602 | LMG  | O2-C2-C1    | -2.16 | 104.92      | 110.08   |
| 30  | 6     | 307 | CHL  | O2D-CGD-O1D | -2.16 | 119.64      | 123.85   |
| 32  | B     | 843 | 8CT  | C11-C10-C03 | -2.16 | 121.22      | 127.00   |
| 33  | b     | 520 | 0UR  | C22-C16-C17 | 2.16  | 121.39      | 118.09   |
| 31  | A     | 852 | CLA  | CMB-C2B-C1B | -2.16 | 122.13      | 125.42   |
| 30  | h     | 608 | CHL  | O1D-CGD-CBD | -2.16 | 121.44      | 124.72   |
| 31  | B     | 806 | CLA  | O2A-CGA-O1A | -2.16 | 118.22      | 123.63   |
| 31  | A     | 830 | CLA  | CHB-C1B-NB  | 2.16  | 127.29      | 124.05   |
| 32  | A     | 854 | 8CT  | C18-C19-C20 | -2.16 | 119.10      | 123.52   |
| 30  | i     | 602 | CHL  | CMB-C2B-C3B | 2.16  | 129.00      | 124.68   |
| 30  | 2     | 307 | CHL  | C5-C3-C4    | 2.16  | 119.56      | 114.59   |
| 30  | 5     | 307 | CHL  | O2A-CGA-CBA | 2.16  | 120.30      | 112.14   |
| 31  | B     | 823 | CLA  | C1-C2-C3    | -2.16 | 122.66      | 126.20   |
| 31  | 9     | 304 | CLA  | O2A-CGA-O1A | -2.16 | 118.23      | 123.63   |
| 30  | a     | 601 | CHL  | O2A-CGA-CBA | 2.16  | 120.30      | 112.14   |
| 31  | a     | 603 | CLA  | O2D-CGD-CBD | 2.16  | 115.00      | 111.23   |
| 36  | A     | 856 | LMG  | O6-C1-C2    | 2.16  | 114.80      | 110.37   |
| 31  | B     | 818 | CLA  | O2A-CGA-O1A | -2.16 | 118.23      | 123.63   |
| 33  | 5     | 501 | 0UR  | C15-C14-C13 | -2.16 | 116.95      | 123.20   |
| 30  | 0     | 301 | CHL  | CMA-C3A-C4A | -2.16 | 109.96      | 114.61   |
| 30  | f     | 606 | CHL  | CMA-C3A-C4A | -2.16 | 109.96      | 114.61   |
| 30  | e     | 605 | CHL  | OMC-CMC-C2C | -2.16 | 121.38      | 125.12   |
| 30  | b     | 609 | CHL  | O2D-CGD-O1D | -2.16 | 119.65      | 123.85   |
| 31  | B     | 808 | CLA  | O2D-CGD-CBD | 2.16  | 115.00      | 111.23   |
| 30  | 4     | 308 | CHL  | OMC-CMC-C2C | -2.16 | 121.38      | 125.12   |
| 34  | G     | 105 | LHG  | C5-O7-C7    | -2.15 | 112.64      | 117.80   |
| 31  | B     | 837 | CLA  | O2A-CGA-O1A | -2.15 | 118.24      | 123.63   |
| 31  | K     | 102 | CLA  | C1-C2-C3    | -2.15 | 122.67      | 126.20   |
| 31  | 4     | 314 | CLA  | CMB-C2B-C1B | -2.15 | 122.14      | 125.42   |
| 31  | A     | 815 | CLA  | O2A-CGA-O1A | -2.15 | 118.24      | 123.63   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | c     | 606 | CHL  | CAC-C3C-C4C | 2.15  | 129.56      | 124.03   |
| 30  | e     | 602 | CHL  | CAC-C3C-C4C | 2.15  | 129.56      | 124.03   |
| 30  | a     | 606 | CHL  | C1-C2-C3    | -2.15 | 123.28      | 126.76   |
| 33  | 9     | 501 | 0UR  | C20-C7-C6   | 2.15  | 121.38      | 118.09   |
| 30  | 5     | 301 | CHL  | CMA-C3A-C4A | -2.15 | 109.98      | 114.61   |
| 30  | b     | 607 | CHL  | O2A-CGA-CBA | 2.15  | 120.27      | 112.14   |
| 30  | i     | 607 | CHL  | O2A-CGA-CBA | 2.15  | 120.27      | 112.14   |
| 31  | 5     | 309 | CLA  | CMB-C2B-C3B | 2.15  | 131.61      | 126.55   |
| 32  | 9     | 401 | 8CT  | C14-C15-C16 | -2.15 | 120.47      | 126.36   |
| 33  | e     | 520 | 0UR  | C9-C10-C11  | -2.15 | 119.12      | 123.52   |
| 31  | A     | 814 | CLA  | C1-C2-C3    | -2.15 | 122.68      | 126.20   |
| 31  | 3     | 309 | CLA  | CMB-C2B-C3B | 2.15  | 131.60      | 126.55   |
| 30  | 6     | 306 | CHL  | C5-C3-C4    | 2.15  | 119.53      | 114.59   |
| 31  | A     | 831 | CLA  | O2A-CGA-O1A | -2.15 | 118.25      | 123.63   |
| 30  | 4     | 302 | CHL  | CAC-C3C-C4C | 2.15  | 129.55      | 124.03   |
| 32  | 3     | 403 | 8CT  | C35-C30-C29 | -2.15 | 110.36      | 112.83   |
| 30  | c     | 602 | CHL  | CMA-C3A-C4A | -2.15 | 109.99      | 114.61   |
| 32  | L     | 209 | 8CT  | C30-C31-C32 | -2.15 | 118.83      | 121.47   |
| 36  | B     | 853 | LMG  | C1-C2-C3    | -2.15 | 105.50      | 110.01   |
| 32  | 1     | 402 | 8CT  | C27-C26-C25 | -2.15 | 119.34      | 122.82   |
| 32  | B     | 848 | 8CT  | C22-C21-C23 | 2.15  | 121.36      | 118.09   |
| 31  | B     | 822 | CLA  | C1-C2-C3    | -2.14 | 122.68      | 126.20   |
| 37  | c     | 522 | 0IE  | C17-C16-C15 | 2.14  | 122.38      | 119.01   |
| 31  | B     | 841 | CLA  | O2A-CGA-O1A | -2.14 | 118.27      | 123.63   |
| 42  | e     | 523 | NEX  | C17-C1-C6   | -2.14 | 108.55      | 110.47   |
| 31  | B     | 801 | CLA  | CHB-C1B-NB  | 2.14  | 127.26      | 124.05   |
| 30  | h     | 614 | CHL  | O2D-CGD-O1D | -2.14 | 119.68      | 123.85   |
| 36  | B     | 853 | LMG  | O7-C10-O9   | -2.14 | 118.70      | 123.70   |
| 31  | B     | 820 | CLA  | O2A-CGA-O1A | -2.14 | 118.27      | 123.63   |
| 31  | B     | 816 | CLA  | CMB-C2B-C1B | -2.14 | 122.16      | 125.42   |
| 31  | A     | 818 | CLA  | O2D-CGD-CBD | 2.14  | 114.97      | 111.23   |
| 30  | 8     | 307 | CHL  | OMC-CMC-C2C | -2.14 | 121.40      | 125.12   |
| 30  | 0     | 305 | CHL  | O2A-CGA-O1A | -2.14 | 118.27      | 123.63   |
| 33  | 6     | 501 | 0UR  | C23-C24-C25 | -2.14 | 108.90      | 113.59   |
| 30  | 0     | 301 | CHL  | O1D-CGD-CBD | -2.14 | 121.48      | 124.72   |
| 30  | 2     | 307 | CHL  | CAA-CBA-CGA | -2.14 | 107.13      | 113.21   |
| 30  | 3     | 307 | CHL  | CMA-C3A-C4A | -2.14 | 110.00      | 114.61   |
| 33  | 2     | 502 | 0UR  | C36-C28-C38 | -2.14 | 104.76      | 107.87   |
| 30  | i     | 607 | CHL  | C1B-CHB-C4A | -2.14 | 119.95      | 121.32   |
| 30  | 5     | 306 | CHL  | CMA-C3A-C4A | -2.14 | 110.00      | 114.61   |
| 30  | h     | 609 | CHL  | O2A-CGA-CBA | 2.14  | 120.22      | 112.14   |
| 30  | f     | 605 | CHL  | C4D-CHA-CBD | -2.14 | 106.81      | 108.97   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | 1     | 402 | 8CT  | C39-C16-C17 | -2.14 | 119.35      | 122.82   |
| 30  | f     | 605 | CHL  | CMA-C3A-C4A | -2.14 | 110.01      | 114.61   |
| 36  | B     | 853 | LMG  | O2-C2-C1    | -2.14 | 104.98      | 110.08   |
| 30  | f     | 608 | CHL  | O2D-CGD-O1D | -2.14 | 119.69      | 123.85   |
| 30  | a     | 602 | CHL  | CAC-C3C-C4C | 2.14  | 129.52      | 124.03   |
| 31  | B     | 817 | CLA  | CAC-C3C-C4C | 2.13  | 127.57      | 124.79   |
| 30  | 8     | 308 | CHL  | OMC-CMC-C2C | -2.13 | 121.41      | 125.12   |
| 30  | d     | 606 | CHL  | CMB-C2B-C3B | 2.13  | 128.95      | 124.68   |
| 30  | 5     | 307 | CHL  | CMA-C3A-C4A | -2.13 | 110.01      | 114.61   |
| 33  | 2     | 501 | 0UR  | C4-C5-C6    | -2.13 | 117.02      | 123.20   |
| 33  | 4     | 501 | 0UR  | C9-C10-C11  | -2.13 | 119.15      | 123.52   |
| 31  | A     | 843 | CLA  | O2A-CGA-O1A | -2.13 | 118.29      | 123.63   |
| 36  | 9     | 602 | LMG  | C42-C41-C40 | -2.13 | 103.59      | 114.37   |
| 31  | A     | 828 | CLA  | CHB-C4A-NA  | 2.13  | 127.48      | 124.40   |
| 30  | a     | 607 | CHL  | O2A-CGA-CBA | 2.13  | 120.19      | 112.14   |
| 32  | A     | 847 | 8CT  | C39-C16-C17 | -2.13 | 119.36      | 122.82   |
| 36  | J     | 105 | LMG  | C1-O6-C5    | -2.13 | 109.56      | 113.72   |
| 38  | B     | 842 | PQN  | C11-C3-C2   | -2.13 | 121.24      | 124.89   |
| 37  | 7     | 502 | 0IE  | C13-C12-C11 | 2.13  | 122.36      | 119.01   |
| 32  | A     | 848 | 8CT  | C39-C16-C15 | 2.13  | 121.34      | 118.09   |
| 31  | 3     | 320 | CLA  | CMB-C2B-C1B | -2.13 | 122.18      | 125.42   |
| 32  | B     | 851 | 8CT  | C35-C30-C29 | -2.13 | 110.38      | 112.83   |
| 30  | d     | 608 | CHL  | CMA-C3A-C4A | -2.13 | 110.03      | 114.61   |
| 30  | e     | 602 | CHL  | CMA-C3A-C4A | -2.13 | 110.03      | 114.61   |
| 37  | f     | 522 | 0IE  | C4-C5-C6    | 2.13  | 129.37      | 123.20   |
| 31  | 2     | 312 | CLA  | CMB-C2B-C3B | 2.13  | 131.55      | 126.55   |
| 31  | B     | 815 | CLA  | CMB-C2B-C3B | 2.13  | 131.55      | 126.55   |
| 31  | A     | 829 | CLA  | O2A-CGA-O1A | -2.13 | 118.31      | 123.63   |
| 30  | 8     | 306 | CHL  | CAC-C3C-C4C | 2.13  | 129.50      | 124.03   |
| 31  | B     | 805 | CLA  | CHB-C4A-NA  | 2.13  | 127.47      | 124.40   |
| 33  | 7     | 501 | 0UR  | C18-C17-C16 | -2.13 | 121.75      | 126.32   |
| 31  | B     | 814 | CLA  | O2A-CGA-O1A | -2.13 | 118.31      | 123.63   |
| 30  | 0     | 302 | CHL  | CAC-C3C-C4C | 2.12  | 129.49      | 124.03   |
| 30  | e     | 614 | CHL  | CED-O2D-CGD | 2.12  | 120.73      | 115.92   |
| 31  | 5     | 303 | CLA  | O2A-CGA-O1A | -2.12 | 118.31      | 123.63   |
| 30  | 1     | 307 | CHL  | O2D-CGD-O1D | -2.12 | 119.71      | 123.85   |
| 30  | h     | 605 | CHL  | CMA-C3A-C4A | -2.12 | 110.03      | 114.61   |
| 31  | B     | 803 | CLA  | CMB-C2B-C1B | -2.12 | 122.19      | 125.42   |
| 30  | f     | 602 | CHL  | OMC-CMC-C2C | -2.12 | 121.43      | 125.12   |
| 31  | B     | 805 | CLA  | O2A-CGA-O1A | -2.12 | 118.32      | 123.63   |
| 30  | e     | 606 | CHL  | CBC-CAC-C3C | -2.12 | 109.83      | 112.87   |
| 30  | 4     | 313 | CHL  | CMA-C3A-C4A | -2.12 | 110.04      | 114.61   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | f     | 602 | CHL  | CMA-C3A-C4A | -2.12 | 110.04      | 114.61   |
| 33  | O     | 204 | 0UR  | C21-C12-C13 | 2.12  | 121.33      | 118.09   |
| 31  | 0     | 309 | CLA  | O2A-CGA-O1A | -2.12 | 118.33      | 123.63   |
| 32  | B     | 847 | 8CT  | C22-C21-C23 | 2.12  | 121.33      | 118.09   |
| 31  | b     | 604 | CLA  | O2A-CGA-O1A | -2.12 | 118.33      | 123.63   |
| 30  | 3     | 307 | CHL  | CMB-C2B-C3B | 2.12  | 128.92      | 124.68   |
| 31  | A     | 833 | CLA  | O2A-CGA-O1A | -2.12 | 118.33      | 123.63   |
| 31  | 3     | 304 | CLA  | O2A-CGA-O1A | -2.12 | 118.33      | 123.63   |
| 31  | 9     | 311 | CLA  | O2A-CGA-O1A | -2.12 | 118.33      | 123.63   |
| 31  | B     | 824 | CLA  | C1-C2-C3    | -2.12 | 122.73      | 126.20   |
| 30  | 4     | 302 | CHL  | CMA-C3A-C4A | -2.12 | 110.05      | 114.61   |
| 30  | 8     | 305 | CHL  | O2A-CGA-CBA | 2.12  | 120.14      | 112.14   |
| 31  | 6     | 312 | CLA  | O2A-CGA-O1A | -2.12 | 118.33      | 123.63   |
| 31  | B     | 810 | CLA  | C1-C2-C3    | -2.12 | 122.73      | 126.20   |
| 37  | d     | 522 | 0IE  | C20-C3-C2   | 2.12  | 119.87      | 115.01   |
| 32  | B     | 848 | 8CT  | C23-C21-C20 | -2.12 | 115.68      | 119.01   |
| 31  | e     | 612 | CLA  | CMB-C2B-C1B | -2.11 | 122.20      | 125.42   |
| 30  | 8     | 307 | CHL  | O2D-CGD-O1D | -2.11 | 119.73      | 123.85   |
| 31  | A     | 824 | CLA  | O2A-CGA-O1A | -2.11 | 118.34      | 123.63   |
| 31  | 3     | 311 | CLA  | CMB-C2B-C1B | -2.11 | 122.20      | 125.42   |
| 37  | g     | 522 | 0IE  | C20-C3-C2   | 2.11  | 119.86      | 115.01   |
| 31  | B     | 808 | CLA  | C1-C2-C3    | -2.11 | 122.74      | 126.20   |
| 30  | a     | 606 | CHL  | C5-C3-C4    | 2.11  | 119.45      | 114.59   |
| 32  | 2     | 402 | 8CT  | C06-C07-C02 | -2.11 | 110.29      | 114.06   |
| 34  | f     | 630 | LHG  | C5-O7-C7    | -2.11 | 112.74      | 117.80   |
| 31  | B     | 830 | CLA  | C2D-C1D-ND  | -2.11 | 108.04      | 110.13   |
| 33  | 9     | 502 | 0UR  | C34-C27-C1  | -2.11 | 121.81      | 124.45   |
| 31  | 7     | 311 | CLA  | O2A-CGA-O1A | -2.11 | 118.35      | 123.63   |
| 33  | 2     | 501 | 0UR  | C14-C15-C16 | -2.11 | 124.32      | 127.28   |
| 33  | a     | 520 | 0UR  | C34-C27-C26 | 2.11  | 118.30      | 114.42   |
| 31  | A     | 828 | CLA  | CMB-C2B-C1B | -2.11 | 122.21      | 125.42   |
| 31  | A     | 802 | CLA  | C1-C2-C3    | -2.11 | 122.74      | 126.20   |
| 30  | b     | 606 | CHL  | CMA-C3A-C4A | -2.11 | 110.07      | 114.61   |
| 32  | B     | 844 | 8CT  | C19-C18-C17 | -2.11 | 119.20      | 123.52   |
| 31  | H     | 204 | CLA  | O2A-CGA-O1A | -2.11 | 118.35      | 123.63   |
| 37  | 3     | 502 | 0IE  | C13-C12-C11 | 2.11  | 122.33      | 119.01   |
| 30  | h     | 606 | CHL  | CAC-C3C-C4C | 2.11  | 129.45      | 124.03   |
| 30  | 9     | 301 | CHL  | O2A-CGA-CBA | 2.11  | 120.10      | 112.14   |
| 30  | f     | 608 | CHL  | OMC-CMC-C2C | -2.11 | 121.46      | 125.12   |
| 30  | g     | 606 | CHL  | OMC-CMC-C2C | -2.11 | 121.46      | 125.12   |
| 30  | f     | 609 | CHL  | O2D-CGD-O1D | -2.11 | 119.75      | 123.85   |
| 32  | A     | 850 | 8CT  | C35-C30-C29 | -2.11 | 110.40      | 112.83   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | a     | 610 | CLA  | O2A-CGA-O1A | -2.11 | 118.36      | 123.63   |
| 30  | 6     | 302 | CHL  | CMA-C3A-C4A | -2.11 | 110.07      | 114.61   |
| 30  | b     | 607 | CHL  | CBC-CAC-C3C | -2.11 | 109.86      | 112.87   |
| 31  | 6     | 311 | CLA  | O2A-CGA-O1A | -2.11 | 118.36      | 123.63   |
| 31  | B     | 807 | CLA  | CMB-C2B-C3B | 2.11  | 131.50      | 126.55   |
| 31  | B     | 812 | CLA  | O2A-CGA-O1A | -2.11 | 118.36      | 123.63   |
| 39  | A     | 857 | CL0  | CMB-C2B-C3B | 2.11  | 128.89      | 124.68   |
| 30  | 4     | 307 | CHL  | C5-C3-C4    | 2.11  | 119.43      | 114.59   |
| 30  | a     | 606 | CHL  | C1B-CHB-C4A | 2.10  | 122.68      | 121.32   |
| 30  | 4     | 308 | CHL  | O2A-CGA-CBA | 2.10  | 120.09      | 112.14   |
| 31  | B     | 819 | CLA  | O2D-CGD-CBD | 2.10  | 114.91      | 111.23   |
| 36  | O     | 207 | LMG  | O1-C7-C8    | -2.10 | 105.70      | 110.82   |
| 30  | 8     | 301 | CHL  | O2A-CGA-O1A | -2.10 | 118.37      | 123.63   |
| 37  | c     | 522 | 0IE  | C4-C5-C6    | 2.10  | 129.29      | 123.20   |
| 31  | A     | 819 | CLA  | CMB-C2B-C3B | 2.10  | 131.49      | 126.55   |
| 30  | 7     | 301 | CHL  | OMC-CMC-C2C | -2.10 | 121.47      | 125.12   |
| 33  | 8     | 501 | 0UR  | C43-C3-C2   | 2.10  | 121.45      | 116.56   |
| 32  | 7     | 402 | 8CT  | C40-C12-C11 | 2.10  | 121.30      | 118.09   |
| 30  | h     | 602 | CHL  | CBC-CAC-C3C | -2.10 | 109.86      | 112.87   |
| 30  | e     | 609 | CHL  | O2D-CGD-O1D | -2.10 | 119.76      | 123.85   |
| 30  | f     | 614 | CHL  | C4D-CHA-CBD | -2.10 | 106.85      | 108.97   |
| 33  | 7     | 501 | 0UR  | C4-C5-C6    | -2.10 | 117.11      | 123.20   |
| 30  | 2     | 308 | CHL  | O2A-CGA-CBA | 2.10  | 120.07      | 112.14   |
| 31  | 9     | 303 | CLA  | O2A-CGA-O1A | -2.10 | 118.38      | 123.63   |
| 32  | L     | 205 | 8CT  | C24-C23-C21 | -2.10 | 120.61      | 126.36   |
| 31  | B     | 826 | CLA  | CMB-C2B-C3B | 2.10  | 131.49      | 126.55   |
| 33  | 9     | 502 | 0UR  | C48-C47-C46 | -2.10 | 121.55      | 125.92   |
| 31  | A     | 803 | CLA  | O2A-CGA-O1A | -2.10 | 118.38      | 123.63   |
| 31  | 6     | 309 | CLA  | CMB-C2B-C3B | 2.10  | 131.49      | 126.55   |
| 33  | a     | 520 | 0UR  | C43-O44-C45 | 2.10  | 119.79      | 116.10   |
| 30  | h     | 608 | CHL  | OMC-CMC-C2C | -2.10 | 121.48      | 125.12   |
| 33  | c     | 520 | 0UR  | C22-C16-C15 | -2.10 | 119.42      | 122.82   |
| 33  | e     | 520 | 0UR  | C10-C9-C8   | -2.10 | 119.23      | 123.52   |
| 30  | c     | 607 | CHL  | CMA-C3A-C4A | -2.10 | 110.09      | 114.61   |
| 33  | 9     | 502 | 0UR  | C43-C3-C4   | -2.10 | 122.56      | 125.03   |
| 31  | e     | 613 | CLA  | C1-C2-C3    | -2.10 | 122.76      | 126.20   |
| 31  | 9     | 312 | CLA  | CMB-C2B-C1B | -2.10 | 122.23      | 125.42   |
| 31  | A     | 825 | CLA  | CMB-C2B-C3B | 2.10  | 131.48      | 126.55   |
| 33  | c     | 520 | 0UR  | C18-C17-C16 | -2.10 | 121.81      | 126.32   |
| 30  | b     | 614 | CHL  | C4D-CHA-CBD | -2.10 | 106.85      | 108.97   |
| 33  | a     | 520 | 0UR  | C18-C17-C16 | -2.10 | 121.81      | 126.32   |
| 31  | 8     | 309 | CLA  | CMB-C2B-C1B | -2.10 | 122.23      | 125.42   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 6     | 314 | CLA  | O2D-CGD-CBD | 2.10  | 114.89      | 111.23   |
| 33  | 8     | 501 | 0UR  | C23-C24-C25 | -2.09 | 109.00      | 113.59   |
| 30  | 5     | 302 | CHL  | CAC-C3C-C4C | 2.09  | 129.41      | 124.03   |
| 31  | A     | 828 | CLA  | O2A-CGA-O1A | -2.09 | 118.39      | 123.63   |
| 31  | B     | 815 | CLA  | O2A-CGA-O1A | -2.09 | 118.39      | 123.63   |
| 31  | A     | 838 | CLA  | O2A-CGA-O1A | -2.09 | 118.39      | 123.63   |
| 31  | A     | 827 | CLA  | CMB-C2B-C3B | 2.09  | 131.47      | 126.55   |
| 37  | b     | 522 | 0IE  | C20-C3-C2   | 2.09  | 119.81      | 115.01   |
| 31  | K     | 102 | CLA  | CAC-C3C-C4C | 2.09  | 127.51      | 124.79   |
| 31  | 7     | 311 | CLA  | C1-C2-C3    | -2.09 | 122.77      | 126.20   |
| 30  | 7     | 313 | CHL  | C1B-CHB-C4A | 2.09  | 122.67      | 121.32   |
| 30  | c     | 607 | CHL  | OMC-CMC-C2C | -2.09 | 121.49      | 125.12   |
| 31  | 2     | 309 | CLA  | CMB-C2B-C1B | -2.09 | 122.24      | 125.42   |
| 33  | c     | 520 | 0UR  | C4-C5-C6    | -2.09 | 117.14      | 123.20   |
| 30  | 9     | 305 | CHL  | CAC-C3C-C4C | 2.09  | 129.40      | 124.03   |
| 33  | h     | 520 | 0UR  | C4-C3-C2    | -2.09 | 118.34      | 120.16   |
| 31  | B     | 837 | CLA  | CMB-C2B-C1B | -2.09 | 122.24      | 125.42   |
| 31  | d     | 610 | CLA  | CMB-C2B-C3B | 2.09  | 131.47      | 126.55   |
| 30  | 0     | 305 | CHL  | CMB-C2B-C3B | 2.09  | 128.86      | 124.68   |
| 31  | B     | 824 | CLA  | O2A-CGA-O1A | -2.09 | 118.40      | 123.63   |
| 37  | a     | 521 | 0IE  | C23-C16-C17 | 2.09  | 121.28      | 118.09   |
| 31  | 2     | 304 | CLA  | O2A-CGA-O1A | -2.09 | 118.40      | 123.63   |
| 33  | 2     | 501 | 0UR  | C41-C2-C3   | 2.09  | 124.81      | 119.12   |
| 31  | B     | 837 | CLA  | O2D-CGD-CBD | 2.09  | 114.88      | 111.23   |
| 31  | A     | 836 | CLA  | O2A-CGA-O1A | -2.09 | 118.40      | 123.63   |
| 30  | h     | 601 | CHL  | O2A-CGA-CBA | 2.09  | 120.03      | 112.14   |
| 30  | h     | 609 | CHL  | CMA-C3A-C4A | -2.09 | 110.11      | 114.61   |
| 30  | 2     | 301 | CHL  | C4-C3-C5    | 2.09  | 118.85      | 115.23   |
| 30  | 2     | 301 | CHL  | CBC-CAC-C3C | -2.09 | 109.88      | 112.87   |
| 33  | f     | 520 | 0UR  | C33-C32-C31 | -2.09 | 118.42      | 123.36   |
| 36  | L     | 211 | LMG  | O1-C7-C8    | -2.09 | 105.74      | 110.82   |
| 31  | B     | 830 | CLA  | CMB-C2B-C3B | 2.09  | 131.46      | 126.55   |
| 32  | B     | 844 | 8CT  | C05-C04-C03 | 2.09  | 113.47      | 110.44   |
| 37  | c     | 521 | 0IE  | C19-C18-C17 | 2.09  | 127.83      | 124.58   |
| 31  | i     | 612 | CLA  | CMB-C2B-C1B | -2.09 | 122.24      | 125.42   |
| 31  | a     | 613 | CLA  | C1-C2-C3    | -2.09 | 122.78      | 126.20   |
| 30  | 2     | 305 | CHL  | CAC-C3C-C4C | 2.09  | 129.39      | 124.03   |
| 31  | 3     | 310 | CLA  | O2A-CGA-O1A | -2.09 | 118.41      | 123.63   |
| 32  | A     | 846 | 8CT  | C39-C16-C17 | -2.09 | 119.44      | 122.82   |
| 31  | 9     | 302 | CLA  | O2A-CGA-O1A | -2.08 | 118.41      | 123.63   |
| 31  | B     | 816 | CLA  | O2A-CGA-O1A | -2.08 | 118.41      | 123.63   |
| 32  | L     | 209 | 8CT  | C39-C16-C15 | 2.08  | 121.27      | 118.09   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 7     | 304 | CLA  | O2A-CGA-O1A | -2.08 | 118.42      | 123.63   |
| 31  | 2     | 309 | CLA  | O2D-CGD-CBD | 2.08  | 114.87      | 111.23   |
| 30  | 1     | 307 | CHL  | CMA-C3A-C4A | -2.08 | 110.12      | 114.61   |
| 30  | b     | 601 | CHL  | OMC-CMC-C2C | -2.08 | 121.50      | 125.12   |
| 30  | 6     | 306 | CHL  | O2D-CGD-O1D | -2.08 | 119.80      | 123.85   |
| 31  | c     | 603 | CLA  | O2A-CGA-O1A | -2.08 | 118.42      | 123.63   |
| 30  | 3     | 305 | CHL  | CAC-C3C-C4C | 2.08  | 129.38      | 124.03   |
| 31  | K     | 101 | CLA  | O2D-CGD-CBD | 2.08  | 114.87      | 111.23   |
| 32  | A     | 847 | 8CT  | C40-C12-C13 | -2.08 | 119.44      | 122.82   |
| 30  | 5     | 301 | CHL  | O2A-CGA-O1A | -2.08 | 118.42      | 123.63   |
| 31  | 1     | 311 | CLA  | CMB-C2B-C1B | -2.08 | 122.25      | 125.42   |
| 30  | 9     | 305 | CHL  | C5-C3-C4    | 2.08  | 119.38      | 114.59   |
| 30  | 5     | 306 | CHL  | O2D-CGD-O1D | -2.08 | 119.80      | 123.85   |
| 31  | A     | 841 | CLA  | O2A-CGA-O1A | -2.08 | 118.42      | 123.63   |
| 42  | e     | 523 | NEX  | C28-C29-C30 | 2.08  | 122.28      | 119.01   |
| 33  | 7     | 501 | 0UR  | C41-C2-C3   | 2.08  | 124.79      | 119.12   |
| 31  | A     | 806 | CLA  | O2A-CGA-O1A | -2.08 | 118.43      | 123.63   |
| 31  | B     | 807 | CLA  | O2A-CGA-O1A | -2.08 | 117.98      | 123.33   |
| 30  | 7     | 313 | CHL  | O2A-CGA-CBA | 2.08  | 119.99      | 112.14   |
| 37  | g     | 521 | 0IE  | C5-C4-C3    | 2.08  | 129.40      | 126.92   |
| 30  | 7     | 307 | CHL  | OMC-CMC-C2C | -2.08 | 121.51      | 125.12   |
| 31  | 9     | 308 | CLA  | O2A-CGA-O1A | -2.08 | 118.43      | 123.63   |
| 30  | g     | 606 | CHL  | CMA-C3A-C4A | -2.08 | 110.13      | 114.61   |
| 31  | g     | 613 | CLA  | O2D-CGD-CBD | 2.08  | 114.86      | 111.23   |
| 31  | B     | 839 | CLA  | CMB-C2B-C1B | -2.08 | 122.25      | 125.42   |
| 36  | 3     | 602 | LMG  | O7-C10-O9   | -2.08 | 118.85      | 123.70   |
| 30  | 6     | 313 | CHL  | O2D-CGD-O1D | -2.08 | 119.80      | 123.85   |
| 31  | 6     | 320 | CLA  | O2A-CGA-O1A | -2.08 | 118.43      | 123.63   |
| 30  | d     | 609 | CHL  | C1B-CHB-C4A | 2.08  | 122.66      | 121.32   |
| 30  | 8     | 305 | CHL  | CAC-C3C-C4C | 2.08  | 129.37      | 124.03   |
| 31  | e     | 610 | CLA  | CMB-C2B-C3B | 2.08  | 131.44      | 126.55   |
| 33  | O     | 204 | 0UR  | C43-C3-C2   | 2.08  | 121.39      | 116.56   |
| 31  | A     | 820 | CLA  | O2A-CGA-O1A | -2.08 | 118.44      | 123.63   |
| 36  | J     | 105 | LMG  | O2-C2-C1    | -2.08 | 105.13      | 110.08   |
| 30  | 0     | 305 | CHL  | OMC-CMC-C2C | -2.08 | 121.52      | 125.12   |
| 30  | e     | 614 | CHL  | O2D-CGD-O1D | -2.08 | 119.81      | 123.85   |
| 30  | 0     | 305 | CHL  | CMA-C3A-C4A | -2.08 | 110.14      | 114.61   |
| 37  | f     | 521 | 0IE  | C23-C16-C17 | 2.08  | 121.26      | 118.09   |
| 31  | 0     | 309 | CLA  | CMB-C2B-C3B | 2.07  | 131.43      | 126.55   |
| 30  | h     | 608 | CHL  | C4D-CHA-CBD | -2.07 | 106.88      | 108.97   |
| 33  | a     | 520 | 0UR  | C20-C7-C6   | 2.07  | 121.26      | 118.09   |
| 32  | A     | 850 | 8CT  | C30-C29-C28 | -2.07 | 121.35      | 124.58   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | h     | 606 | CHL  | OMC-CMC-C2C | -2.07 | 121.52      | 125.12   |
| 33  | 3     | 501 | 0UR  | C4-C5-C6    | -2.07 | 117.19      | 123.20   |
| 30  | 4     | 307 | CHL  | CMA-C3A-C4A | -2.07 | 110.14      | 114.61   |
| 36  | O     | 207 | LMG  | O7-C10-O9   | -2.07 | 118.86      | 123.70   |
| 32  | 2     | 402 | 8CT  | C39-C16-C17 | -2.07 | 119.46      | 122.82   |
| 31  | h     | 604 | CLA  | CMB-C2B-C1B | -2.07 | 122.26      | 125.42   |
| 31  | 0     | 308 | CLA  | O2A-CGA-O1A | -2.07 | 118.44      | 123.63   |
| 31  | A     | 821 | CLA  | O2A-CGA-O1A | -2.07 | 118.44      | 123.63   |
| 31  | A     | 838 | CLA  | C1-C2-C3    | -2.07 | 122.80      | 126.20   |
| 31  | A     | 819 | CLA  | O2A-CGA-O1A | -2.07 | 118.45      | 123.63   |
| 33  | 5     | 502 | 0UR  | C17-C16-C15 | 2.07  | 122.27      | 119.01   |
| 31  | A     | 812 | CLA  | O2A-CGA-O1A | -2.07 | 118.45      | 123.63   |
| 31  | 4     | 311 | CLA  | O2A-CGA-O1A | -2.07 | 118.45      | 123.63   |
| 34  | M     | 104 | LHG  | C5-O7-C7    | -2.07 | 112.84      | 117.80   |
| 30  | f     | 606 | CHL  | CAC-C3C-C4C | 2.07  | 129.35      | 124.03   |
| 34  | A     | 855 | LHG  | C26-C25-C24 | 2.07  | 120.73      | 113.13   |
| 31  | g     | 613 | CLA  | O2A-CGA-O1A | -2.07 | 118.45      | 123.63   |
| 31  | b     | 613 | CLA  | O2A-CGA-O1A | -2.07 | 118.45      | 123.63   |
| 32  | A     | 848 | 8CT  | C28-C26-C25 | -2.07 | 115.75      | 119.01   |
| 31  | A     | 840 | CLA  | C1-C2-C3    | 2.07  | 129.59      | 126.20   |
| 33  | h     | 520 | 0UR  | C48-C47-C46 | -2.07 | 121.61      | 125.92   |
| 30  | l     | 305 | CHL  | CAC-C3C-C4C | 2.07  | 129.34      | 124.03   |
| 31  | a     | 604 | CLA  | CMB-C2B-C1B | -2.07 | 122.27      | 125.42   |
| 30  | 4     | 319 | CHL  | O1D-CGD-CBD | -2.07 | 121.59      | 124.72   |
| 30  | g     | 607 | CHL  | CAC-C3C-C4C | 2.07  | 129.34      | 124.03   |
| 30  | 7     | 306 | CHL  | CMB-C2B-C3B | 2.07  | 128.81      | 124.68   |
| 30  | c     | 614 | CHL  | CMA-C3A-C2A | -2.07 | 111.49      | 116.23   |
| 31  | c     | 604 | CLA  | O2A-CGA-O1A | -2.07 | 118.46      | 123.63   |
| 31  | e     | 611 | CLA  | O2A-CGA-O1A | -2.07 | 118.46      | 123.63   |
| 30  | c     | 605 | CHL  | CMA-C3A-C4A | -2.07 | 110.16      | 114.61   |
| 31  | 8     | 304 | CLA  | O2A-CGA-O1A | -2.07 | 118.46      | 123.63   |
| 30  | i     | 601 | CHL  | O2A-CGA-CBA | 2.07  | 119.94      | 112.14   |
| 30  | f     | 607 | CHL  | CMA-C3A-C4A | -2.06 | 110.16      | 114.61   |
| 31  | 9     | 300 | CLA  | O2D-CGD-CBD | 2.06  | 114.84      | 111.23   |
| 31  | A     | 819 | CLA  | O2D-CGD-CBD | 2.06  | 114.84      | 111.23   |
| 31  | B     | 832 | CLA  | CMB-C2B-C3B | 2.06  | 131.40      | 126.55   |
| 31  | 7     | 304 | CLA  | C1-C2-C3    | -2.06 | 122.82      | 126.20   |
| 32  | B     | 844 | 8CT  | C27-C26-C25 | -2.06 | 119.47      | 122.82   |
| 30  | i     | 601 | CHL  | CMA-C3A-C4A | -2.06 | 110.17      | 114.61   |
| 30  | i     | 607 | CHL  | CAC-C3C-C4C | 2.06  | 129.33      | 124.03   |
| 31  | g     | 611 | CLA  | CMB-C2B-C1B | -2.06 | 122.28      | 125.42   |
| 32  | 1     | 402 | 8CT  | C40-C12-C13 | -2.06 | 119.47      | 122.82   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 33  | 0     | 502 | 0UR  | C29-C30-C31 | -2.06 | 108.12      | 111.18   |
| 30  | b     | 609 | CHL  | CAC-C3C-C4C | 2.06  | 129.33      | 124.03   |
| 31  | B     | 836 | CLA  | O2A-CGA-O1A | -2.06 | 118.47      | 123.63   |
| 32  | A     | 849 | 8CT  | C27-C26-C28 | 2.06  | 121.24      | 118.09   |
| 30  | i     | 606 | CHL  | CAC-C3C-C4C | 2.06  | 129.33      | 124.03   |
| 30  | a     | 606 | CHL  | CMA-C3A-C4A | -2.06 | 110.17      | 114.61   |
| 30  | 8     | 301 | CHL  | C6-C5-C3    | -2.06 | 108.45      | 113.47   |
| 32  | J     | 104 | 8CT  | C01-C02-C07 | 2.06  | 117.99      | 113.60   |
| 31  | B     | 815 | CLA  | C1-C2-C3    | -2.06 | 122.82      | 126.20   |
| 30  | 6     | 313 | CHL  | O2A-CGA-O1A | -2.06 | 118.48      | 123.63   |
| 31  | c     | 613 | CLA  | O2A-CGA-O1A | -2.06 | 118.48      | 123.63   |
| 30  | 9     | 313 | CHL  | OMC-CMC-C2C | -2.06 | 121.54      | 125.12   |
| 31  | 9     | 309 | CLA  | CMB-C2B-C3B | 2.06  | 131.39      | 126.55   |
| 30  | a     | 609 | CHL  | OMC-CMC-C2C | -2.06 | 121.55      | 125.12   |
| 31  | 4     | 304 | CLA  | O2A-CGA-O1A | -2.06 | 118.48      | 123.63   |
| 32  | B     | 848 | 8CT  | C39-C16-C15 | 2.06  | 121.23      | 118.09   |
| 31  | 3     | 303 | CLA  | C1-C2-C3    | -2.06 | 122.82      | 126.20   |
| 30  | b     | 608 | CHL  | CAC-C3C-C4C | 2.06  | 129.32      | 124.03   |
| 31  | A     | 812 | CLA  | CHB-C1B-NB  | 2.06  | 127.14      | 124.05   |
| 31  | O     | 206 | CLA  | O2A-CGA-O1A | -2.06 | 118.48      | 123.63   |
| 30  | a     | 609 | CHL  | CAC-C3C-C4C | 2.06  | 129.32      | 124.03   |
| 31  | K     | 105 | CLA  | O2A-CGA-O1A | -2.06 | 118.48      | 123.63   |
| 31  | H     | 201 | CLA  | CMB-C2B-C3B | 2.06  | 131.39      | 126.55   |
| 30  | 3     | 307 | CHL  | O2A-CGA-O1A | -2.06 | 118.49      | 123.63   |
| 32  | A     | 854 | 8CT  | C40-C12-C13 | -2.05 | 119.49      | 122.82   |
| 32  | K     | 107 | 8CT  | C15-C16-C17 | 2.05  | 122.24      | 119.01   |
| 30  | 7     | 305 | CHL  | CAC-C3C-C4C | 2.05  | 129.31      | 124.03   |
| 32  | A     | 847 | 8CT  | C35-C30-C29 | -2.05 | 110.46      | 112.83   |
| 30  | d     | 606 | CHL  | CAC-C3C-C4C | 2.05  | 129.31      | 124.03   |
| 31  | 2     | 310 | CLA  | O2A-CGA-O1A | -2.05 | 118.49      | 123.63   |
| 33  | 5     | 502 | 0UR  | C34-C27-C26 | 2.05  | 118.19      | 114.42   |
| 30  | a     | 608 | CHL  | OMC-CMC-C2C | -2.05 | 121.56      | 125.12   |
| 31  | A     | 813 | CLA  | CMB-C2B-C3B | 2.05  | 131.38      | 126.55   |
| 31  | B     | 827 | CLA  | O2A-CGA-O1A | -2.05 | 118.50      | 123.63   |
| 30  | g     | 601 | CHL  | CMA-C3A-C4A | -2.05 | 110.19      | 114.61   |
| 32  | O     | 205 | 8CT  | C40-C12-C13 | -2.05 | 119.50      | 122.82   |
| 30  | b     | 608 | CHL  | O2D-CGD-O1D | -2.05 | 119.86      | 123.85   |
| 33  | 6     | 501 | 0UR  | C14-C13-C12 | -2.05 | 120.74      | 126.36   |
| 32  | B     | 843 | 8CT  | C05-C04-C03 | 2.05  | 113.42      | 110.44   |
| 31  | 1     | 304 | CLA  | O2A-CGA-O1A | -2.05 | 118.50      | 123.63   |
| 30  | d     | 607 | CHL  | O2A-CGA-CBA | 2.05  | 119.88      | 112.14   |
| 31  | 7     | 309 | CLA  | CMB-C2B-C3B | 2.05  | 131.37      | 126.55   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 0     | 304 | CLA  | O2A-CGA-O1A | -2.05 | 118.51      | 123.63   |
| 39  | A     | 857 | CL0  | C3C-C4C-NC  | -2.05 | 109.65      | 114.65   |
| 32  | L     | 209 | 8CT  | C27-C26-C28 | 2.05  | 121.21      | 118.09   |
| 33  | 8     | 501 | 0UR  | C20-C7-C6   | 2.05  | 121.21      | 118.09   |
| 30  | 2     | 308 | CHL  | O2D-CGD-O1D | -2.05 | 119.86      | 123.85   |
| 31  | A     | 852 | CLA  | O2A-CGA-O1A | -2.05 | 118.51      | 123.63   |
| 34  | 2     | 601 | LHG  | C26-C25-C24 | 2.05  | 120.64      | 113.13   |
| 30  | i     | 608 | CHL  | O2D-CGD-O1D | -2.05 | 119.87      | 123.85   |
| 30  | e     | 605 | CHL  | CMA-C3A-C4A | -2.04 | 110.20      | 114.61   |
| 30  | i     | 602 | CHL  | CAC-C3C-C4C | 2.04  | 129.28      | 124.03   |
| 31  | B     | 817 | CLA  | CMB-C2B-C3B | 2.04  | 131.36      | 126.55   |
| 31  | 3     | 320 | CLA  | O2A-CGA-O1A | -2.04 | 118.52      | 123.63   |
| 33  | f     | 520 | 0UR  | O44-C45-O57 | -2.04 | 118.66      | 122.96   |
| 32  | B     | 846 | 8CT  | C37-C35-C30 | 2.04  | 112.64      | 109.55   |
| 31  | L     | 201 | CLA  | O2D-CGD-CBD | 2.04  | 114.80      | 111.23   |
| 32  | 7     | 405 | 8CT  | C22-C21-C23 | 2.04  | 121.21      | 118.09   |
| 31  | B     | 833 | CLA  | CAA-CBA-CGA | -2.04 | 107.41      | 113.21   |
| 30  | 2     | 307 | CHL  | O2D-CGD-O1D | -2.04 | 119.87      | 123.85   |
| 30  | b     | 614 | CHL  | CMA-C3A-C2A | -2.04 | 111.55      | 116.23   |
| 30  | 1     | 305 | CHL  | C5-C3-C4    | 2.04  | 119.29      | 114.59   |
| 34  | K     | 106 | LHG  | C5-O7-C7    | -2.04 | 112.91      | 117.80   |
| 31  | f     | 604 | CLA  | O2A-CGA-O1A | -2.04 | 118.52      | 123.63   |
| 30  | 8     | 301 | CHL  | CMA-C3A-C4A | -2.04 | 110.21      | 114.61   |
| 32  | 4     | 402 | 8CT  | C39-C16-C17 | -2.04 | 119.51      | 122.82   |
| 31  | 9     | 300 | CLA  | O2A-CGA-O1A | -2.04 | 118.53      | 123.63   |
| 31  | a     | 604 | CLA  | O2A-CGA-O1A | -2.04 | 118.53      | 123.63   |
| 31  | 0     | 304 | CLA  | C1-C2-C3    | -2.04 | 122.86      | 126.20   |
| 33  | 1     | 501 | 0UR  | C20-C7-C6   | 2.04  | 121.20      | 118.09   |
| 33  | 3     | 501 | 0UR  | C41-C2-C3   | 2.04  | 124.68      | 119.12   |
| 32  | A     | 848 | 8CT  | C22-C21-C23 | 2.04  | 121.20      | 118.09   |
| 33  | 4     | 502 | 0UR  | C34-C27-C26 | 2.04  | 118.17      | 114.42   |
| 32  | L     | 205 | 8CT  | C19-C18-C17 | -2.04 | 119.35      | 123.52   |
| 37  | d     | 521 | 0IE  | C5-C4-C3    | 2.04  | 129.35      | 126.92   |
| 31  | A     | 818 | CLA  | CMB-C2B-C3B | 2.04  | 131.34      | 126.55   |
| 33  | 3     | 501 | 0UR  | C10-C9-C8   | -2.04 | 119.35      | 123.52   |
| 32  | 3     | 403 | 8CT  | C24-C23-C21 | -2.04 | 120.78      | 126.36   |
| 30  | d     | 602 | CHL  | CAC-C3C-C4C | 2.04  | 129.26      | 124.03   |
| 31  | 3     | 303 | CLA  | CMB-C2B-C3B | 2.03  | 131.34      | 126.55   |
| 31  | A     | 803 | CLA  | O2D-CGD-CBD | 2.03  | 114.79      | 111.23   |
| 31  | 0     | 312 | CLA  | O2A-CGA-O1A | -2.03 | 118.54      | 123.63   |
| 31  | f     | 603 | CLA  | O2A-CGA-O1A | -2.03 | 118.54      | 123.63   |
| 31  | B     | 818 | CLA  | C1-C2-C3    | -2.03 | 122.86      | 126.20   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | 4     | 319 | CHL  | CMA-C3A-C4A | -2.03 | 110.23      | 114.61   |
| 34  | 5     | 601 | LHG  | C26-C25-C24 | 2.03  | 120.59      | 113.13   |
| 33  | 0     | 501 | 0UR  | C28-C19-C18 | -2.03 | 110.49      | 112.83   |
| 31  | f     | 610 | CLA  | CMB-C2B-C1B | -2.03 | 122.33      | 125.42   |
| 33  | 4     | 501 | 0UR  | C20-C7-C6   | 2.03  | 121.19      | 118.09   |
| 30  | 1     | 306 | CHL  | CAC-C3C-C4C | 2.03  | 129.25      | 124.03   |
| 36  | A     | 856 | LMG  | O1-C1-C2    | -2.03 | 105.19      | 108.27   |
| 31  | H     | 201 | CLA  | O1D-CGD-CBD | 2.03  | 128.52      | 124.52   |
| 31  | 7     | 316 | CLA  | CMB-C2B-C1B | -2.03 | 122.33      | 125.42   |
| 30  | 8     | 308 | CHL  | O2A-CGA-CBA | 2.03  | 119.81      | 112.14   |
| 30  | 2     | 302 | CHL  | CMA-C3A-C4A | -2.03 | 110.24      | 114.61   |
| 37  | g     | 522 | 0IE  | C17-C16-C15 | 2.03  | 122.20      | 119.01   |
| 30  | d     | 608 | CHL  | O2D-CGD-O1D | -2.03 | 119.90      | 123.85   |
| 31  | 2     | 303 | CLA  | O2A-CGA-O1A | -2.03 | 118.55      | 123.63   |
| 31  | A     | 804 | CLA  | CMB-C2B-C1B | -2.03 | 122.33      | 125.42   |
| 30  | g     | 602 | CHL  | CAC-C3C-C4C | 2.03  | 129.25      | 124.03   |
| 30  | 6     | 313 | CHL  | OMC-CMC-C2C | -2.03 | 121.60      | 125.12   |
| 30  | 3     | 302 | CHL  | CMA-C3A-C4A | -2.03 | 110.24      | 114.61   |
| 31  | g     | 610 | CLA  | CMB-C2B-C1B | -2.03 | 122.33      | 125.42   |
| 32  | 3     | 402 | 8CT  | C14-C15-C16 | 2.03  | 131.92      | 126.36   |
| 30  | h     | 607 | CHL  | CMA-C3A-C4A | -2.03 | 110.25      | 114.61   |
| 31  | B     | 801 | CLA  | O2A-CGA-O1A | -2.03 | 118.56      | 123.63   |
| 34  | g     | 630 | LHG  | C26-C25-C24 | 2.03  | 120.57      | 113.13   |
| 31  | 1     | 304 | CLA  | CMB-C2B-C1B | -2.03 | 122.33      | 125.42   |
| 32  | J     | 101 | 8CT  | C27-C26-C28 | 2.03  | 121.18      | 118.09   |
| 33  | f     | 520 | 0UR  | C20-C7-C6   | 2.03  | 121.18      | 118.09   |
| 30  | 6     | 302 | CHL  | CAC-C3C-C4C | 2.03  | 129.24      | 124.03   |
| 33  | 6     | 502 | 0UR  | C36-C28-C19 | 2.02  | 112.61      | 109.55   |
| 33  | 4     | 501 | 0UR  | C18-C17-C16 | -2.02 | 121.97      | 126.32   |
| 32  | L     | 209 | 8CT  | C05-C04-C03 | 2.02  | 113.38      | 110.44   |
| 30  | i     | 605 | CHL  | OMC-CMC-C2C | -2.02 | 121.61      | 125.12   |
| 31  | A     | 843 | CLA  | CMB-C2B-C3B | 2.02  | 131.31      | 126.55   |
| 31  | 1     | 311 | CLA  | O2A-CGA-O1A | -2.02 | 118.56      | 123.63   |
| 31  | i     | 604 | CLA  | O2A-CGA-O1A | -2.02 | 118.56      | 123.63   |
| 30  | c     | 609 | CHL  | CAC-C3C-C4C | 2.02  | 129.23      | 124.03   |
| 32  | 7     | 404 | 8CT  | C22-C21-C20 | -2.02 | 119.54      | 122.82   |
| 31  | A     | 837 | CLA  | O2D-CGD-CBD | 2.02  | 114.77      | 111.23   |
| 30  | d     | 601 | CHL  | OMC-CMC-C2C | -2.02 | 121.61      | 125.12   |
| 32  | B     | 851 | 8CT  | C25-C24-C23 | -2.02 | 117.34      | 123.20   |
| 30  | a     | 601 | CHL  | CMB-C2B-C3B | 2.02  | 128.72      | 124.68   |
| 37  | i     | 522 | 0IE  | C19-C18-C17 | 2.02  | 127.72      | 124.58   |
| 30  | h     | 602 | CHL  | CAC-C3C-C4C | 2.02  | 129.22      | 124.03   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | B     | 803 | CLA  | CMB-C2B-C3B | 2.02  | 131.30      | 126.55   |
| 32  | 9     | 401 | 8CT  | C10-C03-C02 | -2.02 | 116.90      | 121.56   |
| 31  | a     | 610 | CLA  | CMB-C2B-C1B | -2.02 | 122.34      | 125.42   |
| 31  | c     | 604 | CLA  | CMB-C2B-C1B | -2.02 | 122.34      | 125.42   |
| 31  | A     | 823 | CLA  | O2A-CGA-O1A | -2.02 | 118.58      | 123.63   |
| 31  | a     | 613 | CLA  | O2A-CGA-O1A | -2.02 | 118.58      | 123.63   |
| 30  | h     | 601 | CHL  | OMC-CMC-C2C | -2.02 | 121.61      | 125.12   |
| 32  | A     | 850 | 8CT  | C24-C25-C26 | -2.02 | 124.45      | 127.28   |
| 32  | G     | 104 | 8CT  | C38-C31-C32 | -2.02 | 115.58      | 122.37   |
| 31  | f     | 613 | CLA  | O2A-CGA-O1A | -2.02 | 118.58      | 123.63   |
| 33  | 9     | 501 | 0UR  | C14-C15-C16 | -2.02 | 124.45      | 127.28   |
| 33  | 5     | 502 | 0UR  | C5-C6-C7    | -2.02 | 120.83      | 126.36   |
| 31  | i     | 613 | CLA  | O2A-CGA-O1A | -2.02 | 118.58      | 123.63   |
| 30  | 8     | 305 | CHL  | OMC-CMC-C2C | -2.02 | 121.62      | 125.12   |
| 33  | 5     | 501 | 0UR  | C4-C5-C6    | -2.02 | 117.35      | 123.20   |
| 31  | A     | 830 | CLA  | CMB-C2B-C3B | 2.02  | 131.29      | 126.55   |
| 31  | H     | 205 | CLA  | C1-C2-C3    | -2.02 | 122.89      | 126.20   |
| 30  | 8     | 308 | CHL  | CAC-C3C-C4C | 2.02  | 129.22      | 124.03   |
| 33  | 8     | 502 | 0UR  | C34-C27-C26 | 2.02  | 118.13      | 114.42   |
| 33  | 1     | 501 | 0UR  | C29-C30-C31 | -2.02 | 108.19      | 111.18   |
| 30  | a     | 601 | CHL  | OMC-CMC-C2C | -2.02 | 121.62      | 125.12   |
| 30  | f     | 607 | CHL  | CAC-C3C-C4C | 2.02  | 129.21      | 124.03   |
| 35  | 0     | 603 | SQD  | O2-C2-C3    | -2.02 | 105.63      | 110.38   |
| 30  | 3     | 302 | CHL  | CAC-C3C-C4C | 2.02  | 129.21      | 124.03   |
| 31  | A     | 821 | CLA  | CMB-C2B-C3B | 2.01  | 131.29      | 126.55   |
| 31  | 7     | 315 | CLA  | O2A-CGA-O1A | -2.01 | 118.59      | 123.63   |
| 30  | e     | 601 | CHL  | CMA-C3A-C4A | -2.01 | 110.27      | 114.61   |
| 33  | 0     | 501 | 0UR  | C23-C24-C25 | -2.01 | 109.18      | 113.59   |
| 32  | O     | 205 | 8CT  | C27-C26-C28 | 2.01  | 121.16      | 118.09   |
| 31  | f     | 613 | CLA  | C1-C2-C3    | -2.01 | 122.90      | 126.20   |
| 31  | 1     | 309 | CLA  | CMB-C2B-C1B | -2.01 | 122.36      | 125.42   |
| 30  | c     | 608 | CHL  | CMA-C3A-C4A | -2.01 | 110.28      | 114.61   |
| 30  | a     | 606 | CHL  | CAC-C3C-C4C | 2.01  | 129.20      | 124.03   |
| 30  | 7     | 313 | CHL  | CMA-C3A-C4A | -2.01 | 110.28      | 114.61   |
| 33  | 3     | 501 | 0UR  | C21-C12-C13 | 2.01  | 121.16      | 118.09   |
| 31  | A     | 826 | CLA  | CMB-C2B-C1B | -2.01 | 122.36      | 125.42   |
| 31  | B     | 850 | CLA  | O2A-CGA-O1A | -2.01 | 118.60      | 123.63   |
| 30  | 6     | 306 | CHL  | CAC-C3C-C4C | 2.01  | 129.19      | 124.03   |
| 31  | A     | 802 | CLA  | O2A-CGA-O1A | -2.01 | 118.60      | 123.63   |
| 30  | c     | 608 | CHL  | O2D-CGD-O1D | -2.01 | 119.94      | 123.85   |
| 42  | c     | 523 | NEX  | C24-C23-C22 | -2.01 | 107.03      | 110.79   |
| 31  | b     | 611 | CLA  | O2A-CGA-O1A | -2.01 | 118.61      | 123.63   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 1     | 312 | CLA  | CMB-C2B-C1B | -2.01 | 122.36      | 125.42   |
| 30  | g     | 605 | CHL  | CMA-C3A-C4A | -2.01 | 110.29      | 114.61   |
| 30  | h     | 608 | CHL  | O2D-CGD-O1D | -2.01 | 119.94      | 123.85   |
| 31  | B     | 814 | CLA  | CMB-C2B-C1B | -2.01 | 122.36      | 125.42   |
| 33  | O     | 204 | 0UR  | C34-C27-C26 | 2.01  | 118.11      | 114.42   |
| 31  | i     | 604 | CLA  | C1-C2-C3    | -2.01 | 123.52      | 126.76   |
| 37  | f     | 522 | 0IE  | C19-C18-C17 | 2.01  | 127.70      | 124.58   |
| 31  | A     | 827 | CLA  | O2D-CGD-CBD | 2.01  | 114.74      | 111.23   |
| 31  | A     | 836 | CLA  | CMB-C2B-C3B | 2.01  | 131.27      | 126.55   |
| 33  | 2     | 502 | 0UR  | C48-C47-C46 | -2.01 | 123.56      | 125.84   |
| 31  | H     | 202 | CLA  | O2A-CGA-O1A | -2.01 | 118.61      | 123.63   |
| 31  | 5     | 309 | CLA  | C1-C2-C3    | -2.01 | 122.91      | 126.20   |
| 32  | B     | 847 | 8CT  | C06-C07-C02 | -2.01 | 110.48      | 114.06   |
| 37  | h     | 521 | 0IE  | C19-C18-C17 | 2.00  | 127.70      | 124.58   |
| 30  | b     | 606 | CHL  | CAC-C3C-C4C | 2.00  | 129.18      | 124.03   |
| 31  | B     | 821 | CLA  | CMB-C2B-C3B | 2.00  | 131.26      | 126.55   |
| 30  | d     | 607 | CHL  | CMA-C3A-C4A | -2.00 | 110.29      | 114.61   |
| 32  | L     | 205 | 8CT  | C10-C03-C02 | -2.00 | 116.94      | 121.56   |
| 30  | h     | 608 | CHL  | O2A-CGA-CBA | 2.00  | 120.33      | 114.00   |
| 31  | A     | 804 | CLA  | O2D-CGD-CBD | 2.00  | 114.73      | 111.23   |
| 30  | b     | 607 | CHL  | C1B-CHB-C4A | 2.00  | 122.61      | 121.32   |
| 31  | A     | 853 | CLA  | CAA-CBA-CGA | -2.00 | 107.52      | 113.21   |
| 37  | d     | 522 | 0IE  | C19-C18-C17 | 2.00  | 127.69      | 124.58   |
| 31  | B     | 821 | CLA  | O2A-CGA-O1A | -2.00 | 118.62      | 123.63   |
| 37  | e     | 522 | 0IE  | C23-C16-C17 | 2.00  | 121.14      | 118.09   |
| 33  | 4     | 501 | 0UR  | C14-C13-C12 | -2.00 | 120.88      | 126.36   |
| 32  | J     | 104 | 8CT  | C27-C26-C25 | -2.00 | 119.57      | 122.82   |
| 31  | K     | 102 | CLA  | CMB-C2B-C1B | -2.00 | 122.37      | 125.42   |

All (640) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 30  | 0     | 301 | CHL  | NA   |
| 30  | 0     | 301 | CHL  | ND   |
| 30  | 0     | 301 | CHL  | NC   |
| 30  | 0     | 302 | CHL  | NA   |
| 30  | 0     | 302 | CHL  | ND   |
| 30  | 0     | 302 | CHL  | NC   |
| 30  | 0     | 305 | CHL  | NA   |
| 30  | 0     | 305 | CHL  | ND   |
| 30  | 0     | 305 | CHL  | NC   |
| 30  | 0     | 306 | CHL  | NA   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 30  | 0     | 306 | CHL  | ND   |
| 30  | 0     | 306 | CHL  | NC   |
| 30  | 1     | 302 | CHL  | NA   |
| 30  | 1     | 302 | CHL  | ND   |
| 30  | 1     | 302 | CHL  | NC   |
| 30  | 1     | 305 | CHL  | NA   |
| 30  | 1     | 305 | CHL  | ND   |
| 30  | 1     | 305 | CHL  | NC   |
| 30  | 1     | 306 | CHL  | NA   |
| 30  | 1     | 306 | CHL  | ND   |
| 30  | 1     | 306 | CHL  | NC   |
| 30  | 1     | 307 | CHL  | NA   |
| 30  | 1     | 307 | CHL  | ND   |
| 30  | 1     | 307 | CHL  | NC   |
| 30  | 1     | 313 | CHL  | NA   |
| 30  | 1     | 313 | CHL  | ND   |
| 30  | 1     | 313 | CHL  | NC   |
| 30  | 2     | 301 | CHL  | NA   |
| 30  | 2     | 301 | CHL  | ND   |
| 30  | 2     | 301 | CHL  | NC   |
| 30  | 2     | 302 | CHL  | NA   |
| 30  | 2     | 302 | CHL  | ND   |
| 30  | 2     | 302 | CHL  | NC   |
| 30  | 2     | 305 | CHL  | NA   |
| 30  | 2     | 305 | CHL  | ND   |
| 30  | 2     | 305 | CHL  | NC   |
| 30  | 2     | 306 | CHL  | NA   |
| 30  | 2     | 306 | CHL  | ND   |
| 30  | 2     | 306 | CHL  | NC   |
| 30  | 2     | 307 | CHL  | NA   |
| 30  | 2     | 307 | CHL  | ND   |
| 30  | 2     | 307 | CHL  | NC   |
| 30  | 2     | 308 | CHL  | NA   |
| 30  | 2     | 308 | CHL  | ND   |
| 30  | 2     | 308 | CHL  | NC   |
| 30  | 2     | 313 | CHL  | NA   |
| 30  | 2     | 313 | CHL  | ND   |
| 30  | 2     | 313 | CHL  | NC   |
| 30  | 2     | 319 | CHL  | NA   |
| 30  | 2     | 319 | CHL  | ND   |
| 30  | 2     | 319 | CHL  | NC   |
| 30  | 3     | 302 | CHL  | NA   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 30  | 3     | 302 | CHL  | ND   |
| 30  | 3     | 302 | CHL  | NC   |
| 30  | 3     | 305 | CHL  | NA   |
| 30  | 3     | 305 | CHL  | ND   |
| 30  | 3     | 305 | CHL  | NC   |
| 30  | 3     | 307 | CHL  | NA   |
| 30  | 3     | 307 | CHL  | ND   |
| 30  | 3     | 307 | CHL  | NC   |
| 30  | 5     | 301 | CHL  | NA   |
| 30  | 5     | 301 | CHL  | ND   |
| 30  | 5     | 301 | CHL  | NC   |
| 30  | 5     | 302 | CHL  | NA   |
| 30  | 5     | 302 | CHL  | ND   |
| 30  | 5     | 302 | CHL  | NC   |
| 30  | 5     | 305 | CHL  | NA   |
| 30  | 5     | 305 | CHL  | ND   |
| 30  | 5     | 305 | CHL  | NC   |
| 30  | 5     | 306 | CHL  | NA   |
| 30  | 5     | 306 | CHL  | ND   |
| 30  | 5     | 306 | CHL  | NC   |
| 30  | 5     | 307 | CHL  | NA   |
| 30  | 5     | 307 | CHL  | ND   |
| 30  | 5     | 307 | CHL  | NC   |
| 30  | 5     | 313 | CHL  | NA   |
| 30  | 5     | 313 | CHL  | ND   |
| 30  | 5     | 313 | CHL  | NC   |
| 30  | 6     | 301 | CHL  | NA   |
| 30  | 6     | 301 | CHL  | ND   |
| 30  | 6     | 301 | CHL  | NC   |
| 30  | 6     | 302 | CHL  | NA   |
| 30  | 6     | 302 | CHL  | ND   |
| 30  | 6     | 302 | CHL  | NC   |
| 30  | 6     | 305 | CHL  | NA   |
| 30  | 6     | 305 | CHL  | ND   |
| 30  | 6     | 305 | CHL  | NC   |
| 30  | 6     | 306 | CHL  | NA   |
| 30  | 6     | 306 | CHL  | ND   |
| 30  | 6     | 306 | CHL  | NC   |
| 30  | 6     | 307 | CHL  | NA   |
| 30  | 6     | 307 | CHL  | ND   |
| 30  | 6     | 307 | CHL  | NC   |
| 30  | 6     | 308 | CHL  | NA   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 30  | 6     | 308 | CHL  | ND   |
| 30  | 6     | 308 | CHL  | NC   |
| 30  | 6     | 313 | CHL  | NA   |
| 30  | 6     | 313 | CHL  | ND   |
| 30  | 6     | 313 | CHL  | NC   |
| 30  | 6     | 315 | CHL  | NA   |
| 30  | 6     | 315 | CHL  | ND   |
| 30  | 6     | 315 | CHL  | NC   |
| 30  | 7     | 301 | CHL  | NA   |
| 30  | 7     | 301 | CHL  | ND   |
| 30  | 7     | 301 | CHL  | NC   |
| 30  | 7     | 302 | CHL  | NA   |
| 30  | 7     | 302 | CHL  | ND   |
| 30  | 7     | 302 | CHL  | NC   |
| 30  | 7     | 305 | CHL  | NA   |
| 30  | 7     | 305 | CHL  | ND   |
| 30  | 7     | 305 | CHL  | NC   |
| 30  | 7     | 306 | CHL  | NA   |
| 30  | 7     | 306 | CHL  | ND   |
| 30  | 7     | 306 | CHL  | NC   |
| 30  | 7     | 307 | CHL  | NA   |
| 30  | 7     | 307 | CHL  | ND   |
| 30  | 7     | 307 | CHL  | NC   |
| 30  | 7     | 313 | CHL  | NA   |
| 30  | 7     | 313 | CHL  | ND   |
| 30  | 7     | 313 | CHL  | NC   |
| 30  | 8     | 301 | CHL  | NA   |
| 30  | 8     | 301 | CHL  | ND   |
| 30  | 8     | 301 | CHL  | NC   |
| 30  | 8     | 302 | CHL  | NA   |
| 30  | 8     | 302 | CHL  | ND   |
| 30  | 8     | 302 | CHL  | NC   |
| 30  | 8     | 305 | CHL  | NA   |
| 30  | 8     | 305 | CHL  | ND   |
| 30  | 8     | 305 | CHL  | NC   |
| 30  | 8     | 306 | CHL  | NA   |
| 30  | 8     | 306 | CHL  | ND   |
| 30  | 8     | 306 | CHL  | NC   |
| 30  | 8     | 307 | CHL  | NA   |
| 30  | 8     | 307 | CHL  | ND   |
| 30  | 8     | 307 | CHL  | NC   |
| 30  | 8     | 308 | CHL  | NA   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 30  | 8     | 308 | CHL  | ND   |
| 30  | 8     | 308 | CHL  | NC   |
| 30  | 8     | 313 | CHL  | NA   |
| 30  | 8     | 313 | CHL  | ND   |
| 30  | 8     | 313 | CHL  | NC   |
| 30  | 8     | 315 | CHL  | NA   |
| 30  | 8     | 315 | CHL  | ND   |
| 30  | 8     | 315 | CHL  | NC   |
| 30  | 9     | 301 | CHL  | NA   |
| 30  | 9     | 301 | CHL  | ND   |
| 30  | 9     | 301 | CHL  | NC   |
| 30  | 9     | 305 | CHL  | NA   |
| 30  | 9     | 305 | CHL  | ND   |
| 30  | 9     | 305 | CHL  | NC   |
| 30  | 9     | 306 | CHL  | NA   |
| 30  | 9     | 306 | CHL  | ND   |
| 30  | 9     | 306 | CHL  | NC   |
| 30  | 9     | 313 | CHL  | NA   |
| 30  | 9     | 313 | CHL  | ND   |
| 30  | 9     | 313 | CHL  | NC   |
| 30  | a     | 601 | CHL  | NA   |
| 30  | a     | 601 | CHL  | ND   |
| 30  | a     | 601 | CHL  | NC   |
| 30  | a     | 602 | CHL  | NA   |
| 30  | a     | 602 | CHL  | ND   |
| 30  | a     | 602 | CHL  | NC   |
| 30  | a     | 605 | CHL  | NA   |
| 30  | a     | 605 | CHL  | ND   |
| 30  | a     | 605 | CHL  | NC   |
| 30  | a     | 606 | CHL  | NA   |
| 30  | a     | 606 | CHL  | ND   |
| 30  | a     | 606 | CHL  | NC   |
| 30  | a     | 607 | CHL  | NA   |
| 30  | a     | 607 | CHL  | ND   |
| 30  | a     | 607 | CHL  | NC   |
| 30  | a     | 608 | CHL  | NA   |
| 30  | a     | 608 | CHL  | ND   |
| 30  | a     | 608 | CHL  | NC   |
| 30  | a     | 609 | CHL  | NA   |
| 30  | a     | 609 | CHL  | ND   |
| 30  | a     | 609 | CHL  | NC   |
| 30  | a     | 614 | CHL  | NA   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 30  | a     | 614 | CHL  | ND   |
| 30  | a     | 614 | CHL  | NC   |
| 30  | c     | 601 | CHL  | NA   |
| 30  | c     | 601 | CHL  | ND   |
| 30  | c     | 601 | CHL  | NC   |
| 30  | c     | 602 | CHL  | NA   |
| 30  | c     | 602 | CHL  | ND   |
| 30  | c     | 602 | CHL  | NC   |
| 30  | c     | 605 | CHL  | NA   |
| 30  | c     | 605 | CHL  | ND   |
| 30  | c     | 605 | CHL  | NC   |
| 30  | c     | 606 | CHL  | NA   |
| 30  | c     | 606 | CHL  | ND   |
| 30  | c     | 606 | CHL  | NC   |
| 30  | c     | 607 | CHL  | NA   |
| 30  | c     | 607 | CHL  | ND   |
| 30  | c     | 607 | CHL  | NC   |
| 30  | c     | 608 | CHL  | NA   |
| 30  | c     | 608 | CHL  | ND   |
| 30  | c     | 608 | CHL  | NC   |
| 30  | c     | 609 | CHL  | NA   |
| 30  | c     | 609 | CHL  | ND   |
| 30  | c     | 609 | CHL  | NC   |
| 30  | c     | 614 | CHL  | NA   |
| 30  | c     | 614 | CHL  | ND   |
| 30  | c     | 614 | CHL  | NC   |
| 30  | b     | 601 | CHL  | NA   |
| 30  | b     | 601 | CHL  | ND   |
| 30  | b     | 601 | CHL  | NC   |
| 30  | b     | 602 | CHL  | NA   |
| 30  | b     | 602 | CHL  | ND   |
| 30  | b     | 602 | CHL  | NC   |
| 30  | b     | 606 | CHL  | NA   |
| 30  | b     | 606 | CHL  | ND   |
| 30  | b     | 606 | CHL  | NC   |
| 30  | b     | 607 | CHL  | NA   |
| 30  | b     | 607 | CHL  | ND   |
| 30  | b     | 607 | CHL  | NC   |
| 30  | b     | 608 | CHL  | NA   |
| 30  | b     | 608 | CHL  | ND   |
| 30  | b     | 608 | CHL  | NC   |
| 30  | b     | 609 | CHL  | NA   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 30  | b     | 609 | CHL  | ND   |
| 30  | b     | 609 | CHL  | NC   |
| 30  | b     | 614 | CHL  | NA   |
| 30  | b     | 614 | CHL  | ND   |
| 30  | b     | 614 | CHL  | NC   |
| 30  | d     | 601 | CHL  | NA   |
| 30  | d     | 601 | CHL  | ND   |
| 30  | d     | 601 | CHL  | NC   |
| 30  | d     | 602 | CHL  | NA   |
| 30  | d     | 602 | CHL  | ND   |
| 30  | d     | 602 | CHL  | NC   |
| 30  | d     | 605 | CHL  | NA   |
| 30  | d     | 605 | CHL  | ND   |
| 30  | d     | 605 | CHL  | NC   |
| 30  | d     | 606 | CHL  | NA   |
| 30  | d     | 606 | CHL  | ND   |
| 30  | d     | 606 | CHL  | NC   |
| 30  | d     | 607 | CHL  | NA   |
| 30  | d     | 607 | CHL  | ND   |
| 30  | d     | 607 | CHL  | NC   |
| 30  | d     | 608 | CHL  | NA   |
| 30  | d     | 608 | CHL  | ND   |
| 30  | d     | 608 | CHL  | NC   |
| 30  | d     | 609 | CHL  | NA   |
| 30  | d     | 609 | CHL  | ND   |
| 30  | d     | 609 | CHL  | NC   |
| 30  | d     | 614 | CHL  | NA   |
| 30  | d     | 614 | CHL  | ND   |
| 30  | d     | 614 | CHL  | NC   |
| 30  | f     | 601 | CHL  | NA   |
| 30  | f     | 601 | CHL  | ND   |
| 30  | f     | 601 | CHL  | NC   |
| 30  | f     | 602 | CHL  | NA   |
| 30  | f     | 602 | CHL  | ND   |
| 30  | f     | 602 | CHL  | NC   |
| 30  | f     | 605 | CHL  | NA   |
| 30  | f     | 605 | CHL  | ND   |
| 30  | f     | 605 | CHL  | NC   |
| 30  | f     | 606 | CHL  | NA   |
| 30  | f     | 606 | CHL  | ND   |
| 30  | f     | 606 | CHL  | NC   |
| 30  | f     | 607 | CHL  | NA   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 30  | f     | 607 | CHL  | ND   |
| 30  | f     | 607 | CHL  | NC   |
| 30  | f     | 608 | CHL  | NA   |
| 30  | f     | 608 | CHL  | ND   |
| 30  | f     | 608 | CHL  | NC   |
| 30  | f     | 609 | CHL  | NA   |
| 30  | f     | 609 | CHL  | ND   |
| 30  | f     | 609 | CHL  | NC   |
| 30  | f     | 614 | CHL  | NA   |
| 30  | f     | 614 | CHL  | ND   |
| 30  | f     | 614 | CHL  | NC   |
| 30  | g     | 601 | CHL  | NA   |
| 30  | g     | 601 | CHL  | ND   |
| 30  | g     | 601 | CHL  | NC   |
| 30  | g     | 602 | CHL  | NA   |
| 30  | g     | 602 | CHL  | ND   |
| 30  | g     | 602 | CHL  | NC   |
| 30  | g     | 605 | CHL  | NA   |
| 30  | g     | 605 | CHL  | ND   |
| 30  | g     | 605 | CHL  | NC   |
| 30  | g     | 606 | CHL  | NA   |
| 30  | g     | 606 | CHL  | ND   |
| 30  | g     | 606 | CHL  | NC   |
| 30  | g     | 607 | CHL  | NA   |
| 30  | g     | 607 | CHL  | ND   |
| 30  | g     | 607 | CHL  | NC   |
| 30  | g     | 608 | CHL  | NA   |
| 30  | g     | 608 | CHL  | ND   |
| 30  | g     | 608 | CHL  | NC   |
| 30  | g     | 609 | CHL  | NA   |
| 30  | g     | 609 | CHL  | ND   |
| 30  | g     | 609 | CHL  | NC   |
| 30  | g     | 614 | CHL  | NA   |
| 30  | g     | 614 | CHL  | ND   |
| 30  | g     | 614 | CHL  | NC   |
| 30  | h     | 601 | CHL  | NA   |
| 30  | h     | 601 | CHL  | ND   |
| 30  | h     | 601 | CHL  | NC   |
| 30  | h     | 602 | CHL  | NA   |
| 30  | h     | 602 | CHL  | ND   |
| 30  | h     | 602 | CHL  | NC   |
| 30  | h     | 605 | CHL  | NA   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 30  | h     | 605 | CHL  | ND   |
| 30  | h     | 605 | CHL  | NC   |
| 30  | h     | 606 | CHL  | NA   |
| 30  | h     | 606 | CHL  | ND   |
| 30  | h     | 606 | CHL  | NC   |
| 30  | h     | 607 | CHL  | NA   |
| 30  | h     | 607 | CHL  | ND   |
| 30  | h     | 607 | CHL  | NC   |
| 30  | h     | 608 | CHL  | NA   |
| 30  | h     | 608 | CHL  | ND   |
| 30  | h     | 608 | CHL  | NC   |
| 30  | h     | 609 | CHL  | NA   |
| 30  | h     | 609 | CHL  | ND   |
| 30  | h     | 609 | CHL  | NC   |
| 30  | h     | 614 | CHL  | NA   |
| 30  | h     | 614 | CHL  | ND   |
| 30  | h     | 614 | CHL  | NC   |
| 30  | i     | 601 | CHL  | NA   |
| 30  | i     | 601 | CHL  | ND   |
| 30  | i     | 601 | CHL  | NC   |
| 30  | i     | 602 | CHL  | NA   |
| 30  | i     | 602 | CHL  | ND   |
| 30  | i     | 602 | CHL  | NC   |
| 30  | i     | 605 | CHL  | NA   |
| 30  | i     | 605 | CHL  | ND   |
| 30  | i     | 605 | CHL  | NC   |
| 30  | i     | 606 | CHL  | NA   |
| 30  | i     | 606 | CHL  | ND   |
| 30  | i     | 606 | CHL  | NC   |
| 30  | i     | 607 | CHL  | NA   |
| 30  | i     | 607 | CHL  | ND   |
| 30  | i     | 607 | CHL  | NC   |
| 30  | i     | 608 | CHL  | NA   |
| 30  | i     | 608 | CHL  | ND   |
| 30  | i     | 608 | CHL  | NC   |
| 30  | i     | 609 | CHL  | NA   |
| 30  | i     | 609 | CHL  | ND   |
| 30  | i     | 609 | CHL  | NC   |
| 30  | i     | 614 | CHL  | NA   |
| 30  | i     | 614 | CHL  | ND   |
| 30  | i     | 614 | CHL  | NC   |
| 30  | e     | 601 | CHL  | NA   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 30  | e     | 601 | CHL  | ND   |
| 30  | e     | 601 | CHL  | NC   |
| 30  | e     | 602 | CHL  | NA   |
| 30  | e     | 602 | CHL  | ND   |
| 30  | e     | 602 | CHL  | NC   |
| 30  | e     | 605 | CHL  | NA   |
| 30  | e     | 605 | CHL  | ND   |
| 30  | e     | 605 | CHL  | NC   |
| 30  | e     | 606 | CHL  | NA   |
| 30  | e     | 606 | CHL  | ND   |
| 30  | e     | 606 | CHL  | NC   |
| 30  | e     | 607 | CHL  | NA   |
| 30  | e     | 607 | CHL  | ND   |
| 30  | e     | 607 | CHL  | NC   |
| 30  | e     | 608 | CHL  | NA   |
| 30  | e     | 608 | CHL  | ND   |
| 30  | e     | 608 | CHL  | NC   |
| 30  | e     | 609 | CHL  | NA   |
| 30  | e     | 609 | CHL  | ND   |
| 30  | e     | 609 | CHL  | NC   |
| 30  | e     | 614 | CHL  | NA   |
| 30  | e     | 614 | CHL  | ND   |
| 30  | e     | 614 | CHL  | NC   |
| 30  | 4     | 302 | CHL  | NA   |
| 30  | 4     | 302 | CHL  | ND   |
| 30  | 4     | 302 | CHL  | NC   |
| 30  | 4     | 305 | CHL  | NA   |
| 30  | 4     | 305 | CHL  | ND   |
| 30  | 4     | 305 | CHL  | NC   |
| 30  | 4     | 306 | CHL  | NA   |
| 30  | 4     | 306 | CHL  | ND   |
| 30  | 4     | 306 | CHL  | NC   |
| 30  | 4     | 307 | CHL  | NA   |
| 30  | 4     | 307 | CHL  | ND   |
| 30  | 4     | 307 | CHL  | NC   |
| 30  | 4     | 308 | CHL  | NA   |
| 30  | 4     | 308 | CHL  | ND   |
| 30  | 4     | 308 | CHL  | NC   |
| 30  | 4     | 313 | CHL  | NA   |
| 30  | 4     | 313 | CHL  | ND   |
| 30  | 4     | 313 | CHL  | NC   |
| 30  | 4     | 319 | CHL  | NA   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 30  | 4     | 319 | CHL  | ND   |
| 30  | 4     | 319 | CHL  | NC   |
| 31  | 0     | 303 | CLA  | ND   |
| 31  | 0     | 304 | CLA  | ND   |
| 31  | 0     | 308 | CLA  | ND   |
| 31  | 0     | 309 | CLA  | ND   |
| 31  | 0     | 310 | CLA  | ND   |
| 31  | 0     | 311 | CLA  | ND   |
| 31  | 0     | 312 | CLA  | ND   |
| 31  | 0     | 313 | CLA  | ND   |
| 31  | 0     | 321 | CLA  | ND   |
| 31  | 1     | 303 | CLA  | ND   |
| 31  | 1     | 304 | CLA  | ND   |
| 31  | 1     | 308 | CLA  | ND   |
| 31  | 1     | 309 | CLA  | ND   |
| 31  | 1     | 310 | CLA  | ND   |
| 31  | 1     | 311 | CLA  | ND   |
| 31  | 1     | 312 | CLA  | ND   |
| 31  | 1     | 314 | CLA  | ND   |
| 31  | 2     | 303 | CLA  | ND   |
| 31  | 2     | 304 | CLA  | ND   |
| 31  | 2     | 309 | CLA  | ND   |
| 31  | 2     | 310 | CLA  | ND   |
| 31  | 2     | 311 | CLA  | ND   |
| 31  | 2     | 312 | CLA  | ND   |
| 31  | 2     | 314 | CLA  | ND   |
| 31  | 3     | 303 | CLA  | ND   |
| 31  | 3     | 304 | CLA  | ND   |
| 31  | 3     | 306 | CLA  | ND   |
| 31  | 3     | 308 | CLA  | ND   |
| 31  | 3     | 309 | CLA  | ND   |
| 31  | 3     | 310 | CLA  | ND   |
| 31  | 3     | 311 | CLA  | ND   |
| 31  | 3     | 312 | CLA  | ND   |
| 31  | 3     | 313 | CLA  | ND   |
| 31  | 3     | 318 | CLA  | ND   |
| 31  | 3     | 320 | CLA  | ND   |
| 31  | 5     | 303 | CLA  | ND   |
| 31  | 5     | 304 | CLA  | ND   |
| 31  | 5     | 308 | CLA  | ND   |
| 31  | 5     | 309 | CLA  | ND   |
| 31  | 5     | 310 | CLA  | ND   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 31  | 5     | 311 | CLA  | ND   |
| 31  | 5     | 312 | CLA  | ND   |
| 31  | 5     | 314 | CLA  | ND   |
| 31  | 6     | 303 | CLA  | ND   |
| 31  | 6     | 304 | CLA  | ND   |
| 31  | 6     | 309 | CLA  | ND   |
| 31  | 6     | 310 | CLA  | ND   |
| 31  | 6     | 311 | CLA  | ND   |
| 31  | 6     | 312 | CLA  | ND   |
| 31  | 6     | 314 | CLA  | ND   |
| 31  | 6     | 317 | CLA  | ND   |
| 31  | 6     | 318 | CLA  | ND   |
| 31  | 6     | 320 | CLA  | ND   |
| 31  | 7     | 303 | CLA  | ND   |
| 31  | 7     | 304 | CLA  | ND   |
| 31  | 7     | 308 | CLA  | ND   |
| 31  | 7     | 309 | CLA  | ND   |
| 31  | 7     | 310 | CLA  | ND   |
| 31  | 7     | 311 | CLA  | ND   |
| 31  | 7     | 312 | CLA  | ND   |
| 31  | 7     | 315 | CLA  | ND   |
| 31  | 7     | 316 | CLA  | ND   |
| 31  | 7     | 317 | CLA  | ND   |
| 31  | 7     | 318 | CLA  | ND   |
| 31  | 8     | 303 | CLA  | ND   |
| 31  | 8     | 304 | CLA  | ND   |
| 31  | 8     | 309 | CLA  | ND   |
| 31  | 8     | 310 | CLA  | ND   |
| 31  | 8     | 311 | CLA  | ND   |
| 31  | 8     | 312 | CLA  | ND   |
| 31  | 8     | 314 | CLA  | ND   |
| 31  | 9     | 300 | CLA  | ND   |
| 31  | 9     | 302 | CLA  | ND   |
| 31  | 9     | 303 | CLA  | ND   |
| 31  | 9     | 304 | CLA  | ND   |
| 31  | 9     | 308 | CLA  | ND   |
| 31  | 9     | 309 | CLA  | ND   |
| 31  | 9     | 310 | CLA  | ND   |
| 31  | 9     | 311 | CLA  | ND   |
| 31  | 9     | 312 | CLA  | ND   |
| 31  | A     | 802 | CLA  | ND   |
| 31  | A     | 803 | CLA  | ND   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 31  | A     | 804 | CLA  | ND   |
| 31  | A     | 805 | CLA  | ND   |
| 31  | A     | 806 | CLA  | ND   |
| 31  | A     | 807 | CLA  | ND   |
| 31  | A     | 808 | CLA  | ND   |
| 31  | A     | 809 | CLA  | ND   |
| 31  | A     | 810 | CLA  | ND   |
| 31  | A     | 811 | CLA  | ND   |
| 31  | A     | 812 | CLA  | ND   |
| 31  | A     | 813 | CLA  | ND   |
| 31  | A     | 814 | CLA  | ND   |
| 31  | A     | 815 | CLA  | ND   |
| 31  | A     | 816 | CLA  | ND   |
| 31  | A     | 817 | CLA  | ND   |
| 31  | A     | 818 | CLA  | ND   |
| 31  | A     | 819 | CLA  | ND   |
| 31  | A     | 820 | CLA  | ND   |
| 31  | A     | 821 | CLA  | ND   |
| 31  | A     | 822 | CLA  | ND   |
| 31  | A     | 823 | CLA  | ND   |
| 31  | A     | 824 | CLA  | ND   |
| 31  | A     | 825 | CLA  | ND   |
| 31  | A     | 826 | CLA  | ND   |
| 31  | A     | 827 | CLA  | ND   |
| 31  | A     | 828 | CLA  | ND   |
| 31  | A     | 829 | CLA  | ND   |
| 31  | A     | 830 | CLA  | ND   |
| 31  | A     | 831 | CLA  | ND   |
| 31  | A     | 832 | CLA  | ND   |
| 31  | A     | 833 | CLA  | ND   |
| 31  | A     | 834 | CLA  | ND   |
| 31  | A     | 835 | CLA  | ND   |
| 31  | A     | 836 | CLA  | ND   |
| 31  | A     | 837 | CLA  | ND   |
| 31  | A     | 838 | CLA  | ND   |
| 31  | A     | 839 | CLA  | ND   |
| 31  | A     | 840 | CLA  | ND   |
| 31  | A     | 841 | CLA  | ND   |
| 31  | A     | 843 | CLA  | ND   |
| 31  | A     | 852 | CLA  | ND   |
| 31  | A     | 853 | CLA  | ND   |
| 31  | B     | 801 | CLA  | ND   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 31  | B     | 803 | CLA  | ND   |
| 31  | B     | 805 | CLA  | ND   |
| 31  | B     | 806 | CLA  | ND   |
| 31  | B     | 807 | CLA  | ND   |
| 31  | B     | 808 | CLA  | ND   |
| 31  | B     | 809 | CLA  | ND   |
| 31  | B     | 810 | CLA  | ND   |
| 31  | B     | 811 | CLA  | ND   |
| 31  | B     | 812 | CLA  | ND   |
| 31  | B     | 813 | CLA  | ND   |
| 31  | B     | 814 | CLA  | ND   |
| 31  | B     | 815 | CLA  | ND   |
| 31  | B     | 816 | CLA  | ND   |
| 31  | B     | 817 | CLA  | ND   |
| 31  | B     | 818 | CLA  | ND   |
| 31  | B     | 819 | CLA  | ND   |
| 31  | B     | 820 | CLA  | ND   |
| 31  | B     | 821 | CLA  | ND   |
| 31  | B     | 822 | CLA  | ND   |
| 31  | B     | 823 | CLA  | ND   |
| 31  | B     | 824 | CLA  | ND   |
| 31  | B     | 825 | CLA  | ND   |
| 31  | B     | 826 | CLA  | ND   |
| 31  | B     | 827 | CLA  | ND   |
| 31  | B     | 828 | CLA  | ND   |
| 31  | B     | 829 | CLA  | ND   |
| 31  | B     | 830 | CLA  | ND   |
| 31  | B     | 831 | CLA  | ND   |
| 31  | B     | 832 | CLA  | ND   |
| 31  | B     | 833 | CLA  | ND   |
| 31  | B     | 834 | CLA  | ND   |
| 31  | B     | 835 | CLA  | ND   |
| 31  | B     | 836 | CLA  | ND   |
| 31  | B     | 837 | CLA  | ND   |
| 31  | B     | 838 | CLA  | ND   |
| 31  | B     | 839 | CLA  | ND   |
| 31  | B     | 840 | CLA  | ND   |
| 31  | B     | 841 | CLA  | ND   |
| 31  | B     | 850 | CLA  | ND   |
| 31  | F     | 301 | CLA  | ND   |
| 31  | G     | 101 | CLA  | ND   |
| 31  | G     | 102 | CLA  | ND   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 31  | G     | 103 | CLA  | ND   |
| 31  | J     | 103 | CLA  | ND   |
| 31  | L     | 201 | CLA  | ND   |
| 31  | L     | 202 | CLA  | ND   |
| 31  | L     | 203 | CLA  | ND   |
| 31  | L     | 204 | CLA  | ND   |
| 31  | L     | 207 | CLA  | ND   |
| 31  | K     | 101 | CLA  | ND   |
| 31  | K     | 102 | CLA  | ND   |
| 31  | K     | 104 | CLA  | ND   |
| 31  | K     | 105 | CLA  | ND   |
| 31  | M     | 101 | CLA  | ND   |
| 31  | O     | 201 | CLA  | ND   |
| 31  | O     | 202 | CLA  | ND   |
| 31  | O     | 203 | CLA  | ND   |
| 31  | O     | 206 | CLA  | ND   |
| 31  | a     | 603 | CLA  | ND   |
| 31  | a     | 604 | CLA  | ND   |
| 31  | a     | 610 | CLA  | ND   |
| 31  | a     | 611 | CLA  | ND   |
| 31  | a     | 612 | CLA  | ND   |
| 31  | a     | 613 | CLA  | ND   |
| 31  | c     | 603 | CLA  | ND   |
| 31  | c     | 604 | CLA  | ND   |
| 31  | c     | 610 | CLA  | ND   |
| 31  | c     | 611 | CLA  | ND   |
| 31  | c     | 612 | CLA  | ND   |
| 31  | c     | 613 | CLA  | ND   |
| 31  | b     | 603 | CLA  | ND   |
| 31  | b     | 604 | CLA  | ND   |
| 31  | b     | 610 | CLA  | ND   |
| 31  | b     | 611 | CLA  | ND   |
| 31  | b     | 612 | CLA  | ND   |
| 31  | b     | 613 | CLA  | ND   |
| 31  | d     | 603 | CLA  | ND   |
| 31  | d     | 604 | CLA  | ND   |
| 31  | d     | 610 | CLA  | ND   |
| 31  | d     | 611 | CLA  | ND   |
| 31  | d     | 612 | CLA  | ND   |
| 31  | d     | 613 | CLA  | ND   |
| 31  | f     | 603 | CLA  | ND   |
| 31  | f     | 604 | CLA  | ND   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 31  | f     | 610 | CLA  | ND   |
| 31  | f     | 611 | CLA  | ND   |
| 31  | f     | 612 | CLA  | ND   |
| 31  | f     | 613 | CLA  | ND   |
| 31  | g     | 603 | CLA  | ND   |
| 31  | g     | 604 | CLA  | ND   |
| 31  | g     | 610 | CLA  | ND   |
| 31  | g     | 611 | CLA  | ND   |
| 31  | g     | 612 | CLA  | ND   |
| 31  | g     | 613 | CLA  | ND   |
| 31  | h     | 603 | CLA  | ND   |
| 31  | h     | 604 | CLA  | ND   |
| 31  | h     | 610 | CLA  | ND   |
| 31  | h     | 611 | CLA  | ND   |
| 31  | h     | 612 | CLA  | ND   |
| 31  | h     | 613 | CLA  | ND   |
| 31  | H     | 201 | CLA  | ND   |
| 31  | H     | 202 | CLA  | ND   |
| 31  | H     | 204 | CLA  | ND   |
| 31  | H     | 205 | CLA  | ND   |
| 31  | i     | 603 | CLA  | ND   |
| 31  | i     | 604 | CLA  | ND   |
| 31  | i     | 610 | CLA  | ND   |
| 31  | i     | 611 | CLA  | ND   |
| 31  | i     | 612 | CLA  | ND   |
| 31  | i     | 613 | CLA  | ND   |
| 31  | e     | 603 | CLA  | ND   |
| 31  | e     | 604 | CLA  | ND   |
| 31  | e     | 610 | CLA  | ND   |
| 31  | e     | 611 | CLA  | ND   |
| 31  | e     | 612 | CLA  | ND   |
| 31  | e     | 613 | CLA  | ND   |
| 31  | 4     | 303 | CLA  | ND   |
| 31  | 4     | 304 | CLA  | ND   |
| 31  | 4     | 309 | CLA  | ND   |
| 31  | 4     | 310 | CLA  | ND   |
| 31  | 4     | 311 | CLA  | ND   |
| 31  | 4     | 312 | CLA  | ND   |
| 31  | 4     | 314 | CLA  | ND   |
| 39  | A     | 857 | CL0  | NA   |
| 39  | A     | 857 | CL0  | ND   |
| 39  | A     | 857 | CL0  | NC   |



All (4532) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 30  | 0     | 301 | CHL  | C3A-C2A-CAA-CBA |
| 30  | 0     | 301 | CHL  | C1C-C2C-CMC-OMC |
| 30  | 0     | 301 | CHL  | C3C-C2C-CMC-OMC |
| 30  | 0     | 301 | CHL  | C2-C3-C5-C6     |
| 30  | 0     | 301 | CHL  | C4-C3-C5-C6     |
| 30  | 0     | 302 | CHL  | C12-C13-C15-C16 |
| 30  | 0     | 305 | CHL  | C1A-C2A-CAA-CBA |
| 30  | 0     | 305 | CHL  | C3A-C2A-CAA-CBA |
| 30  | 0     | 305 | CHL  | C1C-C2C-CMC-OMC |
| 30  | 0     | 305 | CHL  | C3C-C2C-CMC-OMC |
| 30  | 0     | 306 | CHL  | C4C-C3C-CAC-CBC |
| 30  | 1     | 302 | CHL  | C1C-C2C-CMC-OMC |
| 30  | 1     | 302 | CHL  | C3C-C2C-CMC-OMC |
| 30  | 1     | 307 | CHL  | C1C-C2C-CMC-OMC |
| 30  | 1     | 307 | CHL  | C3C-C2C-CMC-OMC |
| 30  | 1     | 307 | CHL  | C11-C10-C8-C9   |
| 30  | 1     | 313 | CHL  | C1C-C2C-CMC-OMC |
| 30  | 1     | 313 | CHL  | C3C-C2C-CMC-OMC |
| 30  | 2     | 302 | CHL  | C1C-C2C-CMC-OMC |
| 30  | 2     | 302 | CHL  | C3C-C2C-CMC-OMC |
| 30  | 2     | 302 | CHL  | C6-C7-C8-C9     |
| 30  | 2     | 302 | CHL  | C12-C13-C15-C16 |
| 30  | 2     | 306 | CHL  | C1C-C2C-CMC-OMC |
| 30  | 2     | 306 | CHL  | C3C-C2C-CMC-OMC |
| 30  | 2     | 307 | CHL  | CBD-CGD-O2D-CED |
| 30  | 2     | 319 | CHL  | CAD-CBD-CGD-O1D |
| 30  | 2     | 319 | CHL  | CAD-CBD-CGD-O2D |
| 30  | 3     | 302 | CHL  | C1C-C2C-CMC-OMC |
| 30  | 3     | 302 | CHL  | C3C-C2C-CMC-OMC |
| 30  | 5     | 301 | CHL  | C2-C3-C5-C6     |
| 30  | 5     | 301 | CHL  | C4-C3-C5-C6     |
| 30  | 5     | 302 | CHL  | C1C-C2C-CMC-OMC |
| 30  | 5     | 302 | CHL  | C3C-C2C-CMC-OMC |
| 30  | 5     | 305 | CHL  | C1C-C2C-CMC-OMC |
| 30  | 5     | 305 | CHL  | C3C-C2C-CMC-OMC |
| 30  | 5     | 305 | CHL  | CHA-CBD-CGD-O1D |
| 30  | 5     | 306 | CHL  | C4C-C3C-CAC-CBC |
| 30  | 5     | 307 | CHL  | C1C-C2C-CMC-OMC |
| 30  | 5     | 307 | CHL  | C3C-C2C-CMC-OMC |
| 30  | 5     | 313 | CHL  | CHA-CBD-CGD-O1D |
| 30  | 5     | 313 | CHL  | CHA-CBD-CGD-O2D |
| 30  | 6     | 302 | CHL  | C1C-C2C-CMC-OMC |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 30  | 6     | 302 | CHL  | C3C-C2C-CMC-OMC |
| 30  | 6     | 302 | CHL  | C11-C10-C8-C9   |
| 30  | 6     | 306 | CHL  | C1C-C2C-CMC-OMC |
| 30  | 6     | 306 | CHL  | C3C-C2C-CMC-OMC |
| 30  | 6     | 307 | CHL  | C1C-C2C-CMC-OMC |
| 30  | 6     | 307 | CHL  | C3C-C2C-CMC-OMC |
| 30  | 6     | 313 | CHL  | C2-C3-C5-C6     |
| 30  | 6     | 313 | CHL  | C4-C3-C5-C6     |
| 30  | 7     | 302 | CHL  | C14-C13-C15-C16 |
| 30  | 7     | 307 | CHL  | C3A-C2A-CAA-CBA |
| 30  | 7     | 307 | CHL  | CBD-CGD-O2D-CED |
| 30  | 8     | 302 | CHL  | C1C-C2C-CMC-OMC |
| 30  | 8     | 302 | CHL  | C3C-C2C-CMC-OMC |
| 30  | 8     | 306 | CHL  | C1A-C2A-CAA-CBA |
| 30  | 8     | 306 | CHL  | C1C-C2C-CMC-OMC |
| 30  | 8     | 306 | CHL  | C3C-C2C-CMC-OMC |
| 30  | 8     | 306 | CHL  | CAD-CBD-CGD-O1D |
| 30  | 8     | 306 | CHL  | CAD-CBD-CGD-O2D |
| 30  | 8     | 307 | CHL  | C3A-C2A-CAA-CBA |
| 30  | 8     | 313 | CHL  | C1C-C2C-CMC-OMC |
| 30  | 8     | 313 | CHL  | C3C-C2C-CMC-OMC |
| 30  | 9     | 301 | CHL  | C1C-C2C-CMC-OMC |
| 30  | 9     | 301 | CHL  | C3C-C2C-CMC-OMC |
| 30  | 9     | 306 | CHL  | C1C-C2C-CMC-OMC |
| 30  | 9     | 313 | CHL  | C3A-C2A-CAA-CBA |
| 30  | a     | 601 | CHL  | C1A-C2A-CAA-CBA |
| 30  | a     | 601 | CHL  | C3A-C2A-CAA-CBA |
| 30  | a     | 606 | CHL  | C1C-C2C-CMC-OMC |
| 30  | a     | 607 | CHL  | C3A-C2A-CAA-CBA |
| 30  | a     | 608 | CHL  | CAD-CBD-CGD-O1D |
| 30  | a     | 608 | CHL  | CAD-CBD-CGD-O2D |
| 30  | a     | 608 | CHL  | CBD-CGD-O2D-CED |
| 30  | a     | 609 | CHL  | C6-C7-C8-C9     |
| 30  | c     | 601 | CHL  | C1C-C2C-CMC-OMC |
| 30  | c     | 601 | CHL  | C3C-C2C-CMC-OMC |
| 30  | c     | 601 | CHL  | C4C-C3C-CAC-CBC |
| 30  | c     | 602 | CHL  | C1C-C2C-CMC-OMC |
| 30  | c     | 602 | CHL  | C3C-C2C-CMC-OMC |
| 30  | c     | 607 | CHL  | C1C-C2C-CMC-OMC |
| 30  | c     | 608 | CHL  | C1C-C2C-CMC-OMC |
| 30  | c     | 608 | CHL  | C3C-C2C-CMC-OMC |
| 30  | c     | 614 | CHL  | CAD-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 30  | c     | 614 | CHL  | CAD-CBD-CGD-O2D |
| 30  | b     | 602 | CHL  | C1C-C2C-CMC-OMC |
| 30  | b     | 602 | CHL  | CHA-CBD-CGD-O2D |
| 30  | b     | 608 | CHL  | CBD-CGD-O2D-CED |
| 30  | b     | 609 | CHL  | C1C-C2C-CMC-OMC |
| 30  | d     | 606 | CHL  | CHA-CBD-CGD-O1D |
| 30  | d     | 606 | CHL  | CHA-CBD-CGD-O2D |
| 30  | d     | 607 | CHL  | C1A-C2A-CAA-CBA |
| 30  | d     | 608 | CHL  | C1C-C2C-CMC-OMC |
| 30  | d     | 608 | CHL  | C3C-C2C-CMC-OMC |
| 30  | d     | 608 | CHL  | CBD-CGD-O2D-CED |
| 30  | f     | 606 | CHL  | C1C-C2C-CMC-OMC |
| 30  | f     | 606 | CHL  | C3C-C2C-CMC-OMC |
| 30  | f     | 607 | CHL  | C1A-C2A-CAA-CBA |
| 30  | f     | 608 | CHL  | CBD-CGD-O2D-CED |
| 30  | f     | 609 | CHL  | C14-C13-C15-C16 |
| 30  | f     | 614 | CHL  | C1C-C2C-CMC-OMC |
| 30  | f     | 614 | CHL  | C3C-C2C-CMC-OMC |
| 30  | f     | 614 | CHL  | CAD-CBD-CGD-O1D |
| 30  | f     | 614 | CHL  | CAD-CBD-CGD-O2D |
| 30  | g     | 601 | CHL  | C2-C3-C5-C6     |
| 30  | g     | 601 | CHL  | C4-C3-C5-C6     |
| 30  | g     | 607 | CHL  | C1C-C2C-CMC-OMC |
| 30  | g     | 607 | CHL  | C3C-C2C-CMC-OMC |
| 30  | g     | 608 | CHL  | C3A-C2A-CAA-CBA |
| 30  | g     | 608 | CHL  | C1C-C2C-CMC-OMC |
| 30  | g     | 608 | CHL  | CBD-CGD-O2D-CED |
| 30  | h     | 602 | CHL  | C6-C7-C8-C9     |
| 30  | h     | 614 | CHL  | CAD-CBD-CGD-O2D |
| 30  | i     | 602 | CHL  | C1C-C2C-CMC-OMC |
| 30  | i     | 602 | CHL  | C3C-C2C-CMC-OMC |
| 30  | i     | 606 | CHL  | C1C-C2C-CMC-OMC |
| 30  | i     | 606 | CHL  | C3C-C2C-CMC-OMC |
| 30  | i     | 607 | CHL  | C1C-C2C-CMC-OMC |
| 30  | i     | 607 | CHL  | C3C-C2C-CMC-OMC |
| 30  | i     | 608 | CHL  | C1C-C2C-CMC-OMC |
| 30  | i     | 608 | CHL  | C3C-C2C-CMC-OMC |
| 30  | i     | 614 | CHL  | CAD-CBD-CGD-O1D |
| 30  | i     | 614 | CHL  | CAD-CBD-CGD-O2D |
| 30  | e     | 601 | CHL  | CHA-CBD-CGD-O1D |
| 30  | e     | 608 | CHL  | C1C-C2C-CMC-OMC |
| 30  | e     | 608 | CHL  | C3C-C2C-CMC-OMC |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 30  | e     | 608 | CHL  | C11-C10-C8-C9   |
| 30  | e     | 609 | CHL  | C1C-C2C-CMC-OMC |
| 30  | e     | 609 | CHL  | C3C-C2C-CMC-OMC |
| 30  | e     | 609 | CHL  | CBD-CGD-O2D-CED |
| 30  | e     | 614 | CHL  | C1C-C2C-CMC-OMC |
| 30  | e     | 614 | CHL  | C3C-C2C-CMC-OMC |
| 30  | 4     | 302 | CHL  | C1C-C2C-CMC-OMC |
| 30  | 4     | 302 | CHL  | C3C-C2C-CMC-OMC |
| 30  | 4     | 306 | CHL  | C1C-C2C-CMC-OMC |
| 30  | 4     | 306 | CHL  | C3C-C2C-CMC-OMC |
| 30  | 4     | 307 | CHL  | C1C-C2C-CMC-OMC |
| 30  | 4     | 307 | CHL  | C3C-C2C-CMC-OMC |
| 30  | 4     | 307 | CHL  | CBD-CGD-O2D-CED |
| 30  | 4     | 313 | CHL  | C1C-C2C-CMC-OMC |
| 30  | 4     | 313 | CHL  | C3C-C2C-CMC-OMC |
| 30  | 4     | 319 | CHL  | CAD-CBD-CGD-O1D |
| 30  | 4     | 319 | CHL  | CAD-CBD-CGD-O2D |
| 31  | 0     | 304 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 0     | 304 | CLA  | C3A-C2A-CAA-CBA |
| 31  | 0     | 308 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 0     | 308 | CLA  | C3A-C2A-CAA-CBA |
| 31  | 0     | 309 | CLA  | C2-C3-C5-C6     |
| 31  | 0     | 309 | CLA  | C4-C3-C5-C6     |
| 31  | 0     | 311 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 0     | 312 | CLA  | C6-C7-C8-C9     |
| 31  | 0     | 313 | CLA  | CBA-CGA-O2A-C1  |
| 31  | 0     | 313 | CLA  | CAD-CBD-CGD-O2D |
| 31  | 0     | 313 | CLA  | CBD-CGD-O2D-CED |
| 31  | 0     | 321 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 0     | 321 | CLA  | C3A-C2A-CAA-CBA |
| 31  | 0     | 321 | CLA  | CAD-CBD-CGD-O1D |
| 31  | 0     | 321 | CLA  | CAD-CBD-CGD-O2D |
| 31  | 1     | 311 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 1     | 311 | CLA  | C3A-C2A-CAA-CBA |
| 31  | 3     | 303 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 3     | 306 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 3     | 306 | CLA  | C3A-C2A-CAA-CBA |
| 31  | 3     | 308 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 3     | 308 | CLA  | C3A-C2A-CAA-CBA |
| 31  | 3     | 309 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 3     | 309 | CLA  | C3A-C2A-CAA-CBA |
| 31  | 5     | 304 | CLA  | CAD-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | 5     | 304 | CLA  | CAD-CBD-CGD-O2D |
| 31  | 5     | 304 | CLA  | CBD-CGD-O2D-CED |
| 31  | 5     | 308 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 5     | 308 | CLA  | C3A-C2A-CAA-CBA |
| 31  | 5     | 311 | CLA  | CBD-CGD-O2D-CED |
| 31  | 5     | 312 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 5     | 312 | CLA  | C3A-C2A-CAA-CBA |
| 31  | 5     | 312 | CLA  | CBD-CGD-O2D-CED |
| 31  | 6     | 303 | CLA  | C4-C3-C5-C6     |
| 31  | 6     | 312 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 6     | 317 | CLA  | CAD-CBD-CGD-O1D |
| 31  | 6     | 317 | CLA  | CAD-CBD-CGD-O2D |
| 31  | 6     | 318 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 6     | 318 | CLA  | C3A-C2A-CAA-CBA |
| 31  | 7     | 303 | CLA  | CBD-CGD-O2D-CED |
| 31  | 7     | 304 | CLA  | CHA-CBD-CGD-O1D |
| 31  | 7     | 304 | CLA  | CHA-CBD-CGD-O2D |
| 31  | 7     | 308 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 7     | 308 | CLA  | C3A-C2A-CAA-CBA |
| 31  | 7     | 309 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 7     | 309 | CLA  | C3A-C2A-CAA-CBA |
| 31  | 7     | 315 | CLA  | CBD-CGD-O2D-CED |
| 31  | 7     | 317 | CLA  | CHA-CBD-CGD-O1D |
| 31  | 7     | 317 | CLA  | CHA-CBD-CGD-O2D |
| 31  | 7     | 318 | CLA  | C3A-C2A-CAA-CBA |
| 31  | 8     | 303 | CLA  | CBA-CGA-O2A-C1  |
| 31  | 8     | 304 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 8     | 304 | CLA  | C3A-C2A-CAA-CBA |
| 31  | 8     | 314 | CLA  | C3A-C2A-CAA-CBA |
| 31  | 9     | 300 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 9     | 300 | CLA  | CHA-CBD-CGD-O1D |
| 31  | 9     | 300 | CLA  | CHA-CBD-CGD-O2D |
| 31  | 9     | 302 | CLA  | CHA-CBD-CGD-O1D |
| 31  | 9     | 302 | CLA  | CHA-CBD-CGD-O2D |
| 31  | 9     | 311 | CLA  | CBD-CGD-O2D-CED |
| 31  | A     | 804 | CLA  | C1A-C2A-CAA-CBA |
| 31  | A     | 804 | CLA  | C3A-C2A-CAA-CBA |
| 31  | A     | 804 | CLA  | CHA-CBD-CGD-O1D |
| 31  | A     | 804 | CLA  | CHA-CBD-CGD-O2D |
| 31  | A     | 805 | CLA  | CAD-CBD-CGD-O1D |
| 31  | A     | 805 | CLA  | CAD-CBD-CGD-O2D |
| 31  | A     | 806 | CLA  | C3A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | A     | 806 | CLA  | C4B-C3B-CAB-CBB |
| 31  | A     | 808 | CLA  | C3A-C2A-CAA-CBA |
| 31  | A     | 808 | CLA  | CHA-CBD-CGD-O1D |
| 31  | A     | 808 | CLA  | CHA-CBD-CGD-O2D |
| 31  | A     | 811 | CLA  | C1A-C2A-CAA-CBA |
| 31  | A     | 816 | CLA  | CHA-CBD-CGD-O1D |
| 31  | A     | 816 | CLA  | CHA-CBD-CGD-O2D |
| 31  | A     | 817 | CLA  | CHA-CBD-CGD-O1D |
| 31  | A     | 817 | CLA  | CHA-CBD-CGD-O2D |
| 31  | A     | 818 | CLA  | C3A-C2A-CAA-CBA |
| 31  | A     | 819 | CLA  | C1A-C2A-CAA-CBA |
| 31  | A     | 819 | CLA  | C3A-C2A-CAA-CBA |
| 31  | A     | 820 | CLA  | C1A-C2A-CAA-CBA |
| 31  | A     | 820 | CLA  | C3A-C2A-CAA-CBA |
| 31  | A     | 820 | CLA  | C2B-C3B-CAB-CBB |
| 31  | A     | 820 | CLA  | C4B-C3B-CAB-CBB |
| 31  | A     | 822 | CLA  | C1A-C2A-CAA-CBA |
| 31  | A     | 822 | CLA  | C3A-C2A-CAA-CBA |
| 31  | A     | 828 | CLA  | CBD-CGD-O2D-CED |
| 31  | A     | 830 | CLA  | CHA-CBD-CGD-O1D |
| 31  | A     | 830 | CLA  | CHA-CBD-CGD-O2D |
| 31  | A     | 833 | CLA  | CHA-CBD-CGD-O1D |
| 31  | A     | 833 | CLA  | CHA-CBD-CGD-O2D |
| 31  | A     | 837 | CLA  | C4-C3-C5-C6     |
| 31  | A     | 843 | CLA  | C3A-C2A-CAA-CBA |
| 31  | A     | 843 | CLA  | CBD-CGD-O2D-CED |
| 31  | A     | 852 | CLA  | C12-C13-C15-C16 |
| 31  | A     | 853 | CLA  | CBD-CGD-O2D-CED |
| 31  | A     | 853 | CLA  | O1D-CGD-O2D-CED |
| 31  | B     | 801 | CLA  | CBD-CGD-O2D-CED |
| 31  | B     | 803 | CLA  | CAD-CBD-CGD-O1D |
| 31  | B     | 803 | CLA  | CAD-CBD-CGD-O2D |
| 31  | B     | 808 | CLA  | C1A-C2A-CAA-CBA |
| 31  | B     | 808 | CLA  | C3A-C2A-CAA-CBA |
| 31  | B     | 814 | CLA  | C1A-C2A-CAA-CBA |
| 31  | B     | 817 | CLA  | C1A-C2A-CAA-CBA |
| 31  | B     | 818 | CLA  | C1A-C2A-CAA-CBA |
| 31  | B     | 818 | CLA  | C3A-C2A-CAA-CBA |
| 31  | B     | 818 | CLA  | C2B-C3B-CAB-CBB |
| 31  | B     | 818 | CLA  | C4B-C3B-CAB-CBB |
| 31  | B     | 819 | CLA  | C1A-C2A-CAA-CBA |
| 31  | B     | 819 | CLA  | C3A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | B     | 820 | CLA  | C1A-C2A-CAA-CBA |
| 31  | B     | 820 | CLA  | C2B-C3B-CAB-CBB |
| 31  | B     | 820 | CLA  | C4B-C3B-CAB-CBB |
| 31  | B     | 825 | CLA  | CHA-CBD-CGD-O2D |
| 31  | B     | 827 | CLA  | C1A-C2A-CAA-CBA |
| 31  | B     | 828 | CLA  | C3A-C2A-CAA-CBA |
| 31  | B     | 829 | CLA  | C1A-C2A-CAA-CBA |
| 31  | B     | 829 | CLA  | C3A-C2A-CAA-CBA |
| 31  | B     | 830 | CLA  | C4-C3-C5-C6     |
| 31  | B     | 831 | CLA  | C1A-C2A-CAA-CBA |
| 31  | B     | 831 | CLA  | C3A-C2A-CAA-CBA |
| 31  | B     | 833 | CLA  | C1A-C2A-CAA-CBA |
| 31  | B     | 833 | CLA  | C3A-C2A-CAA-CBA |
| 31  | B     | 833 | CLA  | C4B-C3B-CAB-CBB |
| 31  | B     | 833 | CLA  | CHA-CBD-CGD-O1D |
| 31  | B     | 833 | CLA  | CHA-CBD-CGD-O2D |
| 31  | B     | 834 | CLA  | C1A-C2A-CAA-CBA |
| 31  | B     | 834 | CLA  | C3A-C2A-CAA-CBA |
| 31  | B     | 836 | CLA  | C1A-C2A-CAA-CBA |
| 31  | G     | 101 | CLA  | C1A-C2A-CAA-CBA |
| 31  | G     | 101 | CLA  | C3A-C2A-CAA-CBA |
| 31  | G     | 101 | CLA  | CHA-CBD-CGD-O1D |
| 31  | G     | 101 | CLA  | CHA-CBD-CGD-O2D |
| 31  | G     | 103 | CLA  | CBA-CGA-O2A-C1  |
| 31  | L     | 202 | CLA  | C1A-C2A-CAA-CBA |
| 31  | L     | 203 | CLA  | C1A-C2A-CAA-CBA |
| 31  | L     | 203 | CLA  | CAD-CBD-CGD-O1D |
| 31  | L     | 203 | CLA  | CAD-CBD-CGD-O2D |
| 31  | L     | 204 | CLA  | C1A-C2A-CAA-CBA |
| 31  | L     | 204 | CLA  | C3A-C2A-CAA-CBA |
| 31  | L     | 204 | CLA  | CBA-CGA-O2A-C1  |
| 31  | L     | 207 | CLA  | CHA-CBD-CGD-O1D |
| 31  | L     | 207 | CLA  | CHA-CBD-CGD-O2D |
| 31  | K     | 104 | CLA  | CBA-CGA-O2A-C1  |
| 31  | K     | 104 | CLA  | O1A-CGA-O2A-C1  |
| 31  | K     | 105 | CLA  | C1A-C2A-CAA-CBA |
| 31  | K     | 105 | CLA  | C3A-C2A-CAA-CBA |
| 31  | O     | 201 | CLA  | CAD-CBD-CGD-O1D |
| 31  | O     | 201 | CLA  | CAD-CBD-CGD-O2D |
| 31  | O     | 201 | CLA  | CBD-CGD-O2D-CED |
| 31  | O     | 206 | CLA  | CAD-CBD-CGD-O1D |
| 31  | O     | 206 | CLA  | CAD-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | O     | 206 | CLA  | CBD-CGD-O2D-CED |
| 31  | O     | 206 | CLA  | C2-C3-C5-C6     |
| 31  | O     | 206 | CLA  | C4-C3-C5-C6     |
| 31  | a     | 603 | CLA  | CHA-CBD-CGD-O1D |
| 31  | a     | 603 | CLA  | CHA-CBD-CGD-O2D |
| 31  | a     | 604 | CLA  | C1A-C2A-CAA-CBA |
| 31  | a     | 604 | CLA  | C3A-C2A-CAA-CBA |
| 31  | a     | 610 | CLA  | CBD-CGD-O2D-CED |
| 31  | a     | 613 | CLA  | CAD-CBD-CGD-O1D |
| 31  | a     | 613 | CLA  | CAD-CBD-CGD-O2D |
| 31  | c     | 603 | CLA  | CHA-CBD-CGD-O1D |
| 31  | c     | 603 | CLA  | CHA-CBD-CGD-O2D |
| 31  | c     | 603 | CLA  | CBD-CGD-O2D-CED |
| 31  | c     | 610 | CLA  | CBD-CGD-O2D-CED |
| 31  | c     | 611 | CLA  | C2B-C3B-CAB-CBB |
| 31  | c     | 611 | CLA  | C4B-C3B-CAB-CBB |
| 31  | b     | 604 | CLA  | C1A-C2A-CAA-CBA |
| 31  | d     | 603 | CLA  | CHA-CBD-CGD-O1D |
| 31  | d     | 603 | CLA  | CHA-CBD-CGD-O2D |
| 31  | d     | 603 | CLA  | CBD-CGD-O2D-CED |
| 31  | d     | 612 | CLA  | CBD-CGD-O2D-CED |
| 31  | f     | 610 | CLA  | CBD-CGD-O2D-CED |
| 31  | f     | 612 | CLA  | CHA-CBD-CGD-O1D |
| 31  | f     | 612 | CLA  | CHA-CBD-CGD-O2D |
| 31  | g     | 603 | CLA  | CBD-CGD-O2D-CED |
| 31  | g     | 604 | CLA  | C1A-C2A-CAA-CBA |
| 31  | g     | 604 | CLA  | C3A-C2A-CAA-CBA |
| 31  | g     | 604 | CLA  | CAD-CBD-CGD-O1D |
| 31  | g     | 604 | CLA  | CAD-CBD-CGD-O2D |
| 31  | g     | 612 | CLA  | CHA-CBD-CGD-O1D |
| 31  | g     | 612 | CLA  | CHA-CBD-CGD-O2D |
| 31  | h     | 604 | CLA  | CBD-CGD-O2D-CED |
| 31  | h     | 610 | CLA  | CBD-CGD-O2D-CED |
| 31  | h     | 611 | CLA  | CBD-CGD-O2D-CED |
| 31  | H     | 201 | CLA  | C1A-C2A-CAA-CBA |
| 31  | H     | 201 | CLA  | CAD-CBD-CGD-O1D |
| 31  | H     | 201 | CLA  | CAD-CBD-CGD-O2D |
| 31  | H     | 205 | CLA  | C2-C3-C5-C6     |
| 31  | H     | 205 | CLA  | C4-C3-C5-C6     |
| 31  | i     | 603 | CLA  | CBD-CGD-O2D-CED |
| 31  | i     | 613 | CLA  | CBD-CGD-O2D-CED |
| 31  | i     | 613 | CLA  | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | e     | 604 | CLA  | C1A-C2A-CAA-CBA |
| 31  | e     | 612 | CLA  | CHA-CBD-CGD-O1D |
| 31  | e     | 612 | CLA  | CHA-CBD-CGD-O2D |
| 32  | 0     | 401 | 8CT  | C02-C03-C10-C11 |
| 32  | 1     | 402 | 8CT  | C22-C21-C23-C24 |
| 32  | 1     | 402 | 8CT  | C28-C29-C30-C31 |
| 32  | 1     | 402 | 8CT  | C28-C29-C30-C35 |
| 32  | 2     | 402 | 8CT  | C20-C21-C23-C24 |
| 32  | 2     | 402 | 8CT  | C22-C21-C23-C24 |
| 32  | 3     | 402 | 8CT  | C02-C03-C10-C11 |
| 32  | 3     | 402 | 8CT  | C28-C29-C30-C31 |
| 32  | 3     | 402 | 8CT  | C28-C29-C30-C35 |
| 32  | 3     | 403 | 8CT  | C10-C11-C12-C13 |
| 32  | 3     | 403 | 8CT  | C28-C29-C30-C31 |
| 32  | 6     | 402 | 8CT  | C10-C11-C12-C13 |
| 32  | 6     | 402 | 8CT  | C16-C17-C18-C19 |
| 32  | 7     | 402 | 8CT  | C10-C11-C12-C40 |
| 32  | 7     | 402 | 8CT  | C14-C15-C16-C39 |
| 32  | 7     | 402 | 8CT  | C20-C21-C23-C24 |
| 32  | 7     | 402 | 8CT  | C22-C21-C23-C24 |
| 32  | 7     | 402 | 8CT  | C25-C26-C28-C29 |
| 32  | 7     | 402 | 8CT  | C27-C26-C28-C29 |
| 32  | 7     | 402 | 8CT  | C28-C29-C30-C31 |
| 32  | 7     | 404 | 8CT  | C10-C11-C12-C13 |
| 32  | 7     | 405 | 8CT  | C02-C03-C10-C11 |
| 32  | 8     | 402 | 8CT  | C14-C15-C16-C17 |
| 32  | 8     | 402 | 8CT  | C18-C19-C20-C21 |
| 32  | 8     | 402 | 8CT  | C28-C29-C30-C31 |
| 32  | 8     | 402 | 8CT  | C28-C29-C30-C35 |
| 32  | 8     | 406 | 8CT  | C02-C03-C10-C11 |
| 32  | 8     | 406 | 8CT  | C12-C13-C14-C15 |
| 32  | 9     | 401 | 8CT  | C20-C21-C23-C24 |
| 32  | 9     | 401 | 8CT  | C22-C21-C23-C24 |
| 32  | 9     | 401 | 8CT  | C28-C29-C30-C31 |
| 32  | A     | 847 | 8CT  | C14-C15-C16-C17 |
| 32  | A     | 848 | 8CT  | C10-C11-C12-C13 |
| 32  | A     | 848 | 8CT  | C10-C11-C12-C40 |
| 32  | A     | 848 | 8CT  | C14-C15-C16-C17 |
| 32  | A     | 849 | 8CT  | C16-C17-C18-C19 |
| 32  | A     | 849 | 8CT  | C28-C29-C30-C31 |
| 32  | A     | 850 | 8CT  | C04-C03-C10-C11 |
| 32  | A     | 850 | 8CT  | C14-C15-C16-C17 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 32  | A     | 850 | 8CT  | C18-C19-C20-C21 |
| 32  | A     | 854 | 8CT  | C20-C21-C23-C24 |
| 32  | A     | 854 | 8CT  | C22-C21-C23-C24 |
| 32  | B     | 804 | 8CT  | C10-C11-C12-C13 |
| 32  | B     | 804 | 8CT  | C10-C11-C12-C40 |
| 32  | B     | 804 | 8CT  | C20-C21-C23-C24 |
| 32  | B     | 804 | 8CT  | C28-C29-C30-C31 |
| 32  | B     | 804 | 8CT  | C28-C29-C30-C35 |
| 32  | B     | 843 | 8CT  | C10-C11-C12-C13 |
| 32  | B     | 843 | 8CT  | C20-C21-C23-C24 |
| 32  | B     | 843 | 8CT  | C28-C29-C30-C31 |
| 32  | B     | 843 | 8CT  | C28-C29-C30-C35 |
| 32  | B     | 844 | 8CT  | C10-C11-C12-C13 |
| 32  | B     | 844 | 8CT  | C10-C11-C12-C40 |
| 32  | B     | 845 | 8CT  | C10-C11-C12-C13 |
| 32  | B     | 845 | 8CT  | C10-C11-C12-C40 |
| 32  | B     | 845 | 8CT  | C18-C19-C20-C21 |
| 32  | B     | 846 | 8CT  | C14-C15-C16-C17 |
| 32  | B     | 846 | 8CT  | C14-C15-C16-C39 |
| 32  | B     | 846 | 8CT  | C28-C29-C30-C31 |
| 32  | B     | 846 | 8CT  | C28-C29-C30-C35 |
| 32  | B     | 847 | 8CT  | C28-C29-C30-C31 |
| 32  | B     | 848 | 8CT  | C14-C15-C16-C17 |
| 32  | B     | 848 | 8CT  | C14-C15-C16-C39 |
| 32  | B     | 851 | 8CT  | C14-C15-C16-C17 |
| 32  | B     | 851 | 8CT  | C16-C17-C18-C19 |
| 32  | B     | 851 | 8CT  | C28-C29-C30-C31 |
| 32  | B     | 851 | 8CT  | C28-C29-C30-C35 |
| 32  | F     | 302 | 8CT  | C02-C03-C10-C11 |
| 32  | F     | 302 | 8CT  | C14-C15-C16-C17 |
| 32  | F     | 302 | 8CT  | C14-C15-C16-C39 |
| 32  | F     | 302 | 8CT  | C28-C29-C30-C31 |
| 32  | F     | 302 | 8CT  | C28-C29-C30-C35 |
| 32  | G     | 104 | 8CT  | C10-C11-C12-C13 |
| 32  | G     | 104 | 8CT  | C12-C13-C14-C15 |
| 32  | G     | 104 | 8CT  | C14-C15-C16-C17 |
| 32  | G     | 104 | 8CT  | C14-C15-C16-C39 |
| 32  | G     | 104 | 8CT  | C20-C21-C23-C24 |
| 32  | G     | 104 | 8CT  | C22-C21-C23-C24 |
| 32  | G     | 104 | 8CT  | C25-C26-C28-C29 |
| 32  | G     | 104 | 8CT  | C27-C26-C28-C29 |
| 32  | G     | 104 | 8CT  | C28-C29-C30-C31 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 32  | I     | 101 | 8CT  | C25-C26-C28-C29 |
| 32  | I     | 101 | 8CT  | C27-C26-C28-C29 |
| 32  | I     | 101 | 8CT  | C28-C29-C30-C31 |
| 32  | J     | 101 | 8CT  | C18-C19-C20-C21 |
| 32  | J     | 101 | 8CT  | C20-C21-C23-C24 |
| 32  | J     | 101 | 8CT  | C28-C29-C30-C31 |
| 32  | J     | 101 | 8CT  | C28-C29-C30-C35 |
| 32  | J     | 104 | 8CT  | C18-C19-C20-C21 |
| 32  | J     | 104 | 8CT  | C28-C29-C30-C31 |
| 32  | J     | 104 | 8CT  | C28-C29-C30-C35 |
| 32  | L     | 205 | 8CT  | C25-C26-C28-C29 |
| 32  | L     | 205 | 8CT  | C27-C26-C28-C29 |
| 32  | L     | 205 | 8CT  | C28-C29-C30-C31 |
| 32  | L     | 206 | 8CT  | C28-C29-C30-C31 |
| 32  | L     | 209 | 8CT  | C02-C03-C10-C11 |
| 32  | L     | 209 | 8CT  | C10-C11-C12-C13 |
| 32  | K     | 107 | 8CT  | C10-C11-C12-C13 |
| 32  | K     | 107 | 8CT  | C10-C11-C12-C40 |
| 32  | K     | 107 | 8CT  | C28-C29-C30-C31 |
| 32  | M     | 102 | 8CT  | C25-C26-C28-C29 |
| 32  | O     | 205 | 8CT  | C10-C11-C12-C13 |
| 32  | O     | 205 | 8CT  | C10-C11-C12-C40 |
| 32  | O     | 205 | 8CT  | C14-C15-C16-C17 |
| 32  | 4     | 402 | 8CT  | C20-C21-C23-C24 |
| 32  | 4     | 402 | 8CT  | C22-C21-C23-C24 |
| 33  | 0     | 502 | 0UR  | C2-C3-C43-O44   |
| 33  | 0     | 502 | 0UR  | C4-C3-C43-O44   |
| 33  | 0     | 502 | 0UR  | C46-C45-O44-C43 |
| 33  | 1     | 502 | 0UR  | C17-C18-C19-C28 |
| 33  | 1     | 502 | 0UR  | C17-C18-C19-C32 |
| 33  | 1     | 502 | 0UR  | C46-C45-O44-C43 |
| 33  | 1     | 502 | 0UR  | O57-C45-O44-C43 |
| 33  | 2     | 501 | 0UR  | C2-C3-C43-O44   |
| 33  | 2     | 501 | 0UR  | C4-C3-C43-O44   |
| 33  | 2     | 501 | 0UR  | O42-C2-C3-C4    |
| 33  | 2     | 501 | 0UR  | C46-C45-O44-C43 |
| 33  | 2     | 501 | 0UR  | O57-C45-O44-C43 |
| 33  | 2     | 502 | 0UR  | C2-C3-C43-O44   |
| 33  | 2     | 502 | 0UR  | C4-C3-C43-O44   |
| 33  | 2     | 502 | 0UR  | C41-C2-C3-C4    |
| 33  | 3     | 501 | 0UR  | C2-C3-C43-O44   |
| 33  | 3     | 501 | 0UR  | C4-C3-C43-O44   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 33  | 3     | 501 | 0UR  | C46-C45-O44-C43 |
| 33  | 3     | 501 | 0UR  | O57-C45-O44-C43 |
| 33  | 5     | 501 | 0UR  | O42-C2-C3-C43   |
| 33  | 5     | 501 | 0UR  | C5-C6-C7-C8     |
| 33  | 5     | 502 | 0UR  | C2-C3-C43-O44   |
| 33  | 5     | 502 | 0UR  | C4-C3-C43-O44   |
| 33  | 5     | 502 | 0UR  | C17-C18-C19-C28 |
| 33  | 5     | 502 | 0UR  | C17-C18-C19-C32 |
| 33  | 6     | 501 | 0UR  | C17-C18-C19-C28 |
| 33  | 6     | 501 | 0UR  | C17-C18-C19-C32 |
| 33  | 6     | 501 | 0UR  | C46-C45-O44-C43 |
| 33  | 6     | 502 | 0UR  | C4-C3-C43-O44   |
| 33  | 6     | 502 | 0UR  | C17-C18-C19-C28 |
| 33  | 6     | 502 | 0UR  | C17-C18-C19-C32 |
| 33  | 7     | 501 | 0UR  | C2-C3-C43-O44   |
| 33  | 7     | 501 | 0UR  | C4-C3-C43-O44   |
| 33  | 7     | 501 | 0UR  | C46-C45-O44-C43 |
| 33  | 7     | 501 | 0UR  | O57-C45-O44-C43 |
| 33  | 8     | 502 | 0UR  | C46-C45-O44-C43 |
| 33  | 9     | 502 | 0UR  | C2-C3-C43-O44   |
| 33  | 9     | 502 | 0UR  | C4-C3-C43-O44   |
| 33  | 9     | 502 | 0UR  | O42-C2-C3-C43   |
| 33  | 9     | 502 | 0UR  | C46-C45-O44-C43 |
| 33  | O     | 204 | 0UR  | C46-C45-O44-C43 |
| 33  | a     | 520 | 0UR  | O42-C2-C3-C43   |
| 33  | a     | 520 | 0UR  | C3-C2-C41-C1    |
| 33  | a     | 520 | 0UR  | C5-C6-C7-C20    |
| 33  | a     | 520 | 0UR  | C5-C6-C7-C8     |
| 33  | c     | 520 | 0UR  | C17-C18-C19-C28 |
| 33  | c     | 520 | 0UR  | C17-C18-C19-C32 |
| 33  | b     | 520 | 0UR  | O42-C2-C3-C43   |
| 33  | d     | 520 | 0UR  | O42-C2-C3-C43   |
| 33  | f     | 520 | 0UR  | O42-C2-C3-C4    |
| 33  | f     | 520 | 0UR  | C17-C18-C19-C28 |
| 33  | f     | 520 | 0UR  | C17-C18-C19-C32 |
| 33  | g     | 520 | 0UR  | O42-C2-C3-C43   |
| 33  | h     | 520 | 0UR  | C46-C45-O44-C43 |
| 33  | h     | 520 | 0UR  | O57-C45-O44-C43 |
| 33  | i     | 520 | 0UR  | C46-C47-C48-C49 |
| 33  | e     | 520 | 0UR  | C4-C3-C43-O44   |
| 33  | e     | 520 | 0UR  | O42-C2-C3-C43   |
| 33  | e     | 520 | 0UR  | C46-C45-O44-C43 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 33  | 4     | 501 | 0UR  | C2-C3-C43-O44   |
| 33  | 4     | 501 | 0UR  | C4-C3-C43-O44   |
| 33  | 4     | 501 | 0UR  | C46-C45-O44-C43 |
| 33  | 4     | 501 | 0UR  | O57-C45-O44-C43 |
| 33  | 4     | 502 | 0UR  | C2-C3-C43-O44   |
| 33  | 4     | 502 | 0UR  | C4-C3-C43-O44   |
| 33  | 4     | 502 | 0UR  | C11-C12-C13-C14 |
| 33  | 4     | 502 | 0UR  | C21-C12-C13-C14 |
| 34  | 0     | 601 | LHG  | C3-O3-P-O6      |
| 34  | 0     | 601 | LHG  | C4-O6-P-O3      |
| 34  | 0     | 601 | LHG  | C4-O6-P-O4      |
| 34  | 1     | 601 | LHG  | O2-C2-C3-O3     |
| 34  | 1     | 601 | LHG  | C3-O3-P-O4      |
| 34  | 1     | 601 | LHG  | C3-O3-P-O6      |
| 34  | 2     | 601 | LHG  | O1-C1-C2-C3     |
| 34  | 2     | 601 | LHG  | O2-C2-C3-O3     |
| 34  | 2     | 601 | LHG  | C3-O3-P-O6      |
| 34  | 3     | 601 | LHG  | O1-C1-C2-C3     |
| 34  | 3     | 601 | LHG  | C3-O3-P-O4      |
| 34  | 3     | 601 | LHG  | C3-O3-P-O5      |
| 34  | 3     | 601 | LHG  | C3-O3-P-O6      |
| 34  | 3     | 601 | LHG  | O7-C5-C6-O8     |
| 34  | 3     | 603 | LHG  | O1-C1-C2-C3     |
| 34  | 3     | 603 | LHG  | O2-C2-C3-O3     |
| 34  | 3     | 603 | LHG  | C4-O6-P-O3      |
| 34  | 3     | 603 | LHG  | C4-O6-P-O4      |
| 34  | 3     | 603 | LHG  | C4-O6-P-O5      |
| 34  | 5     | 601 | LHG  | C3-O3-P-O4      |
| 34  | 5     | 601 | LHG  | C3-O3-P-O6      |
| 34  | 6     | 601 | LHG  | C3-O3-P-O4      |
| 34  | 6     | 601 | LHG  | C3-O3-P-O6      |
| 34  | 6     | 603 | LHG  | C4-O6-P-O3      |
| 34  | 6     | 603 | LHG  | C4-O6-P-O5      |
| 34  | 6     | 603 | LHG  | C5-C4-O6-P      |
| 34  | 7     | 601 | LHG  | C1-C2-C3-O3     |
| 34  | 7     | 602 | LHG  | C3-O3-P-O5      |
| 34  | 7     | 602 | LHG  | C3-O3-P-O6      |
| 34  | 7     | 602 | LHG  | C4-O6-P-O3      |
| 34  | 7     | 602 | LHG  | C4-O6-P-O5      |
| 34  | 7     | 602 | LHG  | C8-C7-O7-C5     |
| 34  | 7     | 603 | LHG  | C4-O6-P-O3      |
| 34  | 7     | 603 | LHG  | C4-O6-P-O4      |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 34  | 7     | 603 | LHG  | C4-O6-P-O5      |
| 34  | 8     | 601 | LHG  | C3-O3-P-O5      |
| 34  | 8     | 601 | LHG  | C3-O3-P-O6      |
| 34  | 8     | 601 | LHG  | C4-O6-P-O3      |
| 34  | 8     | 601 | LHG  | C4-O6-P-O5      |
| 34  | 9     | 601 | LHG  | C3-O3-P-O5      |
| 34  | 9     | 601 | LHG  | C4-O6-P-O3      |
| 34  | 9     | 601 | LHG  | C4-O6-P-O5      |
| 34  | 9     | 601 | LHG  | C18-C19-C20-C21 |
| 34  | A     | 845 | LHG  | O2-C2-C3-O3     |
| 34  | A     | 845 | LHG  | C3-O3-P-O4      |
| 34  | A     | 845 | LHG  | C4-O6-P-O3      |
| 34  | A     | 845 | LHG  | C4-O6-P-O4      |
| 34  | A     | 845 | LHG  | C4-O6-P-O5      |
| 34  | A     | 845 | LHG  | O6-C4-C5-O7     |
| 34  | A     | 845 | LHG  | C8-C7-O7-C5     |
| 34  | A     | 855 | LHG  | C3-O3-P-O5      |
| 34  | A     | 855 | LHG  | C3-O3-P-O6      |
| 34  | A     | 855 | LHG  | O9-C7-O7-C5     |
| 34  | A     | 855 | LHG  | C24-C23-O8-C6   |
| 34  | B     | 852 | LHG  | C1-C2-C3-O3     |
| 34  | B     | 852 | LHG  | C3-O3-P-O4      |
| 34  | B     | 852 | LHG  | C3-O3-P-O5      |
| 34  | B     | 852 | LHG  | C3-O3-P-O6      |
| 34  | B     | 852 | LHG  | C4-O6-P-O4      |
| 34  | B     | 852 | LHG  | C8-C7-O7-C5     |
| 34  | B     | 854 | LHG  | C4-O6-P-O5      |
| 34  | G     | 105 | LHG  | C1-C2-C3-O3     |
| 34  | G     | 105 | LHG  | O2-C2-C3-O3     |
| 34  | G     | 105 | LHG  | C3-O3-P-O5      |
| 34  | G     | 105 | LHG  | C3-O3-P-O6      |
| 34  | G     | 105 | LHG  | C4-O6-P-O3      |
| 34  | G     | 105 | LHG  | C4-O6-P-O4      |
| 34  | K     | 106 | LHG  | C5-C4-O6-P      |
| 34  | M     | 104 | LHG  | O1-C1-C2-C3     |
| 34  | M     | 104 | LHG  | O9-C7-O7-C5     |
| 34  | M     | 104 | LHG  | C8-C7-O7-C5     |
| 34  | a     | 630 | LHG  | O2-C2-C3-O3     |
| 34  | a     | 630 | LHG  | C4-O6-P-O3      |
| 34  | a     | 630 | LHG  | C4-O6-P-O4      |
| 34  | a     | 630 | LHG  | C4-O6-P-O5      |
| 34  | c     | 630 | LHG  | O1-C1-C2-C3     |

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| Mol | Chain | Res | Type | Atoms         |
|-----|-------|-----|------|---------------|
| 34  | c     | 630 | LHG  | C4-O6-P-O3    |
| 34  | c     | 630 | LHG  | C4-O6-P-O4    |
| 34  | c     | 630 | LHG  | C4-O6-P-O5    |
| 34  | b     | 630 | LHG  | C1-C2-C3-O3   |
| 34  | b     | 630 | LHG  | O2-C2-C3-O3   |
| 34  | b     | 630 | LHG  | C3-O3-P-O4    |
| 34  | b     | 630 | LHG  | C3-O3-P-O6    |
| 34  | b     | 630 | LHG  | C4-O6-P-O3    |
| 34  | b     | 630 | LHG  | C4-O6-P-O4    |
| 34  | b     | 630 | LHG  | C5-C4-O6-P    |
| 34  | b     | 630 | LHG  | O10-C23-O8-C6 |
| 34  | b     | 630 | LHG  | C24-C23-O8-C6 |
| 34  | d     | 630 | LHG  | C4-O6-P-O3    |
| 34  | d     | 630 | LHG  | C4-O6-P-O4    |
| 34  | d     | 630 | LHG  | O10-C23-O8-C6 |
| 34  | d     | 630 | LHG  | C24-C23-O8-C6 |
| 34  | f     | 630 | LHG  | C3-O3-P-O6    |
| 34  | g     | 630 | LHG  | C1-C2-C3-O3   |
| 34  | g     | 630 | LHG  | O2-C2-C3-O3   |
| 34  | g     | 630 | LHG  | C4-O6-P-O3    |
| 34  | g     | 630 | LHG  | C4-O6-P-O5    |
| 34  | h     | 630 | LHG  | O1-C1-C2-C3   |
| 34  | h     | 630 | LHG  | C3-O3-P-O4    |
| 34  | h     | 630 | LHG  | C3-O3-P-O5    |
| 34  | h     | 630 | LHG  | C3-O3-P-O6    |
| 34  | H     | 203 | LHG  | O1-C1-C2-C3   |
| 34  | i     | 630 | LHG  | O1-C1-C2-C3   |
| 34  | i     | 630 | LHG  | O2-C2-C3-O3   |
| 34  | e     | 630 | LHG  | C1-C2-C3-O3   |
| 34  | e     | 630 | LHG  | O2-C2-C3-O3   |
| 34  | 4     | 601 | LHG  | C3-O3-P-O4    |
| 34  | 4     | 601 | LHG  | C3-O3-P-O6    |
| 35  | 0     | 603 | SQD  | O5-C1-O6-C44  |
| 36  | 2     | 602 | LMG  | O6-C1-O1-C7   |
| 36  | 3     | 602 | LMG  | C2-C1-O1-C7   |
| 36  | 3     | 602 | LMG  | O6-C1-O1-C7   |
| 36  | 3     | 602 | LMG  | O7-C8-C9-O8   |
| 36  | 3     | 602 | LMG  | O9-C10-O7-C8  |
| 36  | A     | 856 | LMG  | C11-C10-O7-C8 |
| 36  | B     | 853 | LMG  | O6-C1-O1-C7   |
| 36  | J     | 102 | LMG  | O6-C1-O1-C7   |
| 36  | L     | 211 | LMG  | O7-C8-C9-O8   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 37  | c     | 522 | 0IE  | O1-C2-C3-C20    |
| 37  | c     | 522 | 0IE  | O29-C20-C3-C4   |
| 37  | c     | 522 | 0IE  | O29-C20-C3-C2   |
| 37  | c     | 522 | 0IE  | C10-C11-C12-C13 |
| 37  | c     | 522 | 0IE  | C10-C11-C12-C22 |
| 37  | c     | 522 | 0IE  | C11-C12-C13-C14 |
| 37  | c     | 522 | 0IE  | C22-C12-C13-C14 |
| 37  | c     | 522 | 0IE  | C17-C18-C19-C24 |
| 37  | c     | 522 | 0IE  | C17-C18-C19-C28 |
| 37  | b     | 522 | 0IE  | O29-C20-C3-C4   |
| 37  | b     | 522 | 0IE  | O29-C20-C3-C2   |
| 37  | b     | 522 | 0IE  | C3-C2-C30-C31   |
| 37  | g     | 521 | 0IE  | C3-C2-C30-C31   |
| 41  | B     | 849 | DGD  | O1B-C1B-O2G-C2G |
| 41  | B     | 849 | DGD  | O6D-C1D-O3G-C3G |
| 42  | a     | 523 | NEX  | O24-C26-C27-C28 |
| 42  | c     | 523 | NEX  | O24-C26-C27-C28 |
| 42  | b     | 523 | NEX  | O24-C26-C27-C28 |
| 42  | d     | 523 | NEX  | O24-C26-C27-C28 |
| 42  | f     | 523 | NEX  | O24-C26-C27-C28 |
| 42  | g     | 523 | NEX  | O24-C26-C27-C28 |
| 42  | h     | 523 | NEX  | O24-C26-C27-C28 |
| 42  | i     | 523 | NEX  | O24-C26-C27-C28 |
| 42  | e     | 523 | NEX  | O24-C26-C27-C28 |
| 31  | 0     | 313 | CLA  | O1D-CGD-O2D-CED |
| 31  | 0     | 321 | CLA  | O1D-CGD-O2D-CED |
| 31  | 7     | 316 | CLA  | O1D-CGD-O2D-CED |
| 31  | B     | 806 | CLA  | O1D-CGD-O2D-CED |
| 31  | a     | 611 | CLA  | O1D-CGD-O2D-CED |
| 31  | d     | 610 | CLA  | O1D-CGD-O2D-CED |
| 31  | h     | 610 | CLA  | O1D-CGD-O2D-CED |
| 31  | e     | 610 | CLA  | O1D-CGD-O2D-CED |
| 30  | e     | 608 | CHL  | O1D-CGD-O2D-CED |
| 31  | 7     | 303 | CLA  | O1D-CGD-O2D-CED |
| 31  | 9     | 309 | CLA  | O1D-CGD-O2D-CED |
| 31  | A     | 843 | CLA  | O1D-CGD-O2D-CED |
| 31  | B     | 805 | CLA  | O1D-CGD-O2D-CED |
| 31  | d     | 603 | CLA  | O1D-CGD-O2D-CED |
| 31  | h     | 604 | CLA  | O1D-CGD-O2D-CED |
| 31  | h     | 611 | CLA  | O1D-CGD-O2D-CED |
| 31  | 4     | 314 | CLA  | O1D-CGD-O2D-CED |
| 30  | 1     | 307 | CHL  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 30  | 5     | 307 | CHL  | CBD-CGD-O2D-CED |
| 30  | 6     | 307 | CHL  | CBD-CGD-O2D-CED |
| 30  | 8     | 307 | CHL  | CBD-CGD-O2D-CED |
| 30  | c     | 608 | CHL  | CBD-CGD-O2D-CED |
| 30  | f     | 609 | CHL  | CBD-CGD-O2D-CED |
| 30  | g     | 607 | CHL  | CBD-CGD-O2D-CED |
| 30  | g     | 609 | CHL  | CBD-CGD-O2D-CED |
| 30  | h     | 608 | CHL  | CBD-CGD-O2D-CED |
| 30  | h     | 614 | CHL  | CBD-CGD-O2D-CED |
| 30  | i     | 608 | CHL  | CBD-CGD-O2D-CED |
| 30  | e     | 608 | CHL  | CBD-CGD-O2D-CED |
| 31  | 0     | 304 | CLA  | CBD-CGD-O2D-CED |
| 31  | 0     | 321 | CLA  | CBD-CGD-O2D-CED |
| 31  | 1     | 311 | CLA  | CBD-CGD-O2D-CED |
| 31  | 1     | 314 | CLA  | CBD-CGD-O2D-CED |
| 31  | 2     | 311 | CLA  | CBD-CGD-O2D-CED |
| 31  | 3     | 303 | CLA  | CBD-CGD-O2D-CED |
| 31  | 5     | 308 | CLA  | CBD-CGD-O2D-CED |
| 31  | 6     | 310 | CLA  | CBD-CGD-O2D-CED |
| 31  | 7     | 316 | CLA  | CBD-CGD-O2D-CED |
| 31  | 8     | 303 | CLA  | CBD-CGD-O2D-CED |
| 31  | 8     | 304 | CLA  | CBD-CGD-O2D-CED |
| 31  | 8     | 311 | CLA  | CBD-CGD-O2D-CED |
| 31  | 8     | 312 | CLA  | CBD-CGD-O2D-CED |
| 31  | 9     | 309 | CLA  | CBD-CGD-O2D-CED |
| 31  | B     | 805 | CLA  | CBD-CGD-O2D-CED |
| 31  | B     | 806 | CLA  | CBD-CGD-O2D-CED |
| 31  | B     | 807 | CLA  | CBD-CGD-O2D-CED |
| 31  | G     | 102 | CLA  | CBD-CGD-O2D-CED |
| 31  | K     | 102 | CLA  | CBD-CGD-O2D-CED |
| 31  | a     | 611 | CLA  | CBD-CGD-O2D-CED |
| 31  | a     | 613 | CLA  | CBD-CGD-O2D-CED |
| 31  | b     | 603 | CLA  | CBD-CGD-O2D-CED |
| 31  | d     | 610 | CLA  | CBD-CGD-O2D-CED |
| 31  | d     | 613 | CLA  | CBD-CGD-O2D-CED |
| 31  | g     | 610 | CLA  | CBD-CGD-O2D-CED |
| 31  | g     | 613 | CLA  | CBD-CGD-O2D-CED |
| 31  | h     | 612 | CLA  | CBD-CGD-O2D-CED |
| 31  | h     | 613 | CLA  | CBD-CGD-O2D-CED |
| 31  | i     | 610 | CLA  | CBD-CGD-O2D-CED |
| 31  | e     | 610 | CLA  | CBD-CGD-O2D-CED |
| 31  | e     | 613 | CLA  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | 4     | 314 | CLA  | CBD-CGD-O2D-CED |
| 31  | 3     | 309 | CLA  | O1A-CGA-O2A-C1  |
| 31  | A     | 805 | CLA  | O1A-CGA-O2A-C1  |
| 31  | A     | 852 | CLA  | O1A-CGA-O2A-C1  |
| 31  | B     | 813 | CLA  | O1A-CGA-O2A-C1  |
| 31  | B     | 823 | CLA  | O1A-CGA-O2A-C1  |
| 34  | 5     | 601 | LHG  | O10-C23-O8-C6   |
| 34  | A     | 855 | LHG  | O10-C23-O8-C6   |
| 34  | K     | 106 | LHG  | O10-C23-O8-C6   |
| 34  | a     | 630 | LHG  | O10-C23-O8-C6   |
| 36  | J     | 102 | LMG  | O10-C28-O8-C9   |
| 31  | 0     | 313 | CLA  | O1A-CGA-O2A-C1  |
| 31  | G     | 103 | CLA  | O1A-CGA-O2A-C1  |
| 31  | L     | 204 | CLA  | O1A-CGA-O2A-C1  |
| 31  | 6     | 304 | CLA  | CBA-CGA-O2A-C1  |
| 30  | c     | 608 | CHL  | O1D-CGD-O2D-CED |
| 31  | 3     | 303 | CLA  | O1D-CGD-O2D-CED |
| 31  | d     | 613 | CLA  | O1D-CGD-O2D-CED |
| 31  | h     | 612 | CLA  | O1D-CGD-O2D-CED |
| 31  | h     | 613 | CLA  | O1D-CGD-O2D-CED |
| 31  | i     | 610 | CLA  | O1D-CGD-O2D-CED |
| 31  | B     | 813 | CLA  | CBA-CGA-O2A-C1  |
| 34  | 5     | 601 | LHG  | C24-C23-O8-C6   |
| 34  | K     | 106 | LHG  | C24-C23-O8-C6   |
| 34  | a     | 630 | LHG  | C24-C23-O8-C6   |
| 36  | J     | 102 | LMG  | C29-C28-O8-C9   |
| 30  | g     | 605 | CHL  | CBD-CGD-O2D-CED |
| 31  | 1     | 308 | CLA  | CBD-CGD-O2D-CED |
| 31  | 9     | 302 | CLA  | CBD-CGD-O2D-CED |
| 31  | i     | 611 | CLA  | CBD-CGD-O2D-CED |
| 31  | 2     | 310 | CLA  | O1A-CGA-O2A-C1  |
| 31  | 7     | 309 | CLA  | O1A-CGA-O2A-C1  |
| 31  | 7     | 315 | CLA  | O1A-CGA-O2A-C1  |
| 31  | B     | 850 | CLA  | O1A-CGA-O2A-C1  |
| 31  | L     | 203 | CLA  | O1A-CGA-O2A-C1  |
| 31  | H     | 202 | CLA  | O1A-CGA-O2A-C1  |
| 34  | 1     | 601 | LHG  | O10-C23-O8-C6   |
| 34  | M     | 104 | LHG  | O10-C23-O8-C6   |
| 34  | g     | 630 | LHG  | O10-C23-O8-C6   |
| 34  | e     | 630 | LHG  | O10-C23-O8-C6   |
| 36  | 9     | 602 | LMG  | O10-C28-O8-C9   |
| 36  | B     | 853 | LMG  | O10-C28-O8-C9   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | 8     | 303 | CLA  | O1A-CGA-O2A-C1  |
| 30  | d     | 608 | CHL  | O1D-CGD-O2D-CED |
| 30  | h     | 608 | CHL  | O1D-CGD-O2D-CED |
| 30  | i     | 608 | CHL  | O1D-CGD-O2D-CED |
| 31  | 7     | 315 | CLA  | O1D-CGD-O2D-CED |
| 31  | O     | 206 | CLA  | O1D-CGD-O2D-CED |
| 31  | a     | 613 | CLA  | O1D-CGD-O2D-CED |
| 31  | c     | 603 | CLA  | O1D-CGD-O2D-CED |
| 31  | f     | 610 | CLA  | O1D-CGD-O2D-CED |
| 31  | g     | 603 | CLA  | O1D-CGD-O2D-CED |
| 31  | g     | 613 | CLA  | O1D-CGD-O2D-CED |
| 30  | 2     | 307 | CHL  | O1D-CGD-O2D-CED |
| 30  | 7     | 307 | CHL  | O1D-CGD-O2D-CED |
| 30  | a     | 608 | CHL  | O1D-CGD-O2D-CED |
| 30  | b     | 608 | CHL  | O1D-CGD-O2D-CED |
| 30  | g     | 608 | CHL  | O1D-CGD-O2D-CED |
| 30  | e     | 609 | CHL  | O1D-CGD-O2D-CED |
| 31  | 5     | 311 | CLA  | O1D-CGD-O2D-CED |
| 31  | 5     | 312 | CLA  | O1D-CGD-O2D-CED |
| 31  | 9     | 311 | CLA  | O1D-CGD-O2D-CED |
| 31  | A     | 828 | CLA  | O1D-CGD-O2D-CED |
| 31  | O     | 201 | CLA  | O1D-CGD-O2D-CED |
| 31  | a     | 610 | CLA  | O1D-CGD-O2D-CED |
| 31  | d     | 612 | CLA  | O1D-CGD-O2D-CED |
| 31  | i     | 603 | CLA  | O1D-CGD-O2D-CED |
| 30  | 6     | 306 | CHL  | CBD-CGD-O2D-CED |
| 34  | 7     | 602 | LHG  | O9-C7-O7-C5     |
| 34  | A     | 845 | LHG  | O9-C7-O7-C5     |
| 34  | B     | 852 | LHG  | O9-C7-O7-C5     |
| 36  | 9     | 602 | LMG  | O9-C10-O7-C8    |
| 36  | A     | 856 | LMG  | O9-C10-O7-C8    |
| 36  | B     | 853 | LMG  | O9-C10-O7-C8    |
| 36  | J     | 102 | LMG  | O9-C10-O7-C8    |
| 36  | L     | 211 | LMG  | O9-C10-O7-C8    |
| 31  | c     | 610 | CLA  | O1D-CGD-O2D-CED |
| 31  | 5     | 314 | CLA  | O1A-CGA-O2A-C1  |
| 33  | 0     | 502 | 0UR  | O57-C45-O44-C43 |
| 33  | 6     | 501 | 0UR  | O57-C45-O44-C43 |
| 33  | 9     | 502 | 0UR  | O57-C45-O44-C43 |
| 33  | e     | 520 | 0UR  | O57-C45-O44-C43 |
| 30  | 2     | 302 | CHL  | C3-C5-C6-C7     |
| 31  | 0     | 303 | CLA  | C3-C5-C6-C7     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | 2     | 303 | CLA  | C3-C5-C6-C7     |
| 31  | 3     | 303 | CLA  | C3-C5-C6-C7     |
| 31  | 5     | 309 | CLA  | C3-C5-C6-C7     |
| 31  | 7     | 308 | CLA  | C3-C5-C6-C7     |
| 31  | 9     | 300 | CLA  | C3-C5-C6-C7     |
| 31  | A     | 806 | CLA  | C3-C5-C6-C7     |
| 31  | A     | 808 | CLA  | C3-C5-C6-C7     |
| 31  | A     | 821 | CLA  | C3-C5-C6-C7     |
| 31  | A     | 832 | CLA  | C3-C5-C6-C7     |
| 31  | B     | 811 | CLA  | C3-C5-C6-C7     |
| 31  | B     | 822 | CLA  | C3-C5-C6-C7     |
| 31  | B     | 836 | CLA  | C3-C5-C6-C7     |
| 31  | L     | 201 | CLA  | C3-C5-C6-C7     |
| 31  | d     | 610 | CLA  | C3-C5-C6-C7     |
| 31  | e     | 611 | CLA  | C3-C5-C6-C7     |
| 38  | B     | 842 | PQN  | C13-C15-C16-C17 |
| 33  | 5     | 501 | 0UR  | C46-C45-O44-C43 |
| 33  | 8     | 501 | 0UR  | C46-C45-O44-C43 |
| 33  | d     | 520 | 0UR  | C46-C45-O44-C43 |
| 33  | g     | 520 | 0UR  | C46-C45-O44-C43 |
| 31  | 8     | 311 | CLA  | O1D-CGD-O2D-CED |
| 31  | 3     | 309 | CLA  | CBA-CGA-O2A-C1  |
| 31  | 3     | 310 | CLA  | CBA-CGA-O2A-C1  |
| 31  | 5     | 303 | CLA  | CBA-CGA-O2A-C1  |
| 31  | A     | 805 | CLA  | CBA-CGA-O2A-C1  |
| 31  | A     | 808 | CLA  | CBA-CGA-O2A-C1  |
| 31  | A     | 852 | CLA  | CBA-CGA-O2A-C1  |
| 31  | B     | 819 | CLA  | CBA-CGA-O2A-C1  |
| 31  | B     | 824 | CLA  | CBA-CGA-O2A-C1  |
| 34  | 1     | 601 | LHG  | C24-C23-O8-C6   |
| 34  | g     | 630 | LHG  | C24-C23-O8-C6   |
| 34  | e     | 630 | LHG  | C24-C23-O8-C6   |
| 36  | 9     | 602 | LMG  | C29-C28-O8-C9   |
| 36  | B     | 853 | LMG  | C29-C28-O8-C9   |
| 30  | 0     | 301 | CHL  | CBD-CGD-O2D-CED |
| 30  | 1     | 306 | CHL  | CBD-CGD-O2D-CED |
| 30  | 3     | 302 | CHL  | CBD-CGD-O2D-CED |
| 30  | 3     | 307 | CHL  | CBD-CGD-O2D-CED |
| 30  | 5     | 302 | CHL  | CBD-CGD-O2D-CED |
| 30  | 5     | 306 | CHL  | CBD-CGD-O2D-CED |
| 30  | 7     | 305 | CHL  | CBD-CGD-O2D-CED |
| 30  | a     | 605 | CHL  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 30  | c     | 601 | CHL  | CBD-CGD-O2D-CED |
| 30  | b     | 601 | CHL  | CBD-CGD-O2D-CED |
| 30  | b     | 607 | CHL  | CBD-CGD-O2D-CED |
| 30  | f     | 614 | CHL  | CBD-CGD-O2D-CED |
| 30  | h     | 607 | CHL  | CBD-CGD-O2D-CED |
| 30  | i     | 614 | CHL  | CBD-CGD-O2D-CED |
| 30  | e     | 605 | CHL  | CBD-CGD-O2D-CED |
| 30  | e     | 614 | CHL  | CBD-CGD-O2D-CED |
| 31  | 0     | 312 | CLA  | CBD-CGD-O2D-CED |
| 31  | 2     | 310 | CLA  | CBD-CGD-O2D-CED |
| 31  | 2     | 312 | CLA  | CBD-CGD-O2D-CED |
| 31  | 5     | 309 | CLA  | CBD-CGD-O2D-CED |
| 31  | 5     | 314 | CLA  | CBD-CGD-O2D-CED |
| 31  | 6     | 317 | CLA  | CBD-CGD-O2D-CED |
| 31  | 7     | 312 | CLA  | CBD-CGD-O2D-CED |
| 31  | A     | 833 | CLA  | CBD-CGD-O2D-CED |
| 31  | A     | 839 | CLA  | CBD-CGD-O2D-CED |
| 31  | B     | 815 | CLA  | CBD-CGD-O2D-CED |
| 31  | B     | 816 | CLA  | CBD-CGD-O2D-CED |
| 31  | B     | 820 | CLA  | CBD-CGD-O2D-CED |
| 31  | F     | 301 | CLA  | CBD-CGD-O2D-CED |
| 31  | G     | 101 | CLA  | CBD-CGD-O2D-CED |
| 31  | c     | 613 | CLA  | CBD-CGD-O2D-CED |
| 31  | b     | 604 | CLA  | CBD-CGD-O2D-CED |
| 31  | b     | 610 | CLA  | CBD-CGD-O2D-CED |
| 31  | g     | 612 | CLA  | CBD-CGD-O2D-CED |
| 31  | h     | 603 | CLA  | CBD-CGD-O2D-CED |
| 31  | 4     | 310 | CLA  | CBD-CGD-O2D-CED |
| 31  | 4     | 312 | CLA  | CBD-CGD-O2D-CED |
| 34  | A     | 855 | LHG  | C8-C7-O7-C5     |
| 35  | 0     | 603 | SQD  | C8-C7-O47-C45   |
| 41  | B     | 849 | DGD  | C2B-C1B-O2G-C2G |
| 30  | 0     | 306 | CHL  | C2C-C3C-CAC-CBC |
| 30  | f     | 608 | CHL  | O1D-CGD-O2D-CED |
| 30  | 4     | 307 | CHL  | O1D-CGD-O2D-CED |
| 31  | 5     | 304 | CLA  | O1D-CGD-O2D-CED |
| 31  | 5     | 308 | CLA  | O1D-CGD-O2D-CED |
| 31  | 8     | 303 | CLA  | O1D-CGD-O2D-CED |
| 31  | 8     | 312 | CLA  | O1D-CGD-O2D-CED |
| 31  | B     | 801 | CLA  | O1D-CGD-O2D-CED |
| 31  | G     | 102 | CLA  | O1D-CGD-O2D-CED |
| 31  | 6     | 304 | CLA  | O1A-CGA-O2A-C1  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | h     | 604 | CLA  | O1A-CGA-O2A-C1  |
| 31  | b     | 603 | CLA  | O1D-CGD-O2D-CED |
| 30  | 2     | 319 | CHL  | C4-C3-C5-C6     |
| 30  | 8     | 313 | CHL  | C4-C3-C5-C6     |
| 30  | c     | 601 | CHL  | C4-C3-C5-C6     |
| 30  | b     | 601 | CHL  | C4-C3-C5-C6     |
| 30  | 4     | 319 | CHL  | C4-C3-C5-C6     |
| 31  | 0     | 303 | CLA  | C4-C3-C5-C6     |
| 31  | 1     | 303 | CLA  | C4-C3-C5-C6     |
| 31  | 1     | 312 | CLA  | C4-C3-C5-C6     |
| 31  | 2     | 303 | CLA  | C4-C3-C5-C6     |
| 31  | 3     | 309 | CLA  | C4-C3-C5-C6     |
| 31  | 7     | 309 | CLA  | C4-C3-C5-C6     |
| 31  | A     | 840 | CLA  | C4-C3-C5-C6     |
| 31  | A     | 841 | CLA  | C4-C3-C5-C6     |
| 31  | B     | 823 | CLA  | C4-C3-C5-C6     |
| 30  | 2     | 319 | CHL  | C2-C3-C5-C6     |
| 30  | 8     | 313 | CHL  | C2-C3-C5-C6     |
| 30  | c     | 601 | CHL  | C2-C3-C5-C6     |
| 30  | b     | 601 | CHL  | C2-C3-C5-C6     |
| 30  | 4     | 319 | CHL  | C2-C3-C5-C6     |
| 31  | 1     | 303 | CLA  | C2-C3-C5-C6     |
| 31  | 2     | 303 | CLA  | C2-C3-C5-C6     |
| 31  | 3     | 309 | CLA  | C2-C3-C5-C6     |
| 31  | 6     | 303 | CLA  | C2-C3-C5-C6     |
| 31  | 7     | 309 | CLA  | C2-C3-C5-C6     |
| 31  | A     | 837 | CLA  | C2-C3-C5-C6     |
| 31  | B     | 823 | CLA  | C2-C3-C5-C6     |
| 31  | B     | 830 | CLA  | C2-C3-C5-C6     |
| 31  | 5     | 314 | CLA  | CBA-CGA-O2A-C1  |
| 31  | 6     | 318 | CLA  | CBA-CGA-O2A-C1  |
| 31  | h     | 604 | CLA  | CBA-CGA-O2A-C1  |
| 30  | b     | 609 | CHL  | CBD-CGD-O2D-CED |
| 31  | A     | 832 | CLA  | CBD-CGD-O2D-CED |
| 31  | H     | 205 | CLA  | CBD-CGD-O2D-CED |
| 30  | h     | 601 | CHL  | C2A-CAA-CBA-CGA |
| 33  | 0     | 502 | 0UR  | O44-C45-C46-C47 |
| 33  | 5     | 502 | 0UR  | O44-C45-C46-C47 |
| 33  | c     | 520 | 0UR  | O44-C45-C46-C47 |
| 34  | 7     | 602 | LHG  | O10-C23-O8-C6   |
| 31  | 0     | 309 | CLA  | C3-C5-C6-C7     |
| 31  | 9     | 308 | CLA  | C3-C5-C6-C7     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | B     | 803 | CLA  | C3-C5-C6-C7     |
| 31  | c     | 613 | CLA  | C3-C5-C6-C7     |
| 31  | f     | 611 | CLA  | C3-C5-C6-C7     |
| 30  | 5     | 302 | CHL  | CBA-CGA-O2A-C1  |
| 31  | 1     | 311 | CLA  | CBA-CGA-O2A-C1  |
| 31  | 2     | 310 | CLA  | CBA-CGA-O2A-C1  |
| 31  | 7     | 309 | CLA  | CBA-CGA-O2A-C1  |
| 31  | 7     | 315 | CLA  | CBA-CGA-O2A-C1  |
| 31  | 9     | 311 | CLA  | CBA-CGA-O2A-C1  |
| 31  | A     | 806 | CLA  | CBA-CGA-O2A-C1  |
| 31  | B     | 822 | CLA  | CBA-CGA-O2A-C1  |
| 31  | B     | 823 | CLA  | CBA-CGA-O2A-C1  |
| 31  | B     | 850 | CLA  | CBA-CGA-O2A-C1  |
| 31  | L     | 203 | CLA  | CBA-CGA-O2A-C1  |
| 31  | H     | 202 | CLA  | CBA-CGA-O2A-C1  |
| 31  | 4     | 310 | CLA  | CBA-CGA-O2A-C1  |
| 34  | M     | 104 | LHG  | C24-C23-O8-C6   |
| 34  | f     | 630 | LHG  | C24-C23-O8-C6   |
| 34  | 4     | 601 | LHG  | C24-C23-O8-C6   |
| 35  | 0     | 603 | SQD  | C24-C23-O48-C46 |
| 34  | 2     | 601 | LHG  | C24-C25-C26-C27 |
| 34  | A     | 855 | LHG  | C24-C25-C26-C27 |
| 34  | B     | 854 | LHG  | C24-C25-C26-C27 |
| 34  | G     | 105 | LHG  | C24-C25-C26-C27 |
| 34  | c     | 630 | LHG  | C24-C25-C26-C27 |
| 34  | b     | 630 | LHG  | C24-C25-C26-C27 |
| 34  | d     | 630 | LHG  | C24-C25-C26-C27 |
| 34  | g     | 630 | LHG  | C24-C25-C26-C27 |
| 34  | e     | 630 | LHG  | C24-C25-C26-C27 |
| 30  | c     | 609 | CHL  | CBD-CGD-O2D-CED |
| 34  | 3     | 603 | LHG  | C24-C25-C26-C27 |
| 34  | f     | 630 | LHG  | C24-C25-C26-C27 |
| 34  | h     | 630 | LHG  | C24-C25-C26-C27 |
| 36  | 9     | 602 | LMG  | C4-C5-C6-O5     |
| 32  | 3     | 403 | 8CT  | C18-C19-C20-C21 |
| 32  | 7     | 402 | 8CT  | C16-C17-C18-C19 |
| 32  | 7     | 404 | 8CT  | C16-C17-C18-C19 |
| 32  | 8     | 402 | 8CT  | C12-C13-C14-C15 |
| 32  | B     | 804 | 8CT  | C12-C13-C14-C15 |
| 32  | F     | 302 | 8CT  | C12-C13-C14-C15 |
| 32  | I     | 101 | 8CT  | C16-C17-C18-C19 |
| 32  | I     | 101 | 8CT  | C18-C19-C20-C21 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 32  | J     | 101 | 8CT  | C23-C24-C25-C26 |
| 32  | K     | 107 | 8CT  | C12-C13-C14-C15 |
| 32  | M     | 102 | 8CT  | C18-C19-C20-C21 |
| 32  | O     | 205 | 8CT  | C18-C19-C20-C21 |
| 37  | c     | 522 | 0IE  | C9-C10-C11-C12  |
| 31  | 1     | 311 | CLA  | O1A-CGA-O2A-C1  |
| 31  | 5     | 303 | CLA  | O1A-CGA-O2A-C1  |
| 31  | A     | 808 | CLA  | O1A-CGA-O2A-C1  |
| 31  | A     | 819 | CLA  | O1A-CGA-O2A-C1  |
| 31  | B     | 819 | CLA  | O1A-CGA-O2A-C1  |
| 31  | B     | 822 | CLA  | O1A-CGA-O2A-C1  |
| 31  | B     | 824 | CLA  | O1A-CGA-O2A-C1  |
| 31  | B     | 833 | CLA  | O1A-CGA-O2A-C1  |
| 31  | 4     | 310 | CLA  | O1A-CGA-O2A-C1  |
| 34  | B     | 854 | LHG  | O10-C23-O8-C6   |
| 34  | G     | 105 | LHG  | O10-C23-O8-C6   |
| 34  | f     | 630 | LHG  | O10-C23-O8-C6   |
| 39  | A     | 857 | CL0  | O1A-CGA-O2A-C1  |
| 35  | 0     | 603 | SQD  | O49-C7-O47-C45  |
| 34  | 0     | 601 | LHG  | C24-C25-C26-C27 |
| 34  | 5     | 601 | LHG  | C24-C25-C26-C27 |
| 34  | K     | 106 | LHG  | C24-C25-C26-C27 |
| 34  | a     | 630 | LHG  | C24-C25-C26-C27 |
| 34  | H     | 203 | LHG  | C24-C25-C26-C27 |
| 34  | i     | 630 | LHG  | C24-C25-C26-C27 |
| 34  | 4     | 601 | LHG  | C24-C25-C26-C27 |
| 33  | 2     | 502 | 0UR  | O57-C45-O44-C43 |
| 33  | 5     | 501 | 0UR  | O57-C45-O44-C43 |
| 33  | 8     | 502 | 0UR  | O57-C45-O44-C43 |
| 33  | O     | 204 | 0UR  | O57-C45-O44-C43 |
| 33  | b     | 520 | 0UR  | O57-C45-O44-C43 |
| 33  | g     | 520 | 0UR  | O57-C45-O44-C43 |
| 33  | 4     | 502 | 0UR  | O57-C45-O44-C43 |
| 30  | 6     | 307 | CHL  | O1D-CGD-O2D-CED |
| 31  | 8     | 304 | CLA  | O1D-CGD-O2D-CED |
| 31  | e     | 613 | CLA  | O1D-CGD-O2D-CED |
| 30  | 1     | 313 | CHL  | C3-C5-C6-C7     |
| 30  | 2     | 301 | CHL  | C3-C5-C6-C7     |
| 30  | c     | 602 | CHL  | C3-C5-C6-C7     |
| 31  | 5     | 303 | CLA  | C3-C5-C6-C7     |
| 31  | 7     | 309 | CLA  | C3-C5-C6-C7     |
| 30  | 9     | 305 | CHL  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 30  | c     | 605 | CHL  | CBD-CGD-O2D-CED |
| 30  | d     | 609 | CHL  | CBD-CGD-O2D-CED |
| 31  | 0     | 310 | CLA  | CBD-CGD-O2D-CED |
| 31  | 6     | 312 | CLA  | CBD-CGD-O2D-CED |
| 31  | 7     | 311 | CLA  | CBD-CGD-O2D-CED |
| 31  | 7     | 318 | CLA  | CBD-CGD-O2D-CED |
| 31  | B     | 803 | CLA  | CBD-CGD-O2D-CED |
| 31  | B     | 824 | CLA  | CBD-CGD-O2D-CED |
| 31  | B     | 836 | CLA  | CBD-CGD-O2D-CED |
| 31  | f     | 604 | CLA  | CBD-CGD-O2D-CED |
| 31  | f     | 612 | CLA  | CBD-CGD-O2D-CED |
| 33  | 2     | 502 | 0UR  | C46-C45-O44-C43 |
| 33  | b     | 520 | 0UR  | C46-C45-O44-C43 |
| 33  | 4     | 502 | 0UR  | C46-C45-O44-C43 |
| 34  | 7     | 601 | LHG  | O2-C2-C3-O3     |
| 34  | 7     | 603 | LHG  | O2-C2-C3-O3     |
| 34  | B     | 854 | LHG  | O2-C2-C3-O3     |
| 30  | 8     | 307 | CHL  | O1D-CGD-O2D-CED |
| 30  | f     | 609 | CHL  | O1D-CGD-O2D-CED |
| 31  | 1     | 311 | CLA  | O1D-CGD-O2D-CED |
| 31  | 2     | 311 | CLA  | O1D-CGD-O2D-CED |
| 31  | 6     | 310 | CLA  | O1D-CGD-O2D-CED |
| 30  | 7     | 301 | CHL  | CBA-CGA-O2A-C1  |
| 31  | A     | 819 | CLA  | CBA-CGA-O2A-C1  |
| 31  | A     | 837 | CLA  | CBA-CGA-O2A-C1  |
| 31  | B     | 833 | CLA  | CBA-CGA-O2A-C1  |
| 31  | B     | 840 | CLA  | CBA-CGA-O2A-C1  |
| 31  | K     | 102 | CLA  | CBA-CGA-O2A-C1  |
| 31  | i     | 604 | CLA  | CBA-CGA-O2A-C1  |
| 31  | 4     | 304 | CLA  | CBA-CGA-O2A-C1  |
| 34  | B     | 854 | LHG  | C24-C23-O8-C6   |
| 39  | A     | 857 | CL0  | CBA-CGA-O2A-C1  |
| 36  | J     | 102 | LMG  | O6-C5-C6-O5     |
| 31  | 3     | 310 | CLA  | O1A-CGA-O2A-C1  |
| 31  | A     | 837 | CLA  | O1A-CGA-O2A-C1  |
| 35  | 0     | 603 | SQD  | O10-C23-O48-C46 |
| 31  | 0     | 304 | CLA  | O1D-CGD-O2D-CED |
| 33  | 6     | 501 | 0UR  | O44-C45-C46-C47 |
| 33  | 7     | 501 | 0UR  | O44-C45-C46-C47 |
| 33  | 9     | 502 | 0UR  | O44-C45-C46-C47 |
| 33  | O     | 204 | 0UR  | O44-C45-C46-C47 |
| 33  | f     | 520 | 0UR  | O44-C45-C46-C47 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 33  | i     | 520 | 0UR  | O44-C45-C46-C47 |
| 36  | B     | 853 | LMG  | O6-C5-C6-O5     |
| 30  | d     | 607 | CHL  | CBD-CGD-O2D-CED |
| 30  | f     | 605 | CHL  | CBD-CGD-O2D-CED |
| 30  | i     | 602 | CHL  | CBD-CGD-O2D-CED |
| 31  | B     | 822 | CLA  | CBD-CGD-O2D-CED |
| 36  | 9     | 602 | LMG  | C11-C10-O7-C8   |
| 36  | B     | 853 | LMG  | C11-C10-O7-C8   |
| 31  | 8     | 311 | CLA  | CBA-CGA-O2A-C1  |
| 31  | c     | 611 | CLA  | CBA-CGA-O2A-C1  |
| 31  | B     | 840 | CLA  | O1A-CGA-O2A-C1  |
| 31  | i     | 604 | CLA  | O1A-CGA-O2A-C1  |
| 34  | 4     | 601 | LHG  | O10-C23-O8-C6   |
| 36  | 3     | 602 | LMG  | O6-C5-C6-O5     |
| 41  | B     | 849 | DGD  | O6E-C5E-C6E-O5E |
| 30  | 5     | 307 | CHL  | O1D-CGD-O2D-CED |
| 30  | g     | 609 | CHL  | O1D-CGD-O2D-CED |
| 30  | 6     | 308 | CHL  | C3-C5-C6-C7     |
| 31  | A     | 838 | CLA  | C3-C5-C6-C7     |
| 31  | B     | 820 | CLA  | C3-C5-C6-C7     |
| 38  | A     | 842 | PQN  | C13-C15-C16-C17 |
| 30  | f     | 607 | CHL  | CBD-CGD-O2D-CED |
| 30  | g     | 602 | CHL  | CBD-CGD-O2D-CED |
| 30  | h     | 606 | CHL  | CBD-CGD-O2D-CED |
| 31  | 1     | 303 | CLA  | CBD-CGD-O2D-CED |
| 31  | 7     | 317 | CLA  | CBD-CGD-O2D-CED |
| 31  | a     | 603 | CLA  | CBD-CGD-O2D-CED |
| 31  | H     | 201 | CLA  | CBD-CGD-O2D-CED |
| 30  | 1     | 307 | CHL  | O1D-CGD-O2D-CED |
| 30  | h     | 614 | CHL  | O1D-CGD-O2D-CED |
| 31  | B     | 807 | CLA  | O1D-CGD-O2D-CED |
| 31  | K     | 102 | CLA  | O1D-CGD-O2D-CED |
| 34  | 7     | 602 | LHG  | C24-C23-O8-C6   |
| 34  | G     | 105 | LHG  | C24-C23-O8-C6   |
| 31  | 1     | 309 | CLA  | C4-C3-C5-C6     |
| 31  | 7     | 304 | CLA  | C4-C3-C5-C6     |
| 31  | A     | 828 | CLA  | C4-C3-C5-C6     |
| 31  | B     | 819 | CLA  | C4-C3-C5-C6     |
| 38  | A     | 842 | PQN  | C14-C13-C15-C16 |
| 31  | 0     | 303 | CLA  | C2-C3-C5-C6     |
| 31  | A     | 828 | CLA  | C2-C3-C5-C6     |
| 31  | A     | 840 | CLA  | C2-C3-C5-C6     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | A     | 841 | CLA  | C2-C3-C5-C6     |
| 31  | B     | 819 | CLA  | C2-C3-C5-C6     |
| 30  | 5     | 302 | CHL  | O1A-CGA-O2A-C1  |
| 31  | 9     | 311 | CLA  | O1A-CGA-O2A-C1  |
| 31  | A     | 806 | CLA  | O1A-CGA-O2A-C1  |
| 31  | K     | 102 | CLA  | O1A-CGA-O2A-C1  |
| 31  | 4     | 304 | CLA  | O1A-CGA-O2A-C1  |
| 36  | 9     | 602 | LMG  | O6-C5-C6-O5     |
| 36  | 3     | 602 | LMG  | C4-C5-C6-O5     |
| 31  | 3     | 320 | CLA  | C2C-C3C-CAC-CBC |
| 30  | d     | 606 | CHL  | CBD-CGD-O2D-CED |
| 30  | h     | 601 | CHL  | CBD-CGD-O2D-CED |
| 31  | 1     | 312 | CLA  | CBD-CGD-O2D-CED |
| 31  | 4     | 304 | CLA  | CBD-CGD-O2D-CED |
| 31  | g     | 610 | CLA  | O1D-CGD-O2D-CED |
| 34  | M     | 104 | LHG  | C2-C3-O3-P      |
| 36  | L     | 210 | LMG  | O6-C5-C6-O5     |
| 30  | 2     | 313 | CHL  | C2A-CAA-CBA-CGA |
| 31  | A     | 824 | CLA  | C2A-CAA-CBA-CGA |
| 33  | 8     | 502 | 0UR  | O44-C45-C46-C47 |
| 33  | b     | 520 | 0UR  | O44-C45-C46-C47 |
| 33  | d     | 520 | 0UR  | O44-C45-C46-C47 |
| 30  | g     | 607 | CHL  | O1D-CGD-O2D-CED |
| 31  | 1     | 314 | CLA  | O1D-CGD-O2D-CED |
| 31  | B     | 834 | CLA  | O1A-CGA-O2A-C1  |
| 36  | 3     | 602 | LMG  | O10-C28-O8-C9   |
| 36  | B     | 853 | LMG  | C4-C5-C6-O5     |
| 31  | 1     | 308 | CLA  | O1D-CGD-O2D-CED |
| 31  | 9     | 302 | CLA  | O1D-CGD-O2D-CED |
| 31  | i     | 611 | CLA  | O1D-CGD-O2D-CED |
| 31  | 2     | 304 | CLA  | CBA-CGA-O2A-C1  |
| 31  | 3     | 304 | CLA  | CBA-CGA-O2A-C1  |
| 31  | A     | 807 | CLA  | CBA-CGA-O2A-C1  |
| 31  | A     | 841 | CLA  | CBA-CGA-O2A-C1  |
| 31  | B     | 831 | CLA  | CBA-CGA-O2A-C1  |
| 31  | B     | 834 | CLA  | CBA-CGA-O2A-C1  |
| 30  | 5     | 313 | CHL  | CBD-CGD-O2D-CED |
| 30  | 8     | 302 | CHL  | CBD-CGD-O2D-CED |
| 30  | 8     | 306 | CHL  | CBD-CGD-O2D-CED |
| 30  | c     | 606 | CHL  | CBD-CGD-O2D-CED |
| 30  | f     | 601 | CHL  | CBD-CGD-O2D-CED |
| 30  | g     | 601 | CHL  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 30  | g     | 614 | CHL  | CBD-CGD-O2D-CED |
| 30  | i     | 607 | CHL  | CBD-CGD-O2D-CED |
| 30  | i     | 609 | CHL  | CBD-CGD-O2D-CED |
| 31  | 2     | 314 | CLA  | CBD-CGD-O2D-CED |
| 31  | A     | 806 | CLA  | CBD-CGD-O2D-CED |
| 31  | A     | 819 | CLA  | CBD-CGD-O2D-CED |
| 31  | L     | 207 | CLA  | CBD-CGD-O2D-CED |
| 36  | O     | 207 | LMG  | O6-C5-C6-O5     |
| 30  | 7     | 301 | CHL  | O1A-CGA-O2A-C1  |
| 34  | A     | 844 | LHG  | C12-C13-C14-C15 |
| 30  | 6     | 315 | CHL  | CBD-CGD-O2D-CED |
| 30  | d     | 605 | CHL  | CBD-CGD-O2D-CED |
| 30  | h     | 605 | CHL  | CBD-CGD-O2D-CED |
| 31  | 3     | 310 | CLA  | CBD-CGD-O2D-CED |
| 31  | 3     | 313 | CLA  | CBD-CGD-O2D-CED |
| 31  | B     | 817 | CLA  | CBD-CGD-O2D-CED |
| 36  | J     | 102 | LMG  | C11-C10-O7-C8   |
| 31  | 6     | 318 | CLA  | O1A-CGA-O2A-C1  |
| 31  | e     | 603 | CLA  | C3-C5-C6-C7     |
| 32  | 0     | 401 | 8CT  | C16-C17-C18-C19 |
| 32  | 0     | 401 | 8CT  | C18-C19-C20-C21 |
| 32  | 7     | 402 | 8CT  | C18-C19-C20-C21 |
| 32  | G     | 104 | 8CT  | C16-C17-C18-C19 |
| 32  | G     | 104 | 8CT  | C18-C19-C20-C21 |
| 32  | J     | 101 | 8CT  | C16-C17-C18-C19 |
| 32  | L     | 209 | 8CT  | C12-C13-C14-C15 |
| 32  | L     | 209 | 8CT  | C18-C19-C20-C21 |
| 31  | 2     | 304 | CLA  | O1A-CGA-O2A-C1  |
| 31  | A     | 841 | CLA  | O1A-CGA-O2A-C1  |
| 34  | 0     | 601 | LHG  | C1-C2-C3-O3     |
| 34  | 2     | 601 | LHG  | C1-C2-C3-O3     |
| 34  | 3     | 603 | LHG  | C1-C2-C3-O3     |
| 34  | 7     | 603 | LHG  | C1-C2-C3-O3     |
| 34  | a     | 630 | LHG  | C1-C2-C3-O3     |
| 30  | 2     | 301 | CHL  | CBA-CGA-O2A-C1  |
| 30  | 2     | 307 | CHL  | CBA-CGA-O2A-C1  |
| 30  | 8     | 306 | CHL  | CBA-CGA-O2A-C1  |
| 30  | 8     | 307 | CHL  | CBA-CGA-O2A-C1  |
| 30  | d     | 602 | CHL  | CBA-CGA-O2A-C1  |
| 30  | 4     | 307 | CHL  | CBA-CGA-O2A-C1  |
| 31  | A     | 804 | CLA  | CBA-CGA-O2A-C1  |
| 31  | A     | 810 | CLA  | CBA-CGA-O2A-C1  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | A     | 817 | CLA  | CBA-CGA-O2A-C1  |
| 31  | A     | 831 | CLA  | CBA-CGA-O2A-C1  |
| 31  | A     | 833 | CLA  | CBA-CGA-O2A-C1  |
| 31  | a     | 613 | CLA  | CBA-CGA-O2A-C1  |
| 31  | d     | 604 | CLA  | CBA-CGA-O2A-C1  |
| 31  | f     | 604 | CLA  | CBA-CGA-O2A-C1  |
| 31  | H     | 205 | CLA  | CBA-CGA-O2A-C1  |
| 36  | 3     | 602 | LMG  | C29-C28-O8-C9   |
| 36  | J     | 105 | LMG  | C29-C28-O8-C9   |
| 31  | 8     | 310 | CLA  | CBA-CGA-O2A-C1  |
| 30  | 0     | 302 | CHL  | CBD-CGD-O2D-CED |
| 30  | 5     | 305 | CHL  | CBD-CGD-O2D-CED |
| 30  | 7     | 306 | CHL  | CBD-CGD-O2D-CED |
| 30  | b     | 614 | CHL  | CBD-CGD-O2D-CED |
| 30  | h     | 602 | CHL  | CBD-CGD-O2D-CED |
| 31  | L     | 204 | CLA  | CBD-CGD-O2D-CED |
| 33  | 1     | 502 | 0UR  | O44-C45-C46-C47 |
| 33  | 6     | 502 | 0UR  | O44-C45-C46-C47 |
| 33  | 8     | 501 | 0UR  | O44-C45-C46-C47 |
| 34  | 0     | 601 | LHG  | C12-C13-C14-C15 |
| 30  | 6     | 306 | CHL  | O1D-CGD-O2D-CED |
| 30  | b     | 607 | CHL  | O1D-CGD-O2D-CED |
| 30  | g     | 605 | CHL  | O1D-CGD-O2D-CED |
| 34  | A     | 855 | LHG  | C12-C13-C14-C15 |
| 34  | M     | 104 | LHG  | C12-C13-C14-C15 |
| 33  | 8     | 501 | 0UR  | O57-C45-O44-C43 |
| 33  | d     | 520 | 0UR  | O57-C45-O44-C43 |
| 30  | 8     | 306 | CHL  | O1A-CGA-O2A-C1  |
| 34  | 1     | 601 | LHG  | C31-C32-C33-C34 |
| 31  | 1     | 312 | CLA  | C2-C3-C5-C6     |
| 31  | 7     | 304 | CLA  | C2-C3-C5-C6     |
| 38  | A     | 842 | PQN  | C12-C13-C15-C16 |
| 31  | B     | 834 | CLA  | C3-C5-C6-C7     |
| 31  | e     | 613 | CLA  | C3-C5-C6-C7     |
| 30  | a     | 609 | CHL  | CBD-CGD-O2D-CED |
| 31  | f     | 611 | CLA  | CBD-CGD-O2D-CED |
| 30  | 2     | 302 | CHL  | C11-C10-C8-C9   |
| 30  | 2     | 319 | CHL  | C6-C7-C8-C9     |
| 30  | 2     | 319 | CHL  | C11-C10-C8-C9   |
| 30  | 5     | 302 | CHL  | C14-C13-C15-C16 |
| 30  | 6     | 301 | CHL  | C11-C10-C8-C9   |
| 30  | 6     | 302 | CHL  | C6-C7-C8-C9     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 30  | 6     | 308 | CHL  | C11-C10-C8-C9   |
| 30  | 7     | 301 | CHL  | C14-C13-C15-C16 |
| 30  | a     | 602 | CHL  | C14-C13-C15-C16 |
| 30  | c     | 602 | CHL  | C6-C7-C8-C9     |
| 30  | c     | 608 | CHL  | C14-C13-C15-C16 |
| 30  | b     | 602 | CHL  | C11-C12-C13-C14 |
| 30  | d     | 609 | CHL  | C6-C7-C8-C9     |
| 30  | f     | 601 | CHL  | C11-C12-C13-C14 |
| 30  | f     | 602 | CHL  | C11-C12-C13-C14 |
| 30  | i     | 602 | CHL  | C6-C7-C8-C9     |
| 30  | e     | 602 | CHL  | C6-C7-C8-C9     |
| 31  | 2     | 303 | CLA  | C6-C7-C8-C9     |
| 31  | 2     | 310 | CLA  | C11-C10-C8-C9   |
| 31  | 3     | 309 | CLA  | C14-C13-C15-C16 |
| 31  | 3     | 310 | CLA  | C6-C7-C8-C9     |
| 31  | 5     | 309 | CLA  | C6-C7-C8-C9     |
| 31  | 6     | 310 | CLA  | C6-C7-C8-C9     |
| 31  | 7     | 308 | CLA  | C11-C12-C13-C14 |
| 31  | 7     | 309 | CLA  | C11-C10-C8-C9   |
| 31  | 9     | 308 | CLA  | C11-C12-C13-C14 |
| 31  | 9     | 309 | CLA  | C6-C7-C8-C9     |
| 31  | A     | 839 | CLA  | C11-C12-C13-C14 |
| 31  | A     | 853 | CLA  | C6-C7-C8-C9     |
| 31  | B     | 806 | CLA  | C11-C12-C13-C14 |
| 31  | B     | 808 | CLA  | C6-C7-C8-C9     |
| 31  | B     | 814 | CLA  | C11-C12-C13-C14 |
| 31  | B     | 836 | CLA  | C11-C10-C8-C9   |
| 31  | L     | 201 | CLA  | C6-C7-C8-C9     |
| 33  | 6     | 502 | 0UR  | C46-C45-O44-C43 |
| 30  | 3     | 307 | CHL  | O1D-CGD-O2D-CED |
| 30  | h     | 607 | CHL  | O1D-CGD-O2D-CED |
| 31  | 5     | 314 | CLA  | O1D-CGD-O2D-CED |
| 31  | b     | 604 | CLA  | O1D-CGD-O2D-CED |
| 36  | B     | 853 | LMG  | C2-C1-O1-C7     |
| 36  | J     | 102 | LMG  | C2-C1-O1-C7     |
| 41  | B     | 849 | DGD  | C2D-C1D-O3G-C3G |
| 34  | 0     | 601 | LHG  | O2-C2-C3-O3     |
| 31  | B     | 815 | CLA  | O1D-CGD-O2D-CED |
| 31  | 4     | 310 | CLA  | O1D-CGD-O2D-CED |
| 33  | O     | 204 | 0UR  | O57-C45-C46-C47 |
| 33  | f     | 520 | 0UR  | O57-C45-C46-C47 |
| 30  | 2     | 301 | CHL  | O1A-CGA-O2A-C1  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 30  | 2     | 307 | CHL  | O1A-CGA-O2A-C1  |
| 30  | 8     | 307 | CHL  | O1A-CGA-O2A-C1  |
| 31  | A     | 817 | CLA  | O1A-CGA-O2A-C1  |
| 41  | B     | 849 | DGD  | C4E-C5E-C6E-O5E |
| 30  | e     | 614 | CHL  | O1D-CGD-O2D-CED |
| 32  | 2     | 402 | 8CT  | C27-C26-C28-C29 |
| 32  | 6     | 402 | 8CT  | C10-C11-C12-C40 |
| 32  | 6     | 402 | 8CT  | C22-C21-C23-C24 |
| 32  | 7     | 404 | 8CT  | C10-C11-C12-C40 |
| 32  | 7     | 405 | 8CT  | C14-C15-C16-C39 |
| 32  | 8     | 402 | 8CT  | C10-C11-C12-C40 |
| 32  | 8     | 402 | 8CT  | C14-C15-C16-C39 |
| 32  | A     | 846 | 8CT  | C10-C11-C12-C40 |
| 32  | A     | 847 | 8CT  | C14-C15-C16-C39 |
| 32  | A     | 847 | 8CT  | C27-C26-C28-C29 |
| 32  | A     | 848 | 8CT  | C14-C15-C16-C39 |
| 32  | A     | 849 | 8CT  | C10-C11-C12-C40 |
| 32  | A     | 850 | 8CT  | C10-C11-C12-C40 |
| 32  | A     | 850 | 8CT  | C14-C15-C16-C39 |
| 32  | A     | 854 | 8CT  | C27-C26-C28-C29 |
| 32  | B     | 804 | 8CT  | C14-C15-C16-C39 |
| 32  | B     | 804 | 8CT  | C22-C21-C23-C24 |
| 32  | B     | 804 | 8CT  | C27-C26-C28-C29 |
| 32  | B     | 843 | 8CT  | C10-C11-C12-C40 |
| 32  | B     | 843 | 8CT  | C22-C21-C23-C24 |
| 32  | B     | 851 | 8CT  | C14-C15-C16-C39 |
| 32  | G     | 104 | 8CT  | C10-C11-C12-C40 |
| 32  | I     | 101 | 8CT  | C10-C11-C12-C40 |
| 32  | J     | 101 | 8CT  | C22-C21-C23-C24 |
| 32  | J     | 101 | 8CT  | C27-C26-C28-C29 |
| 32  | L     | 206 | 8CT  | C10-C11-C12-C40 |
| 32  | L     | 209 | 8CT  | C14-C15-C16-C39 |
| 32  | K     | 107 | 8CT  | C14-C15-C16-C39 |
| 32  | K     | 107 | 8CT  | C22-C21-C23-C24 |
| 32  | M     | 102 | 8CT  | C10-C11-C12-C40 |
| 32  | M     | 102 | 8CT  | C27-C26-C28-C29 |
| 32  | O     | 205 | 8CT  | C14-C15-C16-C39 |
| 32  | 4     | 402 | 8CT  | C27-C26-C28-C29 |
| 33  | 1     | 502 | 0UR  | C22-C16-C17-C18 |
| 33  | 5     | 501 | 0UR  | C5-C6-C7-C20    |
| 33  | c     | 520 | 0UR  | C22-C16-C17-C18 |
| 33  | f     | 520 | 0UR  | C22-C16-C17-C18 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 36  | J     | 105 | LMG  | O6-C5-C6-O5     |
| 32  | 1     | 402 | 8CT  | C20-C21-C23-C24 |
| 32  | 2     | 402 | 8CT  | C25-C26-C28-C29 |
| 32  | 6     | 402 | 8CT  | C20-C21-C23-C24 |
| 32  | 7     | 402 | 8CT  | C10-C11-C12-C13 |
| 32  | 7     | 402 | 8CT  | C14-C15-C16-C17 |
| 32  | 8     | 402 | 8CT  | C10-C11-C12-C13 |
| 32  | 8     | 406 | 8CT  | C14-C15-C16-C17 |
| 32  | A     | 846 | 8CT  | C10-C11-C12-C13 |
| 32  | A     | 849 | 8CT  | C10-C11-C12-C13 |
| 32  | A     | 850 | 8CT  | C20-C21-C23-C24 |
| 32  | A     | 854 | 8CT  | C25-C26-C28-C29 |
| 32  | B     | 804 | 8CT  | C14-C15-C16-C17 |
| 32  | B     | 804 | 8CT  | C25-C26-C28-C29 |
| 32  | B     | 847 | 8CT  | C10-C11-C12-C13 |
| 32  | I     | 101 | 8CT  | C10-C11-C12-C13 |
| 32  | J     | 101 | 8CT  | C25-C26-C28-C29 |
| 32  | L     | 209 | 8CT  | C14-C15-C16-C17 |
| 32  | K     | 107 | 8CT  | C14-C15-C16-C17 |
| 32  | 4     | 402 | 8CT  | C25-C26-C28-C29 |
| 33  | 1     | 502 | 0UR  | C15-C16-C17-C18 |
| 33  | c     | 520 | 0UR  | C15-C16-C17-C18 |
| 33  | f     | 520 | 0UR  | C15-C16-C17-C18 |
| 34  | A     | 855 | LHG  | C10-C11-C12-C13 |
| 30  | 6     | 307 | CHL  | C2A-CAA-CBA-CGA |
| 30  | 4     | 302 | CHL  | C3-C5-C6-C7     |
| 31  | B     | 813 | CLA  | C2A-CAA-CBA-CGA |
| 31  | B     | 823 | CLA  | C3-C5-C6-C7     |
| 31  | M     | 101 | CLA  | C2A-CAA-CBA-CGA |
| 31  | O     | 206 | CLA  | C2A-CAA-CBA-CGA |
| 31  | e     | 604 | CLA  | C2A-CAA-CBA-CGA |
| 31  | A     | 839 | CLA  | O1D-CGD-O2D-CED |
| 31  | F     | 301 | CLA  | O1D-CGD-O2D-CED |
| 31  | 4     | 312 | CLA  | O1D-CGD-O2D-CED |
| 31  | 8     | 311 | CLA  | O1A-CGA-O2A-C1  |
| 31  | A     | 803 | CLA  | C3-C5-C6-C7     |
| 30  | a     | 601 | CHL  | CBD-CGD-O2D-CED |
| 36  | L     | 211 | LMG  | C11-C10-O7-C8   |
| 31  | i     | 603 | CLA  | CBA-CGA-O2A-C1  |
| 34  | 1     | 601 | LHG  | O7-C5-C6-O8     |
| 34  | 7     | 603 | LHG  | O7-C5-C6-O8     |
| 35  | 0     | 603 | SQD  | O47-C45-C46-O48 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 36  | 2     | 602 | LMG  | O7-C8-C9-O8     |
| 30  | b     | 602 | CHL  | CBA-CGA-O2A-C1  |
| 30  | 7     | 302 | CHL  | C5-C6-C7-C8     |
| 31  | A     | 805 | CLA  | C2-C1-O2A-CGA   |
| 39  | A     | 857 | CL0  | C2-C1-O2A-CGA   |
| 34  | A     | 855 | LHG  | C11-C10-C9-C8   |
| 30  | 0     | 301 | CHL  | O1D-CGD-O2D-CED |
| 30  | a     | 605 | CHL  | O1D-CGD-O2D-CED |
| 30  | b     | 601 | CHL  | O1D-CGD-O2D-CED |
| 30  | e     | 605 | CHL  | O1D-CGD-O2D-CED |
| 31  | g     | 612 | CLA  | O1D-CGD-O2D-CED |
| 30  | 8     | 315 | CHL  | CBD-CGD-O2D-CED |
| 30  | 1     | 307 | CHL  | C8-C10-C11-C12  |
| 30  | b     | 602 | CHL  | C5-C6-C7-C8     |
| 30  | f     | 602 | CHL  | C5-C6-C7-C8     |
| 30  | f     | 609 | CHL  | C15-C16-C17-C18 |
| 30  | i     | 602 | CHL  | C5-C6-C7-C8     |
| 31  | 2     | 310 | CLA  | C5-C6-C7-C8     |
| 31  | 9     | 308 | CLA  | C10-C11-C12-C13 |
| 31  | A     | 806 | CLA  | C8-C10-C11-C12  |
| 31  | A     | 809 | CLA  | C8-C10-C11-C12  |
| 31  | A     | 841 | CLA  | C5-C6-C7-C8     |
| 31  | B     | 827 | CLA  | C8-C10-C11-C12  |
| 30  | f     | 614 | CHL  | O1D-CGD-O2D-CED |
| 30  | 7     | 301 | CHL  | C3-C5-C6-C7     |
| 31  | A     | 833 | CLA  | C3-C5-C6-C7     |
| 36  | J     | 102 | LMG  | C4-C5-C6-O5     |
| 34  | 7     | 603 | LHG  | C7-C8-C9-C10    |
| 31  | 5     | 309 | CLA  | O1D-CGD-O2D-CED |
| 31  | 7     | 312 | CLA  | O1D-CGD-O2D-CED |
| 31  | A     | 833 | CLA  | O1D-CGD-O2D-CED |
| 31  | f     | 604 | CLA  | O1A-CGA-O2A-C1  |
| 30  | h     | 602 | CHL  | C13-C15-C16-C17 |
| 31  | B     | 806 | CLA  | C8-C10-C11-C12  |
| 31  | f     | 603 | CLA  | CBD-CGD-O2D-CED |
| 34  | 3     | 603 | LHG  | C28-C29-C30-C31 |
| 34  | 9     | 601 | LHG  | C12-C13-C14-C15 |
| 34  | M     | 104 | LHG  | C28-C29-C30-C31 |
| 30  | 5     | 302 | CHL  | C6-C7-C8-C10    |
| 30  | f     | 601 | CHL  | C6-C7-C8-C10    |
| 31  | 7     | 308 | CLA  | C12-C13-C15-C16 |
| 31  | A     | 803 | CLA  | C11-C10-C8-C7   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | A     | 806 | CLA  | C6-C7-C8-C10    |
| 31  | A     | 817 | CLA  | C11-C12-C13-C15 |
| 31  | B     | 828 | CLA  | C6-C7-C8-C10    |
| 30  | 5     | 306 | CHL  | O1D-CGD-O2D-CED |
| 31  | B     | 820 | CLA  | O1D-CGD-O2D-CED |
| 30  | 7     | 306 | CHL  | CBA-CGA-O2A-C1  |
| 30  | d     | 609 | CHL  | CBA-CGA-O2A-C1  |
| 33  | 5     | 502 | 0UR  | O57-C45-C46-C47 |
| 33  | 6     | 501 | 0UR  | O57-C45-C46-C47 |
| 33  | 6     | 502 | 0UR  | O57-C45-C46-C47 |
| 33  | 7     | 501 | 0UR  | O57-C45-C46-C47 |
| 33  | 8     | 501 | 0UR  | O57-C45-C46-C47 |
| 33  | 9     | 502 | 0UR  | O57-C45-C46-C47 |
| 33  | c     | 520 | 0UR  | O57-C45-C46-C47 |
| 33  | b     | 520 | 0UR  | O57-C45-C46-C47 |
| 33  | i     | 520 | 0UR  | O57-C45-C46-C47 |
| 33  | g     | 520 | 0UR  | O44-C45-C46-C47 |
| 41  | B     | 849 | DGD  | C1B-C2B-C3B-C4B |
| 32  | 6     | 402 | 8CT  | C18-C19-C20-C21 |
| 32  | 8     | 406 | 8CT  | C18-C19-C20-C21 |
| 32  | A     | 854 | 8CT  | C23-C24-C25-C26 |
| 32  | B     | 845 | 8CT  | C12-C13-C14-C15 |
| 32  | J     | 104 | 8CT  | C16-C17-C18-C19 |
| 33  | 4     | 502 | 0UR  | C13-C14-C15-C16 |
| 34  | 0     | 601 | LHG  | C30-C31-C32-C33 |
| 34  | M     | 104 | LHG  | C14-C15-C16-C17 |
| 31  | 2     | 310 | CLA  | O1D-CGD-O2D-CED |
| 31  | h     | 603 | CLA  | O1D-CGD-O2D-CED |
| 34  | 2     | 601 | LHG  | C11-C10-C9-C8   |
| 30  | 1     | 307 | CHL  | C15-C16-C17-C18 |
| 30  | 3     | 307 | CHL  | C13-C15-C16-C17 |
| 30  | 6     | 302 | CHL  | C13-C15-C16-C17 |
| 30  | c     | 609 | CHL  | C15-C16-C17-C18 |
| 30  | d     | 602 | CHL  | C10-C11-C12-C13 |
| 31  | B     | 805 | CLA  | C8-C10-C11-C12  |
| 31  | B     | 808 | CLA  | C15-C16-C17-C18 |
| 31  | 4     | 310 | CLA  | C5-C6-C7-C8     |
| 34  | A     | 844 | LHG  | C28-C29-C30-C31 |
| 34  | 0     | 601 | LHG  | C23-C24-C25-C26 |
| 34  | M     | 104 | LHG  | C7-C8-C9-C10    |
| 34  | f     | 630 | LHG  | C7-C8-C9-C10    |
| 36  | J     | 102 | LMG  | C28-C29-C30-C31 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 30  | 4     | 307 | CHL  | O1A-CGA-O2A-C1  |
| 31  | A     | 804 | CLA  | O1A-CGA-O2A-C1  |
| 30  | 5     | 301 | CHL  | CBD-CGD-O2D-CED |
| 30  | c     | 602 | CHL  | CBD-CGD-O2D-CED |
| 31  | A     | 814 | CLA  | CBD-CGD-O2D-CED |
| 31  | 6     | 317 | CLA  | O1D-CGD-O2D-CED |
| 31  | c     | 613 | CLA  | O1D-CGD-O2D-CED |
| 31  | b     | 610 | CLA  | O1D-CGD-O2D-CED |
| 31  | 0     | 309 | CLA  | CBA-CGA-O2A-C1  |
| 33  | d     | 520 | 0UR  | O57-C45-C46-C47 |
| 30  | 1     | 313 | CHL  | C8-C10-C11-C12  |
| 30  | 8     | 302 | CHL  | C10-C11-C12-C13 |
| 30  | e     | 608 | CHL  | C5-C6-C7-C8     |
| 31  | A     | 803 | CLA  | C8-C10-C11-C12  |
| 31  | A     | 830 | CLA  | C5-C6-C7-C8     |
| 31  | A     | 840 | CLA  | C5-C6-C7-C8     |
| 31  | B     | 809 | CLA  | C5-C6-C7-C8     |
| 31  | B     | 814 | CLA  | C8-C10-C11-C12  |
| 31  | B     | 814 | CLA  | C15-C16-C17-C18 |
| 31  | B     | 819 | CLA  | C5-C6-C7-C8     |
| 31  | B     | 839 | CLA  | C13-C15-C16-C17 |
| 30  | 1     | 305 | CHL  | C2A-CAA-CBA-CGA |
| 30  | 1     | 307 | CHL  | C2A-CAA-CBA-CGA |
| 30  | 5     | 306 | CHL  | C2A-CAA-CBA-CGA |
| 30  | 5     | 313 | CHL  | C2A-CAA-CBA-CGA |
| 30  | 7     | 307 | CHL  | C2A-CAA-CBA-CGA |
| 30  | 9     | 305 | CHL  | C2A-CAA-CBA-CGA |
| 30  | a     | 601 | CHL  | C2A-CAA-CBA-CGA |
| 30  | a     | 607 | CHL  | C2A-CAA-CBA-CGA |
| 30  | b     | 608 | CHL  | C2A-CAA-CBA-CGA |
| 30  | d     | 606 | CHL  | C2A-CAA-CBA-CGA |
| 30  | f     | 606 | CHL  | C2A-CAA-CBA-CGA |
| 30  | f     | 608 | CHL  | C2A-CAA-CBA-CGA |
| 30  | g     | 601 | CHL  | C2A-CAA-CBA-CGA |
| 30  | g     | 607 | CHL  | C2A-CAA-CBA-CGA |
| 30  | h     | 602 | CHL  | C2A-CAA-CBA-CGA |
| 30  | i     | 607 | CHL  | C2A-CAA-CBA-CGA |
| 30  | e     | 607 | CHL  | C2A-CAA-CBA-CGA |
| 30  | e     | 608 | CHL  | C2A-CAA-CBA-CGA |
| 31  | 8     | 304 | CLA  | C2A-CAA-CBA-CGA |
| 31  | 8     | 314 | CLA  | C2A-CAA-CBA-CGA |
| 31  | A     | 822 | CLA  | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | A     | 829 | CLA  | C2A-CAA-CBA-CGA |
| 31  | B     | 834 | CLA  | C2A-CAA-CBA-CGA |
| 31  | i     | 604 | CLA  | C2A-CAA-CBA-CGA |
| 31  | 0     | 312 | CLA  | O1D-CGD-O2D-CED |
| 30  | 2     | 302 | CHL  | C8-C10-C11-C12  |
| 30  | 3     | 302 | CHL  | C8-C10-C11-C12  |
| 30  | 5     | 302 | CHL  | C13-C15-C16-C17 |
| 30  | 8     | 302 | CHL  | C13-C15-C16-C17 |
| 30  | c     | 601 | CHL  | C5-C6-C7-C8     |
| 30  | c     | 608 | CHL  | C15-C16-C17-C18 |
| 30  | b     | 601 | CHL  | C13-C15-C16-C17 |
| 30  | b     | 608 | CHL  | C13-C15-C16-C17 |
| 30  | d     | 609 | CHL  | C15-C16-C17-C18 |
| 30  | f     | 602 | CHL  | C13-C15-C16-C17 |
| 30  | e     | 608 | CHL  | C8-C10-C11-C12  |
| 31  | 1     | 312 | CLA  | C13-C15-C16-C17 |
| 31  | A     | 811 | CLA  | C13-C15-C16-C17 |
| 31  | A     | 829 | CLA  | C15-C16-C17-C18 |
| 31  | A     | 832 | CLA  | C5-C6-C7-C8     |
| 31  | A     | 835 | CLA  | C5-C6-C7-C8     |
| 31  | A     | 852 | CLA  | C13-C15-C16-C17 |
| 31  | B     | 803 | CLA  | C13-C15-C16-C17 |
| 31  | B     | 814 | CLA  | C5-C6-C7-C8     |
| 31  | B     | 827 | CLA  | C15-C16-C17-C18 |
| 31  | d     | 610 | CLA  | C5-C6-C7-C8     |
| 34  | 0     | 601 | LHG  | C7-C8-C9-C10    |
| 34  | 2     | 601 | LHG  | C23-C24-C25-C26 |
| 34  | h     | 630 | LHG  | C23-C24-C25-C26 |
| 30  | 5     | 302 | CHL  | O1D-CGD-O2D-CED |
| 30  | 7     | 305 | CHL  | O1D-CGD-O2D-CED |
| 31  | B     | 816 | CLA  | O1D-CGD-O2D-CED |
| 31  | L     | 202 | CLA  | CBA-CGA-O2A-C1  |
| 31  | A     | 831 | CLA  | O1A-CGA-O2A-C1  |
| 31  | a     | 613 | CLA  | O1A-CGA-O2A-C1  |
| 31  | H     | 205 | CLA  | O1A-CGA-O2A-C1  |
| 31  | 9     | 312 | CLA  | C3-C5-C6-C7     |
| 30  | c     | 608 | CHL  | C8-C10-C11-C12  |
| 30  | c     | 609 | CHL  | C8-C10-C11-C12  |
| 30  | b     | 601 | CHL  | C15-C16-C17-C18 |
| 30  | b     | 602 | CHL  | C8-C10-C11-C12  |
| 30  | b     | 602 | CHL  | C13-C15-C16-C17 |
| 30  | b     | 608 | CHL  | C8-C10-C11-C12  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 30  | f     | 602 | CHL  | C8-C10-C11-C12  |
| 30  | e     | 608 | CHL  | C15-C16-C17-C18 |
| 31  | A     | 811 | CLA  | C8-C10-C11-C12  |
| 31  | A     | 811 | CLA  | C15-C16-C17-C18 |
| 31  | A     | 826 | CLA  | C5-C6-C7-C8     |
| 31  | A     | 853 | CLA  | C5-C6-C7-C8     |
| 31  | B     | 834 | CLA  | C8-C10-C11-C12  |
| 31  | B     | 836 | CLA  | C5-C6-C7-C8     |
| 31  | B     | 836 | CLA  | C8-C10-C11-C12  |
| 31  | L     | 203 | CLA  | C13-C15-C16-C17 |
| 34  | A     | 855 | LHG  | C14-C15-C16-C17 |
| 34  | B     | 852 | LHG  | O2-C2-C3-O3     |
| 34  | c     | 630 | LHG  | O2-C2-C3-O3     |
| 34  | f     | 630 | LHG  | O2-C2-C3-O3     |
| 30  | 4     | 319 | CHL  | CBA-CGA-O2A-C1  |
| 33  | 0     | 502 | 0UR  | O57-C45-C46-C47 |
| 30  | c     | 607 | CHL  | CBD-CGD-O2D-CED |
| 30  | d     | 602 | CHL  | O1A-CGA-O2A-C1  |
| 31  | 3     | 304 | CLA  | O1A-CGA-O2A-C1  |
| 31  | A     | 807 | CLA  | O1A-CGA-O2A-C1  |
| 31  | A     | 810 | CLA  | O1A-CGA-O2A-C1  |
| 31  | A     | 833 | CLA  | O1A-CGA-O2A-C1  |
| 31  | B     | 831 | CLA  | O1A-CGA-O2A-C1  |
| 31  | d     | 604 | CLA  | O1A-CGA-O2A-C1  |
| 30  | 7     | 301 | CHL  | C13-C15-C16-C17 |
| 34  | K     | 106 | LHG  | C23-C24-C25-C26 |
| 36  | 9     | 602 | LMG  | C28-C29-C30-C31 |
| 30  | 2     | 319 | CHL  | C5-C6-C7-C8     |
| 30  | 2     | 319 | CHL  | C8-C10-C11-C12  |
| 30  | b     | 601 | CHL  | C8-C10-C11-C12  |
| 31  | 6     | 317 | CLA  | C10-C11-C12-C13 |
| 31  | A     | 813 | CLA  | C13-C15-C16-C17 |
| 31  | B     | 828 | CLA  | C8-C10-C11-C12  |
| 30  | i     | 614 | CHL  | O1D-CGD-O2D-CED |
| 31  | 2     | 312 | CLA  | C3-C5-C6-C7     |
| 30  | 1     | 306 | CHL  | O1D-CGD-O2D-CED |
| 30  | 3     | 302 | CHL  | O1D-CGD-O2D-CED |
| 30  | 9     | 305 | CHL  | O1D-CGD-O2D-CED |
| 30  | c     | 601 | CHL  | O1D-CGD-O2D-CED |
| 30  | c     | 605 | CHL  | O1D-CGD-O2D-CED |
| 30  | b     | 609 | CHL  | O1D-CGD-O2D-CED |
| 31  | A     | 832 | CLA  | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | B     | 836 | CLA  | O1D-CGD-O2D-CED |
| 31  | G     | 101 | CLA  | O1D-CGD-O2D-CED |
| 31  | f     | 612 | CLA  | O1D-CGD-O2D-CED |
| 31  | H     | 205 | CLA  | O1D-CGD-O2D-CED |
| 30  | c     | 609 | CHL  | C13-C15-C16-C17 |
| 30  | f     | 609 | CHL  | C8-C10-C11-C12  |
| 31  | A     | 818 | CLA  | C13-C15-C16-C17 |
| 31  | A     | 826 | CLA  | C15-C16-C17-C18 |
| 31  | B     | 806 | CLA  | C10-C11-C12-C13 |
| 31  | B     | 830 | CLA  | C5-C6-C7-C8     |
| 30  | 7     | 313 | CHL  | CBD-CGD-O2D-CED |
| 34  | e     | 630 | LHG  | C7-C8-C9-C10    |
| 30  | c     | 609 | CHL  | O1D-CGD-O2D-CED |
| 31  | 0     | 310 | CLA  | O1D-CGD-O2D-CED |
| 31  | 2     | 312 | CLA  | O1D-CGD-O2D-CED |
| 31  | 6     | 312 | CLA  | O1D-CGD-O2D-CED |
| 31  | 7     | 311 | CLA  | O1D-CGD-O2D-CED |
| 31  | f     | 604 | CLA  | O1D-CGD-O2D-CED |
| 31  | c     | 611 | CLA  | O1A-CGA-O2A-C1  |
| 30  | a     | 602 | CHL  | C8-C10-C11-C12  |
| 30  | c     | 602 | CHL  | C8-C10-C11-C12  |
| 30  | b     | 608 | CHL  | C15-C16-C17-C18 |
| 31  | 1     | 303 | CLA  | C5-C6-C7-C8     |
| 31  | 8     | 309 | CLA  | C5-C6-C7-C8     |
| 31  | A     | 829 | CLA  | C8-C10-C11-C12  |
| 30  | 2     | 319 | CHL  | CBA-CGA-O2A-C1  |
| 30  | a     | 602 | CHL  | CBA-CGA-O2A-C1  |
| 30  | f     | 602 | CHL  | CBA-CGA-O2A-C1  |
| 31  | 2     | 312 | CLA  | CBA-CGA-O2A-C1  |
| 33  | 6     | 502 | OUR  | O57-C45-O44-C43 |
| 31  | 6     | 311 | CLA  | O2A-C1-C2-C3    |
| 31  | B     | 806 | CLA  | C2C-C3C-CAC-CBC |
| 31  | B     | 817 | CLA  | C2C-C3C-CAC-CBC |
| 30  | c     | 614 | CHL  | CBD-CGD-O2D-CED |
| 30  | b     | 602 | CHL  | CBD-CGD-O2D-CED |
| 30  | i     | 601 | CHL  | CBD-CGD-O2D-CED |
| 31  | 8     | 314 | CLA  | CBD-CGD-O2D-CED |
| 34  | b     | 630 | LHG  | C28-C29-C30-C31 |
| 30  | b     | 602 | CHL  | O1A-CGA-O2A-C1  |
| 30  | d     | 609 | CHL  | O1A-CGA-O2A-C1  |
| 31  | B     | 803 | CLA  | O1D-CGD-O2D-CED |
| 34  | A     | 855 | LHG  | C28-C29-C30-C31 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 32  | 1     | 402 | 8CT  | C18-C19-C20-C21 |
| 32  | 7     | 404 | 8CT  | C18-C19-C20-C21 |
| 32  | 9     | 401 | 8CT  | C18-C19-C20-C21 |
| 32  | A     | 847 | 8CT  | C12-C13-C14-C15 |
| 32  | A     | 848 | 8CT  | C16-C17-C18-C19 |
| 32  | B     | 848 | 8CT  | C12-C13-C14-C15 |
| 32  | B     | 851 | 8CT  | C18-C19-C20-C21 |
| 37  | d     | 522 | 0IE  | C13-C14-C15-C16 |
| 31  | 3     | 308 | CLA  | C10-C11-C12-C13 |
| 31  | A     | 806 | CLA  | C15-C16-C17-C18 |
| 34  | 1     | 601 | LHG  | C1-C2-C3-O3     |
| 34  | A     | 845 | LHG  | C1-C2-C3-O3     |
| 34  | B     | 854 | LHG  | C1-C2-C3-O3     |
| 34  | c     | 630 | LHG  | C1-C2-C3-O3     |
| 34  | i     | 630 | LHG  | C1-C2-C3-O3     |
| 30  | a     | 602 | CHL  | C2A-CAA-CBA-CGA |
| 30  | a     | 606 | CHL  | C2A-CAA-CBA-CGA |
| 30  | a     | 608 | CHL  | C2A-CAA-CBA-CGA |
| 30  | c     | 608 | CHL  | C2A-CAA-CBA-CGA |
| 30  | b     | 606 | CHL  | C2A-CAA-CBA-CGA |
| 30  | d     | 602 | CHL  | C2A-CAA-CBA-CGA |
| 30  | d     | 608 | CHL  | C2A-CAA-CBA-CGA |
| 30  | g     | 606 | CHL  | C2A-CAA-CBA-CGA |
| 30  | h     | 607 | CHL  | C2A-CAA-CBA-CGA |
| 30  | i     | 602 | CHL  | C2A-CAA-CBA-CGA |
| 30  | e     | 602 | CHL  | C2A-CAA-CBA-CGA |
| 31  | 3     | 306 | CLA  | C2A-CAA-CBA-CGA |
| 31  | 3     | 308 | CLA  | C2A-CAA-CBA-CGA |
| 31  | B     | 823 | CLA  | C2A-CAA-CBA-CGA |
| 31  | L     | 207 | CLA  | C2A-CAA-CBA-CGA |
| 31  | a     | 613 | CLA  | C2A-CAA-CBA-CGA |
| 30  | 0     | 302 | CHL  | CBA-CGA-O2A-C1  |
| 30  | 8     | 302 | CHL  | CBA-CGA-O2A-C1  |
| 31  | 1     | 312 | CLA  | CBA-CGA-O2A-C1  |
| 31  | 9     | 300 | CLA  | CBA-CGA-O2A-C1  |
| 31  | c     | 604 | CLA  | CBA-CGA-O2A-C1  |
| 30  | 1     | 302 | CHL  | C13-C15-C16-C17 |
| 30  | e     | 602 | CHL  | C5-C6-C7-C8     |
| 30  | e     | 609 | CHL  | C8-C10-C11-C12  |
| 31  | 2     | 304 | CLA  | C10-C11-C12-C13 |
| 31  | 3     | 303 | CLA  | C5-C6-C7-C8     |
| 31  | 7     | 308 | CLA  | C5-C6-C7-C8     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | A     | 808 | CLA  | C15-C16-C17-C18 |
| 31  | A     | 852 | CLA  | C10-C11-C12-C13 |
| 31  | B     | 814 | CLA  | C10-C11-C12-C13 |
| 31  | B     | 827 | CLA  | C5-C6-C7-C8     |
| 38  | A     | 842 | PQN  | C15-C16-C17-C18 |
| 38  | B     | 842 | PQN  | C18-C20-C21-C22 |
| 30  | 9     | 301 | CHL  | CBD-CGD-O2D-CED |
| 30  | i     | 606 | CHL  | CBD-CGD-O2D-CED |
| 33  | 2     | 502 | 0UR  | O44-C45-C46-C47 |
| 31  | 5     | 312 | CLA  | C3-C5-C6-C7     |
| 31  | B     | 809 | CLA  | C3-C5-C6-C7     |
| 30  | d     | 607 | CHL  | O1D-CGD-O2D-CED |
| 30  | d     | 609 | CHL  | O1D-CGD-O2D-CED |
| 30  | f     | 605 | CHL  | O1D-CGD-O2D-CED |
| 31  | 7     | 318 | CLA  | O1D-CGD-O2D-CED |
| 31  | B     | 824 | CLA  | O1D-CGD-O2D-CED |
| 34  | 1     | 601 | LHG  | C7-C8-C9-C10    |
| 30  | 2     | 302 | CHL  | C5-C6-C7-C8     |
| 30  | 6     | 302 | CHL  | C8-C10-C11-C12  |
| 30  | h     | 602 | CHL  | C5-C6-C7-C8     |
| 31  | 5     | 312 | CLA  | C5-C6-C7-C8     |
| 31  | 9     | 308 | CLA  | C5-C6-C7-C8     |
| 31  | A     | 852 | CLA  | C8-C10-C11-C12  |
| 30  | 9     | 313 | CHL  | CBD-CGD-O2D-CED |
| 30  | d     | 601 | CHL  | CBD-CGD-O2D-CED |
| 30  | 6     | 302 | CHL  | C5-C6-C7-C8     |
| 30  | 7     | 302 | CHL  | C13-C15-C16-C17 |
| 30  | f     | 601 | CHL  | C13-C15-C16-C17 |
| 31  | 0     | 312 | CLA  | C5-C6-C7-C8     |
| 31  | 1     | 309 | CLA  | C5-C6-C7-C8     |
| 31  | A     | 819 | CLA  | C15-C16-C17-C18 |
| 31  | A     | 852 | CLA  | C5-C6-C7-C8     |
| 31  | B     | 809 | CLA  | C15-C16-C17-C18 |
| 31  | B     | 811 | CLA  | C5-C6-C7-C8     |
| 31  | B     | 839 | CLA  | C15-C16-C17-C18 |
| 31  | L     | 203 | CLA  | C5-C6-C7-C8     |
| 31  | B     | 822 | CLA  | O1D-CGD-O2D-CED |
| 30  | 7     | 302 | CHL  | CBA-CGA-O2A-C1  |
| 33  | 1     | 502 | 0UR  | O57-C45-C46-C47 |
| 33  | 8     | 502 | 0UR  | O57-C45-C46-C47 |
| 30  | c     | 606 | CHL  | C2A-CAA-CBA-CGA |
| 34  | A     | 844 | LHG  | C23-C24-C25-C26 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | A     | 830 | CLA  | C4-C3-C5-C6     |
| 31  | B     | 817 | CLA  | C4-C3-C5-C6     |
| 31  | 1     | 309 | CLA  | C2-C3-C5-C6     |
| 30  | a     | 602 | CHL  | C13-C15-C16-C17 |
| 31  | A     | 815 | CLA  | C13-C15-C16-C17 |
| 31  | f     | 611 | CLA  | C5-C6-C7-C8     |
| 30  | e     | 602 | CHL  | C3-C5-C6-C7     |
| 30  | 7     | 301 | CHL  | CBD-CGD-O2D-CED |
| 30  | i     | 602 | CHL  | O1D-CGD-O2D-CED |
| 30  | a     | 608 | CHL  | O2A-C1-C2-C3    |
| 41  | B     | 849 | DGD  | C2E-C1E-O5D-C6D |
| 31  | A     | 840 | CLA  | C13-C15-C16-C17 |
| 31  | B     | 828 | CLA  | C10-C11-C12-C13 |
| 31  | L     | 201 | CLA  | C5-C6-C7-C8     |
| 33  | 5     | 501 | 0UR  | O44-C45-C46-C47 |
| 30  | 2     | 308 | CHL  | CBA-CGA-O2A-C1  |
| 30  | e     | 602 | CHL  | CBA-CGA-O2A-C1  |
| 31  | 1     | 303 | CLA  | CBA-CGA-O2A-C1  |
| 31  | 1     | 310 | CLA  | CBA-CGA-O2A-C1  |
| 33  | g     | 520 | 0UR  | O57-C45-C46-C47 |
| 34  | 2     | 601 | LHG  | C24-C23-O8-C6   |
| 30  | 7     | 306 | CHL  | O1A-CGA-O2A-C1  |
| 31  | H     | 201 | CLA  | O1D-CGD-O2D-CED |
| 37  | d     | 522 | 0IE  | C14-C15-C16-C23 |
| 31  | 0     | 308 | CLA  | C3-C5-C6-C7     |
| 31  | A     | 837 | CLA  | C5-C6-C7-C8     |
| 32  | 1     | 402 | 8CT  | C10-C11-C12-C40 |
| 32  | 3     | 403 | 8CT  | C10-C11-C12-C40 |
| 32  | 7     | 405 | 8CT  | C27-C26-C28-C29 |
| 32  | 8     | 406 | 8CT  | C14-C15-C16-C39 |
| 32  | 9     | 401 | 8CT  | C10-C11-C12-C40 |
| 32  | 9     | 401 | 8CT  | C27-C26-C28-C29 |
| 32  | A     | 847 | 8CT  | C10-C11-C12-C40 |
| 32  | A     | 850 | 8CT  | C22-C21-C23-C24 |
| 32  | A     | 850 | 8CT  | C27-C26-C28-C29 |
| 32  | B     | 843 | 8CT  | C14-C15-C16-C39 |
| 32  | B     | 847 | 8CT  | C10-C11-C12-C40 |
| 32  | B     | 851 | 8CT  | C10-C11-C12-C40 |
| 32  | L     | 209 | 8CT  | C10-C11-C12-C40 |
| 33  | 2     | 502 | 0UR  | C22-C16-C17-C18 |
| 33  | 5     | 502 | 0UR  | C22-C16-C17-C18 |
| 33  | 6     | 501 | 0UR  | C22-C16-C17-C18 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 33  | 6     | 502 | 0UR  | C22-C16-C17-C18 |
| 34  | B     | 852 | LHG  | C5-C4-O6-P      |
| 32  | 1     | 402 | 8CT  | C10-C11-C12-C13 |
| 32  | 9     | 401 | 8CT  | C10-C11-C12-C13 |
| 32  | 9     | 401 | 8CT  | C25-C26-C28-C29 |
| 32  | A     | 847 | 8CT  | C10-C11-C12-C13 |
| 32  | A     | 850 | 8CT  | C10-C11-C12-C13 |
| 32  | A     | 850 | 8CT  | C25-C26-C28-C29 |
| 32  | F     | 302 | 8CT  | C10-C11-C12-C13 |
| 32  | L     | 206 | 8CT  | C10-C11-C12-C13 |
| 32  | M     | 102 | 8CT  | C10-C11-C12-C13 |
| 33  | 2     | 502 | 0UR  | C15-C16-C17-C18 |
| 33  | 5     | 502 | 0UR  | C15-C16-C17-C18 |
| 33  | 6     | 501 | 0UR  | C15-C16-C17-C18 |
| 30  | 8     | 302 | CHL  | O1A-CGA-O2A-C1  |
| 30  | f     | 602 | CHL  | O1A-CGA-O2A-C1  |
| 31  | 0     | 309 | CLA  | O1A-CGA-O2A-C1  |
| 30  | 0     | 301 | CHL  | C2A-CAA-CBA-CGA |
| 30  | 0     | 302 | CHL  | C2A-CAA-CBA-CGA |
| 30  | 0     | 305 | CHL  | C2A-CAA-CBA-CGA |
| 30  | 1     | 313 | CHL  | C2A-CAA-CBA-CGA |
| 30  | 2     | 302 | CHL  | C2A-CAA-CBA-CGA |
| 30  | 2     | 306 | CHL  | C2A-CAA-CBA-CGA |
| 30  | 3     | 307 | CHL  | C2A-CAA-CBA-CGA |
| 30  | 7     | 302 | CHL  | C2A-CAA-CBA-CGA |
| 30  | 9     | 306 | CHL  | C2A-CAA-CBA-CGA |
| 30  | b     | 602 | CHL  | C2A-CAA-CBA-CGA |
| 30  | f     | 602 | CHL  | C2A-CAA-CBA-CGA |
| 30  | e     | 606 | CHL  | C2A-CAA-CBA-CGA |
| 30  | 4     | 306 | CHL  | C2A-CAA-CBA-CGA |
| 31  | 5     | 304 | CLA  | C2A-CAA-CBA-CGA |
| 31  | 5     | 308 | CLA  | C2A-CAA-CBA-CGA |
| 31  | 5     | 314 | CLA  | C2A-CAA-CBA-CGA |
| 31  | 6     | 318 | CLA  | C2A-CAA-CBA-CGA |
| 31  | 9     | 300 | CLA  | C2A-CAA-CBA-CGA |
| 31  | A     | 840 | CLA  | C2A-CAA-CBA-CGA |
| 31  | B     | 803 | CLA  | C2A-CAA-CBA-CGA |
| 31  | B     | 807 | CLA  | C2A-CAA-CBA-CGA |
| 31  | B     | 816 | CLA  | C2A-CAA-CBA-CGA |
| 31  | B     | 828 | CLA  | C2A-CAA-CBA-CGA |
| 31  | B     | 829 | CLA  | C2A-CAA-CBA-CGA |
| 31  | G     | 103 | CLA  | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | g     | 604 | CLA  | C2A-CAA-CBA-CGA |
| 31  | H     | 202 | CLA  | C2A-CAA-CBA-CGA |
| 30  | b     | 607 | CHL  | CBA-CGA-O2A-C1  |
| 34  | 6     | 601 | LHG  | O1-C1-C2-C3     |
| 34  | 6     | 603 | LHG  | O1-C1-C2-C3     |
| 34  | 7     | 603 | LHG  | O1-C1-C2-C3     |
| 34  | A     | 845 | LHG  | O1-C1-C2-C3     |
| 34  | B     | 852 | LHG  | O1-C1-C2-C3     |
| 34  | g     | 630 | LHG  | O1-C1-C2-C3     |
| 34  | e     | 630 | LHG  | O1-C1-C2-C3     |
| 31  | A     | 807 | CLA  | CBD-CGD-O2D-CED |
| 31  | a     | 603 | CLA  | O1D-CGD-O2D-CED |
| 31  | 3     | 320 | CLA  | C4C-C3C-CAC-CBC |
| 31  | A     | 840 | CLA  | O2A-C1-C2-C3    |
| 35  | 0     | 603 | SQD  | C44-C45-O47-C7  |
| 36  | 9     | 602 | LMG  | C9-C8-O7-C10    |
| 33  | h     | 520 | 0UR  | O44-C45-C46-C47 |
| 32  | 9     | 401 | 8CT  | C16-C17-C18-C19 |
| 33  | g     | 520 | 0UR  | C3-C4-C5-C6     |
| 30  | c     | 609 | CHL  | C16-C17-C18-C19 |
| 30  | b     | 601 | CHL  | C16-C17-C18-C19 |
| 30  | b     | 608 | CHL  | C16-C17-C18-C20 |
| 31  | b     | 611 | CLA  | C11-C12-C13-C15 |
| 30  | h     | 606 | CHL  | O1D-CGD-O2D-CED |
| 31  | 7     | 317 | CLA  | O1D-CGD-O2D-CED |
| 30  | 2     | 319 | CHL  | O1A-CGA-O2A-C1  |
| 30  | 4     | 319 | CHL  | O1A-CGA-O2A-C1  |
| 30  | i     | 602 | CHL  | C3-C5-C6-C7     |
| 31  | 1     | 310 | CLA  | C3-C5-C6-C7     |
| 31  | K     | 102 | CLA  | C3-C5-C6-C7     |
| 41  | B     | 849 | DGD  | O6E-C1E-O5D-C6D |
| 30  | a     | 609 | CHL  | C8-C10-C11-C12  |
| 30  | f     | 607 | CHL  | O1D-CGD-O2D-CED |
| 31  | 1     | 303 | CLA  | O1D-CGD-O2D-CED |
| 31  | 1     | 312 | CLA  | O1D-CGD-O2D-CED |
| 31  | 7     | 311 | CLA  | CBA-CGA-O2A-C1  |
| 31  | 7     | 312 | CLA  | C5-C6-C7-C8     |
| 30  | a     | 607 | CHL  | CBD-CGD-O2D-CED |
| 31  | A     | 826 | CLA  | CBD-CGD-O2D-CED |
| 30  | d     | 606 | CHL  | O1D-CGD-O2D-CED |
| 30  | g     | 602 | CHL  | O1D-CGD-O2D-CED |
| 30  | 1     | 307 | CHL  | C16-C17-C18-C20 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 30  | b     | 608 | CHL  | C16-C17-C18-C19 |
| 30  | f     | 609 | CHL  | C16-C17-C18-C19 |
| 31  | e     | 611 | CLA  | C6-C7-C8-C10    |
| 30  | a     | 602 | CHL  | O1A-CGA-O2A-C1  |
| 31  | 2     | 312 | CLA  | O1A-CGA-O2A-C1  |
| 31  | 9     | 300 | CLA  | O1A-CGA-O2A-C1  |
| 30  | i     | 602 | CHL  | C8-C10-C11-C12  |
| 34  | B     | 854 | LHG  | C34-C35-C36-C37 |
| 34  | h     | 630 | LHG  | C12-C13-C14-C15 |
| 36  | 9     | 602 | LMG  | C14-C15-C16-C17 |
| 33  | 3     | 501 | OUR  | O44-C45-C46-C47 |
| 30  | h     | 601 | CHL  | CBA-CGA-O2A-C1  |
| 30  | i     | 601 | CHL  | CBA-CGA-O2A-C1  |
| 31  | a     | 613 | CLA  | C6-C7-C8-C10    |
| 34  | 8     | 601 | LHG  | C30-C31-C32-C33 |
| 34  | A     | 844 | LHG  | C30-C31-C32-C33 |
| 34  | f     | 630 | LHG  | C11-C12-C13-C14 |
| 35  | 0     | 603 | SQD  | C26-C27-C28-C29 |
| 36  | B     | 853 | LMG  | C16-C17-C18-C19 |
| 41  | B     | 849 | DGD  | C2A-C3A-C4A-C5A |
| 30  | c     | 608 | CHL  | C13-C15-C16-C17 |
| 31  | A     | 838 | CLA  | C11-C10-C8-C9   |
| 30  | 6     | 308 | CHL  | C10-C11-C12-C13 |
| 34  | 8     | 601 | LHG  | C11-C12-C13-C14 |
| 34  | f     | 630 | LHG  | C10-C11-C12-C13 |
| 31  | d     | 613 | CLA  | CBA-CGA-O2A-C1  |
| 41  | B     | 849 | DGD  | C2A-C1A-O1G-C1G |
| 34  | 0     | 601 | LHG  | C15-C16-C17-C18 |
| 34  | 8     | 601 | LHG  | C14-C15-C16-C17 |
| 34  | A     | 844 | LHG  | C10-C11-C12-C13 |
| 36  | 9     | 602 | LMG  | C20-C21-C22-C23 |
| 34  | 2     | 601 | LHG  | O1-C1-C2-O2     |
| 34  | 3     | 601 | LHG  | O1-C1-C2-O2     |
| 34  | 3     | 603 | LHG  | O1-C1-C2-O2     |
| 34  | M     | 104 | LHG  | O1-C1-C2-O2     |
| 34  | c     | 630 | LHG  | O1-C1-C2-O2     |
| 34  | h     | 630 | LHG  | O1-C1-C2-O2     |
| 34  | H     | 203 | LHG  | O1-C1-C2-O2     |
| 31  | 2     | 304 | CLA  | CBD-CGD-O2D-CED |
| 34  | K     | 106 | LHG  | C9-C10-C11-C12  |
| 41  | B     | 849 | DGD  | C4B-C5B-C6B-C7B |
| 30  | g     | 614 | CHL  | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 30  | h     | 601 | CHL  | O1D-CGD-O2D-CED |
| 30  | i     | 607 | CHL  | O1D-CGD-O2D-CED |
| 30  | i     | 609 | CHL  | O1D-CGD-O2D-CED |
| 31  | 2     | 314 | CLA  | O1D-CGD-O2D-CED |
| 31  | A     | 806 | CLA  | O1D-CGD-O2D-CED |
| 31  | 4     | 304 | CLA  | O1D-CGD-O2D-CED |
| 31  | 0     | 312 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 1     | 308 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 1     | 310 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 3     | 310 | CLA  | C4B-C3B-CAB-CBB |
| 31  | A     | 824 | CLA  | C4B-C3B-CAB-CBB |
| 31  | A     | 839 | CLA  | C4B-C3B-CAB-CBB |
| 31  | B     | 824 | CLA  | C4B-C3B-CAB-CBB |
| 31  | G     | 103 | CLA  | C4B-C3B-CAB-CBB |
| 31  | O     | 201 | CLA  | C4B-C3B-CAB-CBB |
| 34  | b     | 630 | LHG  | C12-C13-C14-C15 |
| 30  | c     | 609 | CHL  | C16-C17-C18-C20 |
| 30  | d     | 609 | CHL  | C16-C17-C18-C19 |
| 30  | d     | 609 | CHL  | C16-C17-C18-C20 |
| 30  | f     | 609 | CHL  | C16-C17-C18-C20 |
| 31  | 0     | 309 | CLA  | C11-C12-C13-C14 |
| 31  | A     | 824 | CLA  | C6-C7-C8-C9     |
| 31  | b     | 611 | CLA  | C11-C12-C13-C14 |
| 30  | c     | 606 | CHL  | O1D-CGD-O2D-CED |
| 31  | L     | 207 | CLA  | O1D-CGD-O2D-CED |
| 30  | 1     | 302 | CHL  | C2A-CAA-CBA-CGA |
| 30  | 8     | 307 | CHL  | C2A-CAA-CBA-CGA |
| 30  | d     | 607 | CHL  | C2A-CAA-CBA-CGA |
| 30  | i     | 606 | CHL  | C2A-CAA-CBA-CGA |
| 30  | i     | 608 | CHL  | C2A-CAA-CBA-CGA |
| 31  | 6     | 303 | CLA  | C3-C5-C6-C7     |
| 31  | A     | 808 | CLA  | C2A-CAA-CBA-CGA |
| 31  | h     | 613 | CLA  | C2A-CAA-CBA-CGA |
| 34  | 4     | 601 | LHG  | C10-C11-C12-C13 |
| 30  | 6     | 301 | CHL  | C8-C10-C11-C12  |
| 34  | G     | 105 | LHG  | C8-C7-O7-C5     |
| 36  | 3     | 602 | LMG  | C11-C10-O7-C8   |
| 34  | 8     | 601 | LHG  | C25-C26-C27-C28 |
| 34  | a     | 630 | LHG  | C10-C11-C12-C13 |
| 30  | 1     | 313 | CHL  | C11-C12-C13-C15 |
| 30  | e     | 608 | CHL  | C6-C7-C8-C10    |
| 31  | 0     | 312 | CLA  | C12-C13-C15-C16 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | 5     | 312 | CLA  | C6-C7-C8-C10    |
| 31  | A     | 808 | CLA  | C11-C12-C13-C15 |
| 31  | A     | 830 | CLA  | C12-C13-C15-C16 |
| 31  | B     | 814 | CLA  | C11-C12-C13-C15 |
| 31  | B     | 839 | CLA  | C11-C12-C13-C15 |
| 31  | L     | 201 | CLA  | C6-C7-C8-C10    |
| 39  | A     | 857 | CL0  | C12-C13-C15-C16 |
| 36  | L     | 210 | LMG  | C10-C11-C12-C13 |
| 30  | i     | 602 | CHL  | CBA-CGA-O2A-C1  |
| 30  | 8     | 302 | CHL  | C8-C10-C11-C12  |
| 30  | d     | 609 | CHL  | C8-C10-C11-C12  |
| 31  | 3     | 308 | CLA  | C8-C10-C11-C12  |
| 34  | 5     | 601 | LHG  | C28-C29-C30-C31 |
| 34  | 7     | 602 | LHG  | C15-C16-C17-C18 |
| 34  | A     | 844 | LHG  | C15-C16-C17-C18 |
| 34  | A     | 844 | LHG  | C26-C27-C28-C29 |
| 34  | B     | 854 | LHG  | C25-C26-C27-C28 |
| 34  | a     | 630 | LHG  | C14-C15-C16-C17 |
| 36  | 9     | 602 | LMG  | C34-C35-C36-C37 |
| 41  | B     | 849 | DGD  | C7A-C8A-C9A-CAA |
| 41  | B     | 849 | DGD  | C3B-C4B-C5B-C6B |
| 31  | 1     | 312 | CLA  | O1A-CGA-O2A-C1  |
| 31  | c     | 604 | CLA  | O1A-CGA-O2A-C1  |
| 30  | 4     | 319 | CHL  | C3-C5-C6-C7     |
| 31  | A     | 828 | CLA  | C3-C5-C6-C7     |
| 30  | 6     | 301 | CHL  | C3A-C2A-CAA-CBA |
| 30  | d     | 607 | CHL  | C3A-C2A-CAA-CBA |
| 30  | f     | 607 | CHL  | C3A-C2A-CAA-CBA |
| 30  | i     | 607 | CHL  | C3A-C2A-CAA-CBA |
| 31  | 0     | 303 | CLA  | C3A-C2A-CAA-CBA |
| 31  | 0     | 311 | CLA  | C3A-C2A-CAA-CBA |
| 31  | 0     | 313 | CLA  | C3A-C2A-CAA-CBA |
| 31  | 3     | 303 | CLA  | C3A-C2A-CAA-CBA |
| 31  | 7     | 317 | CLA  | C3A-C2A-CAA-CBA |
| 31  | 9     | 300 | CLA  | C4-C3-C5-C6     |
| 31  | 9     | 311 | CLA  | C3A-C2A-CAA-CBA |
| 31  | A     | 803 | CLA  | C3A-C2A-CAA-CBA |
| 31  | A     | 832 | CLA  | C3A-C2A-CAA-CBA |
| 31  | A     | 836 | CLA  | C3A-C2A-CAA-CBA |
| 31  | B     | 814 | CLA  | C3A-C2A-CAA-CBA |
| 31  | B     | 817 | CLA  | C3A-C2A-CAA-CBA |
| 31  | B     | 827 | CLA  | C3A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | B     | 836 | CLA  | C3A-C2A-CAA-CBA |
| 31  | L     | 202 | CLA  | C3A-C2A-CAA-CBA |
| 31  | H     | 201 | CLA  | C3A-C2A-CAA-CBA |
| 30  | 8     | 306 | CHL  | O1D-CGD-O2D-CED |
| 34  | g     | 630 | LHG  | C26-C27-C28-C29 |
| 36  | 9     | 602 | LMG  | C30-C31-C32-C33 |
| 30  | 7     | 313 | CHL  | CBA-CGA-O2A-C1  |
| 34  | 1     | 601 | LHG  | C15-C16-C17-C18 |
| 36  | J     | 105 | LMG  | C32-C33-C34-C35 |
| 30  | b     | 601 | CHL  | C5-C6-C7-C8     |
| 30  | e     | 608 | CHL  | C13-C15-C16-C17 |
| 31  | A     | 840 | CLA  | C10-C11-C12-C13 |
| 31  | B     | 817 | CLA  | C8-C10-C11-C12  |
| 30  | 5     | 313 | CHL  | O1D-CGD-O2D-CED |
| 30  | 8     | 302 | CHL  | O1D-CGD-O2D-CED |
| 31  | A     | 819 | CLA  | O1D-CGD-O2D-CED |
| 32  | B     | 843 | 8CT  | C18-C19-C20-C21 |
| 32  | B     | 846 | 8CT  | C16-C17-C18-C19 |
| 32  | M     | 102 | 8CT  | C16-C17-C18-C19 |
| 30  | 3     | 307 | CHL  | C16-C17-C18-C20 |
| 30  | 6     | 301 | CHL  | C11-C12-C13-C15 |
| 30  | c     | 608 | CHL  | C16-C17-C18-C19 |
| 30  | b     | 601 | CHL  | C16-C17-C18-C20 |
| 30  | e     | 608 | CHL  | C16-C17-C18-C19 |
| 31  | A     | 824 | CLA  | C6-C7-C8-C10    |
| 31  | e     | 611 | CLA  | C6-C7-C8-C9     |
| 30  | 0     | 302 | CHL  | O1A-CGA-O2A-C1  |
| 30  | 7     | 302 | CHL  | O1A-CGA-O2A-C1  |
| 31  | 8     | 310 | CLA  | O1A-CGA-O2A-C1  |
| 34  | a     | 630 | LHG  | C13-C14-C15-C16 |
| 30  | 3     | 307 | CHL  | C8-C10-C11-C12  |
| 31  | b     | 613 | CLA  | CBD-CGD-O2D-CED |
| 36  | 9     | 602 | LMG  | C33-C34-C35-C36 |
| 34  | A     | 844 | LHG  | C1-C2-C3-O3     |
| 30  | 3     | 307 | CHL  | CBA-CGA-O2A-C1  |
| 31  | 1     | 304 | CLA  | CBA-CGA-O2A-C1  |
| 31  | 4     | 311 | CLA  | CBA-CGA-O2A-C1  |
| 34  | 7     | 601 | LHG  | C4-C5-C6-O8     |
| 34  | e     | 630 | LHG  | C25-C26-C27-C28 |
| 36  | 3     | 602 | LMG  | C12-C13-C14-C15 |
| 41  | B     | 849 | DGD  | C9B-CAB-CBB-CCB |
| 34  | g     | 630 | LHG  | C23-C24-C25-C26 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 34  | i     | 630 | LHG  | C23-C24-C25-C26 |
| 30  | f     | 601 | CHL  | O1D-CGD-O2D-CED |
| 34  | o     | 601 | LHG  | C28-C29-C30-C31 |
| 34  | i     | 630 | LHG  | C26-C27-C28-C29 |
| 34  | e     | 630 | LHG  | C12-C13-C14-C15 |
| 31  | 1     | 303 | CLA  | O1A-CGA-O2A-C1  |
| 36  | J     | 105 | LMG  | O10-C28-O8-C9   |
| 36  | L     | 210 | LMG  | C4-C5-C6-O5     |
| 34  | 3     | 603 | LHG  | C9-C10-C11-C12  |
| 33  | a     | 520 | OUR  | C46-C45-O44-C43 |
| 34  | 3     | 603 | LHG  | C11-C10-C9-C8   |
| 34  | d     | 630 | LHG  | C23-C24-C25-C26 |
| 30  | e     | 602 | CHL  | O1A-CGA-O2A-C1  |
| 31  | 1     | 310 | CLA  | O1A-CGA-O2A-C1  |
| 31  | 0     | 311 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 0     | 312 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 0     | 321 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 1     | 308 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 3     | 310 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 5     | 311 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 6     | 312 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 7     | 317 | CLA  | C2B-C3B-CAB-CBB |
| 31  | A     | 806 | CLA  | C2B-C3B-CAB-CBB |
| 31  | A     | 824 | CLA  | C2B-C3B-CAB-CBB |
| 31  | B     | 824 | CLA  | C2B-C3B-CAB-CBB |
| 31  | B     | 833 | CLA  | C2B-C3B-CAB-CBB |
| 31  | G     | 103 | CLA  | C2B-C3B-CAB-CBB |
| 31  | O     | 201 | CLA  | C2B-C3B-CAB-CBB |
| 32  | 1     | 402 | 8CT  | C02-C03-C10-C11 |
| 32  | 2     | 402 | 8CT  | C02-C03-C10-C11 |
| 32  | 3     | 402 | 8CT  | C04-C03-C10-C11 |
| 32  | 7     | 402 | 8CT  | C04-C03-C10-C11 |
| 32  | 7     | 404 | 8CT  | C02-C03-C10-C11 |
| 32  | 8     | 406 | 8CT  | C04-C03-C10-C11 |
| 32  | A     | 848 | 8CT  | C04-C03-C10-C11 |
| 32  | A     | 854 | 8CT  | C02-C03-C10-C11 |
| 32  | B     | 845 | 8CT  | C02-C03-C10-C11 |
| 32  | B     | 847 | 8CT  | C02-C03-C10-C11 |
| 32  | B     | 847 | 8CT  | C04-C03-C10-C11 |
| 32  | I     | 101 | 8CT  | C02-C03-C10-C11 |
| 32  | J     | 101 | 8CT  | C04-C03-C10-C11 |
| 32  | L     | 206 | 8CT  | C02-C03-C10-C11 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 32  | L     | 206 | 8CT  | C04-C03-C10-C11 |
| 32  | L     | 209 | 8CT  | C04-C03-C10-C11 |
| 32  | K     | 107 | 8CT  | C04-C03-C10-C11 |
| 34  | 1     | 601 | LHG  | C28-C29-C30-C31 |
| 34  | B     | 854 | LHG  | C28-C29-C30-C31 |
| 34  | G     | 105 | LHG  | C13-C14-C15-C16 |
| 30  | f     | 602 | CHL  | CBD-CGD-O2D-CED |
| 30  | 4     | 313 | CHL  | CBD-CGD-O2D-CED |
| 31  | 6     | 303 | CLA  | CBD-CGD-O2D-CED |
| 31  | B     | 825 | CLA  | CBD-CGD-O2D-CED |
| 34  | b     | 630 | LHG  | C8-C7-O7-C5     |
| 31  | 5     | 312 | CLA  | CBA-CGA-O2A-C1  |
| 34  | 3     | 601 | LHG  | C5-C4-O6-P      |
| 30  | h     | 602 | CHL  | C3-C5-C6-C7     |
| 31  | B     | 819 | CLA  | C3-C5-C6-C7     |
| 34  | f     | 630 | LHG  | C9-C10-C11-C12  |
| 34  | 3     | 601 | LHG  | C13-C14-C15-C16 |
| 34  | K     | 106 | LHG  | C31-C32-C33-C34 |
| 30  | 8     | 305 | CHL  | C2A-CAA-CBA-CGA |
| 30  | c     | 602 | CHL  | C2A-CAA-CBA-CGA |
| 30  | g     | 602 | CHL  | C2A-CAA-CBA-CGA |
| 31  | L     | 202 | CLA  | C2A-CAA-CBA-CGA |
| 30  | a     | 602 | CHL  | C10-C11-C12-C13 |
| 34  | f     | 630 | LHG  | C26-C27-C28-C29 |
| 36  | 9     | 602 | LMG  | C12-C13-C14-C15 |
| 31  | 7     | 311 | CLA  | O1A-CGA-O2A-C1  |
| 31  | d     | 613 | CLA  | O1A-CGA-O2A-C1  |
| 34  | 2     | 601 | LHG  | O10-C23-O8-C6   |
| 41  | B     | 849 | DGD  | O1A-C1A-O1G-C1G |
| 34  | 8     | 601 | LHG  | C12-C13-C14-C15 |
| 36  | B     | 853 | LMG  | C14-C15-C16-C17 |
| 36  | J     | 105 | LMG  | C30-C31-C32-C33 |
| 30  | 5     | 302 | CHL  | C8-C10-C11-C12  |
| 31  | 9     | 302 | CLA  | C13-C15-C16-C17 |
| 31  | A     | 830 | CLA  | C2-C3-C5-C6     |
| 31  | B     | 817 | CLA  | C2-C3-C5-C6     |
| 34  | 5     | 601 | LHG  | C26-C27-C28-C29 |
| 34  | A     | 844 | LHG  | C9-C10-C11-C12  |
| 35  | 0     | 603 | SQD  | C11-C10-C9-C8   |
| 30  | d     | 605 | CHL  | O1D-CGD-O2D-CED |
| 30  | 2     | 302 | CHL  | CBA-CGA-O2A-C1  |
| 30  | 6     | 302 | CHL  | CBA-CGA-O2A-C1  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 30  | a     | 609 | CHL  | CBA-CGA-O2A-C1  |
| 30  | h     | 602 | CHL  | CBA-CGA-O2A-C1  |
| 30  | 4     | 302 | CHL  | CBA-CGA-O2A-C1  |
| 31  | 6     | 310 | CLA  | CBA-CGA-O2A-C1  |
| 31  | A     | 840 | CLA  | CBA-CGA-O2A-C1  |
| 33  | 2     | 502 | OUR  | O57-C45-C46-C47 |
| 34  | 0     | 601 | LHG  | C24-C23-O8-C6   |
| 30  | i     | 602 | CHL  | O1A-CGA-O2A-C1  |
| 30  | b     | 601 | CHL  | C11-C10-C8-C9   |
| 30  | h     | 602 | CHL  | C11-C10-C8-C9   |
| 30  | e     | 609 | CHL  | C6-C7-C8-C9     |
| 31  | 7     | 318 | CLA  | C6-C7-C8-C9     |
| 31  | A     | 828 | CLA  | C6-C7-C8-C9     |
| 31  | A     | 840 | CLA  | C11-C10-C8-C9   |
| 34  | K     | 106 | LHG  | C15-C16-C17-C18 |
| 34  | e     | 630 | LHG  | C14-C15-C16-C17 |
| 31  | B     | 820 | CLA  | C5-C6-C7-C8     |
| 31  | i     | 603 | CLA  | O1A-CGA-O2A-C1  |
| 36  | L     | 211 | LMG  | C13-C14-C15-C16 |
| 36  | J     | 105 | LMG  | O6-C1-O1-C7     |
| 34  | 3     | 601 | LHG  | C14-C15-C16-C17 |
| 30  | d     | 609 | CHL  | C13-C15-C16-C17 |
| 31  | f     | 613 | CLA  | C6-C7-C8-C10    |
| 34  | a     | 630 | LHG  | C15-C16-C17-C18 |
| 34  | d     | 630 | LHG  | C25-C26-C27-C28 |
| 31  | K     | 102 | CLA  | C2C-C3C-CAC-CBC |
| 34  | 1     | 601 | LHG  | C14-C15-C16-C17 |
| 30  | d     | 607 | CHL  | CBA-CGA-O2A-C1  |
| 31  | K     | 105 | CLA  | CBA-CGA-O2A-C1  |
| 32  | A     | 846 | 8CT  | C18-C19-C20-C21 |
| 32  | A     | 848 | 8CT  | C18-C19-C20-C21 |
| 32  | A     | 854 | 8CT  | C18-C19-C20-C21 |
| 32  | L     | 205 | 8CT  | C16-C17-C18-C19 |
| 32  | K     | 107 | 8CT  | C16-C17-C18-C19 |
| 30  | b     | 602 | CHL  | C15-C16-C17-C18 |
| 36  | A     | 856 | LMG  | O6-C5-C6-O5     |
| 34  | K     | 106 | LHG  | C14-C15-C16-C17 |
| 34  | K     | 106 | LHG  | C8-C7-O7-C5     |
| 34  | f     | 630 | LHG  | C8-C7-O7-C5     |
| 34  | h     | 630 | LHG  | C8-C7-O7-C5     |
| 36  | L     | 210 | LMG  | C11-C10-O7-C8   |
| 34  | a     | 630 | LHG  | C23-C24-C25-C26 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 34  | 3     | 601 | LHG  | C15-C16-C17-C18 |
| 34  | b     | 630 | LHG  | C30-C31-C32-C33 |
| 34  | H     | 203 | LHG  | C26-C27-C28-C29 |
| 34  | G     | 105 | LHG  | O9-C7-O7-C5     |
| 34  | h     | 630 | LHG  | O9-C7-O7-C5     |
| 34  | M     | 104 | LHG  | C25-C26-C27-C28 |
| 31  | c     | 613 | CLA  | C11-C10-C8-C7   |
| 31  | A     | 828 | CLA  | C5-C6-C7-C8     |
| 31  | B     | 837 | CLA  | C5-C6-C7-C8     |
| 32  | F     | 302 | 8CT  | C10-C11-C12-C40 |
| 32  | J     | 104 | 8CT  | C14-C15-C16-C39 |
| 32  | L     | 205 | 8CT  | C10-C11-C12-C40 |
| 33  | b     | 520 | 0UR  | C5-C6-C7-C20    |
| 34  | 1     | 601 | LHG  | C10-C11-C12-C13 |
| 30  | 2     | 319 | CHL  | C3-C5-C6-C7     |
| 32  | J     | 104 | 8CT  | C14-C15-C16-C17 |
| 32  | L     | 205 | 8CT  | C10-C11-C12-C13 |
| 36  | 3     | 602 | LMG  | C8-C7-O1-C1     |
| 30  | 2     | 307 | CHL  | C2A-CAA-CBA-CGA |
| 30  | 7     | 305 | CHL  | C2A-CAA-CBA-CGA |
| 30  | 8     | 302 | CHL  | C2A-CAA-CBA-CGA |
| 30  | 8     | 306 | CHL  | C2A-CAA-CBA-CGA |
| 30  | h     | 608 | CHL  | C2A-CAA-CBA-CGA |
| 31  | h     | 604 | CLA  | C2A-CAA-CBA-CGA |
| 30  | 3     | 302 | CHL  | C14-C13-C15-C16 |
| 30  | 8     | 313 | CHL  | C6-C7-C8-C9     |
| 30  | c     | 608 | CHL  | C16-C17-C18-C20 |
| 31  | 0     | 309 | CLA  | C11-C12-C13-C15 |
| 31  | A     | 828 | CLA  | C16-C17-C18-C19 |
| 31  | B     | 827 | CLA  | C16-C17-C18-C19 |
| 30  | i     | 605 | CHL  | CBD-CGD-O2D-CED |
| 31  | A     | 817 | CLA  | CBD-CGD-O2D-CED |
| 31  | 3     | 313 | CLA  | O1D-CGD-O2D-CED |
| 30  | f     | 602 | CHL  | C15-C16-C17-C18 |
| 36  | 9     | 602 | LMG  | C13-C14-C15-C16 |
| 30  | f     | 601 | CHL  | C15-C16-C17-C18 |
| 31  | 3     | 304 | CLA  | C15-C16-C17-C18 |
| 31  | f     | 603 | CLA  | C5-C6-C7-C8     |
| 33  | 4     | 502 | 0UR  | O44-C45-C46-C47 |
| 30  | g     | 601 | CHL  | O1D-CGD-O2D-CED |
| 30  | 3     | 307 | CHL  | O1A-CGA-O2A-C1  |
| 31  | 1     | 304 | CLA  | O1A-CGA-O2A-C1  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | 4     | 311 | CLA  | O1A-CGA-O2A-C1  |
| 31  | A     | 835 | CLA  | C3-C5-C6-C7     |
| 30  | d     | 602 | CHL  | C13-C15-C16-C17 |
| 30  | f     | 609 | CHL  | C13-C15-C16-C17 |
| 31  | B     | 801 | CLA  | C10-C11-C12-C13 |
| 34  | 7     | 603 | LHG  | C12-C13-C14-C15 |
| 33  | 3     | 501 | OUR  | O57-C45-C46-C47 |
| 34  | 5     | 601 | LHG  | C23-C24-C25-C26 |
| 34  | G     | 105 | LHG  | C23-C24-C25-C26 |
| 34  | f     | 630 | LHG  | C23-C24-C25-C26 |
| 31  | b     | 613 | CLA  | C6-C7-C8-C10    |
| 30  | 0     | 302 | CHL  | C13-C15-C16-C17 |
| 30  | 7     | 302 | CHL  | C8-C10-C11-C12  |
| 30  | 7     | 306 | CHL  | C8-C10-C11-C12  |
| 30  | i     | 602 | CHL  | C10-C11-C12-C13 |
| 31  | B     | 817 | CLA  | C11-C12-C13-C14 |
| 31  | f     | 613 | CLA  | C5-C6-C7-C8     |
| 34  | b     | 630 | LHG  | C26-C27-C28-C29 |
| 36  | J     | 105 | LMG  | C34-C35-C36-C37 |
| 34  | f     | 630 | LHG  | C12-C13-C14-C15 |
| 36  | B     | 853 | LMG  | C31-C32-C33-C34 |
| 30  | b     | 614 | CHL  | O1D-CGD-O2D-CED |
| 31  | 3     | 310 | CLA  | C3-C5-C6-C7     |
| 31  | A     | 823 | CLA  | CBD-CGD-O2D-CED |
| 31  | B     | 823 | CLA  | CBD-CGD-O2D-CED |
| 34  | 7     | 601 | LHG  | O7-C5-C6-O8     |
| 34  | 1     | 601 | LHG  | C26-C27-C28-C29 |
| 34  | 4     | 601 | LHG  | C9-C10-C11-C12  |
| 31  | B     | 817 | CLA  | O1D-CGD-O2D-CED |
| 30  | 1     | 302 | CHL  | CBA-CGA-O2A-C1  |
| 30  | g     | 606 | CHL  | CBA-CGA-O2A-C1  |
| 31  | B     | 818 | CLA  | CBA-CGA-O2A-C1  |
| 31  | 1     | 312 | CLA  | C8-C10-C11-C12  |
| 31  | 9     | 309 | CLA  | C5-C6-C7-C8     |
| 31  | B     | 811 | CLA  | C8-C10-C11-C12  |
| 36  | B     | 853 | LMG  | C10-C11-C12-C13 |
| 30  | h     | 605 | CHL  | O1D-CGD-O2D-CED |
| 30  | 4     | 308 | CHL  | CBA-CGA-O2A-C1  |
| 31  | L     | 202 | CLA  | O1A-CGA-O2A-C1  |
| 30  | e     | 602 | CHL  | C11-C12-C13-C15 |
| 31  | K     | 101 | CLA  | C11-C12-C13-C14 |
| 34  | 7     | 603 | LHG  | C5-C4-O6-P      |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | c     | 613 | CLA  | C6-C7-C8-C10    |
| 34  | 9     | 601 | LHG  | C11-C10-C9-C8   |
| 34  | e     | 630 | LHG  | C15-C16-C17-C18 |
| 36  | 9     | 602 | LMG  | C38-C39-C40-C41 |
| 30  | 5     | 305 | CHL  | O1D-CGD-O2D-CED |
| 30  | a     | 609 | CHL  | O1D-CGD-O2D-CED |
| 34  | A     | 844 | LHG  | C25-C26-C27-C28 |
| 34  | g     | 630 | LHG  | C25-C26-C27-C28 |
| 30  | 7     | 306 | CHL  | C4-C3-C5-C6     |
| 34  | f     | 630 | LHG  | O9-C7-O7-C5     |
| 30  | 3     | 305 | CHL  | C2A-CAA-CBA-CGA |
| 30  | 5     | 302 | CHL  | C2A-CAA-CBA-CGA |
| 30  | 5     | 305 | CHL  | C2A-CAA-CBA-CGA |
| 30  | b     | 601 | CHL  | C2A-CAA-CBA-CGA |
| 30  | 4     | 302 | CHL  | C2A-CAA-CBA-CGA |
| 31  | 0     | 308 | CLA  | C2A-CAA-CBA-CGA |
| 31  | 7     | 308 | CLA  | C2A-CAA-CBA-CGA |
| 31  | A     | 820 | CLA  | C2A-CAA-CBA-CGA |
| 31  | A     | 841 | CLA  | C2A-CAA-CBA-CGA |
| 31  | B     | 831 | CLA  | C2A-CAA-CBA-CGA |
| 31  | K     | 104 | CLA  | C2A-CAA-CBA-CGA |
| 30  | 8     | 305 | CHL  | CBD-CGD-O2D-CED |
| 30  | a     | 602 | CHL  | CBD-CGD-O2D-CED |
| 30  | e     | 601 | CHL  | CBD-CGD-O2D-CED |
| 31  | B     | 814 | CLA  | CBD-CGD-O2D-CED |
| 30  | 7     | 306 | CHL  | O1D-CGD-O2D-CED |
| 31  | 0     | 311 | CLA  | CBA-CGA-O2A-C1  |
| 31  | A     | 814 | CLA  | CBA-CGA-O2A-C1  |
| 33  | 4     | 502 | OUR  | O57-C45-C46-C47 |
| 34  | 7     | 603 | LHG  | C28-C29-C30-C31 |
| 31  | L     | 204 | CLA  | O1D-CGD-O2D-CED |
| 30  | 1     | 307 | CHL  | C13-C15-C16-C17 |
| 30  | 7     | 301 | CHL  | C10-C11-C12-C13 |
| 31  | 3     | 309 | CLA  | C5-C6-C7-C8     |
| 31  | 3     | 310 | CLA  | O1D-CGD-O2D-CED |
| 36  | 9     | 602 | LMG  | C17-C18-C19-C20 |
| 30  | 0     | 302 | CHL  | O1D-CGD-O2D-CED |
| 30  | 6     | 315 | CHL  | O1D-CGD-O2D-CED |
| 30  | h     | 602 | CHL  | O1D-CGD-O2D-CED |
| 30  | 4     | 302 | CHL  | O1A-CGA-O2A-C1  |
| 31  | 5     | 312 | CLA  | O1A-CGA-O2A-C1  |
| 31  | 6     | 310 | CLA  | O1A-CGA-O2A-C1  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 34  | 0     | 601 | LHG  | O10-C23-O8-C6   |
| 31  | A     | 817 | CLA  | C3-C5-C6-C7     |
| 31  | 4     | 310 | CLA  | C3-C5-C6-C7     |
| 31  | B     | 810 | CLA  | C2C-C3C-CAC-CBC |
| 34  | f     | 630 | LHG  | C14-C15-C16-C17 |
| 31  | 0     | 303 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 0     | 311 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 0     | 313 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 1     | 309 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 5     | 309 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 7     | 317 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 7     | 318 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 8     | 314 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 9     | 308 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 9     | 311 | CLA  | C1A-C2A-CAA-CBA |
| 31  | A     | 803 | CLA  | C1A-C2A-CAA-CBA |
| 31  | A     | 806 | CLA  | C1A-C2A-CAA-CBA |
| 31  | A     | 808 | CLA  | C1A-C2A-CAA-CBA |
| 31  | A     | 818 | CLA  | C1A-C2A-CAA-CBA |
| 31  | A     | 832 | CLA  | C1A-C2A-CAA-CBA |
| 31  | A     | 836 | CLA  | C1A-C2A-CAA-CBA |
| 31  | A     | 843 | CLA  | C1A-C2A-CAA-CBA |
| 31  | B     | 828 | CLA  | C1A-C2A-CAA-CBA |
| 31  | K     | 101 | CLA  | C1A-C2A-CAA-CBA |
| 31  | a     | 610 | CLA  | C1A-C2A-CAA-CBA |
| 31  | b     | 610 | CLA  | C1A-C2A-CAA-CBA |
| 31  | d     | 610 | CLA  | C1A-C2A-CAA-CBA |
| 31  | h     | 610 | CLA  | C1A-C2A-CAA-CBA |
| 31  | H     | 202 | CLA  | C1A-C2A-CAA-CBA |
| 31  | e     | 610 | CLA  | C1A-C2A-CAA-CBA |
| 33  | 5     | 501 | 0UR  | O57-C45-C46-C47 |
| 33  | h     | 520 | 0UR  | O57-C45-C46-C47 |
| 31  | 7     | 309 | CLA  | C5-C6-C7-C8     |
| 31  | B     | 840 | CLA  | C15-C16-C17-C18 |
| 36  | J     | 105 | LMG  | C14-C15-C16-C17 |
| 34  | K     | 106 | LHG  | C27-C28-C29-C30 |
| 36  | O     | 207 | LMG  | C33-C34-C35-C36 |
| 30  | 2     | 302 | CHL  | O1A-CGA-O2A-C1  |
| 30  | 6     | 302 | CHL  | O1A-CGA-O2A-C1  |
| 30  | h     | 602 | CHL  | O1A-CGA-O2A-C1  |
| 31  | A     | 840 | CLA  | O1A-CGA-O2A-C1  |
| 30  | 1     | 313 | CHL  | C10-C11-C12-C13 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 30  | c     | 602 | CHL  | C5-C6-C7-C8     |
| 31  | B     | 816 | CLA  | C10-C11-C12-C13 |
| 38  | B     | 842 | PQN  | C20-C21-C22-C23 |
| 34  | B     | 852 | LHG  | O6-C4-C5-C6     |
| 34  | d     | 630 | LHG  | O6-C4-C5-C6     |
| 34  | b     | 630 | LHG  | O9-C7-O7-C5     |
| 34  | a     | 630 | LHG  | C25-C26-C27-C28 |
| 34  | e     | 630 | LHG  | C23-C24-C25-C26 |
| 30  | 6     | 301 | CHL  | C3-C5-C6-C7     |
| 30  | 1     | 307 | CHL  | C6-C7-C8-C10    |
| 30  | 2     | 301 | CHL  | C6-C7-C8-C10    |
| 30  | 2     | 302 | CHL  | C6-C7-C8-C10    |
| 30  | 3     | 307 | CHL  | C6-C7-C8-C10    |
| 30  | 3     | 307 | CHL  | C12-C13-C15-C16 |
| 30  | 5     | 302 | CHL  | C11-C10-C8-C7   |
| 30  | 5     | 302 | CHL  | C11-C12-C13-C15 |
| 30  | 5     | 302 | CHL  | C12-C13-C15-C16 |
| 30  | 7     | 301 | CHL  | C12-C13-C15-C16 |
| 30  | b     | 601 | CHL  | C12-C13-C15-C16 |
| 30  | d     | 602 | CHL  | C6-C7-C8-C10    |
| 30  | d     | 609 | CHL  | C12-C13-C15-C16 |
| 31  | 1     | 312 | CLA  | C6-C7-C8-C10    |
| 31  | 2     | 304 | CLA  | C11-C10-C8-C7   |
| 31  | 3     | 309 | CLA  | C11-C12-C13-C15 |
| 31  | 3     | 310 | CLA  | C6-C7-C8-C10    |
| 31  | 6     | 317 | CLA  | C11-C10-C8-C7   |
| 31  | 8     | 304 | CLA  | C11-C10-C8-C7   |
| 31  | 9     | 300 | CLA  | C6-C7-C8-C10    |
| 31  | 9     | 309 | CLA  | C11-C10-C8-C7   |
| 31  | A     | 803 | CLA  | C12-C13-C15-C16 |
| 31  | A     | 808 | CLA  | C11-C10-C8-C7   |
| 31  | A     | 813 | CLA  | C6-C7-C8-C10    |
| 31  | A     | 817 | CLA  | C11-C10-C8-C7   |
| 31  | A     | 819 | CLA  | C6-C7-C8-C10    |
| 31  | A     | 819 | CLA  | C11-C10-C8-C7   |
| 31  | A     | 819 | CLA  | C11-C12-C13-C15 |
| 31  | A     | 819 | CLA  | C12-C13-C15-C16 |
| 31  | A     | 825 | CLA  | C11-C10-C8-C7   |
| 31  | A     | 828 | CLA  | C11-C12-C13-C15 |
| 31  | A     | 839 | CLA  | C11-C12-C13-C15 |
| 31  | B     | 801 | CLA  | C11-C10-C8-C7   |
| 31  | B     | 817 | CLA  | C11-C10-C8-C7   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | B     | 834 | CLA  | C6-C7-C8-C10    |
| 31  | B     | 834 | CLA  | C11-C10-C8-C7   |
| 35  | 0     | 603 | SQD  | C9-C10-C11-C12  |
| 30  | f     | 601 | CHL  | C8-C10-C11-C12  |
| 31  | B     | 837 | CLA  | C15-C16-C17-C18 |
| 30  | a     | 609 | CHL  | O1A-CGA-O2A-C1  |
| 31  | K     | 105 | CLA  | O1A-CGA-O2A-C1  |
| 30  | a     | 601 | CHL  | O1D-CGD-O2D-CED |
| 33  | e     | 520 | 0UR  | O57-C45-C46-C47 |
| 33  | e     | 520 | 0UR  | O44-C45-C46-C47 |
| 30  | c     | 609 | CHL  | C5-C6-C7-C8     |
| 31  | 1     | 310 | CLA  | C10-C11-C12-C13 |
| 34  | 4     | 601 | LHG  | C23-C24-C25-C26 |
| 30  | 7     | 306 | CHL  | C2-C3-C5-C6     |
| 30  | 3     | 302 | CHL  | C2A-CAA-CBA-CGA |
| 30  | 6     | 302 | CHL  | C2A-CAA-CBA-CGA |
| 31  | 1     | 304 | CLA  | C2A-CAA-CBA-CGA |
| 31  | 1     | 312 | CLA  | C2A-CAA-CBA-CGA |
| 31  | 7     | 317 | CLA  | C2A-CAA-CBA-CGA |
| 30  | 1     | 307 | CHL  | C6-C7-C8-C9     |
| 30  | 1     | 313 | CHL  | C11-C10-C8-C9   |
| 30  | 2     | 301 | CHL  | C6-C7-C8-C9     |
| 30  | 3     | 307 | CHL  | C6-C7-C8-C9     |
| 30  | 3     | 307 | CHL  | C14-C13-C15-C16 |
| 30  | c     | 608 | CHL  | C6-C7-C8-C9     |
| 30  | b     | 608 | CHL  | C6-C7-C8-C9     |
| 30  | b     | 608 | CHL  | C14-C13-C15-C16 |
| 30  | d     | 602 | CHL  | C6-C7-C8-C9     |
| 31  | 3     | 308 | CLA  | C6-C7-C8-C9     |
| 31  | 3     | 309 | CLA  | C11-C12-C13-C14 |
| 31  | 3     | 310 | CLA  | C11-C12-C13-C14 |
| 31  | 8     | 304 | CLA  | C11-C10-C8-C9   |
| 31  | 9     | 300 | CLA  | C6-C7-C8-C9     |
| 31  | 9     | 309 | CLA  | C11-C10-C8-C9   |
| 31  | A     | 808 | CLA  | C11-C10-C8-C9   |
| 31  | A     | 819 | CLA  | C6-C7-C8-C9     |
| 31  | A     | 819 | CLA  | C11-C10-C8-C9   |
| 31  | A     | 819 | CLA  | C14-C13-C15-C16 |
| 31  | A     | 828 | CLA  | C11-C12-C13-C14 |
| 31  | A     | 829 | CLA  | C11-C12-C13-C14 |
| 31  | A     | 832 | CLA  | C6-C7-C8-C9     |
| 31  | B     | 809 | CLA  | C11-C12-C13-C14 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | B     | 817 | CLA  | C11-C10-C8-C9   |
| 31  | B     | 819 | CLA  | C11-C10-C8-C9   |
| 31  | B     | 839 | CLA  | C11-C12-C13-C14 |
| 31  | B     | 839 | CLA  | C14-C13-C15-C16 |
| 31  | 4     | 310 | CLA  | C11-C10-C8-C9   |
| 34  | c     | 630 | LHG  | C9-C10-C11-C12  |
| 34  | c     | 630 | LHG  | C29-C30-C31-C32 |
| 33  | a     | 520 | OUR  | O57-C45-O44-C43 |
| 41  | B     | 849 | DGD  | CBB-CCB-CDB-CEB |
| 31  | 3     | 308 | CLA  | CBA-CGA-O2A-C1  |
| 31  | A     | 815 | CLA  | CBA-CGA-O2A-C1  |
| 31  | A     | 843 | CLA  | CBA-CGA-O2A-C1  |
| 31  | f     | 611 | CLA  | O1D-CGD-O2D-CED |
| 34  | 7     | 602 | LHG  | C10-C11-C12-C13 |
| 34  | B     | 854 | LHG  | C27-C28-C29-C30 |
| 34  | 1     | 601 | LHG  | C4-C5-C6-O8     |
| 34  | 2     | 601 | LHG  | C4-C5-C6-O8     |
| 34  | 7     | 603 | LHG  | C4-C5-C6-O8     |
| 34  | G     | 105 | LHG  | C4-C5-C6-O8     |
| 35  | 0     | 603 | SQD  | O6-C44-C45-C46  |
| 35  | 0     | 603 | SQD  | C44-C45-C46-O48 |
| 36  | A     | 856 | LMG  | C7-C8-C9-O8     |
| 30  | 5     | 301 | CHL  | O1D-CGD-O2D-CED |
| 30  | 2     | 302 | CHL  | CBD-CGD-O2D-CED |
| 30  | c     | 602 | CHL  | CBA-CGA-O2A-C1  |
| 31  | B     | 830 | CLA  | CBA-CGA-O2A-C1  |
| 30  | 1     | 307 | CHL  | C16-C17-C18-C19 |
| 30  | i     | 602 | CHL  | C11-C12-C13-C15 |
| 30  | e     | 609 | CHL  | C11-C12-C13-C15 |
| 31  | A     | 830 | CLA  | C16-C17-C18-C19 |
| 31  | A     | 830 | CLA  | C16-C17-C18-C20 |
| 31  | K     | 101 | CLA  | C11-C12-C13-C15 |
| 34  | 9     | 601 | LHG  | C31-C32-C33-C34 |
| 34  | H     | 203 | LHG  | C25-C26-C27-C28 |
| 36  | A     | 856 | LMG  | C30-C31-C32-C33 |
| 36  | B     | 853 | LMG  | C15-C16-C17-C18 |
| 36  | B     | 853 | LMG  | C17-C18-C19-C20 |
| 30  | 0     | 306 | CHL  | CHA-CBD-CGD-O1D |
| 30  | 0     | 306 | CHL  | CHA-CBD-CGD-O2D |
| 30  | 1     | 302 | CHL  | CHA-CBD-CGD-O1D |
| 30  | 1     | 302 | CHL  | CHA-CBD-CGD-O2D |
| 30  | 1     | 306 | CHL  | CHA-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 30  | 1     | 306 | CHL  | CHA-CBD-CGD-O2D |
| 30  | 1     | 313 | CHL  | CHA-CBD-CGD-O1D |
| 30  | 1     | 313 | CHL  | CHA-CBD-CGD-O2D |
| 30  | 2     | 302 | CHL  | CHA-CBD-CGD-O1D |
| 30  | 2     | 302 | CHL  | CHA-CBD-CGD-O2D |
| 30  | 3     | 302 | CHL  | CHA-CBD-CGD-O1D |
| 30  | 3     | 302 | CHL  | CHA-CBD-CGD-O2D |
| 30  | 3     | 307 | CHL  | CHA-CBD-CGD-O1D |
| 30  | 3     | 307 | CHL  | CHA-CBD-CGD-O2D |
| 30  | 5     | 305 | CHL  | CHA-CBD-CGD-O2D |
| 30  | 5     | 306 | CHL  | CHA-CBD-CGD-O1D |
| 30  | 5     | 306 | CHL  | CHA-CBD-CGD-O2D |
| 30  | 6     | 306 | CHL  | CHA-CBD-CGD-O1D |
| 30  | 6     | 306 | CHL  | CHA-CBD-CGD-O2D |
| 30  | 6     | 315 | CHL  | CHA-CBD-CGD-O1D |
| 30  | 6     | 315 | CHL  | CHA-CBD-CGD-O2D |
| 30  | 7     | 302 | CHL  | CHA-CBD-CGD-O1D |
| 30  | 7     | 302 | CHL  | CHA-CBD-CGD-O2D |
| 30  | 8     | 302 | CHL  | CHA-CBD-CGD-O1D |
| 30  | 8     | 302 | CHL  | CHA-CBD-CGD-O2D |
| 30  | 8     | 315 | CHL  | CHA-CBD-CGD-O1D |
| 30  | 8     | 315 | CHL  | CHA-CBD-CGD-O2D |
| 30  | 9     | 301 | CHL  | CHA-CBD-CGD-O1D |
| 30  | 9     | 301 | CHL  | CHA-CBD-CGD-O2D |
| 30  | 9     | 306 | CHL  | CHA-CBD-CGD-O1D |
| 30  | a     | 602 | CHL  | CHA-CBD-CGD-O1D |
| 30  | a     | 602 | CHL  | CHA-CBD-CGD-O2D |
| 30  | a     | 605 | CHL  | CHA-CBD-CGD-O1D |
| 30  | c     | 602 | CHL  | CHA-CBD-CGD-O1D |
| 30  | c     | 602 | CHL  | CHA-CBD-CGD-O2D |
| 30  | c     | 608 | CHL  | CHA-CBD-CGD-O2D |
| 30  | b     | 602 | CHL  | CHA-CBD-CGD-O1D |
| 30  | d     | 602 | CHL  | CHA-CBD-CGD-O1D |
| 30  | d     | 602 | CHL  | CHA-CBD-CGD-O2D |
| 30  | f     | 601 | CHL  | CHA-CBD-CGD-O1D |
| 30  | f     | 601 | CHL  | CHA-CBD-CGD-O2D |
| 30  | f     | 602 | CHL  | CHA-CBD-CGD-O1D |
| 30  | f     | 602 | CHL  | CHA-CBD-CGD-O2D |
| 30  | g     | 602 | CHL  | CHA-CBD-CGD-O1D |
| 30  | g     | 602 | CHL  | CHA-CBD-CGD-O2D |
| 30  | h     | 602 | CHL  | CHA-CBD-CGD-O1D |
| 30  | h     | 602 | CHL  | CHA-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 30  | h     | 605 | CHL  | CHA-CBD-CGD-O1D |
| 30  | h     | 605 | CHL  | CHA-CBD-CGD-O2D |
| 30  | h     | 606 | CHL  | CHA-CBD-CGD-O1D |
| 30  | h     | 607 | CHL  | CHA-CBD-CGD-O1D |
| 30  | h     | 607 | CHL  | CHA-CBD-CGD-O2D |
| 30  | i     | 602 | CHL  | CHA-CBD-CGD-O1D |
| 30  | i     | 602 | CHL  | CHA-CBD-CGD-O2D |
| 30  | e     | 601 | CHL  | CHA-CBD-CGD-O2D |
| 30  | e     | 602 | CHL  | CHA-CBD-CGD-O1D |
| 30  | e     | 602 | CHL  | CHA-CBD-CGD-O2D |
| 30  | 4     | 307 | CHL  | CHA-CBD-CGD-O2D |
| 36  | L     | 211 | LMG  | O6-C5-C6-O5     |
| 30  | 1     | 302 | CHL  | O1A-CGA-O2A-C1  |
| 30  | 3     | 307 | CHL  | C2-C3-C5-C6     |
| 31  | 9     | 300 | CLA  | C2-C3-C5-C6     |
| 32  | A     | 854 | 8CT  | C10-C11-C12-C40 |
| 33  | 4     | 502 | 0UR  | C22-C16-C17-C18 |
| 34  | H     | 203 | LHG  | C2-C3-O3-P      |
| 42  | c     | 523 | NEX  | C31-C32-C33-C40 |
| 42  | b     | 523 | NEX  | C31-C32-C33-C40 |
| 42  | h     | 523 | NEX  | C31-C32-C33-C40 |
| 36  | J     | 105 | LMG  | C4-C5-C6-O5     |
| 31  | f     | 603 | CLA  | O1D-CGD-O2D-CED |
| 32  | 0     | 401 | 8CT  | C25-C26-C28-C29 |
| 32  | 7     | 405 | 8CT  | C14-C15-C16-C17 |
| 32  | 8     | 406 | 8CT  | C25-C26-C28-C29 |
| 32  | B     | 848 | 8CT  | C10-C11-C12-C13 |
| 33  | 4     | 502 | 0UR  | C15-C16-C17-C18 |
| 30  | g     | 606 | CHL  | O1A-CGA-O2A-C1  |
| 31  | 3     | 304 | CLA  | C13-C15-C16-C17 |
| 31  | 7     | 308 | CLA  | C8-C10-C11-C12  |
| 31  | A     | 804 | CLA  | C5-C6-C7-C8     |
| 31  | B     | 801 | CLA  | C15-C16-C17-C18 |
| 31  | 4     | 304 | CLA  | C8-C10-C11-C12  |
| 34  | 7     | 603 | LHG  | C26-C27-C28-C29 |
| 30  | c     | 607 | CHL  | C2A-CAA-CBA-CGA |
| 31  | A     | 809 | CLA  | C2A-CAA-CBA-CGA |
| 30  | 5     | 313 | CHL  | CBA-CGA-O2A-C1  |
| 34  | M     | 104 | LHG  | C26-C27-C28-C29 |
| 36  | 2     | 602 | LMG  | C30-C31-C32-C33 |
| 30  | 8     | 315 | CHL  | O1D-CGD-O2D-CED |
| 31  | 2     | 303 | CLA  | CBA-CGA-O2A-C1  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | b     | 604 | CLA  | CBA-CGA-O2A-C1  |
| 31  | i     | 613 | CLA  | CBA-CGA-O2A-C1  |
| 31  | 2     | 311 | CLA  | O2A-C1-C2-C3    |
| 31  | A     | 805 | CLA  | O2A-C1-C2-C3    |
| 34  | B     | 852 | LHG  | C6-C5-O7-C7     |
| 36  | 3     | 602 | LMG  | C7-C8-O7-C10    |
| 34  | G     | 105 | LHG  | C25-C26-C27-C28 |
| 36  | 2     | 602 | LMG  | C32-C33-C34-C35 |
| 34  | 8     | 601 | LHG  | C10-C11-C12-C13 |
| 34  | M     | 104 | LHG  | C30-C31-C32-C33 |
| 34  | f     | 630 | LHG  | C27-C28-C29-C30 |
| 30  | 1     | 306 | CHL  | C3C-C2C-CMC-OMC |
| 30  | 2     | 313 | CHL  | C3C-C2C-CMC-OMC |
| 30  | 7     | 305 | CHL  | C3C-C2C-CMC-OMC |
| 30  | 7     | 306 | CHL  | C3C-C2C-CMC-OMC |
| 30  | 7     | 313 | CHL  | C3C-C2C-CMC-OMC |
| 30  | 8     | 307 | CHL  | C3C-C2C-CMC-OMC |
| 30  | 8     | 308 | CHL  | C3C-C2C-CMC-OMC |
| 30  | 9     | 306 | CHL  | C3C-C2C-CMC-OMC |
| 30  | 9     | 313 | CHL  | C3C-C2C-CMC-OMC |
| 30  | a     | 602 | CHL  | C3C-C2C-CMC-OMC |
| 30  | a     | 606 | CHL  | C3C-C2C-CMC-OMC |
| 30  | c     | 607 | CHL  | C3C-C2C-CMC-OMC |
| 30  | b     | 601 | CHL  | C3C-C2C-CMC-OMC |
| 30  | b     | 602 | CHL  | C3C-C2C-CMC-OMC |
| 30  | b     | 606 | CHL  | C3C-C2C-CMC-OMC |
| 30  | b     | 608 | CHL  | C3C-C2C-CMC-OMC |
| 30  | b     | 609 | CHL  | C3C-C2C-CMC-OMC |
| 30  | b     | 614 | CHL  | C3C-C2C-CMC-OMC |
| 30  | d     | 606 | CHL  | C3C-C2C-CMC-OMC |
| 30  | g     | 602 | CHL  | C3C-C2C-CMC-OMC |
| 30  | g     | 608 | CHL  | C3C-C2C-CMC-OMC |
| 30  | h     | 608 | CHL  | C3C-C2C-CMC-OMC |
| 30  | e     | 601 | CHL  | C3C-C2C-CMC-OMC |
| 32  | 8     | 402 | 8CT  | C16-C17-C18-C19 |
| 36  | A     | 856 | LMG  | C29-C30-C31-C32 |
| 31  | 5     | 308 | CLA  | CBA-CGA-O2A-C1  |
| 31  | B     | 818 | CLA  | O1A-CGA-O2A-C1  |
| 31  | B     | 833 | CLA  | C3-C5-C6-C7     |
| 31  | B     | 819 | CLA  | C10-C11-C12-C13 |
| 37  | d     | 522 | 0IE  | C14-C15-C16-C17 |
| 31  | B     | 839 | CLA  | C5-C6-C7-C8     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 34  | M     | 104 | LHG  | C9-C10-C11-C12  |
| 30  | 3     | 302 | CHL  | CBA-CGA-O2A-C1  |
| 31  | 6     | 320 | CLA  | CBA-CGA-O2A-C1  |
| 31  | K     | 101 | CLA  | CBA-CGA-O2A-C1  |
| 36  | A     | 856 | LMG  | C29-C28-O8-C9   |
| 31  | A     | 852 | CLA  | CBD-CGD-O2D-CED |
| 34  | A     | 855 | LHG  | C23-C24-C25-C26 |
| 34  | a     | 630 | LHG  | C11-C10-C9-C8   |
| 36  | 3     | 602 | LMG  | C32-C33-C34-C35 |
| 31  | L     | 201 | CLA  | C4-C3-C5-C6     |
| 30  | 1     | 307 | CHL  | C2-C3-C5-C6     |
| 30  | c     | 608 | CHL  | C2-C3-C5-C6     |
| 36  | B     | 853 | LMG  | C18-C19-C20-C21 |
| 34  | G     | 105 | LHG  | C9-C10-C11-C12  |
| 34  | 0     | 601 | LHG  | C14-C15-C16-C17 |
| 34  | K     | 106 | LHG  | C32-C33-C34-C35 |
| 34  | b     | 630 | LHG  | C14-C15-C16-C17 |
| 36  | 2     | 602 | LMG  | C12-C13-C14-C15 |
| 34  | A     | 855 | LHG  | O7-C5-C6-O8     |
| 36  | B     | 853 | LMG  | C32-C33-C34-C35 |
| 30  | 2     | 308 | CHL  | O1A-CGA-O2A-C1  |
| 34  | H     | 203 | LHG  | C28-C29-C30-C31 |
| 31  | 3     | 308 | CLA  | O1A-CGA-O2A-C1  |
| 31  | A     | 814 | CLA  | O1D-CGD-O2D-CED |
| 30  | 5     | 302 | CHL  | C15-C16-C17-C18 |
| 30  | 2     | 319 | CHL  | CAA-CBA-CGA-O2A |
| 30  | d     | 607 | CHL  | CAA-CBA-CGA-O2A |
| 31  | 6     | 318 | CLA  | CAA-CBA-CGA-O2A |
| 30  | 4     | 307 | CHL  | C2A-CAA-CBA-CGA |
| 31  | 7     | 303 | CLA  | C2A-CAA-CBA-CGA |
| 30  | 8     | 313 | CHL  | C3-C5-C6-C7     |
| 30  | 8     | 313 | CHL  | C5-C6-C7-C8     |
| 31  | 2     | 310 | CLA  | C8-C10-C11-C12  |
| 31  | 9     | 302 | CLA  | C8-C10-C11-C12  |
| 31  | 9     | 302 | CLA  | C10-C11-C12-C13 |
| 31  | B     | 805 | CLA  | C15-C16-C17-C18 |
| 34  | K     | 106 | LHG  | O9-C7-O7-C5     |
| 31  | 8     | 309 | CLA  | CBD-CGD-O2D-CED |
| 31  | A     | 843 | CLA  | O1A-CGA-O2A-C1  |
| 30  | 3     | 307 | CHL  | C15-C16-C17-C18 |
| 31  | A     | 839 | CLA  | C13-C15-C16-C17 |
| 31  | K     | 101 | CLA  | C10-C11-C12-C13 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 34  | e     | 630 | LHG  | C10-C11-C12-C13 |
| 34  | 7     | 603 | LHG  | C10-C11-C12-C13 |
| 30  | 1     | 306 | CHL  | C1C-C2C-CMC-OMC |
| 30  | 7     | 313 | CHL  | C1C-C2C-CMC-OMC |
| 30  | 8     | 307 | CHL  | C1C-C2C-CMC-OMC |
| 30  | 8     | 308 | CHL  | C1C-C2C-CMC-OMC |
| 30  | 9     | 313 | CHL  | C1C-C2C-CMC-OMC |
| 30  | a     | 602 | CHL  | C1C-C2C-CMC-OMC |
| 30  | b     | 608 | CHL  | C1C-C2C-CMC-OMC |
| 30  | d     | 606 | CHL  | C1C-C2C-CMC-OMC |
| 30  | h     | 608 | CHL  | C1C-C2C-CMC-OMC |
| 31  | A     | 835 | CLA  | CBD-CGD-O2D-CED |
| 31  | J     | 103 | CLA  | CBD-CGD-O2D-CED |
| 30  | 0     | 302 | CHL  | C15-C16-C17-C18 |
| 30  | d     | 602 | CHL  | C15-C16-C17-C18 |
| 41  | B     | 849 | DGD  | CAB-CBB-CCB-CDB |
| 31  | A     | 814 | CLA  | O1A-CGA-O2A-C1  |
| 31  | A     | 815 | CLA  | O1A-CGA-O2A-C1  |
| 30  | 7     | 313 | CHL  | O1D-CGD-O2D-CED |
| 30  | c     | 607 | CHL  | O1D-CGD-O2D-CED |
| 30  | 6     | 308 | CHL  | C8-C10-C11-C12  |
| 30  | i     | 606 | CHL  | O1D-CGD-O2D-CED |
| 30  | 2     | 319 | CHL  | C11-C12-C13-C14 |
| 30  | e     | 606 | CHL  | CBD-CGD-O2D-CED |
| 30  | 3     | 307 | CHL  | C4-C3-C5-C6     |
| 30  | b     | 608 | CHL  | C4-C3-C5-C6     |
| 31  | A     | 839 | CLA  | C4-C3-C5-C6     |
| 31  | 5     | 303 | CLA  | C10-C11-C12-C13 |
| 34  | 7     | 602 | LHG  | C11-C10-C9-C8   |
| 30  | f     | 606 | CHL  | CBA-CGA-O2A-C1  |
| 30  | e     | 609 | CHL  | CBA-CGA-O2A-C1  |
| 31  | A     | 824 | CLA  | CBA-CGA-O2A-C1  |
| 31  | A     | 830 | CLA  | CBA-CGA-O2A-C1  |
| 31  | B     | 829 | CLA  | CBA-CGA-O2A-C1  |
| 31  | B     | 836 | CLA  | CBA-CGA-O2A-C1  |
| 31  | e     | 613 | CLA  | CBA-CGA-O2A-C1  |
| 34  | K     | 106 | LHG  | C30-C31-C32-C33 |
| 36  | 9     | 602 | LMG  | C16-C17-C18-C19 |
| 31  | 8     | 314 | CLA  | O1D-CGD-O2D-CED |
| 35  | 0     | 603 | SQD  | C10-C11-C12-C13 |
| 36  | L     | 211 | LMG  | C17-C18-C19-C20 |
| 34  | 0     | 601 | LHG  | O1-C1-C2-O2     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 34  | i     | 630 | LHG  | O1-C1-C2-O2     |
| 30  | b     | 607 | CHL  | O1A-CGA-O2A-C1  |
| 30  | 1     | 307 | CHL  | C11-C12-C13-C14 |
| 30  | 5     | 302 | CHL  | C6-C7-C8-C9     |
| 30  | 5     | 302 | CHL  | C11-C10-C8-C9   |
| 30  | 5     | 302 | CHL  | C11-C12-C13-C14 |
| 30  | c     | 602 | CHL  | C11-C10-C8-C9   |
| 30  | c     | 609 | CHL  | C6-C7-C8-C9     |
| 30  | c     | 609 | CHL  | C14-C13-C15-C16 |
| 30  | d     | 602 | CHL  | C11-C12-C13-C14 |
| 30  | d     | 609 | CHL  | C11-C12-C13-C14 |
| 30  | d     | 609 | CHL  | C14-C13-C15-C16 |
| 31  | 0     | 312 | CLA  | C14-C13-C15-C16 |
| 31  | 1     | 312 | CLA  | C6-C7-C8-C9     |
| 31  | 2     | 304 | CLA  | C11-C10-C8-C9   |
| 31  | 2     | 310 | CLA  | C6-C7-C8-C9     |
| 31  | 9     | 302 | CLA  | C14-C13-C15-C16 |
| 31  | A     | 803 | CLA  | C14-C13-C15-C16 |
| 31  | A     | 805 | CLA  | C6-C7-C8-C9     |
| 31  | A     | 813 | CLA  | C6-C7-C8-C9     |
| 31  | A     | 815 | CLA  | C14-C13-C15-C16 |
| 31  | A     | 817 | CLA  | C11-C10-C8-C9   |
| 31  | A     | 818 | CLA  | C11-C12-C13-C14 |
| 31  | A     | 819 | CLA  | C11-C12-C13-C14 |
| 31  | A     | 825 | CLA  | C11-C10-C8-C9   |
| 31  | A     | 830 | CLA  | C14-C13-C15-C16 |
| 31  | A     | 833 | CLA  | C6-C7-C8-C9     |
| 31  | B     | 801 | CLA  | C11-C10-C8-C9   |
| 31  | B     | 803 | CLA  | C14-C13-C15-C16 |
| 31  | B     | 809 | CLA  | C14-C13-C15-C16 |
| 31  | B     | 832 | CLA  | C14-C13-C15-C16 |
| 31  | B     | 834 | CLA  | C11-C10-C8-C9   |
| 31  | 4     | 304 | CLA  | C11-C10-C8-C9   |
| 34  | 9     | 601 | LHG  | C27-C28-C29-C30 |
| 30  | 9     | 313 | CHL  | O1D-CGD-O2D-CED |
| 30  | c     | 602 | CHL  | O1D-CGD-O2D-CED |
| 30  | i     | 601 | CHL  | O1D-CGD-O2D-CED |
| 30  | h     | 602 | CHL  | C8-C10-C11-C12  |
| 31  | 6     | 309 | CLA  | C5-C6-C7-C8     |
| 31  | A     | 829 | CLA  | C10-C11-C12-C13 |
| 34  | G     | 105 | LHG  | C2-C3-O3-P      |
| 31  | 0     | 321 | CLA  | C4B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | 2     | 314 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 3     | 306 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 3     | 313 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 5     | 310 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 5     | 311 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 6     | 304 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 6     | 320 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 7     | 317 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 8     | 312 | CLA  | C4B-C3B-CAB-CBB |
| 31  | A     | 809 | CLA  | C4B-C3B-CAB-CBB |
| 31  | A     | 832 | CLA  | C4B-C3B-CAB-CBB |
| 31  | A     | 835 | CLA  | C4B-C3B-CAB-CBB |
| 31  | B     | 805 | CLA  | C4B-C3B-CAB-CBB |
| 31  | K     | 105 | CLA  | C4B-C3B-CAB-CBB |
| 31  | b     | 603 | CLA  | C4B-C3B-CAB-CBB |
| 31  | h     | 612 | CLA  | C4B-C3B-CAB-CBB |
| 31  | H     | 202 | CLA  | C4B-C3B-CAB-CBB |
| 31  | H     | 205 | CLA  | C4B-C3B-CAB-CBB |
| 31  | e     | 603 | CLA  | C4B-C3B-CAB-CBB |
| 34  | 0     | 601 | LHG  | C33-C34-C35-C36 |
| 34  | 7     | 601 | LHG  | C25-C26-C27-C28 |
| 30  | 3     | 307 | CHL  | C5-C6-C7-C8     |
| 31  | 3     | 308 | CLA  | C13-C15-C16-C17 |
| 31  | A     | 826 | CLA  | C13-C15-C16-C17 |
| 30  | a     | 607 | CHL  | CBA-CGA-O2A-C1  |
| 31  | 0     | 311 | CLA  | O1A-CGA-O2A-C1  |
| 30  | 1     | 302 | CHL  | C15-C16-C17-C18 |
| 30  | h     | 602 | CHL  | C15-C16-C17-C18 |
| 31  | 0     | 321 | CLA  | C2A-CAA-CBA-CGA |
| 31  | 5     | 304 | CLA  | C3-C5-C6-C7     |
| 31  | f     | 611 | CLA  | C2A-CAA-CBA-CGA |
| 36  | A     | 856 | LMG  | C32-C33-C34-C35 |
| 35  | 0     | 603 | SQD  | C2-C1-O6-C44    |
| 31  | 6     | 310 | CLA  | C5-C6-C7-C8     |
| 31  | B     | 841 | CLA  | C13-C15-C16-C17 |
| 34  | 1     | 601 | LHG  | C27-C28-C29-C30 |
| 36  | 9     | 602 | LMG  | C37-C38-C39-C40 |
| 31  | B     | 832 | CLA  | C3-C5-C6-C7     |
| 34  | b     | 630 | LHG  | C15-C16-C17-C18 |
| 36  | J     | 105 | LMG  | C42-C43-C44-C45 |
| 34  | f     | 630 | LHG  | O6-C4-C5-C6     |
| 34  | 8     | 601 | LHG  | C28-C29-C30-C31 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 30  | 5     | 306 | CHL  | CAA-CBA-CGA-O2A |
| 30  | 1     | 307 | CHL  | C11-C10-C8-C7   |
| 30  | 1     | 307 | CHL  | C11-C12-C13-C15 |
| 30  | 1     | 313 | CHL  | C11-C10-C8-C7   |
| 30  | 6     | 302 | CHL  | C6-C7-C8-C10    |
| 30  | 6     | 302 | CHL  | C11-C10-C8-C7   |
| 30  | 7     | 301 | CHL  | C11-C12-C13-C15 |
| 30  | 7     | 302 | CHL  | C12-C13-C15-C16 |
| 30  | 8     | 302 | CHL  | C12-C13-C15-C16 |
| 30  | a     | 602 | CHL  | C11-C12-C13-C15 |
| 30  | c     | 608 | CHL  | C6-C7-C8-C10    |
| 30  | c     | 609 | CHL  | C12-C13-C15-C16 |
| 30  | b     | 608 | CHL  | C6-C7-C8-C10    |
| 30  | f     | 609 | CHL  | C12-C13-C15-C16 |
| 30  | h     | 602 | CHL  | C6-C7-C8-C10    |
| 30  | e     | 608 | CHL  | C11-C10-C8-C7   |
| 31  | 0     | 308 | CLA  | C11-C10-C8-C7   |
| 31  | 0     | 312 | CLA  | C6-C7-C8-C10    |
| 31  | 3     | 310 | CLA  | C11-C12-C13-C15 |
| 31  | 6     | 310 | CLA  | C6-C7-C8-C10    |
| 31  | 7     | 308 | CLA  | C11-C12-C13-C15 |
| 31  | 8     | 309 | CLA  | C11-C10-C8-C7   |
| 31  | 9     | 302 | CLA  | C12-C13-C15-C16 |
| 31  | A     | 805 | CLA  | C6-C7-C8-C10    |
| 31  | A     | 811 | CLA  | C11-C10-C8-C7   |
| 31  | A     | 811 | CLA  | C11-C12-C13-C15 |
| 31  | A     | 815 | CLA  | C6-C7-C8-C10    |
| 31  | A     | 818 | CLA  | C11-C12-C13-C15 |
| 31  | A     | 829 | CLA  | C11-C12-C13-C15 |
| 31  | A     | 833 | CLA  | C6-C7-C8-C10    |
| 31  | A     | 840 | CLA  | C6-C7-C8-C10    |
| 31  | B     | 803 | CLA  | C12-C13-C15-C16 |
| 31  | B     | 809 | CLA  | C11-C12-C13-C15 |
| 31  | B     | 809 | CLA  | C12-C13-C15-C16 |
| 31  | B     | 819 | CLA  | C11-C10-C8-C7   |
| 31  | B     | 820 | CLA  | C6-C7-C8-C10    |
| 31  | B     | 832 | CLA  | C12-C13-C15-C16 |
| 31  | B     | 839 | CLA  | C12-C13-C15-C16 |
| 31  | 4     | 304 | CLA  | C11-C10-C8-C7   |
| 31  | A     | 828 | CLA  | C15-C16-C17-C18 |
| 31  | B     | 830 | CLA  | O1A-CGA-O2A-C1  |
| 30  | 8     | 302 | CHL  | C15-C16-C17-C18 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | L     | 203 | CLA  | C15-C16-C17-C18 |
| 34  | c     | 630 | LHG  | C14-C15-C16-C17 |
| 34  | 4     | 601 | LHG  | C12-C13-C14-C15 |
| 30  | 8     | 305 | CHL  | CBA-CGA-O2A-C1  |
| 33  | 4     | 501 | OUR  | O44-C45-C46-C47 |
| 30  | 6     | 302 | CHL  | C15-C16-C17-C18 |
| 30  | 6     | 308 | CHL  | C11-C12-C13-C15 |
| 30  | a     | 602 | CHL  | C15-C16-C17-C18 |
| 36  | 9     | 602 | LMG  | C36-C37-C38-C39 |
| 30  | h     | 601 | CHL  | O1A-CGA-O2A-C1  |
| 30  | c     | 602 | CHL  | O1A-CGA-O2A-C1  |
| 30  | 8     | 301 | CHL  | C3-C5-C6-C7     |
| 30  | 1     | 307 | CHL  | C4-C3-C5-C6     |
| 30  | 6     | 306 | CHL  | C3A-C2A-CAA-CBA |
| 30  | 6     | 307 | CHL  | C3A-C2A-CAA-CBA |
| 30  | c     | 601 | CHL  | C3A-C2A-CAA-CBA |
| 30  | c     | 608 | CHL  | C4-C3-C5-C6     |
| 30  | b     | 601 | CHL  | C3A-C2A-CAA-CBA |
| 30  | f     | 608 | CHL  | C3A-C2A-CAA-CBA |
| 30  | h     | 608 | CHL  | C3A-C2A-CAA-CBA |
| 30  | 4     | 308 | CHL  | C3A-C2A-CAA-CBA |
| 31  | 5     | 314 | CLA  | C3A-C2A-CAA-CBA |
| 31  | 6     | 317 | CLA  | C3A-C2A-CAA-CBA |
| 31  | 9     | 308 | CLA  | C3A-C2A-CAA-CBA |
| 31  | A     | 853 | CLA  | C4-C3-C5-C6     |
| 31  | B     | 816 | CLA  | C3A-C2A-CAA-CBA |
| 31  | B     | 820 | CLA  | C3A-C2A-CAA-CBA |
| 31  | L     | 203 | CLA  | C3A-C2A-CAA-CBA |
| 31  | a     | 611 | CLA  | C3A-C2A-CAA-CBA |
| 31  | b     | 604 | CLA  | C3A-C2A-CAA-CBA |
| 31  | e     | 604 | CLA  | C3A-C2A-CAA-CBA |
| 30  | 1     | 307 | CHL  | C5-C6-C7-C8     |
| 31  | B     | 819 | CLA  | C8-C10-C11-C12  |
| 31  | A     | 839 | CLA  | C2-C3-C5-C6     |
| 30  | c     | 607 | CHL  | CBA-CGA-O2A-C1  |
| 30  | 9     | 301 | CHL  | O1D-CGD-O2D-CED |
| 30  | a     | 607 | CHL  | O1D-CGD-O2D-CED |
| 30  | d     | 601 | CHL  | O1D-CGD-O2D-CED |
| 36  | 9     | 602 | LMG  | O6-C1-O1-C7     |
| 30  | 5     | 301 | CHL  | CBA-CGA-O2A-C1  |
| 31  | 0     | 312 | CLA  | CBA-CGA-O2A-C1  |
| 31  | 7     | 304 | CLA  | CBA-CGA-O2A-C1  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | 7     | 312 | CLA  | CBA-CGA-O2A-C1  |
| 32  | 3     | 403 | 8CT  | C16-C17-C18-C19 |
| 32  | 7     | 402 | 8CT  | C23-C24-C25-C26 |
| 32  | 7     | 405 | 8CT  | C12-C13-C14-C15 |
| 32  | A     | 846 | 8CT  | C16-C17-C18-C19 |
| 32  | A     | 849 | 8CT  | C18-C19-C20-C21 |
| 32  | B     | 848 | 8CT  | C18-C19-C20-C21 |
| 32  | L     | 206 | 8CT  | C16-C17-C18-C19 |
| 32  | K     | 107 | 8CT  | C18-C19-C20-C21 |
| 32  | O     | 205 | 8CT  | C16-C17-C18-C19 |
| 33  | 5     | 502 | 0UR  | C3-C4-C5-C6     |
| 30  | 6     | 302 | CHL  | C3-C5-C6-C7     |
| 31  | A     | 840 | CLA  | C3-C5-C6-C7     |
| 32  | 0     | 401 | 8CT  | C27-C26-C28-C29 |
| 32  | 2     | 402 | 8CT  | C14-C15-C16-C39 |
| 32  | 8     | 406 | 8CT  | C27-C26-C28-C29 |
| 32  | B     | 848 | 8CT  | C10-C11-C12-C40 |
| 42  | a     | 523 | NEX  | C31-C32-C33-C40 |
| 42  | d     | 523 | NEX  | C31-C32-C33-C40 |
| 42  | f     | 523 | NEX  | C31-C32-C33-C40 |
| 42  | g     | 523 | NEX  | C31-C32-C33-C40 |
| 42  | i     | 523 | NEX  | C31-C32-C33-C40 |
| 30  | 3     | 302 | CHL  | O1A-CGA-O2A-C1  |
| 31  | 2     | 303 | CLA  | O1A-CGA-O2A-C1  |
| 30  | c     | 614 | CHL  | O1D-CGD-O2D-CED |
| 31  | 9     | 308 | CLA  | C13-C15-C16-C17 |
| 30  | i     | 601 | CHL  | C2A-CAA-CBA-CGA |
| 31  | A     | 852 | CLA  | C2A-CAA-CBA-CGA |
| 36  | L     | 210 | LMG  | C30-C31-C32-C33 |
| 30  | 8     | 301 | CHL  | C10-C11-C12-C13 |
| 34  | 8     | 601 | LHG  | C4-C5-C6-O8     |
| 34  | 4     | 601 | LHG  | C4-C5-C6-O8     |
| 36  | 2     | 602 | LMG  | C7-C8-C9-O8     |
| 36  | L     | 211 | LMG  | O1-C7-C8-C9     |
| 31  | A     | 841 | CLA  | CBD-CGD-O2D-CED |
| 30  | 2     | 319 | CHL  | C11-C12-C13-C15 |
| 30  | f     | 601 | CHL  | C16-C17-C18-C20 |
| 36  | J     | 105 | LMG  | C13-C14-C15-C16 |
| 30  | b     | 601 | CHL  | C1A-C2A-CAA-CBA |
| 30  | i     | 607 | CHL  | C1A-C2A-CAA-CBA |
| 34  | a     | 630 | LHG  | C12-C13-C14-C15 |
| 36  | O     | 207 | LMG  | C32-C33-C34-C35 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 30  | 1     | 313 | CHL  | C4-C3-C5-C6     |
| 31  | 3     | 310 | CLA  | C4-C3-C5-C6     |
| 31  | A     | 835 | CLA  | C4-C3-C5-C6     |
| 30  | b     | 608 | CHL  | C2-C3-C5-C6     |
| 31  | A     | 853 | CLA  | C2-C3-C5-C6     |
| 31  | b     | 604 | CLA  | O1A-CGA-O2A-C1  |
| 31  | 5     | 303 | CLA  | C11-C12-C13-C15 |
| 30  | b     | 602 | CHL  | O1D-CGD-O2D-CED |
| 31  | 9     | 310 | CLA  | CBD-CGD-O2D-CED |
| 36  | 3     | 602 | LMG  | C30-C31-C32-C33 |
| 36  | B     | 853 | LMG  | C11-C12-C13-C14 |
| 30  | f     | 601 | CHL  | C16-C17-C18-C19 |
| 34  | c     | 630 | LHG  | O6-C4-C5-O7     |
| 34  | g     | 630 | LHG  | O6-C4-C5-O7     |
| 31  | 2     | 314 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 3     | 306 | CLA  | C2B-C3B-CAB-CBB |
| 31  | A     | 832 | CLA  | C2B-C3B-CAB-CBB |
| 31  | K     | 105 | CLA  | C2B-C3B-CAB-CBB |
| 31  | h     | 612 | CLA  | C2B-C3B-CAB-CBB |
| 31  | H     | 205 | CLA  | C2B-C3B-CAB-CBB |
| 32  | 3     | 403 | 8CT  | C04-C03-C10-C11 |
| 32  | 7     | 405 | 8CT  | C04-C03-C10-C11 |
| 32  | 9     | 401 | 8CT  | C02-C03-C10-C11 |
| 34  | d     | 630 | LHG  | C11-C10-C9-C8   |
| 31  | A     | 807 | CLA  | O1D-CGD-O2D-CED |
| 31  | 1     | 312 | CLA  | C3-C5-C6-C7     |
| 34  | 8     | 601 | LHG  | C26-C27-C28-C29 |
| 33  | d     | 520 | 0UR  | C45-C46-C47-C48 |
| 33  | f     | 520 | 0UR  | C45-C46-C47-C48 |
| 31  | i     | 613 | CLA  | O1A-CGA-O2A-C1  |
| 31  | 2     | 309 | CLA  | C10-C11-C12-C13 |
| 34  | f     | 630 | LHG  | C28-C29-C30-C31 |
| 30  | e     | 608 | CHL  | C16-C17-C18-C20 |
| 34  | H     | 203 | LHG  | O8-C23-C24-C25  |
| 31  | 0     | 309 | CLA  | C5-C6-C7-C8     |
| 34  | 0     | 601 | LHG  | O7-C5-C6-O8     |
| 34  | 2     | 601 | LHG  | O7-C5-C6-O8     |
| 34  | 5     | 601 | LHG  | O7-C5-C6-O8     |
| 34  | B     | 854 | LHG  | O7-C5-C6-O8     |
| 34  | G     | 105 | LHG  | O7-C5-C6-O8     |
| 34  | 4     | 601 | LHG  | O7-C5-C6-O8     |
| 35  | 0     | 603 | SQD  | O6-C44-C45-O47  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 36  | A     | 856 | LMG  | O1-C7-C8-O7     |
| 36  | L     | 211 | LMG  | O1-C7-C8-O7     |
| 41  | B     | 849 | DGD  | O2G-C2G-C3G-O3G |
| 36  | J     | 105 | LMG  | C37-C38-C39-C40 |
| 30  | 7     | 301 | CHL  | O1D-CGD-O2D-CED |
| 31  | 2     | 304 | CLA  | O1D-CGD-O2D-CED |
| 31  | A     | 838 | CLA  | C11-C10-C8-C7   |
| 31  | 4     | 310 | CLA  | C8-C10-C11-C12  |
| 30  | 1     | 313 | CHL  | C2-C3-C5-C6     |
| 31  | A     | 835 | CLA  | C2-C3-C5-C6     |
| 36  | L     | 211 | LMG  | C18-C19-C20-C21 |
| 34  | h     | 630 | LHG  | C26-C27-C28-C29 |
| 33  | g     | 520 | 0UR  | C46-C47-C48-C49 |
| 34  | B     | 854 | LHG  | C26-C27-C28-C29 |
| 30  | 3     | 302 | CHL  | C11-C12-C13-C14 |
| 30  | 6     | 301 | CHL  | C6-C7-C8-C9     |
| 30  | 7     | 301 | CHL  | C11-C12-C13-C14 |
| 30  | a     | 602 | CHL  | C11-C12-C13-C14 |
| 31  | 2     | 312 | CLA  | C11-C10-C8-C9   |
| 31  | A     | 837 | CLA  | C6-C7-C8-C9     |
| 34  | B     | 854 | LHG  | C31-C32-C33-C34 |
| 31  | A     | 809 | CLA  | C5-C6-C7-C8     |
| 31  | 6     | 320 | CLA  | O1A-CGA-O2A-C1  |
| 31  | K     | 101 | CLA  | O1A-CGA-O2A-C1  |
| 34  | 4     | 601 | LHG  | C11-C12-C13-C14 |
| 34  | K     | 106 | LHG  | C10-C11-C12-C13 |
| 31  | 7     | 309 | CLA  | C11-C12-C13-C14 |
| 30  | i     | 601 | CHL  | O1A-CGA-O2A-C1  |
| 30  | 3     | 307 | CHL  | C16-C17-C18-C19 |
| 30  | 8     | 313 | CHL  | C6-C7-C8-C10    |
| 31  | B     | 817 | CLA  | C11-C12-C13-C15 |
| 31  | B     | 827 | CLA  | C16-C17-C18-C20 |
| 30  | i     | 605 | CHL  | O1D-CGD-O2D-CED |
| 31  | A     | 826 | CLA  | O1D-CGD-O2D-CED |
| 31  | A     | 814 | CLA  | C3-C5-C6-C7     |
| 31  | B     | 810 | CLA  | C3-C5-C6-C7     |
| 30  | 7     | 313 | CHL  | C2A-CAA-CBA-CGA |
| 34  | 0     | 601 | LHG  | C18-C19-C20-C21 |
| 33  | 1     | 502 | 0UR  | C46-C47-C48-C49 |
| 34  | 6     | 601 | LHG  | C11-C10-C9-C8   |
| 34  | 1     | 601 | LHG  | C23-C24-C25-C26 |
| 31  | A     | 818 | CLA  | C15-C16-C17-C18 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 34  | B     | 852 | LHG  | O1-C1-C2-O2     |
| 32  | A     | 854 | 8CT  | C16-C17-C18-C19 |
| 32  | L     | 209 | 8CT  | C16-C17-C18-C19 |
| 30  | 6     | 301 | CHL  | C11-C12-C13-C14 |
| 30  | c     | 602 | CHL  | C11-C12-C13-C15 |
| 31  | b     | 613 | CLA  | O1D-CGD-O2D-CED |
| 33  | 0     | 501 | 0UR  | O42-C2-C3-C4    |
| 33  | 0     | 502 | 0UR  | O42-C2-C3-C4    |
| 33  | 1     | 501 | 0UR  | O42-C2-C3-C4    |
| 33  | 2     | 502 | 0UR  | O42-C2-C3-C4    |
| 33  | 3     | 501 | 0UR  | O42-C2-C3-C4    |
| 33  | 5     | 501 | 0UR  | O42-C2-C3-C4    |
| 33  | 6     | 501 | 0UR  | O42-C2-C3-C4    |
| 33  | 7     | 501 | 0UR  | O42-C2-C3-C4    |
| 33  | 8     | 501 | 0UR  | O42-C2-C3-C4    |
| 33  | 9     | 501 | 0UR  | O42-C2-C3-C4    |
| 33  | 9     | 502 | 0UR  | O42-C2-C3-C4    |
| 33  | a     | 520 | 0UR  | O42-C2-C3-C4    |
| 33  | c     | 520 | 0UR  | O42-C2-C3-C4    |
| 33  | b     | 520 | 0UR  | O42-C2-C3-C4    |
| 33  | d     | 520 | 0UR  | O42-C2-C3-C4    |
| 33  | g     | 520 | 0UR  | O42-C2-C3-C4    |
| 33  | h     | 520 | 0UR  | O42-C2-C3-C4    |
| 33  | i     | 520 | 0UR  | O42-C2-C3-C4    |
| 33  | e     | 520 | 0UR  | O42-C2-C3-C4    |
| 33  | 4     | 501 | 0UR  | O42-C2-C3-C4    |
| 37  | 3     | 502 | 0IE  | O1-C2-C3-C4     |
| 37  | 7     | 502 | 0IE  | O1-C2-C3-C4     |
| 37  | a     | 521 | 0IE  | O1-C2-C3-C4     |
| 37  | c     | 521 | 0IE  | O1-C2-C3-C4     |
| 37  | b     | 521 | 0IE  | O1-C2-C3-C4     |
| 37  | d     | 521 | 0IE  | O1-C2-C3-C4     |
| 37  | f     | 521 | 0IE  | O1-C2-C3-C4     |
| 37  | g     | 521 | 0IE  | O1-C2-C3-C4     |
| 37  | h     | 521 | 0IE  | O1-C2-C3-C4     |
| 37  | i     | 521 | 0IE  | O1-C2-C3-C4     |
| 37  | e     | 521 | 0IE  | O1-C2-C3-C4     |
| 30  | 7     | 306 | CHL  | C12-C13-C15-C16 |
| 36  | O     | 207 | LMG  | C31-C32-C33-C34 |
| 34  | 9     | 601 | LHG  | C10-C11-C12-C13 |
| 34  | f     | 630 | LHG  | O8-C23-C24-C25  |
| 30  | 1     | 305 | CHL  | CBA-CGA-O2A-C1  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | 7     | 308 | CLA  | CBA-CGA-O2A-C1  |
| 30  | 2     | 301 | CHL  | C10-C11-C12-C13 |
| 34  | h     | 630 | LHG  | C10-C11-C12-C13 |
| 34  | 0     | 601 | LHG  | O6-C4-C5-C6     |
| 34  | 6     | 601 | LHG  | O6-C4-C5-C6     |
| 34  | 6     | 603 | LHG  | O6-C4-C5-C6     |
| 34  | a     | 630 | LHG  | O6-C4-C5-C6     |
| 34  | c     | 630 | LHG  | O6-C4-C5-C6     |
| 31  | A     | 828 | CLA  | C16-C17-C18-C20 |
| 31  | 7     | 304 | CLA  | O1A-CGA-O2A-C1  |
| 30  | 2     | 302 | CHL  | C13-C15-C16-C17 |
| 31  | 8     | 304 | CLA  | C13-C15-C16-C17 |
| 32  | B     | 847 | 8CT  | C27-C26-C28-C29 |
| 32  | B     | 851 | 8CT  | C27-C26-C28-C29 |
| 33  | 8     | 502 | 0UR  | C22-C16-C17-C18 |
| 30  | 1     | 307 | CHL  | C12-C13-C15-C16 |
| 30  | 3     | 302 | CHL  | C11-C12-C13-C15 |
| 30  | b     | 602 | CHL  | C12-C13-C15-C16 |
| 30  | f     | 602 | CHL  | C12-C13-C15-C16 |
| 30  | f     | 609 | CHL  | C11-C12-C13-C15 |
| 31  | 2     | 303 | CLA  | C6-C7-C8-C10    |
| 31  | 2     | 312 | CLA  | C11-C10-C8-C7   |
| 31  | 5     | 303 | CLA  | C6-C7-C8-C10    |
| 31  | A     | 826 | CLA  | C6-C7-C8-C10    |
| 31  | A     | 837 | CLA  | C6-C7-C8-C10    |
| 31  | A     | 853 | CLA  | C12-C13-C15-C16 |
| 31  | a     | 611 | CLA  | C11-C10-C8-C7   |
| 30  | 7     | 302 | CHL  | C15-C16-C17-C18 |
| 30  | 8     | 305 | CHL  | O1D-CGD-O2D-CED |
| 34  | 9     | 601 | LHG  | C34-C35-C36-C37 |
| 34  | A     | 844 | LHG  | C27-C28-C29-C30 |
| 31  | 4     | 312 | CLA  | C3-C5-C6-C7     |
| 30  | 1     | 313 | CHL  | CBD-CGD-O2D-CED |
| 31  | A     | 808 | CLA  | C8-C10-C11-C12  |
| 32  | 7     | 405 | 8CT  | C25-C26-C28-C29 |
| 32  | A     | 847 | 8CT  | C25-C26-C28-C29 |
| 32  | A     | 854 | 8CT  | C10-C11-C12-C13 |
| 32  | B     | 843 | 8CT  | C14-C15-C16-C17 |
| 32  | B     | 847 | 8CT  | C25-C26-C28-C29 |
| 32  | B     | 851 | 8CT  | C10-C11-C12-C13 |
| 32  | B     | 851 | 8CT  | C25-C26-C28-C29 |
| 32  | K     | 107 | 8CT  | C20-C21-C23-C24 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 33  | 6     | 502 | 0UR  | C15-C16-C17-C18 |
| 33  | 8     | 502 | 0UR  | C15-C16-C17-C18 |
| 31  | B     | 812 | CLA  | CBA-CGA-O2A-C1  |
| 31  | B     | 817 | CLA  | CBA-CGA-O2A-C1  |
| 31  | f     | 613 | CLA  | CBA-CGA-O2A-C1  |
| 30  | e     | 609 | CHL  | O1A-CGA-O2A-C1  |
| 31  | A     | 830 | CLA  | O1A-CGA-O2A-C1  |
| 31  | B     | 836 | CLA  | O1A-CGA-O2A-C1  |
| 30  | 7     | 306 | CHL  | C11-C12-C13-C15 |
| 31  | A     | 825 | CLA  | C15-C16-C17-C18 |
| 30  | 5     | 307 | CHL  | C2A-CAA-CBA-CGA |
| 30  | 6     | 301 | CHL  | C2A-CAA-CBA-CGA |
| 30  | h     | 606 | CHL  | C2A-CAA-CBA-CGA |
| 30  | 2     | 302 | CHL  | C15-C16-C17-C18 |
| 34  | 7     | 601 | LHG  | C9-C10-C11-C12  |
| 34  | i     | 630 | LHG  | C11-C10-C9-C8   |
| 31  | e     | 613 | CLA  | C6-C7-C8-C10    |
| 34  | b     | 630 | LHG  | C27-C28-C29-C30 |
| 30  | i     | 602 | CHL  | C11-C12-C13-C14 |
| 36  | 2     | 602 | LMG  | C11-C10-O7-C8   |
| 31  | A     | 817 | CLA  | O1D-CGD-O2D-CED |
| 34  | 8     | 601 | LHG  | C13-C14-C15-C16 |
| 30  | 5     | 301 | CHL  | O1A-CGA-O2A-C1  |
| 30  | f     | 606 | CHL  | O1A-CGA-O2A-C1  |
| 31  | 7     | 312 | CLA  | O1A-CGA-O2A-C1  |
| 31  | B     | 829 | CLA  | O1A-CGA-O2A-C1  |
| 30  | f     | 602 | CHL  | O1D-CGD-O2D-CED |
| 41  | B     | 849 | DGD  | C3G-C2G-O2G-C1B |
| 31  | e     | 613 | CLA  | O1A-CGA-O2A-C1  |
| 30  | i     | 607 | CHL  | CBA-CGA-O2A-C1  |
| 33  | h     | 520 | 0UR  | C47-C48-C49-C50 |
| 41  | B     | 849 | DGD  | C5A-C6A-C7A-C8A |
| 32  | 7     | 402 | 8CT  | C12-C13-C14-C15 |
| 32  | B     | 804 | 8CT  | C16-C17-C18-C19 |
| 30  | 4     | 313 | CHL  | O1D-CGD-O2D-CED |
| 30  | e     | 602 | CHL  | C11-C12-C13-C14 |
| 30  | e     | 609 | CHL  | C11-C12-C13-C14 |
| 31  | B     | 819 | CLA  | C11-C12-C13-C15 |
| 31  | 0     | 312 | CLA  | O1A-CGA-O2A-C1  |
| 31  | A     | 824 | CLA  | O1A-CGA-O2A-C1  |
| 30  | 3     | 307 | CHL  | C3-C5-C6-C7     |
| 31  | 3     | 304 | CLA  | C8-C10-C11-C12  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 34  | b     | 630 | LHG  | C10-C11-C12-C13 |
| 33  | d     | 520 | 0UR  | C4-C3-C43-O44   |
| 34  | 9     | 601 | LHG  | C30-C31-C32-C33 |
| 36  | 2     | 602 | LMG  | C13-C14-C15-C16 |
| 31  | 6     | 303 | CLA  | O1D-CGD-O2D-CED |
| 30  | i     | 607 | CHL  | CAA-CBA-CGA-O2A |
| 34  | 0     | 601 | LHG  | O6-C4-C5-O7     |
| 34  | 6     | 601 | LHG  | O6-C4-C5-O7     |
| 34  | 6     | 603 | LHG  | O6-C4-C5-O7     |
| 34  | 7     | 603 | LHG  | O6-C4-C5-O7     |
| 34  | 8     | 601 | LHG  | O6-C4-C5-O7     |
| 34  | B     | 852 | LHG  | O6-C4-C5-O7     |
| 34  | G     | 105 | LHG  | O6-C4-C5-O7     |
| 34  | a     | 630 | LHG  | O6-C4-C5-O7     |
| 34  | d     | 630 | LHG  | O6-C4-C5-O7     |
| 34  | H     | 203 | LHG  | O6-C4-C5-O7     |
| 30  | a     | 602 | CHL  | O1D-CGD-O2D-CED |
| 30  | e     | 601 | CHL  | O1D-CGD-O2D-CED |
| 34  | 3     | 601 | LHG  | C4-C5-C6-O8     |
| 34  | 7     | 602 | LHG  | C4-C5-C6-O8     |
| 34  | a     | 630 | LHG  | C4-C5-C6-O8     |
| 34  | d     | 630 | LHG  | C4-C5-C6-O8     |
| 36  | 3     | 602 | LMG  | C7-C8-C9-O8     |
| 36  | A     | 856 | LMG  | O1-C7-C8-C9     |
| 31  | A     | 819 | CLA  | C13-C15-C16-C17 |
| 30  | c     | 602 | CHL  | C11-C12-C13-C14 |
| 31  | 7     | 308 | CLA  | O1A-CGA-O2A-C1  |
| 31  | A     | 823 | CLA  | O1D-CGD-O2D-CED |
| 34  | 7     | 602 | LHG  | C14-C15-C16-C17 |
| 31  | A     | 805 | CLA  | C4-C3-C5-C6     |
| 31  | A     | 806 | CLA  | C4-C3-C5-C6     |
| 31  | c     | 604 | CLA  | C2A-CAA-CBA-CGA |
| 33  | 6     | 502 | 0UR  | C2-C3-C43-O44   |
| 33  | d     | 520 | 0UR  | C2-C3-C43-O44   |
| 33  | e     | 520 | 0UR  | C2-C3-C43-O44   |
| 31  | B     | 825 | CLA  | O1D-CGD-O2D-CED |
| 34  | 8     | 601 | LHG  | O7-C5-C6-O8     |
| 34  | a     | 630 | LHG  | O7-C5-C6-O8     |
| 36  | A     | 856 | LMG  | O7-C8-C9-O8     |
| 36  | J     | 105 | LMG  | O7-C8-C9-O8     |
| 31  | B     | 829 | CLA  | C8-C10-C11-C12  |
| 30  | 3     | 302 | CHL  | C6-C7-C8-C9     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 30  | b     | 602 | CHL  | C14-C13-C15-C16 |
| 30  | d     | 609 | CHL  | C11-C10-C8-C9   |
| 30  | f     | 602 | CHL  | C14-C13-C15-C16 |
| 31  | 2     | 304 | CLA  | C6-C7-C8-C9     |
| 31  | 6     | 317 | CLA  | C11-C10-C8-C9   |
| 31  | A     | 811 | CLA  | C11-C10-C8-C9   |
| 31  | A     | 825 | CLA  | C11-C12-C13-C14 |
| 31  | A     | 826 | CLA  | C14-C13-C15-C16 |
| 31  | A     | 833 | CLA  | C11-C10-C8-C9   |
| 31  | B     | 801 | CLA  | C11-C12-C13-C14 |
| 31  | B     | 827 | CLA  | C11-C12-C13-C14 |
| 38  | A     | 842 | PQN  | C24-C23-C25-C26 |
| 30  | 5     | 307 | CHL  | CBA-CGA-O2A-C1  |
| 30  | e     | 606 | CHL  | CBA-CGA-O2A-C1  |
| 36  | 9     | 602 | LMG  | C41-C42-C43-C44 |
| 30  | 1     | 305 | CHL  | O1A-CGA-O2A-C1  |
| 34  | h     | 630 | LHG  | C11-C10-C9-C8   |
| 31  | A     | 817 | CLA  | C8-C10-C11-C12  |
| 31  | A     | 853 | CLA  | C13-C15-C16-C17 |
| 31  | B     | 825 | CLA  | C5-C6-C7-C8     |
| 32  | 2     | 402 | 8CT  | C26-C28-C29-C30 |
| 32  | 4     | 402 | 8CT  | C26-C28-C29-C30 |
| 31  | B     | 817 | CLA  | C10-C11-C12-C13 |
| 36  | B     | 853 | LMG  | C34-C35-C36-C37 |
| 30  | 7     | 313 | CHL  | O1A-CGA-O2A-C1  |
| 34  | A     | 855 | LHG  | C2-C3-O3-P      |
| 34  | 5     | 601 | LHG  | C12-C13-C14-C15 |
| 41  | B     | 849 | DGD  | C2B-C3B-C4B-C5B |
| 34  | a     | 630 | LHG  | C26-C27-C28-C29 |
| 33  | 2     | 501 | 0UR  | O42-C2-C3-C43   |
| 33  | f     | 520 | 0UR  | O42-C2-C3-C43   |
| 37  | g     | 521 | 0IE  | O1-C2-C3-C20    |
| 31  | 3     | 320 | CLA  | C4-C3-C5-C6     |
| 31  | A     | 805 | CLA  | C2-C3-C5-C6     |
| 31  | A     | 806 | CLA  | C5-C6-C7-C8     |
| 34  | A     | 844 | LHG  | O2-C2-C3-O3     |
| 31  | 3     | 320 | CLA  | C2A-CAA-CBA-CGA |
| 31  | 6     | 317 | CLA  | C16-C17-C18-C20 |
| 31  | B     | 817 | CLA  | O1A-CGA-O2A-C1  |
| 36  | O     | 207 | LMG  | C4-C5-C6-O5     |
| 31  | A     | 841 | CLA  | C3-C5-C6-C7     |
| 31  | B     | 813 | CLA  | C3-C5-C6-C7     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 30  | 2     | 308 | CHL  | C4C-C3C-CAC-CBC |
| 30  | 8     | 302 | CHL  | C4C-C3C-CAC-CBC |
| 30  | a     | 609 | CHL  | C4C-C3C-CAC-CBC |
| 30  | c     | 607 | CHL  | C4C-C3C-CAC-CBC |
| 30  | c     | 609 | CHL  | C4C-C3C-CAC-CBC |
| 30  | b     | 609 | CHL  | C4C-C3C-CAC-CBC |
| 30  | h     | 602 | CHL  | C4C-C3C-CAC-CBC |
| 30  | h     | 609 | CHL  | C4C-C3C-CAC-CBC |
| 30  | i     | 609 | CHL  | C4C-C3C-CAC-CBC |
| 30  | e     | 607 | CHL  | C4C-C3C-CAC-CBC |
| 30  | 4     | 302 | CHL  | C4C-C3C-CAC-CBC |
| 31  | 8     | 312 | CLA  | C11-C10-C8-C9   |
| 37  | c     | 522 | 0IE  | C12-C13-C14-C15 |
| 30  | f     | 609 | CHL  | CBA-CGA-O2A-C1  |
| 31  | B     | 837 | CLA  | C16-C17-C18-C19 |
| 30  | 9     | 313 | CHL  | CAA-CBA-CGA-O2A |
| 30  | e     | 606 | CHL  | O1D-CGD-O2D-CED |
| 34  | g     | 630 | LHG  | O1-C1-C2-O2     |
| 34  | e     | 630 | LHG  | O1-C1-C2-O2     |
| 34  | G     | 105 | LHG  | C15-C16-C17-C18 |
| 32  | A     | 849 | 8CT  | C14-C15-C16-C39 |
| 33  | 0     | 502 | 0UR  | C22-C16-C17-C18 |
| 30  | d     | 607 | CHL  | O1A-CGA-O2A-C1  |
| 31  | 0     | 309 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 2     | 303 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 2     | 310 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 2     | 310 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 3     | 312 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 5     | 314 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 5     | 314 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 6     | 309 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 6     | 310 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 6     | 317 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 6     | 318 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 7     | 310 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 7     | 311 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 7     | 312 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 7     | 315 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 8     | 309 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 8     | 310 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 8     | 311 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 9     | 310 | CLA  | C4B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | A     | 823 | CLA  | C4B-C3B-CAB-CBB |
| 31  | A     | 824 | CLA  | C1A-C2A-CAA-CBA |
| 31  | A     | 840 | CLA  | C4B-C3B-CAB-CBB |
| 31  | B     | 809 | CLA  | C4B-C3B-CAB-CBB |
| 31  | B     | 811 | CLA  | C4B-C3B-CAB-CBB |
| 31  | B     | 822 | CLA  | C4B-C3B-CAB-CBB |
| 31  | B     | 834 | CLA  | C4B-C3B-CAB-CBB |
| 31  | B     | 850 | CLA  | C4B-C3B-CAB-CBB |
| 31  | F     | 301 | CLA  | C4B-C3B-CAB-CBB |
| 31  | L     | 207 | CLA  | C4B-C3B-CAB-CBB |
| 31  | K     | 101 | CLA  | C4B-C3B-CAB-CBB |
| 31  | O     | 206 | CLA  | C4B-C3B-CAB-CBB |
| 31  | a     | 611 | CLA  | C1A-C2A-CAA-CBA |
| 31  | a     | 611 | CLA  | C4B-C3B-CAB-CBB |
| 31  | d     | 611 | CLA  | C4B-C3B-CAB-CBB |
| 31  | d     | 612 | CLA  | C4B-C3B-CAB-CBB |
| 31  | f     | 603 | CLA  | C4B-C3B-CAB-CBB |
| 31  | i     | 610 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 4     | 303 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 4     | 309 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 4     | 310 | CLA  | C4B-C3B-CAB-CBB |
| 37  | h     | 521 | 0IE  | O29-C20-C3-C2   |
| 37  | i     | 521 | 0IE  | O29-C20-C3-C2   |
| 31  | B     | 823 | CLA  | O1D-CGD-O2D-CED |
| 31  | 1     | 310 | CLA  | C4-C3-C5-C6     |
| 31  | A     | 829 | CLA  | C4-C3-C5-C6     |
| 36  | L     | 210 | LMG  | O7-C10-C11-C12  |
| 34  | c     | 630 | LHG  | C31-C32-C33-C34 |
| 32  | 2     | 402 | 8CT  | C14-C15-C16-C17 |
| 32  | A     | 849 | 8CT  | C14-C15-C16-C17 |
| 31  | 3     | 308 | CLA  | C16-C17-C18-C19 |
| 31  | 9     | 302 | CLA  | C16-C17-C18-C20 |
| 31  | B     | 806 | CLA  | C4C-C3C-CAC-CBC |
| 31  | B     | 812 | CLA  | O1A-CGA-O2A-C1  |
| 31  | B     | 810 | CLA  | C2A-CAA-CBA-CGA |
| 31  | d     | 613 | CLA  | C2A-CAA-CBA-CGA |
| 34  | 9     | 601 | LHG  | C25-C26-C27-C28 |
| 34  | f     | 630 | LHG  | C11-C10-C9-C8   |
| 31  | A     | 811 | CLA  | C10-C11-C12-C13 |
| 31  | B     | 810 | CLA  | C5-C6-C7-C8     |
| 31  | B     | 824 | CLA  | C8-C10-C11-C12  |
| 34  | 7     | 603 | LHG  | O6-C4-C5-C6     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 34  | 8     | 601 | LHG  | O6-C4-C5-C6     |
| 34  | A     | 845 | LHG  | O6-C4-C5-C6     |
| 34  | G     | 105 | LHG  | O6-C4-C5-C6     |
| 34  | g     | 630 | LHG  | O6-C4-C5-C6     |
| 34  | H     | 203 | LHG  | O6-C4-C5-C6     |
| 36  | 2     | 602 | LMG  | C33-C34-C35-C36 |
| 31  | 0     | 303 | CLA  | CBD-CGD-O2D-CED |
| 30  | e     | 607 | CHL  | CBA-CGA-O2A-C1  |
| 31  | 6     | 320 | CLA  | C2-C3-C5-C6     |
| 31  | A     | 836 | CLA  | C2-C3-C5-C6     |
| 31  | B     | 826 | CLA  | C2-C3-C5-C6     |
| 31  | B     | 811 | CLA  | C10-C11-C12-C13 |
| 34  | 9     | 601 | LHG  | C28-C29-C30-C31 |
| 31  | L     | 203 | CLA  | C3-C5-C6-C7     |
| 30  | 1     | 302 | CHL  | C11-C12-C13-C15 |
| 30  | 3     | 307 | CHL  | C11-C12-C13-C15 |
| 30  | c     | 608 | CHL  | C11-C12-C13-C15 |
| 30  | c     | 608 | CHL  | C12-C13-C15-C16 |
| 30  | c     | 609 | CHL  | C11-C12-C13-C15 |
| 30  | b     | 601 | CHL  | C11-C12-C13-C15 |
| 30  | b     | 608 | CHL  | C11-C12-C13-C15 |
| 30  | d     | 602 | CHL  | C12-C13-C15-C16 |
| 30  | e     | 602 | CHL  | C6-C7-C8-C10    |
| 31  | 1     | 303 | CLA  | C6-C7-C8-C10    |
| 31  | 3     | 308 | CLA  | C11-C10-C8-C7   |
| 31  | 5     | 309 | CLA  | C6-C7-C8-C10    |
| 31  | 9     | 308 | CLA  | C12-C13-C15-C16 |
| 31  | 9     | 309 | CLA  | C6-C7-C8-C10    |
| 31  | B     | 808 | CLA  | C11-C10-C8-C7   |
| 31  | B     | 810 | CLA  | C6-C7-C8-C10    |
| 31  | B     | 817 | CLA  | C6-C7-C8-C10    |
| 31  | B     | 841 | CLA  | C12-C13-C15-C16 |
| 30  | 8     | 301 | CHL  | C11-C12-C13-C15 |
| 31  | J     | 103 | CLA  | O1D-CGD-O2D-CED |
| 34  | A     | 844 | LHG  | C19-C20-C21-C22 |
| 30  | 0     | 306 | CHL  | CBA-CGA-O2A-C1  |
| 31  | b     | 613 | CLA  | CBA-CGA-O2A-C1  |
| 31  | g     | 603 | CLA  | CBA-CGA-O2A-C1  |
| 31  | e     | 611 | CLA  | CBA-CGA-O2A-C1  |
| 30  | e     | 606 | CHL  | O1A-CGA-O2A-C1  |
| 31  | f     | 613 | CLA  | O1A-CGA-O2A-C1  |
| 31  | g     | 603 | CLA  | O1A-CGA-O2A-C1  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | 0     | 308 | CLA  | C8-C10-C11-C12  |
| 31  | 9     | 312 | CLA  | C5-C6-C7-C8     |
| 36  | B     | 853 | LMG  | C35-C36-C37-C38 |
| 34  | 0     | 601 | LHG  | C17-C18-C19-C20 |
| 34  | 8     | 601 | LHG  | C15-C16-C17-C18 |
| 30  | h     | 609 | CHL  | C3A-C2A-CAA-CBA |
| 31  | B     | 803 | CLA  | C16-C17-C18-C19 |
| 36  | 9     | 602 | LMG  | C11-C12-C13-C14 |
| 31  | A     | 806 | CLA  | C2-C3-C5-C6     |
| 34  | f     | 630 | LHG  | O6-C4-C5-O7     |
| 34  | 6     | 601 | LHG  | C11-C12-C13-C14 |
| 34  | a     | 630 | LHG  | C8-C7-O7-C5     |
| 31  | c     | 613 | CLA  | C2A-CAA-CBA-CGA |
| 31  | H     | 205 | CLA  | C2A-CAA-CBA-CGA |
| 30  | 1     | 302 | CHL  | C14-C13-C15-C16 |
| 30  | 1     | 307 | CHL  | C14-C13-C15-C16 |
| 30  | f     | 609 | CHL  | C11-C12-C13-C14 |
| 31  | 0     | 308 | CLA  | C11-C10-C8-C9   |
| 31  | 5     | 303 | CLA  | C6-C7-C8-C9     |
| 31  | 7     | 308 | CLA  | C14-C13-C15-C16 |
| 31  | A     | 811 | CLA  | C11-C12-C13-C14 |
| 31  | A     | 817 | CLA  | C11-C12-C13-C14 |
| 31  | A     | 853 | CLA  | C14-C13-C15-C16 |
| 30  | 4     | 308 | CHL  | O1A-CGA-O2A-C1  |
| 31  | B     | 818 | CLA  | C8-C10-C11-C12  |
| 31  | B     | 814 | CLA  | O1D-CGD-O2D-CED |
| 36  | 9     | 602 | LMG  | C32-C33-C34-C35 |
| 32  | 7     | 405 | 8CT  | C16-C17-C18-C19 |
| 32  | 8     | 406 | 8CT  | C16-C17-C18-C19 |
| 32  | A     | 847 | 8CT  | C18-C19-C20-C21 |
| 32  | L     | 206 | 8CT  | C18-C19-C20-C21 |
| 31  | B     | 805 | CLA  | C16-C17-C18-C19 |
| 30  | 2     | 302 | CHL  | O1D-CGD-O2D-CED |
| 31  | 8     | 309 | CLA  | O1D-CGD-O2D-CED |
| 34  | A     | 855 | LHG  | C27-C28-C29-C30 |
| 34  | B     | 854 | LHG  | C32-C33-C34-C35 |
| 30  | i     | 608 | CHL  | C1-C2-C3-C4     |
| 31  | A     | 822 | CLA  | C1-C2-C3-C4     |
| 31  | h     | 603 | CLA  | C1-C2-C3-C4     |
| 32  | 9     | 401 | 8CT  | C28-C29-C30-C35 |
| 33  | 0     | 502 | 0UR  | C17-C18-C19-C28 |
| 33  | O     | 204 | 0UR  | C17-C18-C19-C28 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 33  | h     | 520 | 0UR  | C17-C18-C19-C28 |
| 31  | 9     | 310 | CLA  | O1D-CGD-O2D-CED |
| 34  | 6     | 601 | LHG  | C25-C26-C27-C28 |
| 31  | A     | 852 | CLA  | O1D-CGD-O2D-CED |
| 34  | 0     | 601 | LHG  | C10-C11-C12-C13 |
| 30  | f     | 609 | CHL  | O1A-CGA-O2A-C1  |
| 34  | 7     | 602 | LHG  | O7-C5-C6-O8     |
| 34  | K     | 106 | LHG  | O7-C5-C6-O8     |
| 34  | d     | 630 | LHG  | O7-C5-C6-O8     |
| 36  | 2     | 602 | LMG  | O1-C7-C8-O7     |
| 36  | 9     | 602 | LMG  | O7-C8-C9-O8     |
| 36  | B     | 853 | LMG  | O7-C8-C9-O8     |
| 31  | A     | 808 | CLA  | C5-C6-C7-C8     |
| 34  | K     | 106 | LHG  | C4-C5-C6-O8     |
| 36  | 2     | 602 | LMG  | O1-C7-C8-C9     |
| 36  | 9     | 602 | LMG  | C7-C8-C9-O8     |
| 36  | B     | 853 | LMG  | C7-C8-C9-O8     |
| 36  | J     | 105 | LMG  | C7-C8-C9-O8     |
| 36  | L     | 210 | LMG  | O1-C7-C8-C9     |
| 36  | L     | 210 | LMG  | C7-C8-C9-O8     |
| 36  | L     | 211 | LMG  | C7-C8-C9-O8     |
| 36  | O     | 207 | LMG  | C7-C8-C9-O8     |
| 31  | A     | 814 | CLA  | C4-C3-C5-C6     |
| 30  | 6     | 313 | CHL  | O1A-CGA-O2A-C1  |
| 30  | 2     | 301 | CHL  | CAD-CBD-CGD-O2D |
| 30  | 6     | 301 | CHL  | CAD-CBD-CGD-O2D |
| 31  | A     | 835 | CLA  | CAD-CBD-CGD-O2D |
| 31  | d     | 604 | CLA  | CAD-CBD-CGD-O2D |
| 31  | f     | 604 | CLA  | CAD-CBD-CGD-O2D |
| 31  | h     | 604 | CLA  | CAD-CBD-CGD-O2D |
| 31  | i     | 604 | CLA  | CAD-CBD-CGD-O2D |
| 31  | b     | 613 | CLA  | O1A-CGA-O2A-C1  |
| 31  | e     | 611 | CLA  | O1A-CGA-O2A-C1  |
| 31  | B     | 822 | CLA  | C4C-C3C-CAC-CBC |
| 30  | 6     | 313 | CHL  | CBA-CGA-O2A-C1  |
| 33  | 0     | 501 | 0UR  | C46-C47-C48-C49 |
| 31  | A     | 821 | CLA  | C13-C15-C16-C17 |
| 30  | c     | 608 | CHL  | C3-C5-C6-C7     |
| 31  | a     | 610 | CLA  | C2A-CAA-CBA-CGA |
| 35  | 0     | 603 | SQD  | O5-C5-C6-S      |
| 34  | 7     | 601 | LHG  | C26-C27-C28-C29 |
| 30  | 0     | 306 | CHL  | O1A-CGA-O2A-C1  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 34  | K     | 106 | LHG  | C26-C27-C28-C29 |
| 34  | K     | 106 | LHG  | C7-C8-C9-C10    |
| 33  | 4     | 501 | OUR  | O57-C45-C46-C47 |
| 30  | 0     | 301 | CHL  | CHA-CBD-CGD-O1D |
| 30  | 0     | 301 | CHL  | CHA-CBD-CGD-O2D |
| 30  | 0     | 302 | CHL  | CHA-CBD-CGD-O1D |
| 30  | 0     | 302 | CHL  | CHA-CBD-CGD-O2D |
| 30  | 2     | 301 | CHL  | CAD-CBD-CGD-O1D |
| 30  | 2     | 307 | CHL  | CHA-CBD-CGD-O2D |
| 30  | 6     | 301 | CHL  | CAD-CBD-CGD-O1D |
| 30  | 7     | 301 | CHL  | CHA-CBD-CGD-O1D |
| 30  | 7     | 301 | CHL  | CHA-CBD-CGD-O2D |
| 30  | 7     | 305 | CHL  | CHA-CBD-CGD-O2D |
| 30  | 7     | 313 | CHL  | CHA-CBD-CGD-O2D |
| 30  | 8     | 301 | CHL  | CHA-CBD-CGD-O1D |
| 30  | 8     | 301 | CHL  | CHA-CBD-CGD-O2D |
| 30  | 9     | 306 | CHL  | CHA-CBD-CGD-O2D |
| 30  | a     | 601 | CHL  | CHA-CBD-CGD-O2D |
| 30  | a     | 605 | CHL  | CHA-CBD-CGD-O2D |
| 30  | a     | 607 | CHL  | CHA-CBD-CGD-O2D |
| 30  | c     | 601 | CHL  | CHA-CBD-CGD-O1D |
| 30  | c     | 601 | CHL  | CHA-CBD-CGD-O2D |
| 30  | c     | 607 | CHL  | CHA-CBD-CGD-O2D |
| 30  | c     | 608 | CHL  | CHA-CBD-CGD-O1D |
| 30  | c     | 609 | CHL  | CHA-CBD-CGD-O1D |
| 30  | c     | 609 | CHL  | CHA-CBD-CGD-O2D |
| 30  | b     | 601 | CHL  | CHA-CBD-CGD-O1D |
| 30  | b     | 601 | CHL  | CHA-CBD-CGD-O2D |
| 30  | d     | 601 | CHL  | CHA-CBD-CGD-O2D |
| 30  | d     | 607 | CHL  | CHA-CBD-CGD-O1D |
| 30  | d     | 607 | CHL  | CHA-CBD-CGD-O2D |
| 30  | d     | 609 | CHL  | CHA-CBD-CGD-O1D |
| 30  | d     | 609 | CHL  | CHA-CBD-CGD-O2D |
| 30  | g     | 609 | CHL  | O1A-CGA-O2A-C1  |
| 30  | h     | 606 | CHL  | CHA-CBD-CGD-O2D |
| 30  | h     | 614 | CHL  | CAD-CBD-CGD-O1D |
| 30  | i     | 601 | CHL  | CHA-CBD-CGD-O1D |
| 30  | i     | 601 | CHL  | CHA-CBD-CGD-O2D |
| 30  | e     | 609 | CHL  | CHA-CBD-CGD-O2D |
| 30  | 4     | 302 | CHL  | CHA-CBD-CGD-O1D |
| 30  | 4     | 302 | CHL  | CHA-CBD-CGD-O2D |
| 30  | 4     | 307 | CHL  | CHA-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | 0     | 313 | CLA  | CAD-CBD-CGD-O1D |
| 31  | 1     | 303 | CLA  | CHA-CBD-CGD-O1D |
| 31  | 1     | 303 | CLA  | CHA-CBD-CGD-O2D |
| 31  | 2     | 310 | CLA  | CHA-CBD-CGD-O1D |
| 31  | 2     | 310 | CLA  | CHA-CBD-CGD-O2D |
| 31  | 3     | 304 | CLA  | CHA-CBD-CGD-O1D |
| 31  | 3     | 304 | CLA  | CHA-CBD-CGD-O2D |
| 31  | 5     | 303 | CLA  | CHA-CBD-CGD-O1D |
| 31  | 5     | 303 | CLA  | CHA-CBD-CGD-O2D |
| 31  | 6     | 304 | CLA  | CHA-CBD-CGD-O1D |
| 31  | 6     | 304 | CLA  | CHA-CBD-CGD-O2D |
| 31  | 9     | 303 | CLA  | CHA-CBD-CGD-O1D |
| 31  | 9     | 303 | CLA  | CHA-CBD-CGD-O2D |
| 31  | A     | 806 | CLA  | CHA-CBD-CGD-O1D |
| 31  | A     | 806 | CLA  | CHA-CBD-CGD-O2D |
| 31  | A     | 835 | CLA  | CAD-CBD-CGD-O1D |
| 31  | A     | 840 | CLA  | CHA-CBD-CGD-O1D |
| 31  | B     | 825 | CLA  | CHA-CBD-CGD-O1D |
| 31  | J     | 103 | CLA  | CHA-CBD-CGD-O1D |
| 31  | K     | 105 | CLA  | CAD-CBD-CGD-O1D |
| 31  | O     | 202 | CLA  | CHA-CBD-CGD-O2D |
| 31  | O     | 202 | CLA  | CAD-CBD-CGD-O2D |
| 31  | c     | 612 | CLA  | CHA-CBD-CGD-O1D |
| 31  | c     | 612 | CLA  | CHA-CBD-CGD-O2D |
| 31  | b     | 612 | CLA  | CHA-CBD-CGD-O1D |
| 31  | b     | 612 | CLA  | CHA-CBD-CGD-O2D |
| 31  | d     | 604 | CLA  | CAD-CBD-CGD-O1D |
| 31  | f     | 604 | CLA  | CAD-CBD-CGD-O1D |
| 31  | h     | 604 | CLA  | CAD-CBD-CGD-O1D |
| 31  | i     | 604 | CLA  | CAD-CBD-CGD-O1D |
| 31  | 4     | 310 | CLA  | CHA-CBD-CGD-O1D |
| 31  | 4     | 310 | CLA  | CHA-CBD-CGD-O2D |
| 32  | B     | 846 | 8CT  | C18-C19-C20-C21 |
| 33  | 5     | 501 | 0UR  | C41-C2-C3-C4    |
| 33  | 5     | 501 | 0UR  | C3-C2-C41-C1    |
| 33  | b     | 520 | 0UR  | C41-C2-C3-C4    |
| 33  | d     | 520 | 0UR  | C41-C2-C3-C4    |
| 33  | g     | 520 | 0UR  | C41-C2-C3-C4    |
| 33  | e     | 520 | 0UR  | C41-C2-C3-C4    |
| 34  | 3     | 603 | LHG  | C3-O3-P-O4      |
| 34  | 3     | 603 | LHG  | C3-O3-P-O5      |
| 34  | 3     | 603 | LHG  | C3-O3-P-O6      |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 34  | 6     | 601 | LHG  | C4-O6-P-O3      |
| 34  | 6     | 601 | LHG  | C4-O6-P-O4      |
| 34  | 6     | 601 | LHG  | C4-O6-P-O5      |
| 34  | 6     | 603 | LHG  | C4-O6-P-O4      |
| 34  | 7     | 602 | LHG  | C4-O6-P-O4      |
| 34  | 8     | 601 | LHG  | C3-O3-P-O4      |
| 34  | 9     | 601 | LHG  | C4-O6-P-O4      |
| 34  | A     | 844 | LHG  | C4-O6-P-O3      |
| 34  | A     | 845 | LHG  | C3-O3-P-O5      |
| 34  | A     | 845 | LHG  | C3-O3-P-O6      |
| 34  | A     | 855 | LHG  | C3-O3-P-O4      |
| 34  | A     | 855 | LHG  | C4-O6-P-O4      |
| 34  | B     | 852 | LHG  | C4-O6-P-O3      |
| 34  | B     | 852 | LHG  | C4-O6-P-O5      |
| 34  | G     | 105 | LHG  | C4-O6-P-O5      |
| 34  | K     | 106 | LHG  | C4-O6-P-O5      |
| 34  | d     | 630 | LHG  | C3-O3-P-O6      |
| 34  | g     | 630 | LHG  | C3-O3-P-O6      |
| 34  | i     | 630 | LHG  | C3-O3-P-O5      |
| 34  | e     | 630 | LHG  | C4-O6-P-O4      |
| 39  | A     | 857 | CL0  | CHA-CBD-CGD-O1D |
| 39  | A     | 857 | CL0  | CHA-CBD-CGD-O2D |
| 31  | 8     | 312 | CLA  | C3-C5-C6-C7     |
| 31  | A     | 827 | CLA  | C3-C5-C6-C7     |
| 34  | M     | 104 | LHG  | C34-C35-C36-C37 |
| 31  | A     | 830 | CLA  | C13-C15-C16-C17 |
| 31  | B     | 827 | CLA  | C10-C11-C12-C13 |
| 31  | 1     | 310 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 3     | 312 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 3     | 313 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 5     | 314 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 6     | 304 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 7     | 310 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 8     | 311 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 8     | 312 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 9     | 310 | CLA  | C2B-C3B-CAB-CBB |
| 31  | A     | 835 | CLA  | C2B-C3B-CAB-CBB |
| 31  | A     | 839 | CLA  | C2B-C3B-CAB-CBB |
| 31  | B     | 850 | CLA  | C2B-C3B-CAB-CBB |
| 31  | H     | 202 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 4     | 303 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 4     | 310 | CLA  | C2B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 32  | B     | 804 | 8CT  | C02-C03-C10-C11 |
| 30  | f     | 607 | CHL  | CAA-CBA-CGA-O2A |
| 31  | B     | 840 | CLA  | C13-C15-C16-C17 |
| 32  | 3     | 403 | 8CT  | C22-C21-C23-C24 |
| 34  | 3     | 601 | LHG  | C2-C3-O3-P      |
| 34  | 3     | 603 | LHG  | C5-C4-O6-P      |
| 34  | 7     | 601 | LHG  | C2-C3-O3-P      |
| 34  | 8     | 601 | LHG  | C2-C3-O3-P      |
| 34  | A     | 855 | LHG  | C5-C4-O6-P      |
| 34  | B     | 852 | LHG  | C2-C3-O3-P      |
| 34  | B     | 854 | LHG  | C2-C3-O3-P      |
| 34  | c     | 630 | LHG  | C2-C3-O3-P      |
| 31  | A     | 841 | CLA  | O1D-CGD-O2D-CED |
| 34  | K     | 106 | LHG  | C12-C13-C14-C15 |
| 31  | B     | 817 | CLA  | C4C-C3C-CAC-CBC |
| 34  | 1     | 601 | LHG  | C12-C13-C14-C15 |
| 36  | 9     | 602 | LMG  | C21-C22-C23-C24 |
| 34  | 1     | 601 | LHG  | C35-C36-C37-C38 |
| 31  | 0     | 308 | CLA  | C10-C11-C12-C13 |
| 35  | 0     | 603 | SQD  | C4-C5-C6-S      |
| 31  | A     | 817 | CLA  | C12-C13-C15-C16 |
| 30  | 1     | 305 | CHL  | O2A-C1-C2-C3    |
| 36  | B     | 853 | LMG  | C9-C8-O7-C10    |
| 34  | h     | 630 | LHG  | C25-C26-C27-C28 |
| 30  | 5     | 313 | CHL  | O1A-CGA-O2A-C1  |
| 31  | 5     | 308 | CLA  | O1A-CGA-O2A-C1  |
| 32  | 3     | 402 | 8CT  | C13-C14-C15-C16 |
| 32  | 6     | 402 | 8CT  | C21-C23-C24-C25 |
| 32  | B     | 843 | 8CT  | C13-C14-C15-C16 |
| 32  | B     | 843 | 8CT  | C21-C23-C24-C25 |
| 32  | B     | 844 | 8CT  | C13-C14-C15-C16 |
| 32  | B     | 844 | 8CT  | C21-C23-C24-C25 |
| 32  | B     | 845 | 8CT  | C13-C14-C15-C16 |
| 32  | B     | 846 | 8CT  | C13-C14-C15-C16 |
| 32  | B     | 846 | 8CT  | C21-C23-C24-C25 |
| 31  | 9     | 300 | CLA  | CAA-CBA-CGA-O2A |
| 30  | c     | 608 | CHL  | C10-C11-C12-C13 |
| 31  | 3     | 312 | CLA  | C6-C7-C8-C10    |
| 31  | 6     | 317 | CLA  | C16-C17-C18-C19 |
| 31  | 4     | 304 | CLA  | C10-C11-C12-C13 |
| 30  | 8     | 302 | CHL  | C14-C13-C15-C16 |
| 30  | b     | 601 | CHL  | C11-C12-C13-C14 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 30  | f     | 601 | CHL  | C6-C7-C8-C9     |
| 31  | 8     | 309 | CLA  | C11-C10-C8-C9   |
| 31  | A     | 806 | CLA  | C14-C13-C15-C16 |
| 31  | A     | 811 | CLA  | C14-C13-C15-C16 |
| 31  | A     | 815 | CLA  | C6-C7-C8-C9     |
| 31  | A     | 821 | CLA  | C14-C13-C15-C16 |
| 31  | A     | 828 | CLA  | C14-C13-C15-C16 |
| 31  | B     | 820 | CLA  | C6-C7-C8-C9     |
| 30  | 6     | 302 | CHL  | C12-C13-C15-C16 |
| 31  | A     | 828 | CLA  | C12-C13-C15-C16 |
| 31  | B     | 806 | CLA  | C11-C12-C13-C15 |
| 31  | L     | 203 | CLA  | C11-C10-C8-C7   |
| 34  | b     | 630 | LHG  | C23-C24-C25-C26 |
| 31  | 0     | 311 | CLA  | CBD-CGD-O2D-CED |
| 34  | 0     | 601 | LHG  | C31-C32-C33-C34 |
| 34  | M     | 104 | LHG  | C13-C14-C15-C16 |
| 34  | b     | 630 | LHG  | C11-C12-C13-C14 |
| 31  | 3     | 308 | CLA  | C16-C17-C18-C20 |
| 31  | 2     | 304 | CLA  | C8-C10-C11-C12  |
| 30  | c     | 601 | CHL  | C2C-C3C-CAC-CBC |
| 31  | A     | 853 | CLA  | C15-C16-C17-C18 |
| 36  | 9     | 602 | LMG  | C15-C16-C17-C18 |
| 30  | 1     | 305 | CHL  | CBD-CGD-O2D-CED |
| 30  | 1     | 305 | CHL  | O1D-CGD-O2D-CED |
| 31  | 0     | 303 | CLA  | O1D-CGD-O2D-CED |
| 30  | 4     | 319 | CHL  | CAA-CBA-CGA-O2A |
| 31  | L     | 201 | CLA  | C2-C3-C5-C6     |
| 34  | 6     | 601 | LHG  | C27-C28-C29-C30 |
| 34  | G     | 105 | LHG  | C12-C13-C14-C15 |
| 31  | 7     | 312 | CLA  | C3-C5-C6-C7     |
| 31  | 9     | 302 | CLA  | C16-C17-C18-C19 |
| 31  | B     | 805 | CLA  | C16-C17-C18-C20 |
| 34  | G     | 105 | LHG  | C7-C8-C9-C10    |
| 34  | a     | 630 | LHG  | O9-C7-O7-C5     |
| 30  | 1     | 313 | CHL  | O1D-CGD-O2D-CED |
| 31  | b     | 611 | CLA  | C8-C10-C11-C12  |
| 36  | L     | 210 | LMG  | O7-C8-C9-O8     |
| 30  | 9     | 306 | CHL  | CAA-CBA-CGA-O2A |
| 34  | 6     | 603 | LHG  | O8-C23-C24-C25  |
| 33  | 2     | 502 | OUR  | C46-C47-C48-C49 |
| 34  | 6     | 603 | LHG  | C24-C23-O8-C6   |
| 32  | A     | 847 | 8CT  | C23-C24-C25-C26 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 32  | B     | 804 | 8CT  | C18-C19-C20-C21 |
| 31  | B     | 822 | CLA  | C2C-C3C-CAC-CBC |
| 31  | A     | 818 | CLA  | CAA-CBA-CGA-O2A |
| 31  | A     | 802 | CLA  | C2A-CAA-CBA-CGA |
| 31  | A     | 817 | CLA  | C2A-CAA-CBA-CGA |
| 31  | K     | 105 | CLA  | C2A-CAA-CBA-CGA |
| 30  | g     | 606 | CHL  | CBD-CGD-O2D-CED |
| 34  | A     | 855 | LHG  | C15-C16-C17-C18 |
| 31  | L     | 203 | CLA  | C2-C1-O2A-CGA   |
| 31  | 9     | 312 | CLA  | C4-C3-C5-C6     |
| 34  | K     | 106 | LHG  | C29-C30-C31-C32 |
| 34  | M     | 104 | LHG  | C15-C16-C17-C18 |
| 34  | A     | 855 | LHG  | C4-C5-C6-O8     |
| 41  | B     | 849 | DGD  | C1G-C2G-C3G-O3G |
| 34  | 6     | 601 | LHG  | O8-C23-C24-C25  |
| 32  | 3     | 402 | 8CT  | C10-C11-C12-C40 |
| 34  | 2     | 601 | LHG  | C10-C11-C12-C13 |
| 31  | B     | 814 | CLA  | C16-C17-C18-C19 |
| 30  | 2     | 313 | CHL  | C1C-C2C-CMC-OMC |
| 30  | 7     | 305 | CHL  | C1C-C2C-CMC-OMC |
| 30  | 7     | 306 | CHL  | C1C-C2C-CMC-OMC |
| 30  | e     | 601 | CHL  | C1C-C2C-CMC-OMC |
| 30  | e     | 605 | CHL  | C1C-C2C-CMC-OMC |
| 33  | b     | 520 | 0UR  | C5-C6-C7-C8     |
| 31  | B     | 805 | CLA  | CAA-CBA-CGA-O2A |
| 31  | d     | 613 | CLA  | C11-C10-C8-C7   |
| 30  | 5     | 301 | CHL  | C2A-CAA-CBA-CGA |
| 31  | 2     | 312 | CLA  | C2A-CAA-CBA-CGA |
| 31  | A     | 837 | CLA  | C2A-CAA-CBA-CGA |
| 31  | A     | 839 | CLA  | C2A-CAA-CBA-CGA |
| 31  | b     | 613 | CLA  | C2A-CAA-CBA-CGA |
| 31  | f     | 613 | CLA  | C2A-CAA-CBA-CGA |
| 31  | g     | 610 | CLA  | C2A-CAA-CBA-CGA |
| 31  | i     | 613 | CLA  | C2A-CAA-CBA-CGA |
| 31  | e     | 610 | CLA  | C2A-CAA-CBA-CGA |
| 32  | B     | 847 | 8CT  | C23-C24-C25-C26 |
| 36  | L     | 211 | LMG  | C14-C15-C16-C17 |
| 31  | B     | 808 | CLA  | C4-C3-C5-C6     |
| 31  | 1     | 310 | CLA  | C2-C3-C5-C6     |
| 31  | A     | 829 | CLA  | C2-C3-C5-C6     |
| 31  | B     | 824 | CLA  | C5-C6-C7-C8     |
| 36  | 2     | 602 | LMG  | C10-C11-C12-C13 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 30  | 2     | 319 | CHL  | CAA-CBA-CGA-O1A |
| 30  | d     | 607 | CHL  | CAA-CBA-CGA-O1A |
| 34  | A     | 845 | LHG  | O1-C1-C2-O2     |
| 31  | A     | 803 | CLA  | C16-C17-C18-C20 |
| 30  | 8     | 305 | CHL  | O1A-CGA-O2A-C1  |
| 30  | a     | 607 | CHL  | O1A-CGA-O2A-C1  |
| 30  | 1     | 313 | CHL  | C6-C7-C8-C9     |
| 30  | e     | 608 | CHL  | C6-C7-C8-C9     |
| 31  | 6     | 317 | CLA  | C11-C12-C13-C14 |
| 31  | B     | 803 | CLA  | C11-C12-C13-C14 |
| 31  | B     | 808 | CLA  | C11-C10-C8-C9   |
| 31  | B     | 817 | CLA  | C6-C7-C8-C9     |
| 38  | B     | 842 | PQN  | C21-C22-C23-C24 |
| 39  | A     | 857 | CL0  | C14-C13-C15-C16 |
| 34  | 6     | 603 | LHG  | C2-C3-O3-P      |
| 31  | 8     | 303 | CLA  | C4B-C3B-CAB-CBB |
| 31  | B     | 840 | CLA  | C4B-C3B-CAB-CBB |
| 34  | A     | 855 | LHG  | C11-C12-C13-C14 |
| 30  | 6     | 308 | CHL  | C5-C6-C7-C8     |
| 31  | A     | 829 | CLA  | C16-C17-C18-C20 |
| 31  | A     | 813 | CLA  | CBA-CGA-O2A-C1  |
| 34  | 8     | 601 | LHG  | C24-C23-O8-C6   |
| 34  | 2     | 601 | LHG  | C7-C8-C9-C10    |
| 31  | i     | 612 | CLA  | CAA-CBA-CGA-O2A |
| 30  | f     | 609 | CHL  | C10-C11-C12-C13 |
| 30  | 9     | 301 | CHL  | C2A-CAA-CBA-CGA |
| 31  | 3     | 312 | CLA  | C2A-CAA-CBA-CGA |
| 31  | A     | 835 | CLA  | C2A-CAA-CBA-CGA |
| 31  | d     | 611 | CLA  | C2A-CAA-CBA-CGA |
| 30  | 2     | 302 | CHL  | C4-C3-C5-C6     |
| 30  | 4     | 302 | CHL  | C4-C3-C5-C6     |
| 31  | A     | 819 | CLA  | C4-C3-C5-C6     |
| 30  | 5     | 313 | CHL  | CAA-CBA-CGA-O2A |
| 33  | 8     | 502 | OUR  | C46-C47-C48-C49 |
| 30  | c     | 607 | CHL  | O1A-CGA-O2A-C1  |
| 34  | 3     | 601 | LHG  | C25-C26-C27-C28 |
| 34  | 6     | 603 | LHG  | O10-C23-O8-C6   |
| 31  | A     | 829 | CLA  | C16-C17-C18-C19 |
| 30  | 2     | 302 | CHL  | C11-C10-C8-C7   |
| 30  | 7     | 306 | CHL  | C11-C10-C8-C7   |
| 30  | a     | 602 | CHL  | C12-C13-C15-C16 |
| 30  | c     | 602 | CHL  | C6-C7-C8-C10    |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 30  | f     | 602 | CHL  | C11-C12-C13-C15 |
| 31  | 0     | 308 | CLA  | C6-C7-C8-C10    |
| 31  | 9     | 302 | CLA  | C11-C10-C8-C7   |
| 31  | 9     | 308 | CLA  | C11-C10-C8-C7   |
| 31  | A     | 806 | CLA  | C12-C13-C15-C16 |
| 31  | A     | 818 | CLA  | C12-C13-C15-C16 |
| 31  | A     | 827 | CLA  | C6-C7-C8-C10    |
| 30  | f     | 609 | CHL  | C5-C6-C7-C8     |
| 31  | A     | 813 | CLA  | O1A-CGA-O2A-C1  |
| 34  | 2     | 601 | LHG  | C12-C13-C14-C15 |
| 31  | 5     | 309 | CLA  | CBA-CGA-O2A-C1  |
| 31  | 7     | 317 | CLA  | CAA-CBA-CGA-O2A |
| 34  | e     | 630 | LHG  | C11-C12-C13-C14 |
| 31  | 8     | 304 | CLA  | C16-C17-C18-C20 |
| 31  | A     | 835 | CLA  | O1D-CGD-O2D-CED |
| 33  | 6     | 501 | 0UR  | C46-C47-C48-C49 |
| 33  | 8     | 501 | 0UR  | C46-C47-C48-C49 |
| 33  | c     | 520 | 0UR  | C46-C47-C48-C49 |
| 33  | b     | 520 | 0UR  | C46-C47-C48-C49 |
| 33  | e     | 520 | 0UR  | C46-C47-C48-C49 |
| 34  | 8     | 601 | LHG  | O10-C23-O8-C6   |
| 36  | O     | 207 | LMG  | C12-C13-C14-C15 |
| 36  | O     | 207 | LMG  | O7-C8-C9-O8     |
| 30  | 3     | 307 | CHL  | C3A-C2A-CAA-CBA |
| 30  | 9     | 306 | CHL  | C3A-C2A-CAA-CBA |
| 30  | f     | 609 | CHL  | C4-C3-C5-C6     |
| 30  | i     | 608 | CHL  | C3A-C2A-CAA-CBA |
| 31  | 5     | 304 | CLA  | C3A-C2A-CAA-CBA |
| 31  | A     | 828 | CLA  | C3A-C2A-CAA-CBA |
| 31  | B     | 829 | CLA  | C4-C3-C5-C6     |
| 31  | F     | 301 | CLA  | C3A-C2A-CAA-CBA |
| 31  | K     | 102 | CLA  | C4-C3-C5-C6     |
| 31  | 9     | 312 | CLA  | C2-C3-C5-C6     |
| 31  | B     | 808 | CLA  | C2-C3-C5-C6     |
| 36  | L     | 211 | LMG  | C30-C31-C32-C33 |
| 31  | 0     | 303 | CLA  | C10-C11-C12-C13 |
| 31  | 2     | 304 | CLA  | C5-C6-C7-C8     |
| 31  | 6     | 320 | CLA  | O1D-CGD-O2D-CED |
| 32  | 2     | 402 | 8CT  | C19-C20-C21-C22 |
| 32  | 3     | 402 | 8CT  | C40-C12-C13-C14 |
| 32  | 7     | 404 | 8CT  | C24-C25-C26-C27 |
| 32  | 7     | 405 | 8CT  | C24-C25-C26-C27 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 32  | 8     | 406 | 8CT  | C24-C25-C26-C27 |
| 32  | B     | 843 | 8CT  | C39-C16-C17-C18 |
| 32  | B     | 844 | 8CT  | C39-C16-C17-C18 |
| 32  | B     | 844 | 8CT  | C19-C20-C21-C22 |
| 32  | B     | 844 | 8CT  | C24-C25-C26-C27 |
| 32  | B     | 845 | 8CT  | C39-C16-C17-C18 |
| 32  | B     | 845 | 8CT  | C24-C25-C26-C27 |
| 32  | B     | 846 | 8CT  | C40-C12-C13-C14 |
| 32  | B     | 846 | 8CT  | C39-C16-C17-C18 |
| 32  | B     | 848 | 8CT  | C24-C25-C26-C27 |
| 32  | B     | 851 | 8CT  | C40-C12-C13-C14 |
| 32  | J     | 104 | 8CT  | C40-C12-C13-C14 |
| 32  | 4     | 402 | 8CT  | C19-C20-C21-C22 |
| 42  | a     | 523 | NEX  | C39-C29-C30-C31 |
| 42  | c     | 523 | NEX  | C39-C29-C30-C31 |
| 42  | b     | 523 | NEX  | C39-C29-C30-C31 |
| 42  | d     | 523 | NEX  | C39-C29-C30-C31 |
| 42  | f     | 523 | NEX  | C39-C29-C30-C31 |
| 42  | g     | 523 | NEX  | C39-C29-C30-C31 |
| 42  | h     | 523 | NEX  | C39-C29-C30-C31 |
| 42  | i     | 523 | NEX  | C39-C29-C30-C31 |
| 42  | e     | 523 | NEX  | C39-C29-C30-C31 |
| 31  | B     | 834 | CLA  | C10-C11-C12-C13 |
| 31  | B     | 830 | CLA  | C11-C10-C8-C9   |
| 31  | g     | 612 | CLA  | CAA-CBA-CGA-O2A |
| 30  | 6     | 301 | CHL  | C5-C6-C7-C8     |
| 30  | g     | 606 | CHL  | O1D-CGD-O2D-CED |
| 30  | 1     | 305 | CHL  | C2-C1-O2A-CGA   |
| 30  | 7     | 306 | CHL  | C2-C1-O2A-CGA   |
| 30  | 9     | 305 | CHL  | C2-C1-O2A-CGA   |
| 30  | f     | 602 | CHL  | C2-C1-O2A-CGA   |
| 32  | B     | 847 | 8CT  | C12-C13-C14-C15 |
| 33  | 8     | 502 | 0UR  | C3-C4-C5-C6     |
| 31  | 0     | 311 | CLA  | O1D-CGD-O2D-CED |
| 34  | 7     | 602 | LHG  | C13-C14-C15-C16 |
| 34  | h     | 630 | LHG  | C28-C29-C30-C31 |
| 31  | 3     | 308 | CLA  | C5-C6-C7-C8     |
| 31  | B     | 806 | CLA  | C15-C16-C17-C18 |
| 32  | 2     | 402 | 8CT  | C10-C11-C12-C40 |
| 33  | 4     | 502 | 0UR  | C5-C6-C7-C20    |
| 31  | 8     | 314 | CLA  | CAA-CBA-CGA-O1A |
| 31  | i     | 612 | CLA  | CAA-CBA-CGA-O1A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 30  | g     | 602 | CHL  | C4-C3-C5-C6     |
| 31  | 6     | 320 | CLA  | C4-C3-C5-C6     |
| 31  | A     | 836 | CLA  | C4-C3-C5-C6     |
| 30  | 2     | 308 | CHL  | C2C-C3C-CAC-CBC |
| 31  | A     | 829 | CLA  | CBA-CGA-O2A-C1  |
| 31  | a     | 611 | CLA  | C8-C10-C11-C12  |
| 36  | A     | 856 | LMG  | C33-C34-C35-C36 |
| 30  | 5     | 306 | CHL  | C2C-C3C-CAC-CBC |
| 31  | B     | 832 | CLA  | C15-C16-C17-C18 |
| 33  | 0     | 502 | 0UR  | C15-C16-C17-C18 |
| 31  | e     | 613 | CLA  | C4-C3-C5-C6     |
| 36  | 9     | 602 | LMG  | C31-C32-C33-C34 |
| 31  | 8     | 304 | CLA  | C16-C17-C18-C19 |
| 30  | 1     | 313 | CHL  | C5-C6-C7-C8     |
| 31  | 9     | 300 | CLA  | C5-C6-C7-C8     |
| 31  | A     | 816 | CLA  | O1D-CGD-O2D-CED |
| 34  | 0     | 601 | LHG  | C9-C10-C11-C12  |
| 31  | 5     | 311 | CLA  | C2A-CAA-CBA-CGA |
| 31  | K     | 102 | CLA  | C5-C6-C7-C8     |
| 31  | 6     | 318 | CLA  | CAA-CBA-CGA-O1A |
| 31  | 6     | 320 | CLA  | CBD-CGD-O2D-CED |
| 31  | 7     | 317 | CLA  | CAA-CBA-CGA-O1A |
| 31  | e     | 612 | CLA  | CAA-CBA-CGA-O1A |
| 31  | A     | 829 | CLA  | O1A-CGA-O2A-C1  |
| 30  | 7     | 306 | CHL  | C11-C10-C8-C9   |
| 30  | a     | 609 | CHL  | C11-C10-C8-C9   |
| 30  | c     | 608 | CHL  | C11-C12-C13-C14 |
| 30  | b     | 608 | CHL  | C11-C12-C13-C14 |
| 30  | e     | 602 | CHL  | C11-C10-C8-C9   |
| 30  | e     | 609 | CHL  | C11-C10-C8-C9   |
| 31  | 0     | 308 | CLA  | C6-C7-C8-C9     |
| 31  | 1     | 310 | CLA  | C11-C12-C13-C14 |
| 31  | 7     | 308 | CLA  | C11-C10-C8-C9   |
| 31  | 9     | 302 | CLA  | C11-C10-C8-C9   |
| 31  | A     | 809 | CLA  | C11-C10-C8-C9   |
| 31  | B     | 806 | CLA  | C14-C13-C15-C16 |
| 31  | B     | 816 | CLA  | C6-C7-C8-C9     |
| 31  | B     | 827 | CLA  | C11-C10-C8-C9   |
| 31  | B     | 813 | CLA  | C6-C7-C8-C10    |
| 31  | A     | 820 | CLA  | C5-C6-C7-C8     |
| 34  | 2     | 601 | LHG  | C9-C10-C11-C12  |
| 31  | h     | 612 | CLA  | CAA-CBA-CGA-O1A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 30  | 9     | 305 | CHL  | O2A-C1-C2-C3    |
| 36  | J     | 102 | LMG  | C7-C8-O7-C10    |
| 31  | A     | 829 | CLA  | C5-C6-C7-C8     |
| 30  | 1     | 302 | CHL  | C1A-C2A-CAA-CBA |
| 30  | 2     | 302 | CHL  | C1A-C2A-CAA-CBA |
| 30  | 5     | 306 | CHL  | C1A-C2A-CAA-CBA |
| 30  | 5     | 313 | CHL  | C1A-C2A-CAA-CBA |
| 30  | 6     | 301 | CHL  | C1A-C2A-CAA-CBA |
| 30  | 7     | 302 | CHL  | C1A-C2A-CAA-CBA |
| 30  | 9     | 313 | CHL  | C1A-C2A-CAA-CBA |
| 30  | c     | 601 | CHL  | C1A-C2A-CAA-CBA |
| 30  | f     | 602 | CHL  | C1A-C2A-CAA-CBA |
| 30  | e     | 602 | CHL  | C1A-C2A-CAA-CBA |
| 30  | 4     | 307 | CHL  | C1A-C2A-CAA-CBA |
| 31  | c     | 612 | CLA  | CAA-CBA-CGA-O1A |
| 34  | 6     | 601 | LHG  | C23-C24-C25-C26 |
| 31  | B     | 840 | CLA  | C16-C17-C18-C20 |
| 33  | 6     | 502 | OUR  | C46-C47-C48-C49 |
| 31  | A     | 816 | CLA  | CBD-CGD-O2D-CED |
| 34  | 6     | 603 | LHG  | O1-C1-C2-O2     |
| 31  | g     | 612 | CLA  | CAA-CBA-CGA-O1A |
| 31  | 6     | 312 | CLA  | C2A-CAA-CBA-CGA |
| 31  | 7     | 312 | CLA  | C2A-CAA-CBA-CGA |
| 31  | 9     | 312 | CLA  | C2A-CAA-CBA-CGA |
| 31  | A     | 818 | CLA  | C2A-CAA-CBA-CGA |
| 34  | 9     | 601 | LHG  | C29-C30-C31-C32 |
| 31  | 5     | 310 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 6     | 310 | CLA  | C1A-C2A-CAA-CBA |
| 31  | A     | 802 | CLA  | C1A-C2A-CAA-CBA |
| 31  | A     | 828 | CLA  | C1A-C2A-CAA-CBA |
| 31  | B     | 813 | CLA  | C1A-C2A-CAA-CBA |
| 31  | B     | 816 | CLA  | C1A-C2A-CAA-CBA |
| 31  | c     | 610 | CLA  | C1A-C2A-CAA-CBA |
| 31  | d     | 604 | CLA  | C1A-C2A-CAA-CBA |
| 32  | 2     | 402 | 8CT  | C19-C20-C21-C23 |
| 32  | 3     | 402 | 8CT  | C11-C12-C13-C14 |
| 32  | 7     | 404 | 8CT  | C24-C25-C26-C28 |
| 32  | 7     | 405 | 8CT  | C24-C25-C26-C28 |
| 32  | 8     | 406 | 8CT  | C24-C25-C26-C28 |
| 32  | B     | 843 | 8CT  | C15-C16-C17-C18 |
| 32  | B     | 844 | 8CT  | C15-C16-C17-C18 |
| 32  | B     | 844 | 8CT  | C19-C20-C21-C23 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 32  | B     | 844 | 8CT  | C24-C25-C26-C28 |
| 32  | B     | 845 | 8CT  | C15-C16-C17-C18 |
| 32  | B     | 845 | 8CT  | C24-C25-C26-C28 |
| 32  | B     | 846 | 8CT  | C11-C12-C13-C14 |
| 32  | B     | 846 | 8CT  | C15-C16-C17-C18 |
| 32  | B     | 848 | 8CT  | C24-C25-C26-C28 |
| 32  | B     | 851 | 8CT  | C11-C12-C13-C14 |
| 32  | J     | 104 | 8CT  | C11-C12-C13-C14 |
| 32  | 4     | 402 | 8CT  | C19-C20-C21-C23 |
| 37  | g     | 522 | 0IE  | O1-C2-C30-C31   |
| 42  | a     | 523 | NEX  | C28-C29-C30-C31 |
| 42  | c     | 523 | NEX  | C28-C29-C30-C31 |
| 42  | b     | 523 | NEX  | C28-C29-C30-C31 |
| 42  | d     | 523 | NEX  | C28-C29-C30-C31 |
| 42  | f     | 523 | NEX  | C28-C29-C30-C31 |
| 42  | g     | 523 | NEX  | C28-C29-C30-C31 |
| 42  | h     | 523 | NEX  | C28-C29-C30-C31 |
| 42  | i     | 523 | NEX  | C28-C29-C30-C31 |
| 42  | e     | 523 | NEX  | C28-C29-C30-C31 |
| 31  | A     | 804 | CLA  | C6-C7-C8-C10    |
| 34  | c     | 630 | LHG  | C23-C24-C25-C26 |
| 34  | h     | 630 | LHG  | C27-C28-C29-C30 |
| 34  | A     | 855 | LHG  | O6-C4-C5-O7     |
| 31  | 2     | 303 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 2     | 310 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 6     | 310 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 6     | 318 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 7     | 311 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 7     | 312 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 7     | 315 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 8     | 303 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 8     | 310 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 8     | 314 | CLA  | C2B-C3B-CAB-CBB |
| 31  | A     | 815 | CLA  | C2B-C3B-CAB-CBB |
| 31  | A     | 823 | CLA  | C2B-C3B-CAB-CBB |
| 31  | A     | 837 | CLA  | C2B-C3B-CAB-CBB |
| 31  | A     | 840 | CLA  | C2B-C3B-CAB-CBB |
| 31  | B     | 805 | CLA  | C2B-C3B-CAB-CBB |
| 31  | B     | 809 | CLA  | C2B-C3B-CAB-CBB |
| 31  | B     | 811 | CLA  | C2B-C3B-CAB-CBB |
| 31  | B     | 822 | CLA  | C2B-C3B-CAB-CBB |
| 31  | B     | 831 | CLA  | C2B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | B     | 834 | CLA  | C2B-C3B-CAB-CBB |
| 31  | B     | 840 | CLA  | C2B-C3B-CAB-CBB |
| 31  | F     | 301 | CLA  | C2B-C3B-CAB-CBB |
| 31  | L     | 207 | CLA  | C2B-C3B-CAB-CBB |
| 31  | K     | 101 | CLA  | C2B-C3B-CAB-CBB |
| 31  | O     | 206 | CLA  | C2B-C3B-CAB-CBB |
| 31  | a     | 611 | CLA  | C2B-C3B-CAB-CBB |
| 31  | b     | 603 | CLA  | C2B-C3B-CAB-CBB |
| 31  | d     | 611 | CLA  | C2B-C3B-CAB-CBB |
| 31  | d     | 612 | CLA  | C2B-C3B-CAB-CBB |
| 31  | d     | 613 | CLA  | C2B-C3B-CAB-CBB |
| 31  | f     | 603 | CLA  | C2B-C3B-CAB-CBB |
| 31  | e     | 603 | CLA  | C2B-C3B-CAB-CBB |
| 32  | 6     | 402 | 8CT  | C02-C03-C10-C11 |
| 32  | 8     | 402 | 8CT  | C02-C03-C10-C11 |
| 32  | A     | 847 | 8CT  | C04-C03-C10-C11 |
| 32  | B     | 843 | 8CT  | C04-C03-C10-C11 |
| 32  | B     | 844 | 8CT  | C04-C03-C10-C11 |
| 32  | B     | 848 | 8CT  | C02-C03-C10-C11 |
| 32  | B     | 851 | 8CT  | C02-C03-C10-C11 |
| 32  | F     | 302 | 8CT  | C04-C03-C10-C11 |
| 32  | G     | 104 | 8CT  | C02-C03-C10-C11 |
| 32  | 4     | 402 | 8CT  | C02-C03-C10-C11 |
| 31  | 8     | 314 | CLA  | CAA-CBA-CGA-O2A |
| 31  | 4     | 303 | CLA  | CAA-CBA-CGA-O2A |
| 31  | 5     | 309 | CLA  | O1A-CGA-O2A-C1  |
| 34  | 8     | 601 | LHG  | C9-C10-C11-C12  |
| 30  | 1     | 313 | CHL  | C14-C13-C15-C16 |
| 31  | 5     | 310 | CLA  | CBD-CGD-O2D-CED |
| 34  | 0     | 601 | LHG  | C16-C17-C18-C19 |
| 31  | c     | 612 | CLA  | CAA-CBA-CGA-O2A |
| 30  | 6     | 302 | CHL  | C4-C3-C5-C6     |
| 30  | i     | 602 | CHL  | C4-C3-C5-C6     |
| 31  | B     | 813 | CLA  | C4-C3-C5-C6     |
| 31  | B     | 822 | CLA  | C4-C3-C5-C6     |
| 34  | b     | 630 | LHG  | O6-C4-C5-C6     |
| 31  | 4     | 312 | CLA  | O1A-CGA-O2A-C1  |
| 30  | f     | 609 | CHL  | C2-C3-C5-C6     |
| 30  | 4     | 302 | CHL  | C2-C3-C5-C6     |
| 31  | e     | 613 | CLA  | C2-C3-C5-C6     |
| 34  | 6     | 601 | LHG  | C28-C29-C30-C31 |
| 34  | 6     | 601 | LHG  | C7-C8-C9-C10    |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 30  | i     | 608 | CHL  | O2A-C1-C2-C3    |
| 31  | 5     | 303 | CLA  | C8-C10-C11-C12  |
| 30  | 1     | 313 | CHL  | C6-C7-C8-C10    |
| 30  | 2     | 302 | CHL  | C11-C12-C13-C15 |
| 30  | i     | 602 | CHL  | C6-C7-C8-C10    |
| 31  | 3     | 309 | CLA  | C12-C13-C15-C16 |
| 31  | 6     | 317 | CLA  | C11-C12-C13-C15 |
| 31  | 9     | 308 | CLA  | C11-C12-C13-C15 |
| 31  | 9     | 312 | CLA  | C6-C7-C8-C10    |
| 31  | B     | 801 | CLA  | C12-C13-C15-C16 |
| 38  | B     | 842 | PQN  | C21-C22-C23-C25 |
| 31  | A     | 837 | CLA  | CBD-CGD-O2D-CED |
| 34  | 7     | 603 | LHG  | C9-C10-C11-C12  |
| 30  | 9     | 313 | CHL  | C2A-CAA-CBA-CGA |
| 31  | 1     | 303 | CLA  | C2A-CAA-CBA-CGA |
| 31  | A     | 840 | CLA  | C15-C16-C17-C18 |
| 33  | 3     | 501 | OUR  | C46-C47-C48-C49 |
| 31  | b     | 611 | CLA  | C10-C11-C12-C13 |
| 34  | H     | 203 | LHG  | C24-C23-O8-C6   |
| 31  | K     | 101 | CLA  | CBD-CGD-O2D-CED |
| 31  | 2     | 309 | CLA  | C11-C12-C13-C15 |
| 34  | 2     | 601 | LHG  | C25-C26-C27-C28 |
| 34  | 6     | 601 | LHG  | C10-C11-C12-C13 |
| 30  | 1     | 313 | CHL  | C12-C13-C15-C16 |
| 30  | 3     | 302 | CHL  | C12-C13-C15-C16 |
| 31  | 8     | 312 | CLA  | C11-C10-C8-C7   |
| 31  | B     | 830 | CLA  | C11-C10-C8-C7   |
| 30  | 7     | 302 | CHL  | C4-C3-C5-C6     |
| 30  | d     | 609 | CHL  | C4-C3-C5-C6     |
| 30  | e     | 609 | CHL  | C4-C3-C5-C6     |
| 31  | A     | 817 | CLA  | C4-C3-C5-C6     |
| 31  | L     | 203 | CLA  | C4-C3-C5-C6     |
| 30  | 2     | 301 | CHL  | C8-C10-C11-C12  |
| 30  | 2     | 302 | CHL  | C2-C3-C5-C6     |
| 30  | i     | 602 | CHL  | C2-C3-C5-C6     |
| 31  | 3     | 310 | CLA  | C2-C3-C5-C6     |
| 31  | A     | 819 | CLA  | C2-C3-C5-C6     |
| 31  | L     | 203 | CLA  | C2-C3-C5-C6     |
| 30  | 1     | 302 | CHL  | C2-C1-O2A-CGA   |
| 30  | 5     | 307 | CHL  | O1A-CGA-O2A-C1  |
| 31  | B     | 841 | CLA  | CBD-CGD-O2D-CED |
| 31  | A     | 825 | CLA  | C8-C10-C11-C12  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | A     | 828 | CLA  | C8-C10-C11-C12  |
| 30  | 4     | 306 | CHL  | O1D-CGD-O2D-CED |
| 31  | B     | 832 | CLA  | C13-C15-C16-C17 |
| 31  | 4     | 309 | CLA  | C10-C11-C12-C13 |
| 31  | 4     | 303 | CLA  | CAA-CBA-CGA-O1A |
| 30  | 0     | 302 | CHL  | C14-C13-C15-C16 |
| 30  | 2     | 302 | CHL  | C14-C13-C15-C16 |
| 30  | 6     | 308 | CHL  | C6-C7-C8-C9     |
| 31  | A     | 818 | CLA  | C11-C10-C8-C9   |
| 31  | A     | 826 | CLA  | C11-C12-C13-C14 |
| 31  | B     | 814 | CLA  | C14-C13-C15-C16 |
| 30  | 5     | 306 | CHL  | C2-C1-O2A-CGA   |
| 32  | K     | 107 | 8CT  | C23-C24-C25-C26 |
| 31  | B     | 818 | CLA  | C11-C12-C13-C14 |
| 31  | K     | 102 | CLA  | C4C-C3C-CAC-CBC |
| 31  | 7     | 303 | CLA  | CAA-CBA-CGA-O2A |
| 31  | e     | 612 | CLA  | CAA-CBA-CGA-O2A |
| 30  | d     | 602 | CHL  | C5-C6-C7-C8     |
| 30  | c     | 609 | CHL  | C4-C3-C5-C6     |
| 30  | b     | 609 | CHL  | C4-C3-C5-C6     |
| 30  | f     | 601 | CHL  | C4-C3-C5-C6     |
| 31  | A     | 808 | CLA  | C4-C3-C5-C6     |
| 31  | A     | 809 | CLA  | C4-C3-C5-C6     |
| 31  | A     | 810 | CLA  | C4-C3-C5-C6     |
| 31  | h     | 612 | CLA  | CAA-CBA-CGA-O2A |
| 31  | 3     | 320 | CLA  | C2-C3-C5-C6     |
| 30  | a     | 601 | CHL  | CBA-CGA-O2A-C1  |
| 30  | d     | 602 | CHL  | C8-C10-C11-C12  |
| 39  | A     | 857 | CL0  | C8-C10-C11-C12  |
| 30  | i     | 607 | CHL  | O1A-CGA-O2A-C1  |
| 31  | B     | 813 | CLA  | C6-C7-C8-C9     |
| 31  | 1     | 309 | CLA  | CBA-CGA-O2A-C1  |
| 31  | A     | 836 | CLA  | C2C-C3C-CAC-CBC |
| 31  | h     | 603 | CLA  | O2A-C1-C2-C3    |
| 30  | 5     | 306 | CHL  | CAA-CBA-CGA-O1A |
| 31  | B     | 813 | CLA  | C5-C6-C7-C8     |
| 31  | B     | 808 | CLA  | CAA-CBA-CGA-O2A |
| 34  | A     | 845 | LHG  | C4-C5-C6-O8     |
| 34  | H     | 203 | LHG  | O10-C23-O8-C6   |
| 31  | B     | 806 | CLA  | C2A-CAA-CBA-CGA |
| 31  | c     | 603 | CLA  | C2A-CAA-CBA-CGA |
| 31  | 0     | 321 | CLA  | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | b     | 612 | CLA  | CAA-CBA-CGA-O2A |
| 31  | 1     | 309 | CLA  | O1A-CGA-O2A-C1  |
| 34  | 7     | 603 | LHG  | O1-C1-C2-O2     |
| 34  | b     | 630 | LHG  | O1-C1-C2-O2     |
| 34  | b     | 630 | LHG  | C25-C26-C27-C28 |
| 30  | a     | 609 | CHL  | C4-C3-C5-C6     |
| 31  | B     | 811 | CLA  | C4-C3-C5-C6     |
| 31  | G     | 102 | CLA  | CAA-CBA-CGA-O2A |
| 31  | B     | 811 | CLA  | C2-C3-C5-C6     |
| 34  | A     | 855 | LHG  | C9-C10-C11-C12  |
| 34  | G     | 105 | LHG  | C10-C11-C12-C13 |
| 34  | M     | 104 | LHG  | C10-C11-C12-C13 |
| 31  | 1     | 314 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 5     | 303 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 8     | 314 | CLA  | C4B-C3B-CAB-CBB |
| 31  | A     | 815 | CLA  | C4B-C3B-CAB-CBB |
| 31  | A     | 837 | CLA  | C4B-C3B-CAB-CBB |
| 31  | B     | 831 | CLA  | C4B-C3B-CAB-CBB |
| 31  | L     | 203 | CLA  | C4B-C3B-CAB-CBB |
| 31  | d     | 613 | CLA  | C4B-C3B-CAB-CBB |
| 31  | i     | 611 | CLA  | C4B-C3B-CAB-CBB |
| 33  | 4     | 502 | 0UR  | O42-C2-C3-C4    |
| 37  | c     | 522 | 0IE  | O1-C2-C3-C4     |
| 30  | 0     | 301 | CHL  | O1A-CGA-O2A-C1  |
| 30  | 1     | 306 | CHL  | C2-C1-O2A-CGA   |
| 31  | A     | 837 | CLA  | O1D-CGD-O2D-CED |
| 31  | e     | 604 | CLA  | CBD-CGD-O2D-CED |
| 34  | 9     | 601 | LHG  | C26-C27-C28-C29 |
| 31  | 6     | 312 | CLA  | O1A-CGA-O2A-C1  |
| 31  | A     | 803 | CLA  | C16-C17-C18-C19 |
| 31  | 6     | 318 | CLA  | CBD-CGD-O2D-CED |
| 30  | e     | 607 | CHL  | O1A-CGA-O2A-C1  |
| 34  | f     | 630 | LHG  | C1-C2-C3-O3     |
| 34  | a     | 630 | LHG  | C17-C18-C19-C20 |
| 30  | 7     | 306 | CHL  | CHA-CBD-CGD-O2D |
| 30  | 7     | 313 | CHL  | CHA-CBD-CGD-O1D |
| 30  | d     | 601 | CHL  | CHA-CBD-CGD-O1D |
| 30  | f     | 607 | CHL  | CHA-CBD-CGD-O1D |
| 30  | f     | 607 | CHL  | CHA-CBD-CGD-O2D |
| 30  | g     | 601 | CHL  | CHA-CBD-CGD-O1D |
| 30  | g     | 601 | CHL  | CHA-CBD-CGD-O2D |
| 30  | g     | 605 | CHL  | CHA-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 30  | g     | 605 | CHL  | CHA-CBD-CGD-O2D |
| 30  | g     | 609 | CHL  | CHA-CBD-CGD-O1D |
| 30  | g     | 609 | CHL  | CHA-CBD-CGD-O2D |
| 30  | e     | 609 | CHL  | CHA-CBD-CGD-O1D |
| 30  | 4     | 319 | CHL  | CHA-CBD-CGD-O1D |
| 30  | 4     | 319 | CHL  | CHA-CBD-CGD-O2D |
| 30  | g     | 602 | CHL  | O1A-CGA-O2A-C1  |
| 31  | 7     | 304 | CLA  | C3-C5-C6-C7     |
| 30  | 5     | 305 | CHL  | CAA-CBA-CGA-O2A |
| 34  | d     | 630 | LHG  | C9-C10-C11-C12  |
| 36  | 9     | 602 | LMG  | C35-C36-C37-C38 |
| 31  | A     | 808 | CLA  | C16-C17-C18-C19 |
| 31  | d     | 603 | CLA  | C6-C7-C8-C10    |
| 36  | L     | 210 | LMG  | O1-C7-C8-O7     |
| 30  | e     | 602 | CHL  | C8-C10-C11-C12  |
| 34  | 3     | 601 | LHG  | C12-C13-C14-C15 |
| 30  | c     | 609 | CHL  | C2-C3-C5-C6     |
| 33  | 2     | 501 | 0UR  | C46-C47-C48-C49 |
| 33  | 9     | 501 | 0UR  | C46-C47-C48-C49 |
| 33  | h     | 520 | 0UR  | C46-C47-C48-C49 |
| 31  | e     | 604 | CLA  | O1D-CGD-O2D-CED |
| 30  | e     | 608 | CHL  | C11-C12-C13-C15 |
| 31  | A     | 818 | CLA  | C11-C10-C8-C7   |
| 31  | A     | 821 | CLA  | C6-C7-C8-C10    |
| 31  | B     | 808 | CLA  | C6-C7-C8-C10    |
| 31  | i     | 611 | CLA  | CAA-CBA-CGA-O2A |
| 31  | 4     | 314 | CLA  | CAA-CBA-CGA-O2A |
| 41  | B     | 849 | DGD  | C6A-C7A-C8A-C9A |
| 31  | A     | 808 | CLA  | C13-C15-C16-C17 |
| 30  | 1     | 307 | CHL  | C3-C5-C6-C7     |
| 31  | 7     | 303 | CLA  | CAA-CBA-CGA-O1A |
| 32  | 3     | 402 | 8CT  | C10-C11-C12-C13 |
| 31  | 4     | 312 | CLA  | CBA-CGA-O2A-C1  |
| 30  | c     | 609 | CHL  | C11-C12-C13-C14 |
| 31  | 0     | 303 | CLA  | C11-C12-C13-C14 |
| 31  | 1     | 303 | CLA  | C6-C7-C8-C9     |
| 31  | 5     | 312 | CLA  | C6-C7-C8-C9     |
| 31  | A     | 821 | CLA  | C6-C7-C8-C9     |
| 31  | A     | 852 | CLA  | C14-C13-C15-C16 |
| 31  | 4     | 309 | CLA  | C6-C7-C8-C9     |
| 31  | B     | 840 | CLA  | C2C-C3C-CAC-CBC |
| 31  | A     | 841 | CLA  | C8-C10-C11-C12  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 36  | 2     | 602 | LMG  | C8-C7-O1-C1     |
| 31  | A     | 828 | CLA  | CAA-CBA-CGA-O2A |
| 36  | L     | 211 | LMG  | C29-C30-C31-C32 |
| 31  | a     | 612 | CLA  | CAA-CBA-CGA-O2A |
| 33  | 5     | 501 | 0UR  | C46-C47-C48-C49 |
| 33  | 4     | 501 | 0UR  | C46-C47-C48-C49 |
| 31  | 0     | 312 | CLA  | C2A-CAA-CBA-CGA |
| 31  | 7     | 318 | CLA  | C2A-CAA-CBA-CGA |
| 31  | 8     | 312 | CLA  | C2A-CAA-CBA-CGA |
| 31  | A     | 836 | CLA  | C2A-CAA-CBA-CGA |
| 31  | 4     | 312 | CLA  | C2A-CAA-CBA-CGA |
| 30  | 3     | 302 | CHL  | C2-C1-O2A-CGA   |
| 30  | 5     | 301 | CHL  | C2-C1-O2A-CGA   |
| 30  | 6     | 313 | CHL  | C2-C1-O2A-CGA   |
| 30  | 7     | 302 | CHL  | C2-C1-O2A-CGA   |
| 30  | 8     | 302 | CHL  | C2-C1-O2A-CGA   |
| 30  | a     | 606 | CHL  | C2-C1-O2A-CGA   |
| 30  | b     | 602 | CHL  | C2-C1-O2A-CGA   |
| 30  | f     | 609 | CHL  | C2-C1-O2A-CGA   |
| 30  | 4     | 302 | CHL  | C2-C1-O2A-CGA   |
| 31  | A     | 821 | CLA  | C2-C1-O2A-CGA   |
| 31  | K     | 102 | CLA  | C2-C1-O2A-CGA   |
| 30  | 3     | 305 | CHL  | O1A-CGA-O2A-C1  |
| 34  | B     | 854 | LHG  | C35-C36-C37-C38 |
| 39  | A     | 857 | CL0  | C13-C15-C16-C17 |
| 30  | 0     | 301 | CHL  | CBA-CGA-O2A-C1  |
| 30  | 3     | 305 | CHL  | CBA-CGA-O2A-C1  |
| 31  | 6     | 312 | CLA  | CBA-CGA-O2A-C1  |
| 30  | f     | 601 | CHL  | C3A-C2A-CAA-CBA |
| 30  | h     | 601 | CHL  | C3A-C2A-CAA-CBA |
| 31  | 3     | 313 | CLA  | C3A-C2A-CAA-CBA |
| 31  | A     | 802 | CLA  | C3A-C2A-CAA-CBA |
| 31  | A     | 821 | CLA  | C4-C3-C5-C6     |
| 31  | d     | 611 | CLA  | C3A-C2A-CAA-CBA |
| 31  | i     | 604 | CLA  | C3A-C2A-CAA-CBA |
| 31  | e     | 611 | CLA  | C3A-C2A-CAA-CBA |
| 31  | b     | 612 | CLA  | CAA-CBA-CGA-O1A |
| 31  | A     | 814 | CLA  | C2-C3-C5-C6     |
| 34  | G     | 105 | LHG  | C14-C15-C16-C17 |
| 34  | 7     | 602 | LHG  | C11-C12-C13-C14 |
| 34  | H     | 203 | LHG  | O10-C23-C24-C25 |
| 31  | B     | 807 | CLA  | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | f     | 612 | CLA  | CAA-CBA-CGA-O2A |
| 30  | i     | 609 | CHL  | C2-C1-O2A-CGA   |
| 31  | 7     | 318 | CLA  | C11-C12-C13-C14 |
| 31  | 6     | 318 | CLA  | O1D-CGD-O2D-CED |
| 33  | 0     | 502 | 0UR  | C46-C47-C48-C49 |
| 33  | 1     | 501 | 0UR  | C46-C47-C48-C49 |
| 33  | 5     | 502 | 0UR  | C46-C47-C48-C49 |
| 30  | 0     | 306 | CHL  | C3C-C2C-CMC-OMC |
| 30  | 6     | 313 | CHL  | C3C-C2C-CMC-OMC |
| 30  | 7     | 301 | CHL  | C3C-C2C-CMC-OMC |
| 30  | 8     | 305 | CHL  | C3C-C2C-CMC-OMC |
| 30  | d     | 605 | CHL  | C3C-C2C-CMC-OMC |
| 30  | h     | 606 | CHL  | C3C-C2C-CMC-OMC |
| 30  | e     | 602 | CHL  | C3C-C2C-CMC-OMC |
| 30  | e     | 605 | CHL  | C3C-C2C-CMC-OMC |
| 30  | e     | 606 | CHL  | C3C-C2C-CMC-OMC |
| 31  | 0     | 321 | CLA  | CAA-CBA-CGA-O1A |
| 34  | 8     | 601 | LHG  | C31-C32-C33-C34 |
| 34  | 8     | 601 | LHG  | O2-C2-C3-O3     |
| 31  | A     | 832 | CLA  | C13-C15-C16-C17 |
| 30  | 5     | 305 | CHL  | CAA-CBA-CGA-O1A |
| 31  | 6     | 314 | CLA  | CAA-CBA-CGA-O2A |
| 31  | 9     | 302 | CLA  | C15-C16-C17-C18 |
| 34  | b     | 630 | LHG  | C9-C10-C11-C12  |
| 31  | B     | 819 | CLA  | C11-C12-C13-C14 |
| 33  | 1     | 502 | 0UR  | C4-C3-C43-O44   |
| 31  | G     | 102 | CLA  | CAA-CBA-CGA-O1A |
| 34  | 9     | 601 | LHG  | C5-C4-O6-P      |
| 30  | 7     | 305 | CHL  | C2-C1-O2A-CGA   |
| 31  | A     | 822 | CLA  | O2A-C1-C2-C3    |
| 34  | 5     | 601 | LHG  | C27-C28-C29-C30 |
| 36  | O     | 207 | LMG  | O6-C1-O1-C7     |
| 30  | 3     | 307 | CHL  | C10-C11-C12-C13 |
| 30  | g     | 602 | CHL  | CBA-CGA-O2A-C1  |
| 31  | a     | 612 | CLA  | CAA-CBA-CGA-O1A |
| 34  | 0     | 601 | LHG  | C4-C5-C6-O8     |
| 34  | B     | 854 | LHG  | C4-C5-C6-O8     |
| 36  | J     | 102 | LMG  | O1-C7-C8-C9     |
| 31  | A     | 836 | CLA  | CBD-CGD-O2D-CED |
| 30  | b     | 609 | CHL  | C5-C6-C7-C8     |
| 30  | 4     | 319 | CHL  | C5-C6-C7-C8     |
| 30  | b     | 602 | CHL  | C10-C11-C12-C13 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 34  | A     | 845 | LHG  | C10-C11-C12-C13 |
| 31  | A     | 821 | CLA  | CBA-CGA-O2A-C1  |
| 31  | A     | 813 | CLA  | C4-C3-C5-C6     |
| 31  | B     | 815 | CLA  | C2A-CAA-CBA-CGA |
| 31  | b     | 604 | CLA  | C2A-CAA-CBA-CGA |
| 31  | d     | 612 | CLA  | CAA-CBA-CGA-O1A |
| 30  | b     | 609 | CHL  | C2C-C3C-CAC-CBC |
| 31  | 4     | 309 | CLA  | C11-C12-C13-C15 |
| 38  | B     | 842 | PQN  | C15-C16-C17-C18 |
| 31  | B     | 807 | CLA  | CAA-CBA-CGA-O1A |
| 31  | A     | 817 | CLA  | C14-C13-C15-C16 |
| 31  | K     | 105 | CLA  | CAA-CBA-CGA-O2A |
| 36  | 2     | 602 | LMG  | O8-C28-C29-C30  |
| 30  | g     | 607 | CHL  | O1A-CGA-O2A-C1  |
| 31  | i     | 611 | CLA  | CAA-CBA-CGA-O1A |
| 30  | 1     | 302 | CHL  | C11-C12-C13-C14 |
| 30  | 3     | 302 | CHL  | C11-C10-C8-C9   |
| 30  | 3     | 307 | CHL  | C11-C12-C13-C14 |
| 30  | f     | 609 | CHL  | C6-C7-C8-C9     |
| 31  | 3     | 308 | CLA  | C11-C10-C8-C9   |
| 31  | A     | 853 | CLA  | C11-C12-C13-C14 |
| 31  | B     | 832 | CLA  | C6-C7-C8-C9     |
| 31  | B     | 841 | CLA  | C14-C13-C15-C16 |
| 38  | A     | 842 | PQN  | C21-C22-C23-C24 |
| 31  | 0     | 313 | CLA  | CAA-CBA-CGA-O2A |
| 34  | 7     | 602 | LHG  | O7-C7-C8-C9     |
| 31  | f     | 612 | CLA  | CAA-CBA-CGA-O1A |
| 31  | 4     | 314 | CLA  | CAA-CBA-CGA-O1A |
| 42  | a     | 523 | NEX  | C31-C32-C33-C34 |
| 42  | c     | 523 | NEX  | C31-C32-C33-C34 |
| 42  | b     | 523 | NEX  | C31-C32-C33-C34 |
| 42  | d     | 523 | NEX  | C31-C32-C33-C34 |
| 42  | g     | 523 | NEX  | C31-C32-C33-C34 |
| 42  | h     | 523 | NEX  | C31-C32-C33-C34 |
| 42  | i     | 523 | NEX  | C31-C32-C33-C34 |
| 34  | c     | 630 | LHG  | C25-C26-C27-C28 |
| 34  | 8     | 601 | LHG  | C11-C10-C9-C8   |
| 31  | A     | 820 | CLA  | CAA-CBA-CGA-O2A |
| 34  | b     | 630 | LHG  | O7-C7-C8-C9     |
| 30  | 6     | 302 | CHL  | C2-C3-C5-C6     |
| 30  | e     | 609 | CHL  | C2-C3-C5-C6     |
| 30  | 0     | 306 | CHL  | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 30  | 8     | 313 | CHL  | C2A-CAA-CBA-CGA |
| 30  | 2     | 319 | CHL  | C6-C7-C8-C10    |
| 30  | 6     | 308 | CHL  | C6-C7-C8-C10    |
| 30  | 7     | 302 | CHL  | C6-C7-C8-C10    |
| 30  | a     | 609 | CHL  | C6-C7-C8-C10    |
| 30  | b     | 602 | CHL  | C11-C12-C13-C15 |
| 30  | d     | 609 | CHL  | C6-C7-C8-C10    |
| 30  | f     | 601 | CHL  | C11-C12-C13-C15 |
| 31  | 7     | 309 | CLA  | C11-C10-C8-C7   |
| 31  | 9     | 308 | CLA  | C6-C7-C8-C10    |
| 31  | A     | 826 | CLA  | C11-C12-C13-C15 |
| 31  | B     | 803 | CLA  | C6-C7-C8-C10    |
| 31  | B     | 814 | CLA  | C12-C13-C15-C16 |
| 31  | B     | 816 | CLA  | C6-C7-C8-C10    |
| 31  | A     | 805 | CLA  | C3-C5-C6-C7     |
| 30  | c     | 609 | CHL  | C2C-C3C-CAC-CBC |
| 34  | K     | 106 | LHG  | C35-C36-C37-C38 |
| 31  | d     | 612 | CLA  | CAA-CBA-CGA-O2A |
| 31  | 1     | 314 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 5     | 310 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 6     | 320 | CLA  | C2B-C3B-CAB-CBB |
| 31  | A     | 809 | CLA  | C2B-C3B-CAB-CBB |
| 31  | B     | 841 | CLA  | C2B-C3B-CAB-CBB |
| 32  | 7     | 402 | 8CT  | C02-C03-C10-C11 |
| 32  | J     | 101 | 8CT  | C02-C03-C10-C11 |
| 32  | M     | 102 | 8CT  | C02-C03-C10-C11 |
| 34  | A     | 845 | LHG  | O8-C23-C24-C25  |
| 31  | 5     | 303 | CLA  | CAA-CBA-CGA-O2A |
| 33  | 7     | 501 | 0UR  | C46-C47-C48-C49 |
| 34  | 8     | 601 | LHG  | C27-C28-C29-C30 |
| 30  | 1     | 313 | CHL  | C2-C1-O2A-CGA   |
| 30  | 8     | 307 | CHL  | C2-C1-O2A-CGA   |
| 30  | c     | 602 | CHL  | C2-C1-O2A-CGA   |
| 30  | d     | 609 | CHL  | C2-C1-O2A-CGA   |
| 31  | 7     | 308 | CLA  | C2-C1-O2A-CGA   |
| 31  | A     | 839 | CLA  | C2-C1-O2A-CGA   |
| 31  | A     | 853 | CLA  | C2-C1-O2A-CGA   |
| 31  | B     | 812 | CLA  | C2-C1-O2A-CGA   |
| 31  | h     | 613 | CLA  | CAA-CBA-CGA-O2A |
| 30  | 9     | 305 | CHL  | CAA-CBA-CGA-O2A |
| 30  | a     | 606 | CHL  | CAA-CBA-CGA-O2A |
| 31  | L     | 203 | CLA  | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 34  | A     | 844 | LHG  | O8-C23-C24-C25  |
| 30  | 4     | 306 | CHL  | CBD-CGD-O2D-CED |
| 31  | K     | 101 | CLA  | O1D-CGD-O2D-CED |
| 33  | 0     | 501 | 0UR  | O42-C2-C3-C43   |
| 33  | 0     | 502 | 0UR  | O42-C2-C3-C43   |
| 33  | 1     | 501 | 0UR  | O42-C2-C3-C43   |
| 33  | 3     | 501 | 0UR  | O42-C2-C3-C43   |
| 33  | 6     | 501 | 0UR  | O42-C2-C3-C43   |
| 33  | 7     | 501 | 0UR  | O42-C2-C3-C43   |
| 33  | 8     | 501 | 0UR  | O42-C2-C3-C43   |
| 33  | 9     | 501 | 0UR  | O42-C2-C3-C43   |
| 33  | c     | 520 | 0UR  | O42-C2-C3-C43   |
| 33  | h     | 520 | 0UR  | O42-C2-C3-C43   |
| 33  | i     | 520 | 0UR  | O42-C2-C3-C43   |
| 33  | 4     | 501 | 0UR  | O42-C2-C3-C43   |
| 37  | 3     | 502 | 0IE  | O1-C2-C3-C20    |
| 37  | 7     | 502 | 0IE  | O1-C2-C3-C20    |
| 37  | a     | 521 | 0IE  | O1-C2-C3-C20    |
| 37  | c     | 521 | 0IE  | O1-C2-C3-C20    |
| 37  | b     | 521 | 0IE  | O1-C2-C3-C20    |
| 37  | d     | 521 | 0IE  | O1-C2-C3-C20    |
| 37  | f     | 521 | 0IE  | O1-C2-C3-C20    |
| 37  | h     | 521 | 0IE  | O1-C2-C3-C20    |
| 37  | i     | 521 | 0IE  | O1-C2-C3-C20    |
| 37  | e     | 521 | 0IE  | O1-C2-C3-C20    |
| 30  | c     | 609 | CHL  | CBA-CGA-O2A-C1  |
| 30  | g     | 607 | CHL  | CBA-CGA-O2A-C1  |
| 31  | e     | 604 | CLA  | CBA-CGA-O2A-C1  |
| 31  | e     | 604 | CLA  | O1A-CGA-O2A-C1  |
| 31  | B     | 840 | CLA  | C16-C17-C18-C19 |
| 34  | e     | 630 | LHG  | C28-C29-C30-C31 |
| 36  | 3     | 602 | LMG  | C33-C34-C35-C36 |
| 30  | 0     | 305 | CHL  | CAA-CBA-CGA-O2A |
| 30  | 5     | 301 | CHL  | CAA-CBA-CGA-O2A |
| 34  | A     | 844 | LHG  | O7-C7-C8-C9     |
| 31  | A     | 821 | CLA  | C2-C3-C5-C6     |
| 31  | 7     | 317 | CLA  | C2C-C3C-CAC-CBC |
| 31  | A     | 802 | CLA  | C13-C15-C16-C17 |
| 31  | B     | 839 | CLA  | C8-C10-C11-C12  |
| 41  | B     | 849 | DGD  | C3A-C4A-C5A-C6A |
| 31  | B     | 840 | CLA  | C4C-C3C-CAC-CBC |
| 30  | b     | 601 | CHL  | C1C-C2C-CMC-OMC |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 30  | b     | 606 | CHL  | C1C-C2C-CMC-OMC |
| 30  | b     | 614 | CHL  | C1C-C2C-CMC-OMC |
| 30  | g     | 602 | CHL  | C1C-C2C-CMC-OMC |
| 31  | B     | 801 | CLA  | C2A-CAA-CBA-CGA |
| 31  | b     | 610 | CLA  | C2A-CAA-CBA-CGA |
| 31  | 4     | 309 | CLA  | C2A-CAA-CBA-CGA |
| 34  | 1     | 601 | LHG  | C16-C17-C18-C19 |
| 30  | 0     | 302 | CHL  | CAA-CBA-CGA-O2A |
| 30  | 7     | 306 | CHL  | CAA-CBA-CGA-O2A |
| 30  | e     | 602 | CHL  | CAA-CBA-CGA-O2A |
| 31  | 1     | 303 | CLA  | CAA-CBA-CGA-O2A |
| 31  | b     | 603 | CLA  | CAA-CBA-CGA-O2A |
| 34  | e     | 630 | LHG  | O8-C23-C24-C25  |
| 31  | e     | 613 | CLA  | C11-C10-C8-C7   |
| 31  | B     | 837 | CLA  | C13-C15-C16-C17 |
| 31  | A     | 805 | CLA  | CAA-CBA-CGA-O2A |
| 34  | 7     | 603 | LHG  | O7-C7-C8-C9     |
| 34  | a     | 630 | LHG  | O8-C23-C24-C25  |
| 30  | b     | 608 | CHL  | O1A-CGA-O2A-C1  |
| 31  | A     | 821 | CLA  | O1A-CGA-O2A-C1  |
| 30  | 3     | 307 | CHL  | CAA-CBA-CGA-O2A |
| 30  | 8     | 306 | CHL  | CAA-CBA-CGA-O2A |
| 31  | A     | 825 | CLA  | CAA-CBA-CGA-O2A |
| 31  | H     | 204 | CLA  | CAA-CBA-CGA-O2A |
| 34  | 3     | 603 | LHG  | O8-C23-C24-C25  |
| 34  | 7     | 601 | LHG  | O8-C23-C24-C25  |
| 31  | f     | 613 | CLA  | C11-C10-C8-C7   |
| 31  | B     | 829 | CLA  | C2-C3-C5-C6     |
| 31  | K     | 102 | CLA  | C2-C3-C5-C6     |
| 31  | f     | 613 | CLA  | C2-C3-C5-C6     |
| 31  | A     | 818 | CLA  | C10-C11-C12-C13 |
| 30  | 4     | 313 | CHL  | C2A-CAA-CBA-CGA |
| 31  | 1     | 310 | CLA  | C2A-CAA-CBA-CGA |
| 31  | 5     | 311 | CLA  | CAA-CBA-CGA-O1A |
| 31  | 6     | 314 | CLA  | CAA-CBA-CGA-O1A |
| 31  | 2     | 311 | CLA  | CAA-CBA-CGA-O2A |
| 34  | 8     | 601 | LHG  | O8-C23-C24-C25  |
| 31  | A     | 839 | CLA  | C15-C16-C17-C18 |
| 41  | B     | 849 | DGD  | O6D-C5D-C6D-O5D |
| 34  | e     | 630 | LHG  | C31-C32-C33-C34 |
| 30  | d     | 602 | CHL  | C14-C13-C15-C16 |
| 31  | 0     | 303 | CLA  | C6-C7-C8-C9     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | A     | 835 | CLA  | C11-C10-C8-C9   |
| 31  | L     | 203 | CLA  | C11-C10-C8-C9   |
| 31  | L     | 203 | CLA  | C14-C13-C15-C16 |
| 30  | 2     | 302 | CHL  | CAA-CBA-CGA-O2A |
| 31  | B     | 838 | CLA  | CAA-CBA-CGA-O2A |
| 31  | d     | 603 | CLA  | CAA-CBA-CGA-O2A |
| 34  | c     | 630 | LHG  | O8-C23-C24-C25  |
| 34  | 5     | 601 | LHG  | C4-C5-C6-O8     |
| 36  | J     | 105 | LMG  | O1-C7-C8-C9     |
| 31  | d     | 603 | CLA  | C6-C7-C8-C9     |
| 31  | 0     | 308 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 3     | 313 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 5     | 311 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 7     | 303 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 9     | 303 | CLA  | C4B-C3B-CAB-CBB |
| 31  | A     | 816 | CLA  | C4B-C3B-CAB-CBB |
| 31  | A     | 826 | CLA  | C1A-C2A-CAA-CBA |
| 31  | B     | 841 | CLA  | C4B-C3B-CAB-CBB |
| 31  | F     | 301 | CLA  | C1A-C2A-CAA-CBA |
| 31  | d     | 603 | CLA  | C4B-C3B-CAB-CBB |
| 31  | d     | 612 | CLA  | C1A-C2A-CAA-CBA |
| 31  | f     | 610 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 4     | 310 | CLA  | C1A-C2A-CAA-CBA |
| 37  | h     | 521 | 0IE  | O29-C20-C3-C4   |
| 37  | i     | 521 | 0IE  | O29-C20-C3-C4   |
| 31  | 5     | 311 | CLA  | CAA-CBA-CGA-O2A |
| 34  | G     | 105 | LHG  | C28-C29-C30-C31 |
| 31  | 5     | 310 | CLA  | O1D-CGD-O2D-CED |
| 30  | b     | 608 | CHL  | CBA-CGA-O2A-C1  |
| 34  | f     | 630 | LHG  | O10-C23-C24-C25 |
| 31  | 6     | 317 | CLA  | C8-C10-C11-C12  |
| 31  | 3     | 308 | CLA  | CAA-CBA-CGA-O2A |
| 31  | 7     | 315 | CLA  | CAA-CBA-CGA-O2A |
| 31  | B     | 809 | CLA  | CAA-CBA-CGA-O2A |
| 31  | B     | 823 | CLA  | CAA-CBA-CGA-O2A |
| 31  | f     | 603 | CLA  | CAA-CBA-CGA-O2A |
| 32  | 3     | 403 | 8CT  | C20-C21-C23-C24 |
| 42  | f     | 523 | NEX  | C31-C32-C33-C34 |
| 36  | O     | 207 | LMG  | C28-C29-C30-C31 |
| 30  | c     | 609 | CHL  | O1A-CGA-O2A-C1  |
| 31  | 1     | 308 | CLA  | CAA-CBA-CGA-O2A |
| 30  | 1     | 302 | CHL  | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 30  | f     | 602 | CHL  | CAA-CBA-CGA-O2A |
| 31  | 2     | 312 | CLA  | CAA-CBA-CGA-O2A |
| 31  | A     | 808 | CLA  | CAA-CBA-CGA-O2A |
| 31  | A     | 833 | CLA  | CAA-CBA-CGA-O2A |
| 31  | K     | 104 | CLA  | CAA-CBA-CGA-O2A |
| 34  | 0     | 601 | LHG  | O8-C23-C24-C25  |
| 34  | A     | 855 | LHG  | O7-C7-C8-C9     |
| 34  | d     | 630 | LHG  | O7-C7-C8-C9     |
| 34  | f     | 630 | LHG  | O7-C7-C8-C9     |
| 34  | h     | 630 | LHG  | O8-C23-C24-C25  |
| 31  | B     | 829 | CLA  | C10-C11-C12-C13 |
| 31  | 7     | 318 | CLA  | O1A-CGA-O2A-C1  |
| 39  | A     | 857 | CL0  | C16-C17-C18-C19 |
| 31  | A     | 814 | CLA  | CAA-CBA-CGA-O2A |
| 34  | 3     | 601 | LHG  | O8-C23-C24-C25  |
| 31  | B     | 841 | CLA  | O1D-CGD-O2D-CED |
| 34  | 8     | 601 | LHG  | C1-C2-C3-O3     |
| 30  | 2     | 306 | CHL  | O1D-CGD-O2D-CED |
| 31  | 2     | 304 | CLA  | C4-C3-C5-C6     |
| 31  | f     | 613 | CLA  | C4-C3-C5-C6     |
| 30  | 0     | 302 | CHL  | C2-C1-O2A-CGA   |
| 30  | a     | 609 | CHL  | C2-C1-O2A-CGA   |
| 30  | c     | 609 | CHL  | C2-C1-O2A-CGA   |
| 30  | b     | 609 | CHL  | C2-C1-O2A-CGA   |
| 30  | d     | 601 | CHL  | C2-C1-O2A-CGA   |
| 30  | d     | 606 | CHL  | C2-C1-O2A-CGA   |
| 30  | i     | 606 | CHL  | C2-C1-O2A-CGA   |
| 30  | e     | 602 | CHL  | C2-C1-O2A-CGA   |
| 31  | 0     | 308 | CLA  | C2-C1-O2A-CGA   |
| 31  | 6     | 320 | CLA  | C2-C1-O2A-CGA   |
| 31  | 7     | 311 | CLA  | C2-C1-O2A-CGA   |
| 31  | A     | 814 | CLA  | C2-C1-O2A-CGA   |
| 31  | A     | 831 | CLA  | C2-C1-O2A-CGA   |
| 31  | 8     | 311 | CLA  | CAA-CBA-CGA-O2A |
| 34  | a     | 630 | LHG  | O7-C7-C8-C9     |
| 30  | 3     | 302 | CHL  | C11-C10-C8-C7   |
| 30  | 6     | 301 | CHL  | C11-C10-C8-C7   |
| 30  | b     | 601 | CHL  | C6-C7-C8-C10    |
| 31  | A     | 852 | CLA  | C6-C7-C8-C10    |
| 31  | B     | 825 | CLA  | C6-C7-C8-C10    |
| 31  | B     | 832 | CLA  | C6-C7-C8-C10    |
| 31  | B     | 836 | CLA  | C11-C10-C8-C7   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | A     | 809 | CLA  | C13-C15-C16-C17 |
| 31  | A     | 840 | CLA  | C16-C17-C18-C19 |
| 31  | 4     | 310 | CLA  | C11-C12-C13-C14 |
| 30  | a     | 606 | CHL  | O2A-C1-C2-C3    |
| 36  | J     | 102 | LMG  | C9-C8-O7-C10    |
| 30  | 3     | 305 | CHL  | O1D-CGD-O2D-CED |
| 31  | h     | 613 | CLA  | CAA-CBA-CGA-O1A |
| 34  | 0     | 601 | LHG  | O7-C7-C8-C9     |
| 41  | B     | 849 | DGD  | C7B-C8B-C9B-CAB |
| 36  | 9     | 602 | LMG  | C19-C20-C21-C22 |
| 30  | i     | 607 | CHL  | CAA-CBA-CGA-O1A |
| 31  | 6     | 320 | CLA  | C2A-CAA-CBA-CGA |
| 31  | a     | 604 | CLA  | C2A-CAA-CBA-CGA |
| 31  | H     | 204 | CLA  | C2A-CAA-CBA-CGA |
| 36  | L     | 210 | LMG  | O9-C10-O7-C8    |
| 31  | 3     | 309 | CLA  | C15-C16-C17-C18 |
| 31  | B     | 811 | CLA  | C13-C15-C16-C17 |
| 30  | 9     | 301 | CHL  | CBA-CGA-O2A-C1  |
| 31  | A     | 811 | CLA  | C16-C17-C18-C20 |
| 38  | A     | 842 | PQN  | C26-C27-C28-C30 |
| 31  | L     | 201 | CLA  | C8-C10-C11-C12  |
| 30  | 0     | 305 | CHL  | CAA-CBA-CGA-O1A |
| 31  | K     | 105 | CLA  | CAA-CBA-CGA-O1A |
| 31  | 6     | 303 | CLA  | O1A-CGA-O2A-C1  |
| 30  | 5     | 301 | CHL  | C3A-C2A-CAA-CBA |
| 30  | 8     | 306 | CHL  | C3A-C2A-CAA-CBA |
| 31  | 3     | 312 | CLA  | C4-C3-C5-C6     |
| 31  | A     | 811 | CLA  | C3A-C2A-CAA-CBA |
| 31  | 9     | 303 | CLA  | O1A-CGA-O2A-C1  |
| 31  | B     | 832 | CLA  | C16-C17-C18-C20 |
| 31  | B     | 813 | CLA  | C2-C3-C5-C6     |
| 36  | L     | 210 | LMG  | C28-C29-C30-C31 |
| 31  | 7     | 317 | CLA  | C4C-C3C-CAC-CBC |
| 31  | 2     | 310 | CLA  | C3-C5-C6-C7     |
| 31  | A     | 825 | CLA  | CAA-CBA-CGA-O1A |
| 31  | 7     | 318 | CLA  | CBA-CGA-O2A-C1  |
| 34  | 5     | 601 | LHG  | O6-C4-C5-O7     |
| 34  | b     | 630 | LHG  | O6-C4-C5-O7     |
| 36  | L     | 211 | LMG  | O6-C1-O1-C7     |
| 30  | h     | 609 | CHL  | C2C-C3C-CAC-CBC |
| 30  | 9     | 305 | CHL  | CAA-CBA-CGA-O1A |
| 31  | 0     | 313 | CLA  | CAA-CBA-CGA-O1A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 34  | e     | 630 | LHG  | O10-C23-C24-C25 |
| 30  | a     | 602 | CHL  | C3-C5-C6-C7     |
| 30  | 2     | 306 | CHL  | C2-C1-O2A-CGA   |
| 31  | 6     | 317 | CLA  | C2A-CAA-CBA-CGA |
| 31  | A     | 812 | CLA  | C2A-CAA-CBA-CGA |
| 31  | B     | 814 | CLA  | C2A-CAA-CBA-CGA |
| 30  | 6     | 302 | CHL  | C14-C13-C15-C16 |
| 31  | 9     | 308 | CLA  | C14-C13-C15-C16 |
| 31  | A     | 808 | CLA  | C11-C12-C13-C14 |
| 31  | B     | 801 | CLA  | C14-C13-C15-C16 |
| 31  | B     | 825 | CLA  | C6-C7-C8-C9     |
| 34  | A     | 844 | LHG  | C17-C18-C19-C20 |
| 30  | 9     | 313 | CHL  | CAA-CBA-CGA-O1A |
| 30  | f     | 602 | CHL  | CAA-CBA-CGA-O1A |
| 31  | 1     | 303 | CLA  | CAA-CBA-CGA-O1A |
| 31  | 2     | 311 | CLA  | CAA-CBA-CGA-O1A |
| 31  | B     | 823 | CLA  | CAA-CBA-CGA-O1A |
| 34  | 7     | 601 | LHG  | O10-C23-C24-C25 |
| 34  | f     | 630 | LHG  | O9-C7-C8-C9     |
| 31  | 3     | 308 | CLA  | CAA-CBA-CGA-O1A |
| 31  | A     | 808 | CLA  | CAA-CBA-CGA-O1A |
| 31  | b     | 603 | CLA  | CAA-CBA-CGA-O1A |
| 31  | 9     | 303 | CLA  | CBA-CGA-O2A-C1  |
| 31  | B     | 822 | CLA  | C2-C3-C5-C6     |
| 31  | O     | 203 | CLA  | CAD-CBD-CGD-O1D |
| 32  | 3     | 403 | 8CT  | C28-C29-C30-C35 |
| 32  | L     | 205 | 8CT  | C28-C29-C30-C35 |
| 32  | L     | 206 | 8CT  | C28-C29-C30-C35 |
| 32  | M     | 102 | 8CT  | C28-C29-C30-C35 |
| 30  | b     | 609 | CHL  | O1A-CGA-O2A-C1  |
| 31  | 5     | 303 | CLA  | CAA-CBA-CGA-O1A |
| 34  | A     | 855 | LHG  | O9-C7-C8-C9     |
| 31  | 3     | 303 | CLA  | CAA-CBA-CGA-O2A |
| 31  | B     | 834 | CLA  | CAA-CBA-CGA-O2A |
| 31  | 1     | 308 | CLA  | CAA-CBA-CGA-O1A |
| 32  | 2     | 402 | 8CT  | C10-C11-C12-C13 |
| 42  | e     | 523 | NEX  | C11-C12-C13-C14 |
| 30  | b     | 609 | CHL  | CBA-CGA-O2A-C1  |
| 30  | a     | 606 | CHL  | CAA-CBA-CGA-O1A |
| 31  | A     | 814 | CLA  | CAA-CBA-CGA-O1A |
| 31  | A     | 820 | CLA  | CAA-CBA-CGA-O1A |
| 34  | 7     | 602 | LHG  | O9-C7-C8-C9     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 34  | 7     | 603 | LHG  | O9-C7-C8-C9     |
| 34  | A     | 844 | LHG  | O10-C23-C24-C25 |
| 34  | b     | 630 | LHG  | O9-C7-C8-C9     |
| 36  | L     | 211 | LMG  | O9-C10-C11-C12  |
| 36  | A     | 856 | LMG  | C11-C12-C13-C14 |
| 36  | B     | 853 | LMG  | C8-C7-O1-C1     |
| 36  | L     | 210 | LMG  | C8-C7-O1-C1     |
| 31  | 4     | 311 | CLA  | O2A-C1-C2-C3    |
| 31  | B     | 838 | CLA  | CAA-CBA-CGA-O1A |
| 34  | c     | 630 | LHG  | O10-C23-C24-C25 |
| 31  | A     | 825 | CLA  | C13-C15-C16-C17 |
| 31  | 2     | 309 | CLA  | C2A-CAA-CBA-CGA |
| 31  | 9     | 302 | CLA  | C2A-CAA-CBA-CGA |
| 31  | B     | 803 | CLA  | C16-C17-C18-C20 |
| 34  | 3     | 603 | LHG  | C26-C27-C28-C29 |
| 30  | 2     | 302 | CHL  | CAA-CBA-CGA-O1A |
| 30  | 7     | 306 | CHL  | CAA-CBA-CGA-O1A |
| 31  | 2     | 312 | CLA  | CAA-CBA-CGA-O1A |
| 31  | B     | 809 | CLA  | CAA-CBA-CGA-O1A |
| 31  | H     | 204 | CLA  | CAA-CBA-CGA-O1A |
| 34  | 8     | 601 | LHG  | O10-C23-C24-C25 |
| 34  | d     | 630 | LHG  | O9-C7-C8-C9     |
| 34  | f     | 630 | LHG  | C25-C26-C27-C28 |
| 30  | 6     | 301 | CHL  | C10-C11-C12-C13 |
| 30  | 7     | 302 | CHL  | CAA-CBA-CGA-O2A |
| 31  | g     | 613 | CLA  | CAA-CBA-CGA-O2A |
| 31  | A     | 809 | CLA  | C2-C3-C5-C6     |
| 34  | d     | 630 | LHG  | C31-C32-C33-C34 |
| 32  | B     | 846 | 8CT  | C23-C24-C25-C26 |
| 30  | 1     | 302 | CHL  | CAA-CBA-CGA-O1A |
| 30  | 3     | 307 | CHL  | CAA-CBA-CGA-O1A |
| 31  | L     | 203 | CLA  | CAA-CBA-CGA-O1A |
| 34  | A     | 844 | LHG  | O9-C7-C8-C9     |
| 30  | d     | 606 | CHL  | O1A-CGA-O2A-C1  |
| 30  | 6     | 302 | CHL  | CAD-CBD-CGD-O2D |
| 31  | 6     | 310 | CLA  | CAD-CBD-CGD-O2D |
| 31  | 6     | 311 | CLA  | CAD-CBD-CGD-O2D |
| 31  | 7     | 311 | CLA  | CAD-CBD-CGD-O2D |
| 31  | A     | 813 | CLA  | CAD-CBD-CGD-O2D |
| 31  | A     | 852 | CLA  | CAD-CBD-CGD-O2D |
| 31  | B     | 814 | CLA  | CAD-CBD-CGD-O2D |
| 31  | K     | 105 | CLA  | CAD-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | e     | 603 | CLA  | CAD-CBD-CGD-O2D |
| 31  | 4     | 311 | CLA  | CAD-CBD-CGD-O2D |
| 30  | 4     | 306 | CHL  | C2-C1-O2A-CGA   |
| 31  | 2     | 314 | CLA  | CAA-CBA-CGA-O2A |
| 30  | 8     | 306 | CHL  | CAA-CBA-CGA-O1A |
| 31  | 8     | 311 | CLA  | CAA-CBA-CGA-O1A |
| 31  | d     | 603 | CLA  | CAA-CBA-CGA-O1A |
| 30  | c     | 609 | CHL  | C10-C11-C12-C13 |
| 34  | 7     | 602 | LHG  | O6-C4-C5-C6     |
| 31  | G     | 101 | CLA  | C2-C1-O2A-CGA   |
| 31  | A     | 805 | CLA  | CAA-CBA-CGA-O1A |
| 34  | 0     | 601 | LHG  | O10-C23-C24-C25 |
| 34  | 3     | 603 | LHG  | O10-C23-C24-C25 |
| 34  | a     | 630 | LHG  | O10-C23-C24-C25 |
| 34  | h     | 630 | LHG  | O10-C23-C24-C25 |
| 30  | 6     | 307 | CHL  | CAA-CBA-CGA-O2A |
| 31  | 3     | 311 | CLA  | CAA-CBA-CGA-O2A |
| 31  | 6     | 311 | CLA  | CAA-CBA-CGA-O2A |
| 31  | 7     | 308 | CLA  | CAA-CBA-CGA-O2A |
| 31  | A     | 808 | CLA  | C16-C17-C18-C20 |
| 31  | B     | 810 | CLA  | C4C-C3C-CAC-CBC |
| 31  | A     | 833 | CLA  | CAA-CBA-CGA-O1A |
| 31  | H     | 201 | CLA  | C5-C6-C7-C8     |
| 30  | d     | 602 | CHL  | CAA-CBA-CGA-O2A |
| 31  | 7     | 312 | CLA  | CAA-CBA-CGA-O2A |
| 34  | 9     | 601 | LHG  | O8-C23-C24-C25  |
| 31  | A     | 836 | CLA  | O1D-CGD-O2D-CED |
| 30  | 0     | 302 | CHL  | CAA-CBA-CGA-O1A |
| 30  | e     | 602 | CHL  | CAA-CBA-CGA-O1A |
| 31  | 7     | 315 | CLA  | CAA-CBA-CGA-O1A |
| 30  | i     | 606 | CHL  | CAA-CBA-CGA-O2A |
| 30  | 4     | 302 | CHL  | CAA-CBA-CGA-O2A |
| 34  | 1     | 601 | LHG  | O8-C23-C24-C25  |
| 34  | M     | 104 | LHG  | O8-C23-C24-C25  |
| 31  | 3     | 313 | CLA  | CAA-CBA-CGA-O2A |
| 31  | B     | 834 | CLA  | CAA-CBA-CGA-O1A |
| 31  | K     | 104 | CLA  | CAA-CBA-CGA-O1A |
| 31  | f     | 603 | CLA  | CAA-CBA-CGA-O1A |

There are no ring outliers.

411 monomers are involved in 1119 short contacts:



| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 31  | B     | 825 | CLA  | 5       | 0            |
| 30  | 7     | 307 | CHL  | 7       | 0            |
| 31  | 2     | 309 | CLA  | 2       | 0            |
| 36  | A     | 856 | LMG  | 3       | 0            |
| 41  | B     | 849 | DGD  | 3       | 0            |
| 30  | 8     | 302 | CHL  | 1       | 0            |
| 31  | c     | 613 | CLA  | 4       | 0            |
| 31  | 0     | 311 | CLA  | 2       | 0            |
| 35  | 0     | 603 | SQD  | 2       | 0            |
| 30  | h     | 607 | CHL  | 1       | 0            |
| 37  | b     | 522 | 0IE  | 1       | 0            |
| 31  | 4     | 309 | CLA  | 5       | 0            |
| 31  | L     | 202 | CLA  | 2       | 0            |
| 30  | 6     | 306 | CHL  | 2       | 0            |
| 31  | i     | 613 | CLA  | 1       | 0            |
| 31  | e     | 604 | CLA  | 1       | 0            |
| 31  | A     | 811 | CLA  | 6       | 0            |
| 31  | 6     | 309 | CLA  | 1       | 0            |
| 31  | g     | 603 | CLA  | 3       | 0            |
| 31  | 6     | 312 | CLA  | 3       | 0            |
| 31  | K     | 105 | CLA  | 2       | 0            |
| 30  | 5     | 313 | CHL  | 1       | 0            |
| 31  | B     | 840 | CLA  | 1       | 0            |
| 42  | e     | 523 | NEX  | 3       | 0            |
| 31  | 0     | 309 | CLA  | 3       | 0            |
| 31  | h     | 612 | CLA  | 3       | 0            |
| 30  | b     | 607 | CHL  | 3       | 0            |
| 30  | 5     | 306 | CHL  | 1       | 0            |
| 34  | a     | 630 | LHG  | 4       | 0            |
| 31  | 3     | 308 | CLA  | 4       | 0            |
| 31  | f     | 613 | CLA  | 4       | 0            |
| 31  | 6     | 304 | CLA  | 2       | 0            |
| 31  | 1     | 303 | CLA  | 2       | 0            |
| 31  | 6     | 318 | CLA  | 1       | 0            |
| 31  | B     | 817 | CLA  | 8       | 0            |
| 31  | i     | 611 | CLA  | 4       | 0            |
| 31  | 7     | 308 | CLA  | 7       | 0            |
| 33  | h     | 520 | 0UR  | 1       | 0            |
| 31  | 7     | 312 | CLA  | 5       | 0            |
| 30  | a     | 605 | CHL  | 2       | 0            |
| 31  | B     | 827 | CLA  | 3       | 0            |
| 31  | H     | 201 | CLA  | 3       | 0            |
| 31  | 6     | 310 | CLA  | 2       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 30  | 4     | 305 | CHL  | 3       | 0            |
| 33  | b     | 520 | OUR  | 3       | 0            |
| 30  | e     | 607 | CHL  | 2       | 0            |
| 32  | B     | 804 | 8CT  | 1       | 0            |
| 30  | 2     | 307 | CHL  | 3       | 0            |
| 31  | a     | 611 | CLA  | 1       | 0            |
| 31  | B     | 822 | CLA  | 4       | 0            |
| 31  | J     | 103 | CLA  | 2       | 0            |
| 38  | A     | 842 | PQN  | 5       | 0            |
| 30  | 7     | 305 | CHL  | 3       | 0            |
| 31  | 3     | 306 | CLA  | 2       | 0            |
| 31  | 1     | 308 | CLA  | 2       | 0            |
| 31  | 4     | 311 | CLA  | 4       | 0            |
| 42  | c     | 523 | NEX  | 5       | 0            |
| 31  | B     | 836 | CLA  | 3       | 0            |
| 34  | A     | 855 | LHG  | 1       | 0            |
| 30  | 4     | 308 | CHL  | 3       | 0            |
| 31  | G     | 102 | CLA  | 1       | 0            |
| 31  | 8     | 311 | CLA  | 2       | 0            |
| 34  | 7     | 602 | LHG  | 2       | 0            |
| 31  | g     | 604 | CLA  | 6       | 0            |
| 30  | a     | 601 | CHL  | 1       | 0            |
| 30  | i     | 608 | CHL  | 2       | 0            |
| 30  | h     | 608 | CHL  | 5       | 0            |
| 31  | B     | 830 | CLA  | 6       | 0            |
| 31  | 0     | 303 | CLA  | 4       | 0            |
| 31  | B     | 828 | CLA  | 3       | 0            |
| 30  | a     | 606 | CHL  | 4       | 0            |
| 31  | B     | 816 | CLA  | 1       | 0            |
| 31  | 3     | 320 | CLA  | 1       | 0            |
| 34  | 7     | 601 | LHG  | 2       | 0            |
| 30  | 8     | 307 | CHL  | 4       | 0            |
| 31  | a     | 603 | CLA  | 2       | 0            |
| 31  | B     | 834 | CLA  | 7       | 0            |
| 32  | 3     | 402 | 8CT  | 1       | 0            |
| 30  | 1     | 305 | CHL  | 4       | 0            |
| 30  | 3     | 307 | CHL  | 5       | 0            |
| 31  | A     | 839 | CLA  | 5       | 0            |
| 31  | 9     | 309 | CLA  | 4       | 0            |
| 30  | d     | 608 | CHL  | 5       | 0            |
| 31  | B     | 832 | CLA  | 3       | 0            |
| 42  | g     | 523 | NEX  | 8       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 33  | O     | 204 | 0UR  | 1       | 0            |
| 40  | B     | 802 | SF4  | 1       | 0            |
| 31  | A     | 808 | CLA  | 7       | 0            |
| 31  | A     | 809 | CLA  | 8       | 0            |
| 31  | B     | 826 | CLA  | 3       | 0            |
| 30  | e     | 608 | CHL  | 7       | 0            |
| 37  | b     | 521 | 0IE  | 1       | 0            |
| 30  | 9     | 301 | CHL  | 1       | 0            |
| 30  | c     | 605 | CHL  | 1       | 0            |
| 31  | 5     | 303 | CLA  | 3       | 0            |
| 31  | K     | 102 | CLA  | 3       | 0            |
| 42  | i     | 523 | NEX  | 35      | 0            |
| 30  | c     | 614 | CHL  | 3       | 0            |
| 34  | c     | 630 | LHG  | 5       | 0            |
| 33  | 0     | 501 | 0UR  | 1       | 0            |
| 31  | B     | 831 | CLA  | 3       | 0            |
| 30  | 6     | 315 | CHL  | 1       | 0            |
| 31  | 8     | 309 | CLA  | 1       | 0            |
| 31  | L     | 201 | CLA  | 2       | 0            |
| 31  | 0     | 321 | CLA  | 4       | 0            |
| 30  | h     | 601 | CHL  | 1       | 0            |
| 30  | 1     | 306 | CHL  | 3       | 0            |
| 33  | 1     | 501 | 0UR  | 1       | 0            |
| 31  | A     | 820 | CLA  | 1       | 0            |
| 31  | d     | 603 | CLA  | 3       | 0            |
| 31  | 2     | 304 | CLA  | 1       | 0            |
| 31  | A     | 828 | CLA  | 8       | 0            |
| 30  | 7     | 302 | CHL  | 3       | 0            |
| 31  | 3     | 312 | CLA  | 2       | 0            |
| 31  | 1     | 312 | CLA  | 9       | 0            |
| 30  | 8     | 308 | CHL  | 3       | 0            |
| 30  | d     | 601 | CHL  | 2       | 0            |
| 30  | 6     | 307 | CHL  | 3       | 0            |
| 31  | A     | 817 | CLA  | 1       | 0            |
| 31  | e     | 612 | CLA  | 3       | 0            |
| 42  | f     | 523 | NEX  | 26      | 0            |
| 31  | 1     | 311 | CLA  | 2       | 0            |
| 36  | 9     | 602 | LMG  | 4       | 0            |
| 30  | 2     | 319 | CHL  | 6       | 0            |
| 31  | B     | 814 | CLA  | 5       | 0            |
| 36  | 3     | 602 | LMG  | 1       | 0            |
| 31  | 1     | 304 | CLA  | 1       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 30  | 7     | 301 | CHL  | 3       | 0            |
| 30  | 0     | 306 | CHL  | 4       | 0            |
| 30  | h     | 602 | CHL  | 5       | 0            |
| 30  | i     | 609 | CHL  | 4       | 0            |
| 30  | h     | 609 | CHL  | 1       | 0            |
| 34  | G     | 105 | LHG  | 2       | 0            |
| 31  | 2     | 310 | CLA  | 3       | 0            |
| 31  | 7     | 315 | CLA  | 2       | 0            |
| 30  | 2     | 302 | CHL  | 2       | 0            |
| 30  | d     | 606 | CHL  | 8       | 0            |
| 34  | 9     | 601 | LHG  | 5       | 0            |
| 30  | d     | 602 | CHL  | 2       | 0            |
| 30  | c     | 601 | CHL  | 8       | 0            |
| 30  | d     | 609 | CHL  | 4       | 0            |
| 31  | 6     | 303 | CLA  | 1       | 0            |
| 31  | B     | 809 | CLA  | 9       | 0            |
| 33  | 2     | 501 | OUR  | 3       | 0            |
| 30  | e     | 602 | CHL  | 5       | 0            |
| 31  | K     | 101 | CLA  | 1       | 0            |
| 30  | e     | 609 | CHL  | 6       | 0            |
| 31  | A     | 807 | CLA  | 2       | 0            |
| 30  | g     | 608 | CHL  | 3       | 0            |
| 30  | f     | 602 | CHL  | 1       | 0            |
| 30  | a     | 608 | CHL  | 4       | 0            |
| 31  | A     | 813 | CLA  | 5       | 0            |
| 30  | 3     | 302 | CHL  | 3       | 0            |
| 31  | g     | 610 | CLA  | 5       | 0            |
| 30  | 8     | 313 | CHL  | 3       | 0            |
| 31  | f     | 611 | CLA  | 3       | 0            |
| 30  | i     | 614 | CHL  | 2       | 0            |
| 30  | b     | 602 | CHL  | 7       | 0            |
| 31  | A     | 827 | CLA  | 2       | 0            |
| 31  | h     | 613 | CLA  | 3       | 0            |
| 30  | f     | 614 | CHL  | 2       | 0            |
| 31  | 3     | 318 | CLA  | 3       | 0            |
| 34  | f     | 630 | LHG  | 5       | 0            |
| 31  | A     | 852 | CLA  | 3       | 0            |
| 30  | g     | 602 | CHL  | 2       | 0            |
| 31  | B     | 803 | CLA  | 7       | 0            |
| 30  | c     | 602 | CHL  | 2       | 0            |
| 31  | d     | 610 | CLA  | 1       | 0            |
| 30  | b     | 608 | CHL  | 5       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 31  | d     | 613 | CLA  | 2       | 0            |
| 31  | H     | 204 | CLA  | 1       | 0            |
| 31  | 2     | 314 | CLA  | 1       | 0            |
| 32  | A     | 850 | 8CT  | 1       | 0            |
| 31  | f     | 604 | CLA  | 4       | 0            |
| 30  | 1     | 307 | CHL  | 5       | 0            |
| 31  | A     | 826 | CLA  | 3       | 0            |
| 30  | i     | 606 | CHL  | 21      | 0            |
| 31  | d     | 611 | CLA  | 1       | 0            |
| 31  | B     | 823 | CLA  | 4       | 0            |
| 31  | B     | 818 | CLA  | 12      | 0            |
| 30  | 6     | 305 | CHL  | 2       | 0            |
| 30  | 4     | 319 | CHL  | 8       | 0            |
| 31  | A     | 814 | CLA  | 2       | 0            |
| 31  | B     | 838 | CLA  | 3       | 0            |
| 30  | i     | 605 | CHL  | 1       | 0            |
| 42  | d     | 523 | NEX  | 10      | 0            |
| 31  | 7     | 318 | CLA  | 1       | 0            |
| 34  | A     | 844 | LHG  | 4       | 0            |
| 30  | h     | 606 | CHL  | 5       | 0            |
| 31  | e     | 613 | CLA  | 3       | 0            |
| 31  | A     | 803 | CLA  | 5       | 0            |
| 30  | e     | 601 | CHL  | 2       | 0            |
| 31  | 0     | 308 | CLA  | 1       | 0            |
| 30  | f     | 601 | CHL  | 6       | 0            |
| 31  | 9     | 300 | CLA  | 1       | 0            |
| 31  | 7     | 317 | CLA  | 5       | 0            |
| 31  | i     | 603 | CLA  | 2       | 0            |
| 30  | 6     | 302 | CHL  | 3       | 0            |
| 32  | 4     | 402 | 8CT  | 1       | 0            |
| 30  | g     | 609 | CHL  | 2       | 0            |
| 31  | b     | 610 | CLA  | 3       | 0            |
| 30  | 4     | 302 | CHL  | 2       | 0            |
| 30  | c     | 609 | CHL  | 5       | 0            |
| 31  | 5     | 308 | CLA  | 2       | 0            |
| 31  | A     | 804 | CLA  | 1       | 0            |
| 31  | A     | 821 | CLA  | 9       | 0            |
| 31  | B     | 835 | CLA  | 1       | 0            |
| 31  | 5     | 304 | CLA  | 2       | 0            |
| 30  | 2     | 301 | CHL  | 2       | 0            |
| 34  | 0     | 601 | LHG  | 4       | 0            |
| 30  | 1     | 302 | CHL  | 4       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 31  | A     | 823 | CLA  | 1       | 0            |
| 30  | 8     | 315 | CHL  | 3       | 0            |
| 38  | B     | 842 | PQN  | 1       | 0            |
| 31  | 5     | 311 | CLA  | 2       | 0            |
| 31  | 9     | 303 | CLA  | 1       | 0            |
| 31  | 4     | 304 | CLA  | 1       | 0            |
| 31  | A     | 853 | CLA  | 5       | 0            |
| 30  | b     | 609 | CHL  | 3       | 0            |
| 31  | 0     | 313 | CLA  | 2       | 0            |
| 33  | 6     | 502 | 0UR  | 1       | 0            |
| 30  | a     | 607 | CHL  | 3       | 0            |
| 33  | 9     | 502 | 0UR  | 1       | 0            |
| 30  | 4     | 313 | CHL  | 3       | 0            |
| 30  | 6     | 308 | CHL  | 4       | 0            |
| 34  | i     | 630 | LHG  | 4       | 0            |
| 34  | h     | 630 | LHG  | 4       | 0            |
| 31  | 4     | 314 | CLA  | 1       | 0            |
| 30  | 1     | 313 | CHL  | 3       | 0            |
| 30  | 9     | 305 | CHL  | 1       | 0            |
| 31  | F     | 301 | CLA  | 3       | 0            |
| 30  | 9     | 306 | CHL  | 2       | 0            |
| 31  | A     | 818 | CLA  | 10      | 0            |
| 30  | 5     | 301 | CHL  | 5       | 0            |
| 34  | d     | 630 | LHG  | 5       | 0            |
| 31  | B     | 813 | CLA  | 3       | 0            |
| 34  | M     | 104 | LHG  | 4       | 0            |
| 31  | h     | 610 | CLA  | 2       | 0            |
| 31  | 9     | 312 | CLA  | 2       | 0            |
| 31  | 0     | 312 | CLA  | 8       | 0            |
| 31  | A     | 832 | CLA  | 6       | 0            |
| 37  | i     | 521 | 0IE  | 4       | 0            |
| 34  | e     | 630 | LHG  | 5       | 0            |
| 33  | a     | 520 | 0UR  | 2       | 0            |
| 34  | 3     | 603 | LHG  | 3       | 0            |
| 30  | i     | 607 | CHL  | 1       | 0            |
| 31  | B     | 837 | CLA  | 1       | 0            |
| 34  | 2     | 601 | LHG  | 3       | 0            |
| 31  | A     | 841 | CLA  | 5       | 0            |
| 31  | h     | 611 | CLA  | 1       | 0            |
| 31  | A     | 838 | CLA  | 3       | 0            |
| 31  | e     | 610 | CLA  | 2       | 0            |
| 31  | 9     | 311 | CLA  | 2       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 30  | 4     | 306 | CHL  | 2       | 0            |
| 31  | K     | 104 | CLA  | 3       | 0            |
| 33  | 4     | 501 | OUR  | 3       | 0            |
| 30  | h     | 614 | CHL  | 1       | 0            |
| 30  | f     | 609 | CHL  | 6       | 0            |
| 30  | 5     | 305 | CHL  | 4       | 0            |
| 31  | g     | 612 | CLA  | 1       | 0            |
| 31  | B     | 820 | CLA  | 4       | 0            |
| 30  | d     | 605 | CHL  | 2       | 0            |
| 37  | c     | 522 | OIE  | 1       | 0            |
| 31  | 3     | 309 | CLA  | 4       | 0            |
| 31  | B     | 824 | CLA  | 5       | 0            |
| 30  | b     | 614 | CHL  | 2       | 0            |
| 30  | a     | 609 | CHL  | 5       | 0            |
| 31  | B     | 806 | CLA  | 8       | 0            |
| 33  | 9     | 501 | OUR  | 2       | 0            |
| 31  | B     | 810 | CLA  | 5       | 0            |
| 34  | 3     | 601 | LHG  | 1       | 0            |
| 31  | 9     | 302 | CLA  | 5       | 0            |
| 30  | b     | 606 | CHL  | 2       | 0            |
| 31  | G     | 103 | CLA  | 1       | 0            |
| 30  | 6     | 301 | CHL  | 5       | 0            |
| 30  | c     | 607 | CHL  | 3       | 0            |
| 31  | b     | 603 | CLA  | 2       | 0            |
| 30  | 0     | 305 | CHL  | 4       | 0            |
| 31  | A     | 843 | CLA  | 4       | 0            |
| 39  | A     | 857 | CL0  | 7       | 0            |
| 30  | 0     | 302 | CHL  | 3       | 0            |
| 30  | g     | 601 | CHL  | 1       | 0            |
| 31  | a     | 604 | CLA  | 2       | 0            |
| 34  | A     | 845 | LHG  | 3       | 0            |
| 31  | 0     | 310 | CLA  | 2       | 0            |
| 31  | B     | 811 | CLA  | 7       | 0            |
| 30  | b     | 601 | CHL  | 4       | 0            |
| 30  | d     | 607 | CHL  | 3       | 0            |
| 30  | 4     | 307 | CHL  | 2       | 0            |
| 31  | d     | 612 | CLA  | 4       | 0            |
| 30  | 5     | 302 | CHL  | 4       | 0            |
| 31  | c     | 610 | CLA  | 2       | 0            |
| 31  | 6     | 317 | CLA  | 4       | 0            |
| 31  | f     | 610 | CLA  | 1       | 0            |
| 31  | A     | 816 | CLA  | 1       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 31  | 1     | 309 | CLA  | 2       | 0            |
| 31  | 7     | 309 | CLA  | 4       | 0            |
| 30  | f     | 606 | CHL  | 5       | 0            |
| 30  | g     | 607 | CHL  | 2       | 0            |
| 30  | 8     | 301 | CHL  | 4       | 0            |
| 34  | g     | 630 | LHG  | 3       | 0            |
| 31  | b     | 613 | CLA  | 2       | 0            |
| 36  | J     | 102 | LMG  | 1       | 0            |
| 30  | 8     | 305 | CHL  | 3       | 0            |
| 31  | A     | 822 | CLA  | 3       | 0            |
| 33  | 5     | 501 | 0UR  | 4       | 0            |
| 31  | 9     | 308 | CLA  | 5       | 0            |
| 32  | B     | 847 | 8CT  | 1       | 0            |
| 31  | A     | 819 | CLA  | 4       | 0            |
| 31  | a     | 613 | CLA  | 1       | 0            |
| 31  | B     | 850 | CLA  | 1       | 0            |
| 34  | 6     | 601 | LHG  | 5       | 0            |
| 33  | d     | 520 | 0UR  | 1       | 0            |
| 31  | a     | 610 | CLA  | 4       | 0            |
| 31  | O     | 206 | CLA  | 3       | 0            |
| 31  | B     | 805 | CLA  | 4       | 0            |
| 31  | B     | 808 | CLA  | 6       | 0            |
| 37  | h     | 521 | 0IE  | 1       | 0            |
| 31  | B     | 812 | CLA  | 1       | 0            |
| 30  | 2     | 308 | CHL  | 1       | 0            |
| 31  | 5     | 314 | CLA  | 1       | 0            |
| 31  | B     | 801 | CLA  | 8       | 0            |
| 31  | 4     | 312 | CLA  | 2       | 0            |
| 36  | O     | 207 | LMG  | 1       | 0            |
| 30  | e     | 605 | CHL  | 2       | 0            |
| 31  | 3     | 303 | CLA  | 2       | 0            |
| 30  | 6     | 313 | CHL  | 2       | 0            |
| 31  | h     | 604 | CLA  | 2       | 0            |
| 31  | 8     | 304 | CLA  | 2       | 0            |
| 31  | 3     | 313 | CLA  | 1       | 0            |
| 33  | c     | 520 | 0UR  | 1       | 0            |
| 31  | L     | 203 | CLA  | 5       | 0            |
| 31  | A     | 836 | CLA  | 1       | 0            |
| 36  | B     | 853 | LMG  | 1       | 0            |
| 31  | 7     | 304 | CLA  | 4       | 0            |
| 31  | e     | 603 | CLA  | 5       | 0            |
| 30  | 8     | 306 | CHL  | 1       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 30  | c     | 608 | CHL  | 7       | 0            |
| 31  | A     | 815 | CLA  | 3       | 0            |
| 30  | 2     | 313 | CHL  | 6       | 0            |
| 31  | B     | 833 | CLA  | 6       | 0            |
| 30  | f     | 608 | CHL  | 3       | 0            |
| 31  | O     | 203 | CLA  | 4       | 0            |
| 31  | A     | 829 | CLA  | 4       | 0            |
| 31  | i     | 610 | CLA  | 2       | 0            |
| 34  | B     | 854 | LHG  | 2       | 0            |
| 30  | 2     | 306 | CHL  | 1       | 0            |
| 30  | 5     | 307 | CHL  | 2       | 0            |
| 33  | 8     | 501 | 0UR  | 3       | 0            |
| 31  | c     | 604 | CLA  | 1       | 0            |
| 31  | A     | 805 | CLA  | 2       | 0            |
| 31  | 5     | 309 | CLA  | 4       | 0            |
| 32  | L     | 205 | 8CT  | 1       | 0            |
| 31  | A     | 802 | CLA  | 2       | 0            |
| 31  | 2     | 312 | CLA  | 2       | 0            |
| 34  | B     | 852 | LHG  | 2       | 0            |
| 34  | 5     | 601 | LHG  | 1       | 0            |
| 34  | 1     | 601 | LHG  | 6       | 0            |
| 31  | A     | 810 | CLA  | 3       | 0            |
| 36  | L     | 211 | LMG  | 3       | 0            |
| 31  | b     | 604 | CLA  | 3       | 0            |
| 31  | A     | 824 | CLA  | 1       | 0            |
| 31  | B     | 819 | CLA  | 5       | 0            |
| 34  | K     | 106 | LHG  | 4       | 0            |
| 30  | f     | 607 | CHL  | 2       | 0            |
| 33  | i     | 520 | 0UR  | 2       | 0            |
| 31  | 4     | 310 | CLA  | 3       | 0            |
| 30  | e     | 606 | CHL  | 1       | 0            |
| 30  | c     | 606 | CHL  | 3       | 0            |
| 31  | 3     | 304 | CLA  | 3       | 0            |
| 31  | A     | 831 | CLA  | 3       | 0            |
| 31  | A     | 830 | CLA  | 5       | 0            |
| 31  | B     | 829 | CLA  | 4       | 0            |
| 42  | b     | 523 | NEX  | 3       | 0            |
| 32  | 7     | 404 | 8CT  | 1       | 0            |
| 31  | B     | 839 | CLA  | 5       | 0            |
| 30  | 7     | 306 | CHL  | 4       | 0            |
| 33  | 7     | 501 | 0UR  | 2       | 0            |
| 42  | a     | 523 | NEX  | 7       | 0            |

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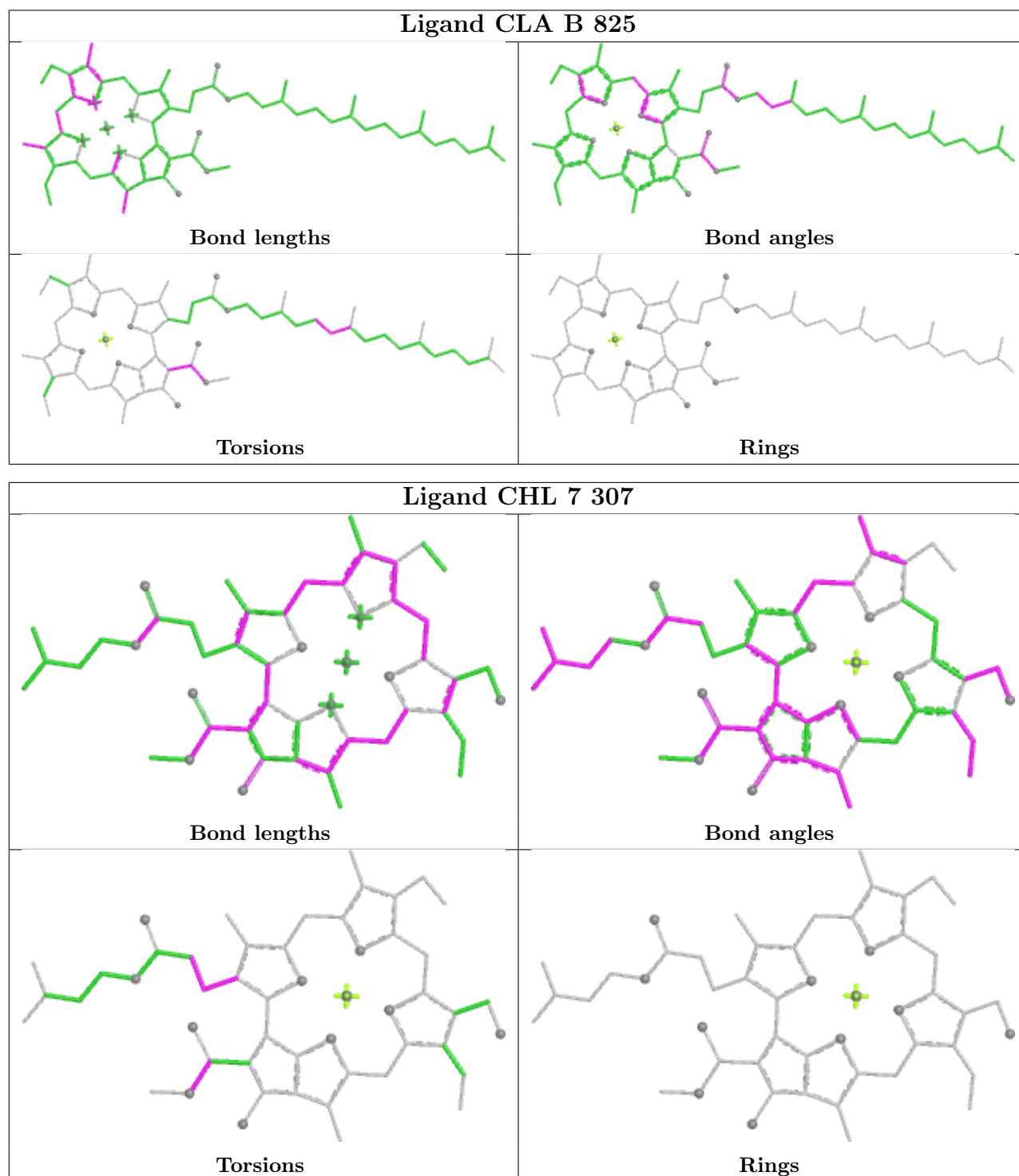
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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 31  | i     | 612 | CLA  | 1       | 0            |
| 31  | L     | 204 | CLA  | 3       | 0            |
| 36  | J     | 105 | LMG  | 2       | 0            |
| 31  | 0     | 304 | CLA  | 1       | 0            |
| 30  | 0     | 301 | CHL  | 6       | 0            |
| 31  | A     | 825 | CLA  | 6       | 0            |
| 31  | 6     | 311 | CLA  | 1       | 0            |
| 31  | i     | 604 | CLA  | 28      | 0            |
| 31  | 8     | 312 | CLA  | 1       | 0            |
| 31  | A     | 837 | CLA  | 3       | 0            |
| 31  | B     | 821 | CLA  | 1       | 0            |
| 31  | g     | 613 | CLA  | 3       | 0            |
| 30  | g     | 605 | CHL  | 3       | 0            |
| 31  | 5     | 312 | CLA  | 2       | 0            |
| 42  | h     | 523 | NEX  | 15      | 0            |
| 31  | b     | 612 | CLA  | 1       | 0            |
| 31  | c     | 603 | CLA  | 2       | 0            |
| 32  | 8     | 402 | 8CT  | 1       | 0            |
| 31  | A     | 806 | CLA  | 3       | 0            |
| 30  | 3     | 305 | CHL  | 1       | 0            |
| 31  | 3     | 311 | CLA  | 1       | 0            |
| 30  | g     | 606 | CHL  | 2       | 0            |
| 33  | 3     | 501 | 0UR  | 1       | 0            |
| 31  | A     | 840 | CLA  | 7       | 0            |
| 30  | i     | 602 | CHL  | 3       | 0            |
| 30  | a     | 602 | CHL  | 3       | 0            |
| 31  | B     | 841 | CLA  | 4       | 0            |
| 37  | h     | 522 | 0IE  | 1       | 0            |
| 31  | g     | 611 | CLA  | 1       | 0            |
| 31  | d     | 604 | CLA  | 1       | 0            |
| 34  | b     | 630 | LHG  | 2       | 0            |
| 32  | J     | 104 | 8CT  | 1       | 0            |

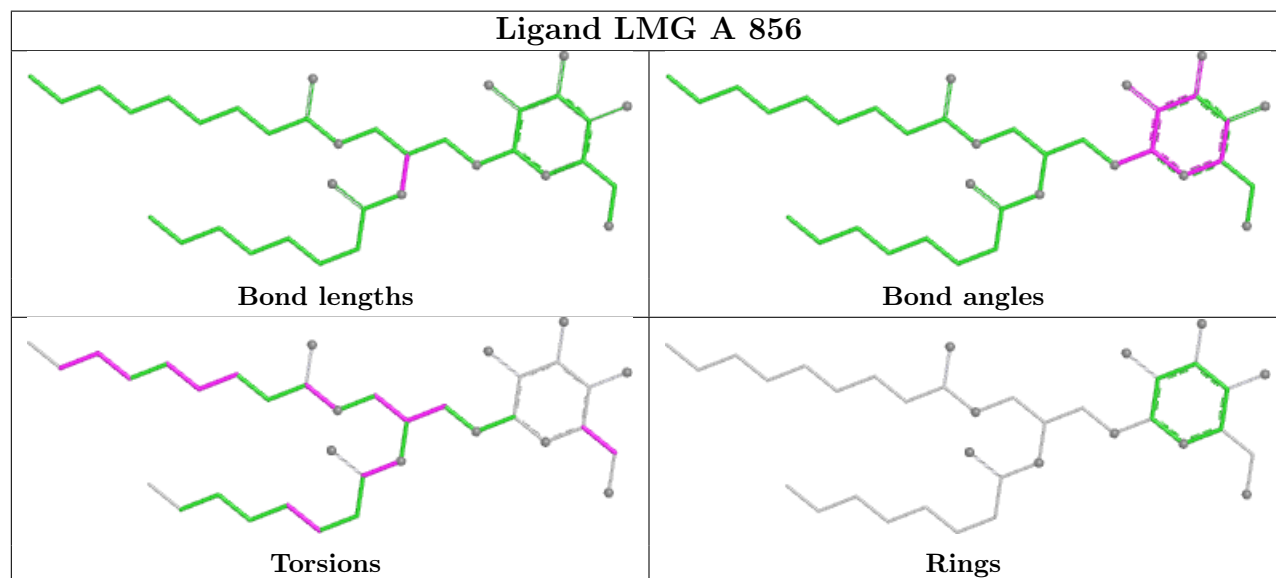
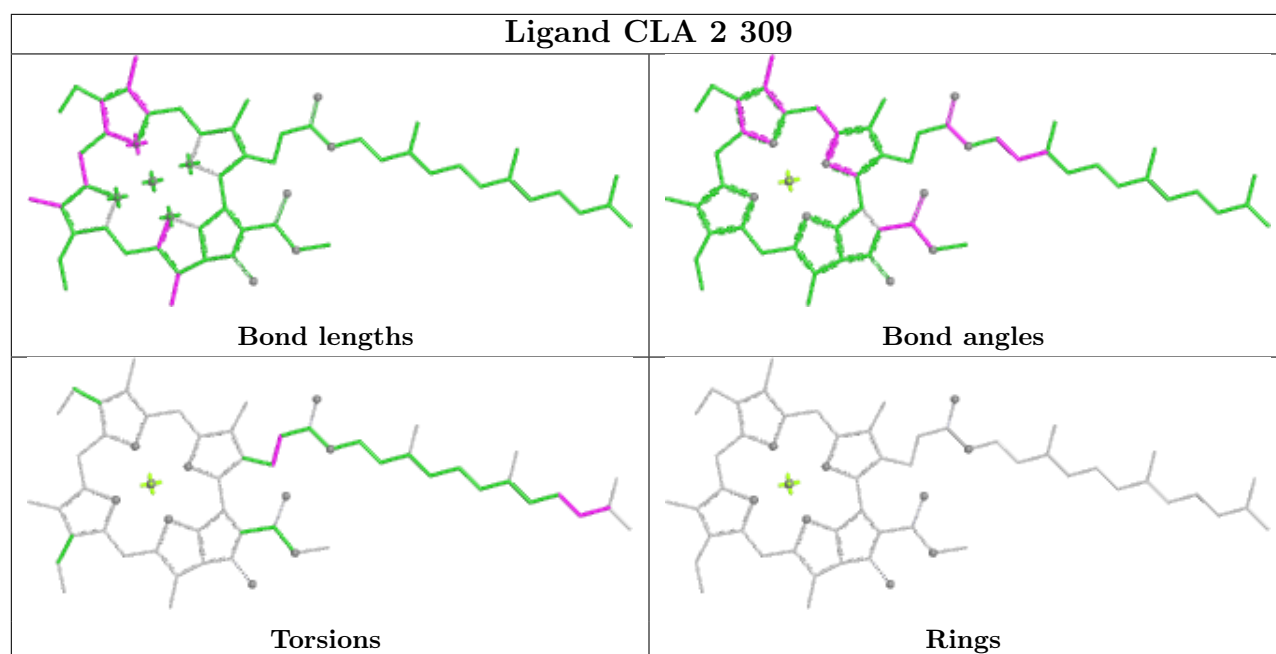
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.



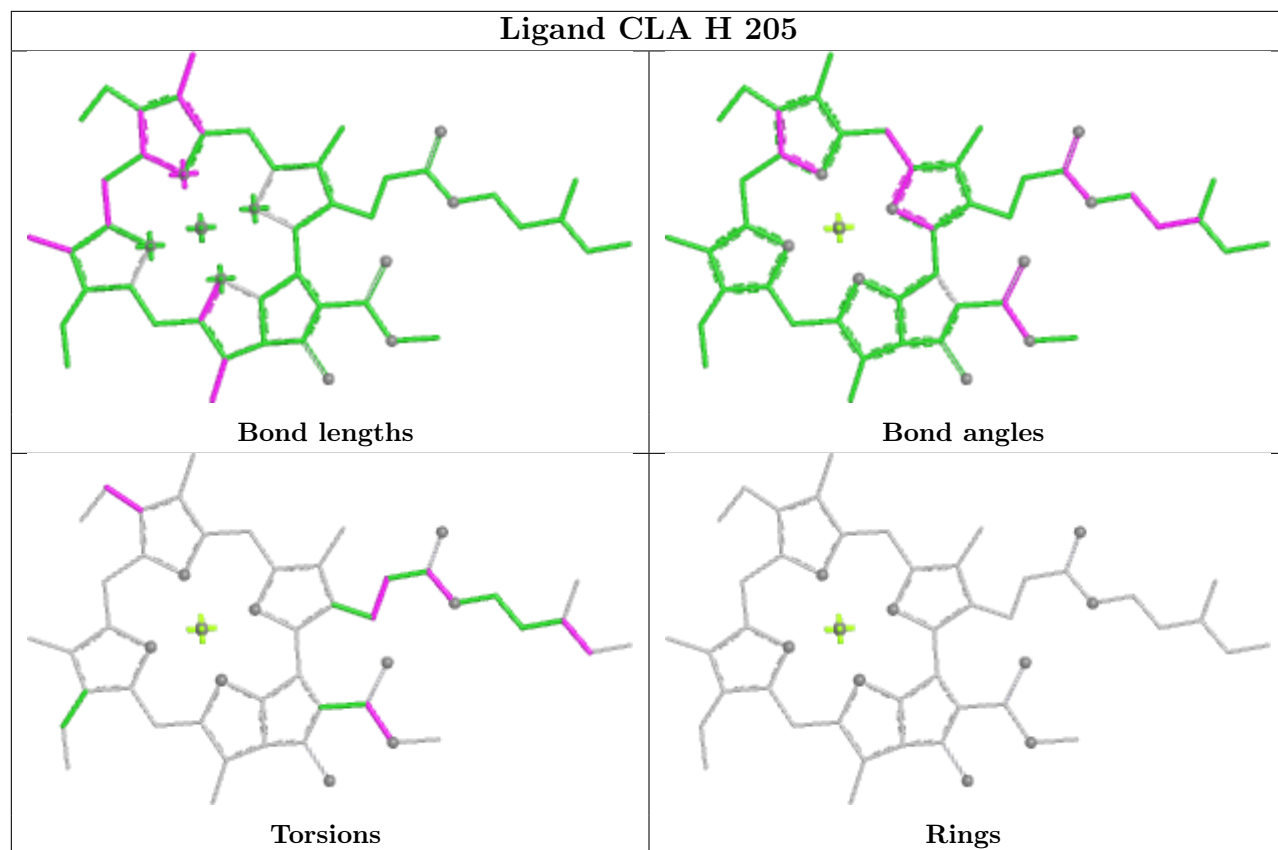
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





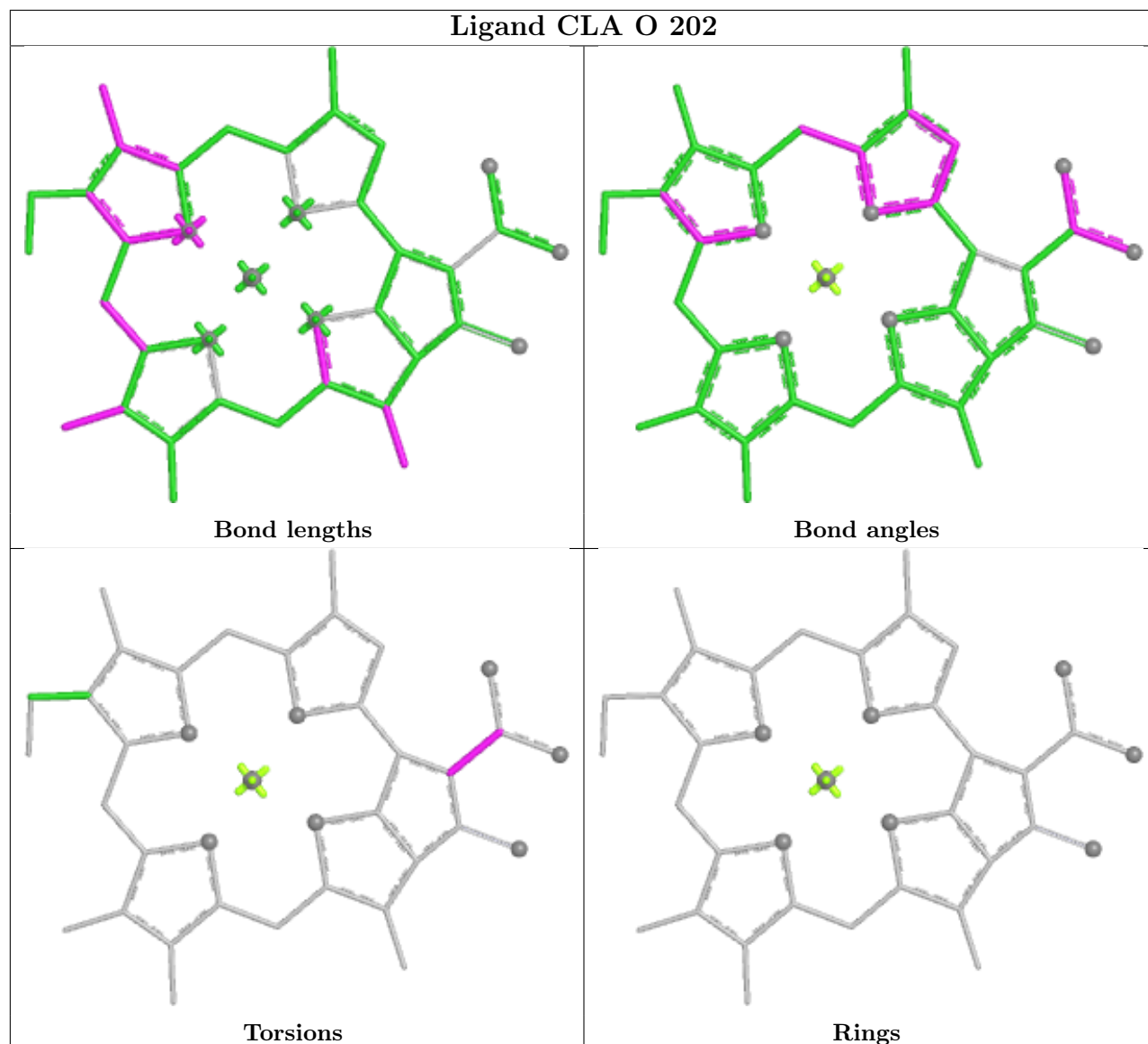




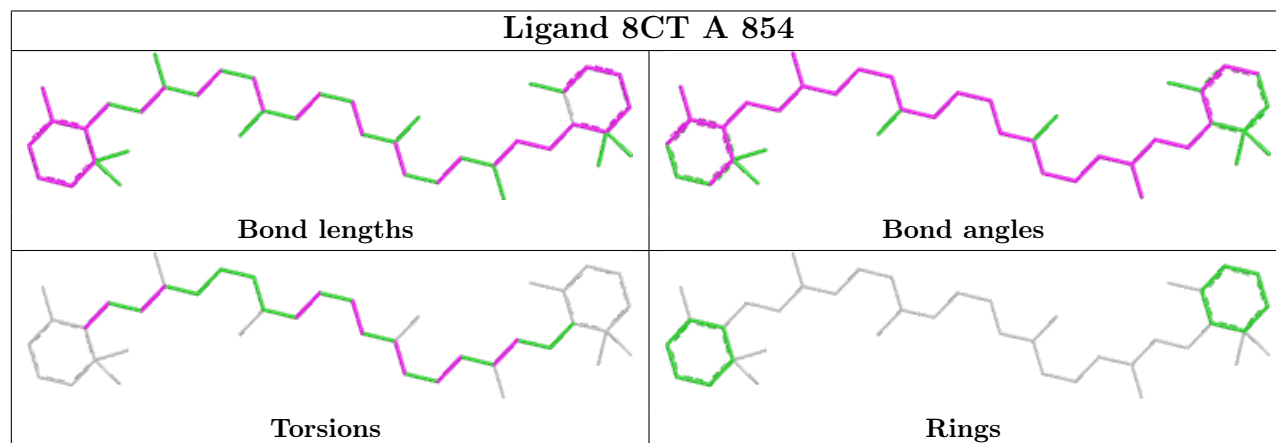




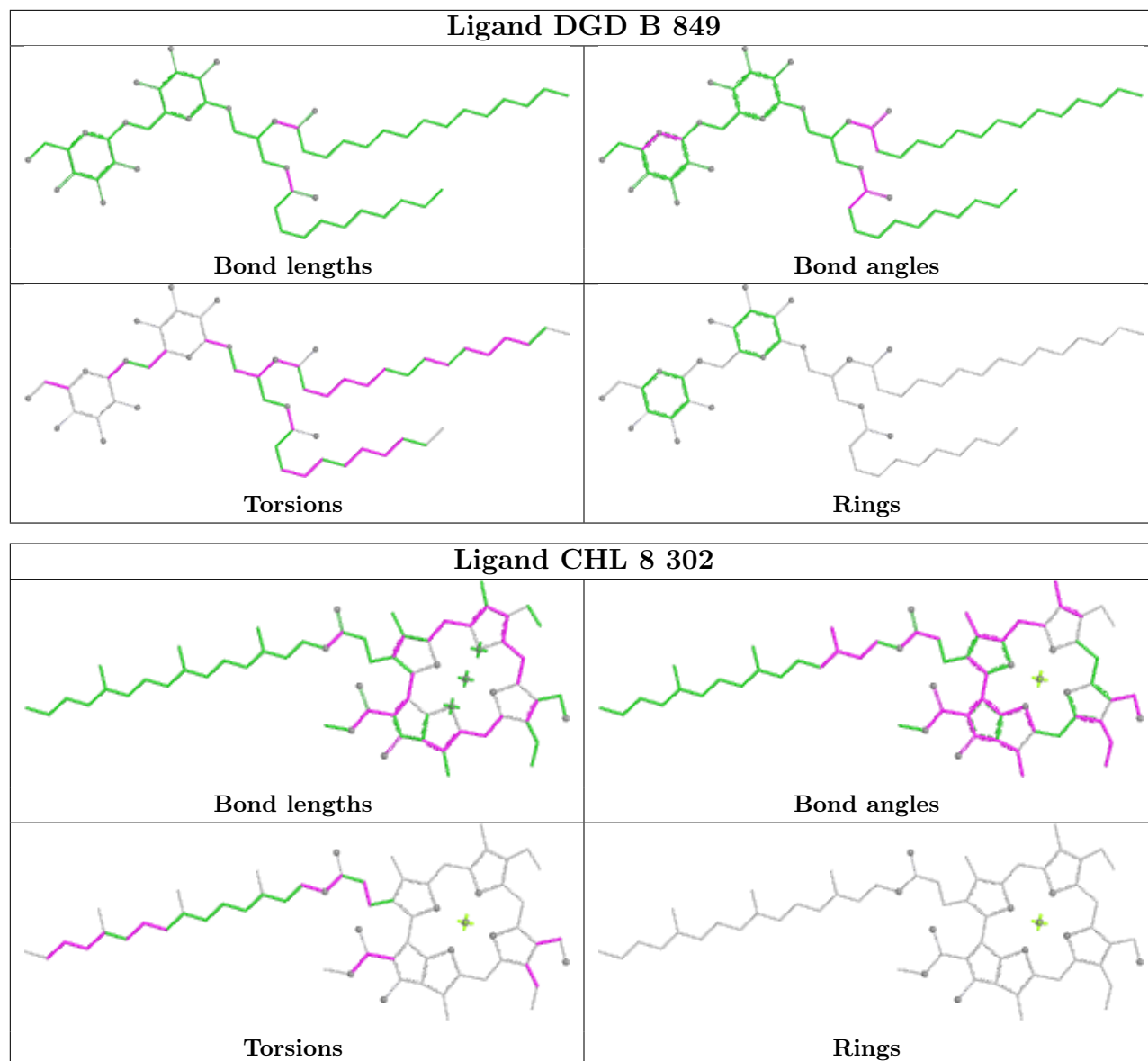
## Ligand CLA O 202



## Ligand 8CT A 854

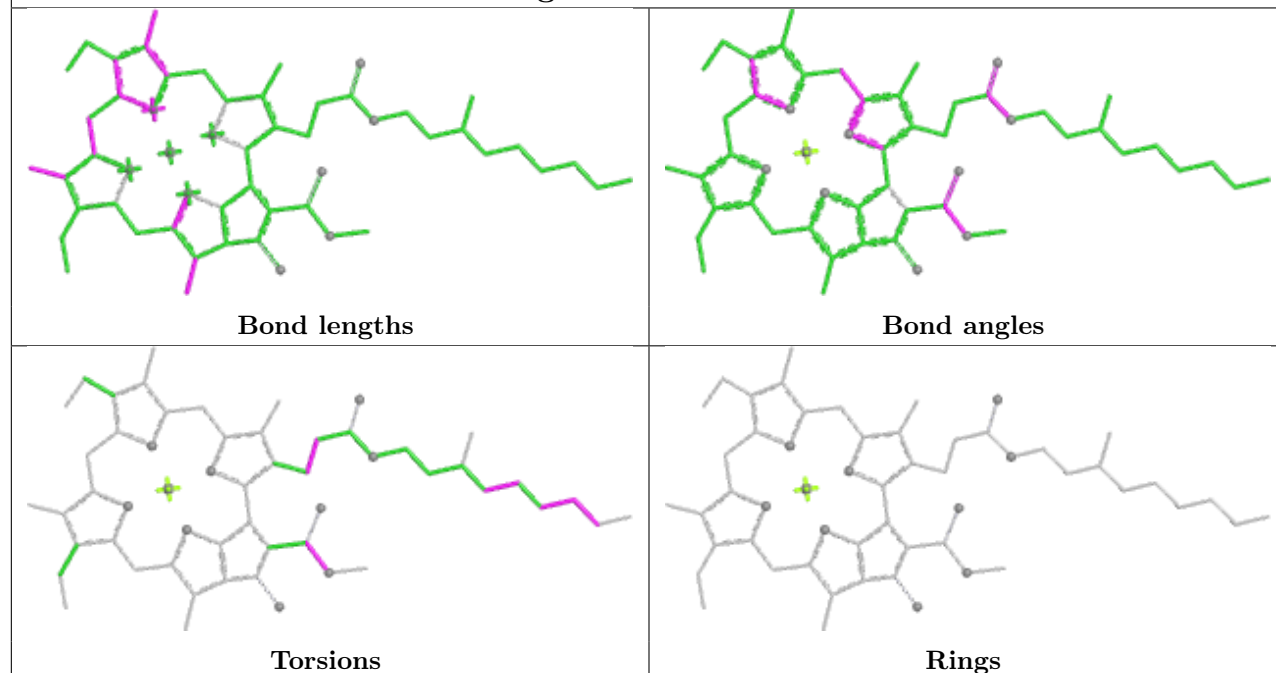




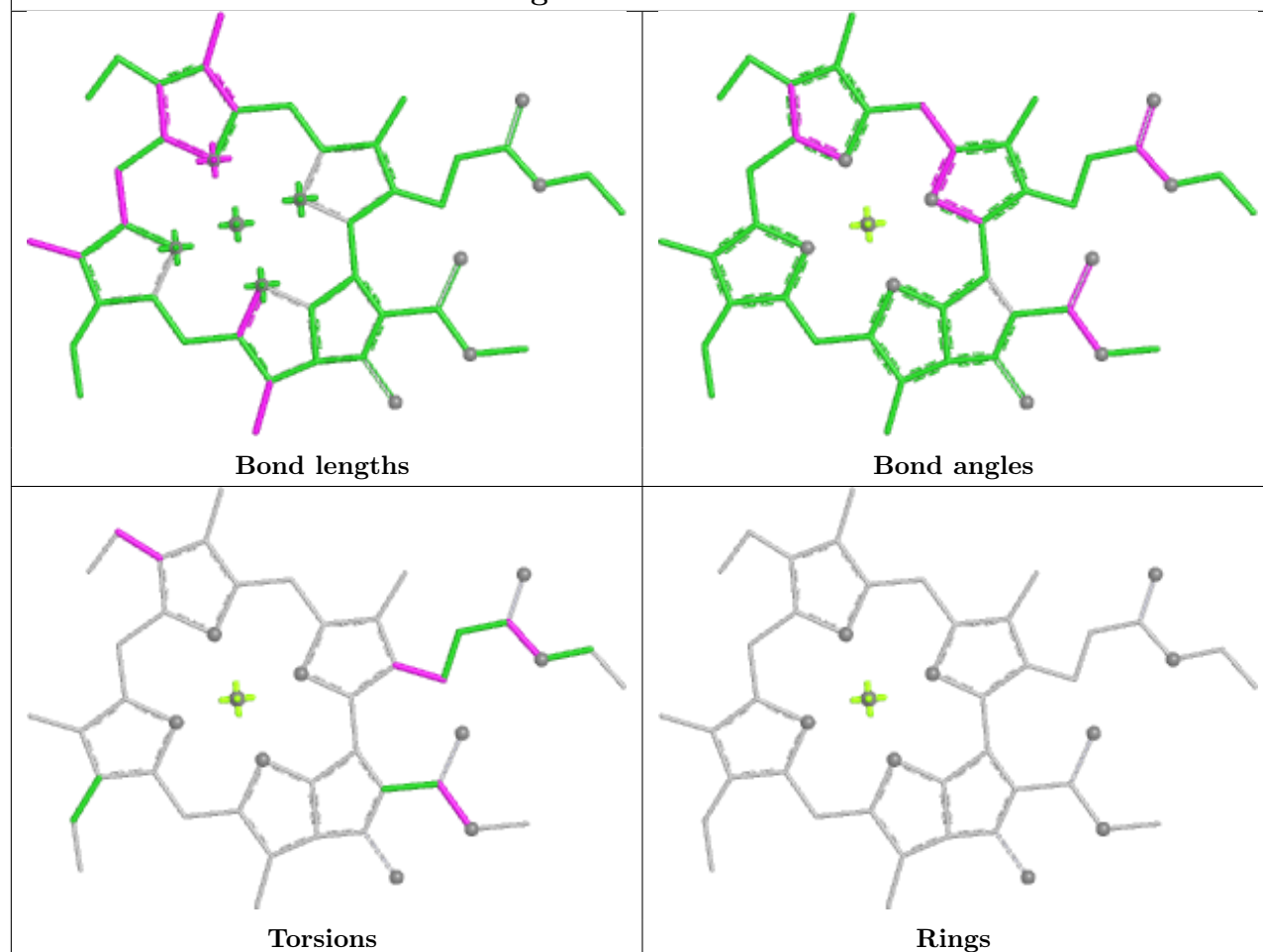




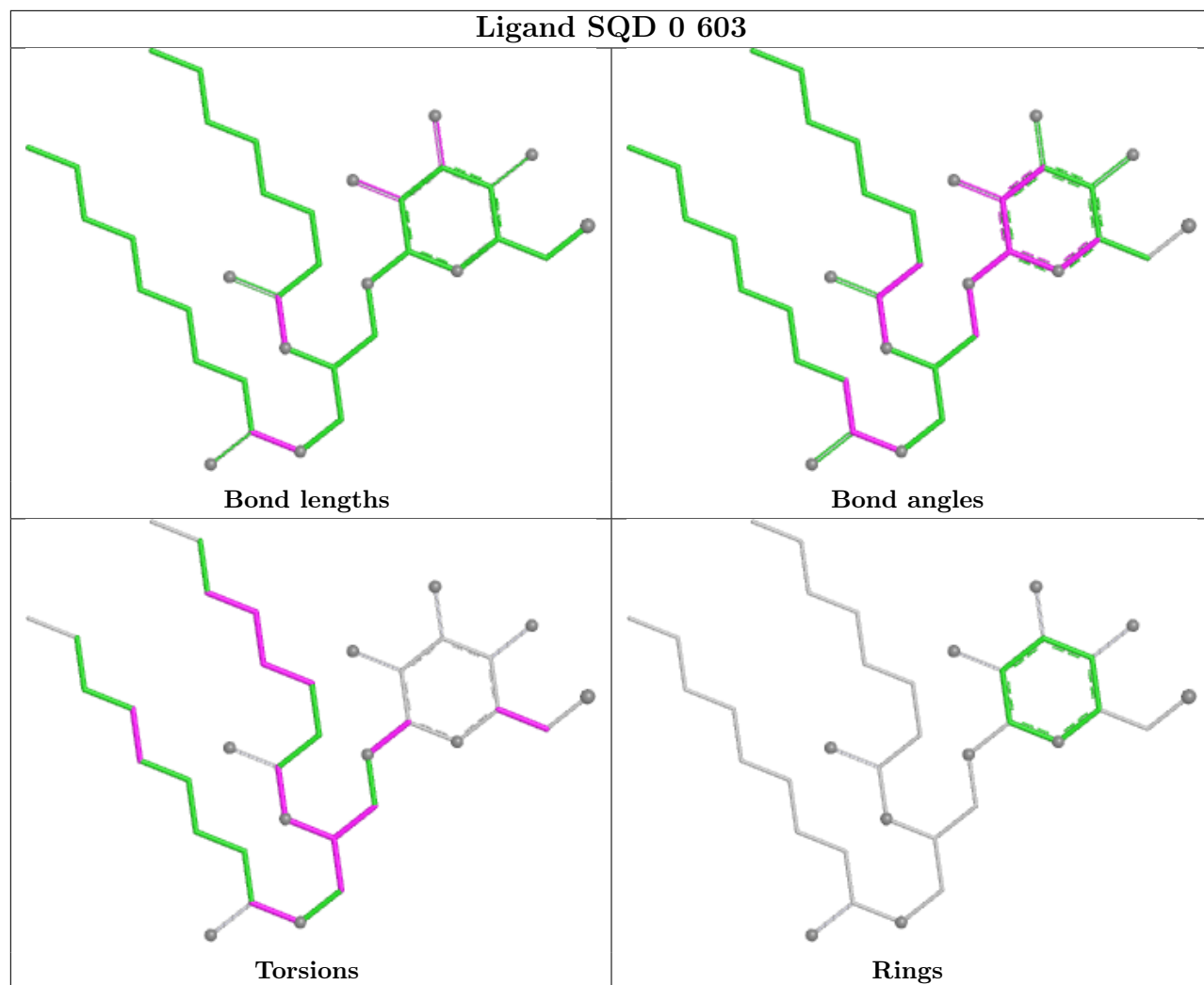
## Ligand CLA c 613



## Ligand CLA 0 311

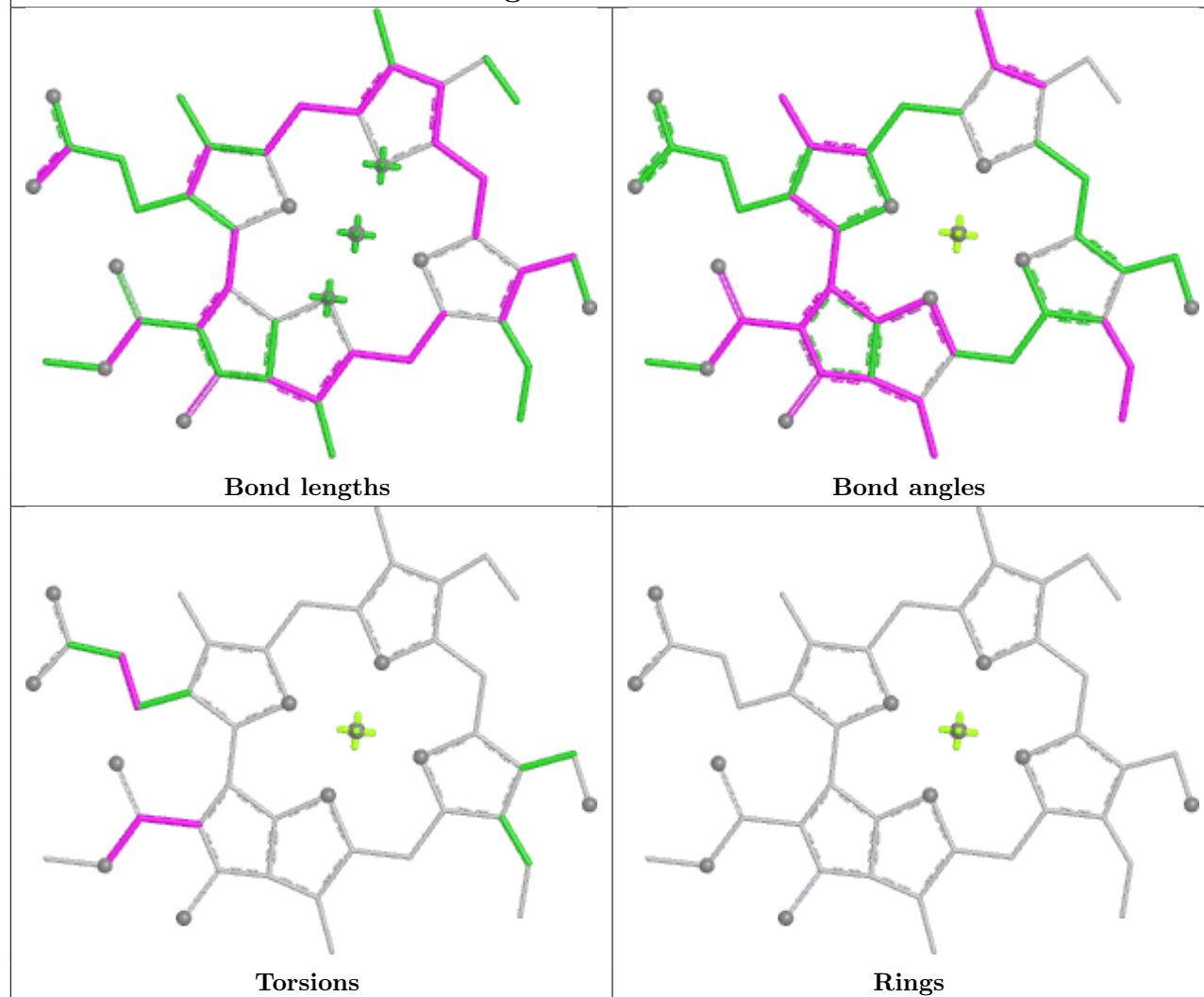




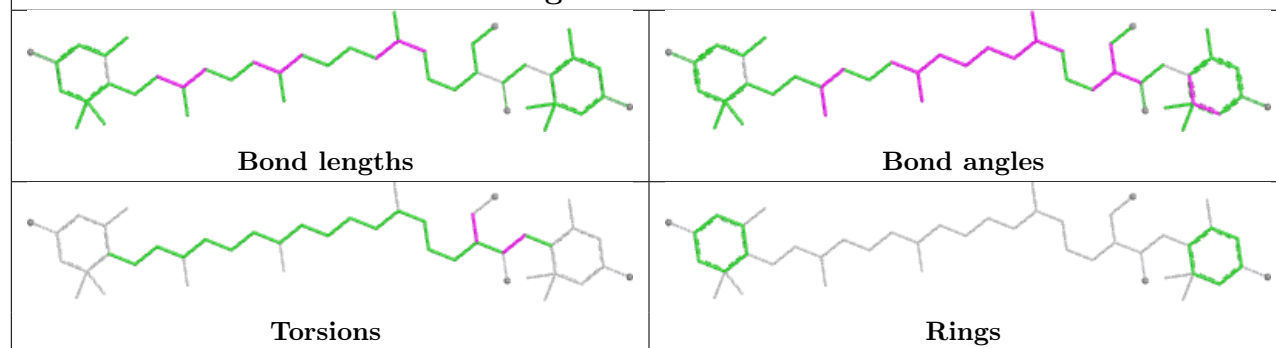




## Ligand CHL h 607

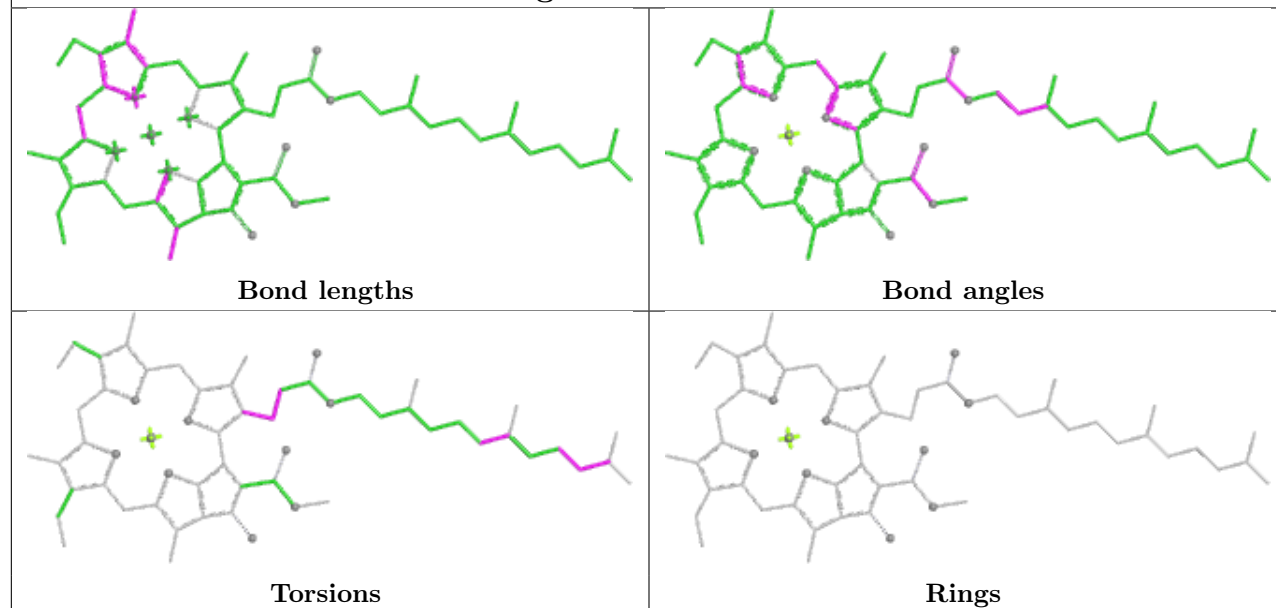


## Ligand OIE b 522

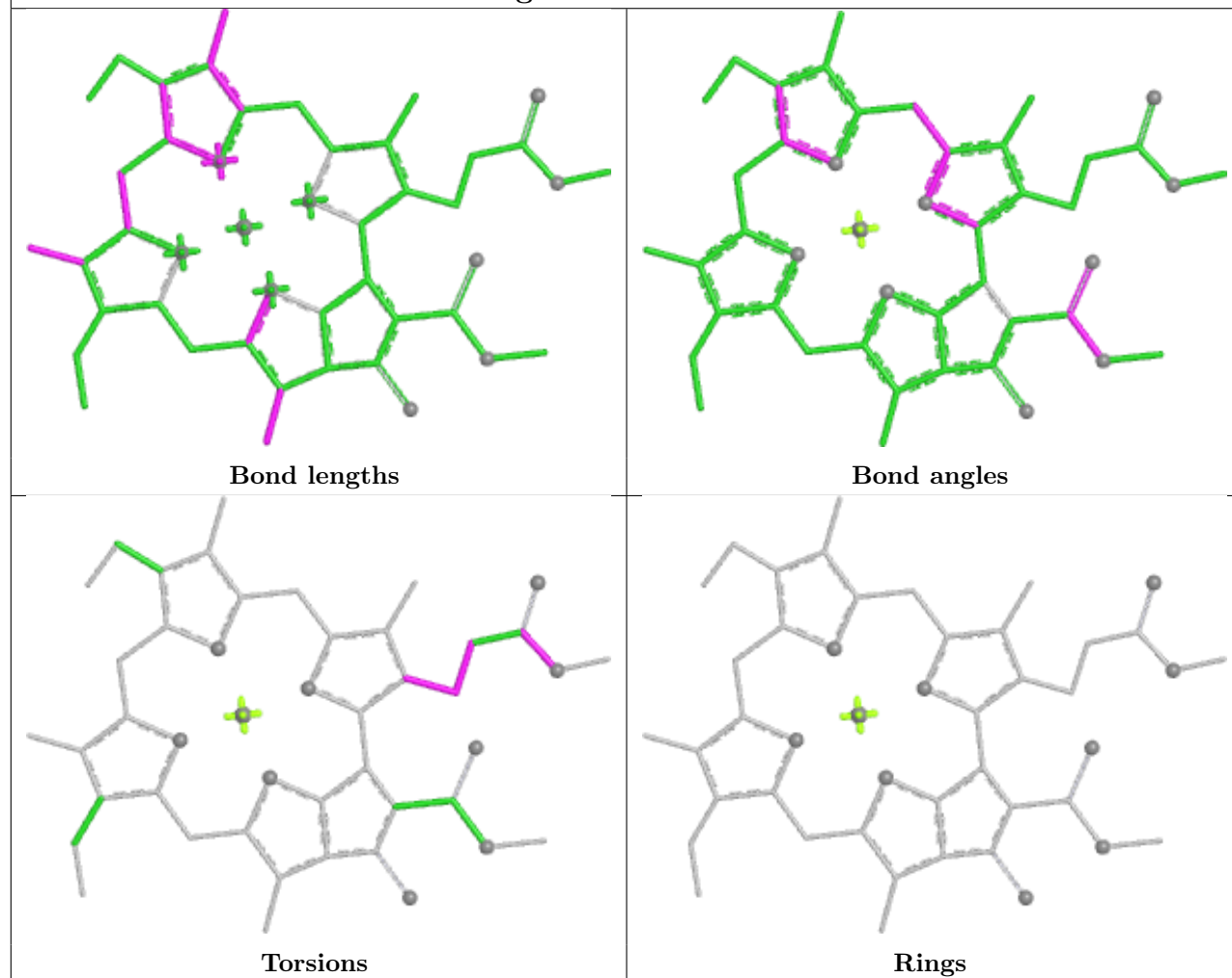




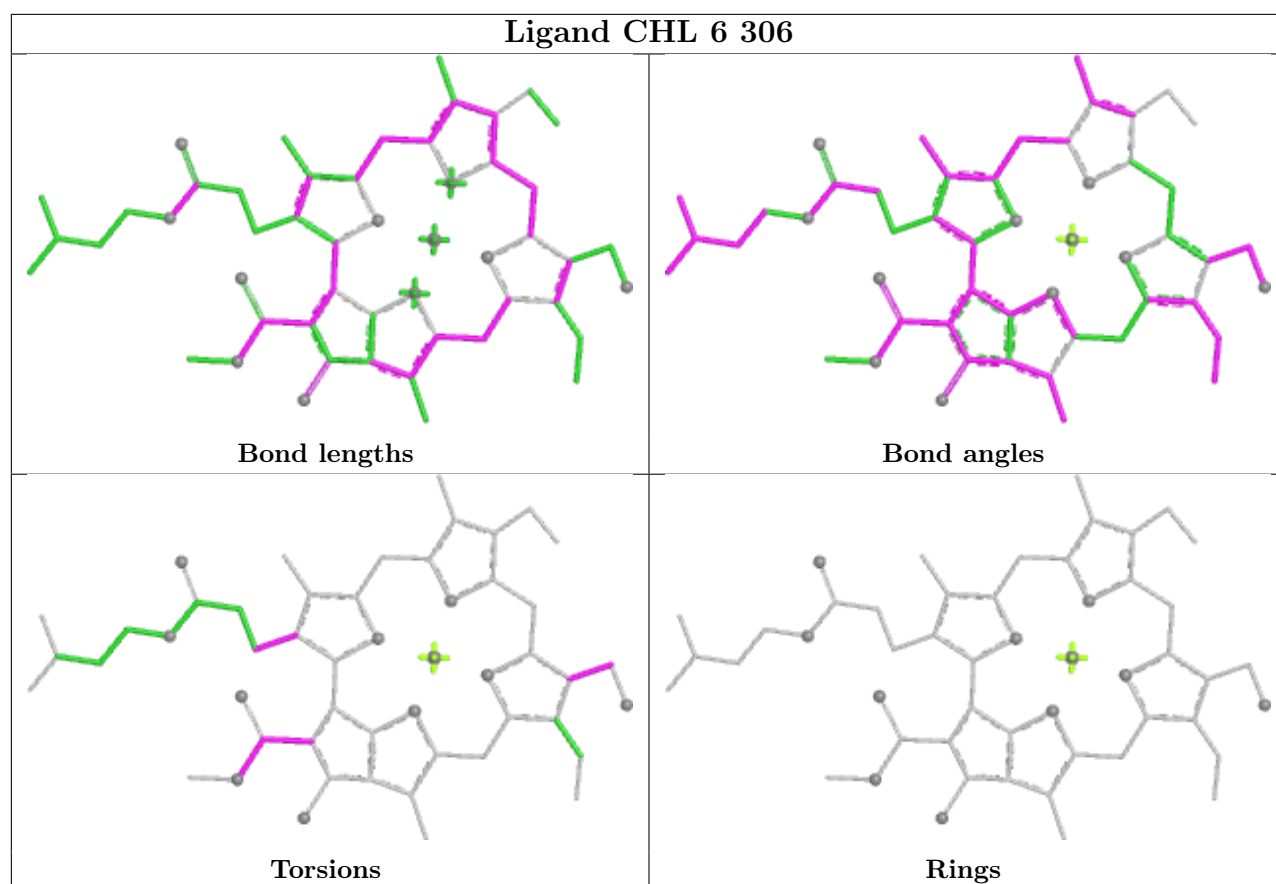
## Ligand CLA 4 309



## Ligand CLA L 202

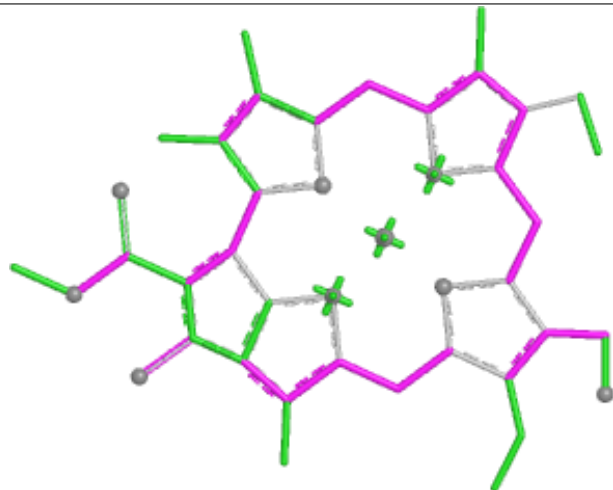




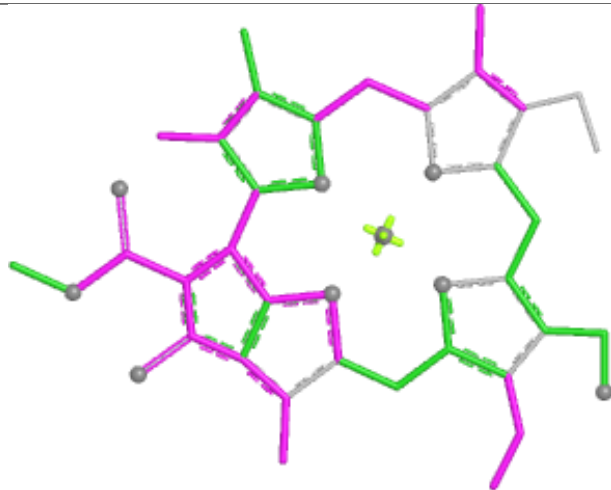




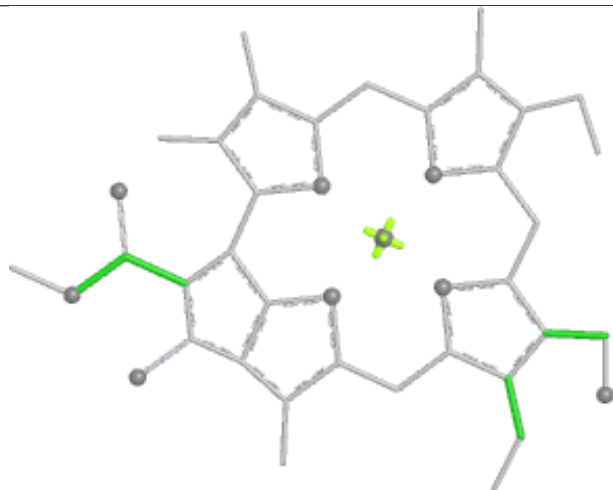
## Ligand CHL d 614



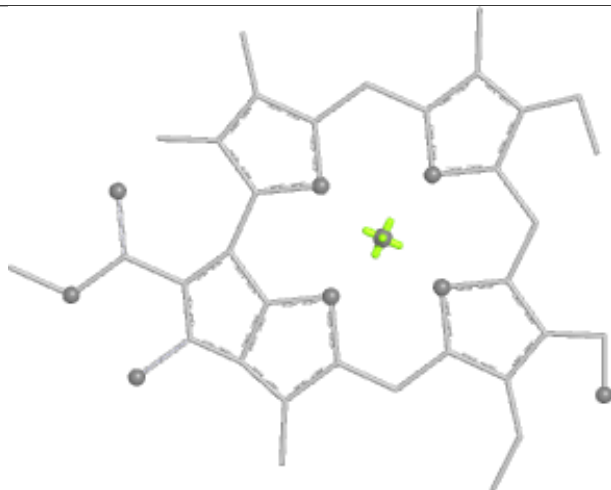
Bond lengths



Bond angles



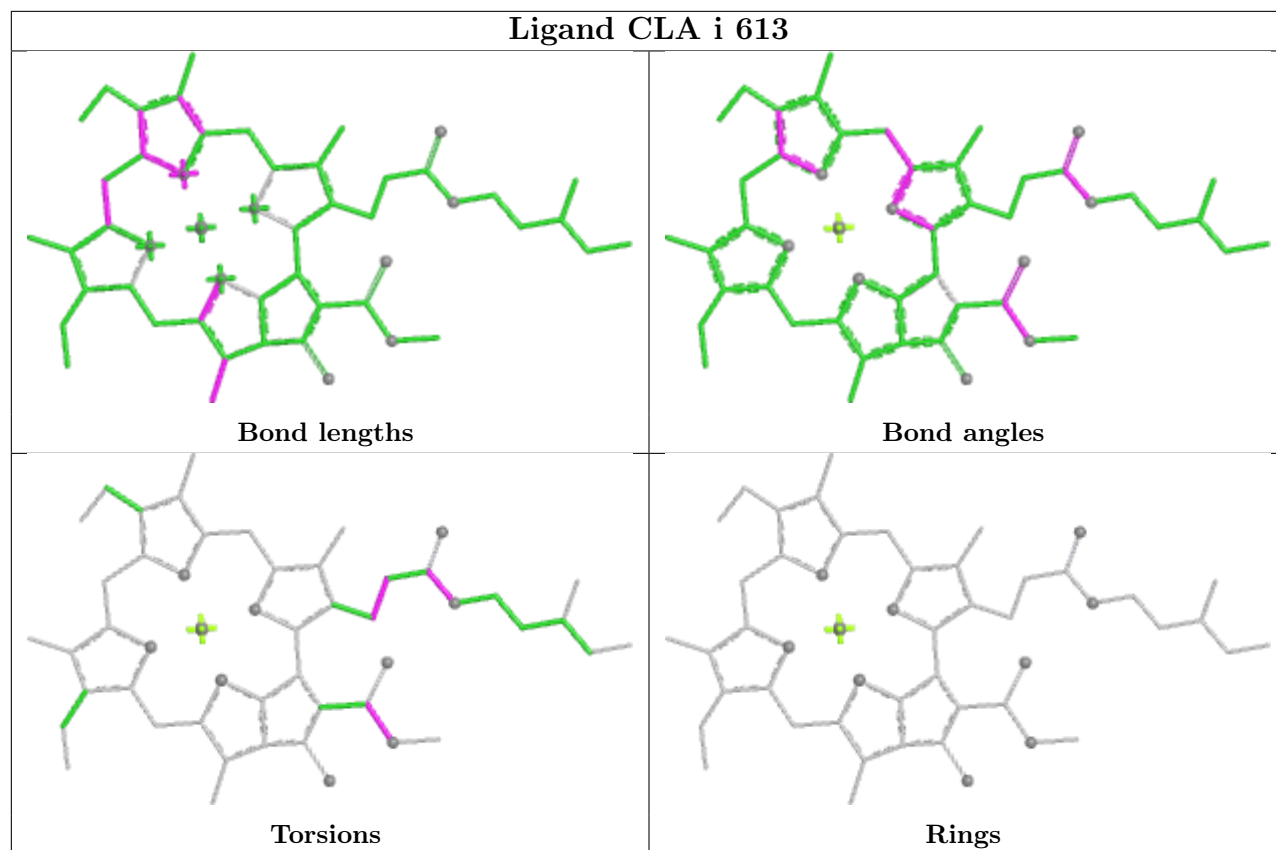
Torsions



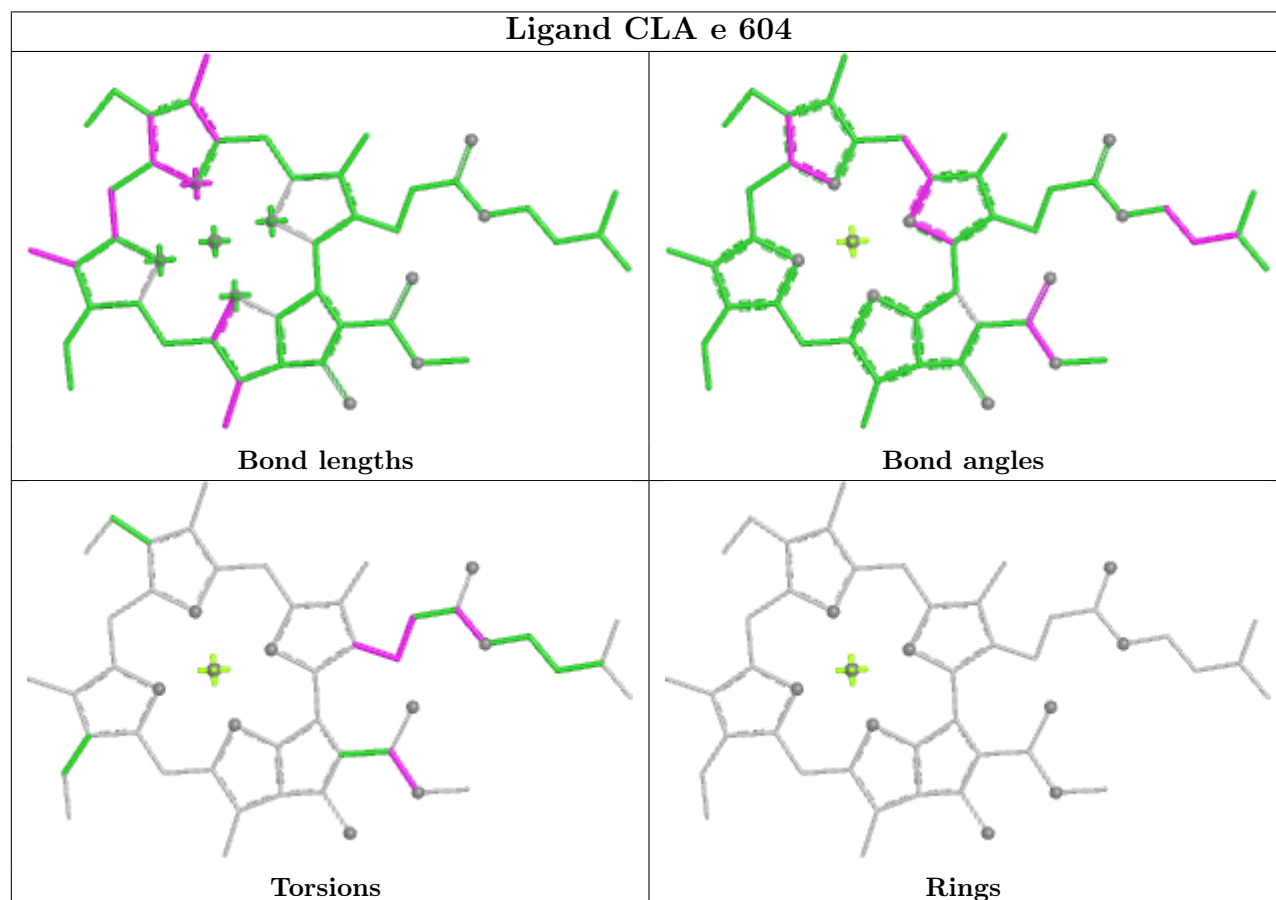
Rings



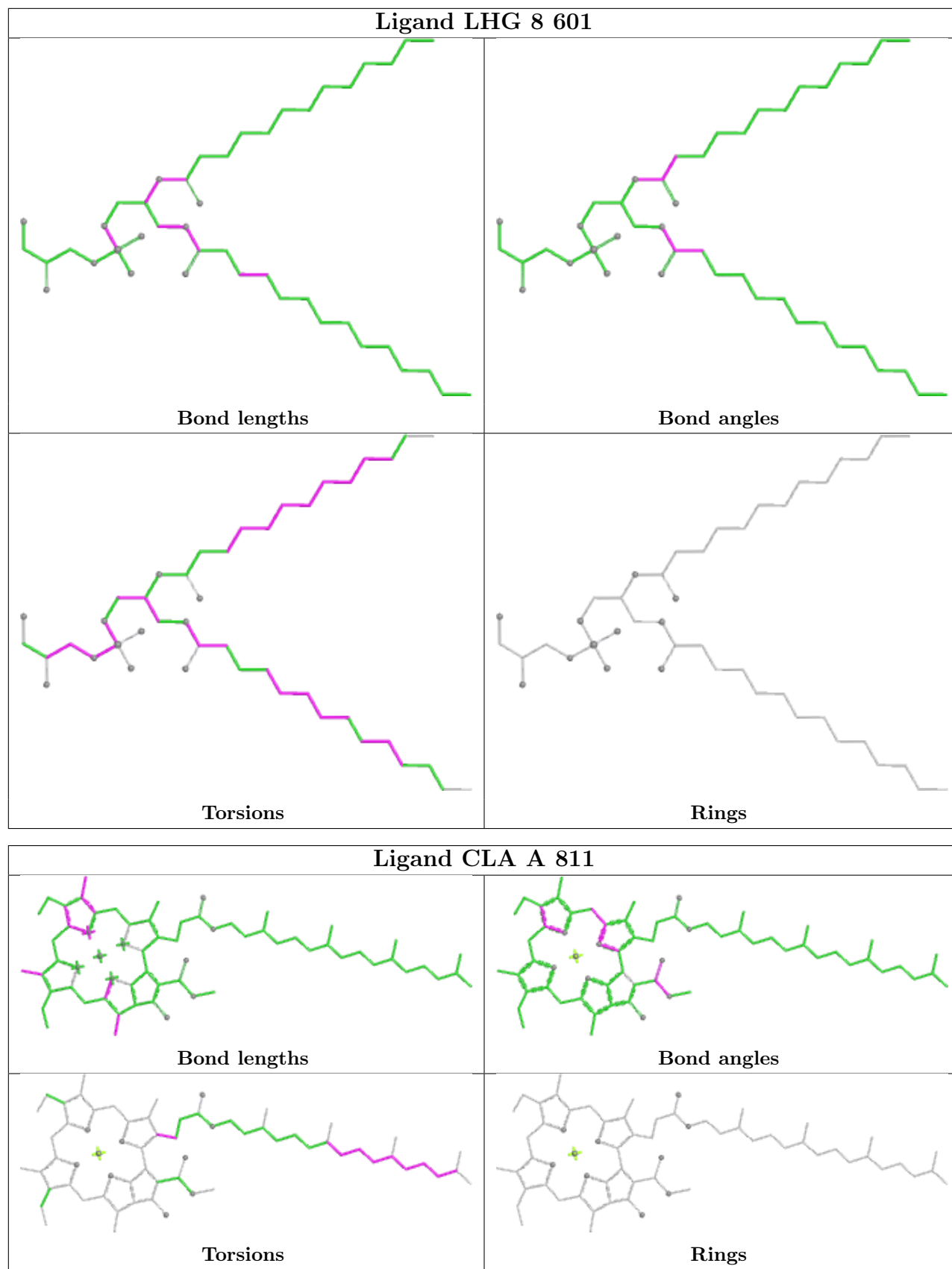
## Ligand CLA i 613



## Ligand CLA e 604

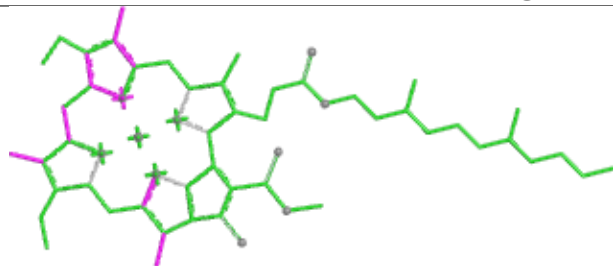




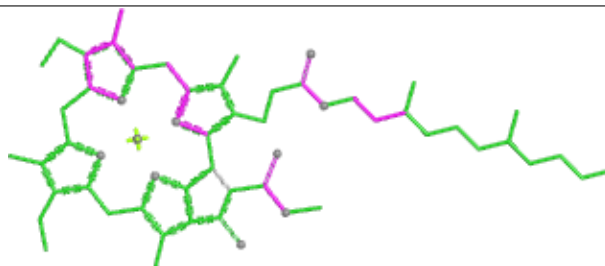




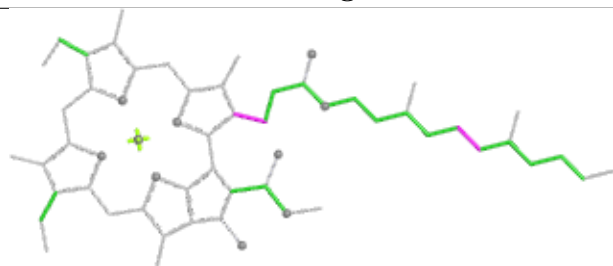
## Ligand CLA 6 309



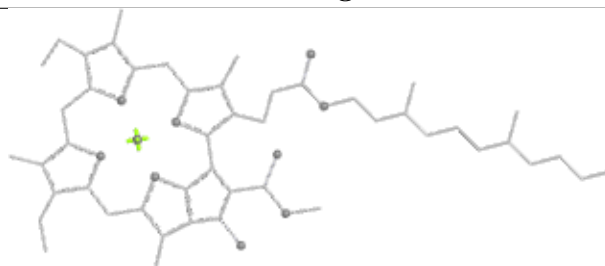
Bond lengths



Bond angles

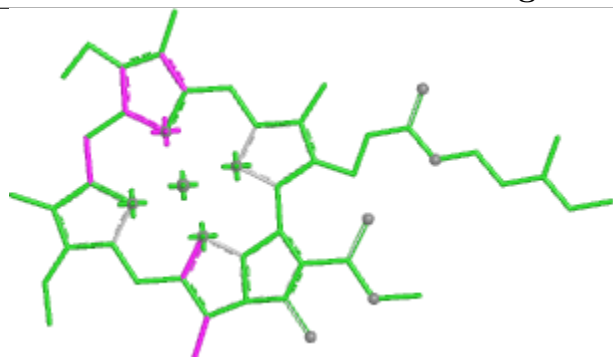


Torsions

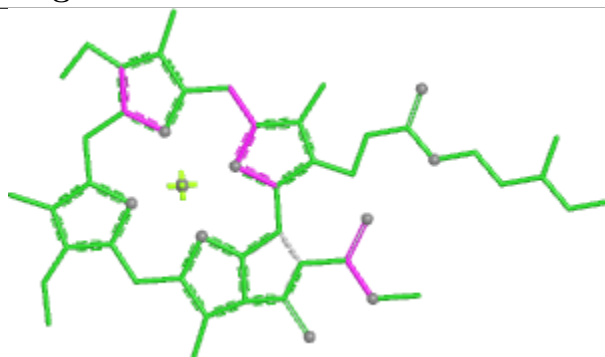


Rings

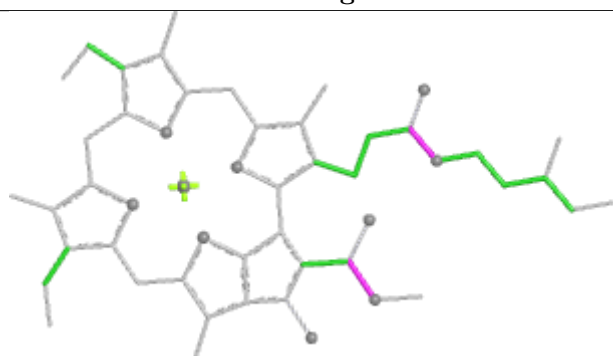
## Ligand CLA g 603



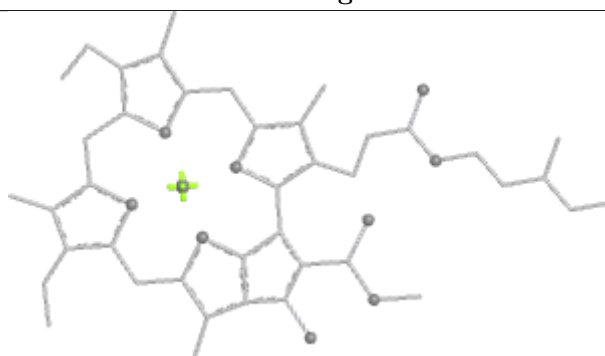
Bond lengths



Bond angles



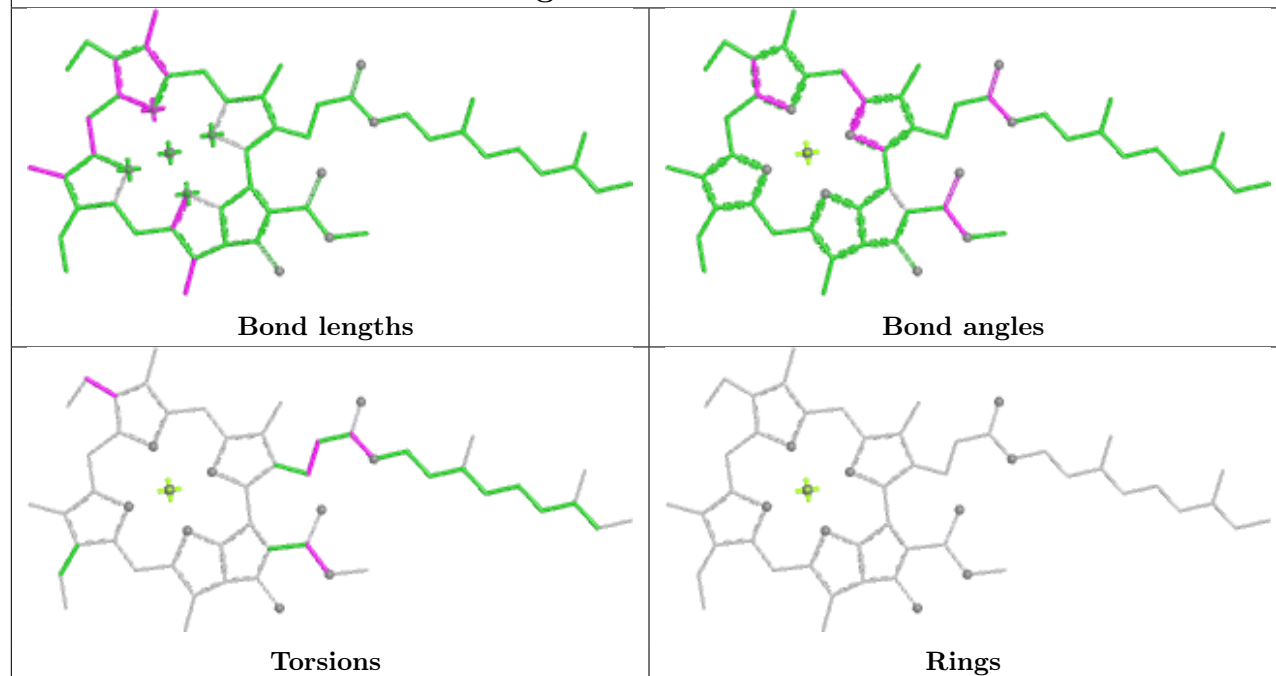
Torsions



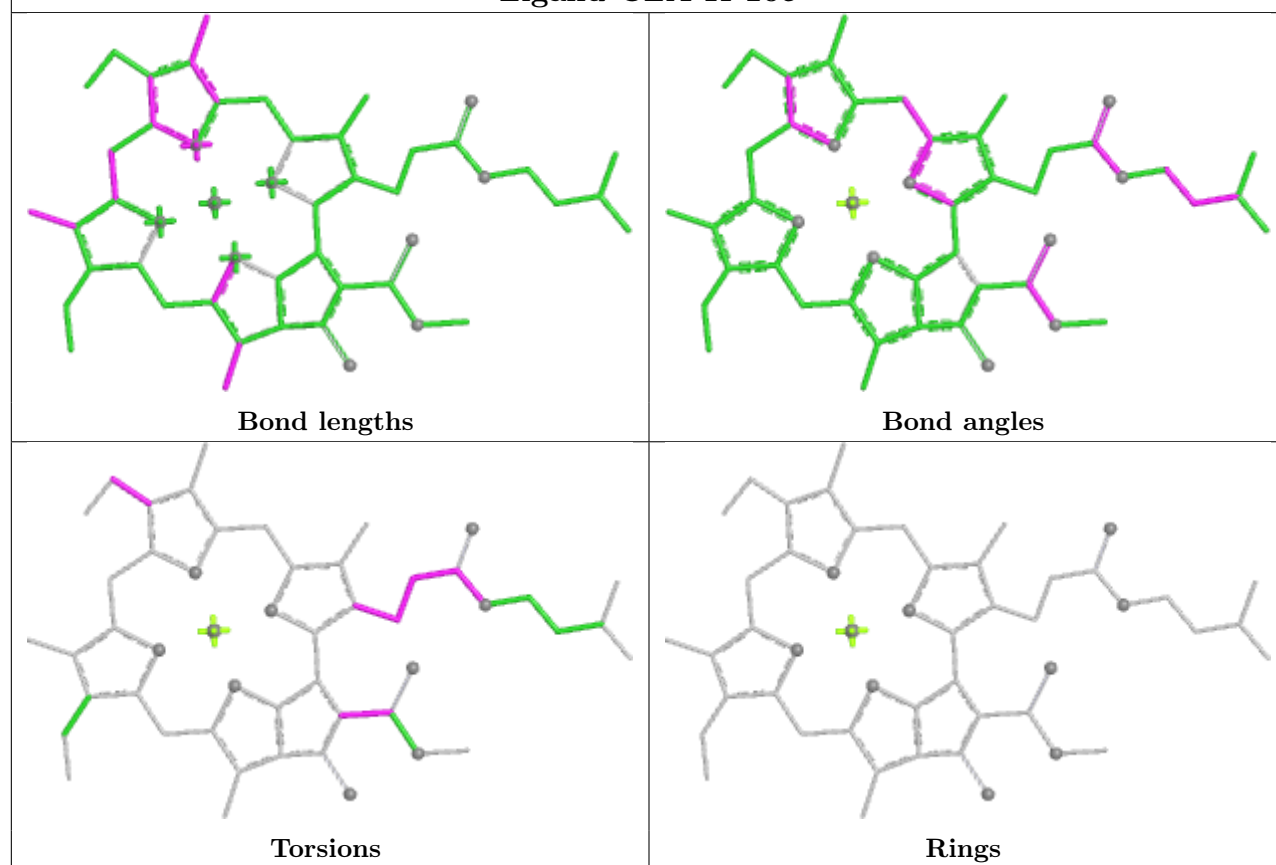
Rings



## Ligand CLA 6 312

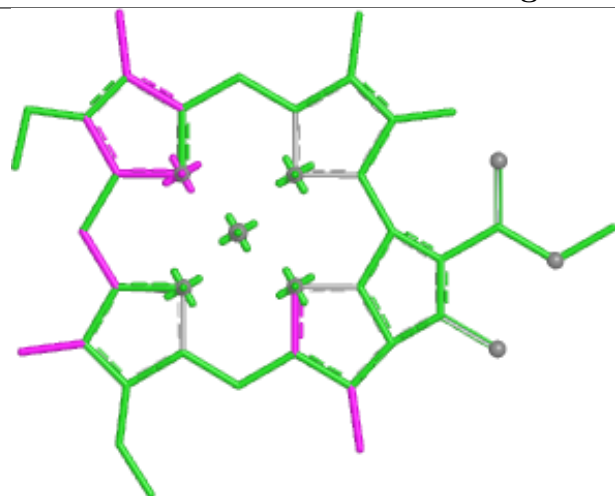


## Ligand CLA K 105

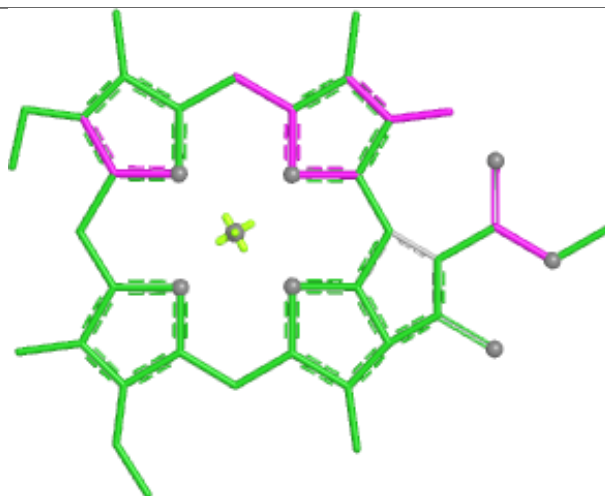




## Ligand CLA 9 310



Bond lengths



Bond angles



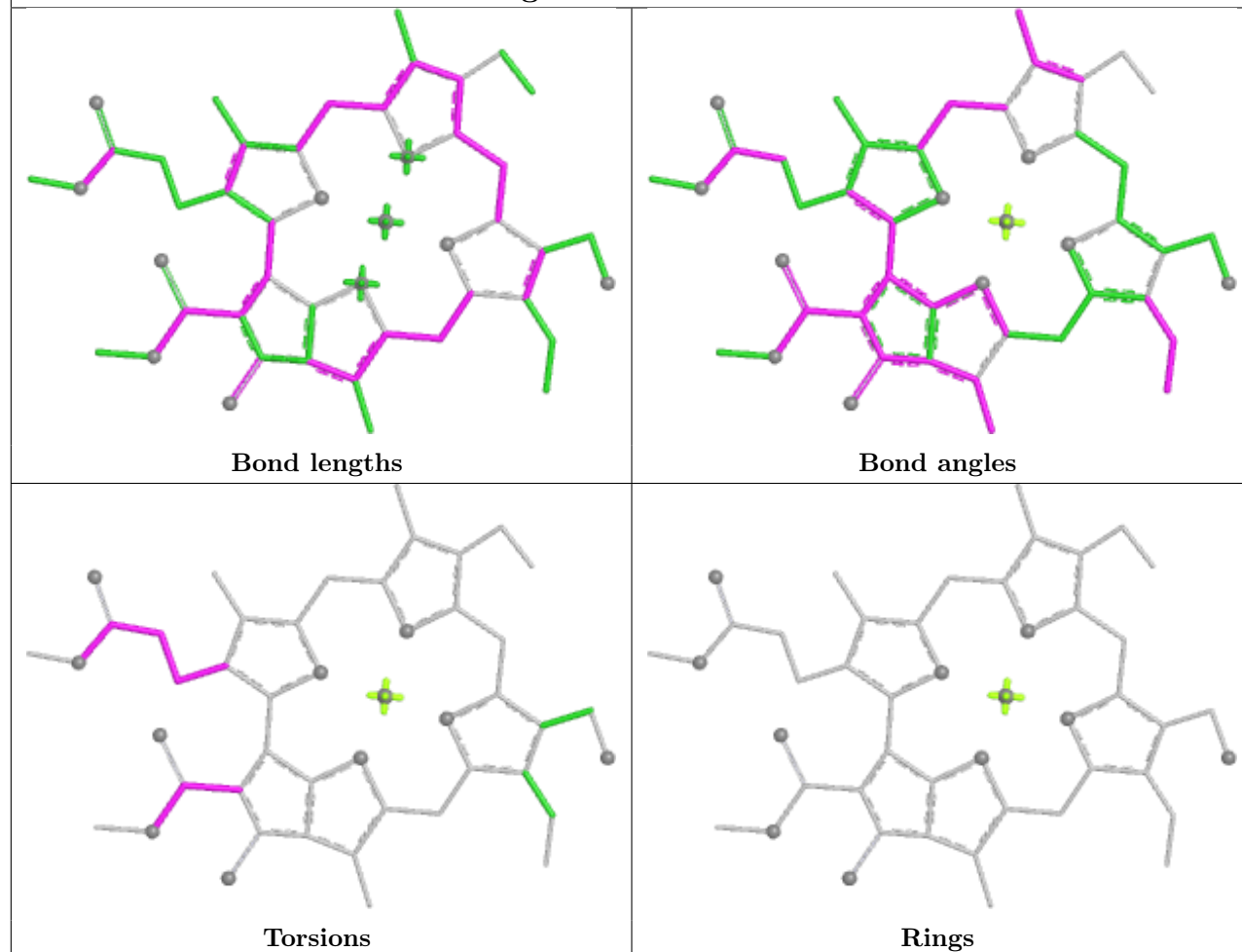
Torsions



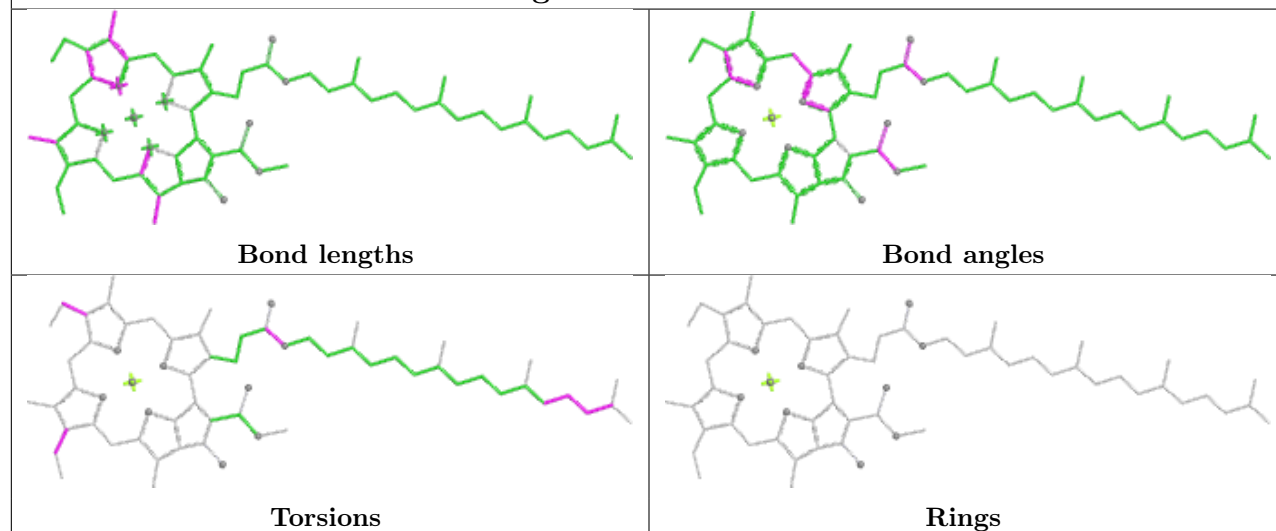
Rings



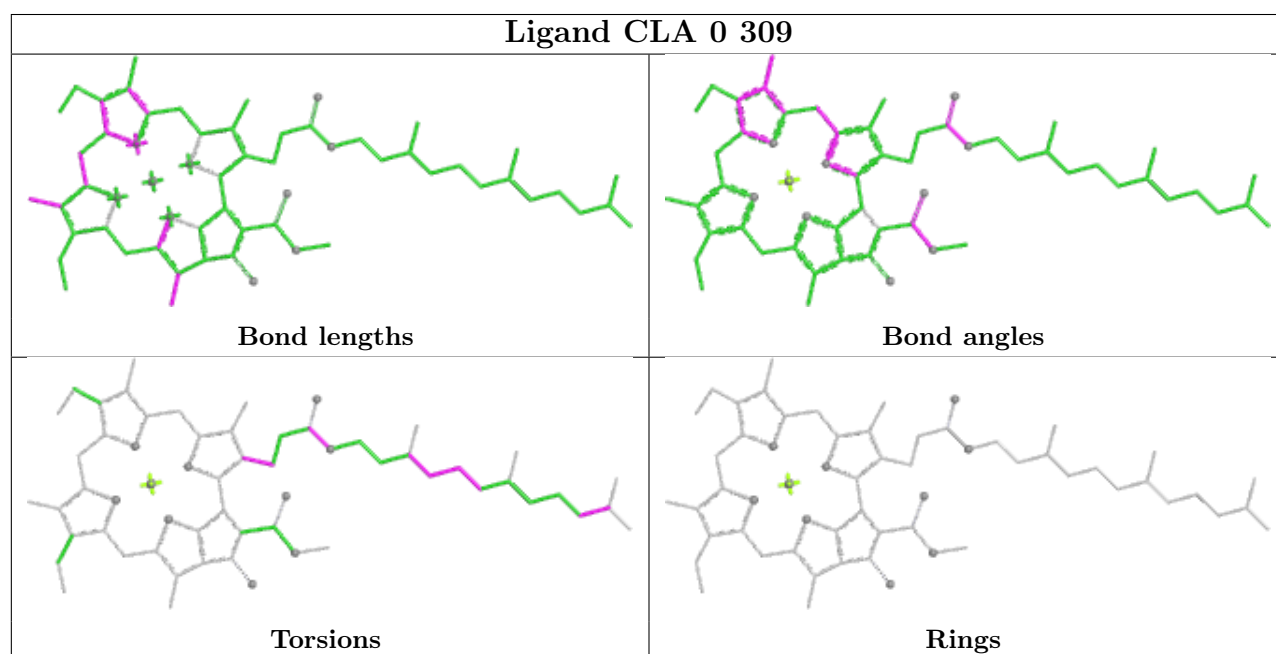
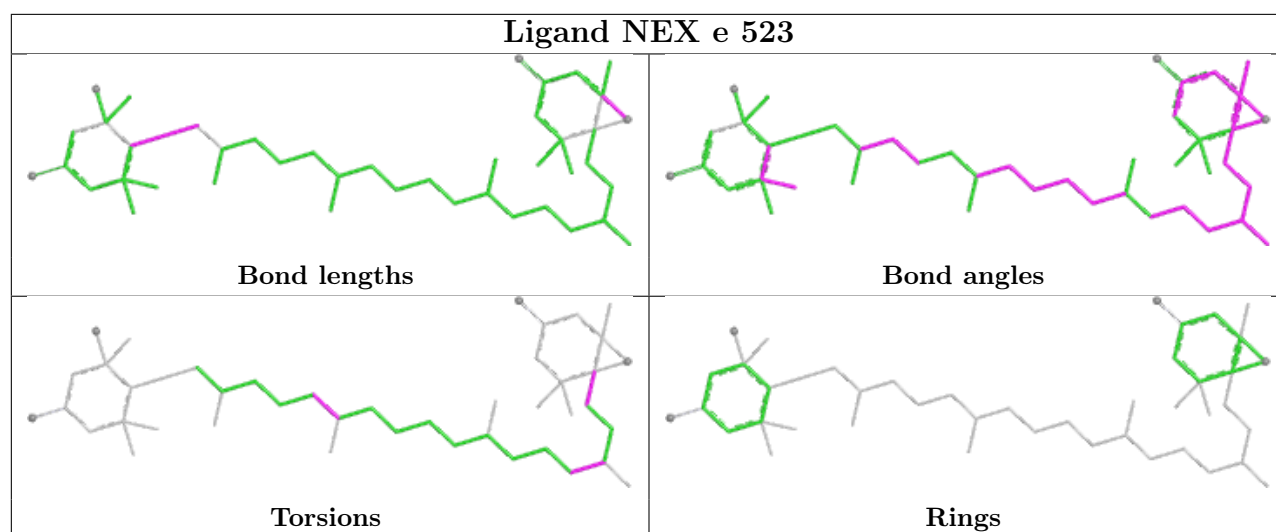
## Ligand CHL 5 313



## Ligand CLA B 840

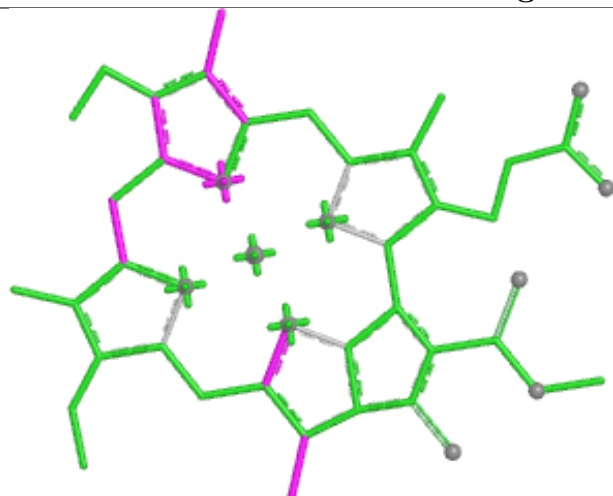




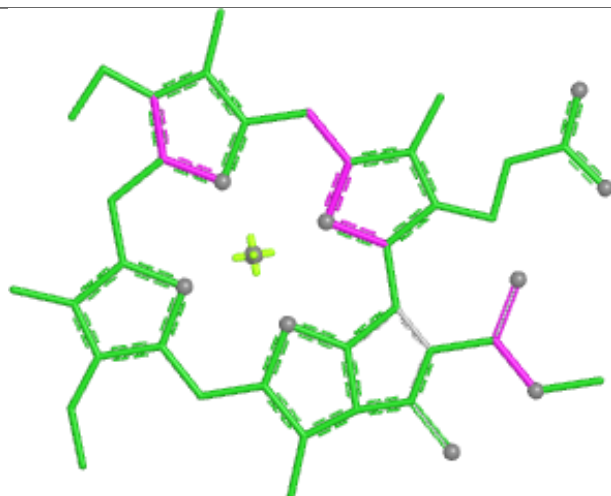




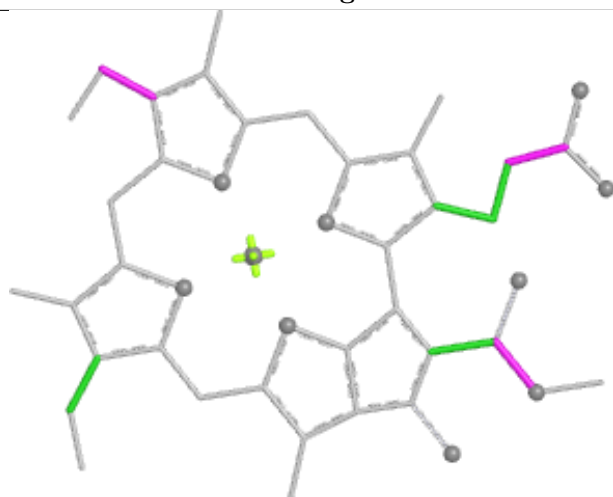
## Ligand CLA h 612



Bond lengths



Bond angles



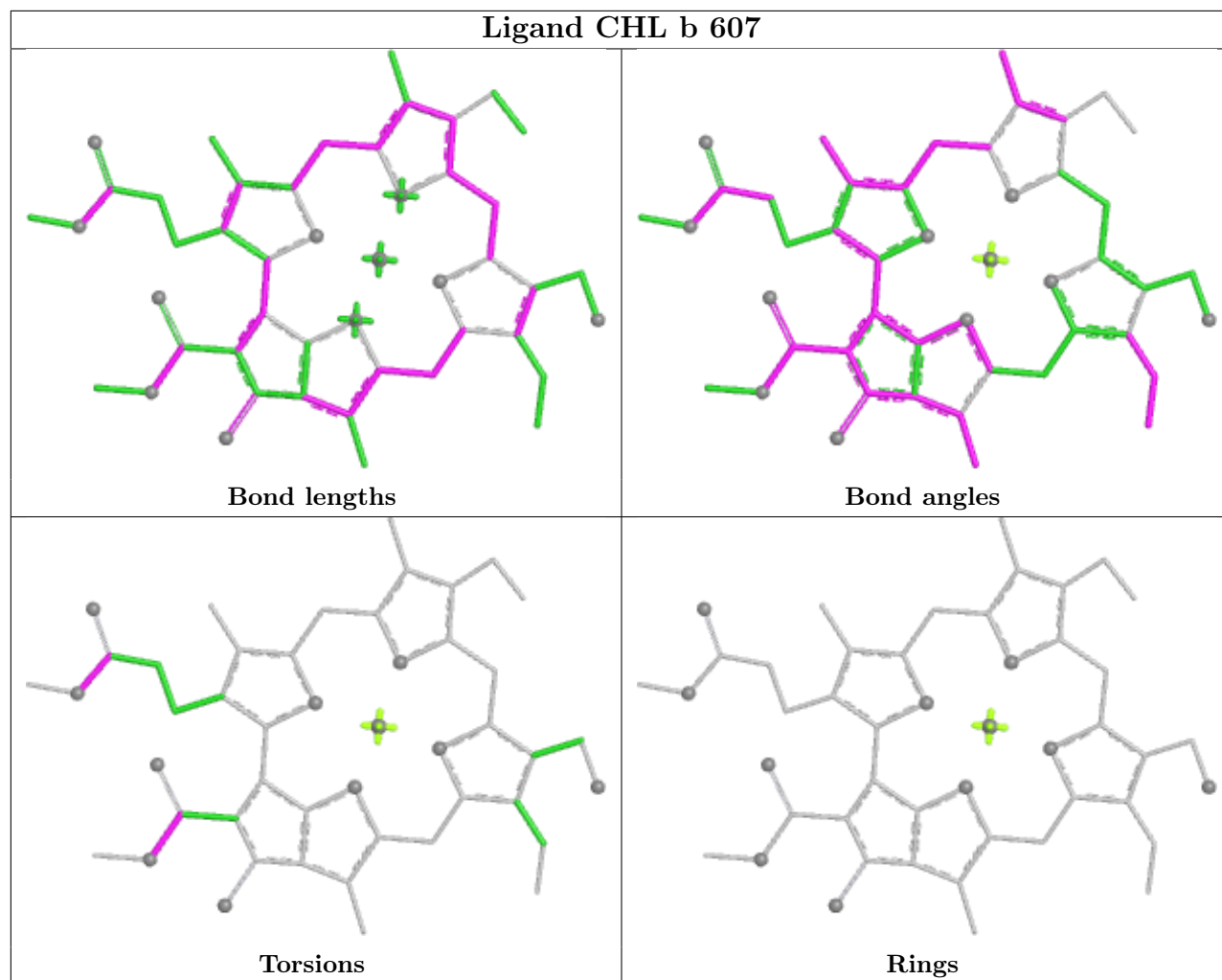
Torsions



Rings

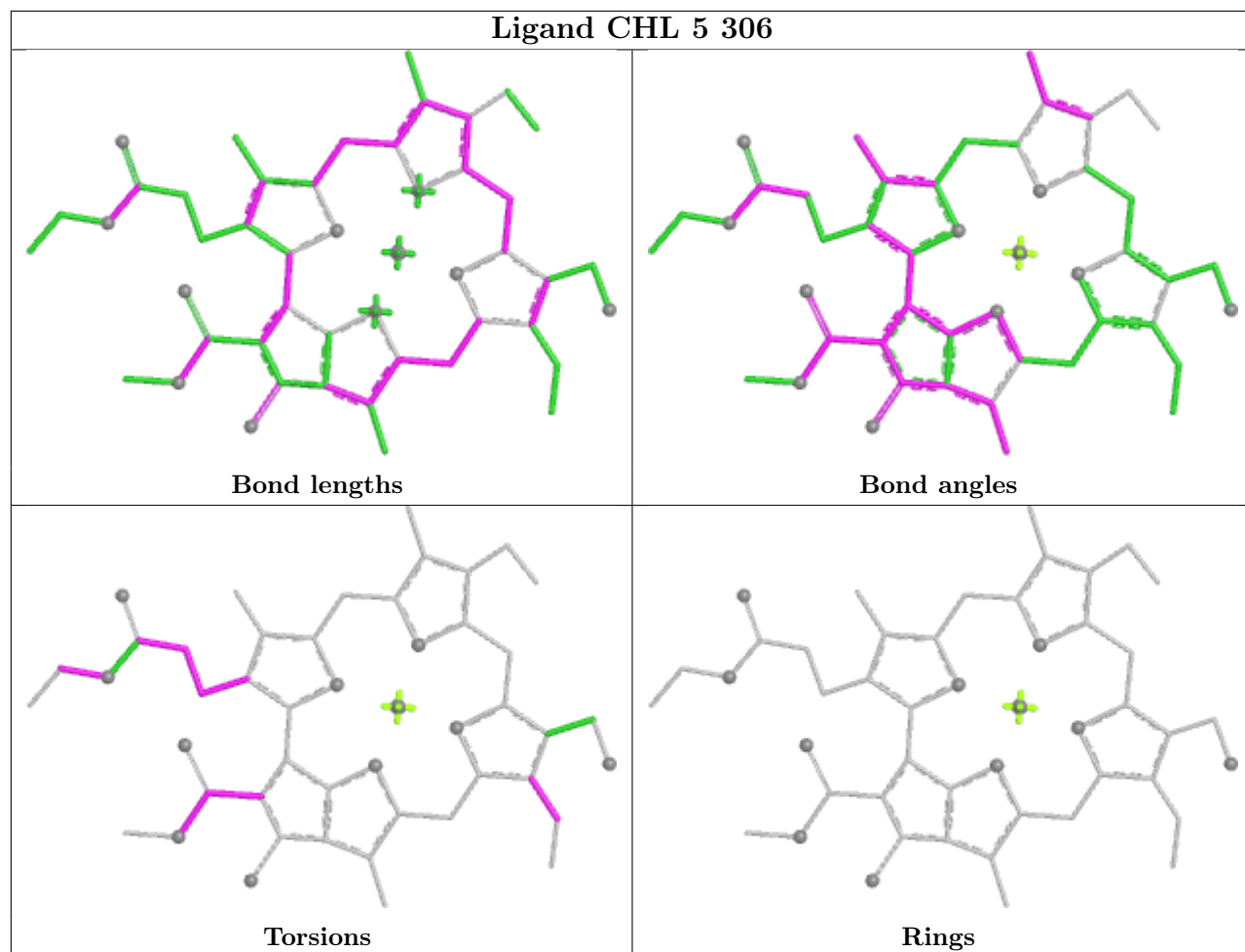


## Ligand CHL b 607



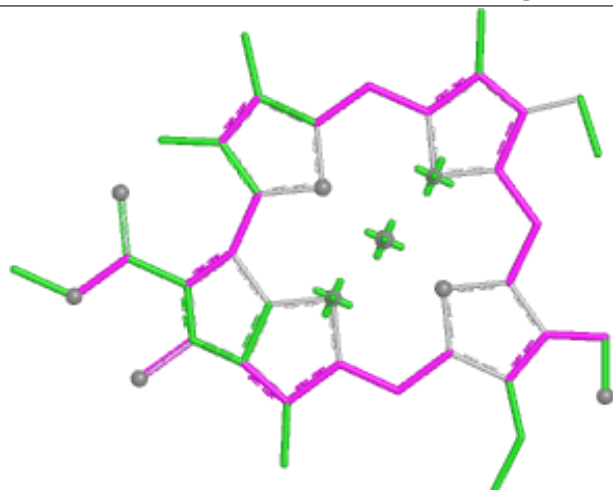


## Ligand CHL 5 306

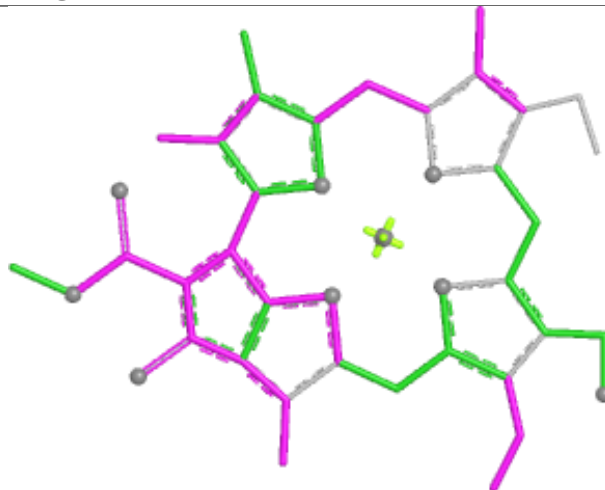




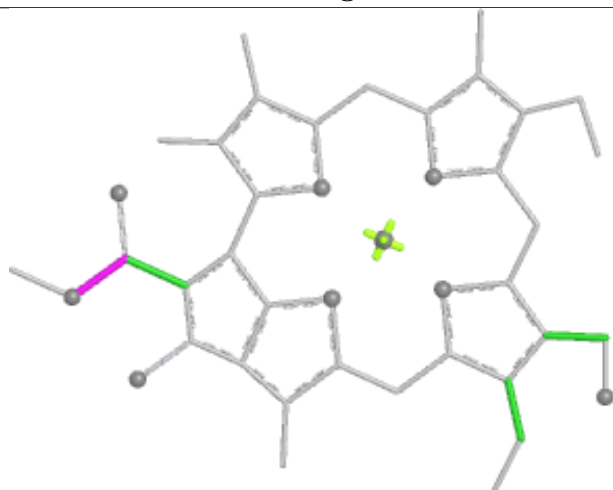
## Ligand CHL g 614



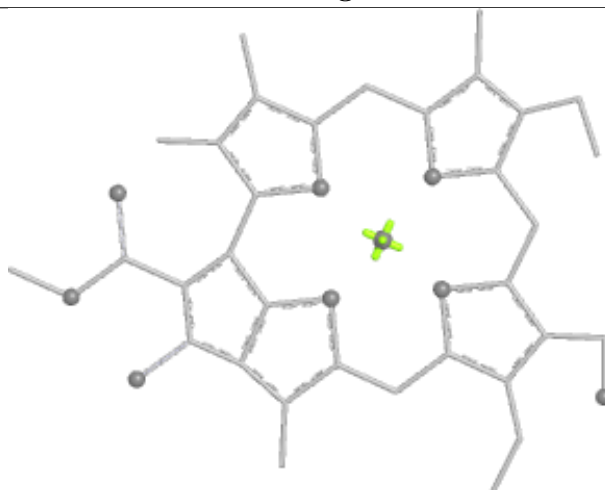
Bond lengths



Bond angles



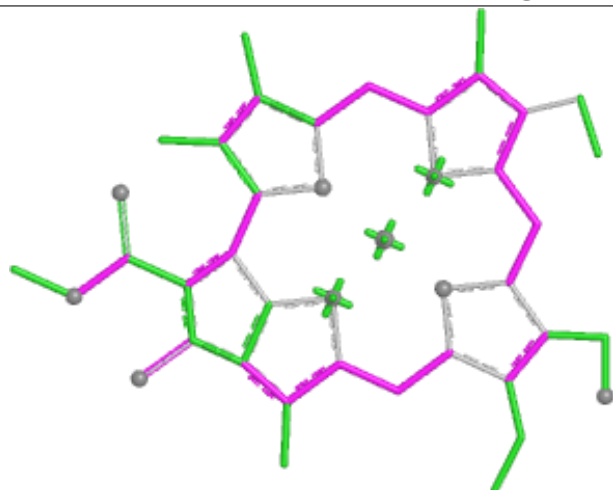
Torsions



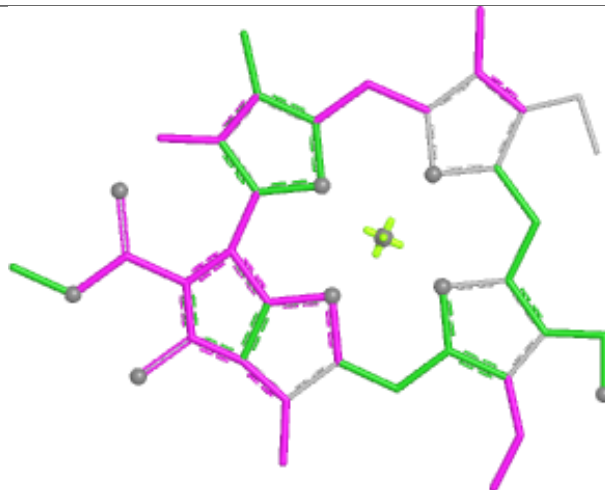
Rings



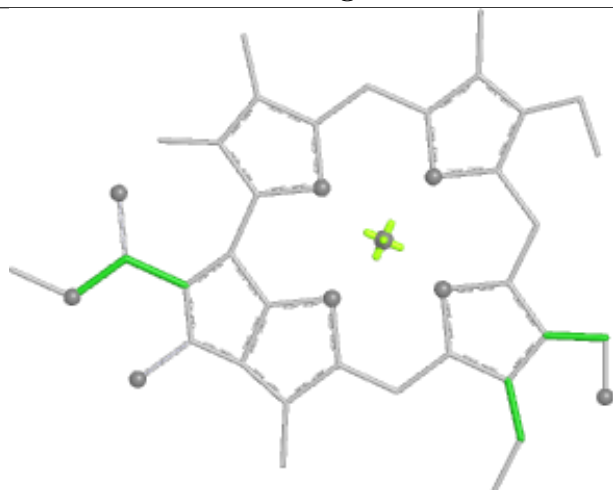
## Ligand CHL a 614



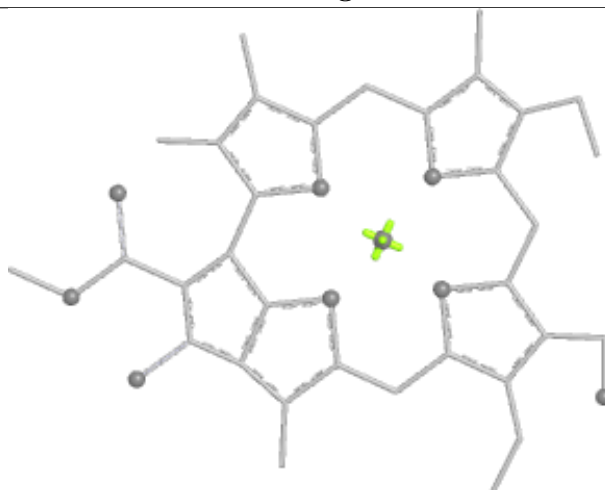
Bond lengths



Bond angles



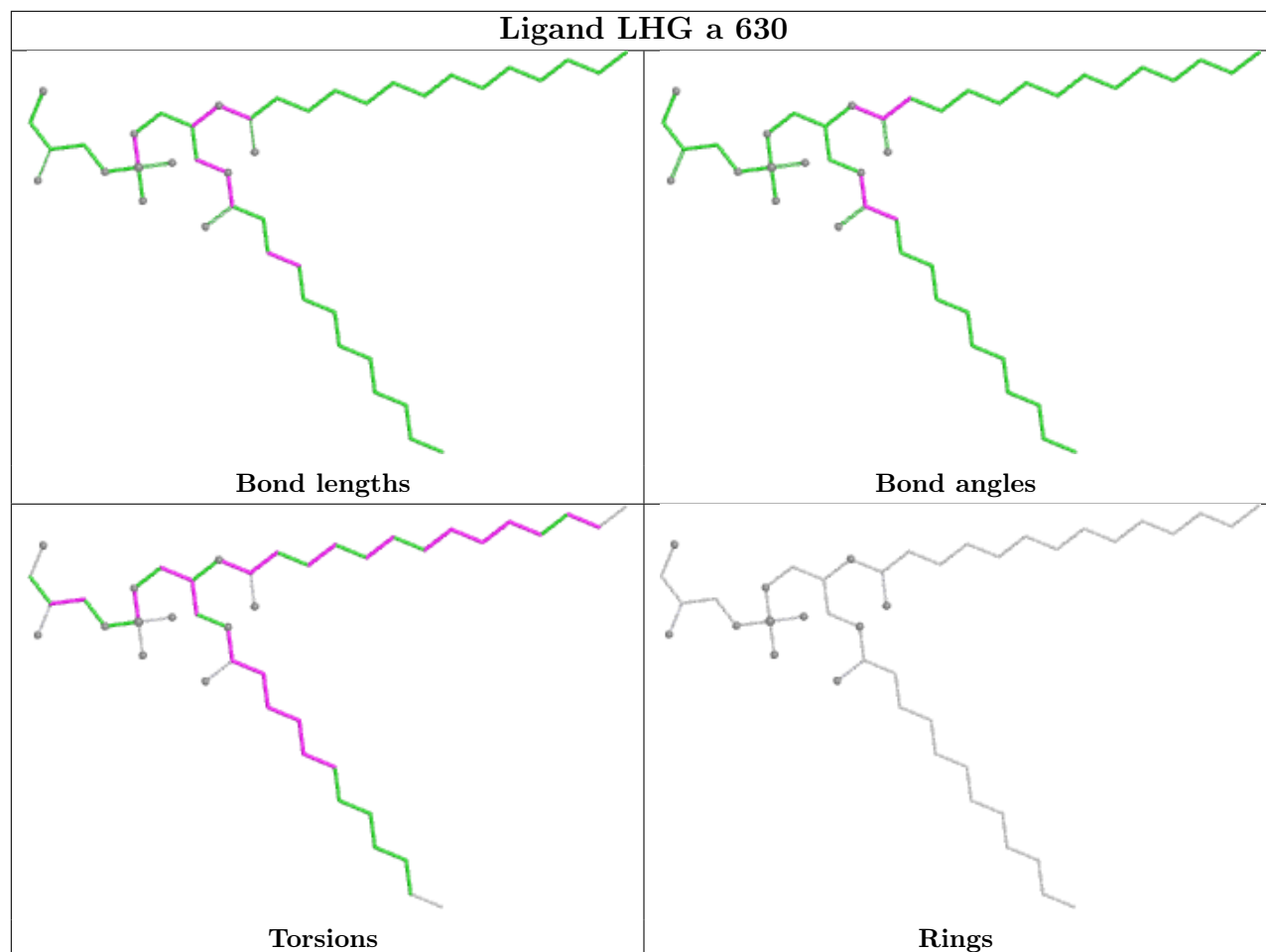
Torsions



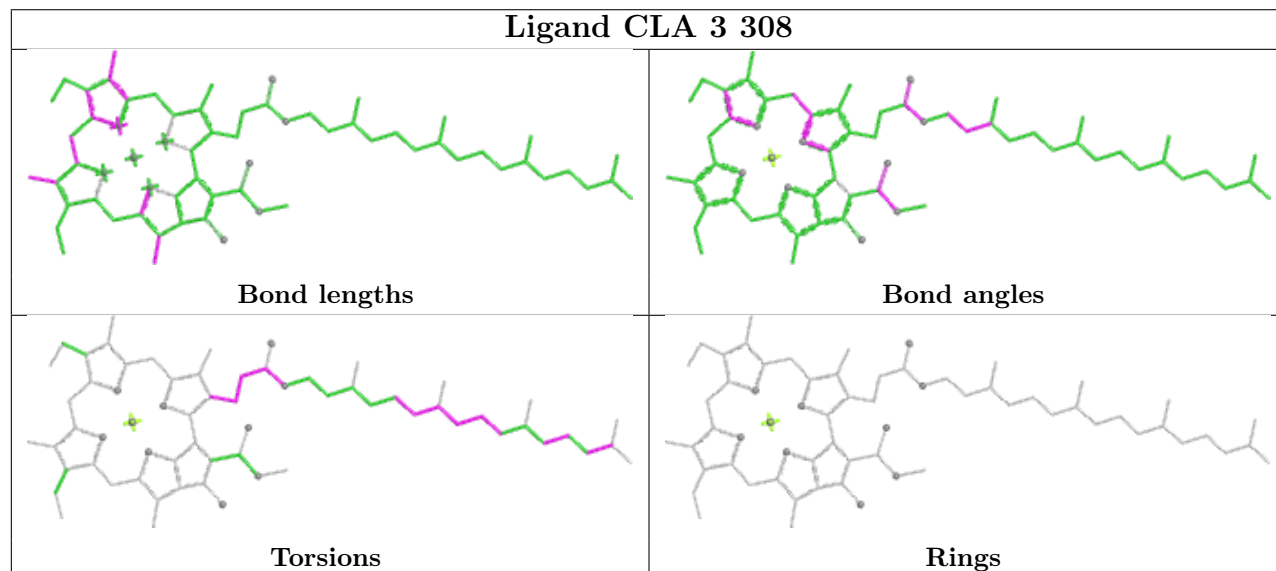
Rings



## Ligand LHG a 630

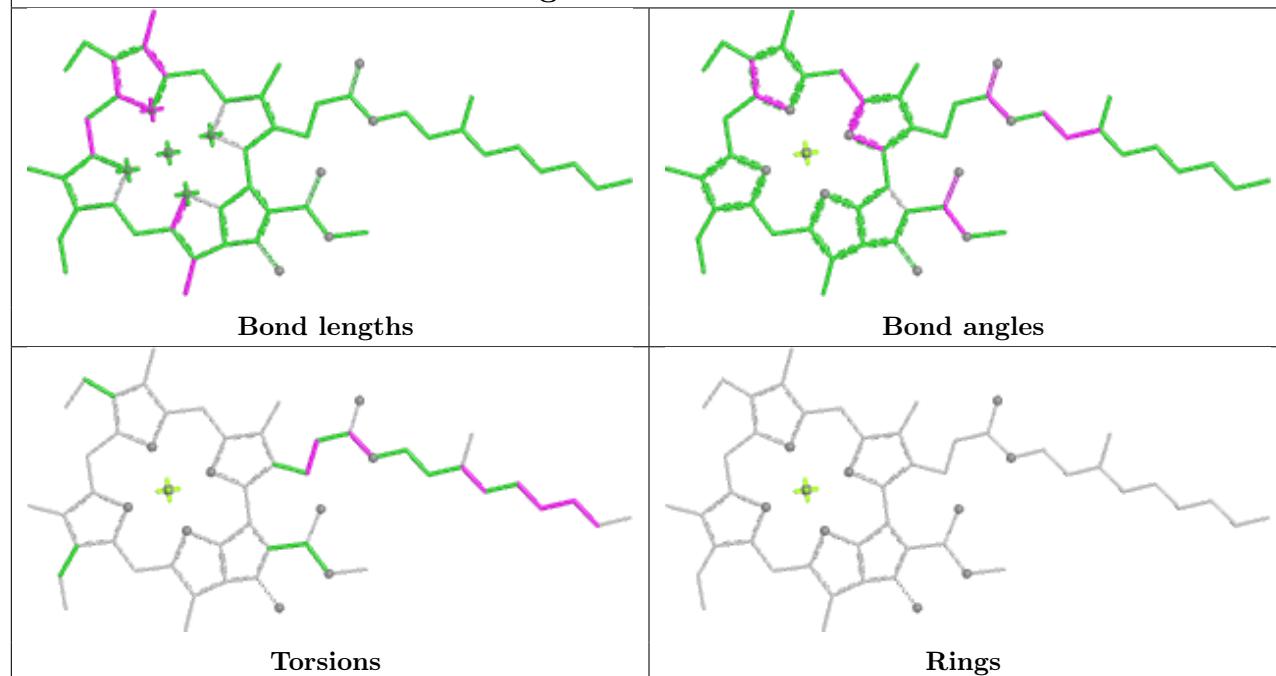


## Ligand CLA 3 308

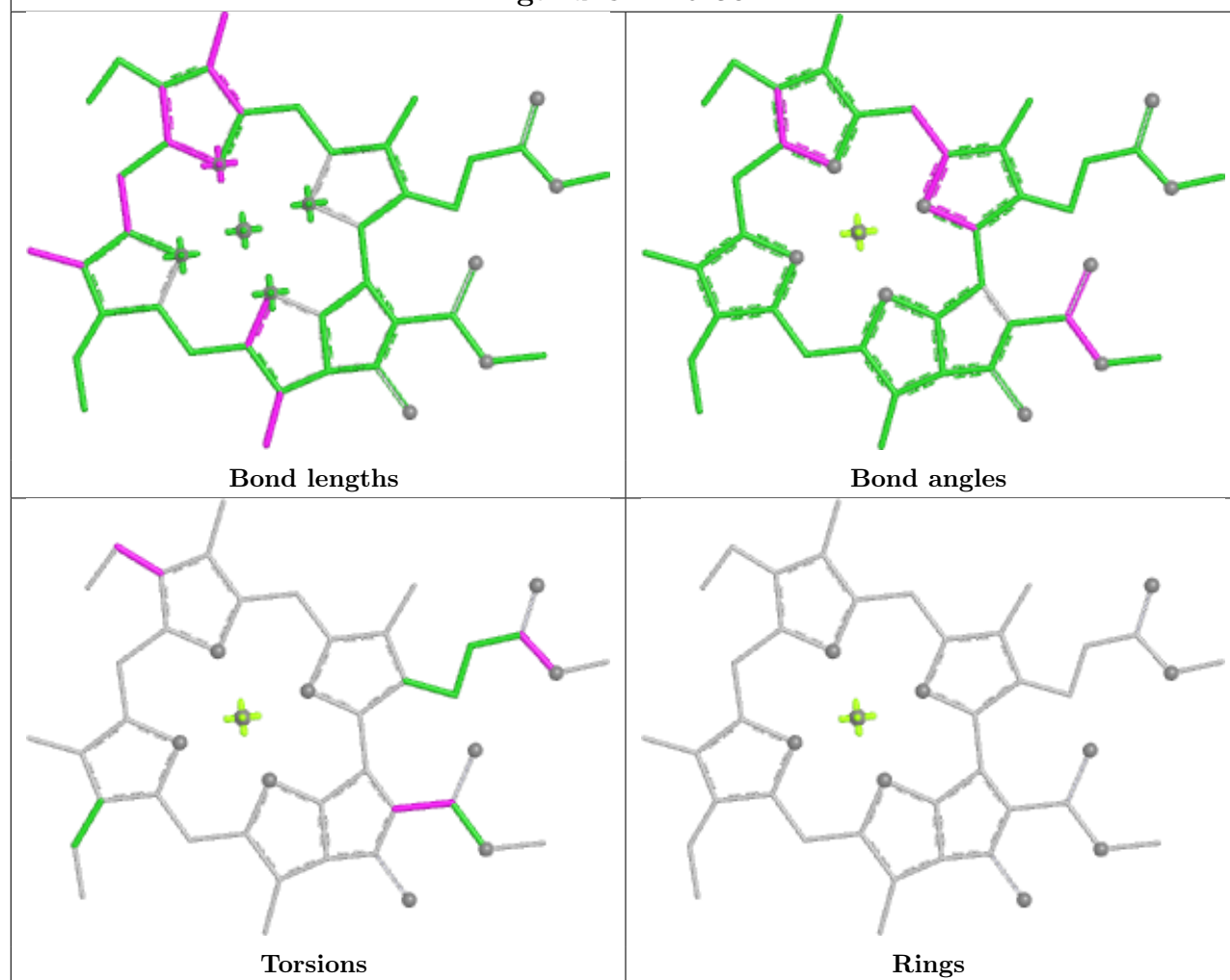




## Ligand CLA f 613

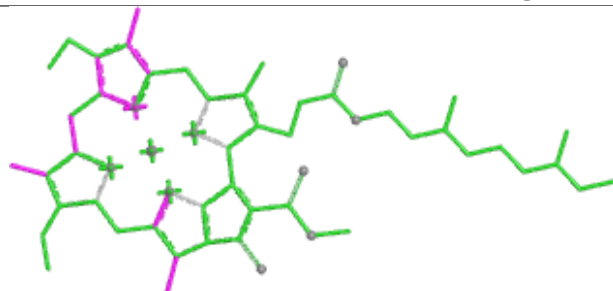


## Ligand CLA 6 304

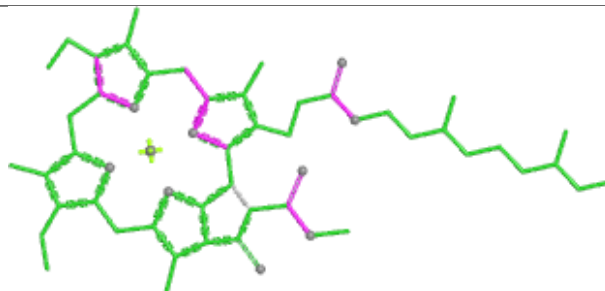




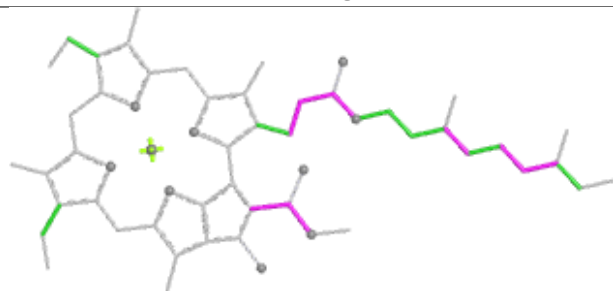
## Ligand CLA 1 303



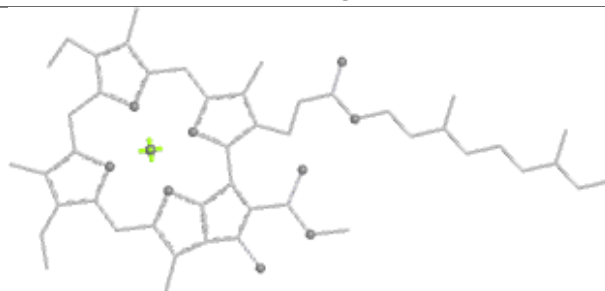
Bond lengths



Bond angles

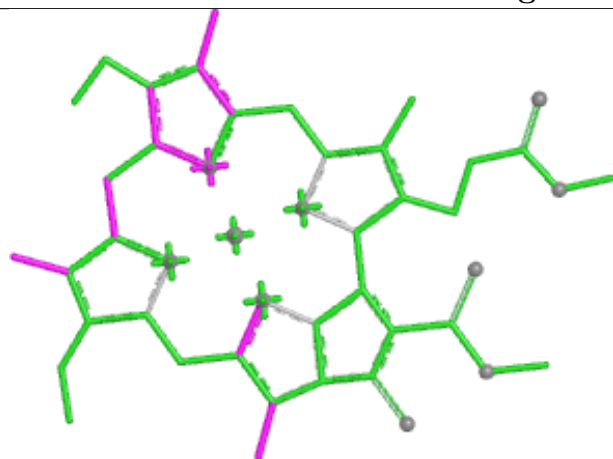


Torsions

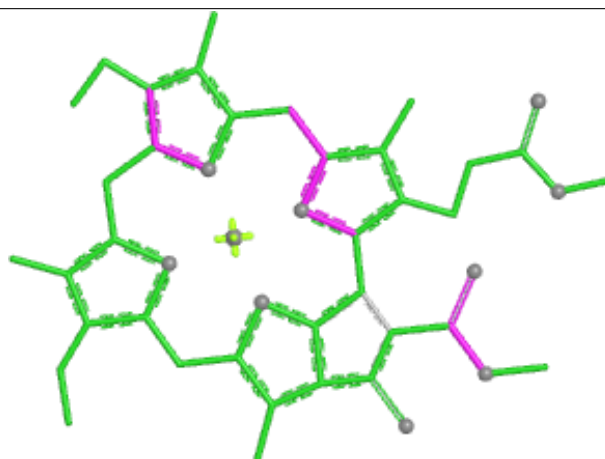


Rings

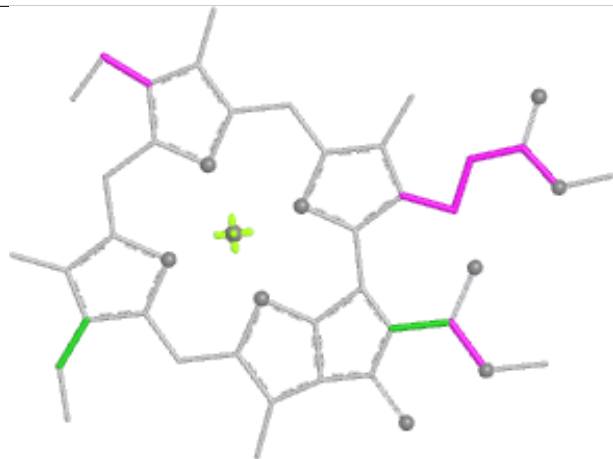
## Ligand CLA 6 318



Bond lengths



Bond angles

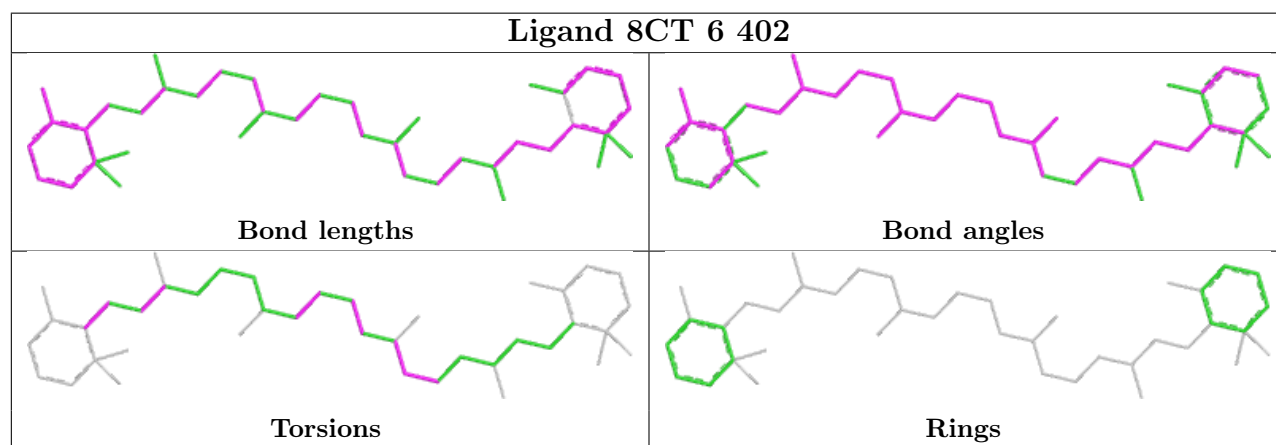
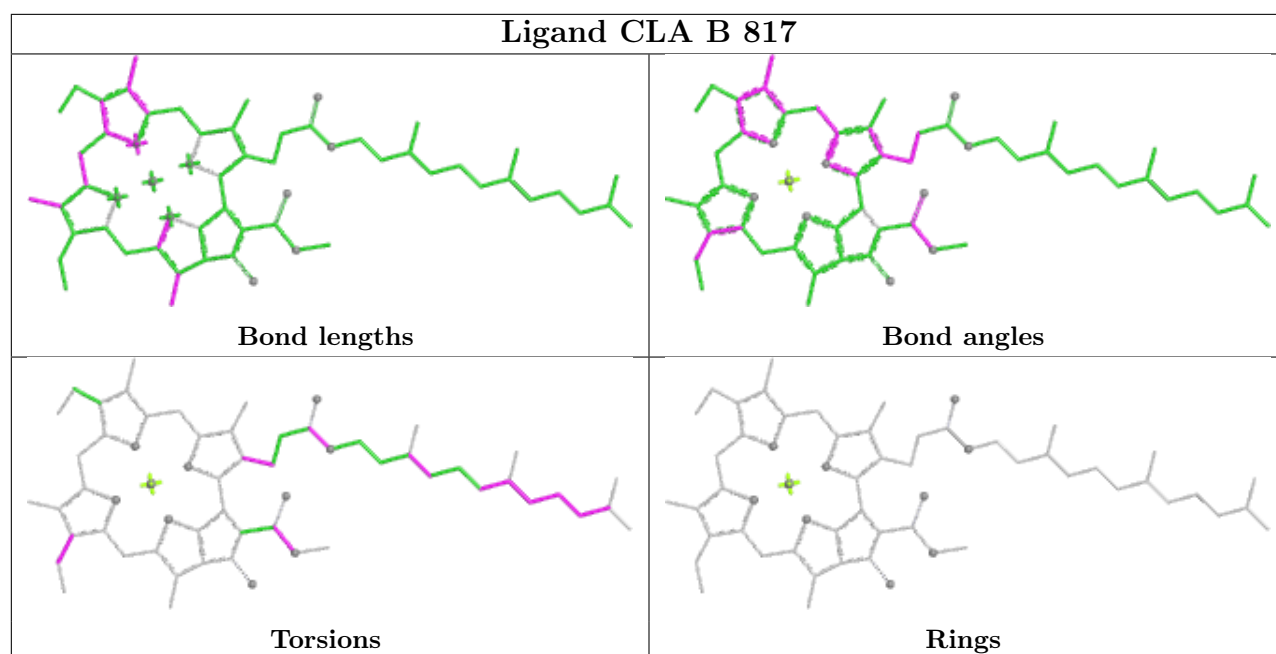


Torsions



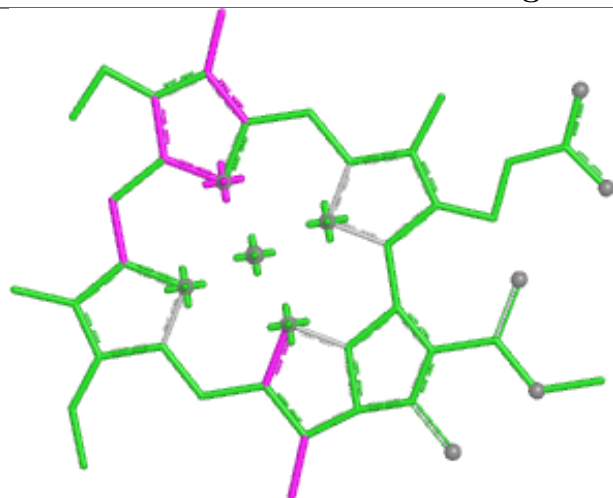
Rings



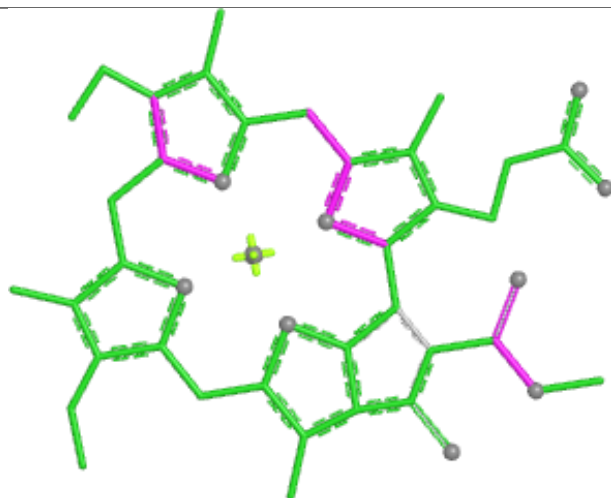




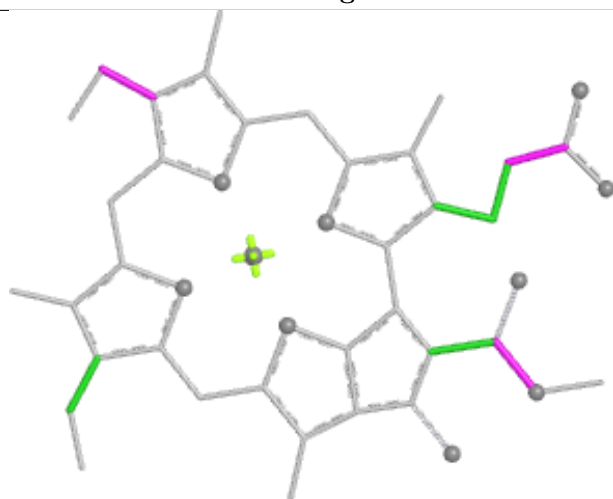
## Ligand CLA i 611



Bond lengths



Bond angles

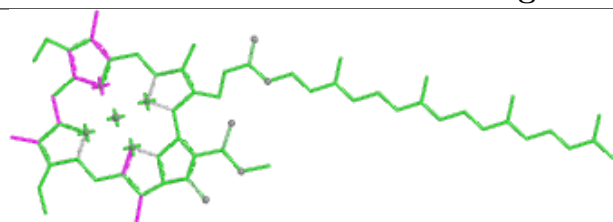


Torsions

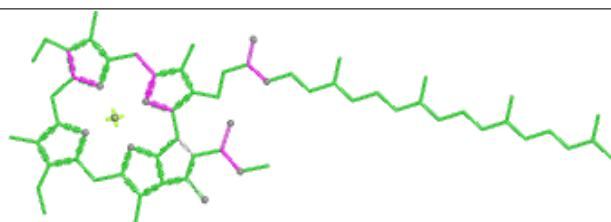


Rings

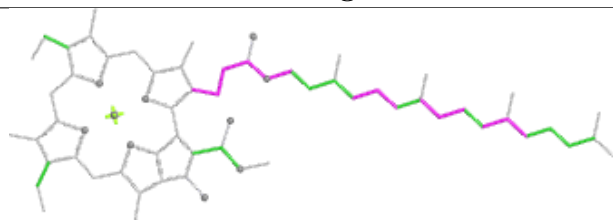
## Ligand CLA 7 308



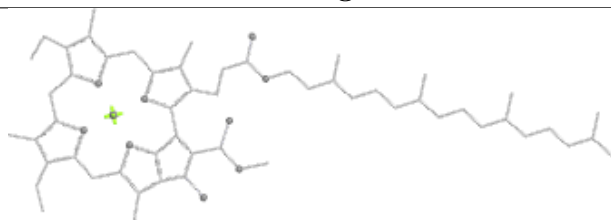
Bond lengths



Bond angles

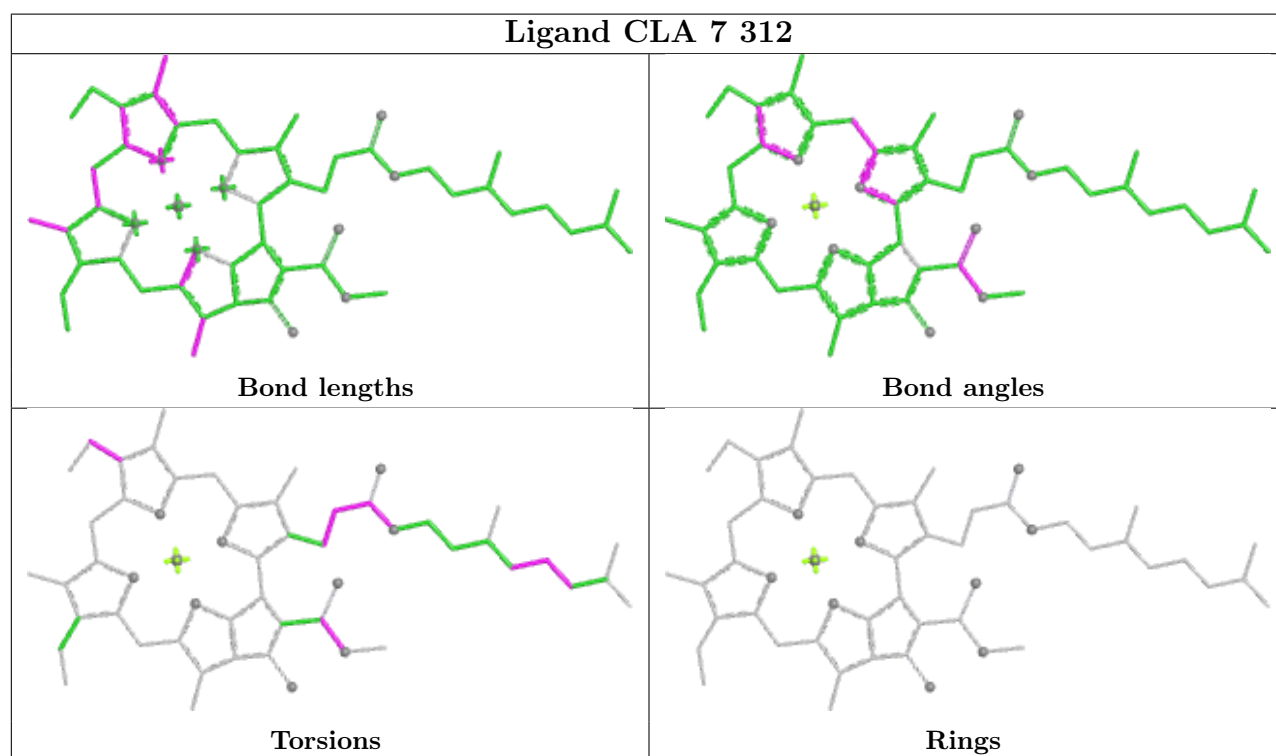
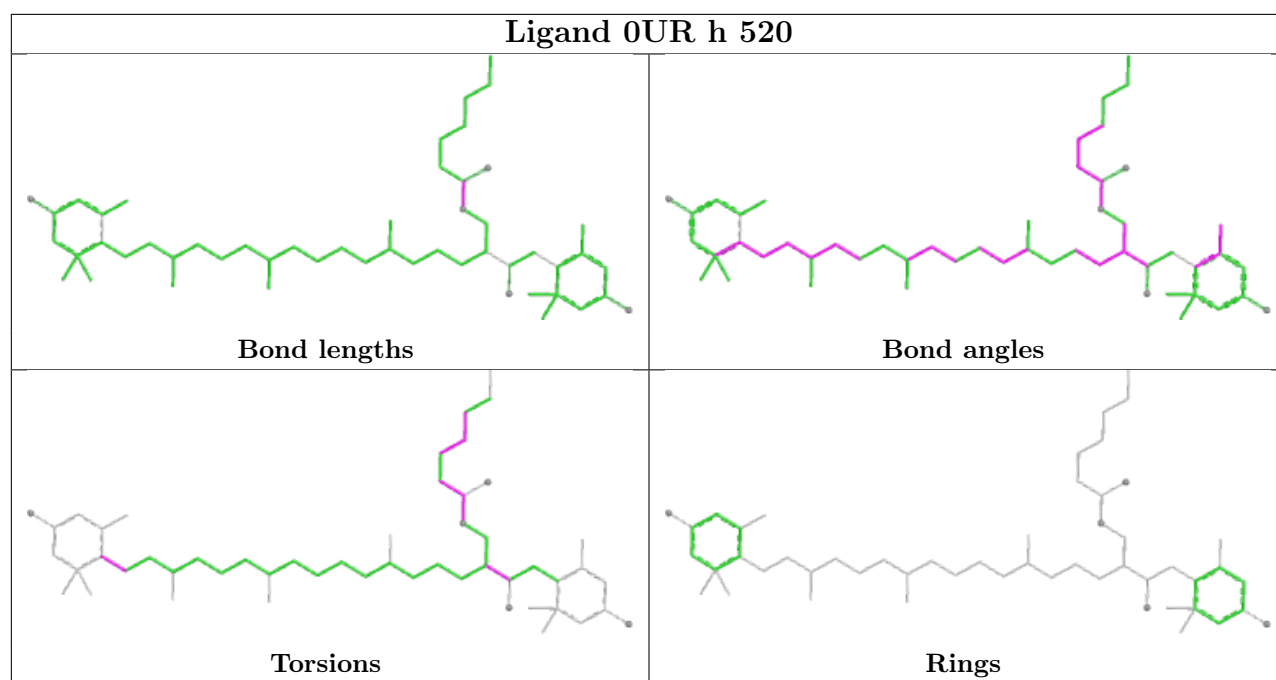


Torsions



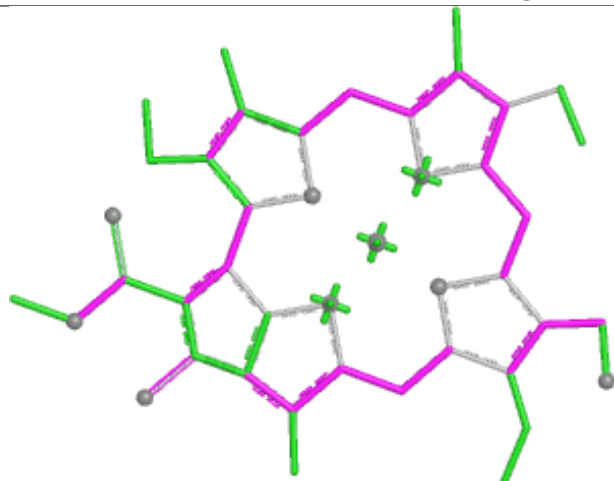
Rings



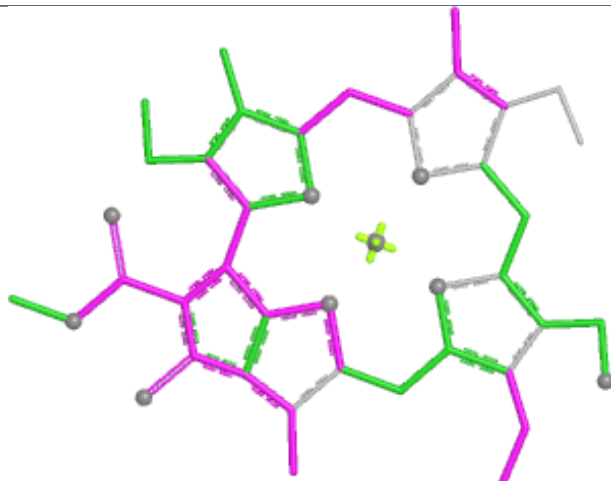




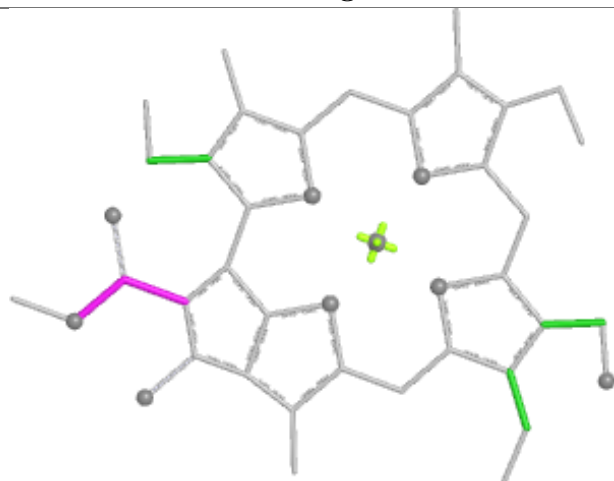
## Ligand CHL a 605



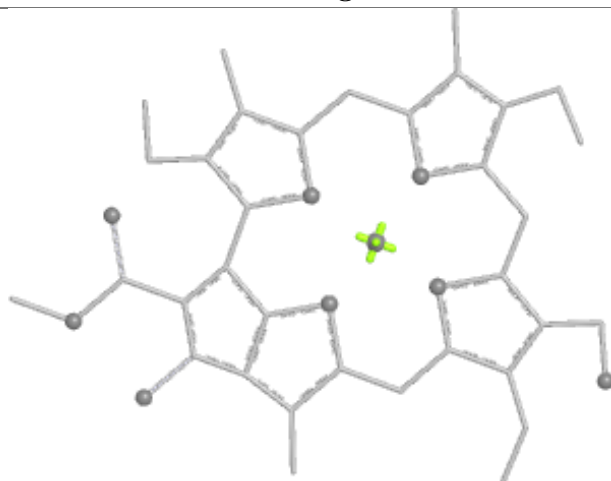
Bond lengths



Bond angles

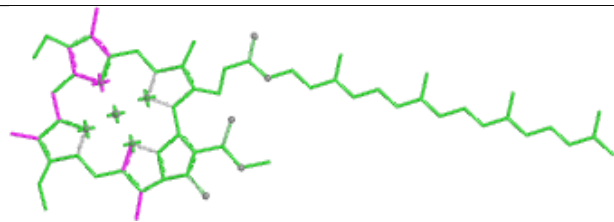


Torsions

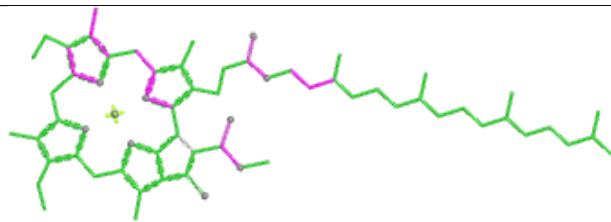


Rings

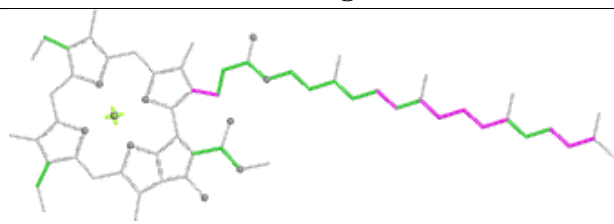
## Ligand CLA B 827



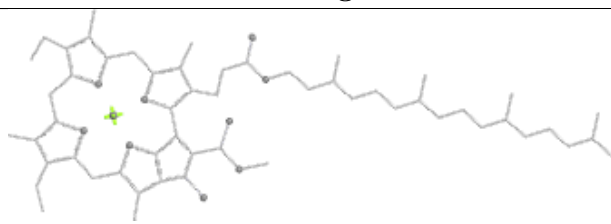
Bond lengths



Bond angles

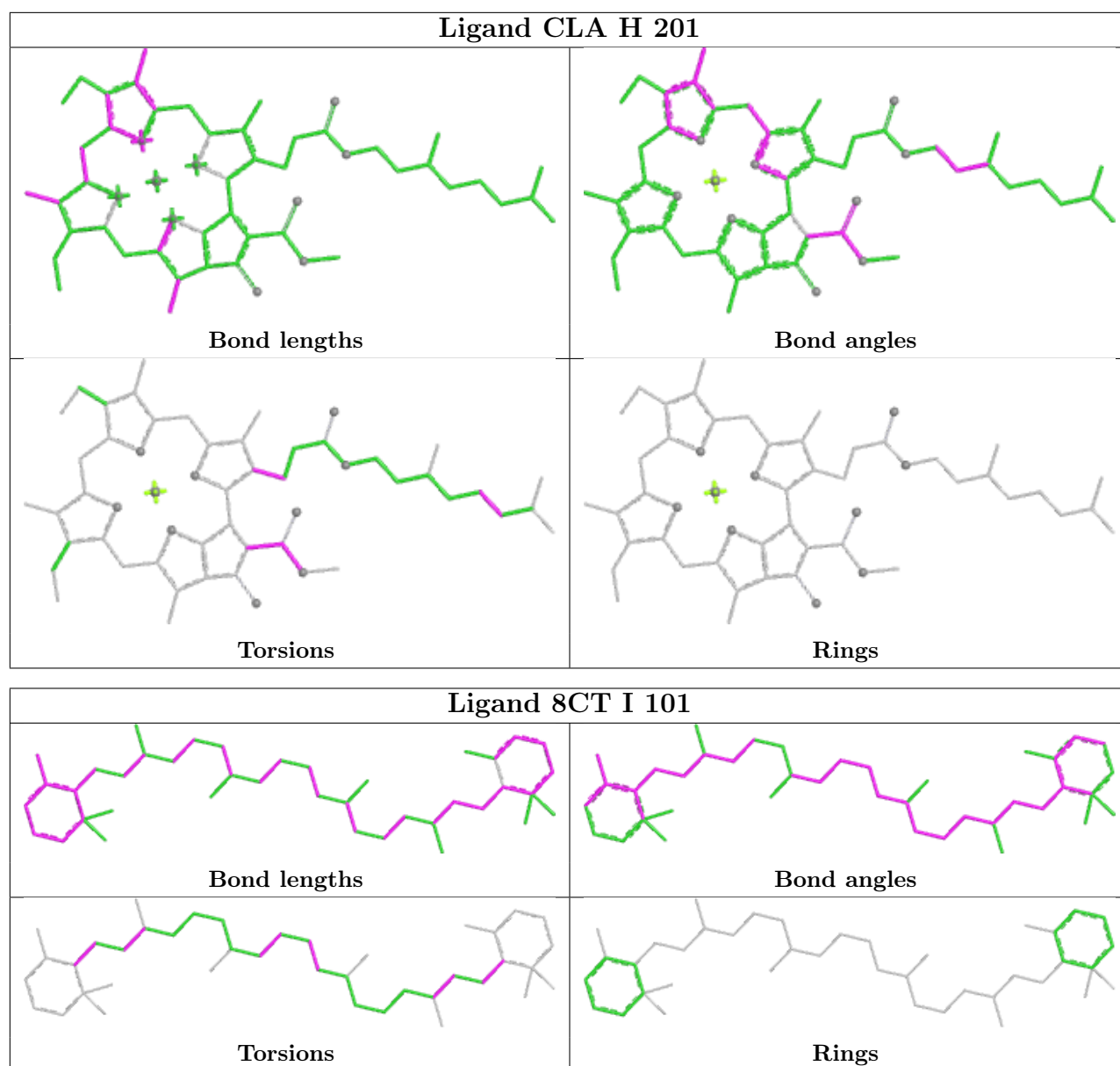


Torsions



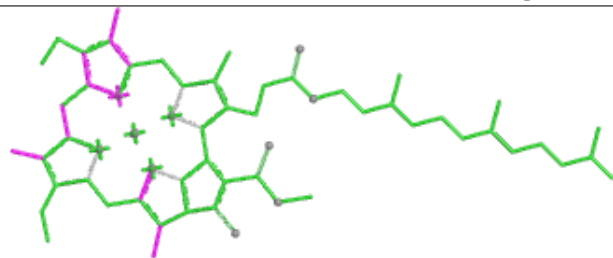
Rings



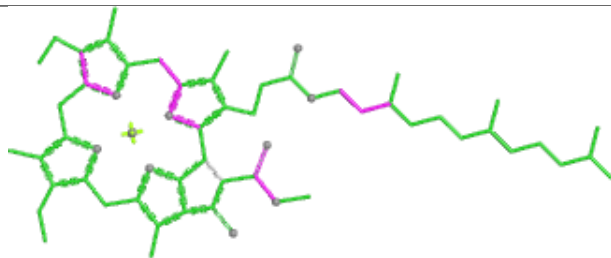




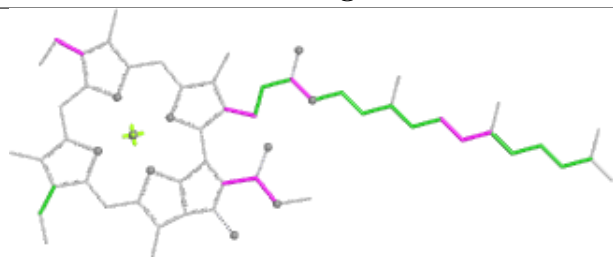
## Ligand CLA 6 310



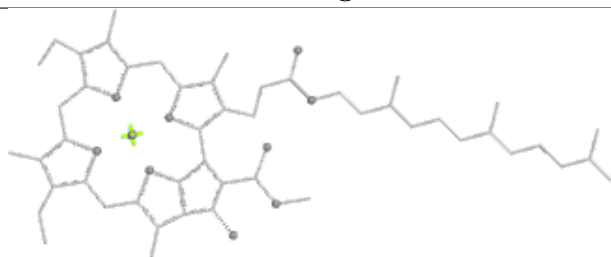
Bond lengths



Bond angles

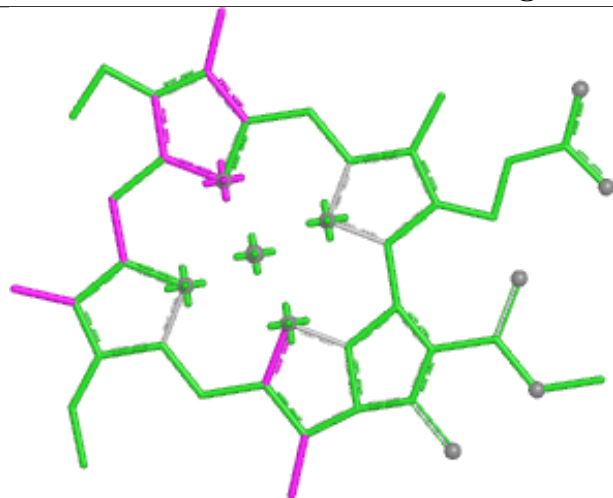


Torsions

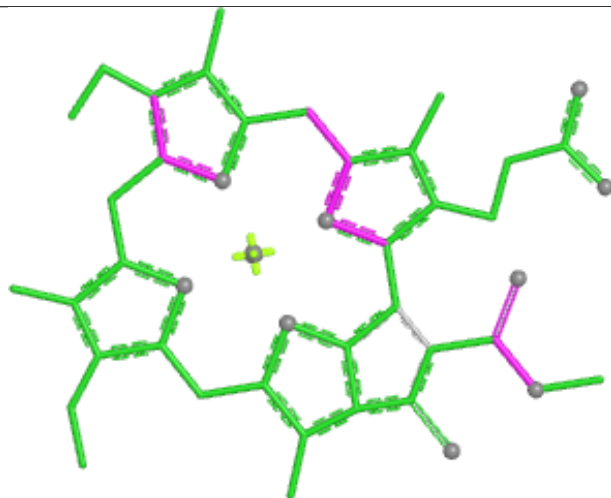


Rings

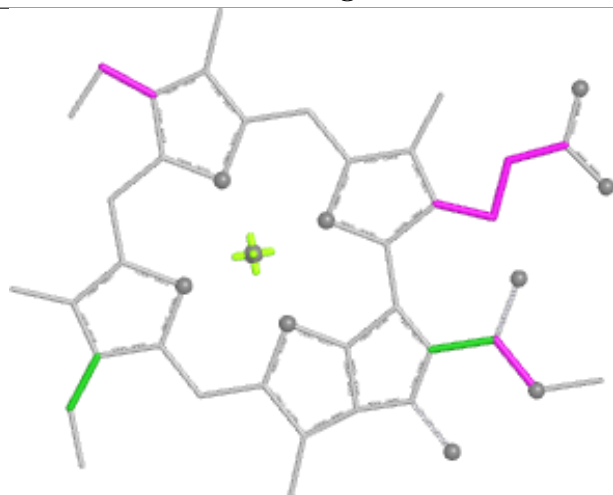
## Ligand CLA 8 314



Bond lengths



Bond angles

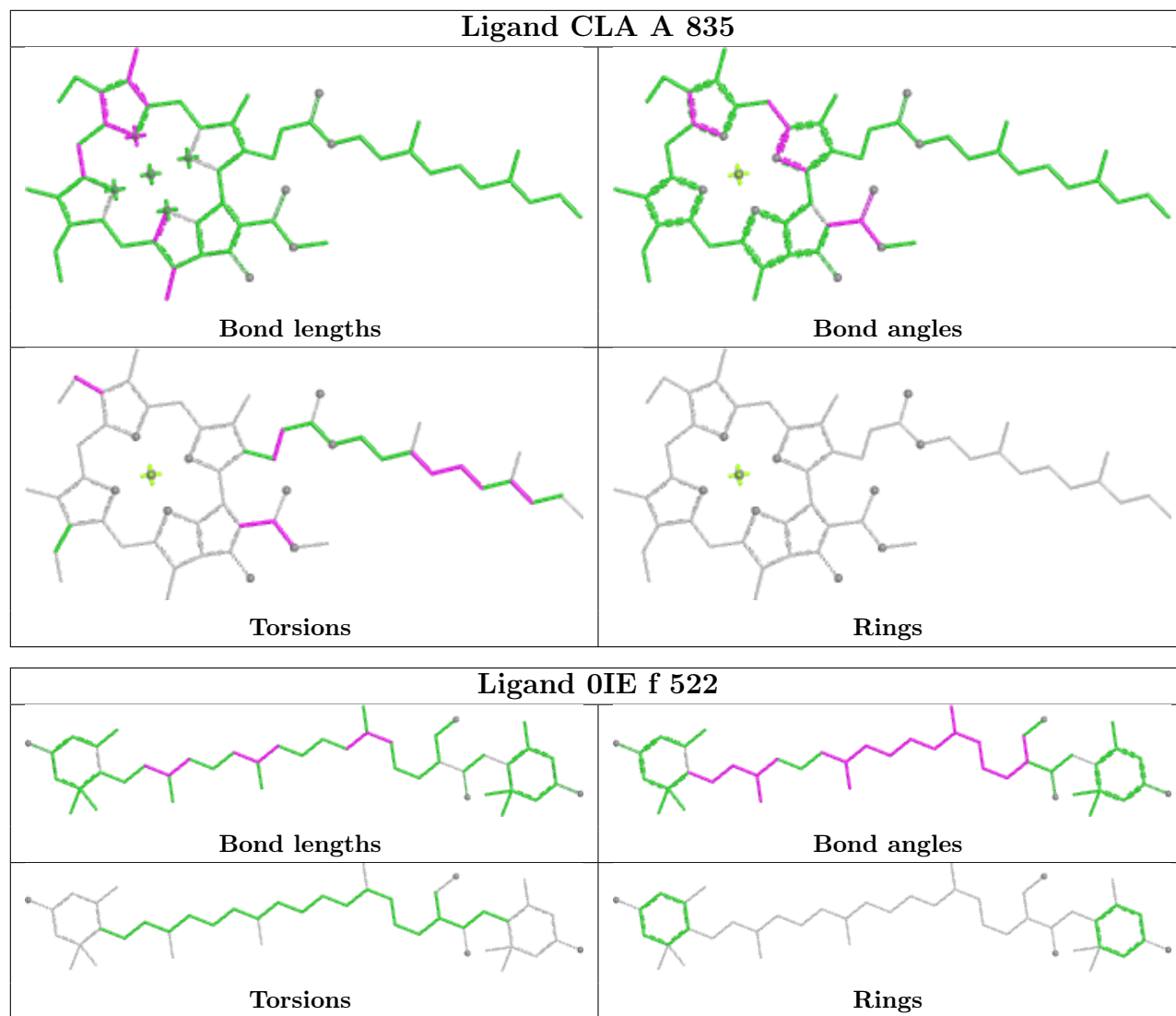


Torsions



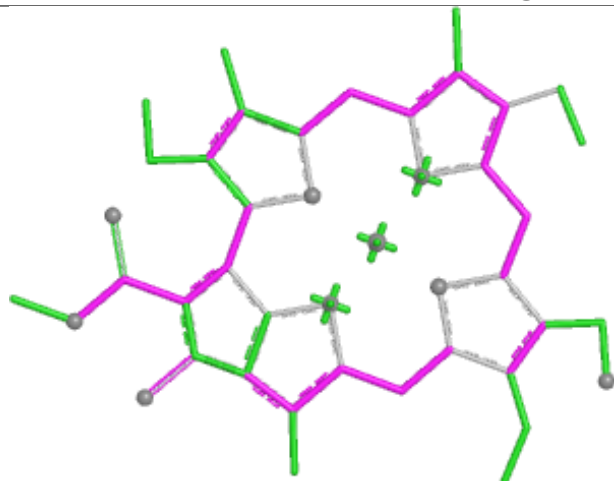
Rings



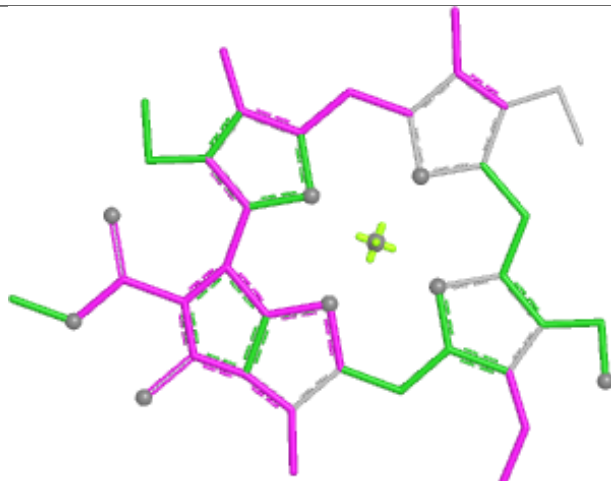




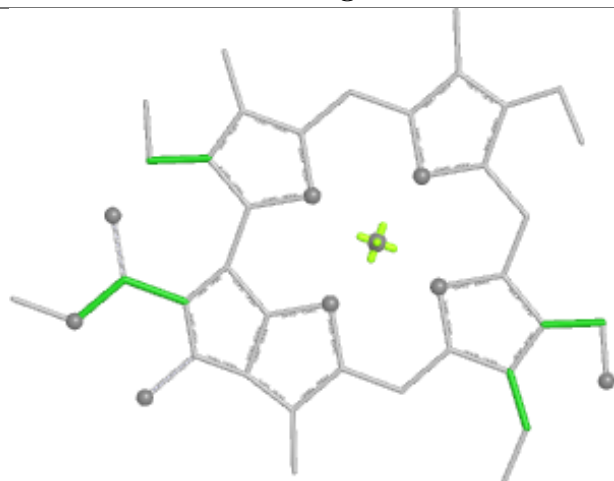
## Ligand CHL 4 305



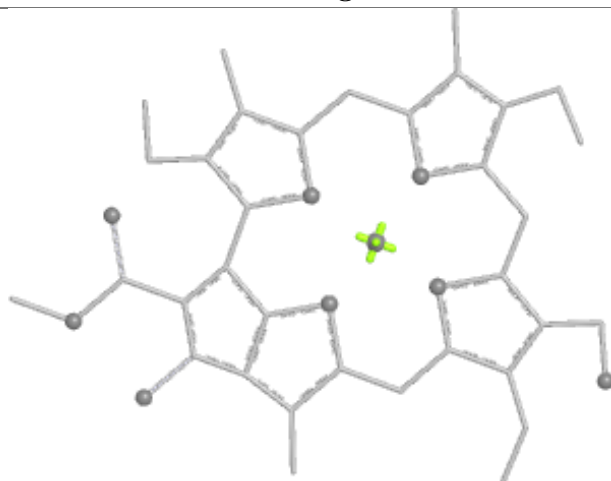
Bond lengths



Bond angles

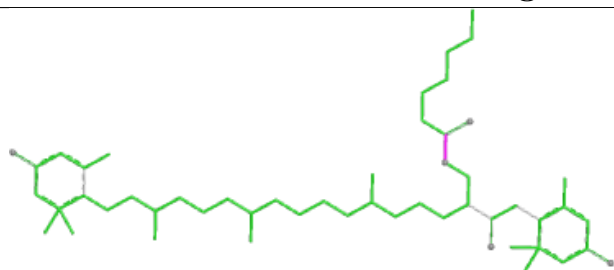


Torsions

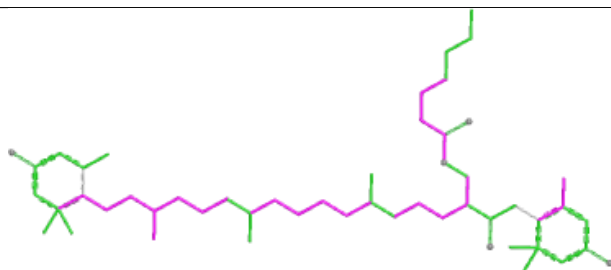


Rings

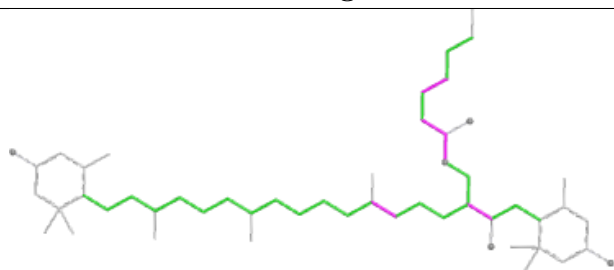
## Ligand OUR b 520



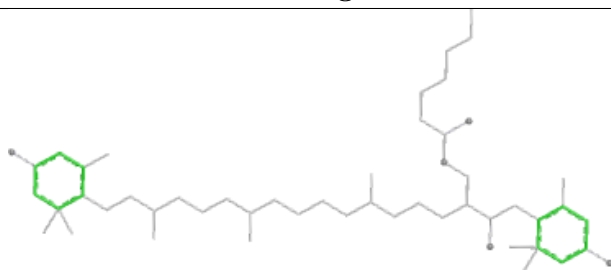
Bond lengths



Bond angles



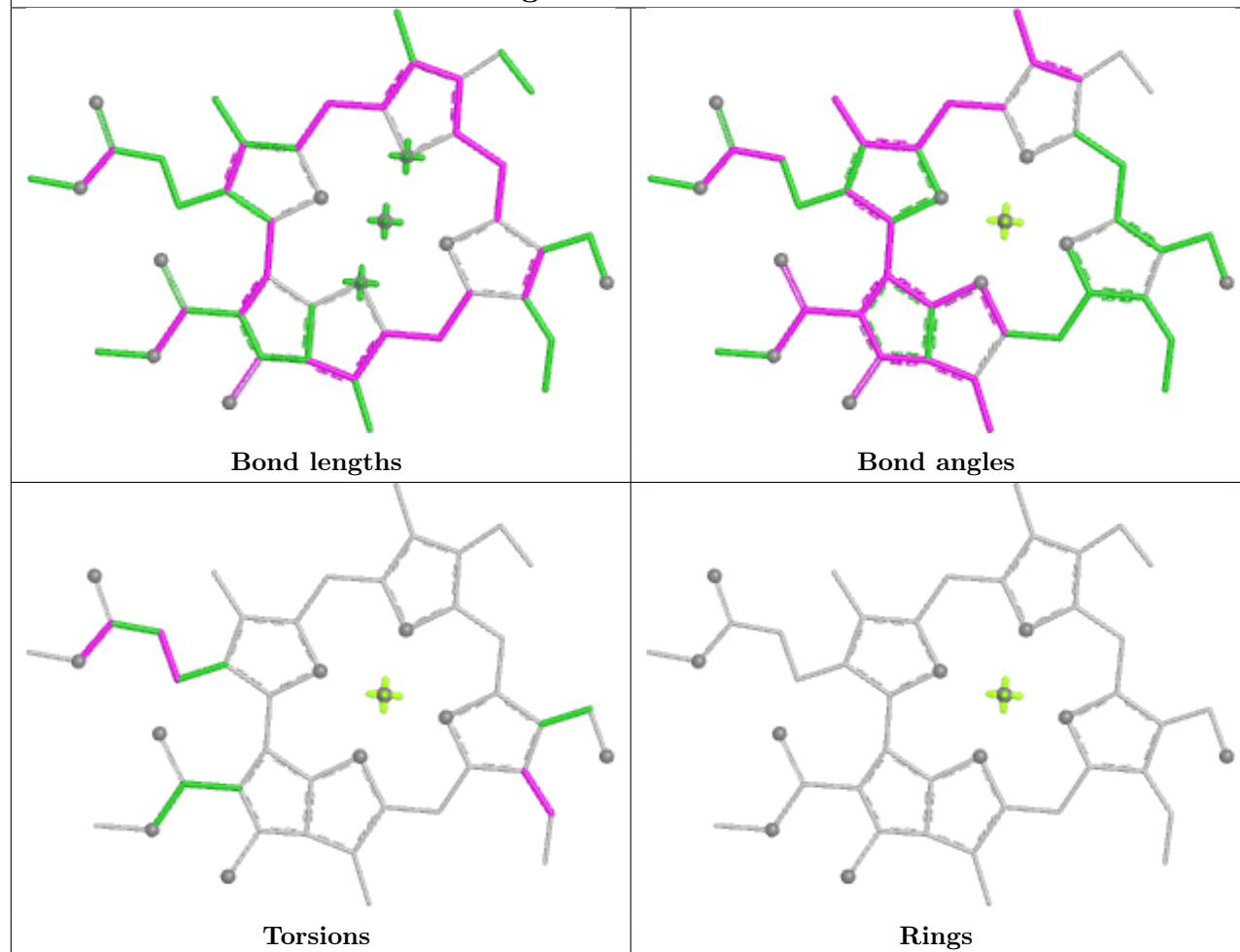
Torsions



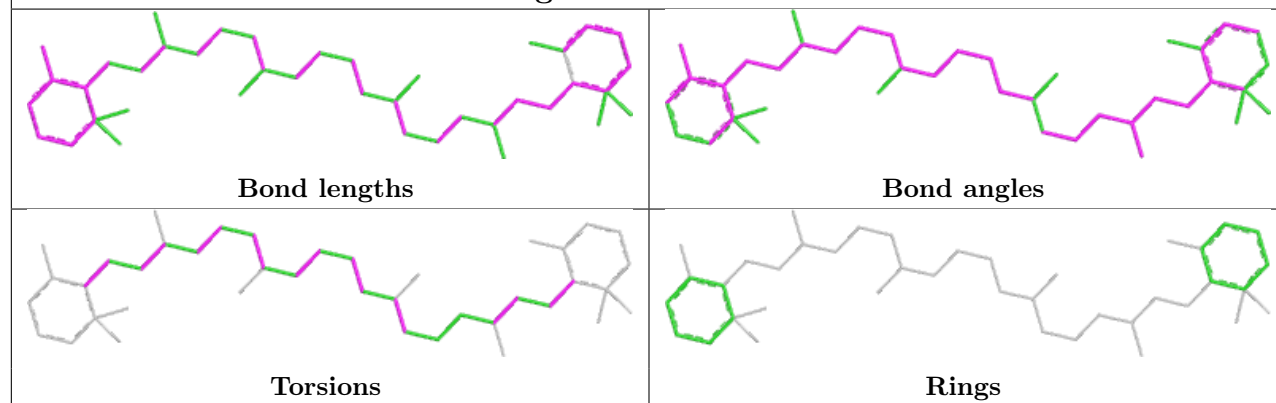
Rings



## Ligand CHL e 607

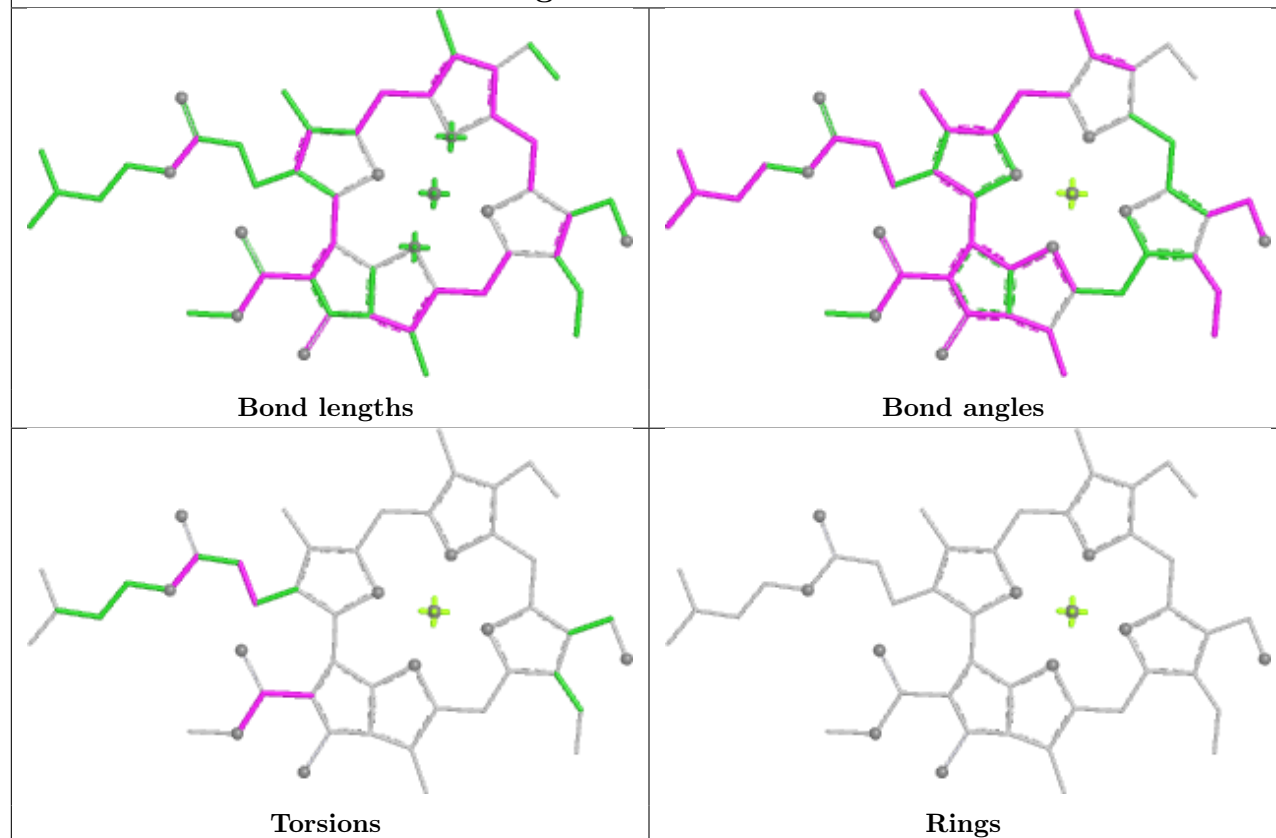


## Ligand 8CT B 804

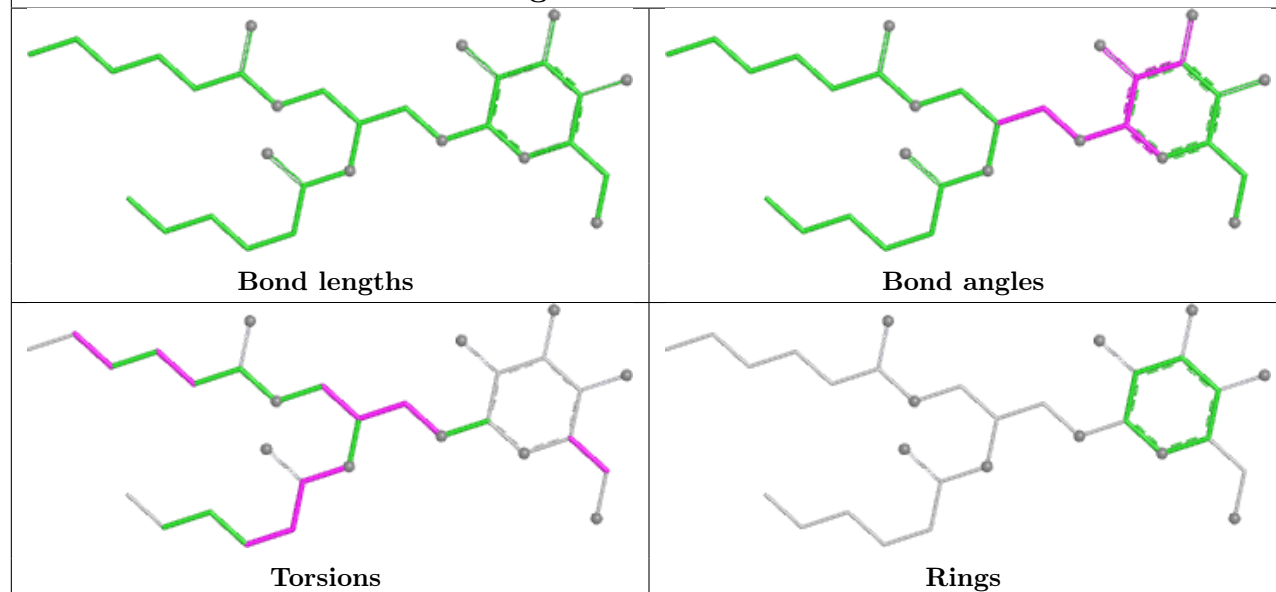




## Ligand CHL 2 307

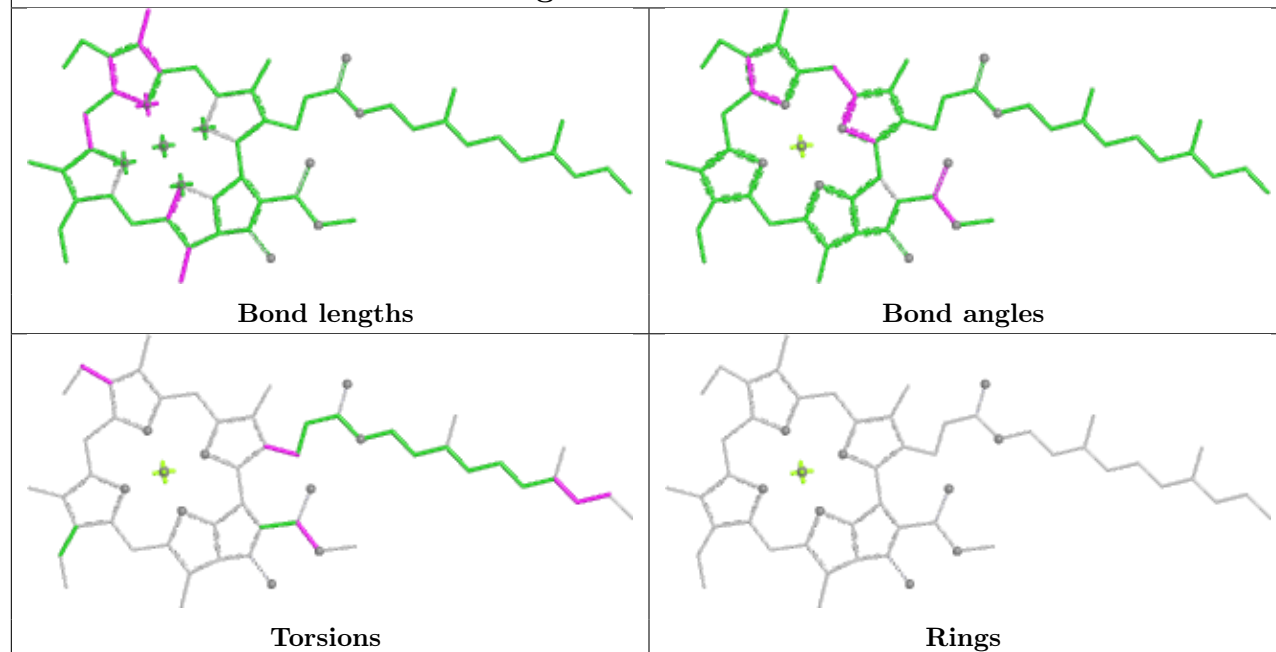


## Ligand LMG L 210

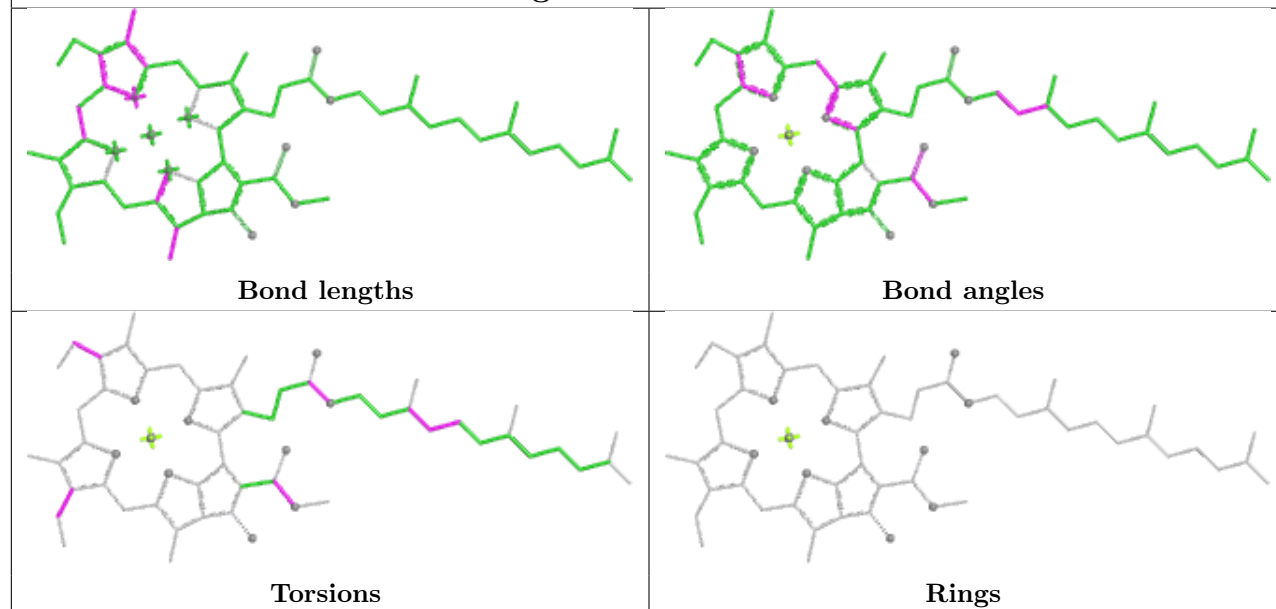




## Ligand CLA a 611

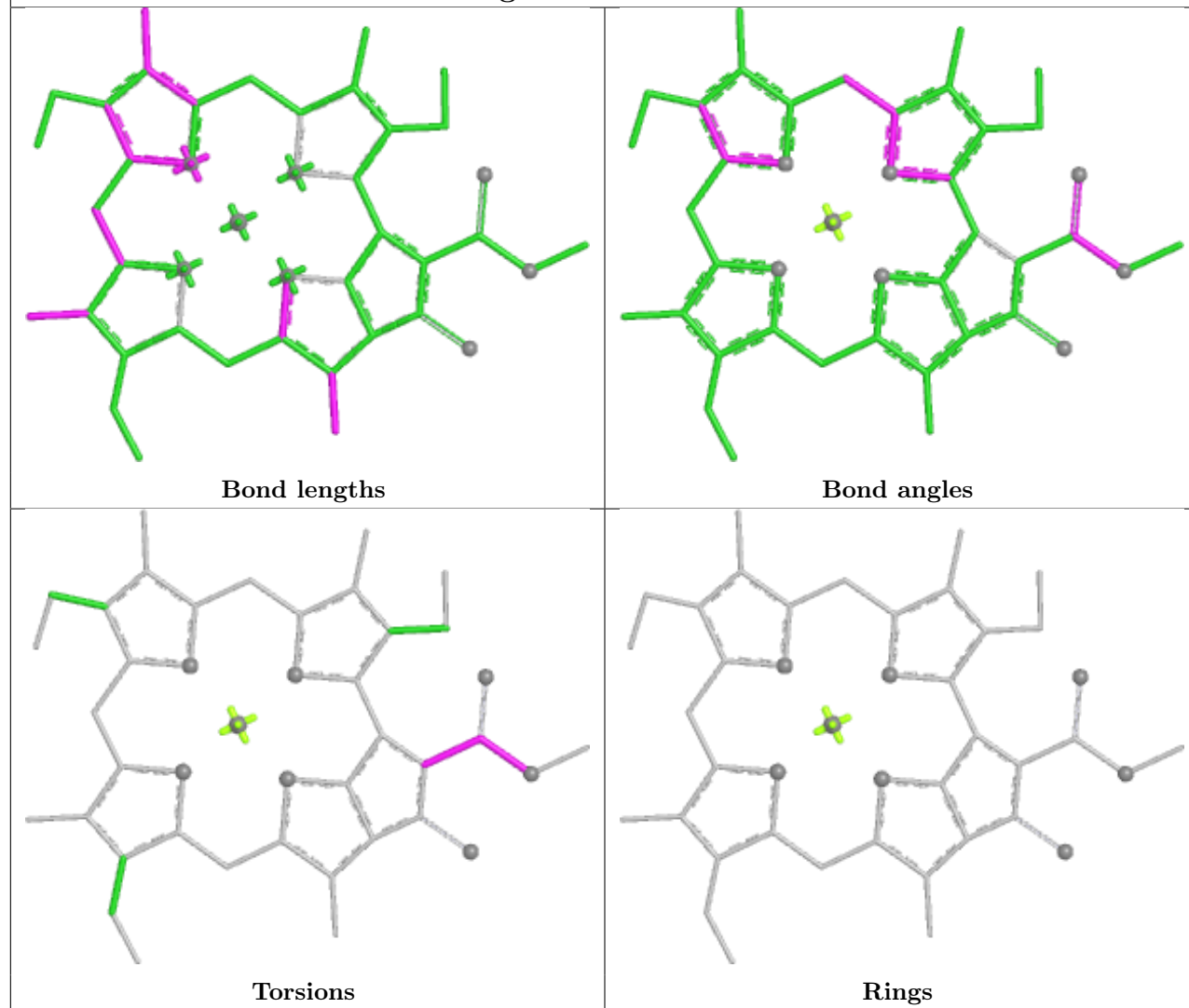


## Ligand CLA B 822

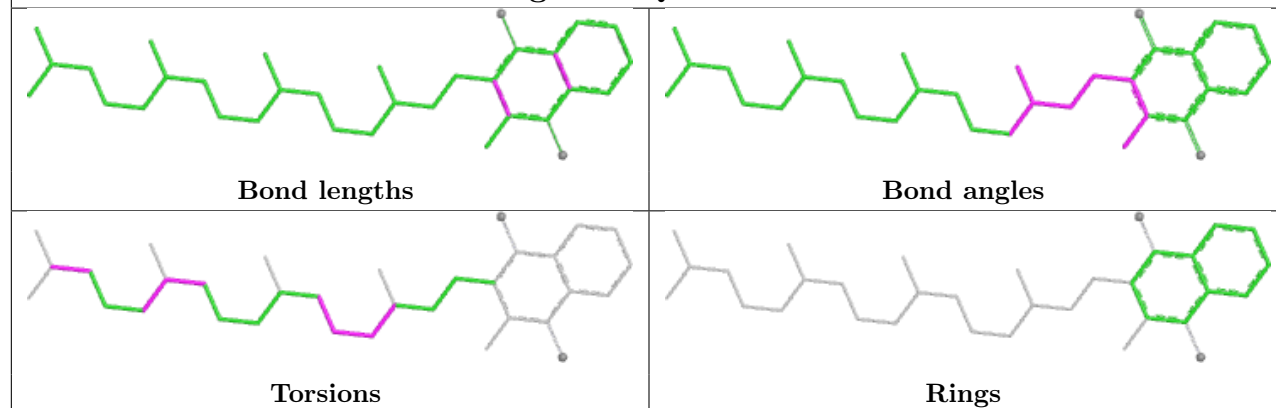




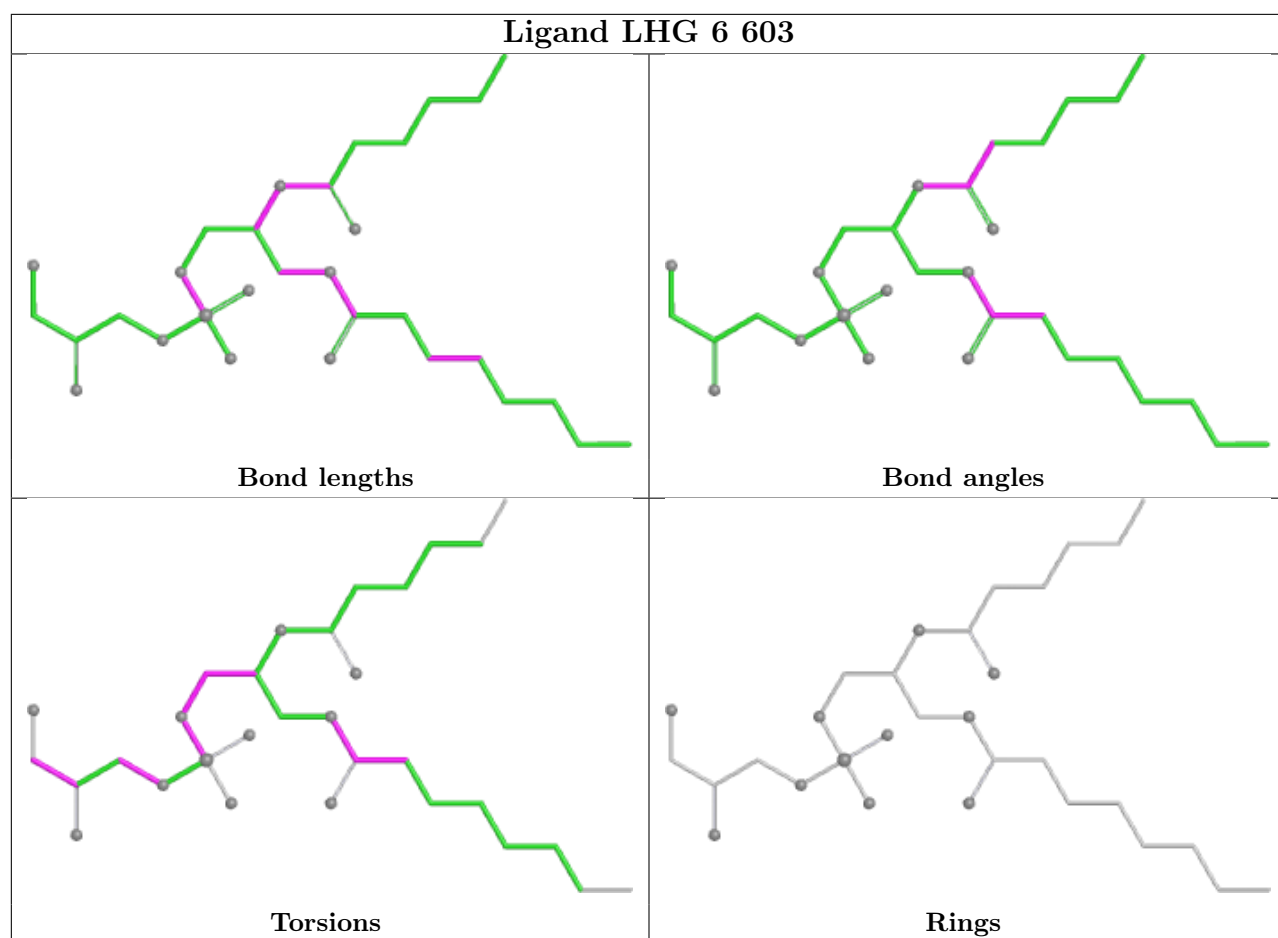
## Ligand CLA J 103



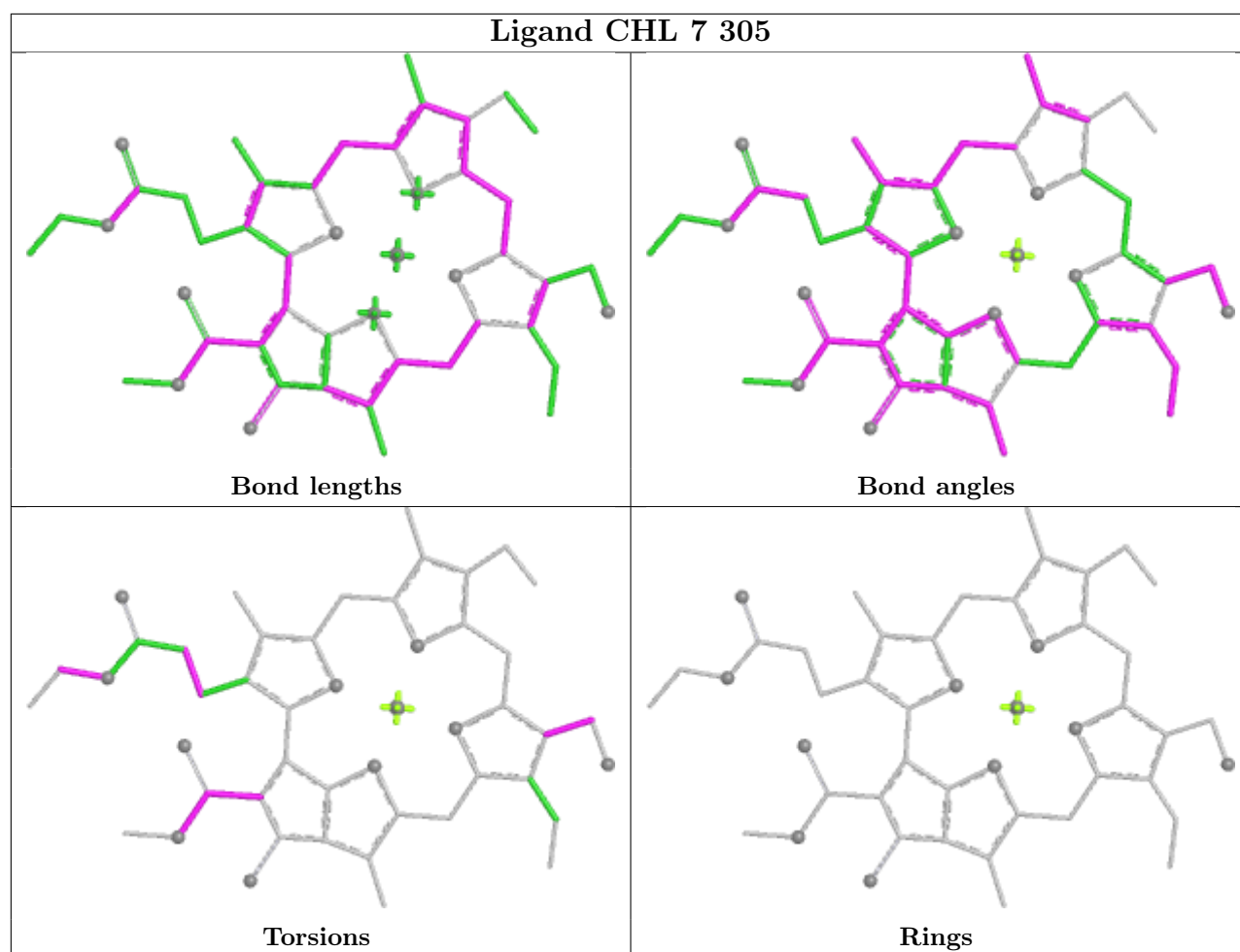
## Ligand PQN A 842





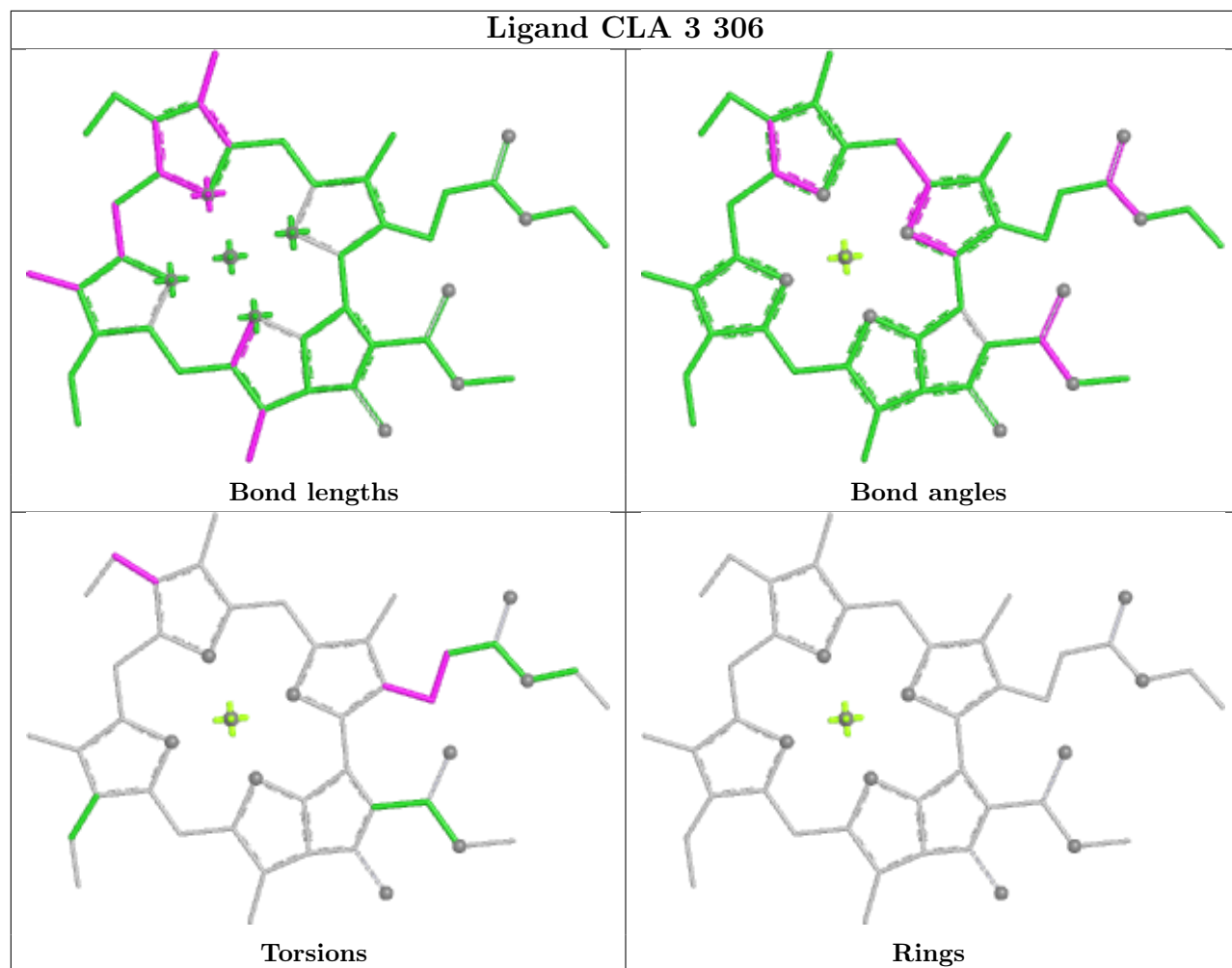






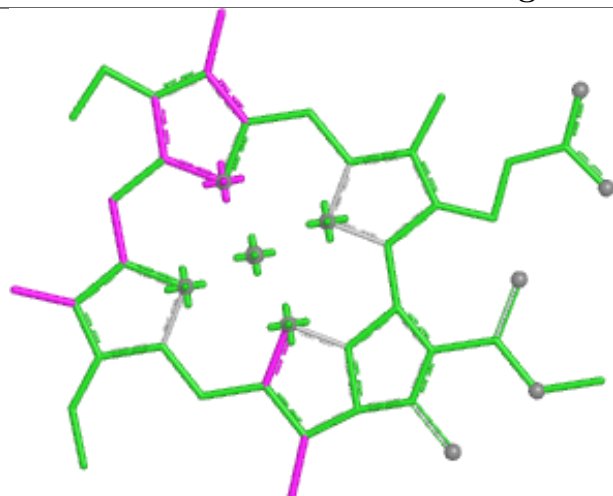


## Ligand CLA 3 306

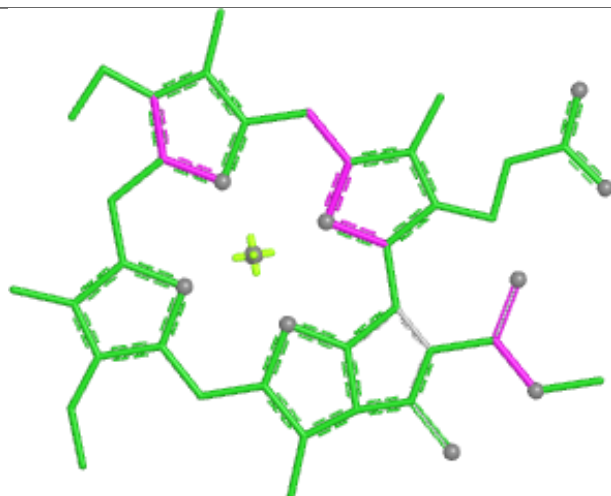




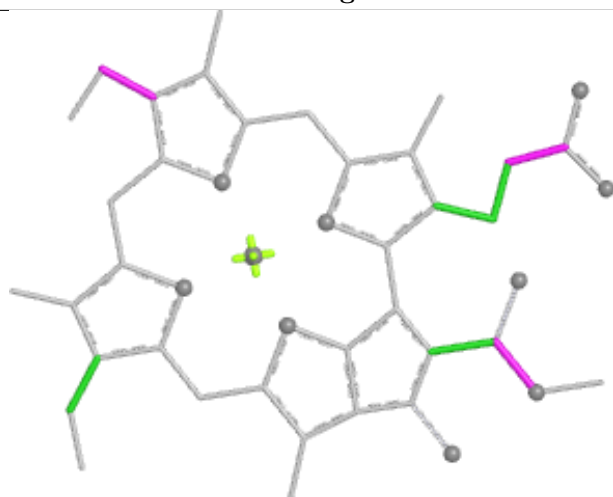
## Ligand CLA 1 308



Bond lengths



Bond angles



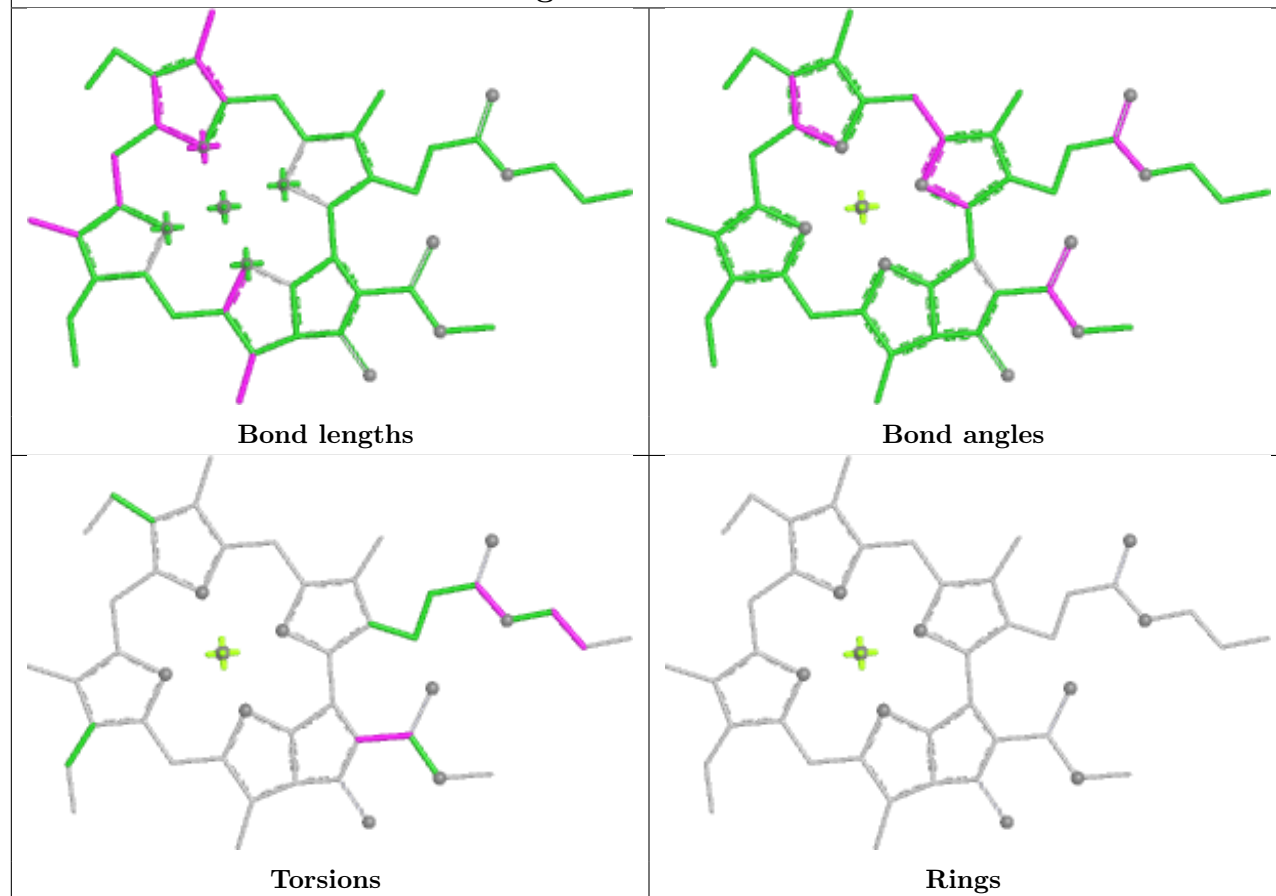
Torsions



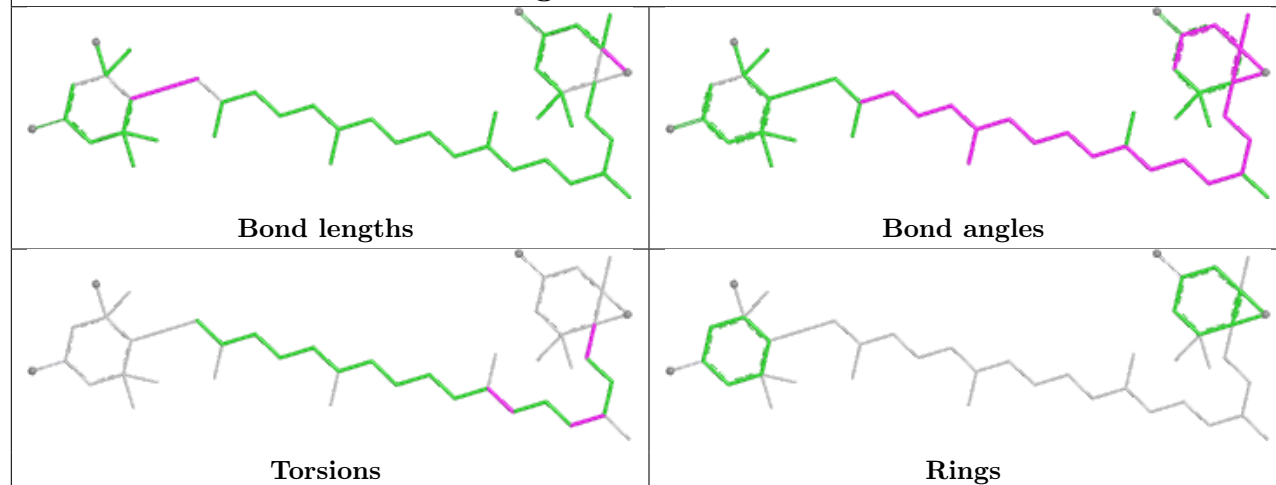
Rings



## Ligand CLA 4 311

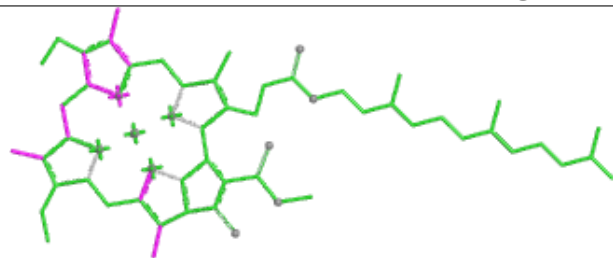


## Ligand NEX c 523

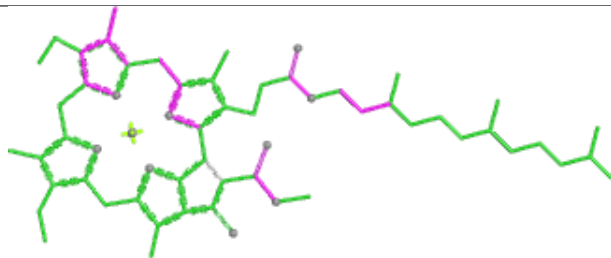




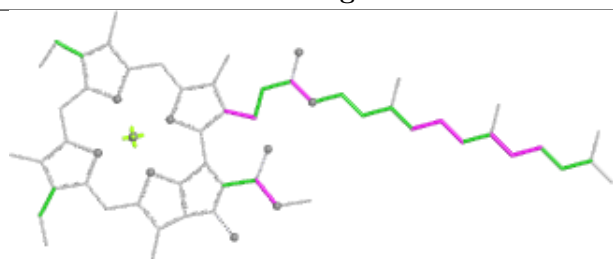
## Ligand CLA B 836



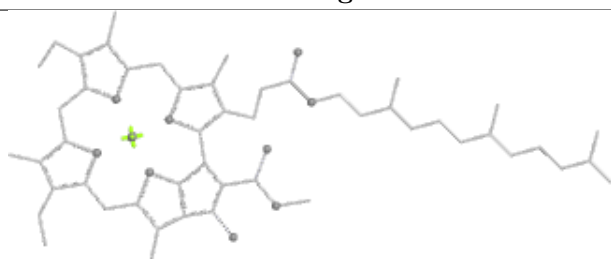
Bond lengths



Bond angles

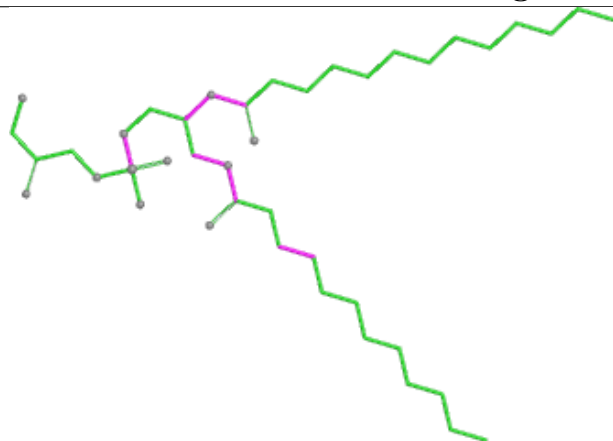


Torsions

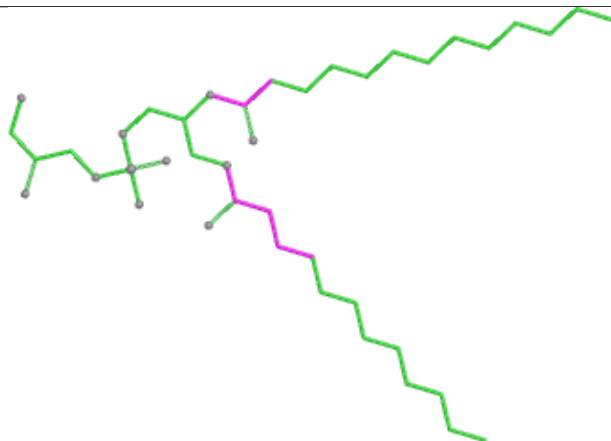


Rings

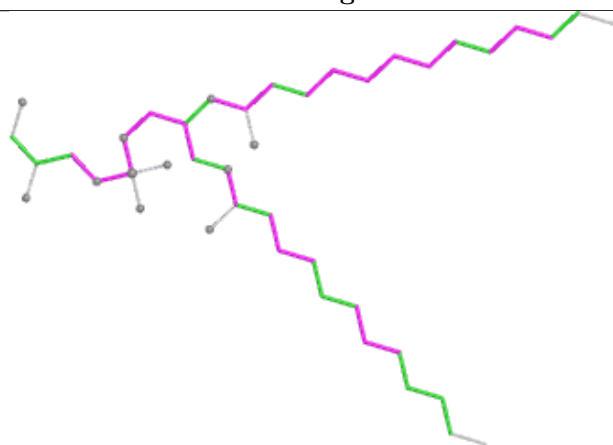
## Ligand LHG A 855



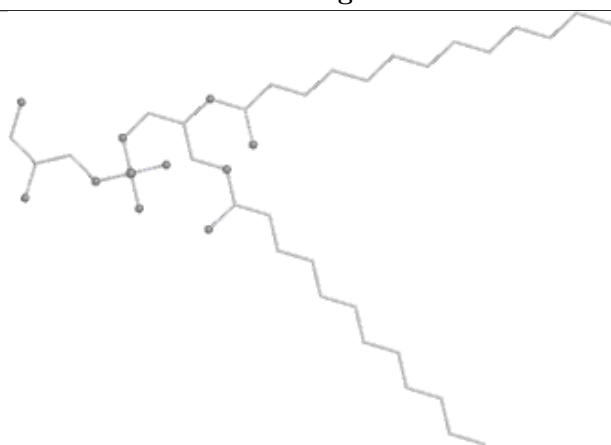
Bond lengths



Bond angles



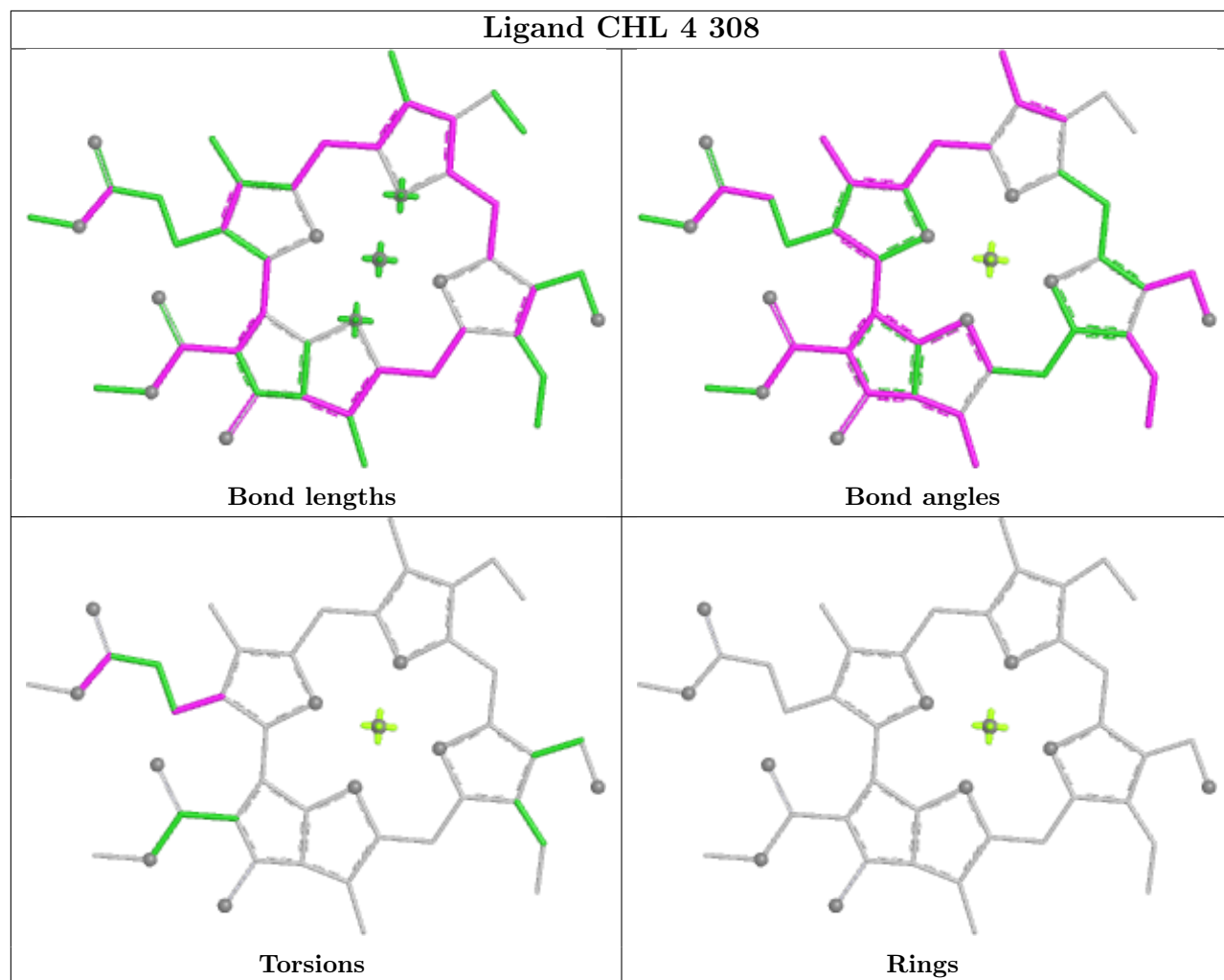
Torsions



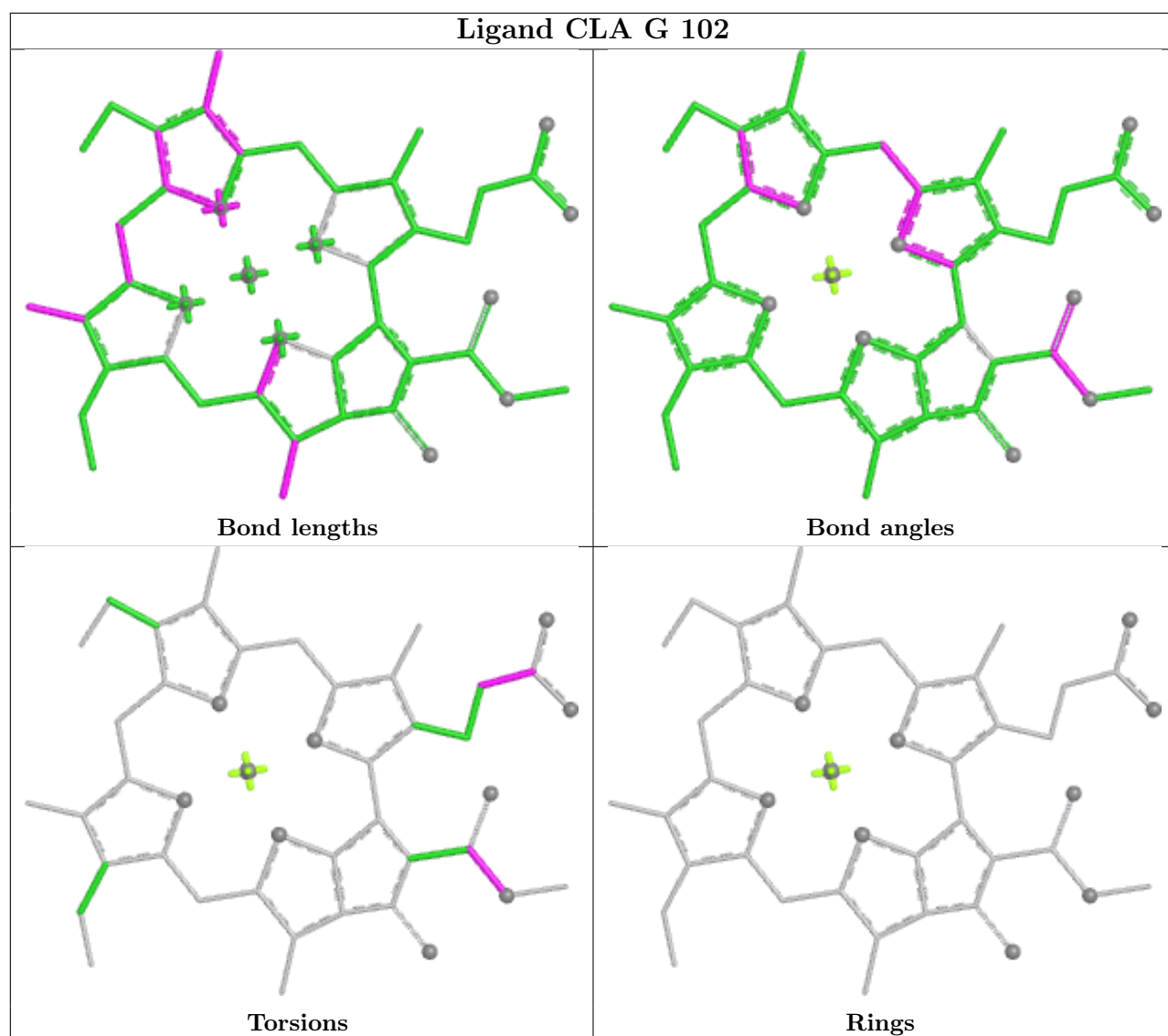
Rings



## Ligand CHL 4 308

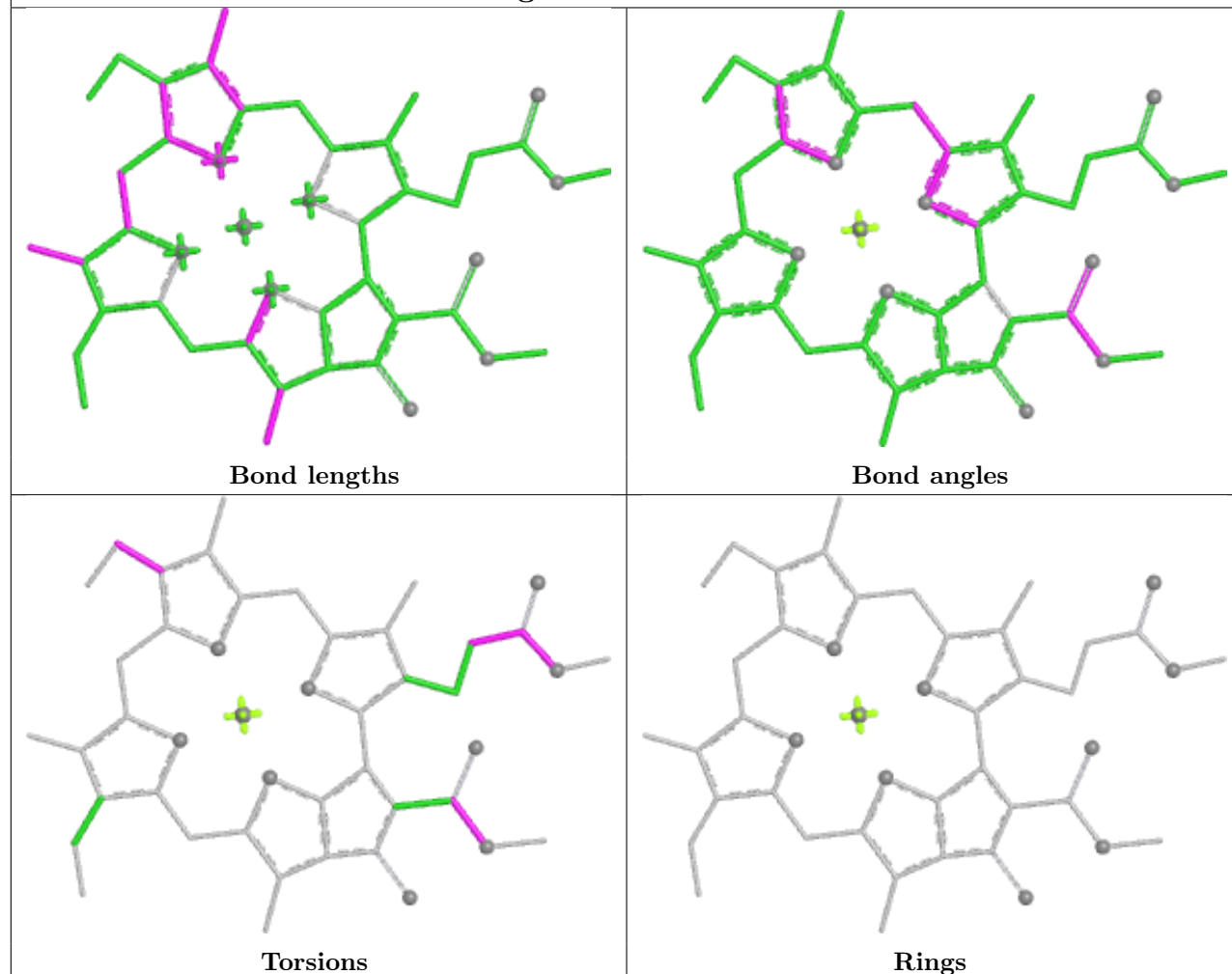




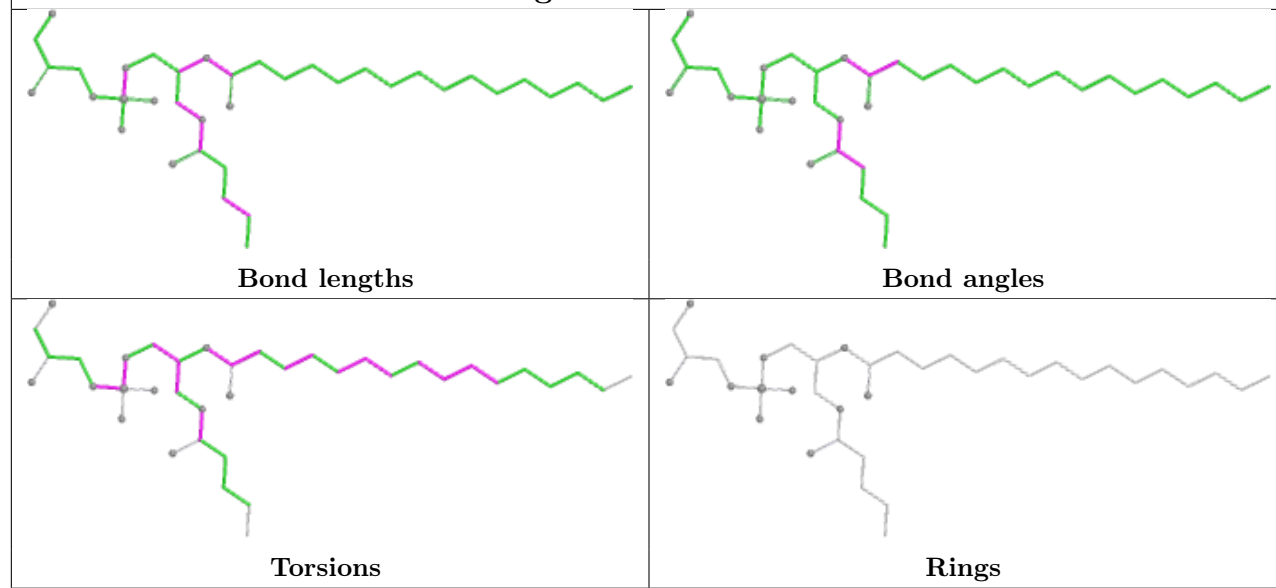




## Ligand CLA 8 311

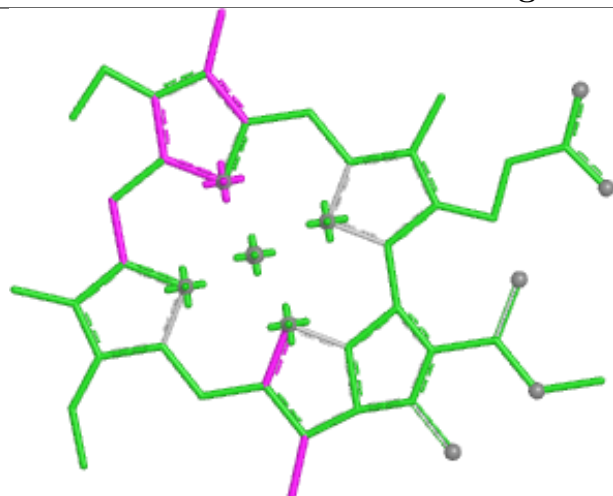


## Ligand LHG 7 602

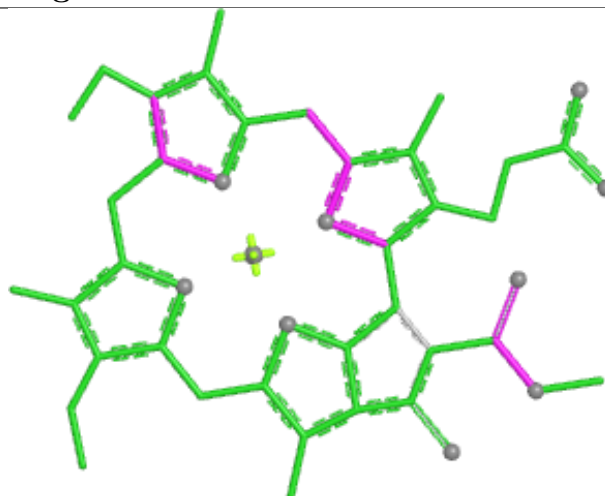




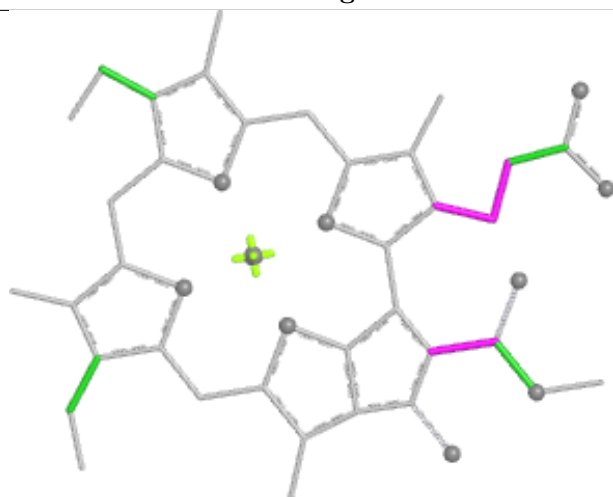
## Ligand CLA g 604



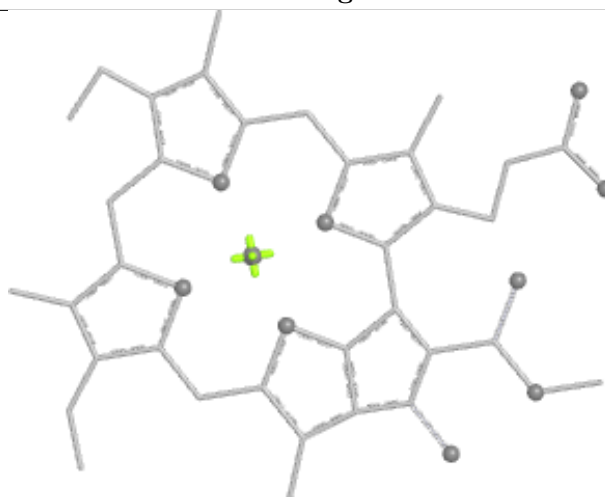
Bond lengths



Bond angles



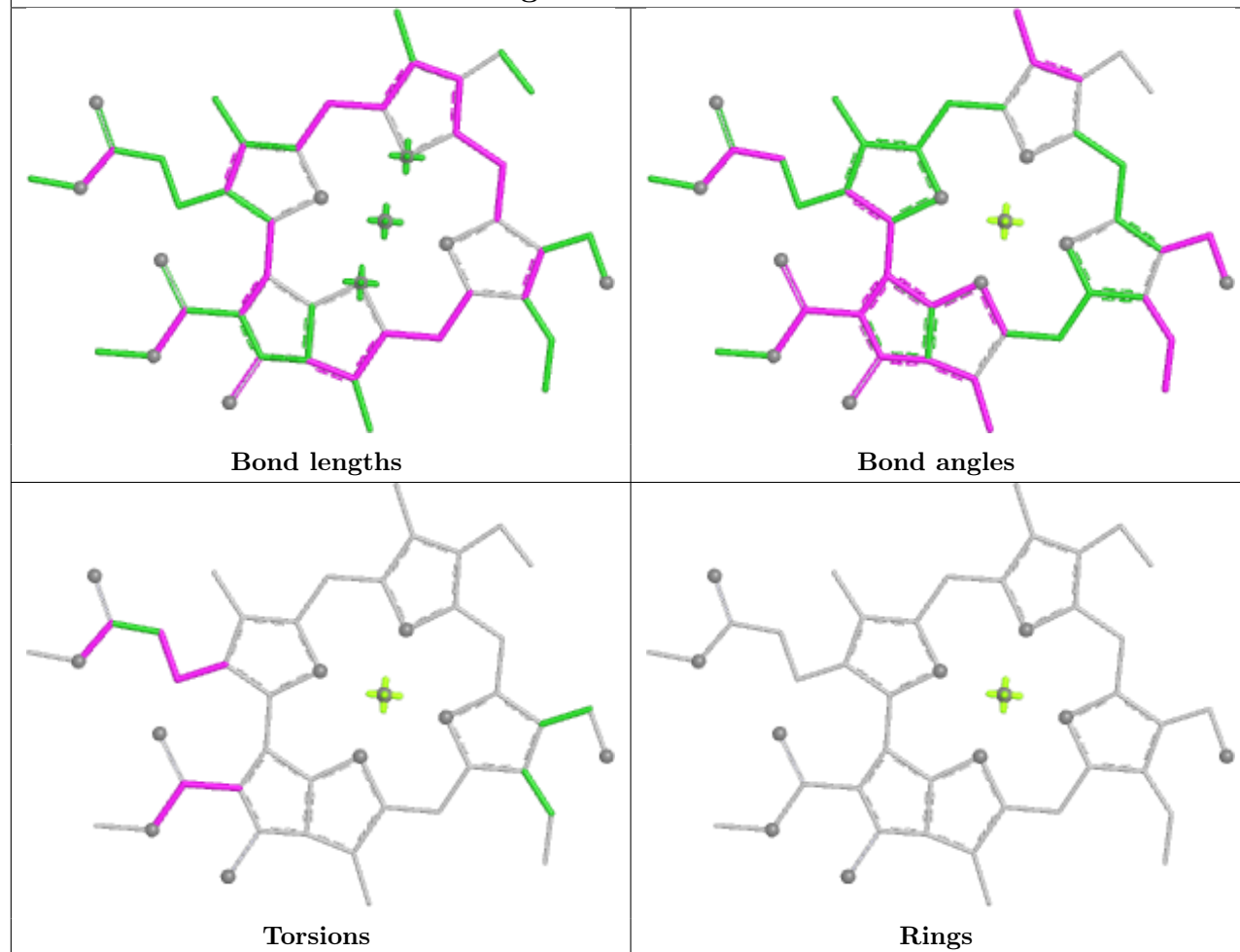
Torsions



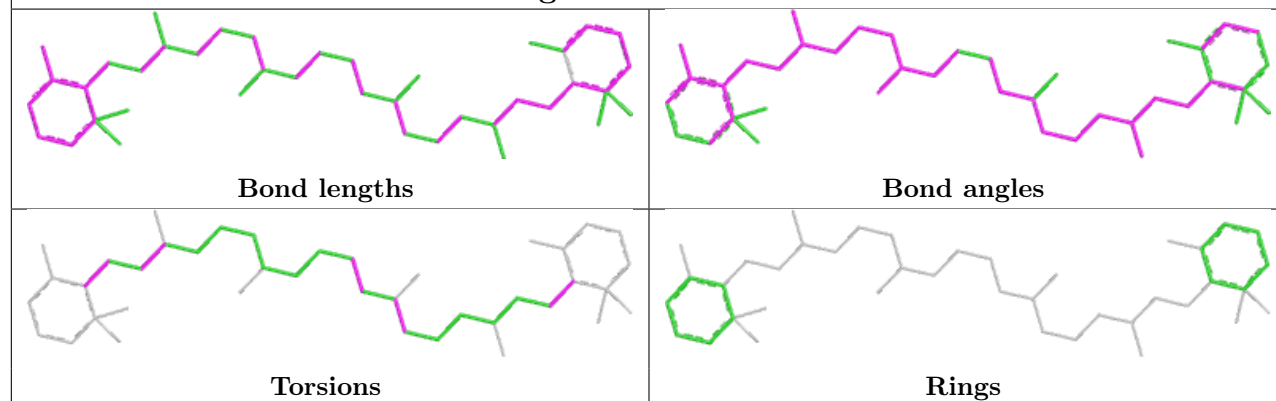
Rings



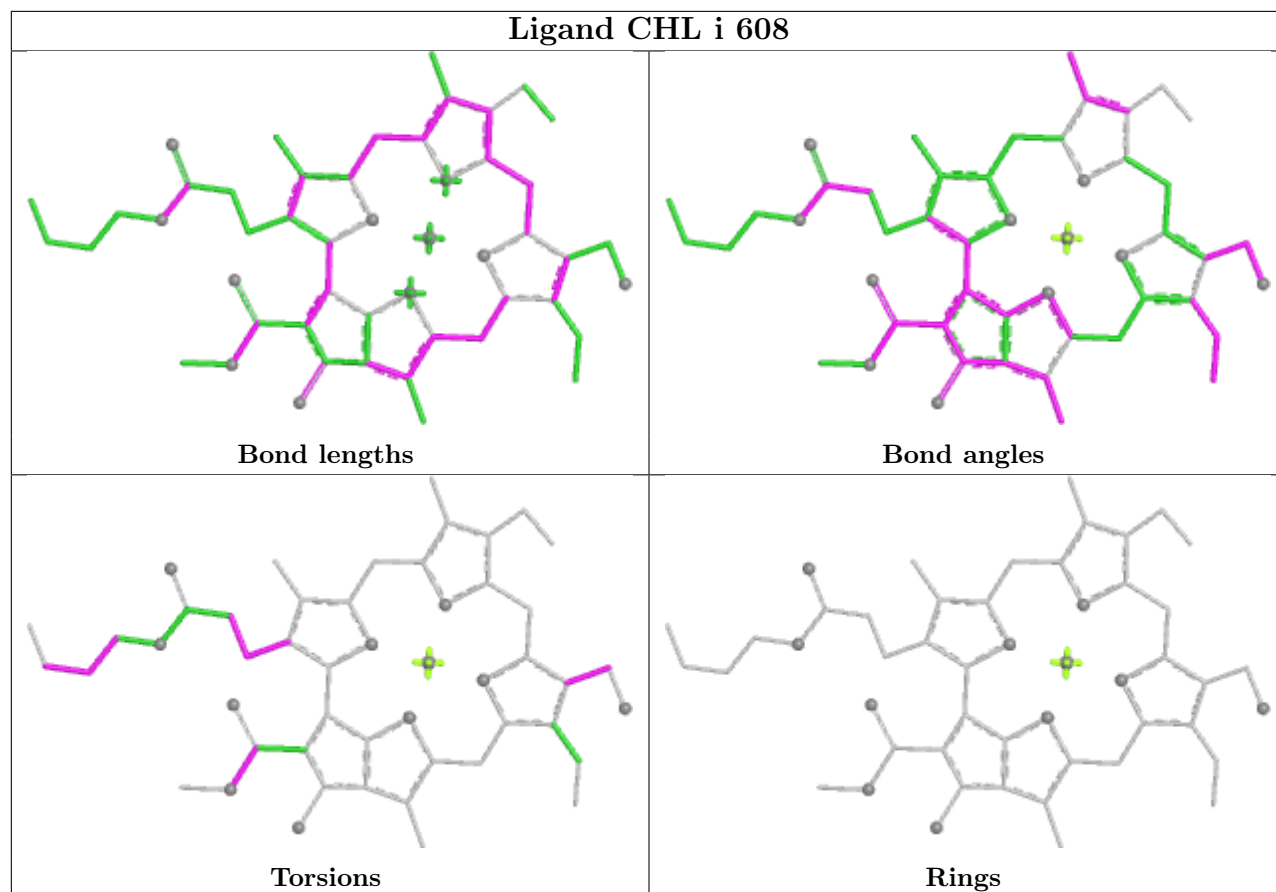
## Ligand CHL a 601



## Ligand 8CT 1 402

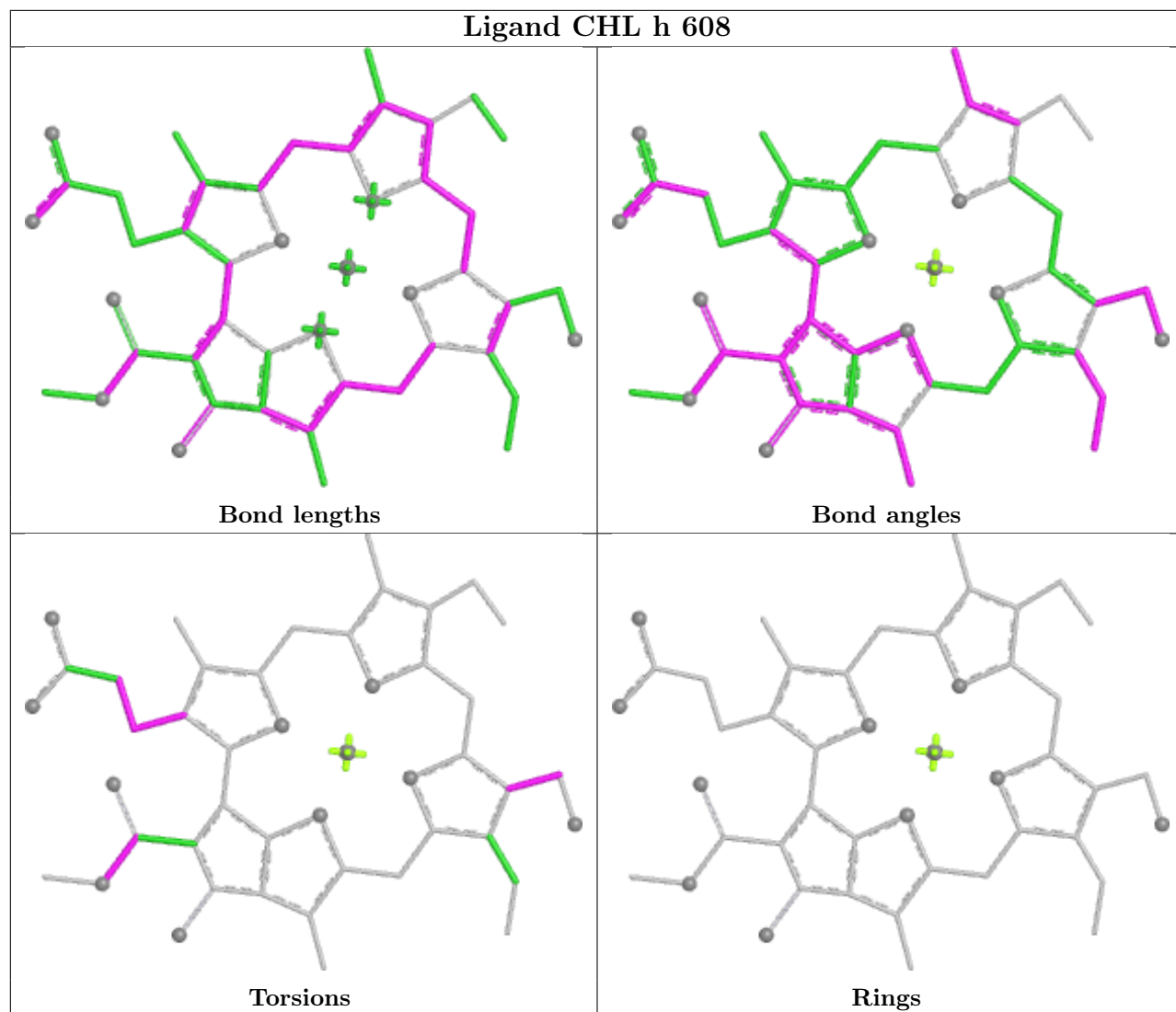




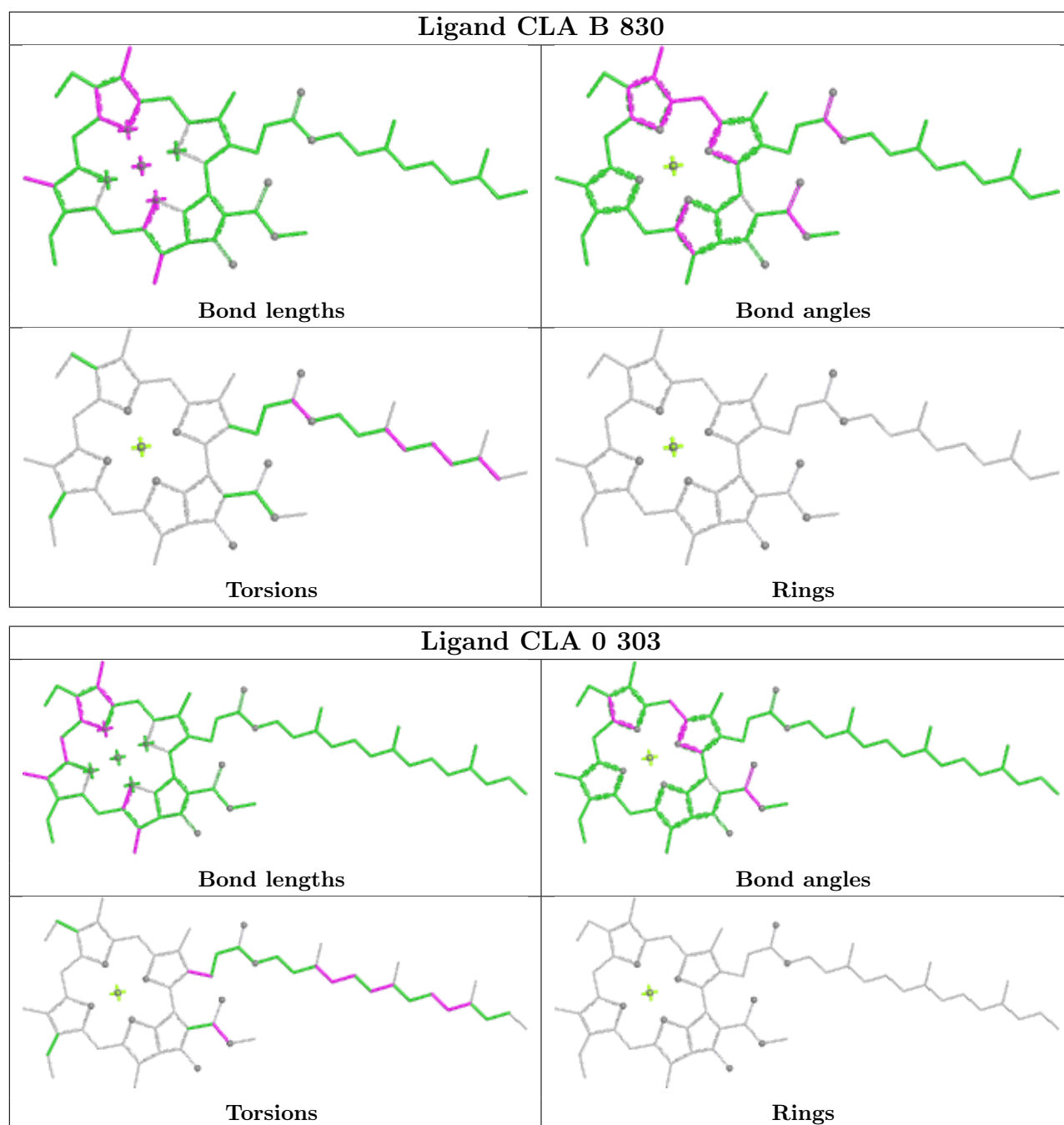




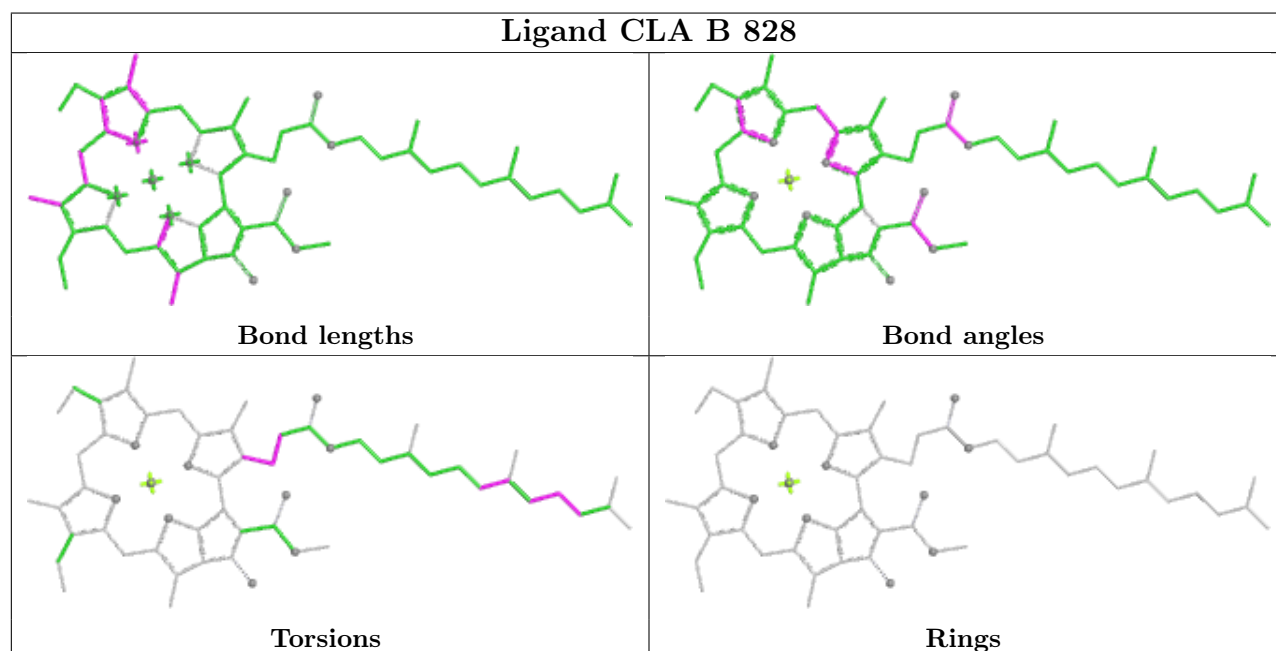
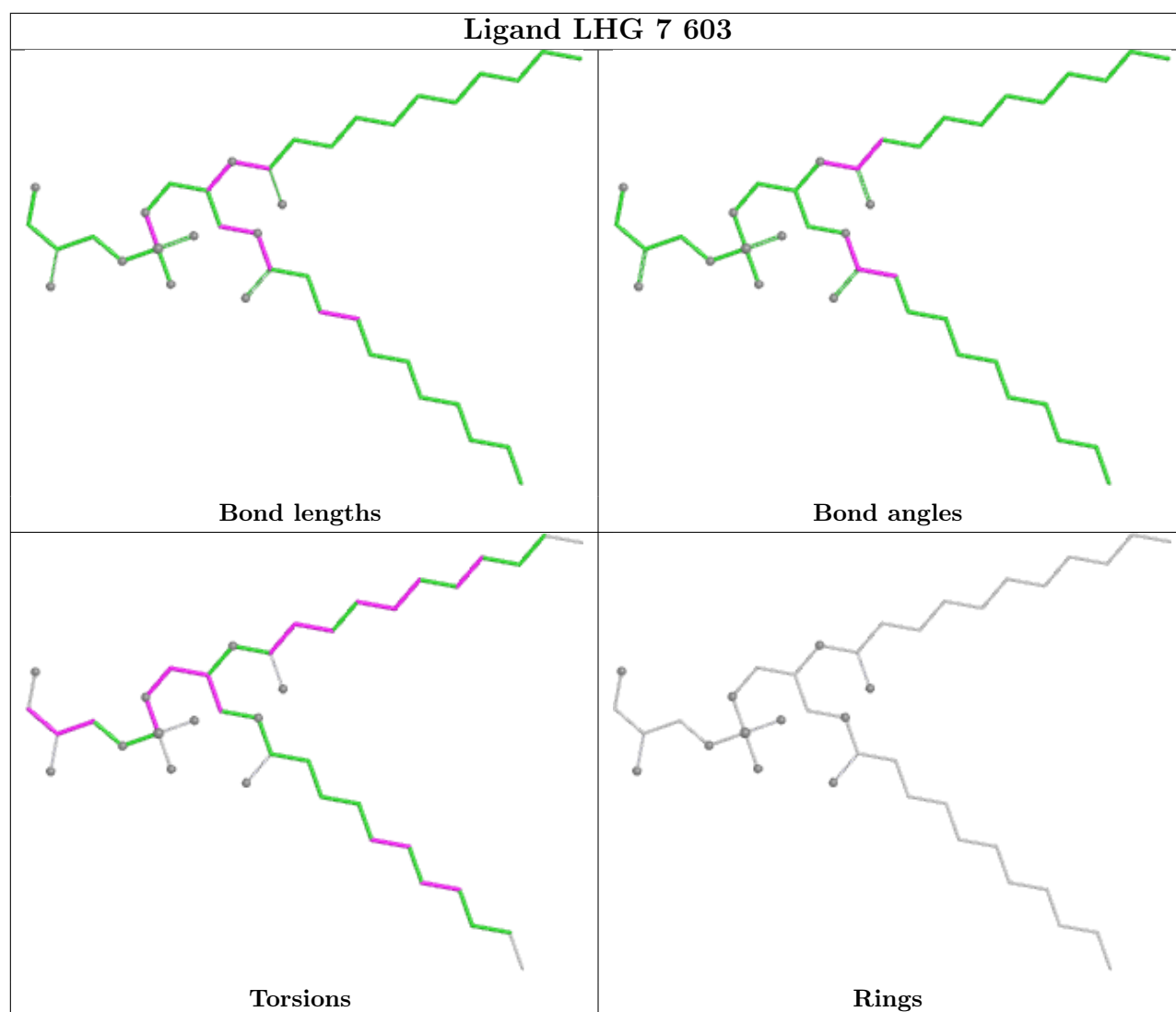
## Ligand CHL h 608





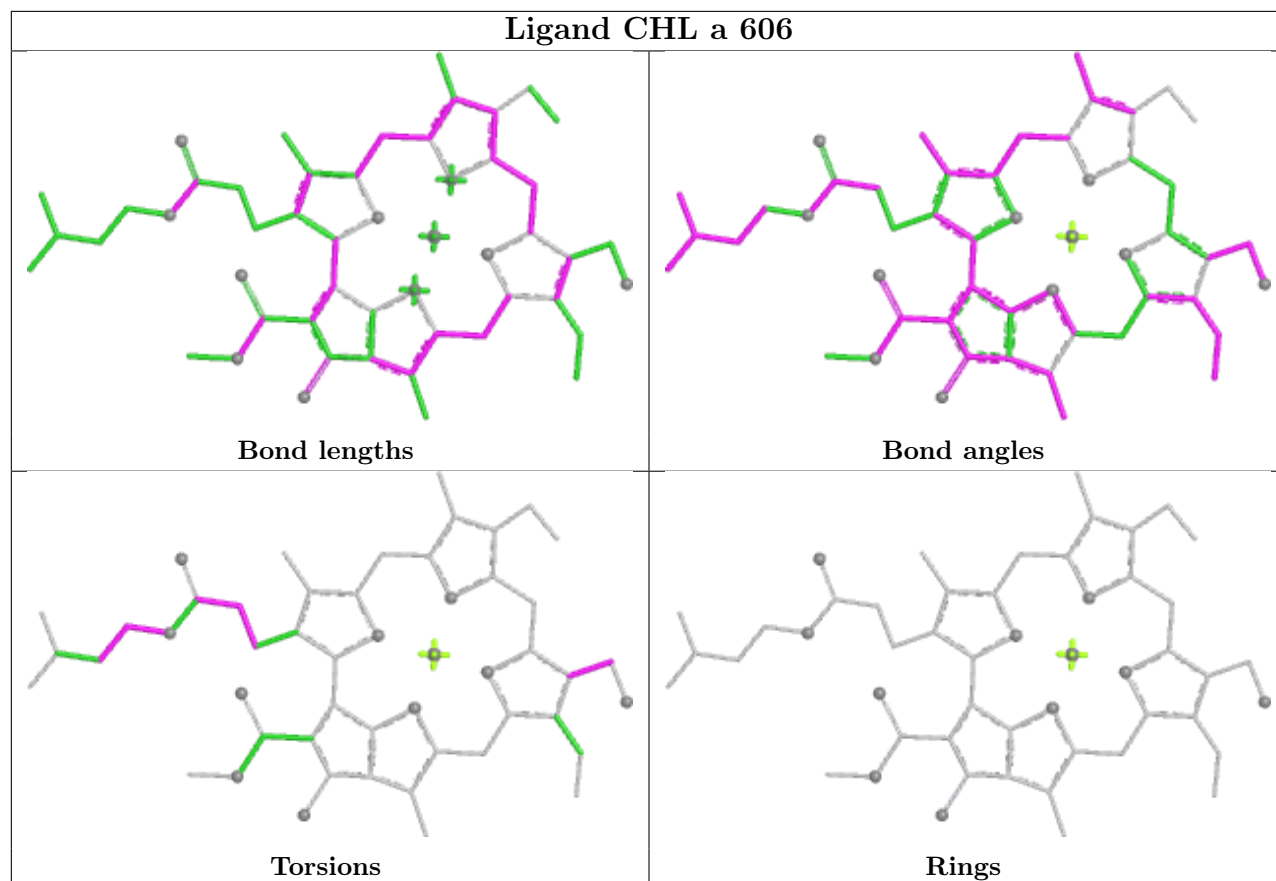




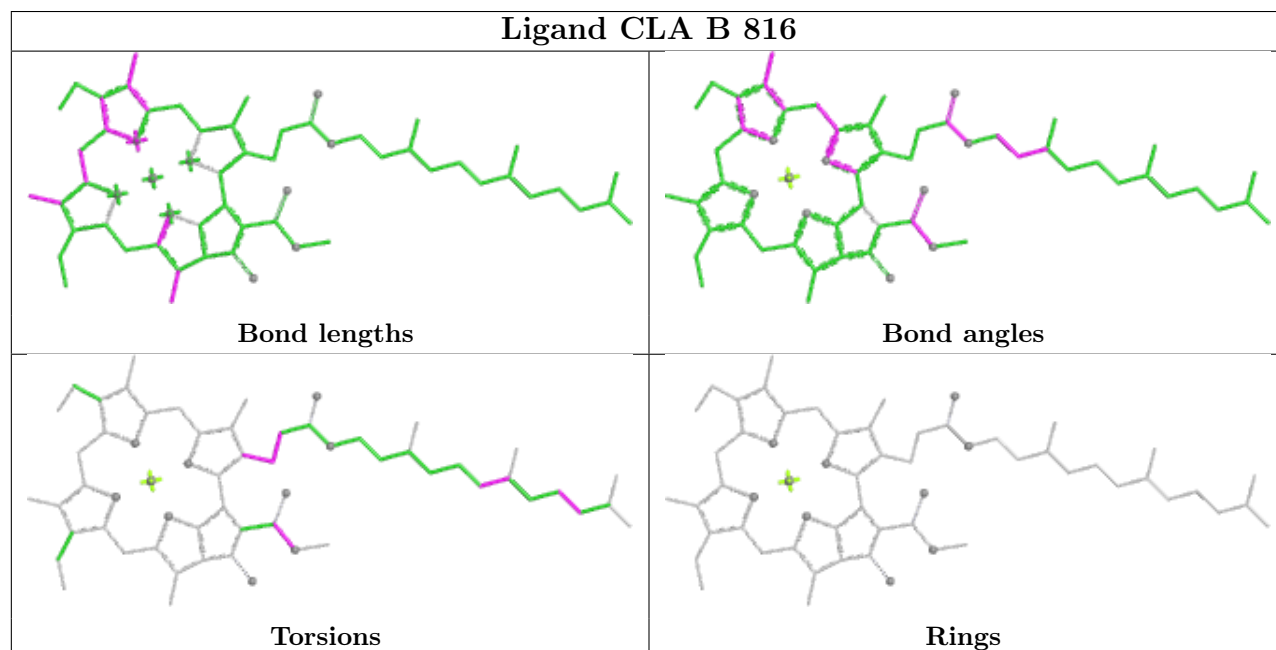




## Ligand CHL a 606

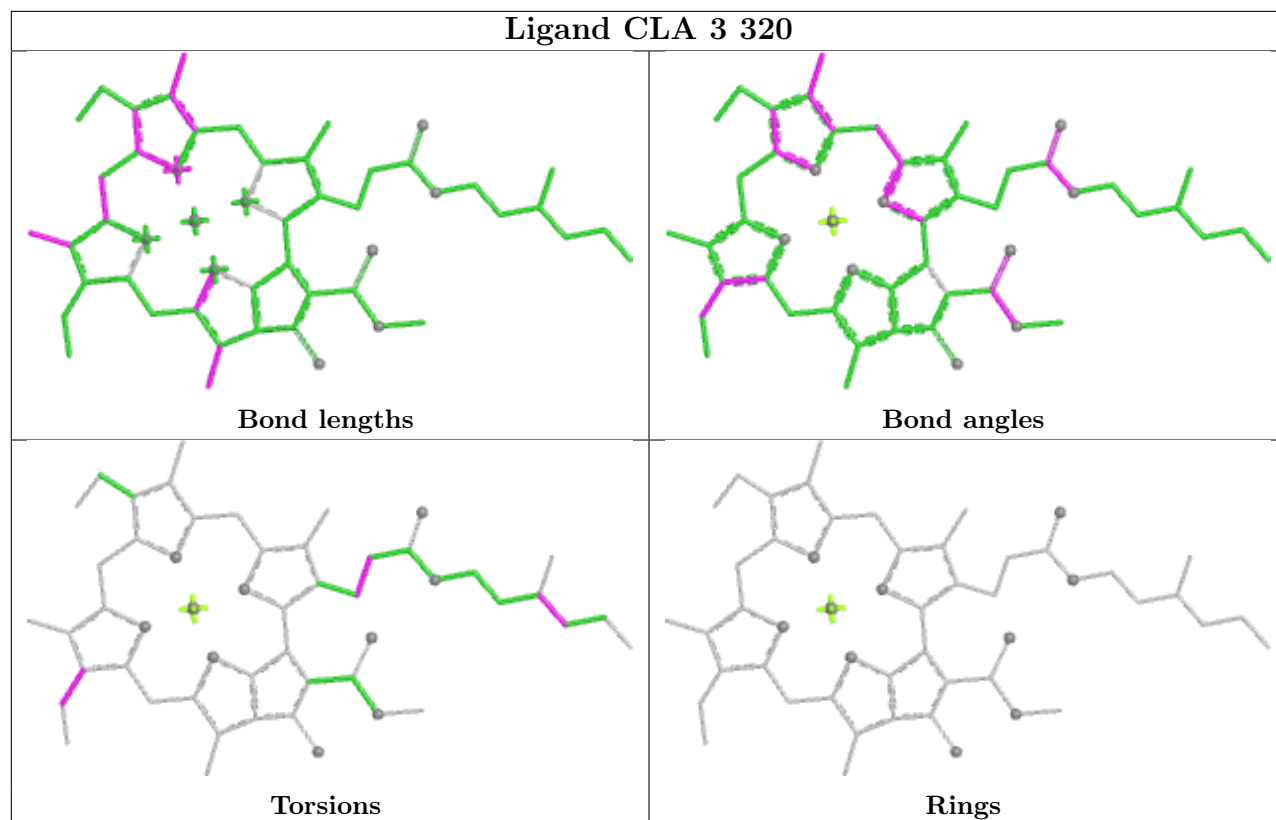


## Ligand CLA B 816

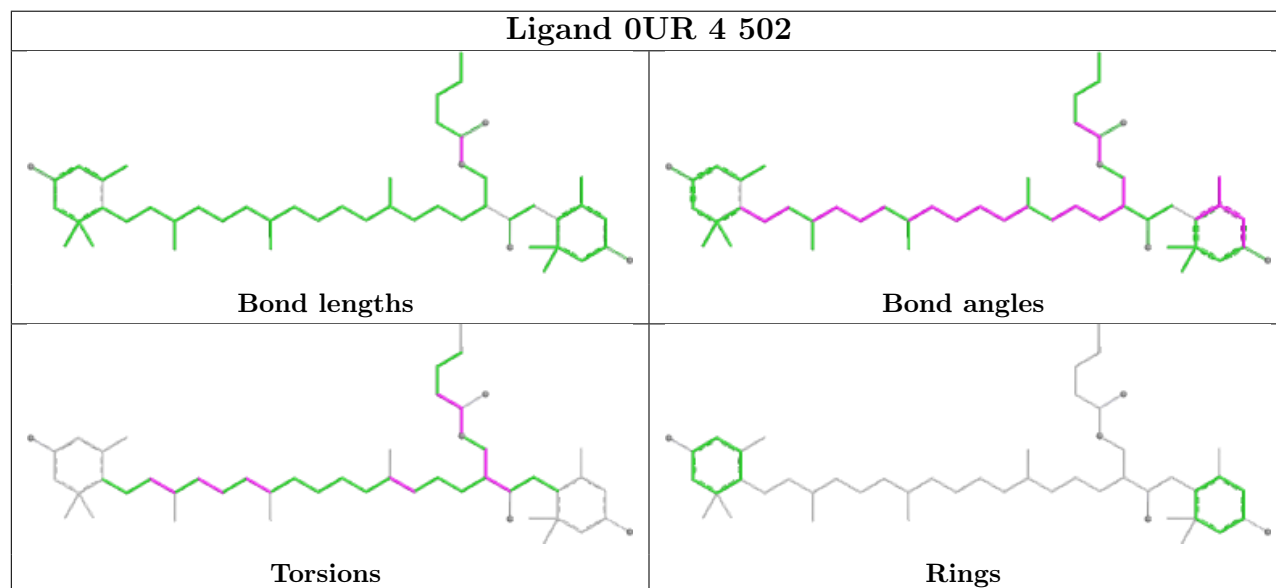




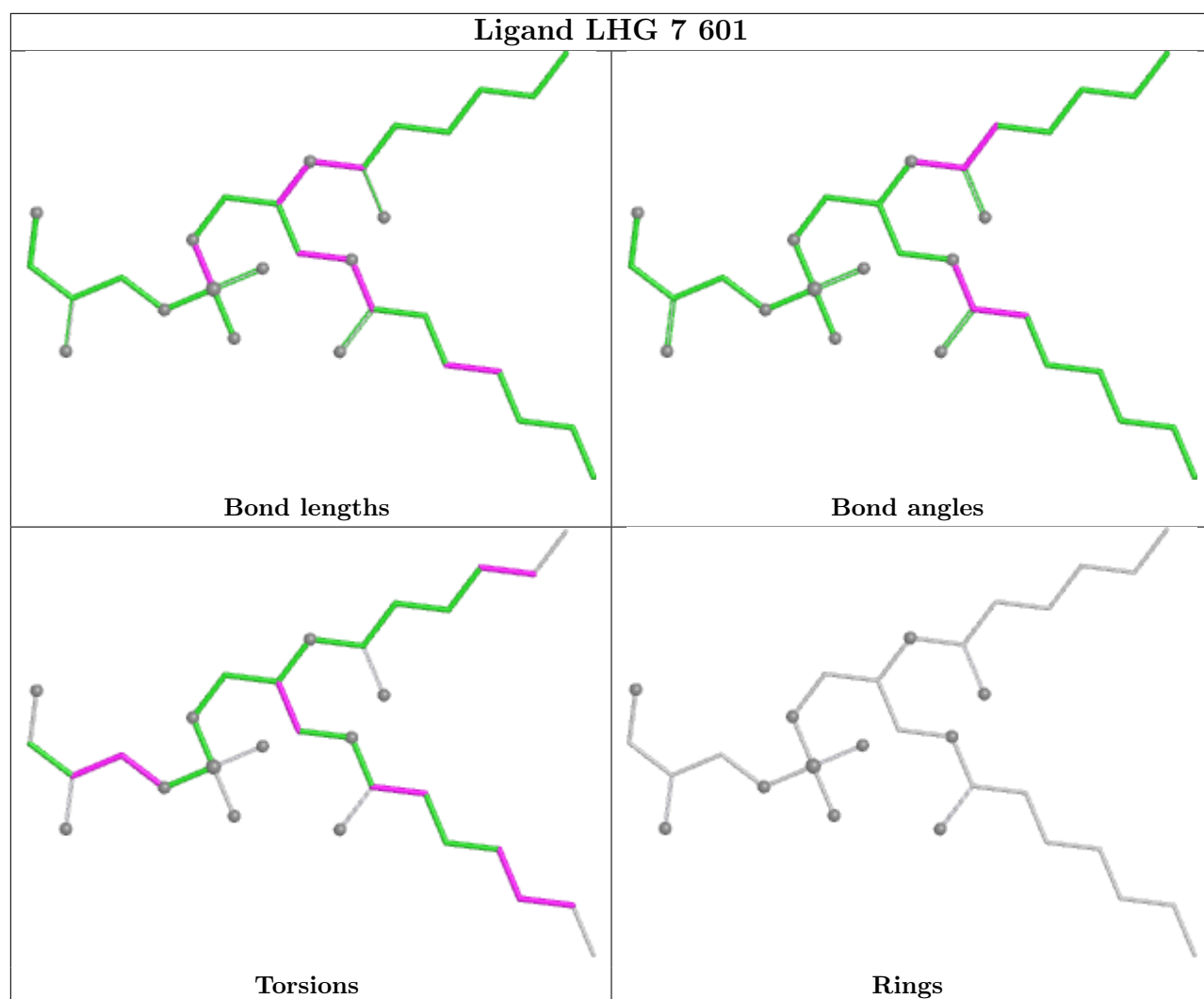
## Ligand CLA 3 320



## Ligand 0UR 4 502

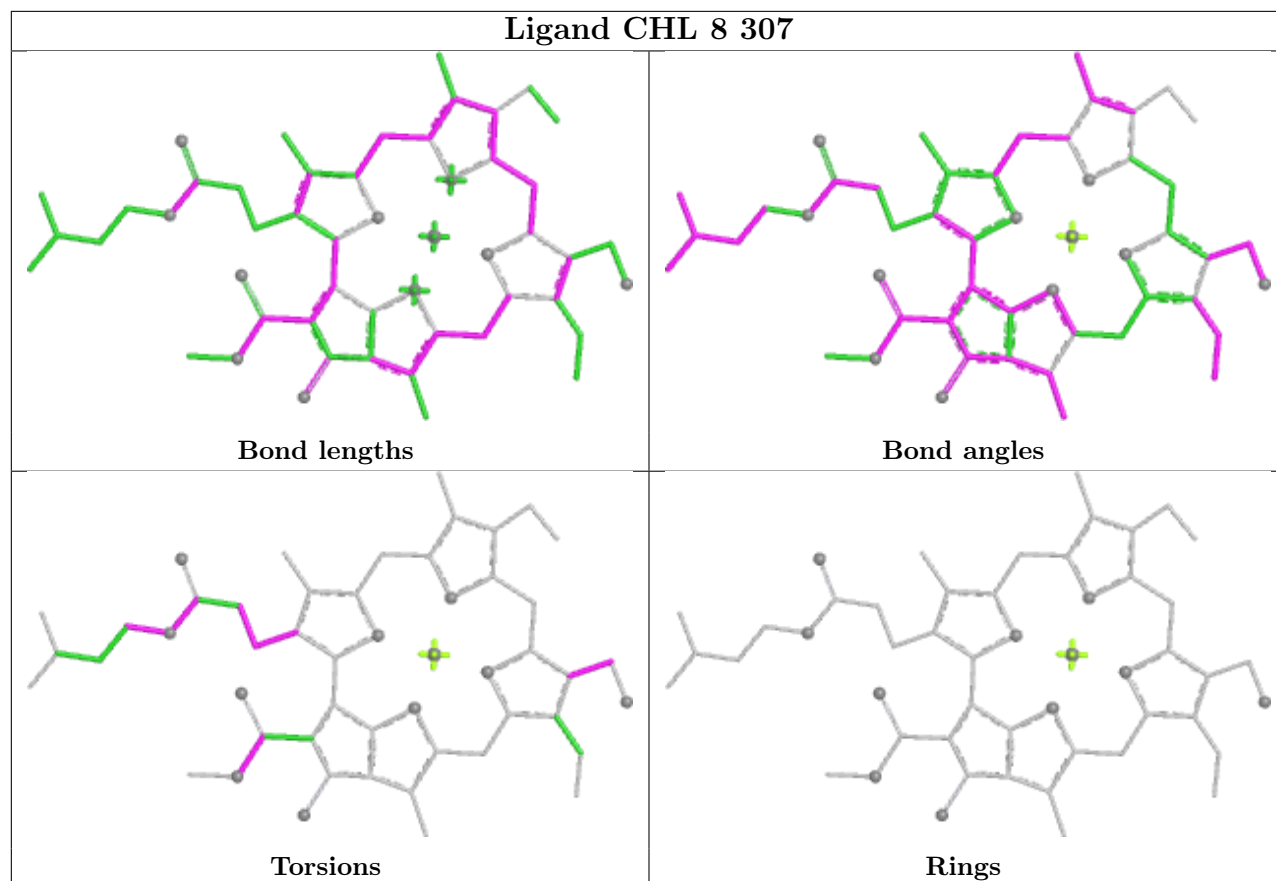




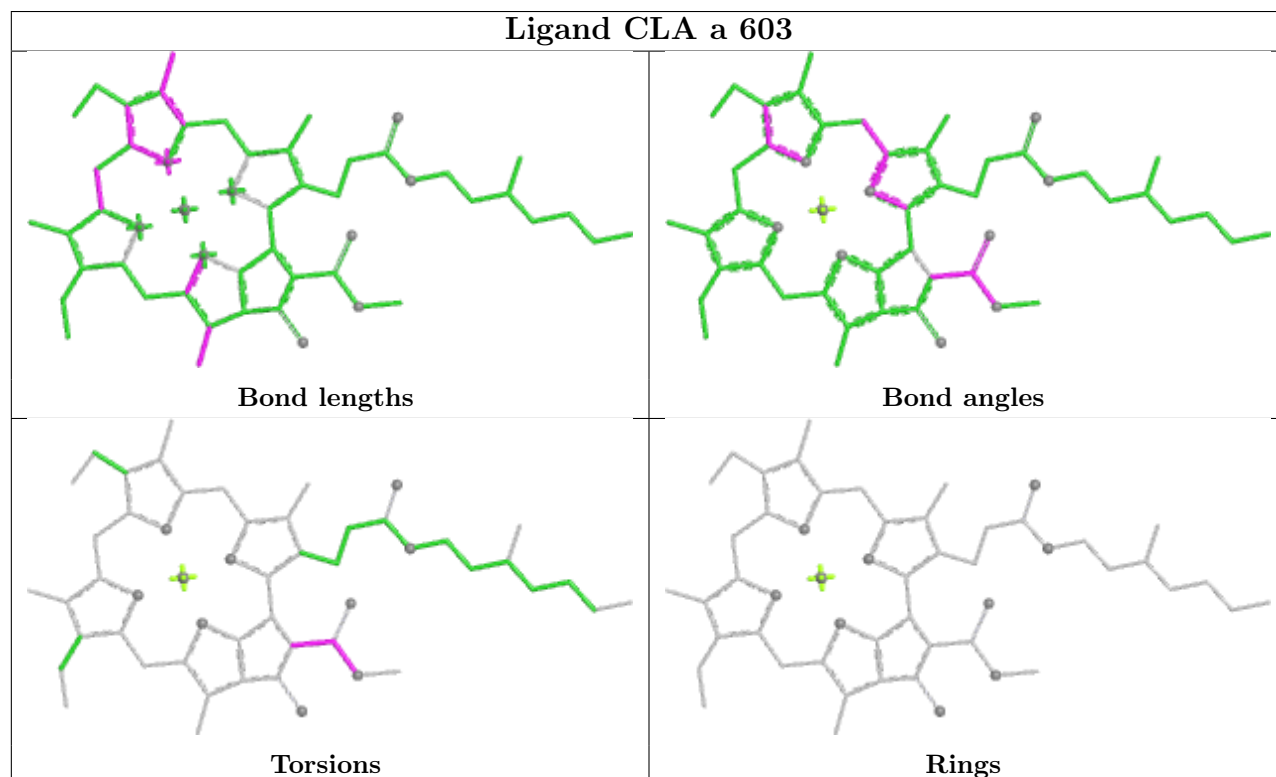




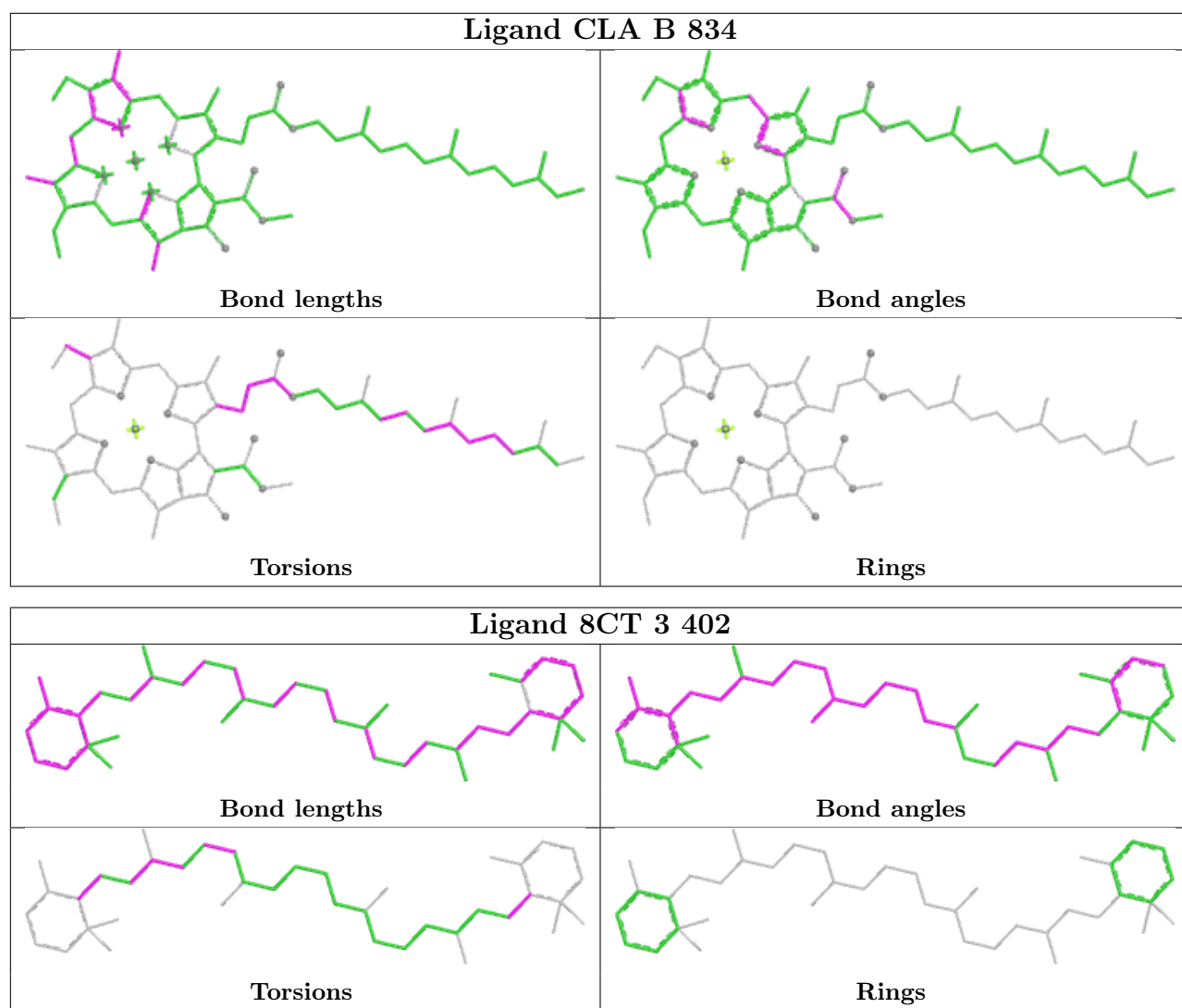
## Ligand CHL 8 307



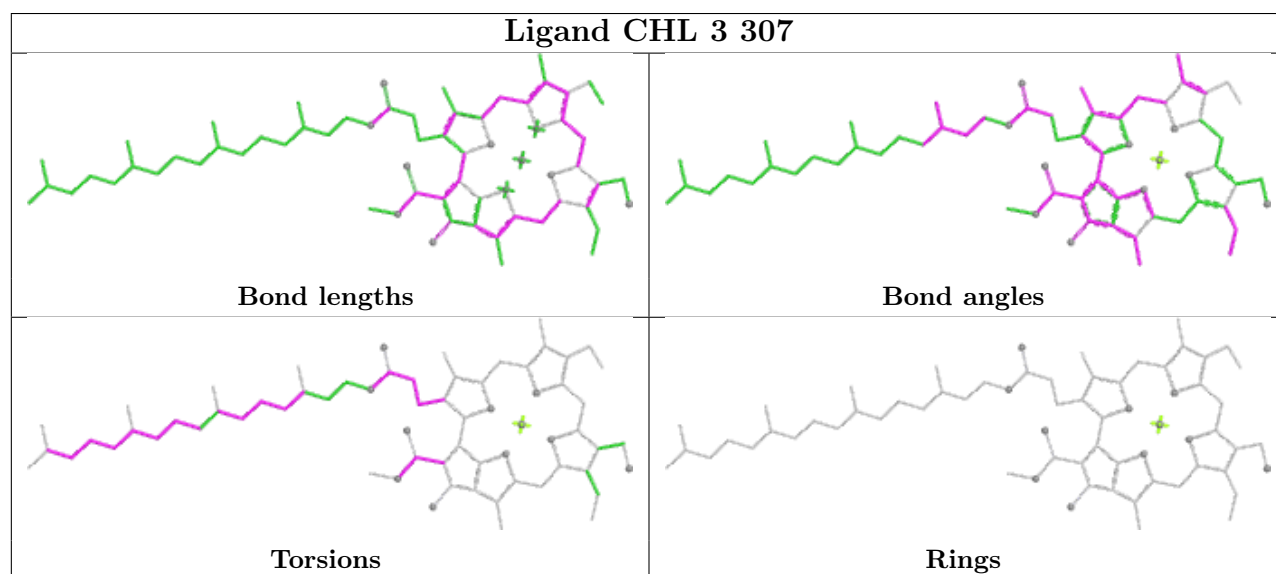
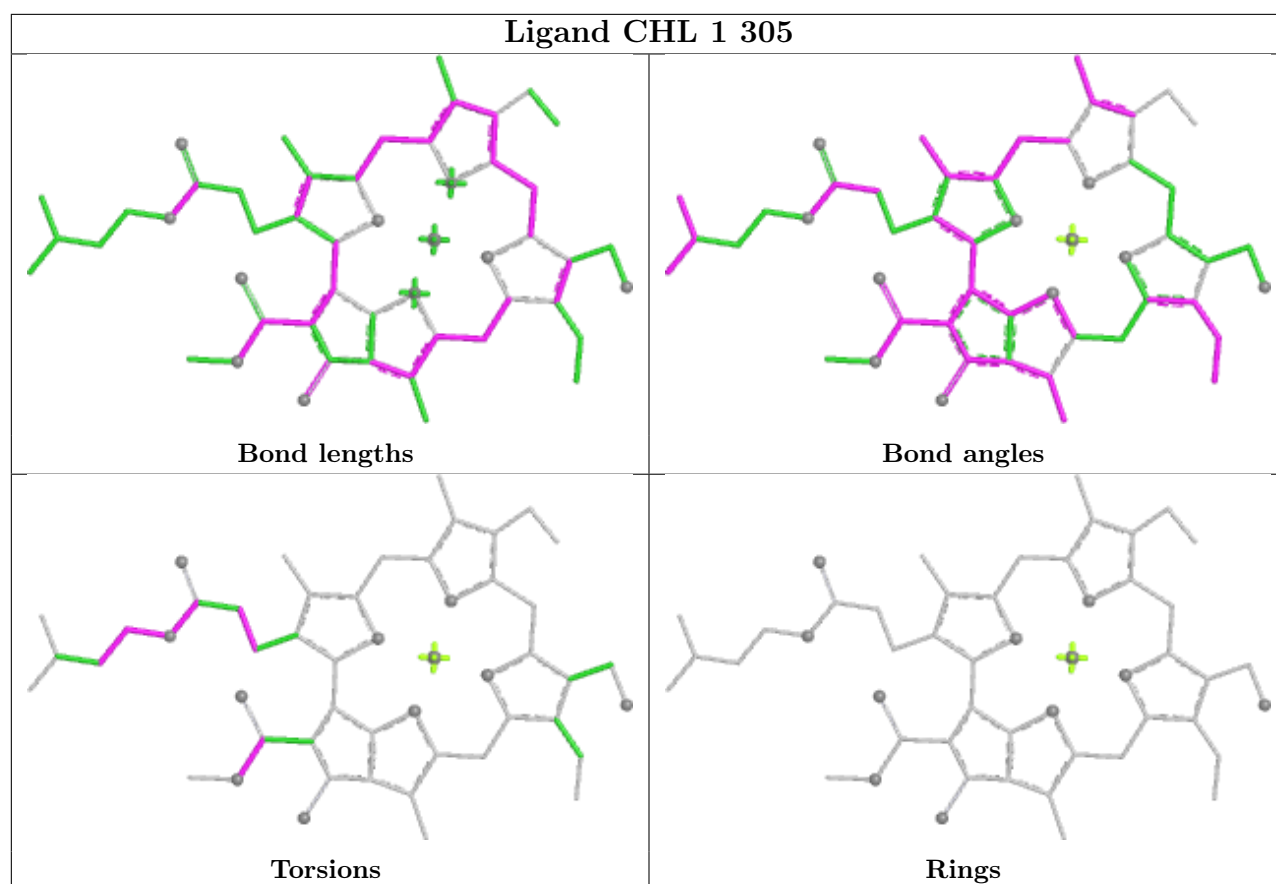
## Ligand CLA a 603



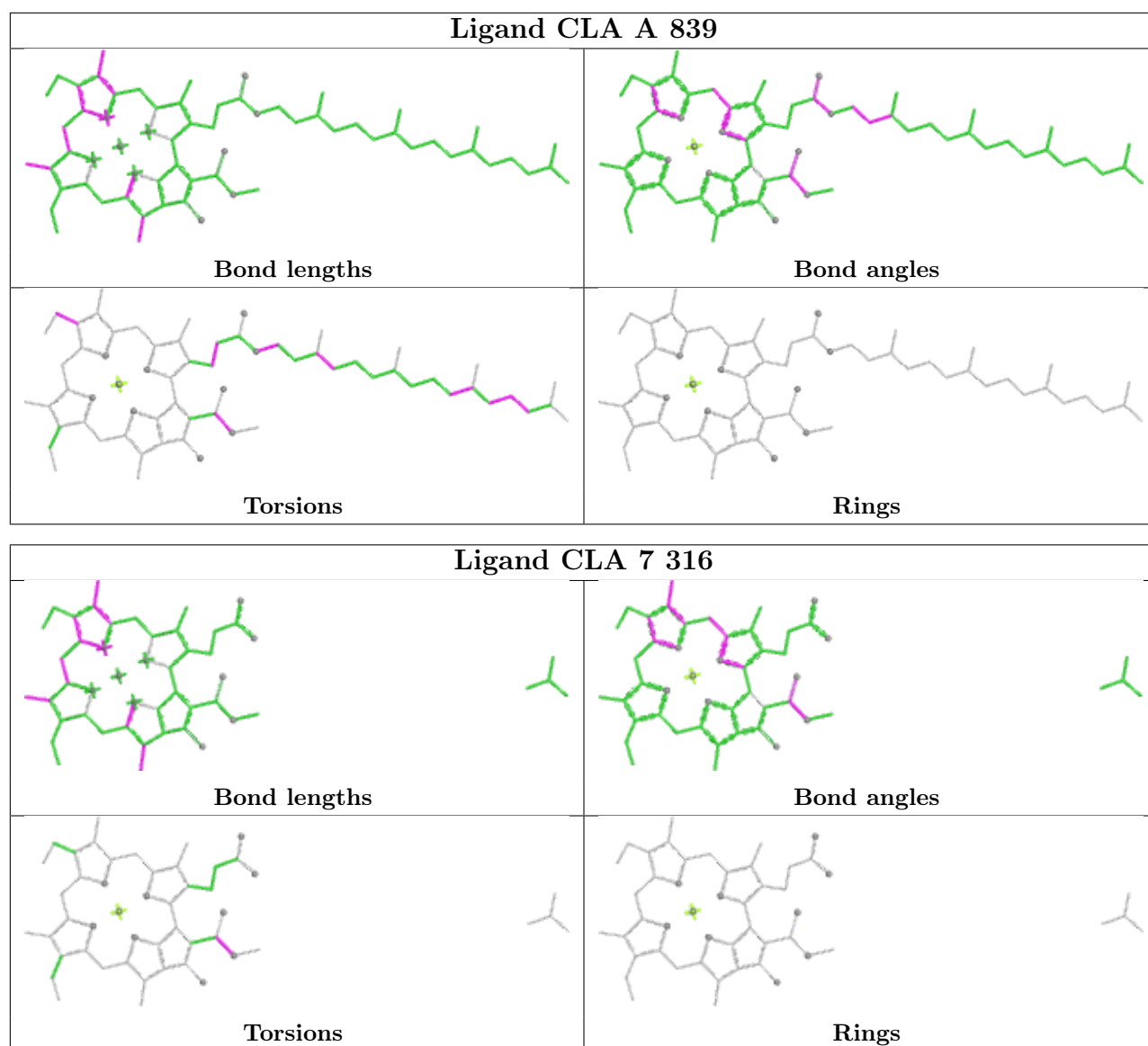




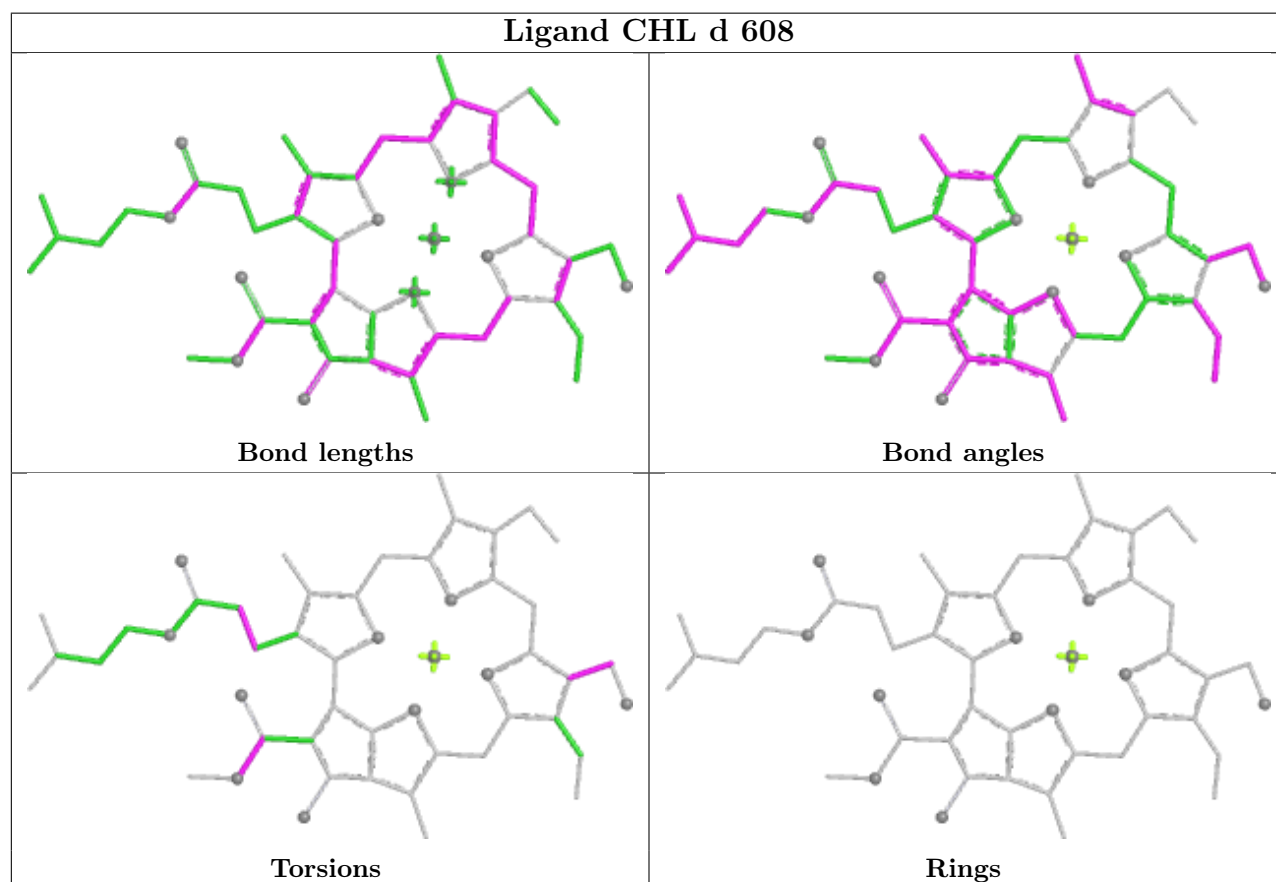
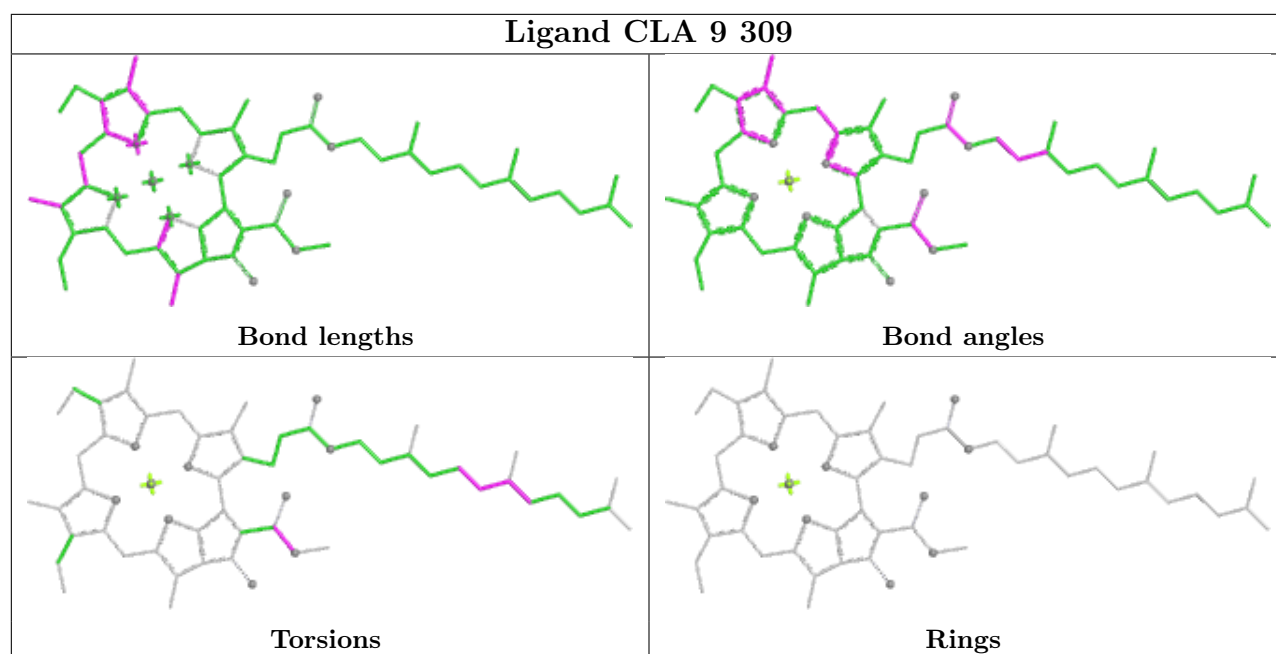




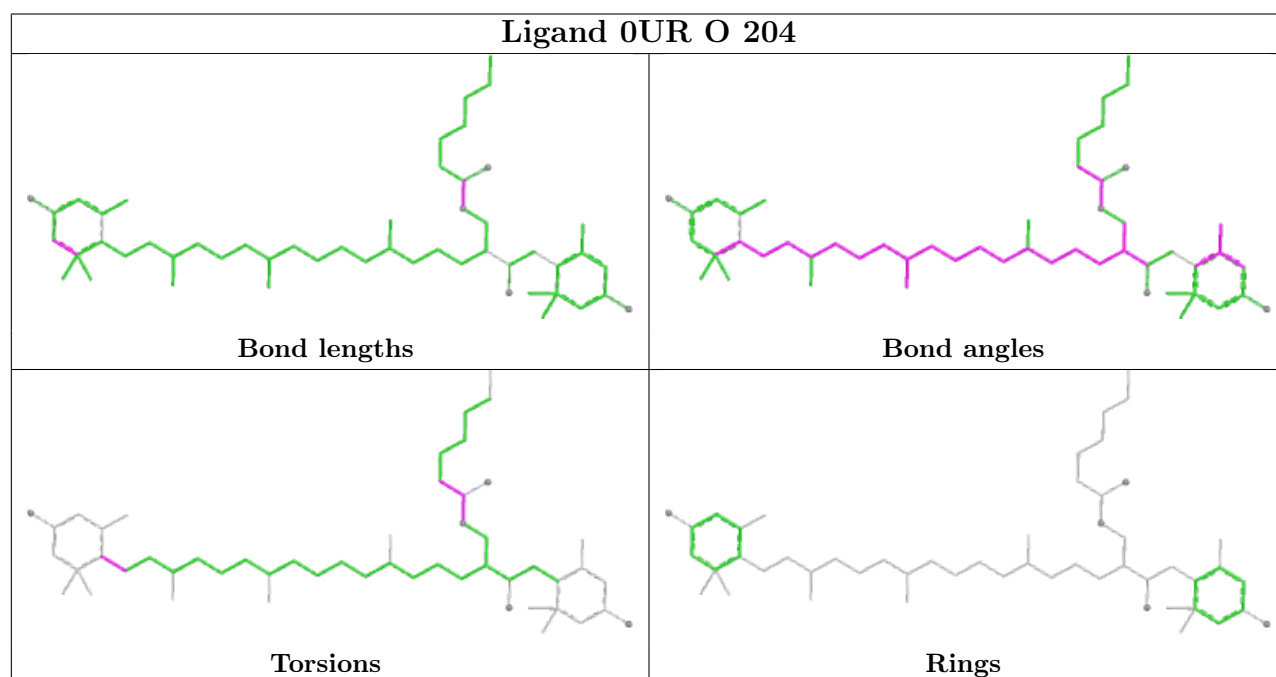
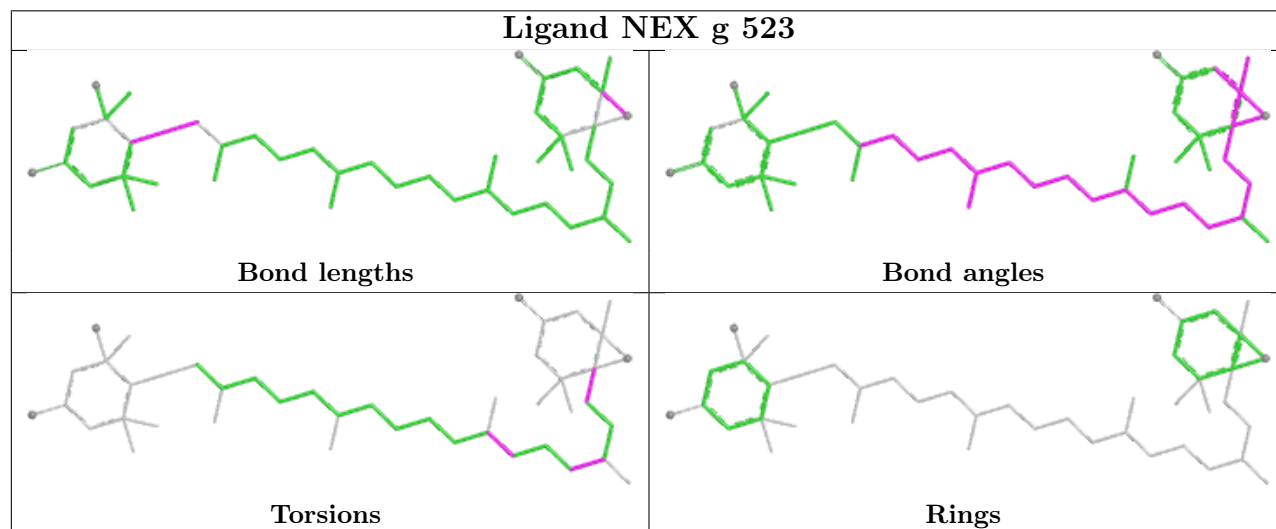
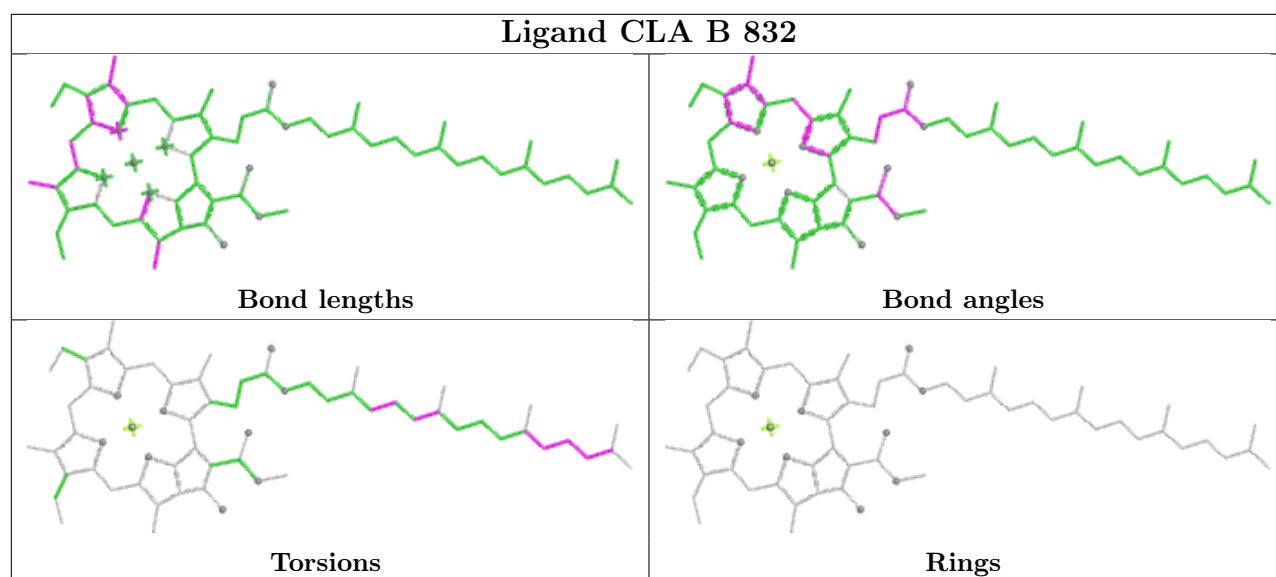




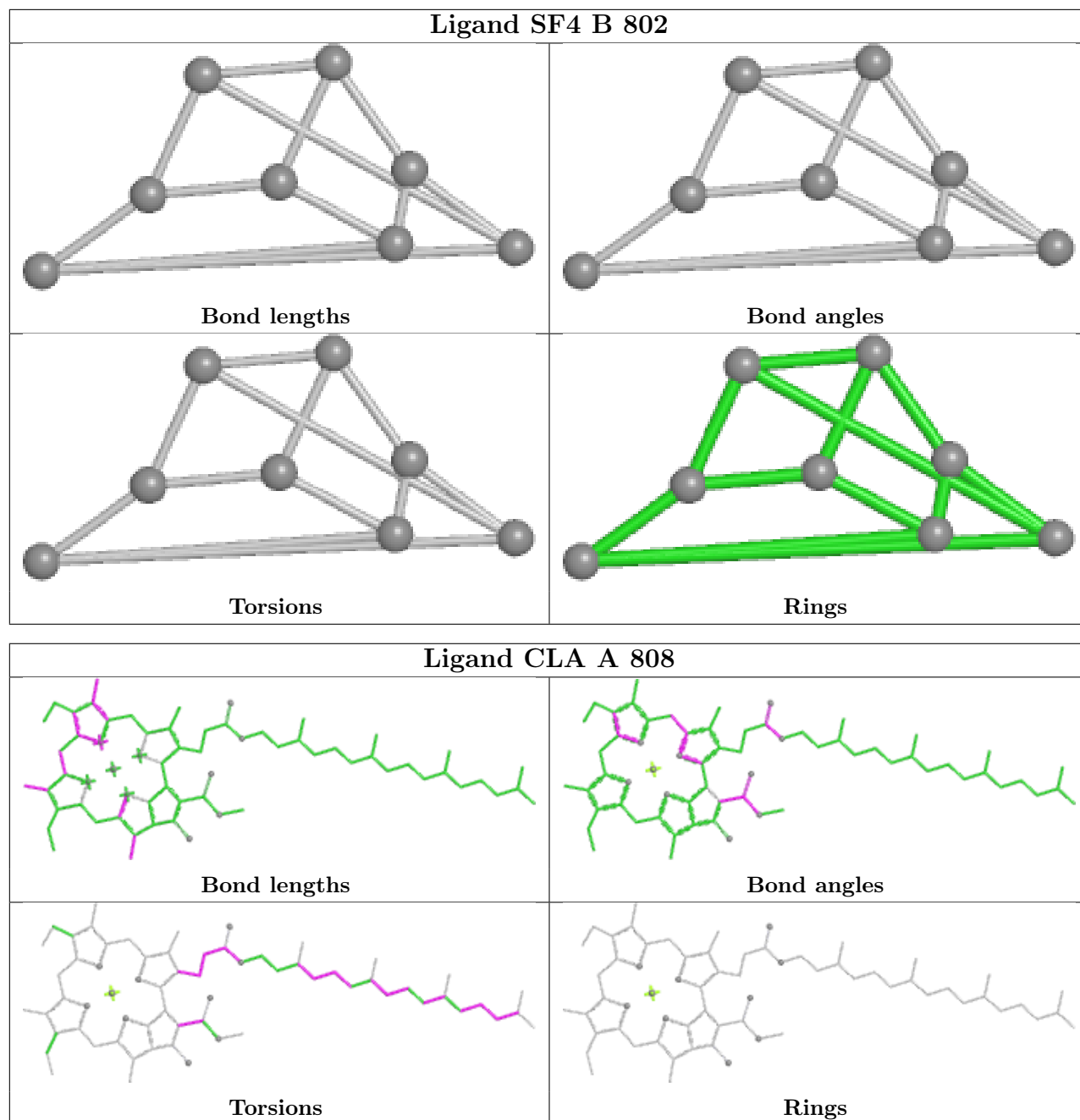




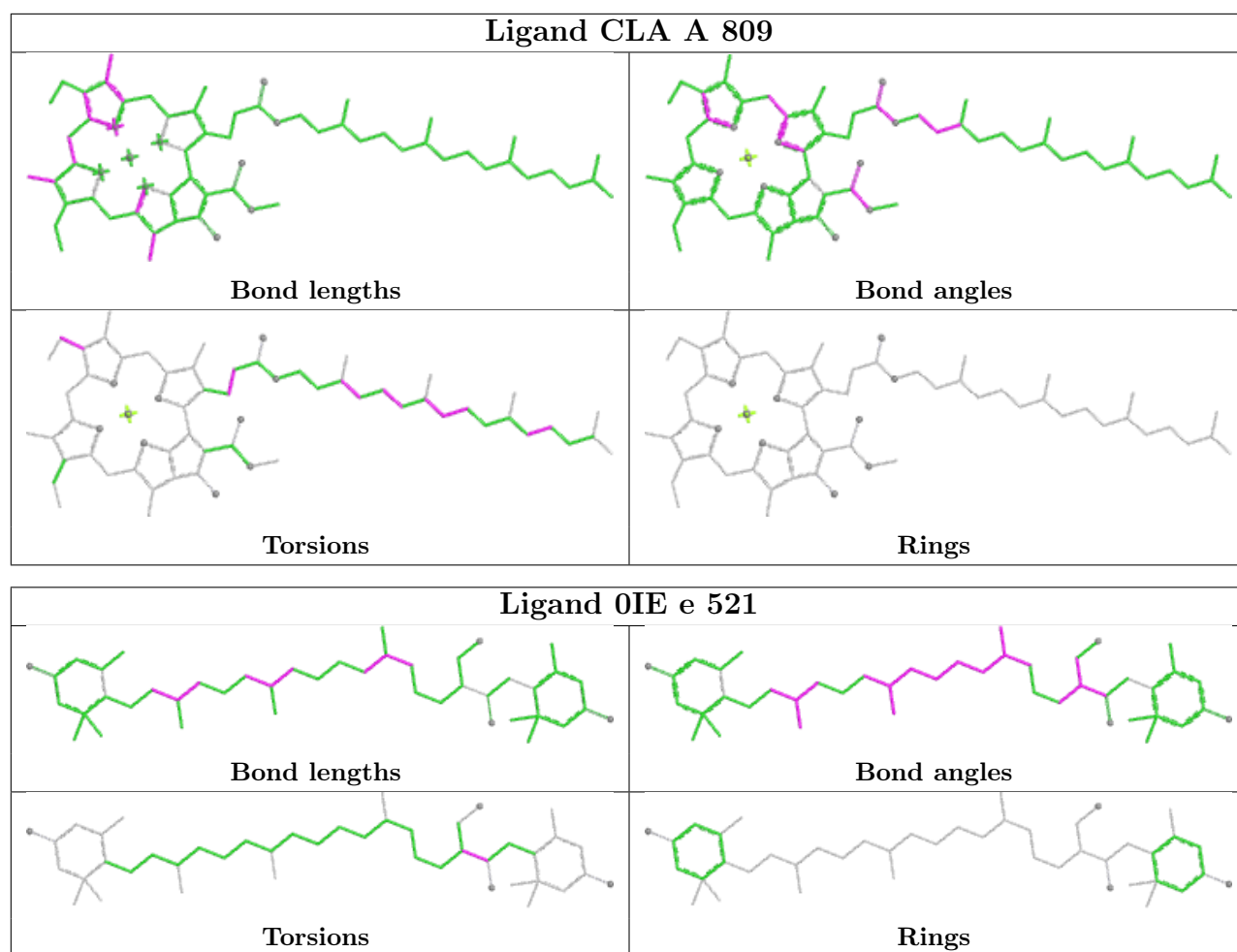






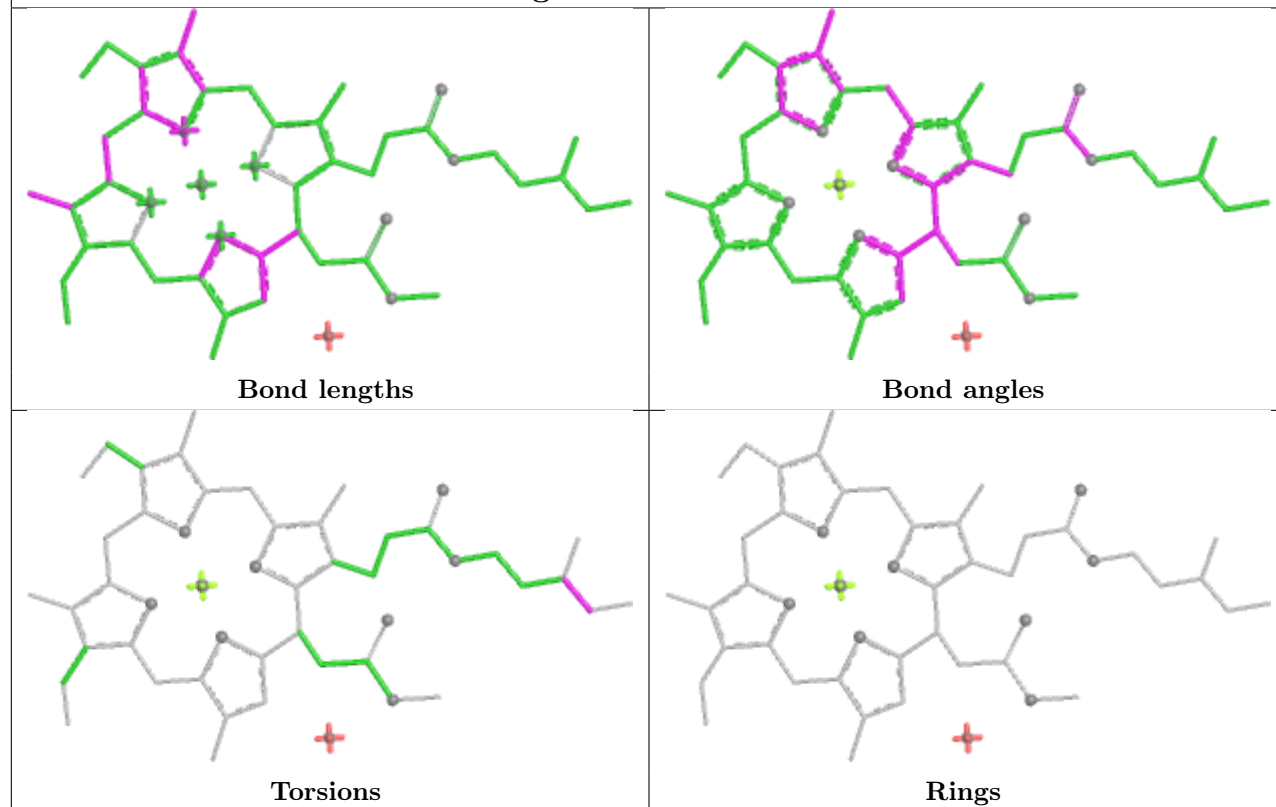




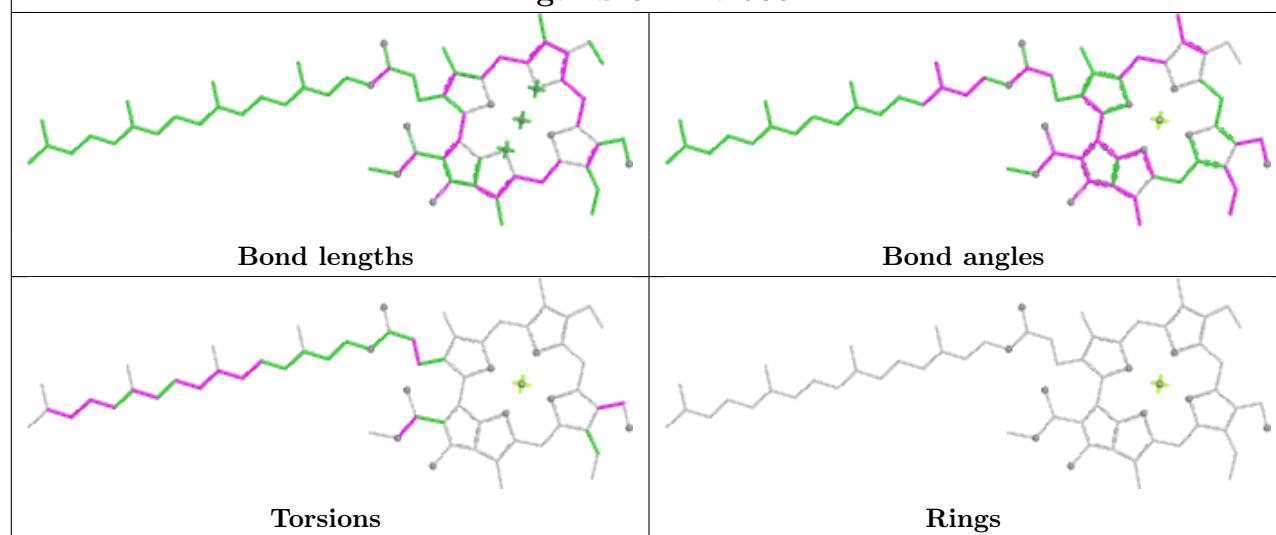




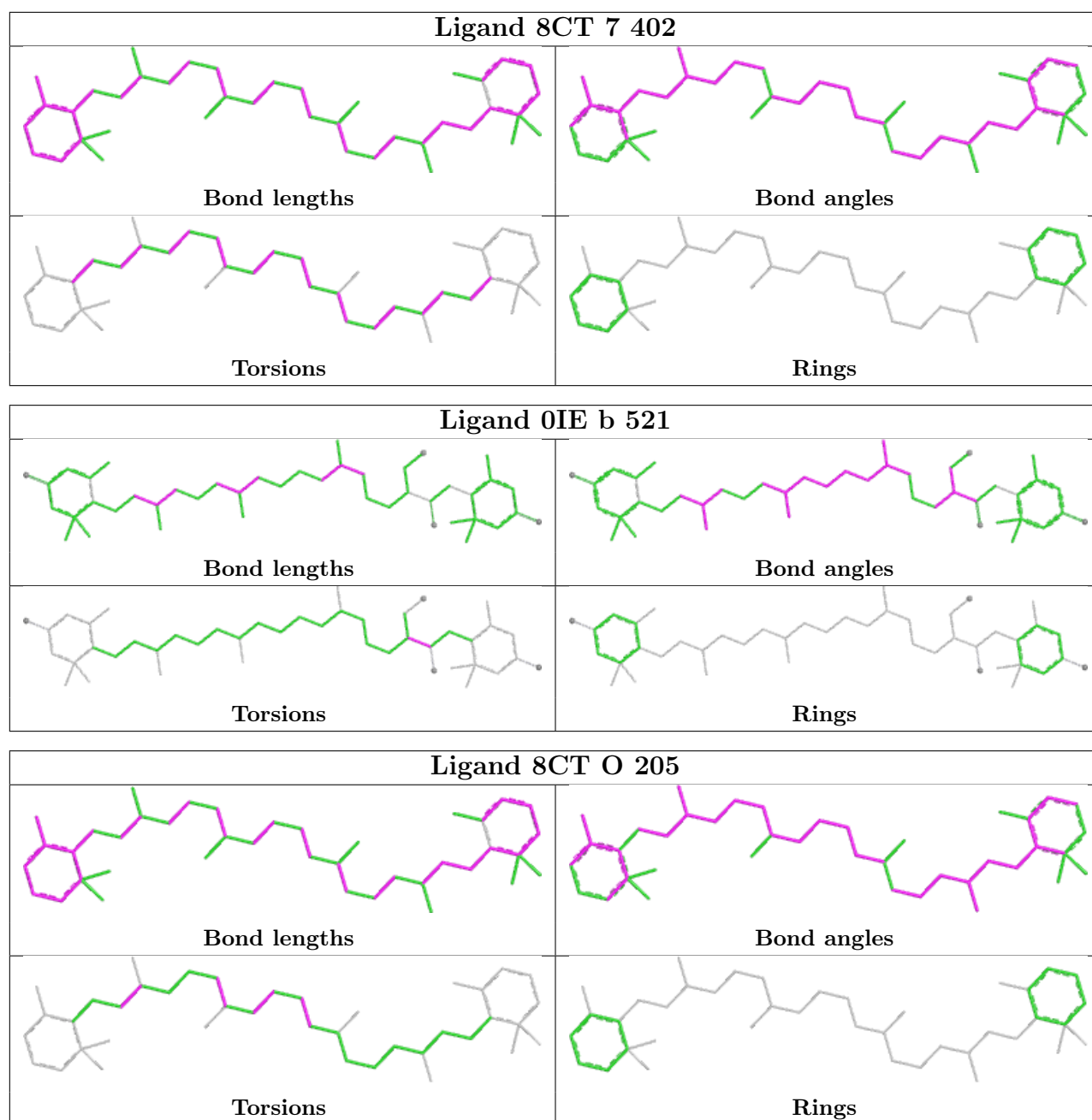
## Ligand CLA B 826



## Ligand CHL e 608

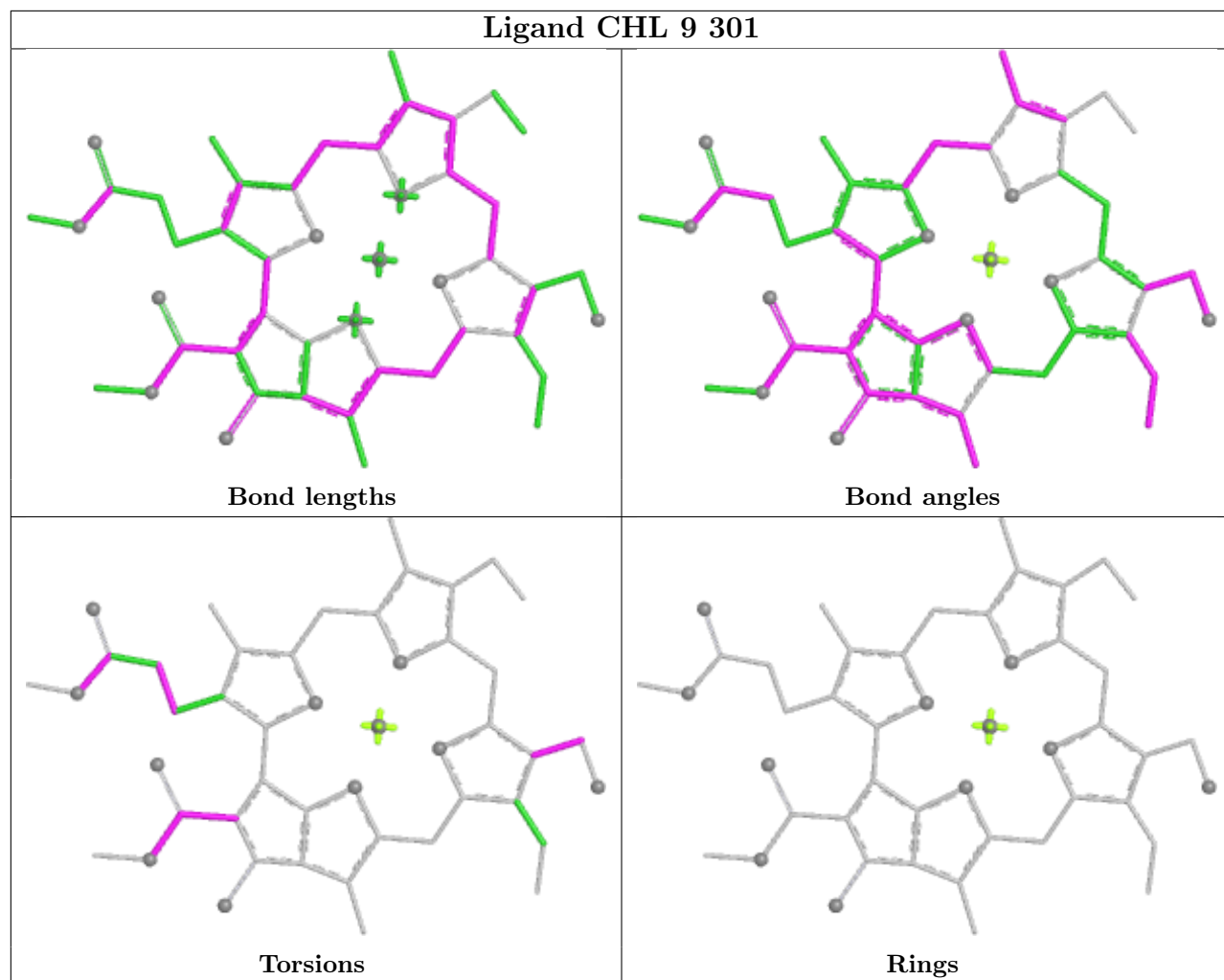






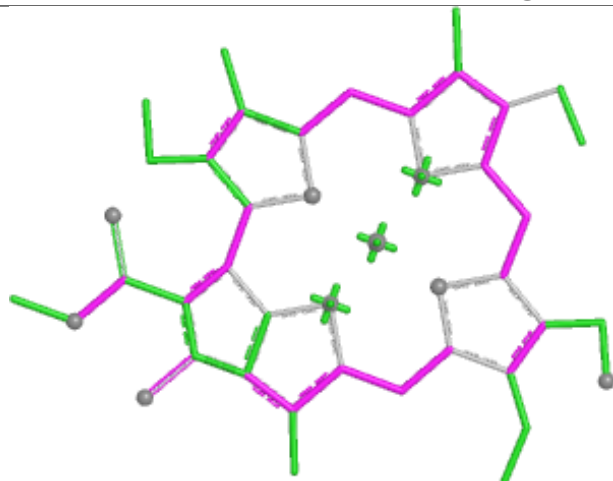


## Ligand CHL 9 301





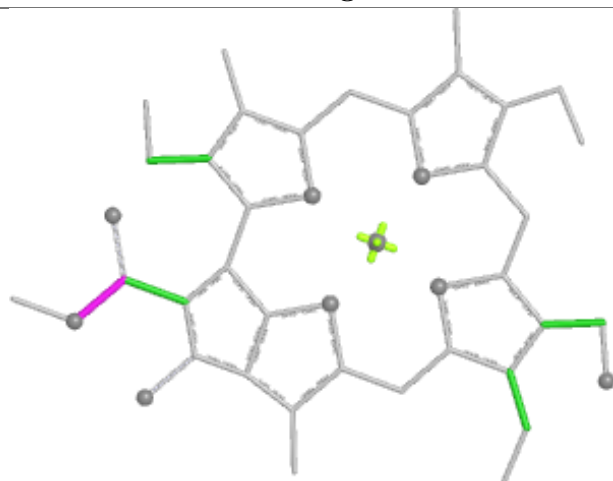
## Ligand CHL c 605



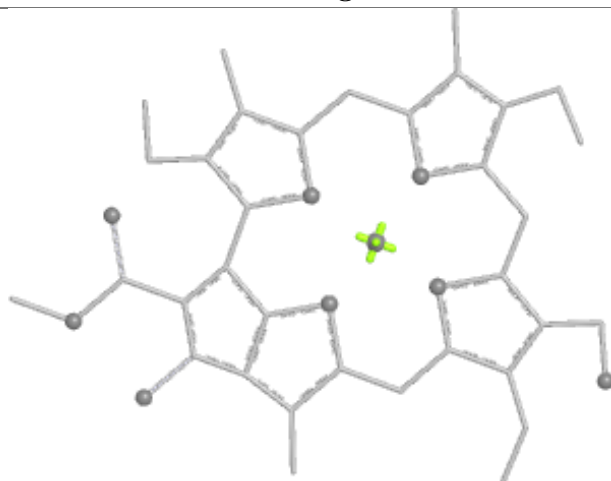
Bond lengths



Bond angles

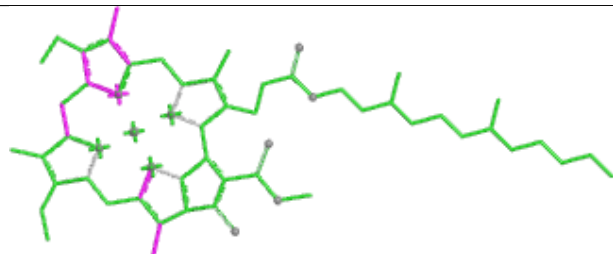


Torsions

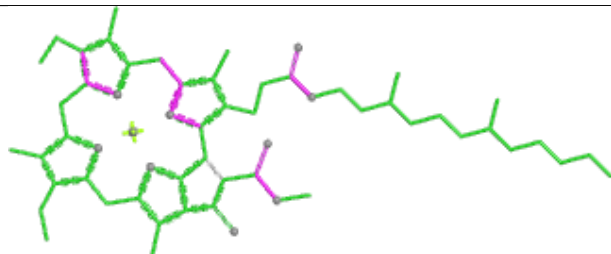


Rings

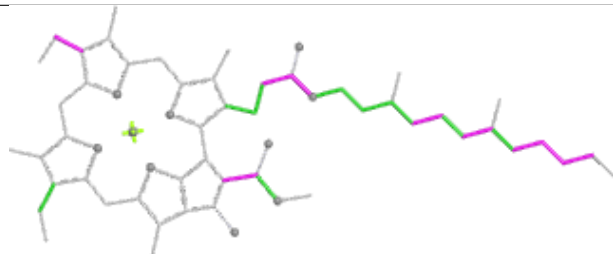
## Ligand CLA 5 303



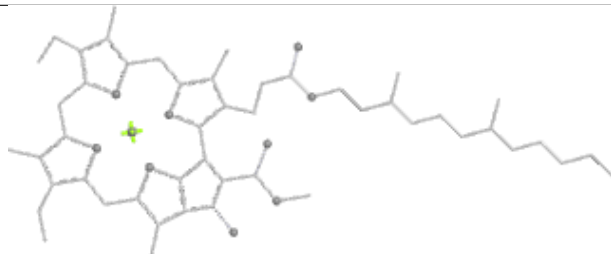
Bond lengths



Bond angles

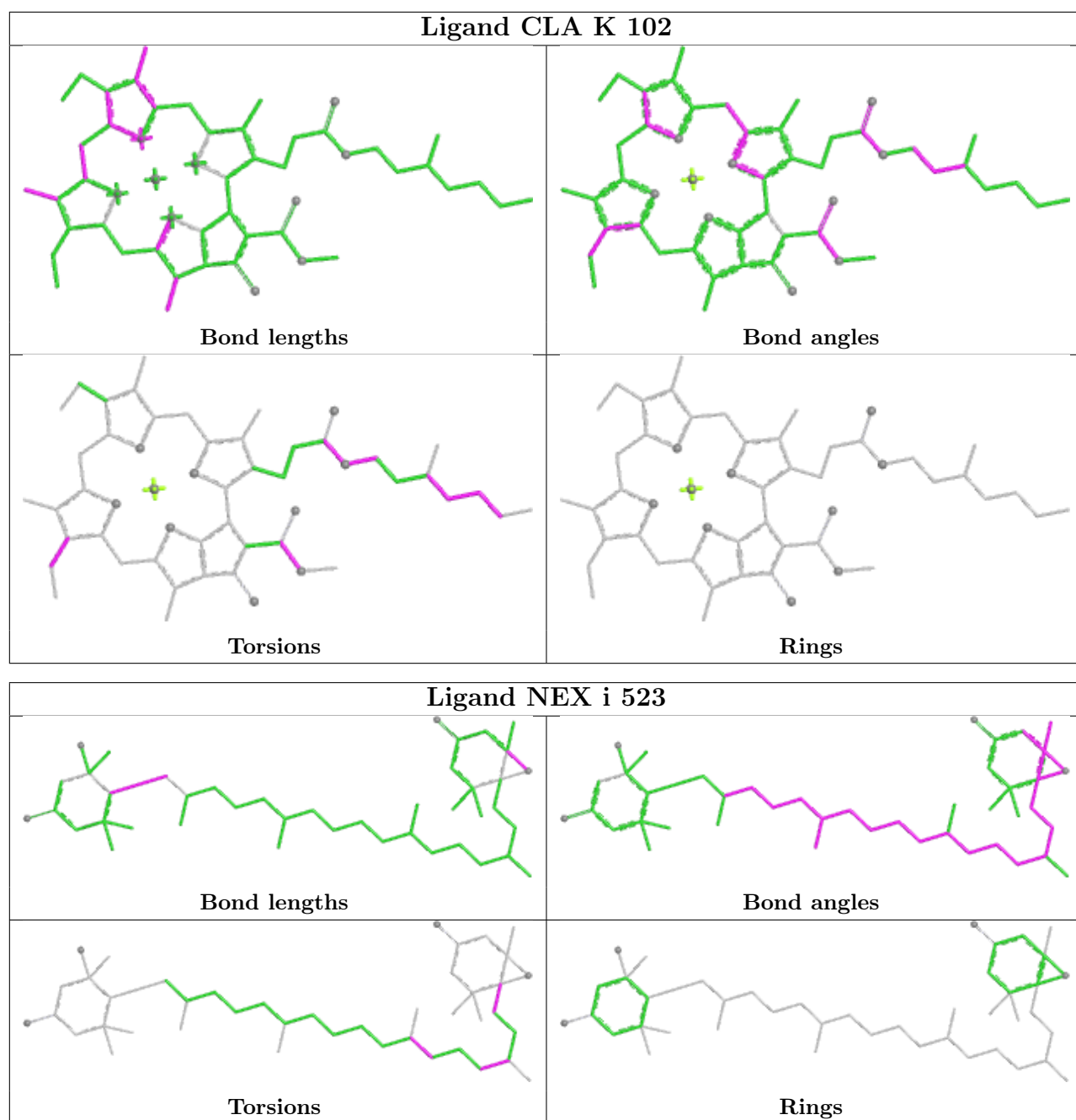


Torsions



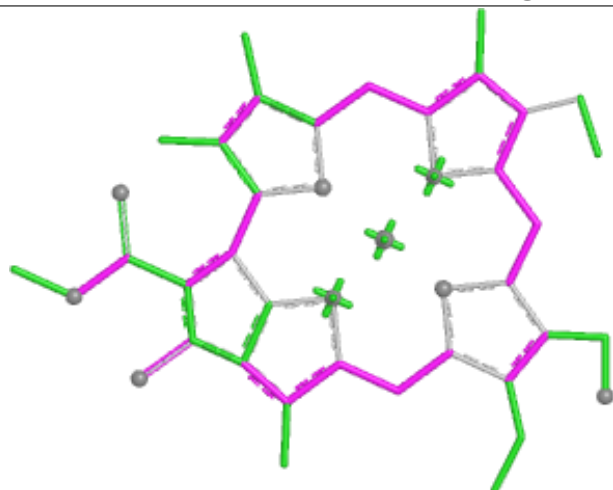
Rings



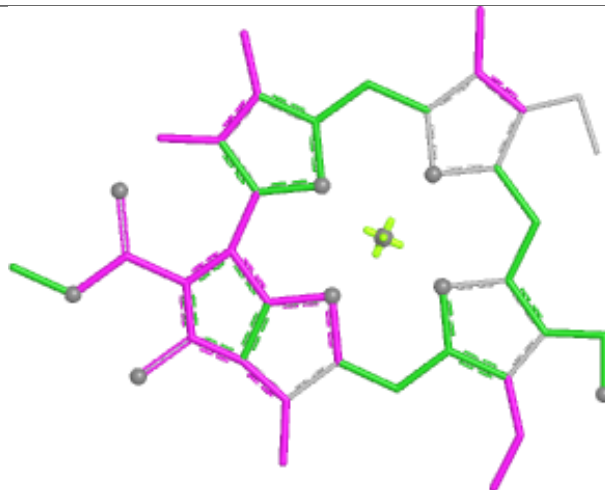




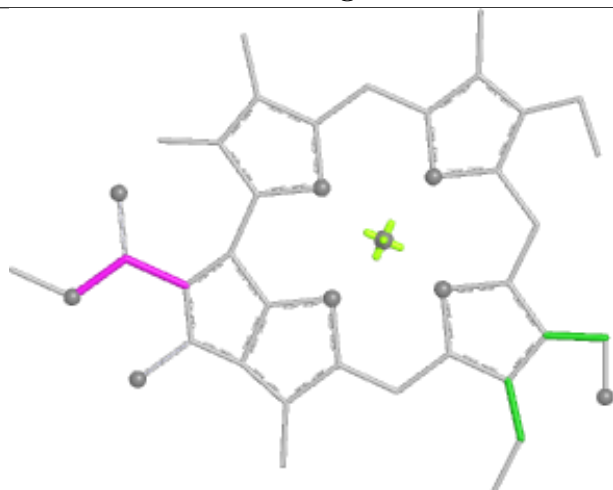
## Ligand CHL c 614



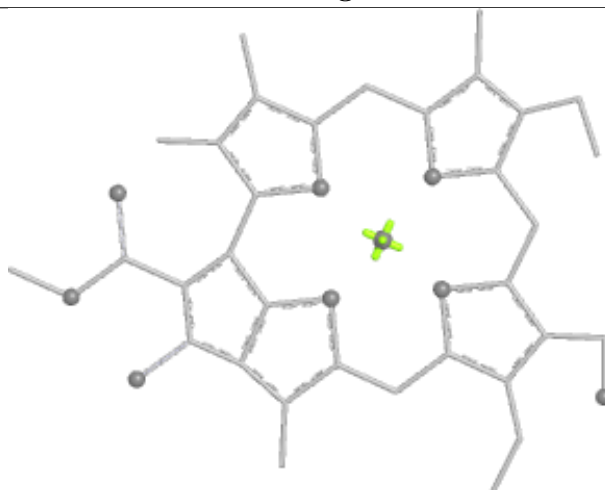
Bond lengths



Bond angles

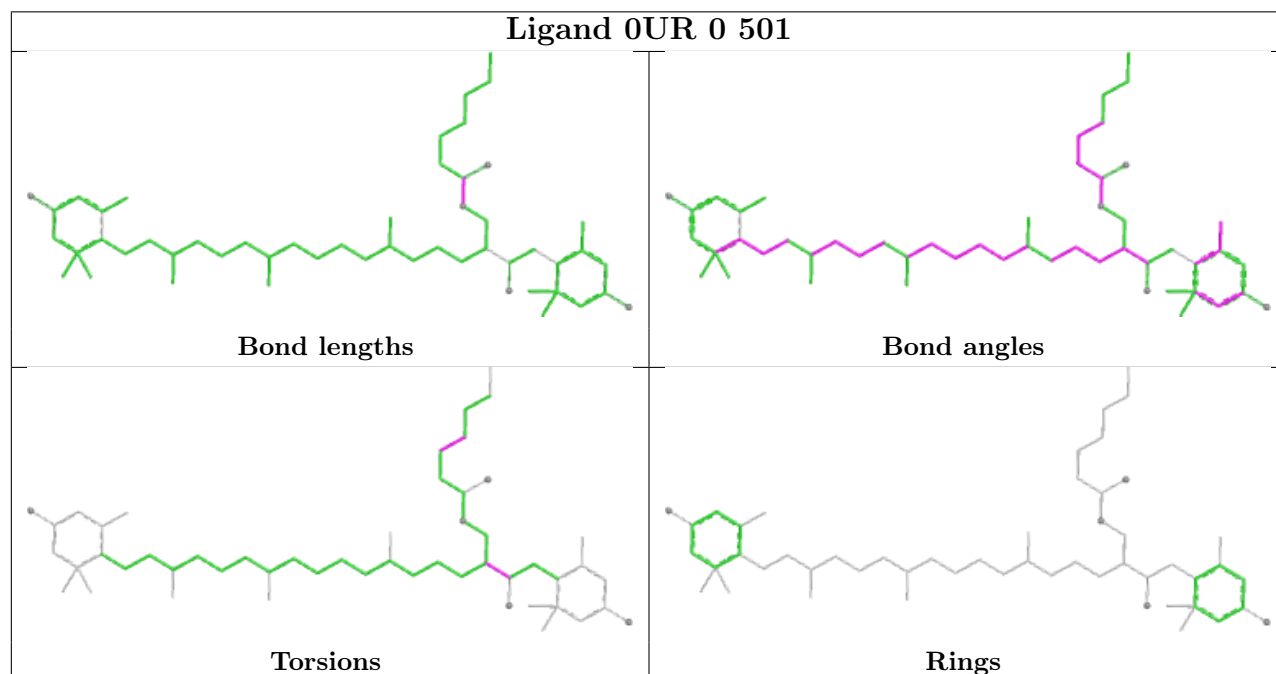
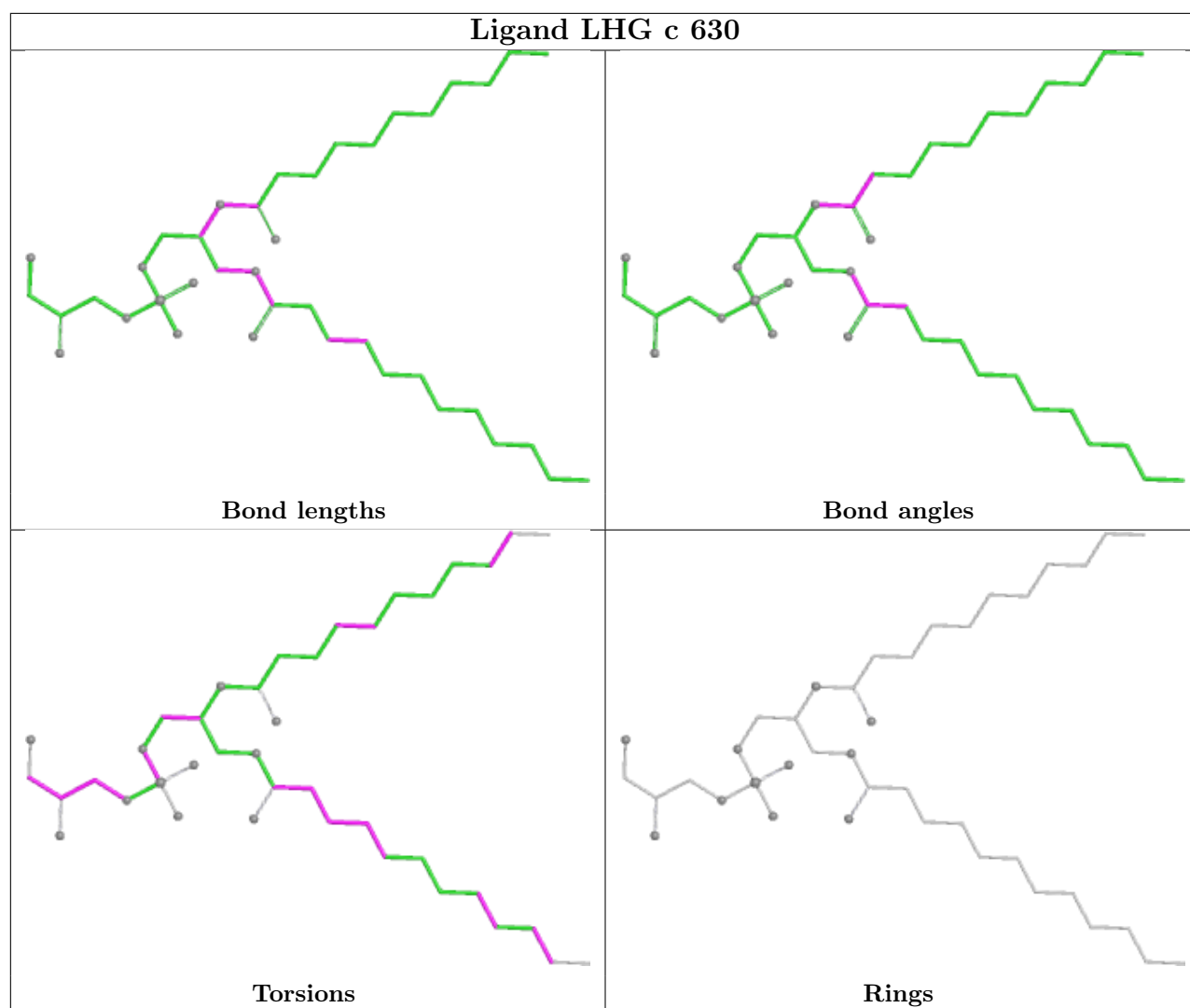


Torsions

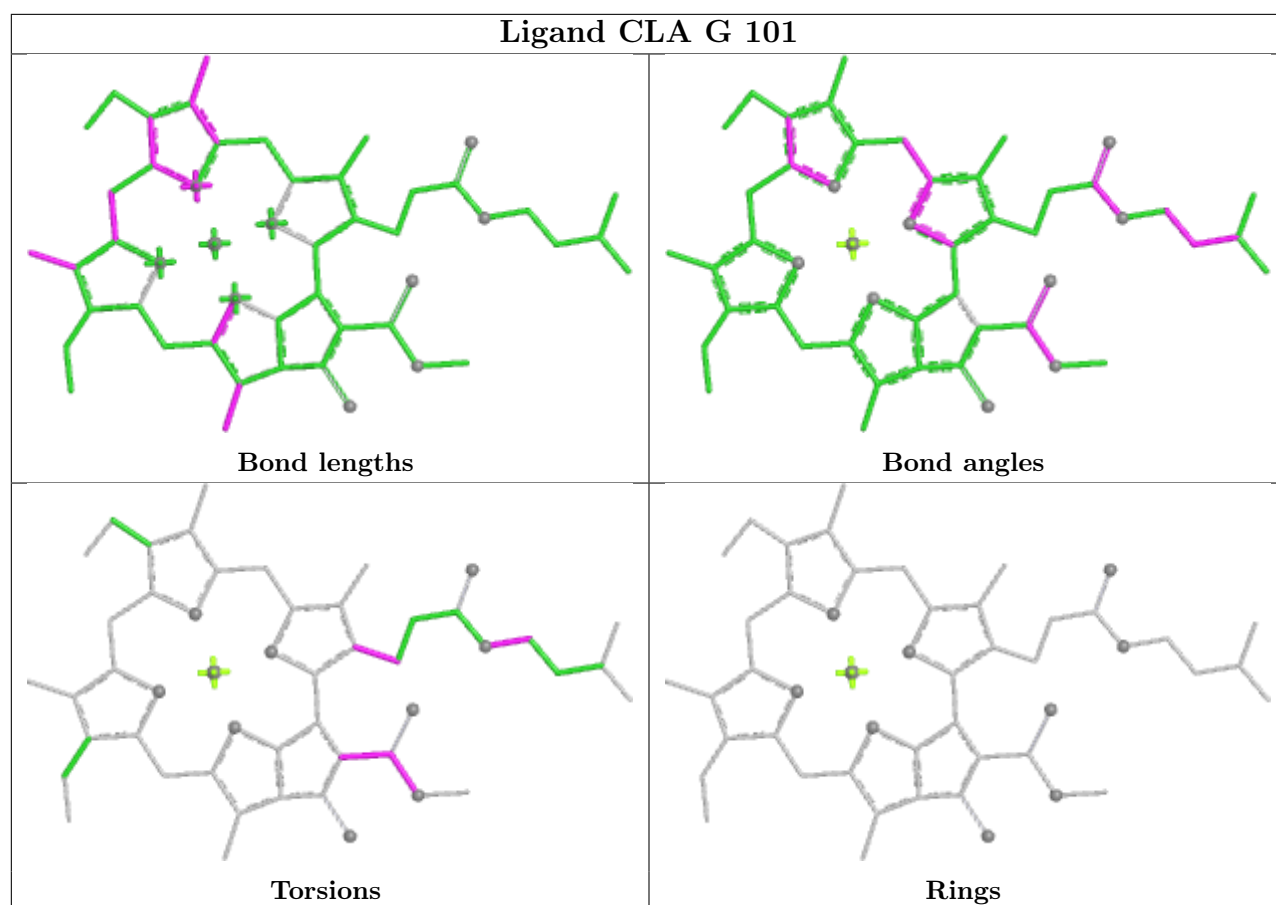


Rings

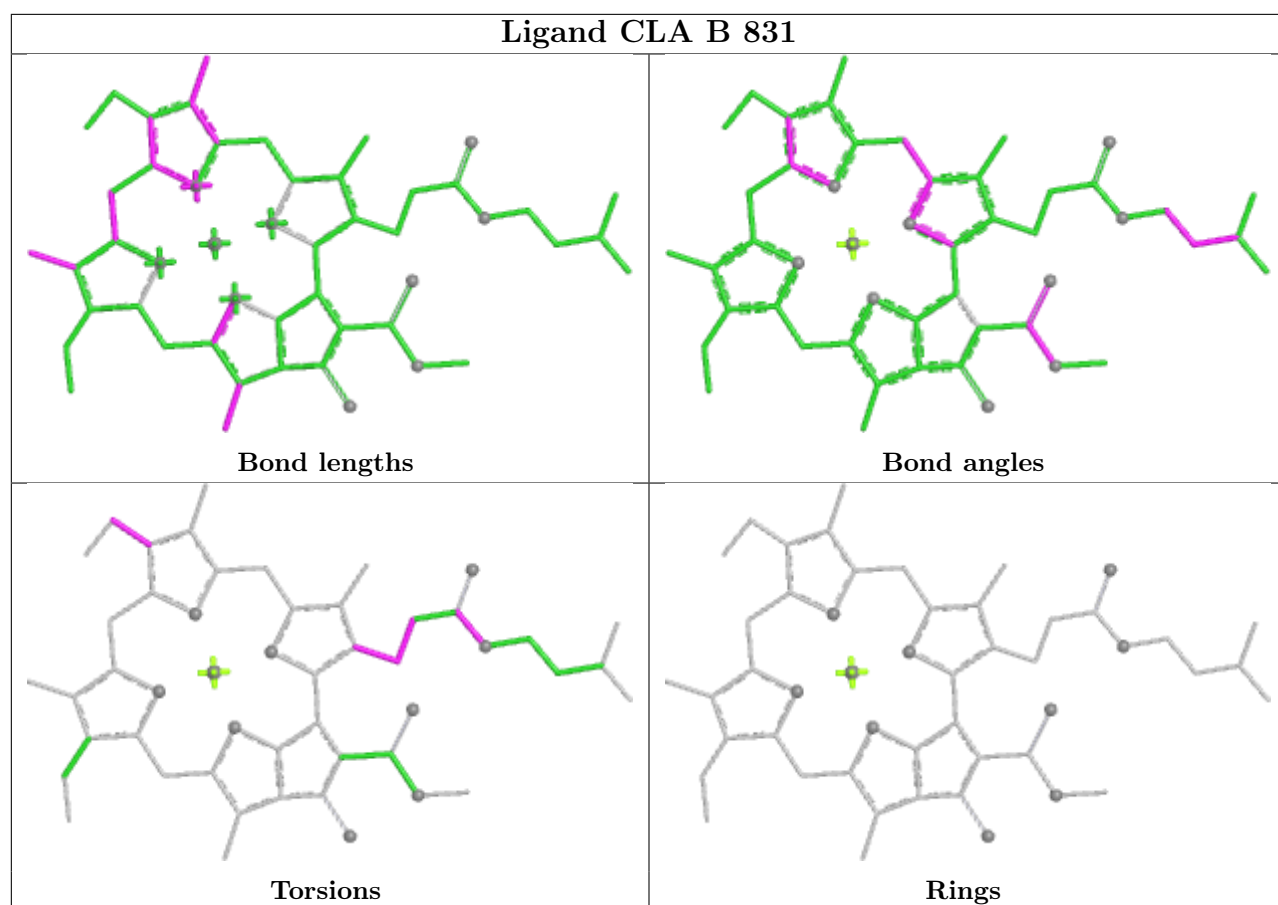






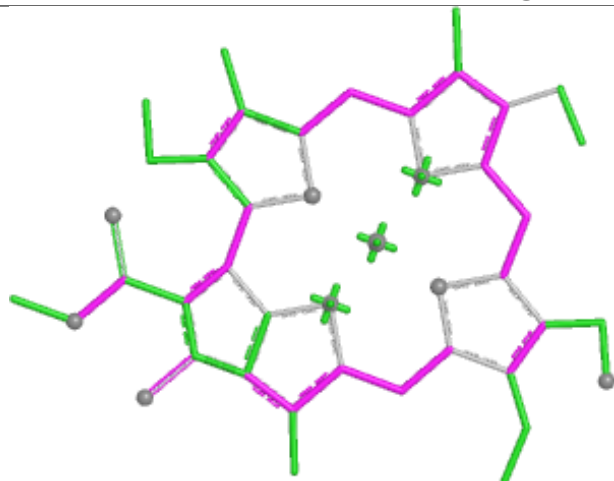




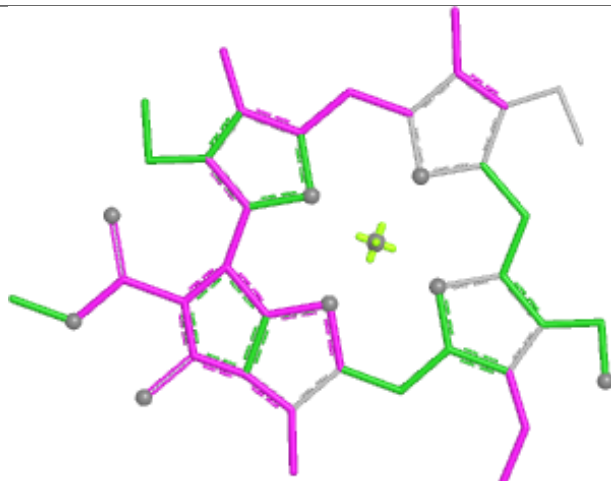




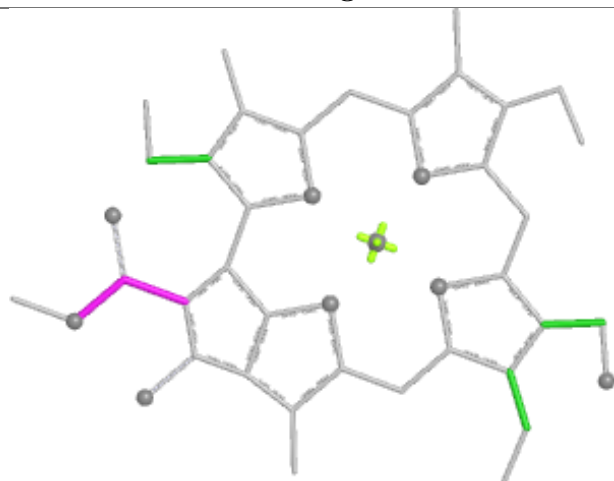
## Ligand CHL 6 315



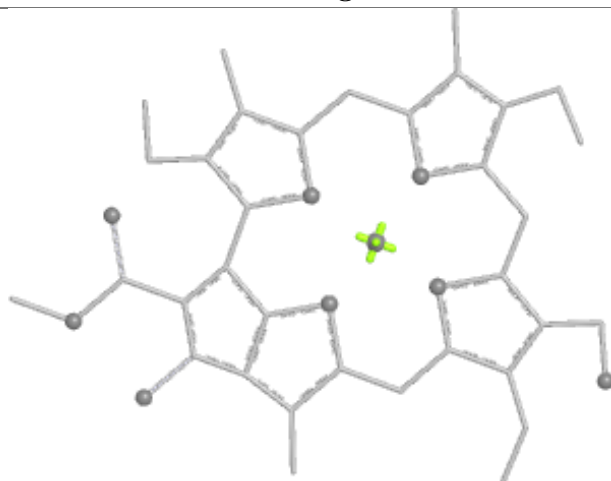
Bond lengths



Bond angles

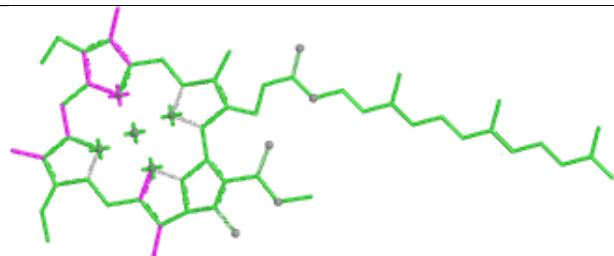


Torsions

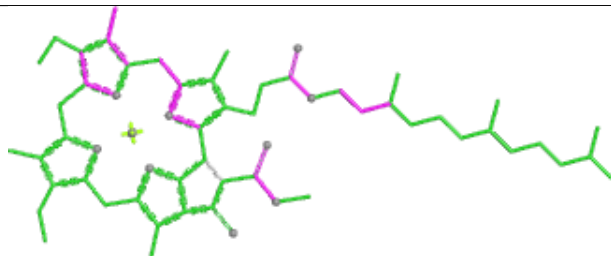


Rings

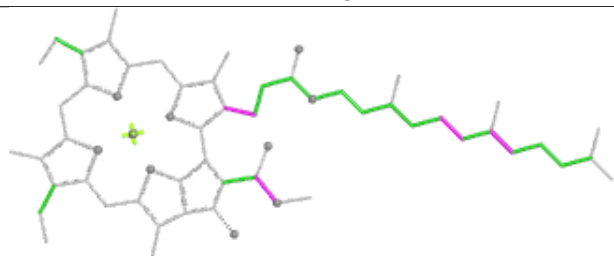
## Ligand CLA 8 309



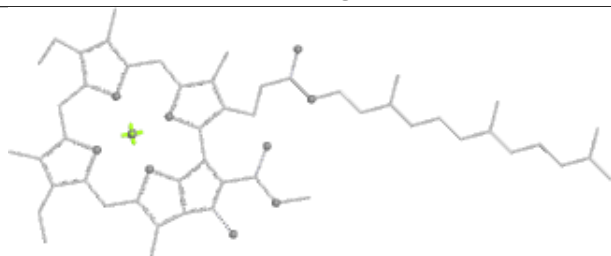
Bond lengths



Bond angles



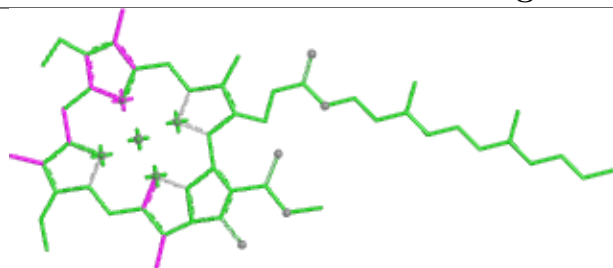
Torsions



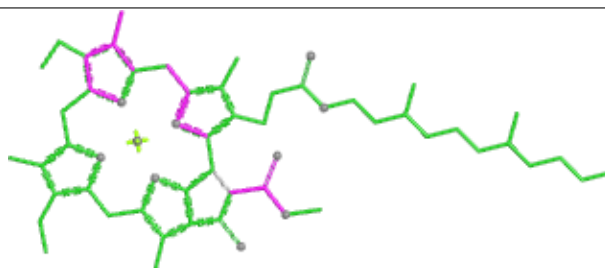
Rings



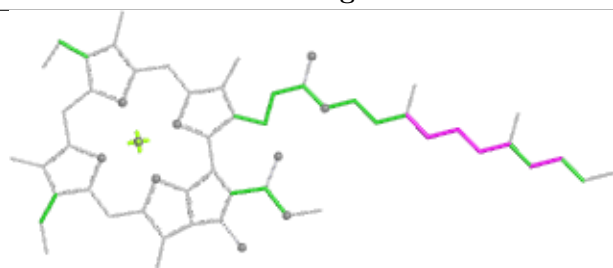
## Ligand CLA L 201



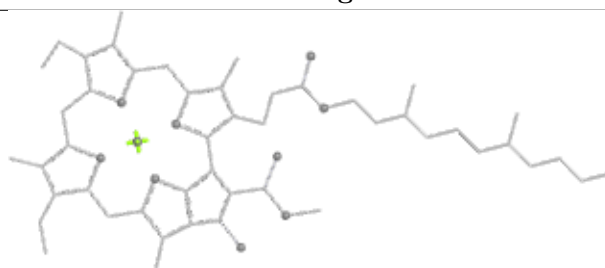
Bond lengths



Bond angles

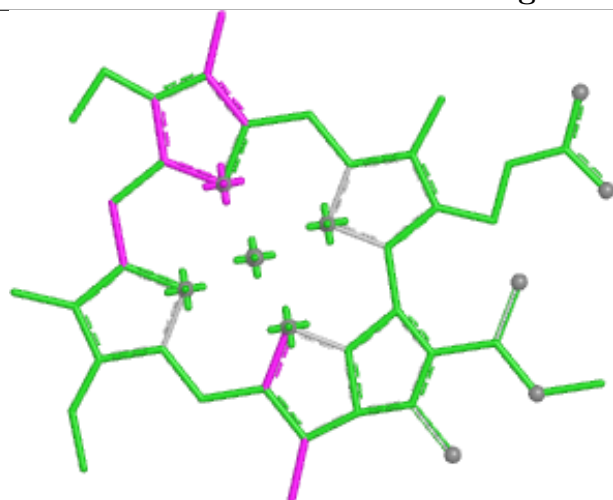


Torsions

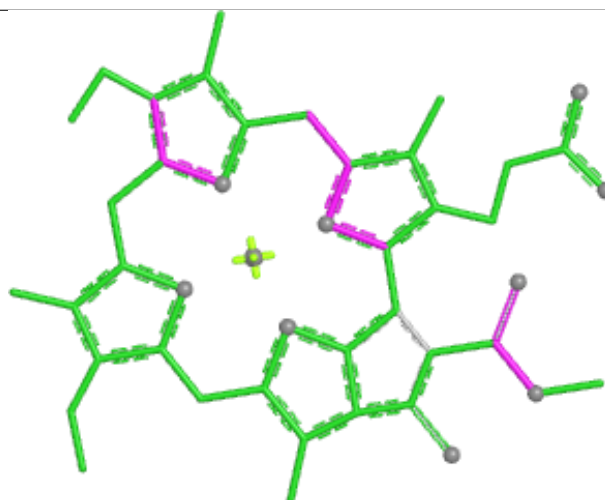


Rings

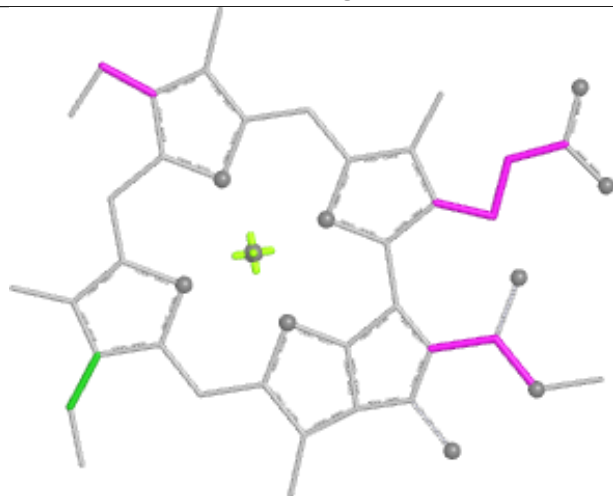
## Ligand CLA 0 321



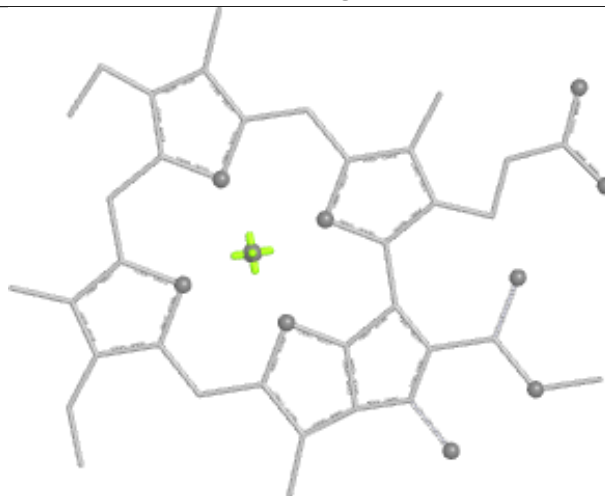
Bond lengths



Bond angles



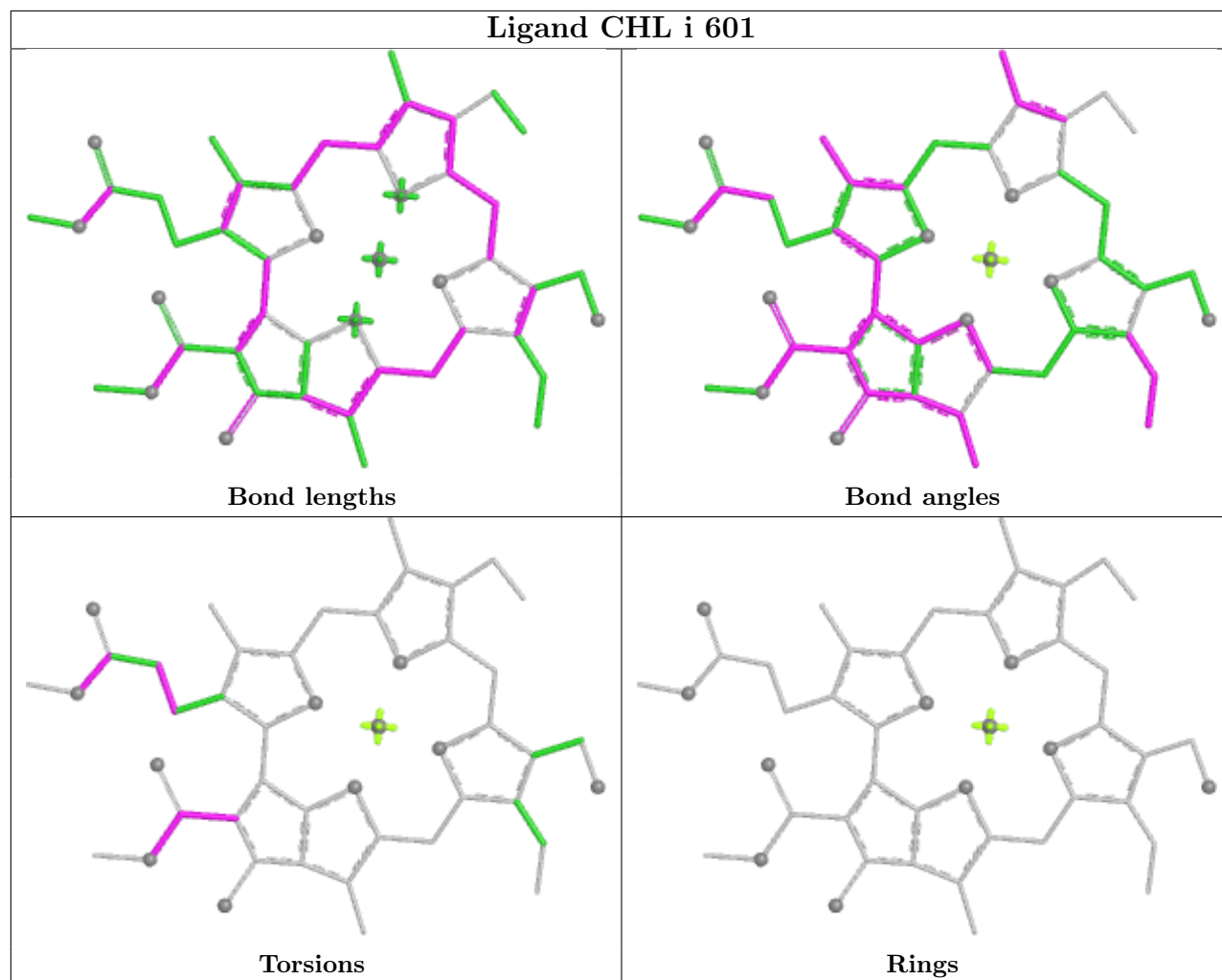
Torsions



Rings

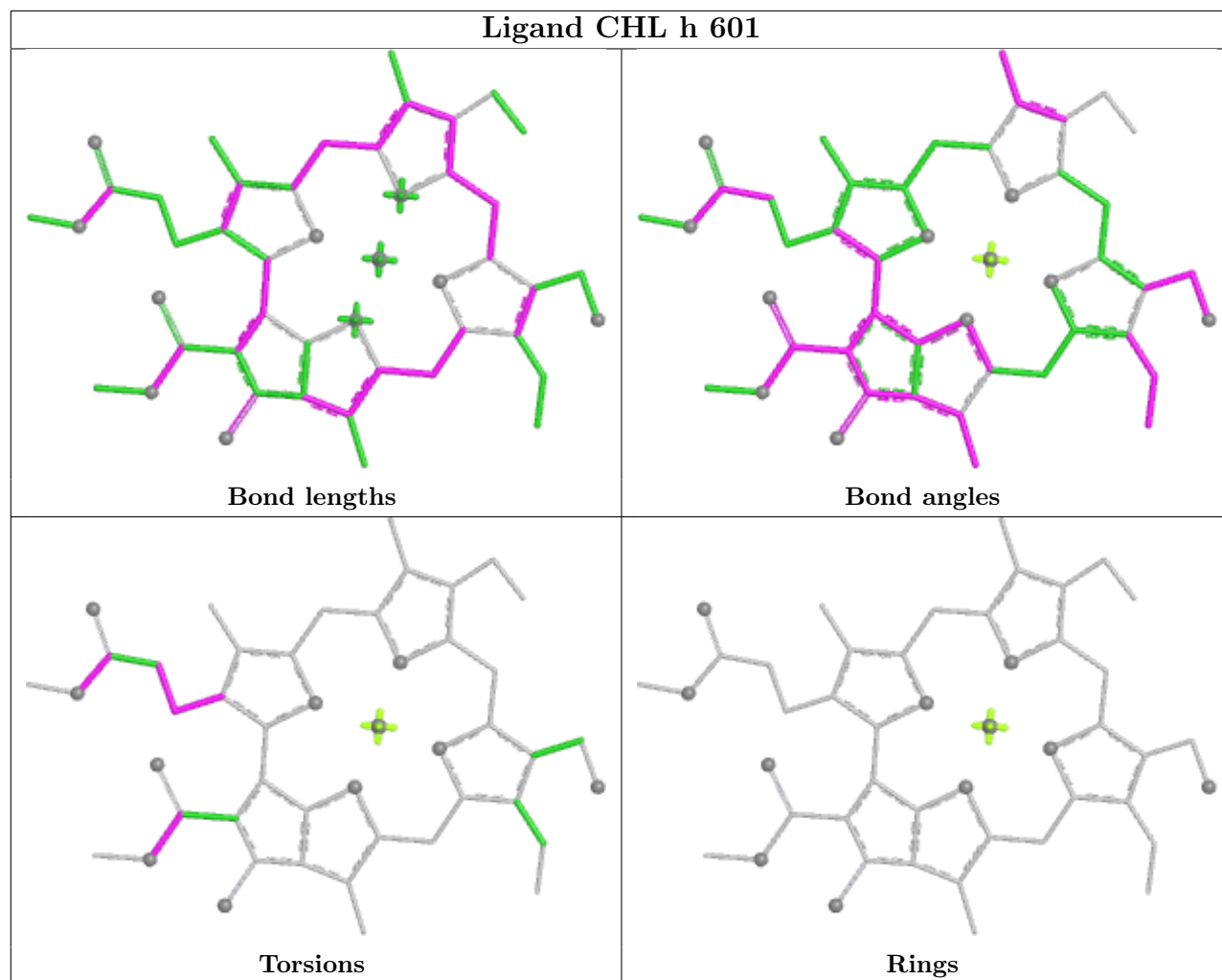


## Ligand CHL i 601



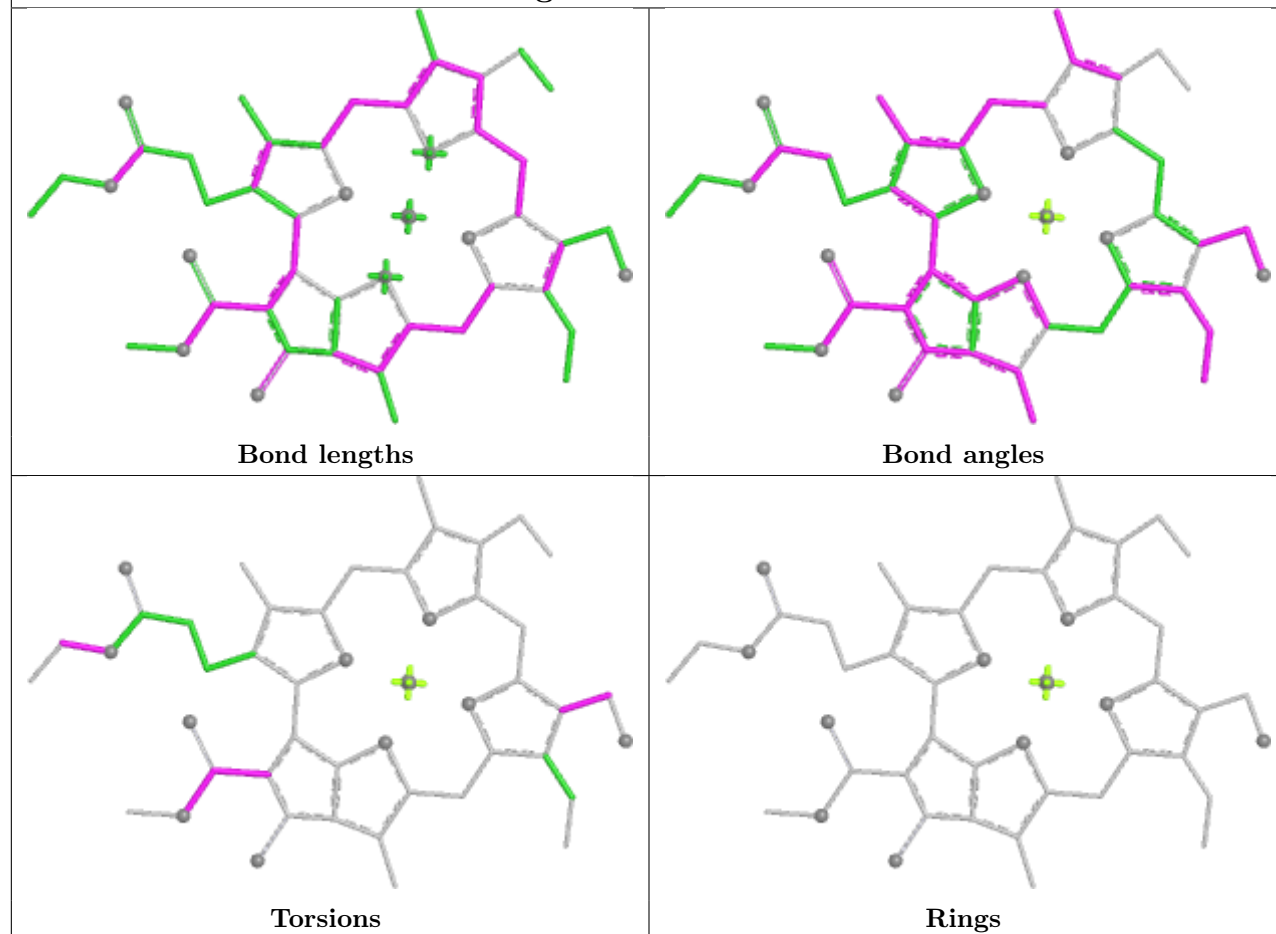


## Ligand CHL h 601

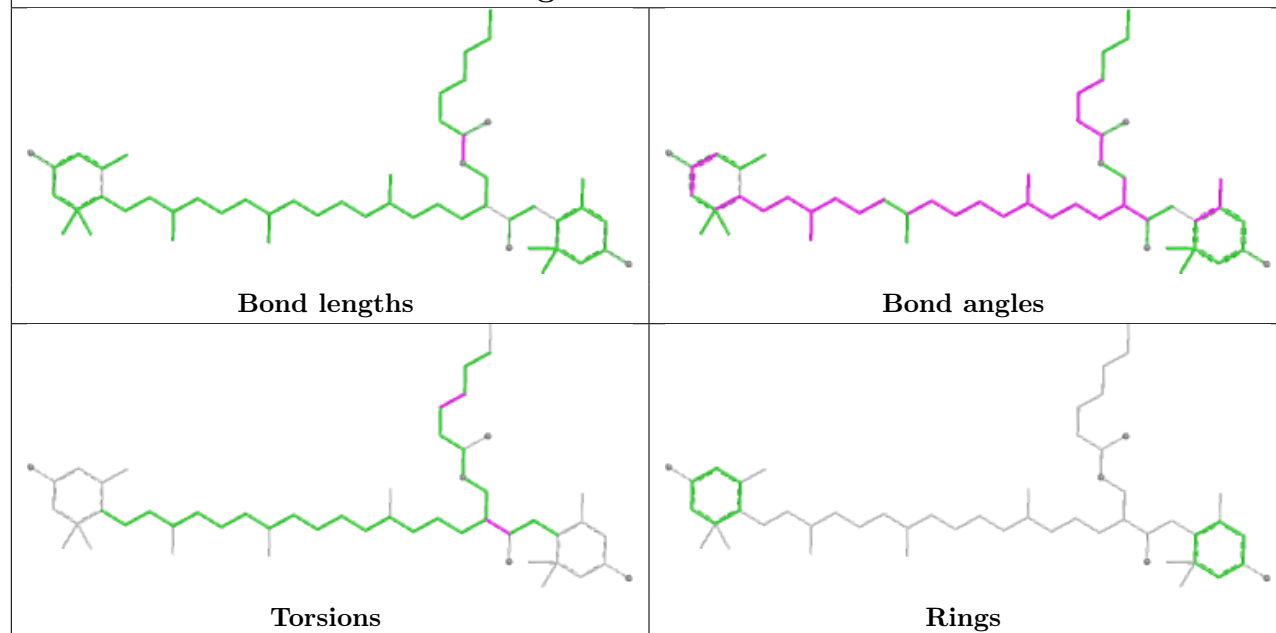




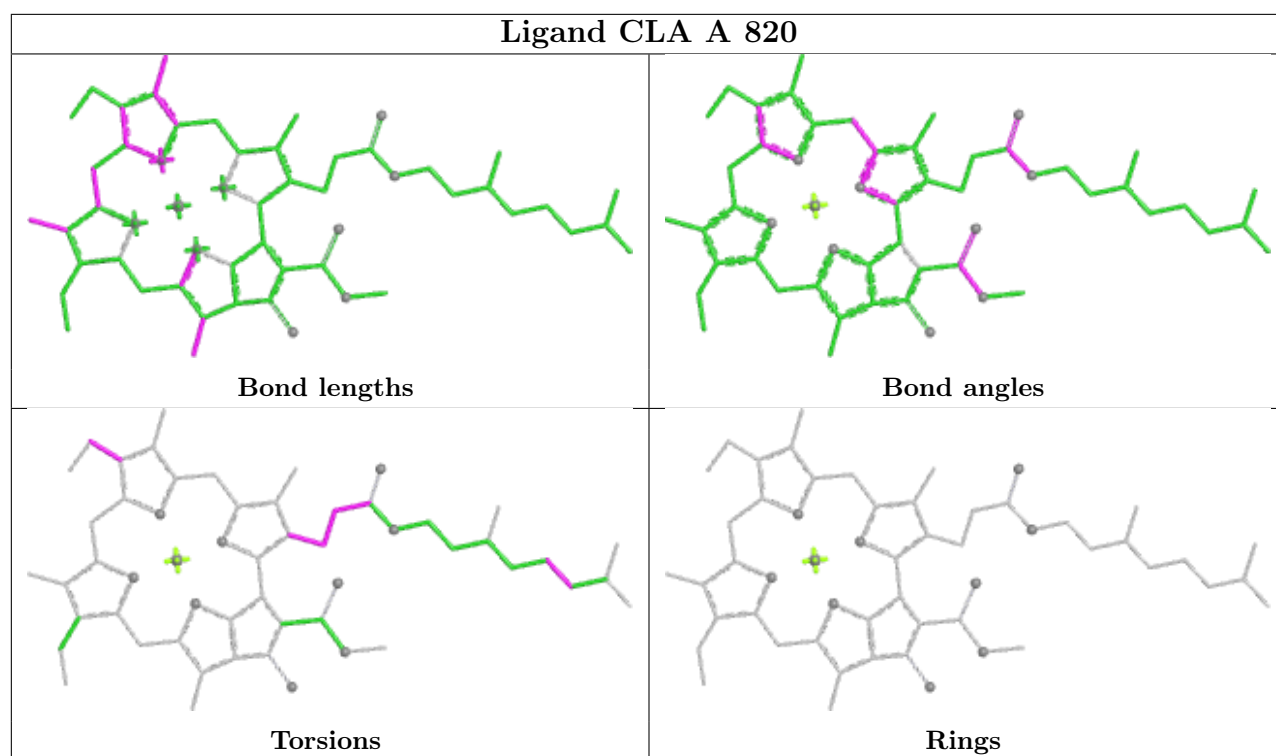
## Ligand CHL 1 306



## Ligand OUR 1 501

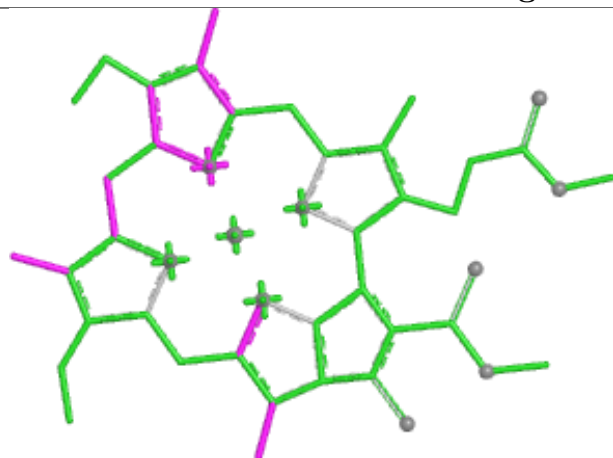




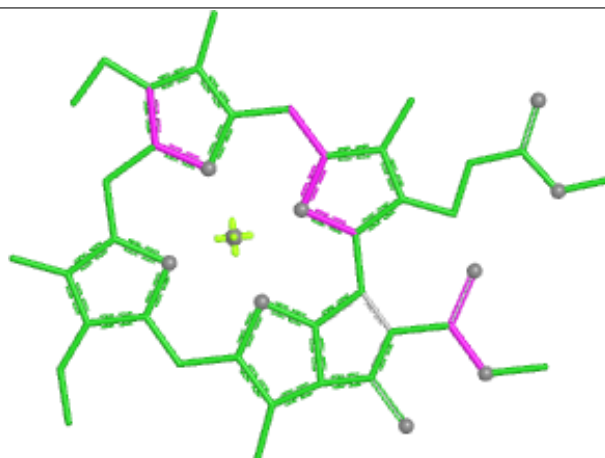




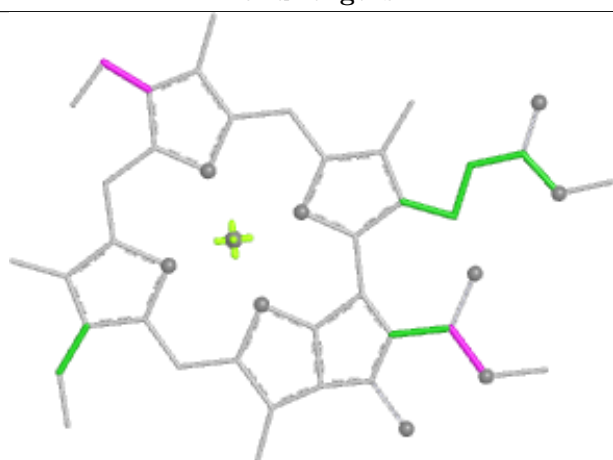
## Ligand CLA 1 314



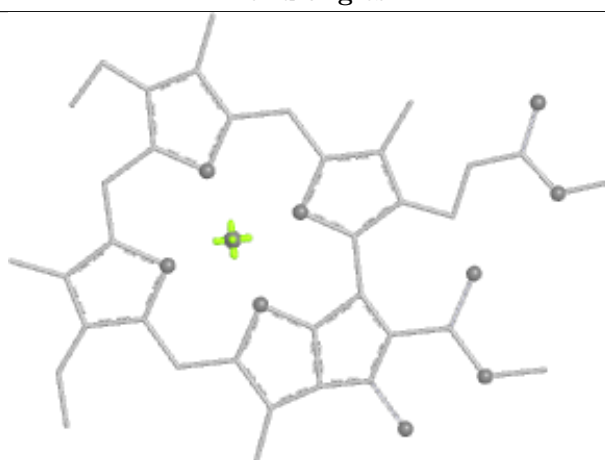
Bond lengths



Bond angles



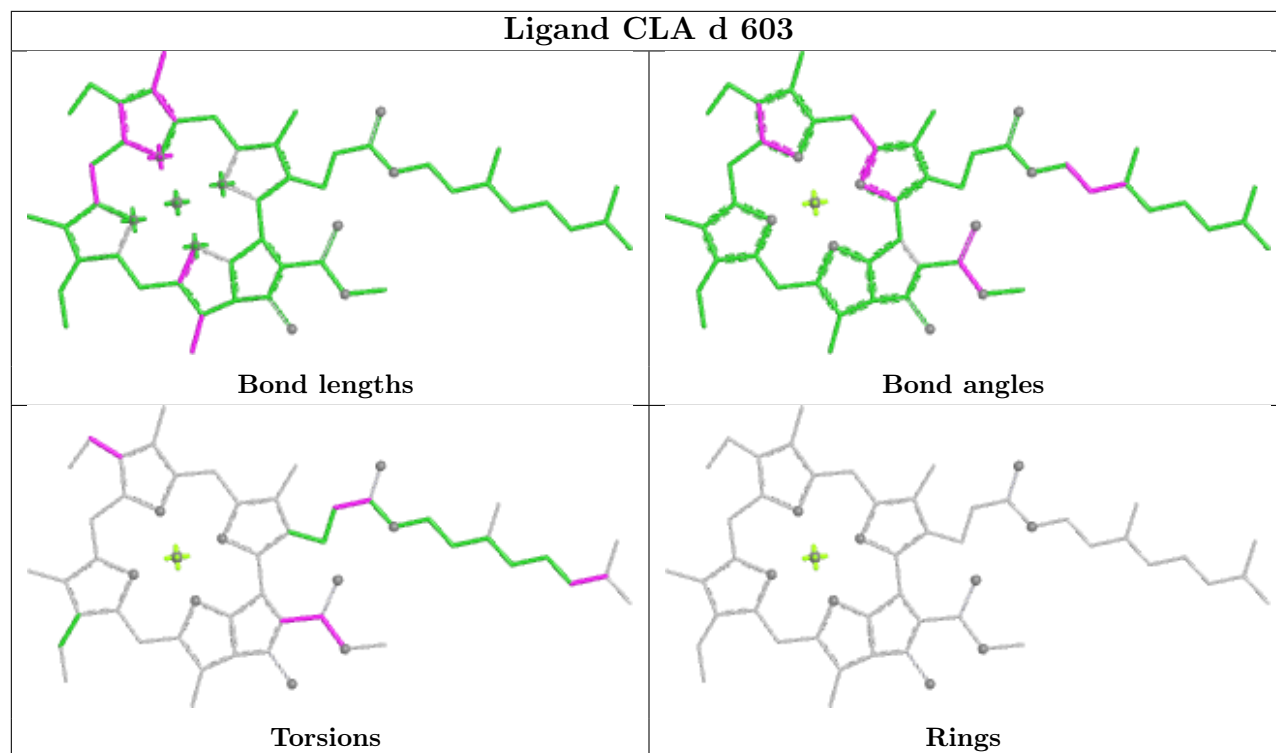
Torsions



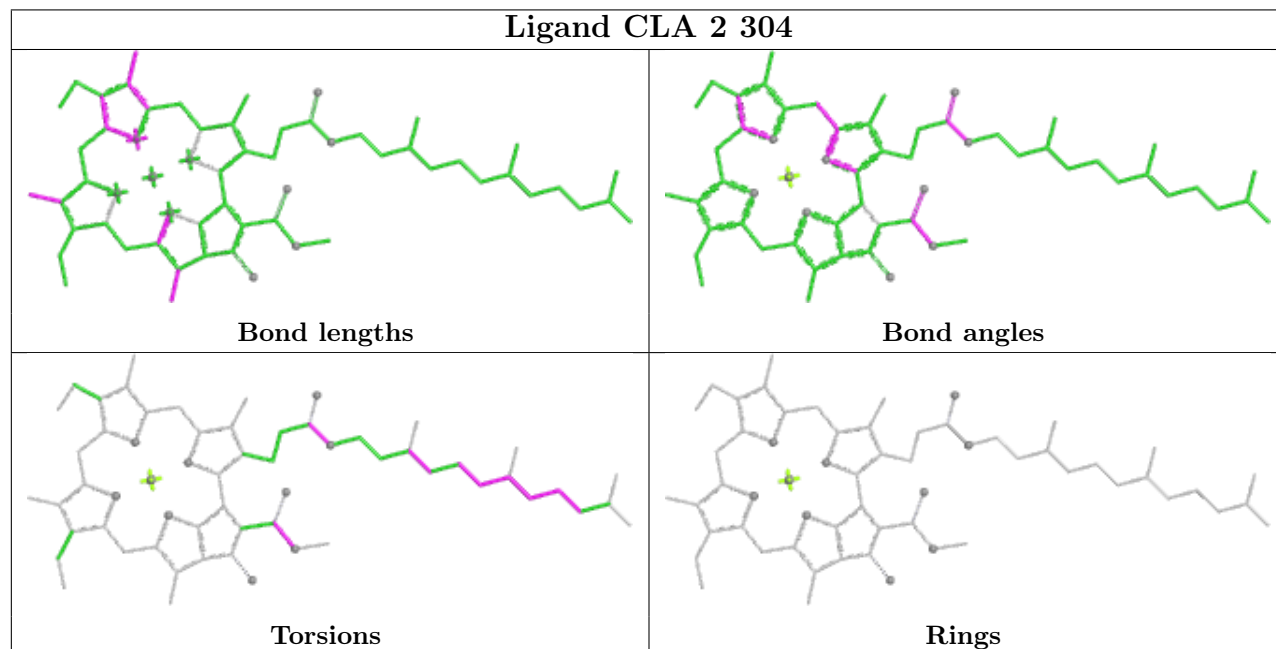
Rings



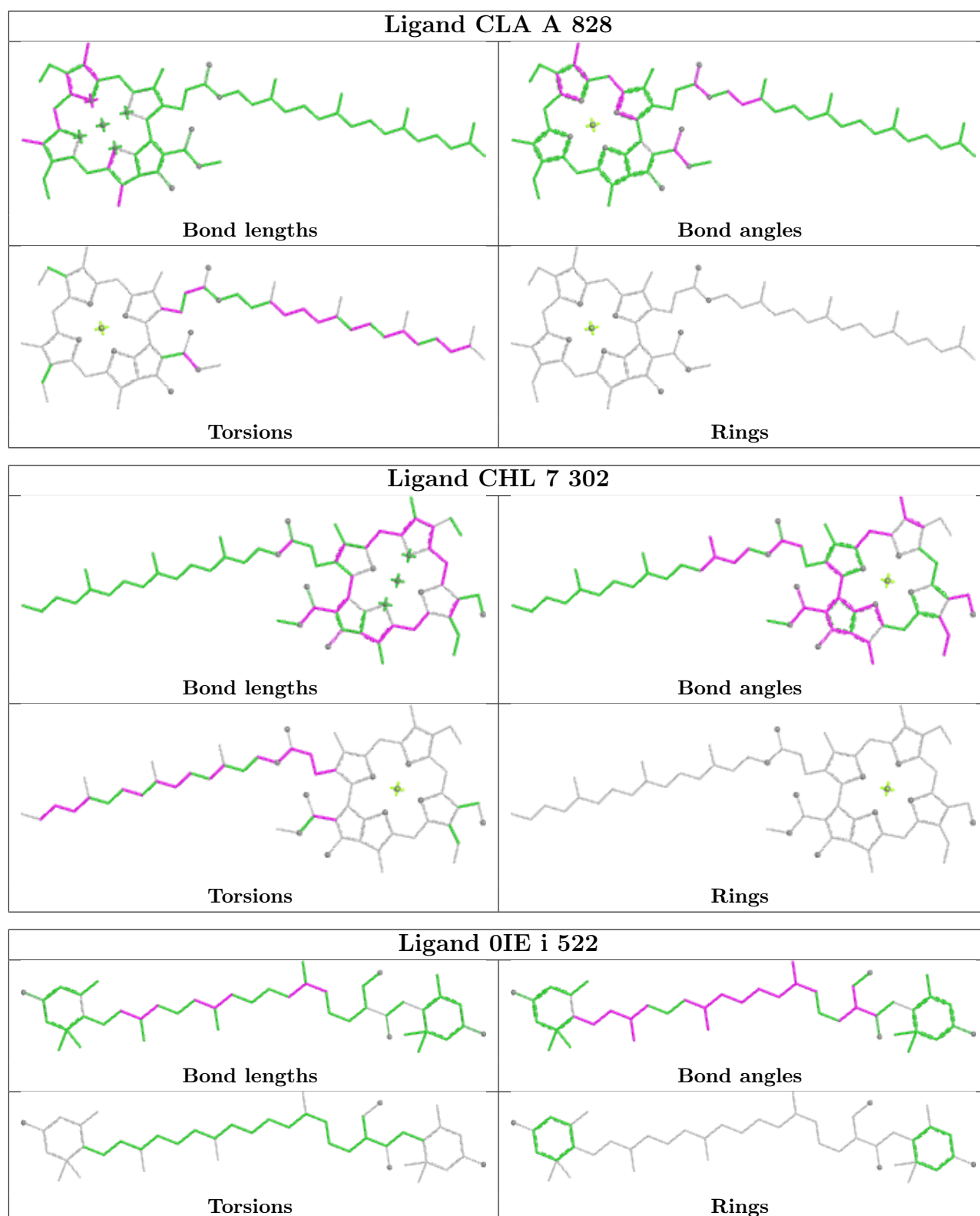
## Ligand CLA d 603



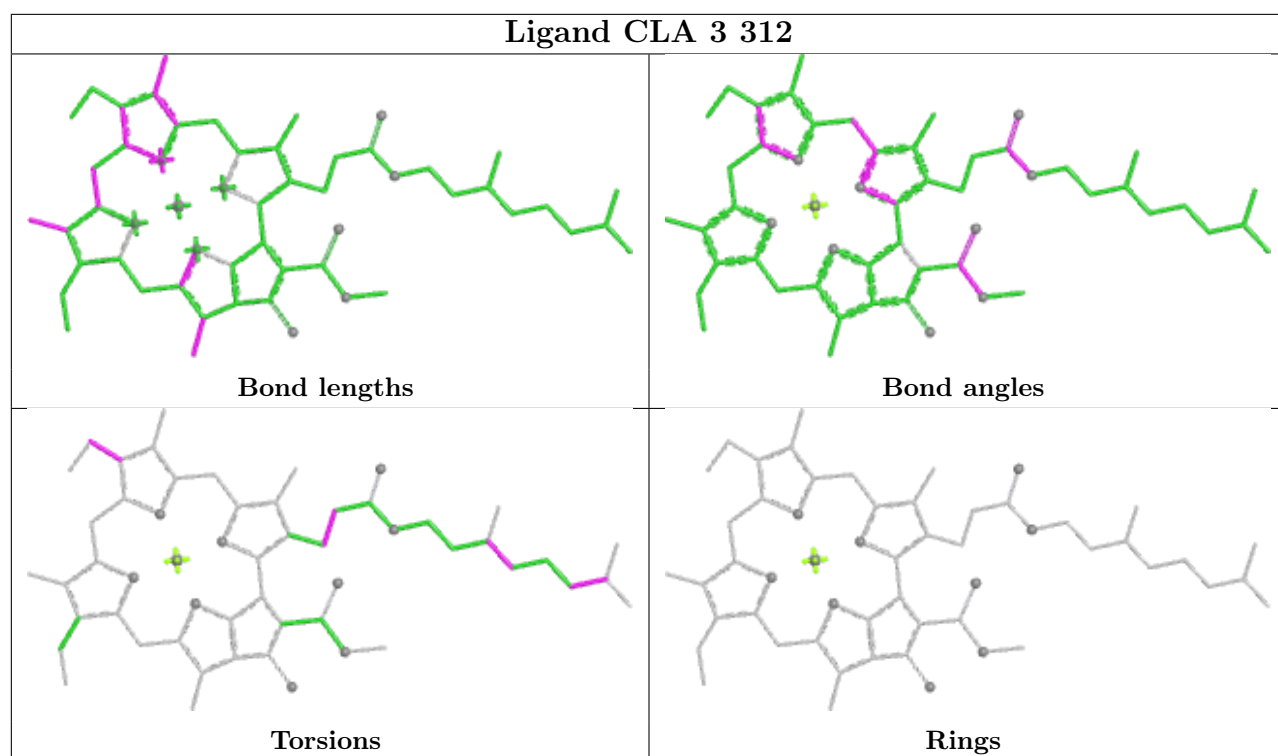
## Ligand CLA 2 304





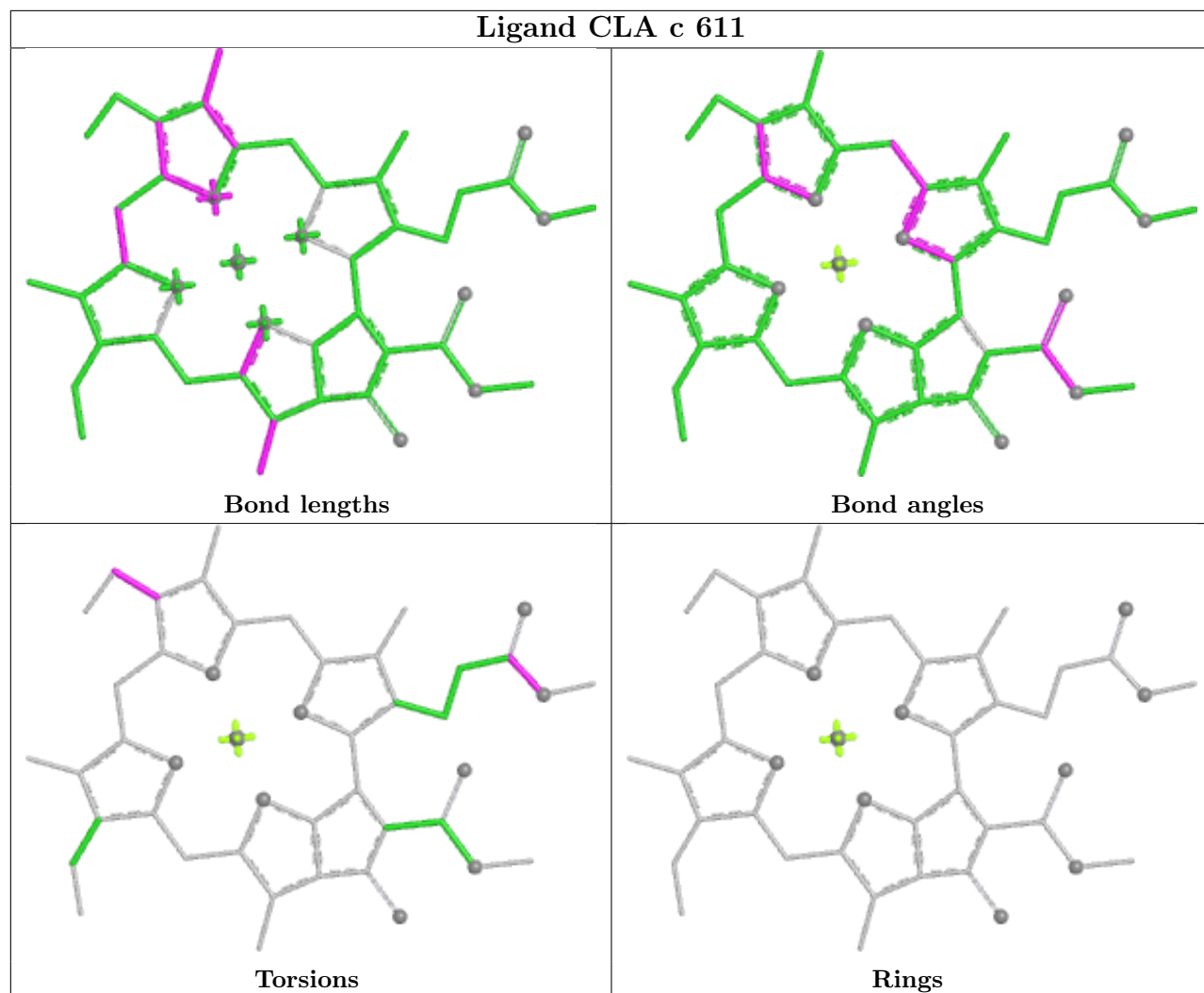






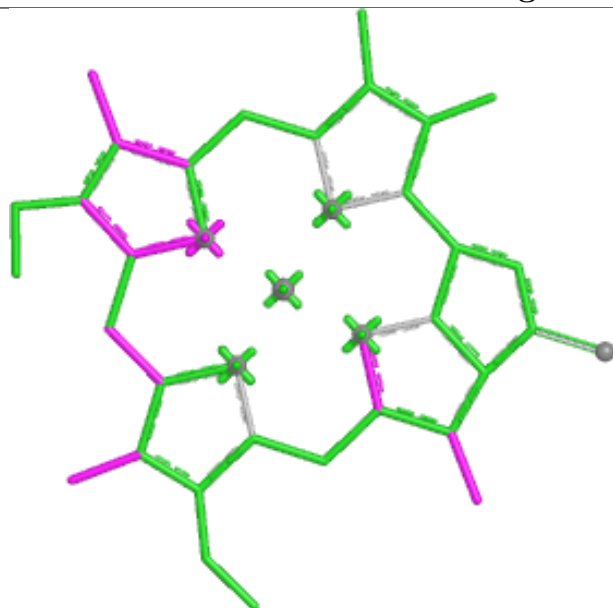


## Ligand CLA c 611

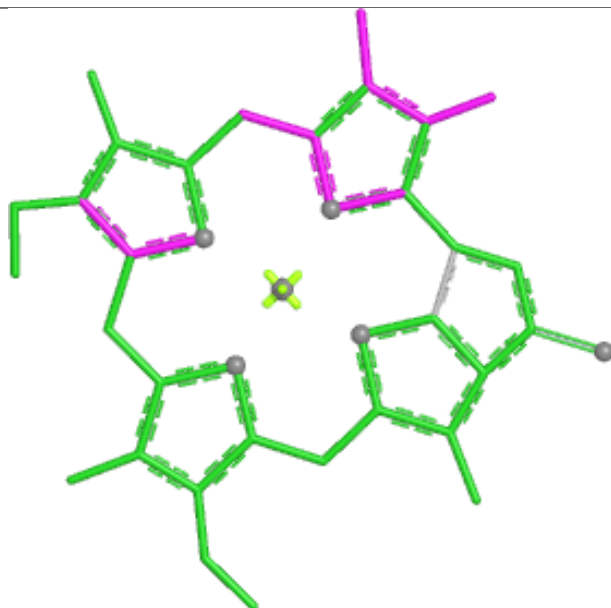




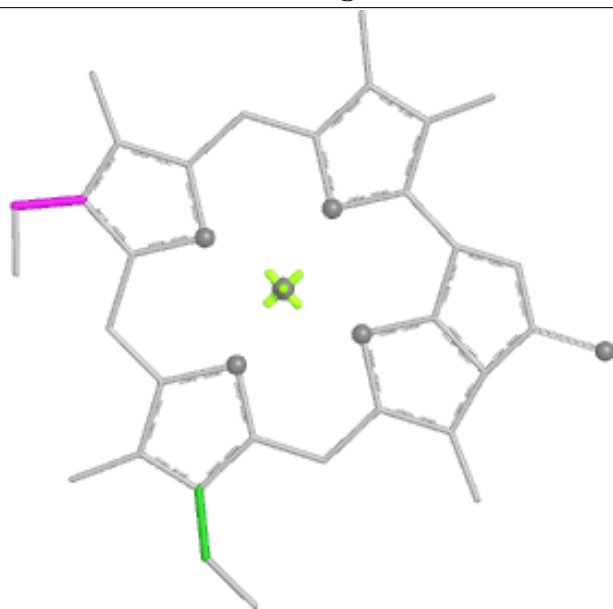
## Ligand CLA 7 310



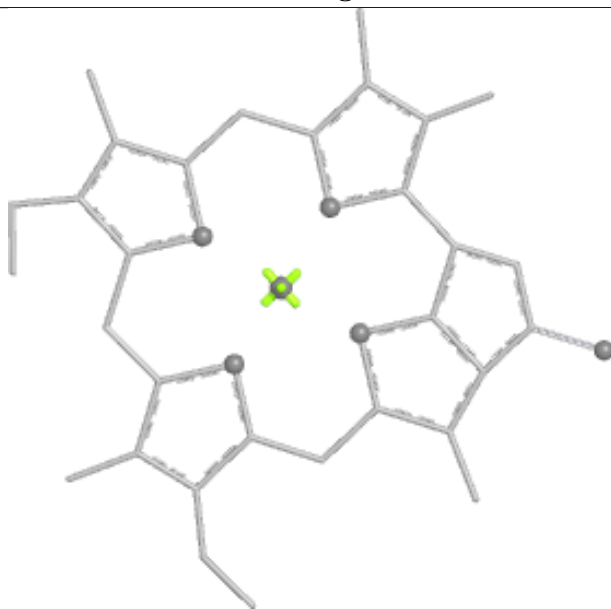
Bond lengths



Bond angles



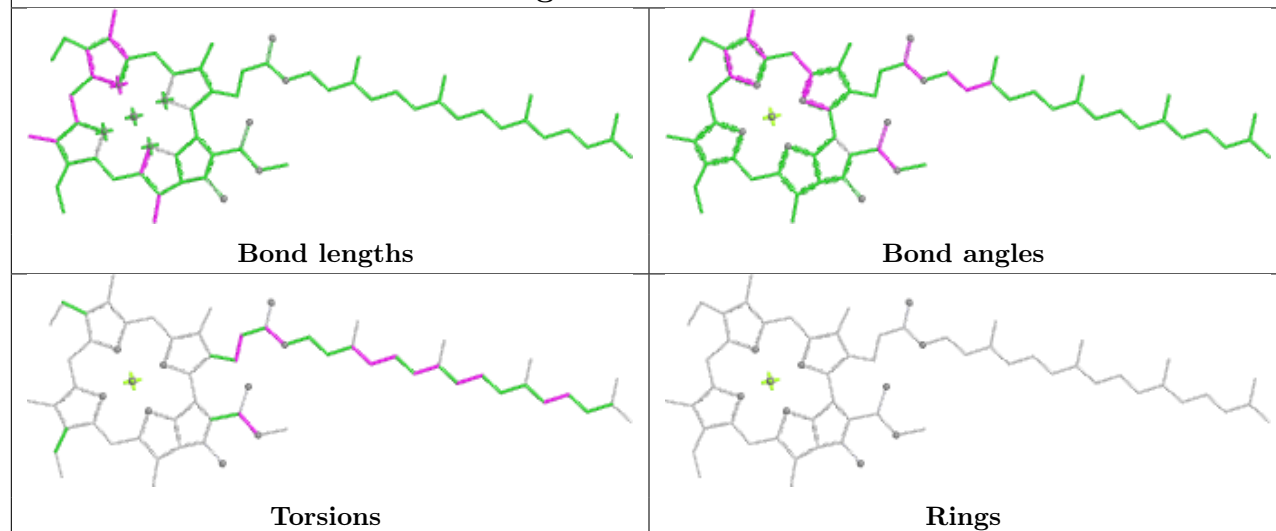
Torsions



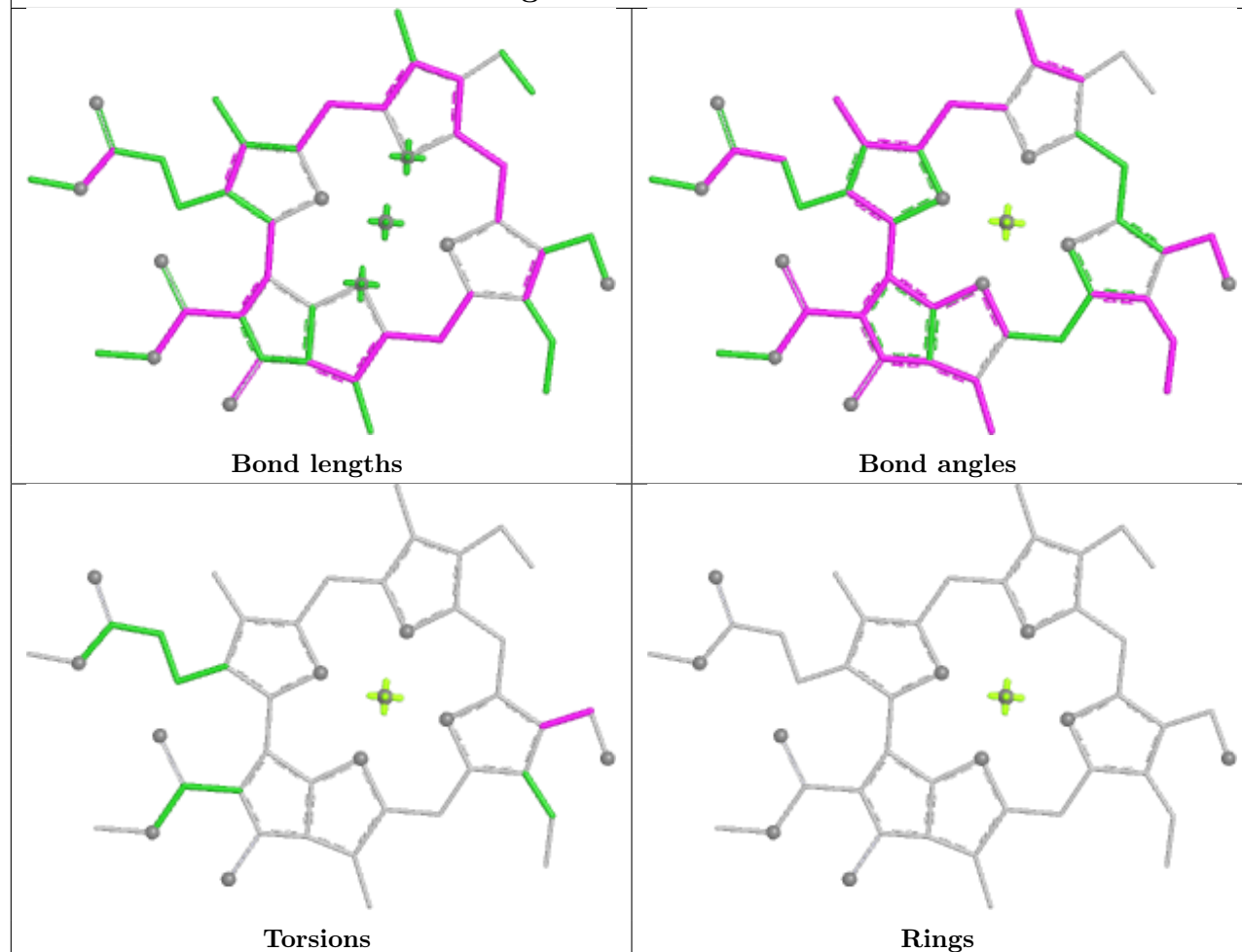
Rings



## Ligand CLA 1 312

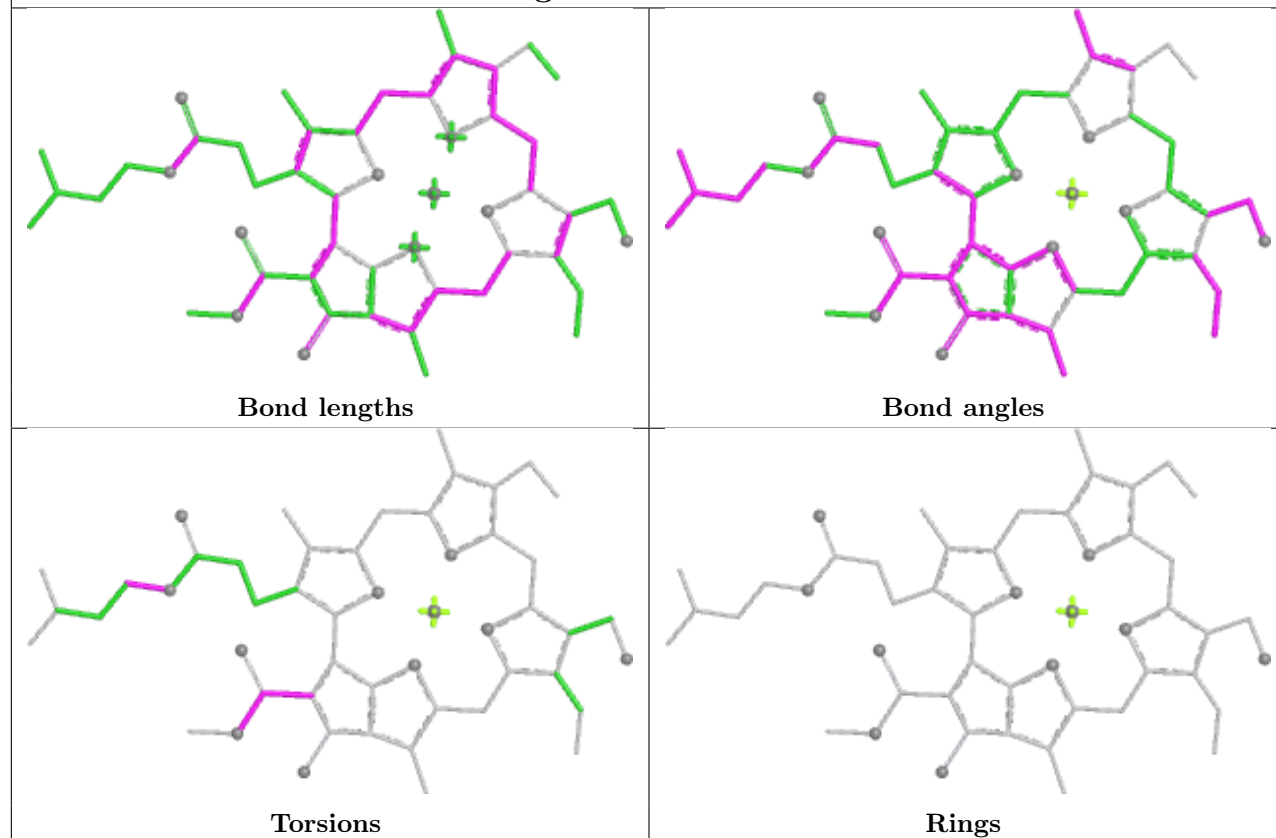


## Ligand CHL 8 308

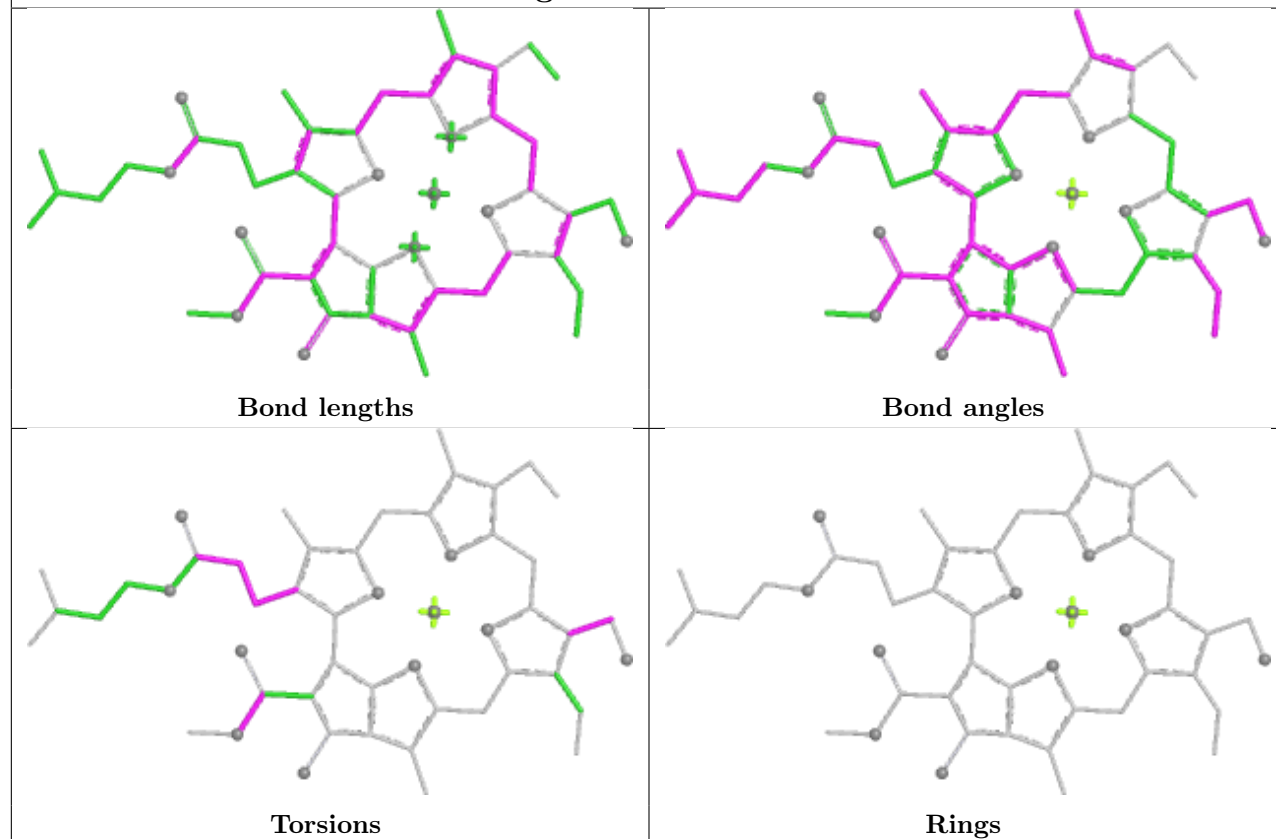




## Ligand CHL d 601

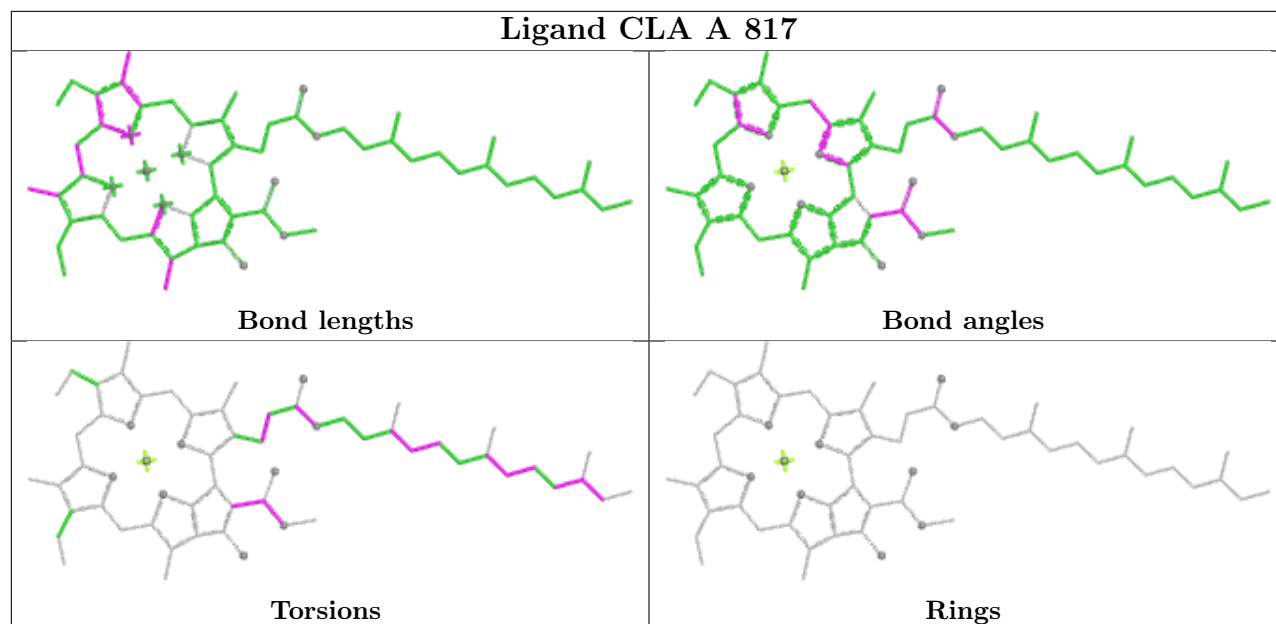


## Ligand CHL 6 307

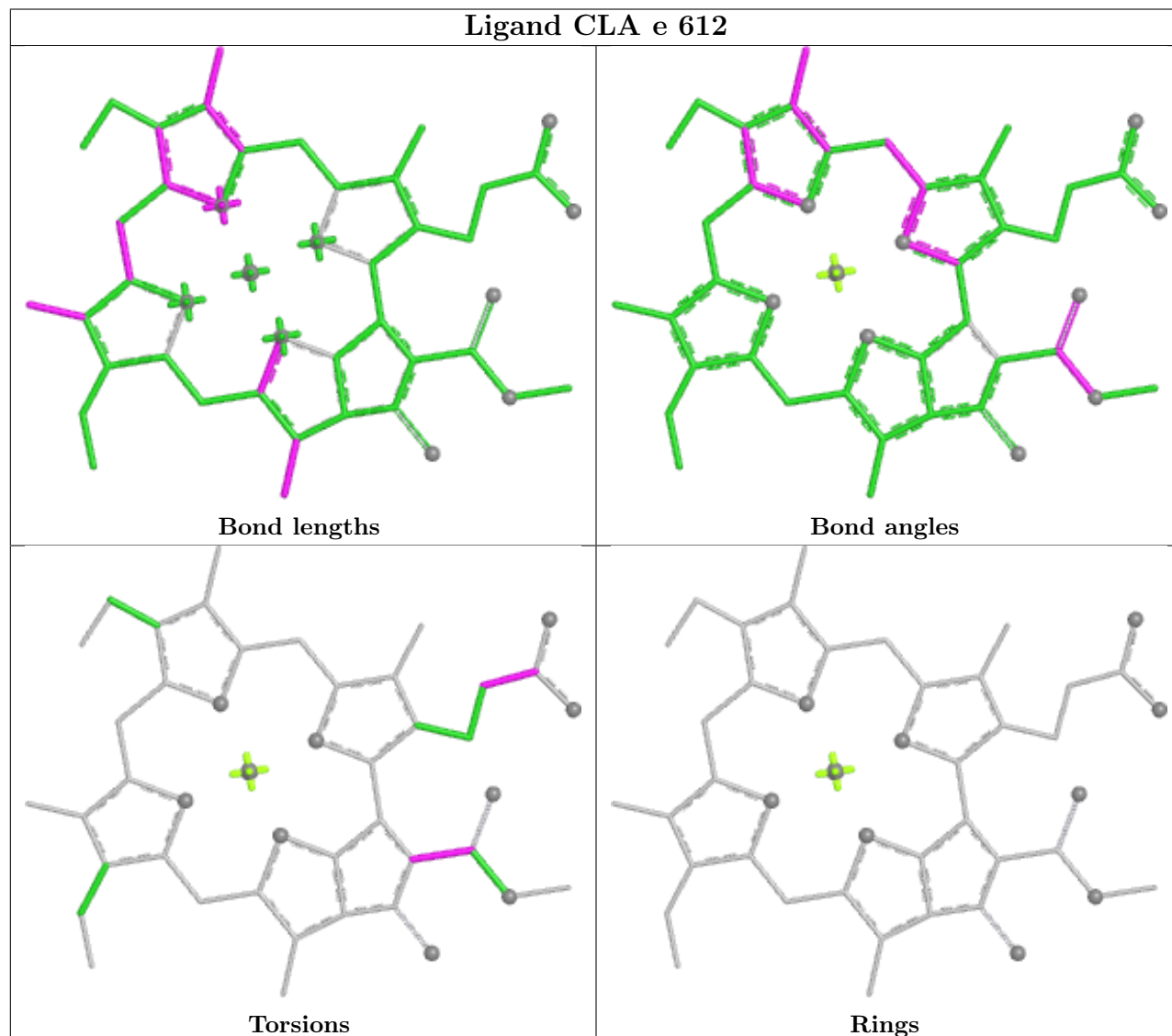




## Ligand CLA A 817

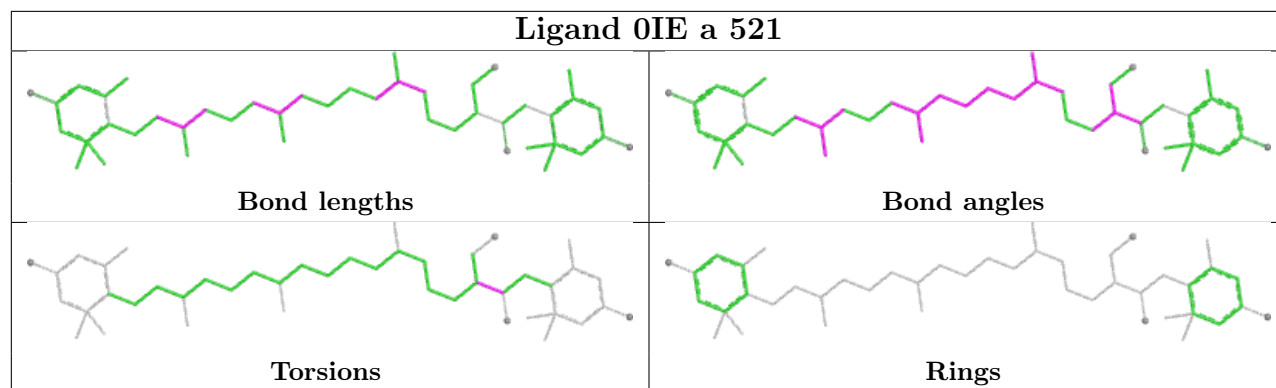


## Ligand CLA e 612

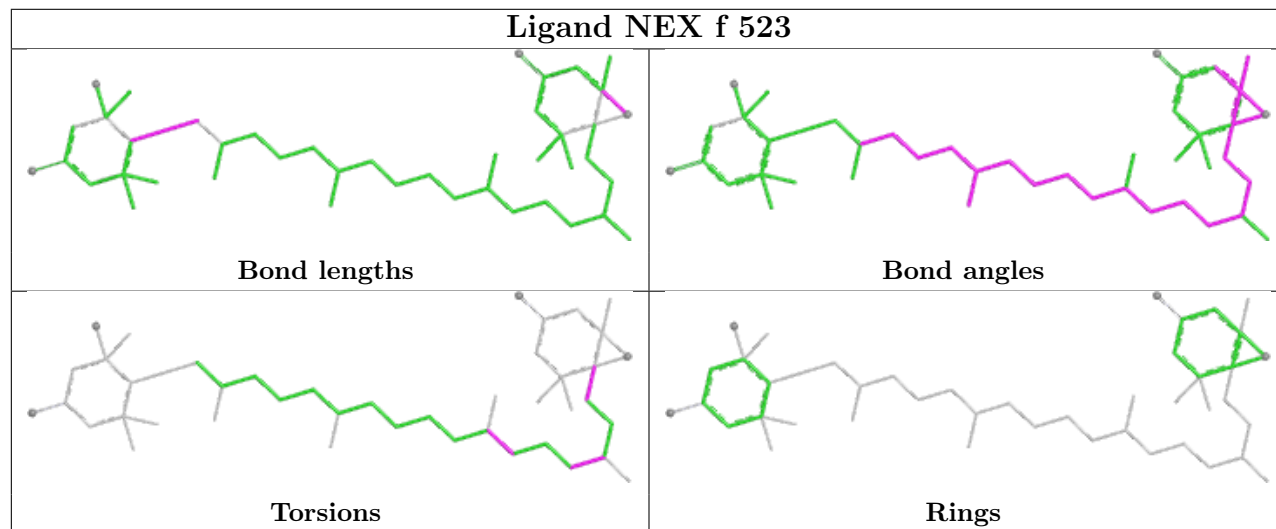




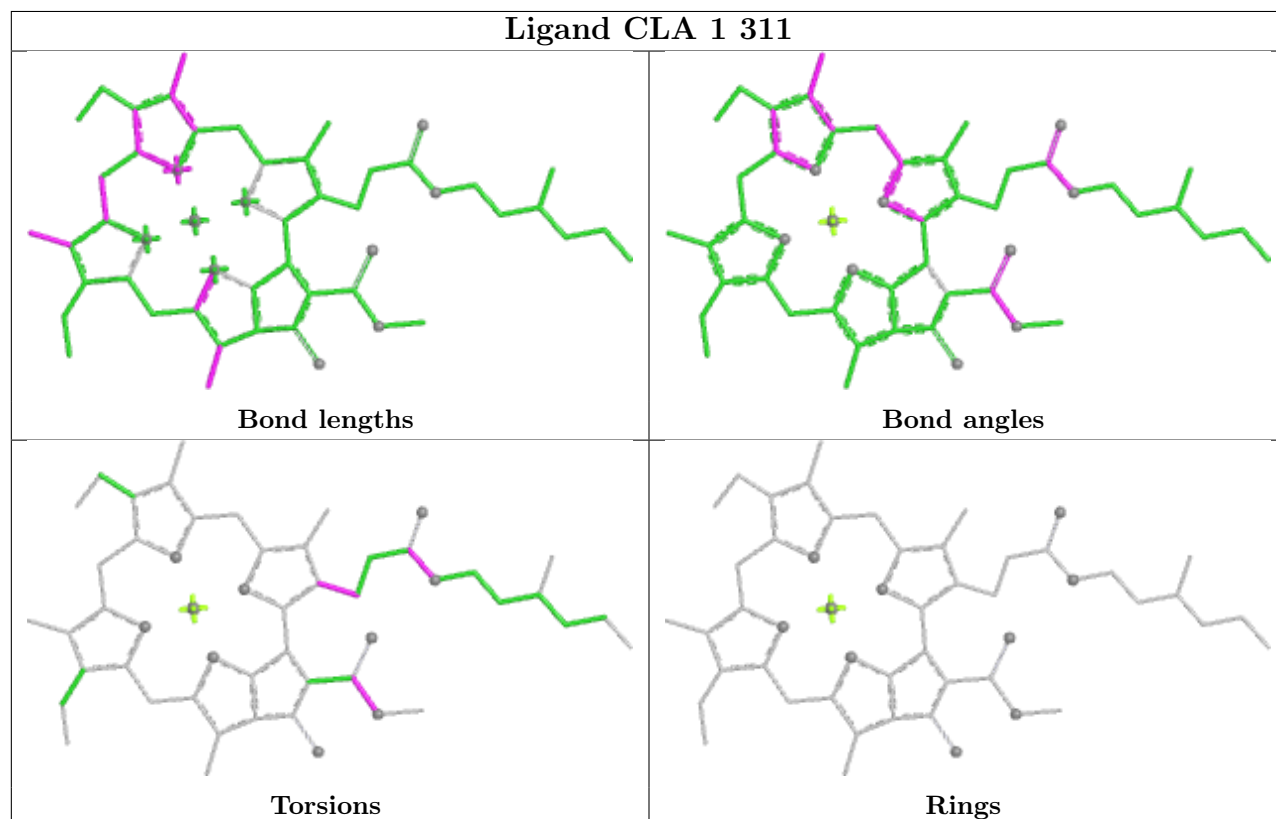
## Ligand OIE a 521



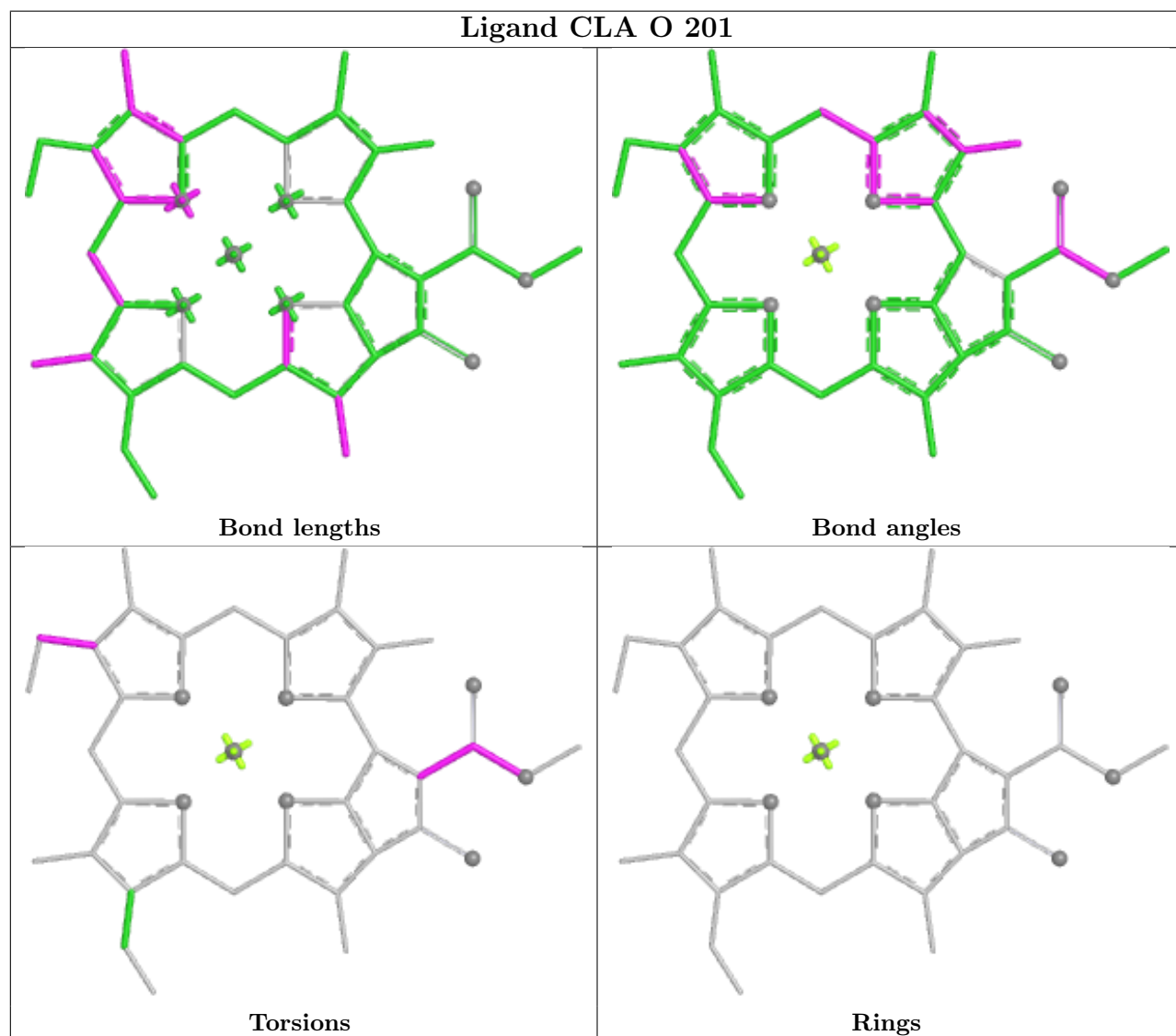
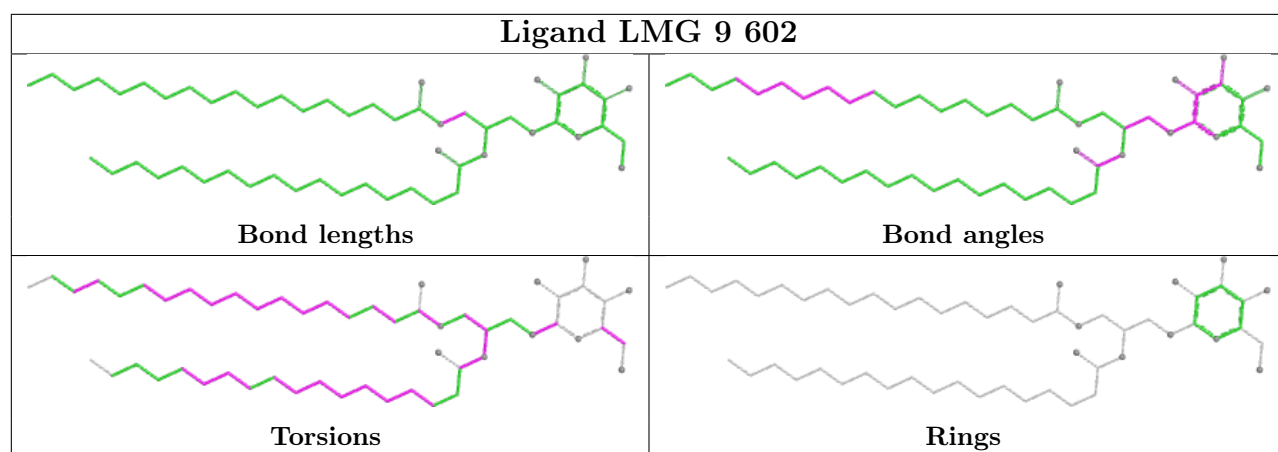
## Ligand NEX f 523



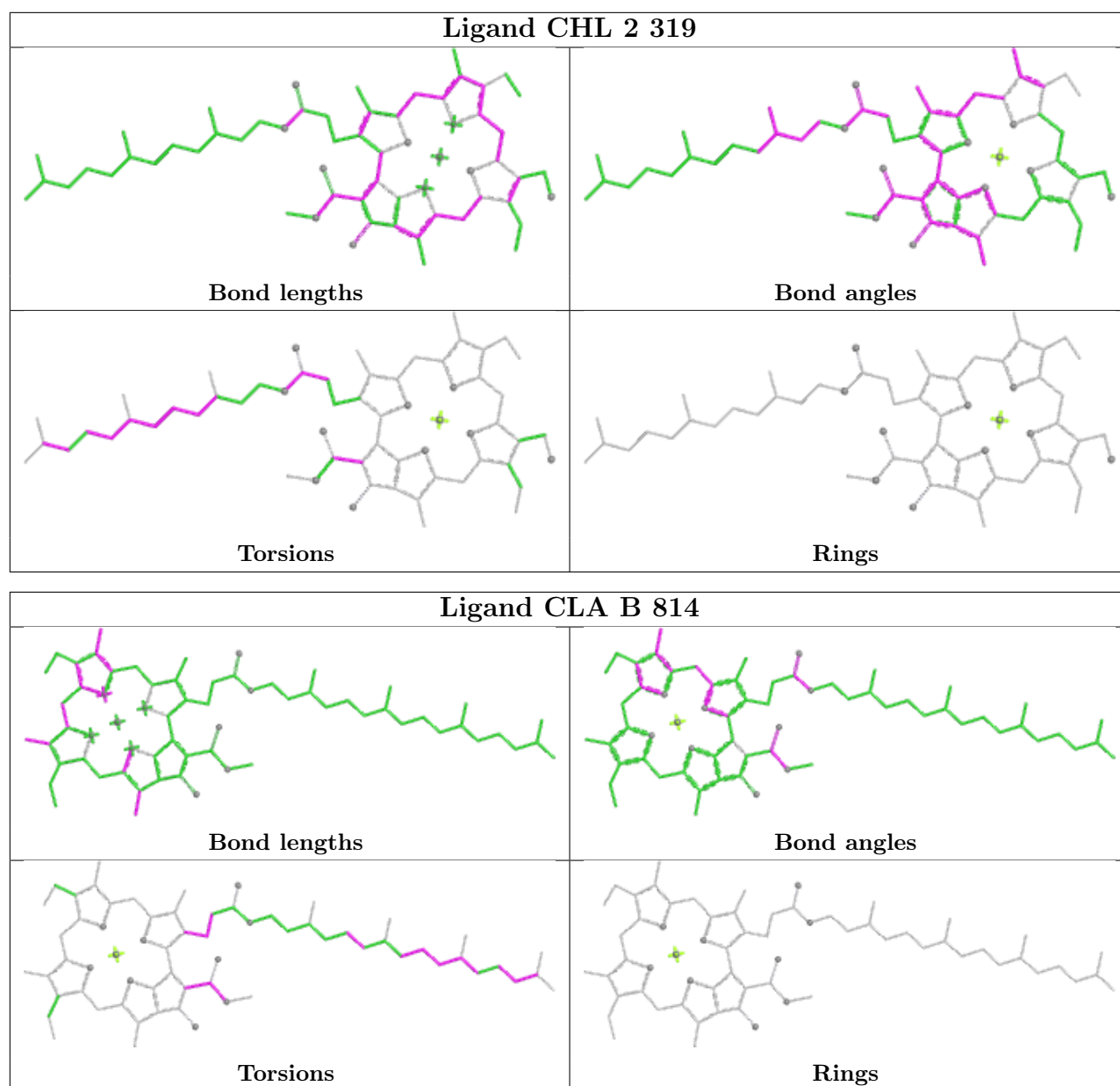
## Ligand CLA 1 311



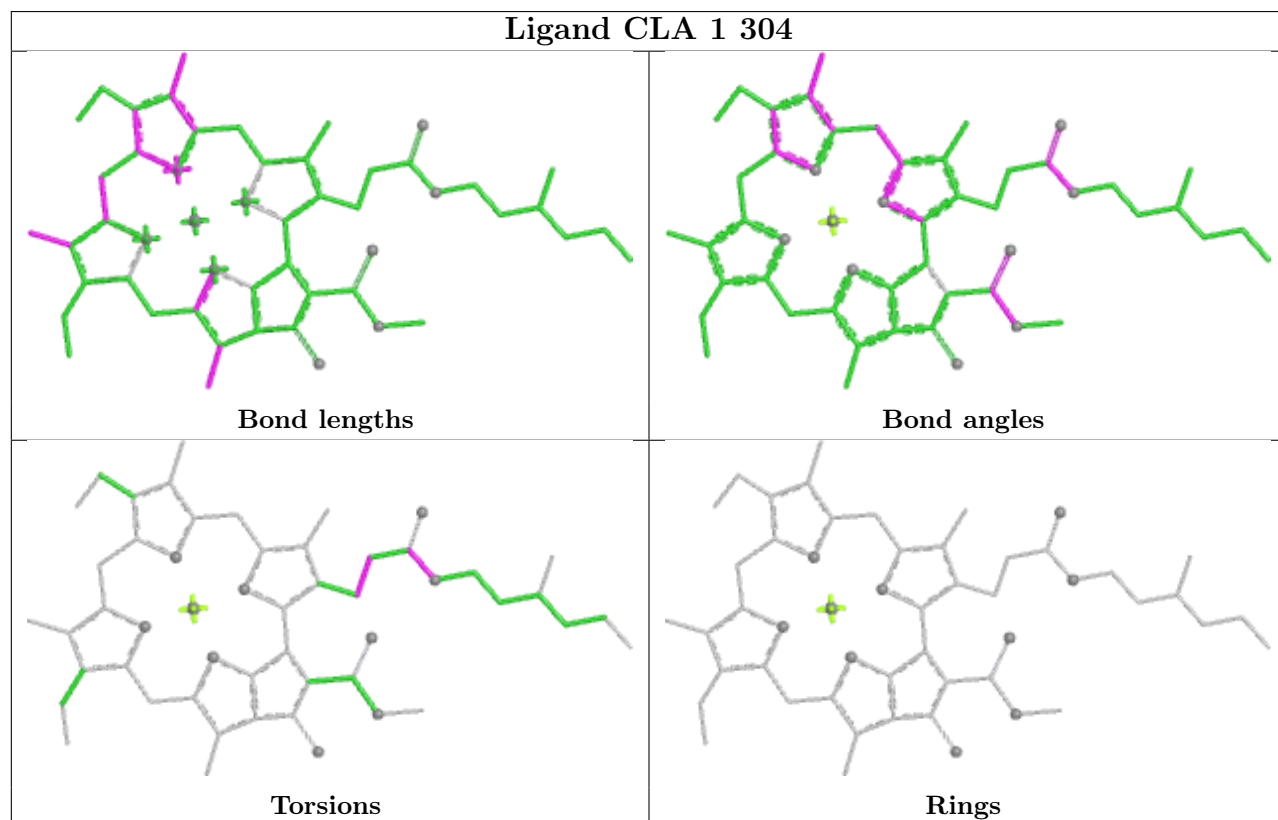
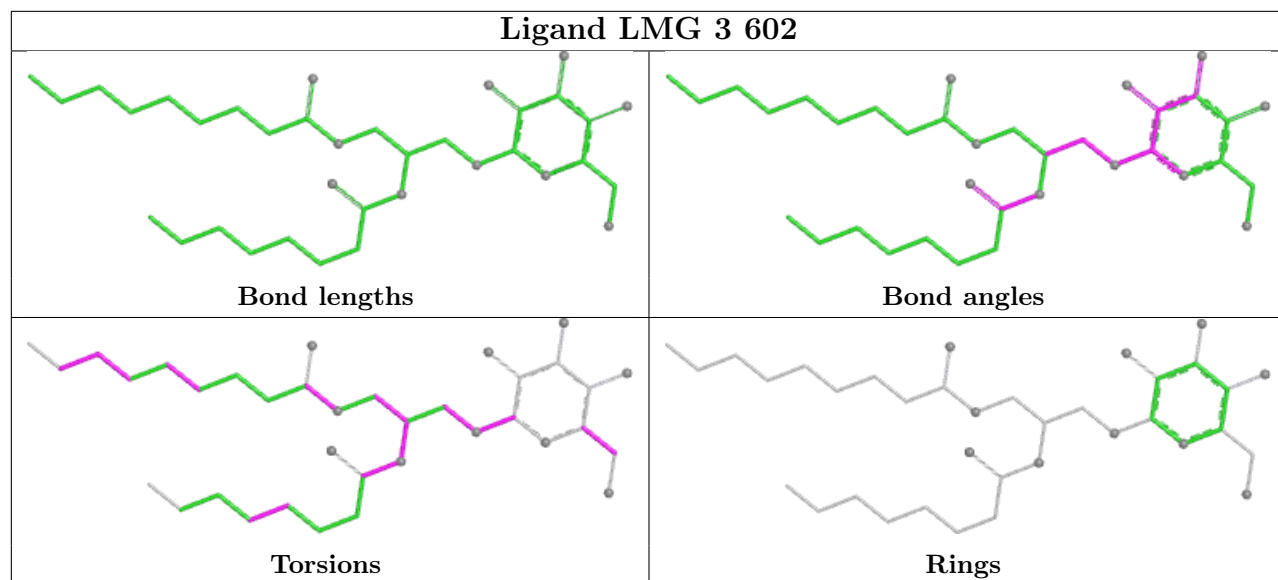




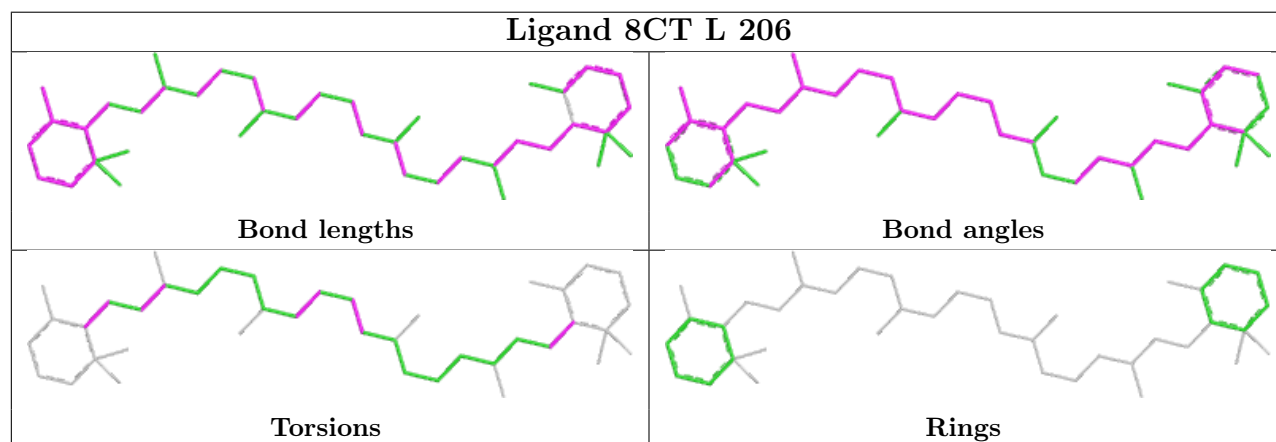
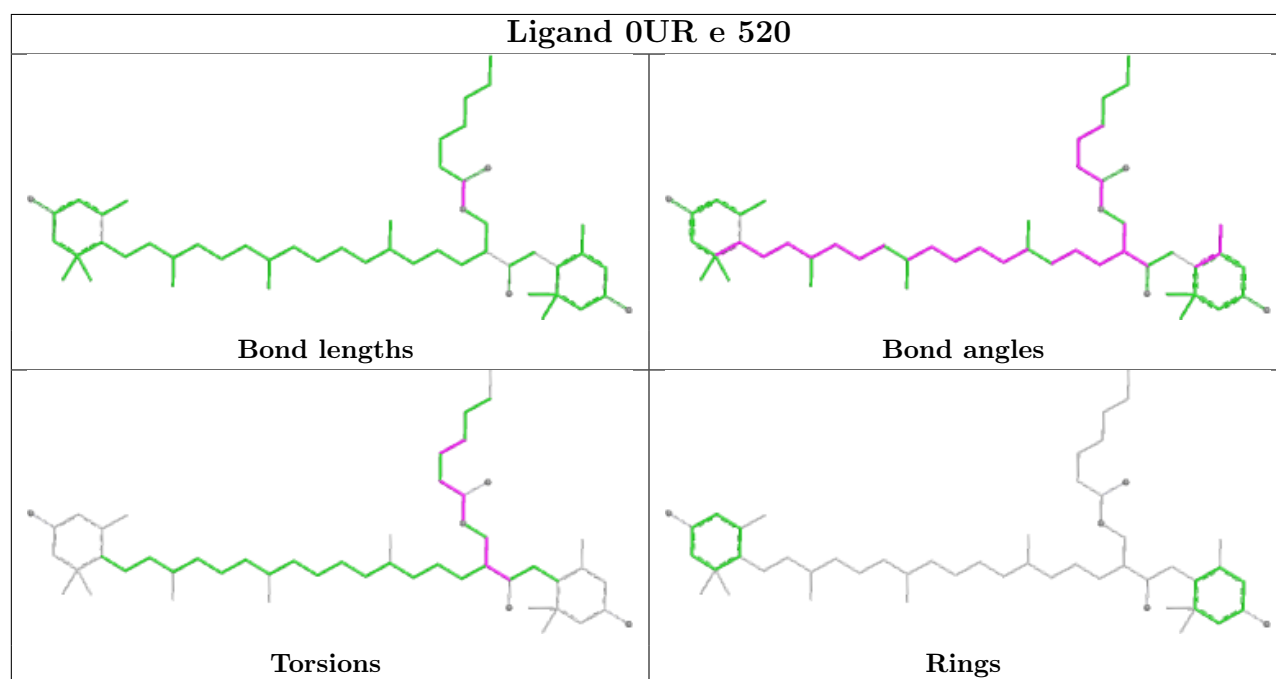
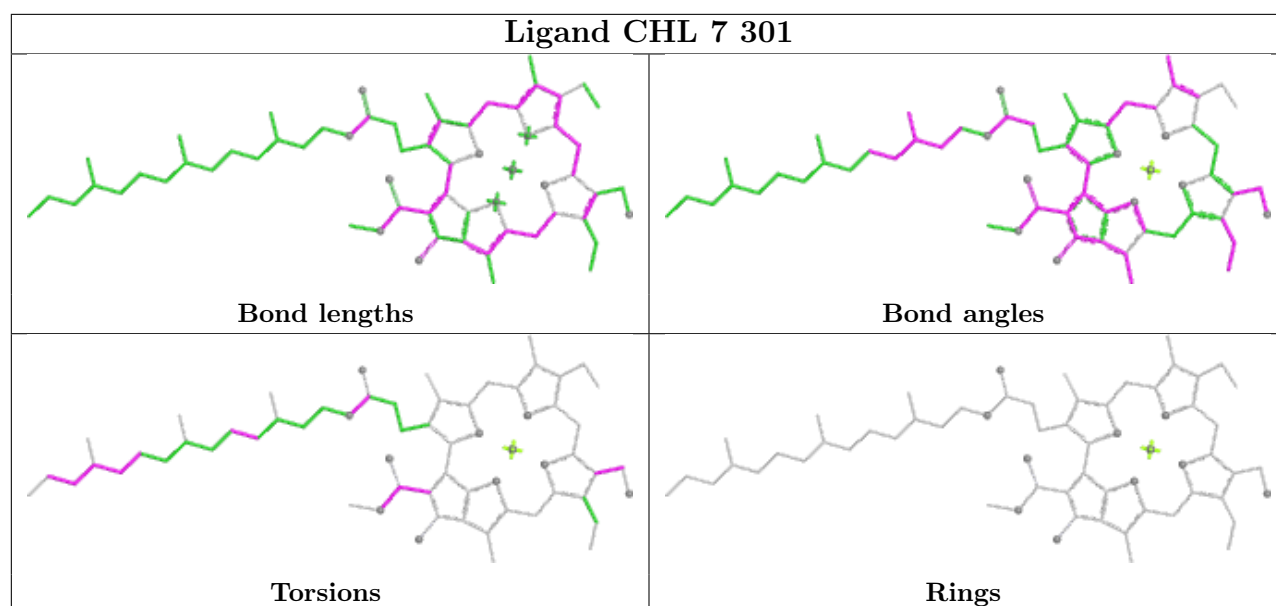






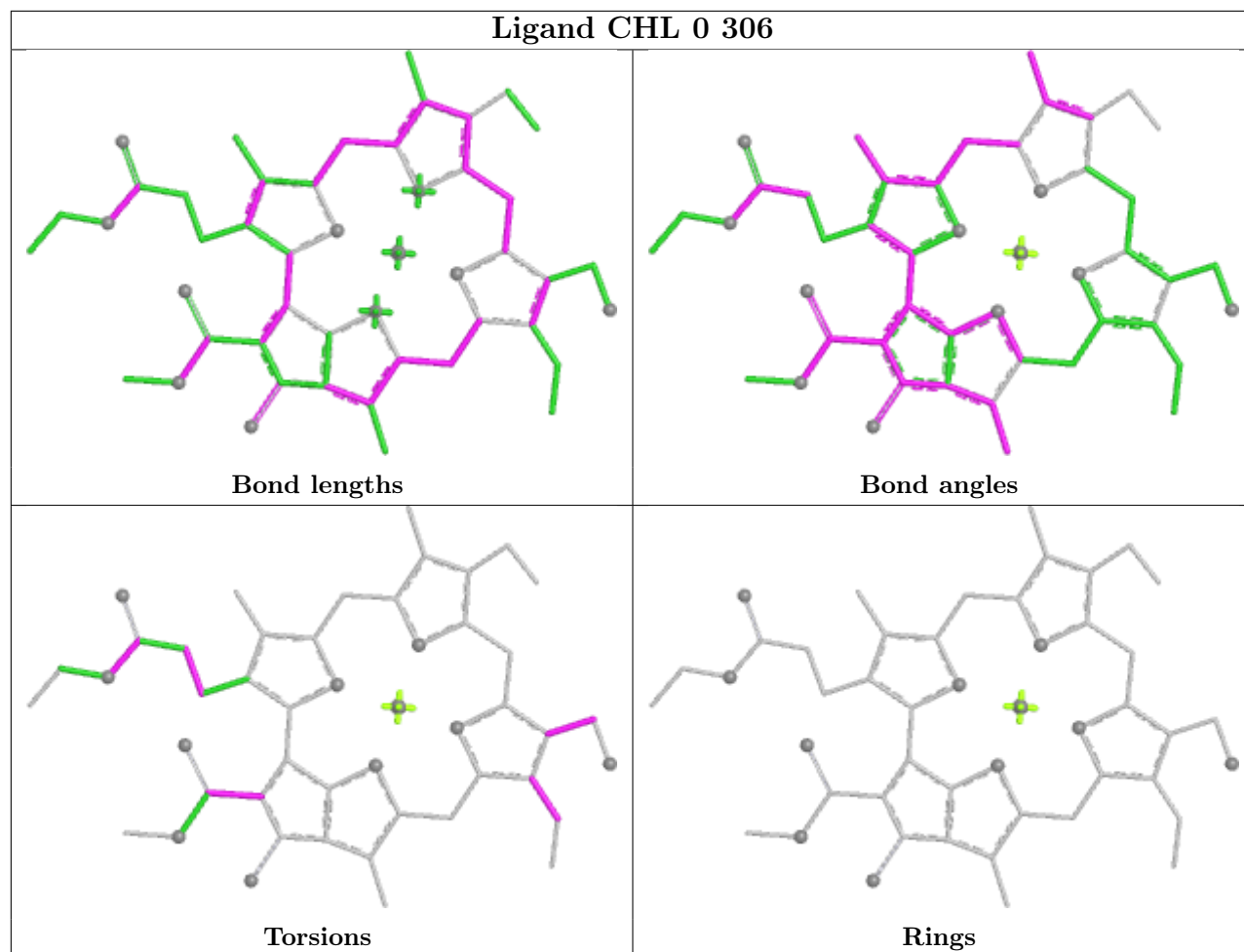




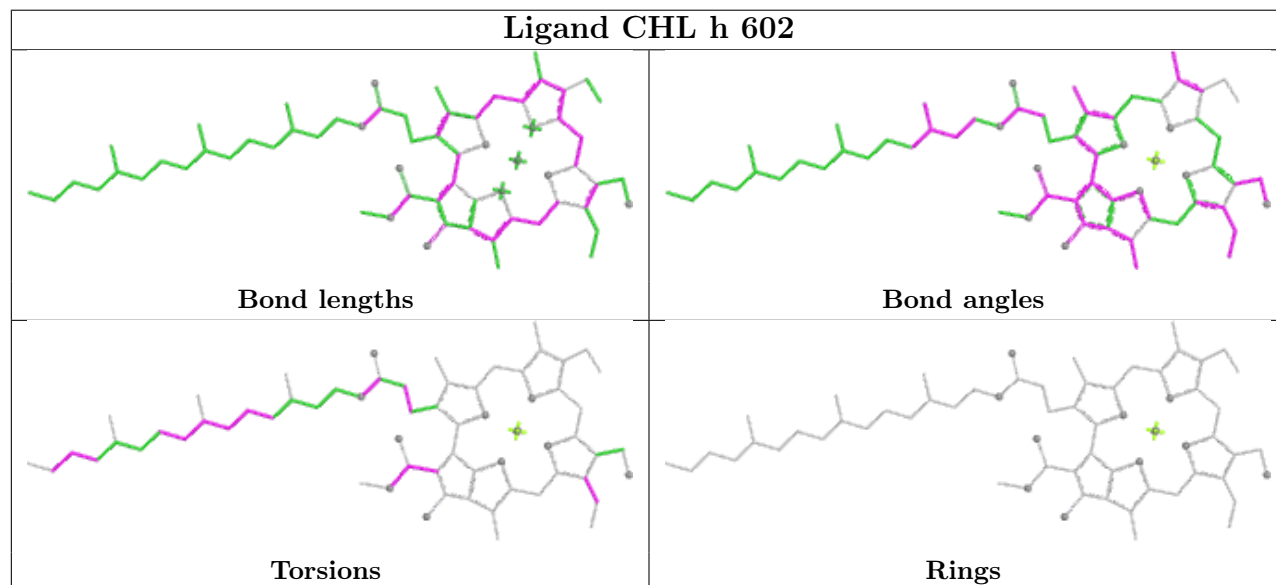




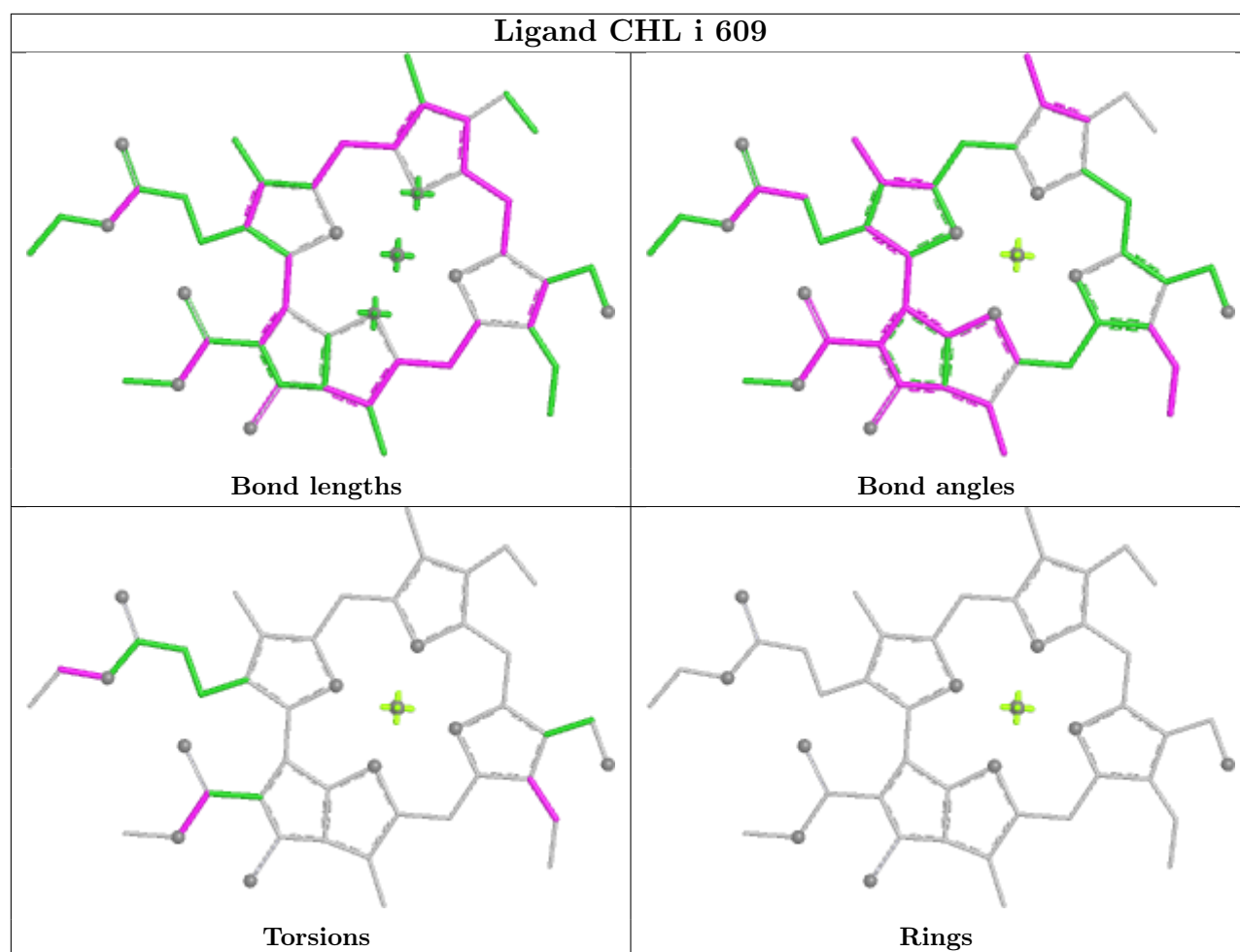
## Ligand CHL 0 306



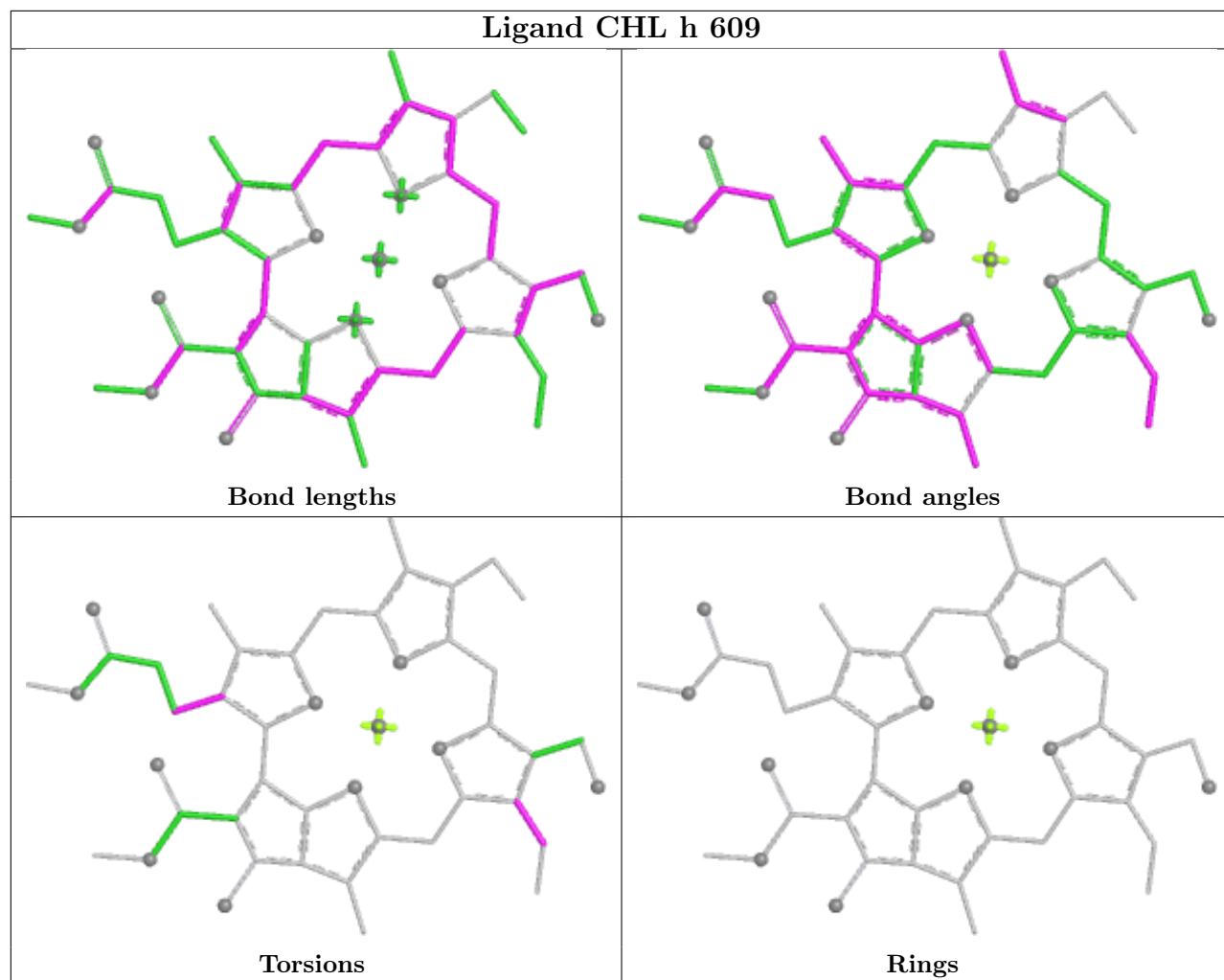
## Ligand CHL h 602



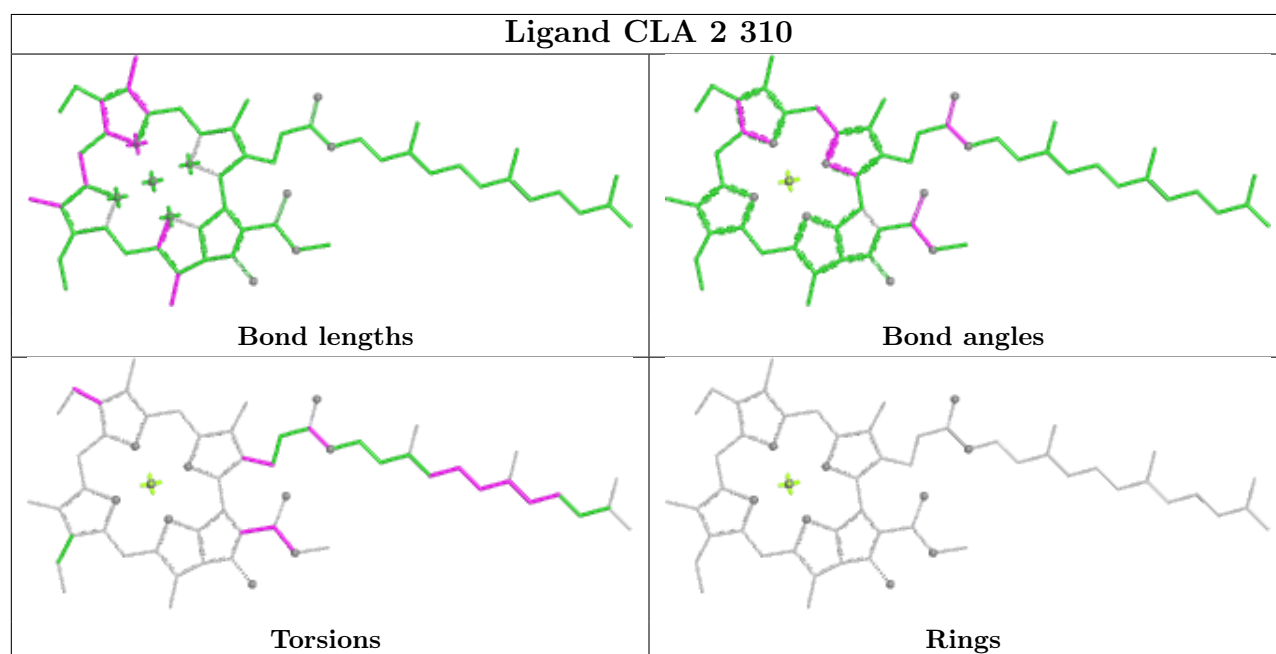
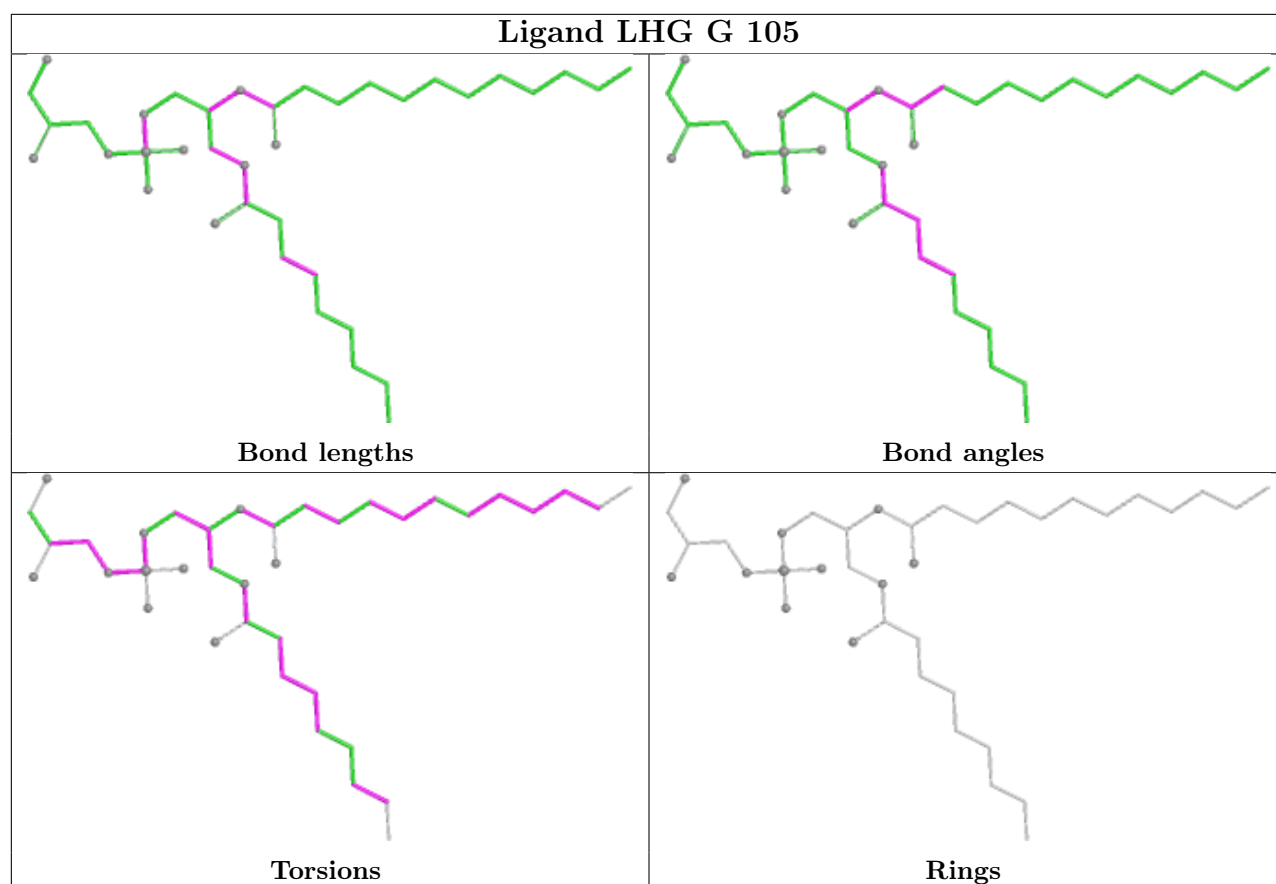






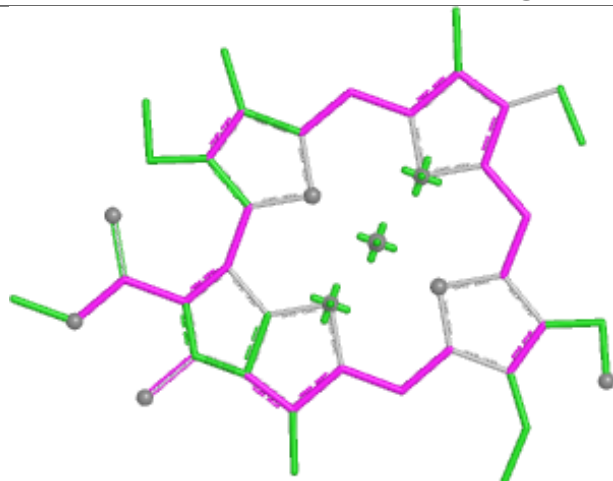




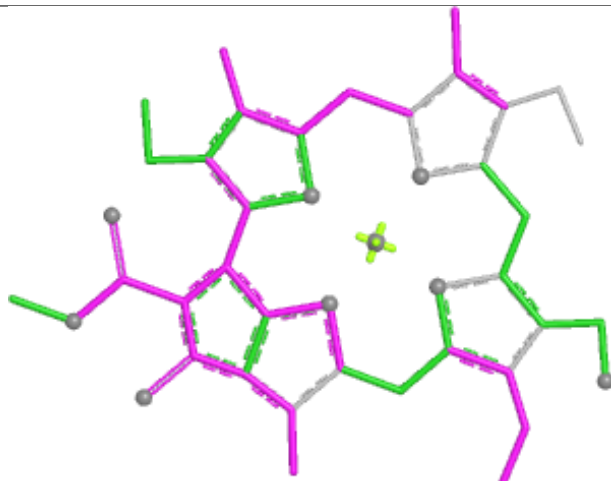




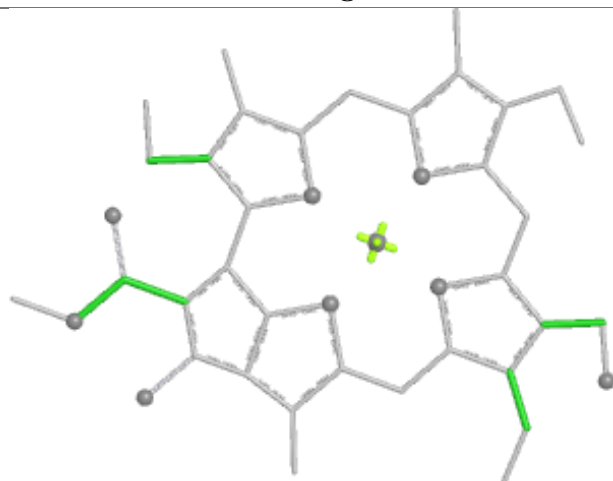
## Ligand CHL 2 305



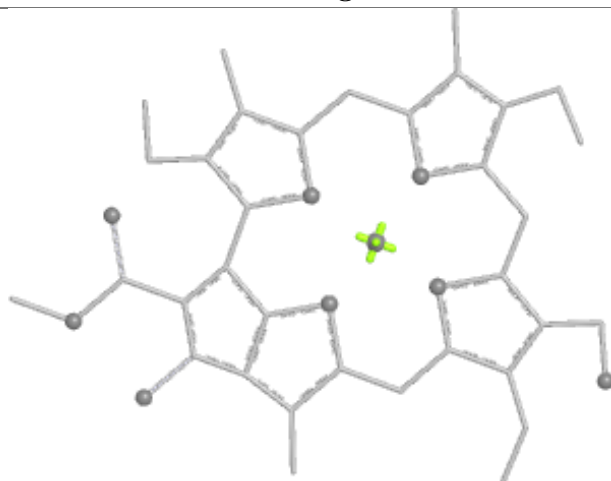
Bond lengths



Bond angles

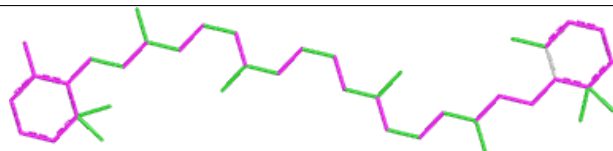


Torsions

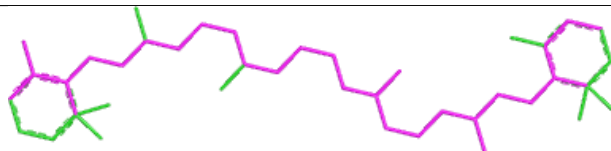


Rings

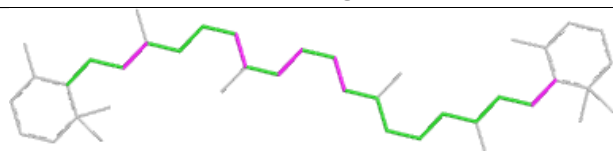
## Ligand 8CT A 849



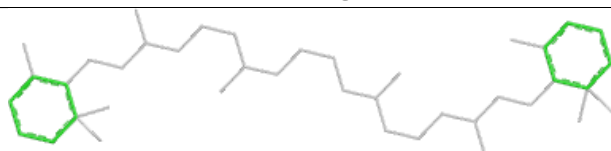
Bond lengths



Bond angles



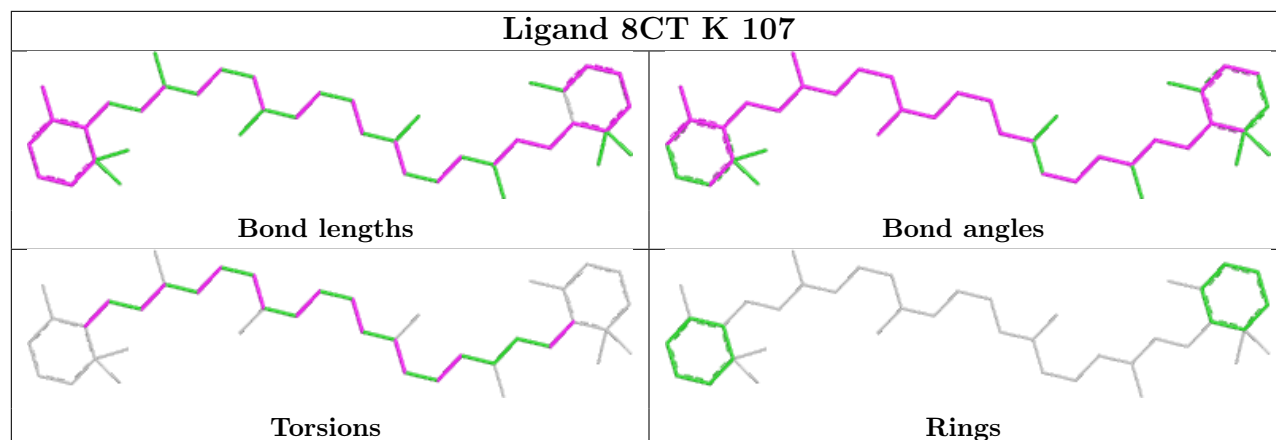
Torsions



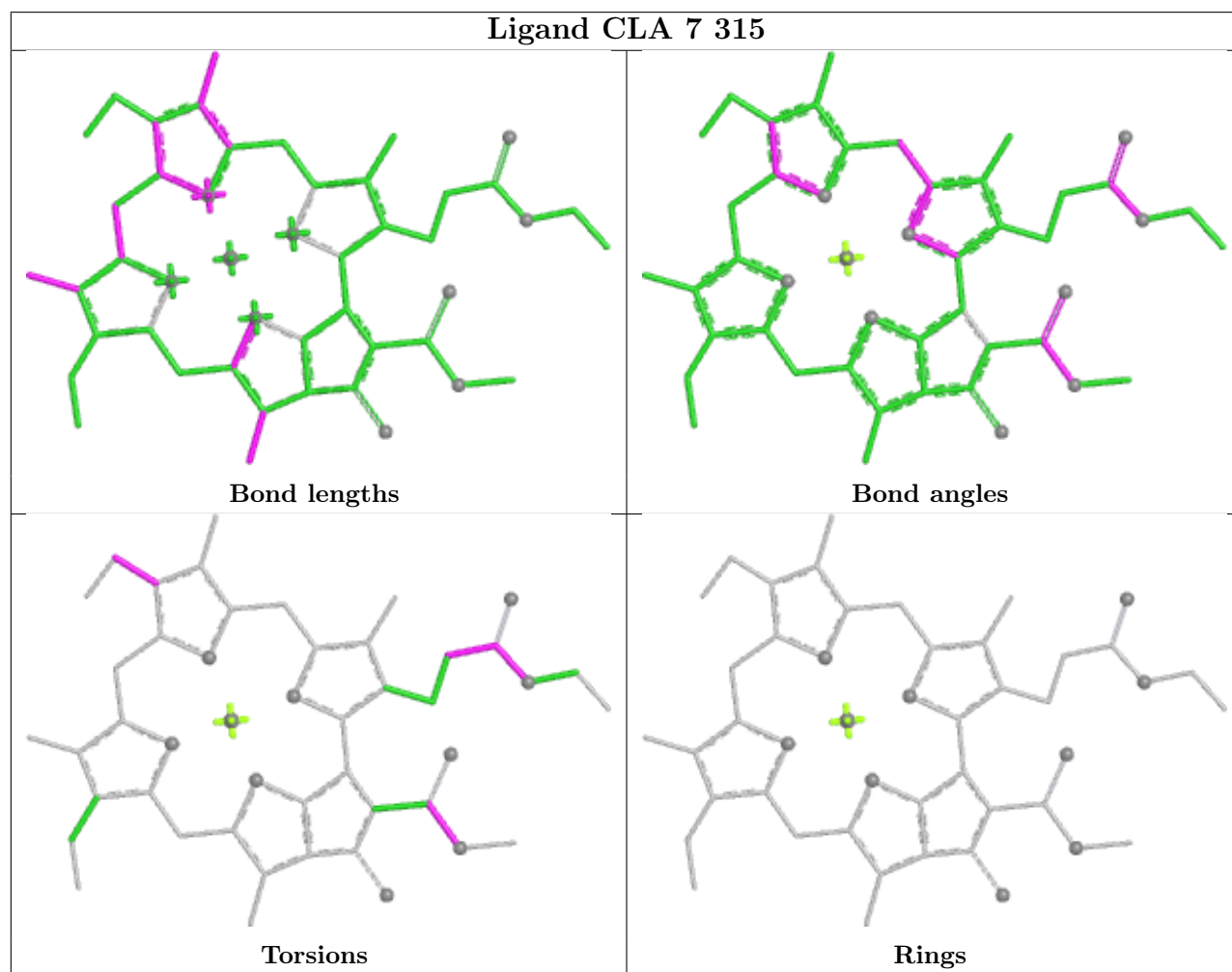
Rings



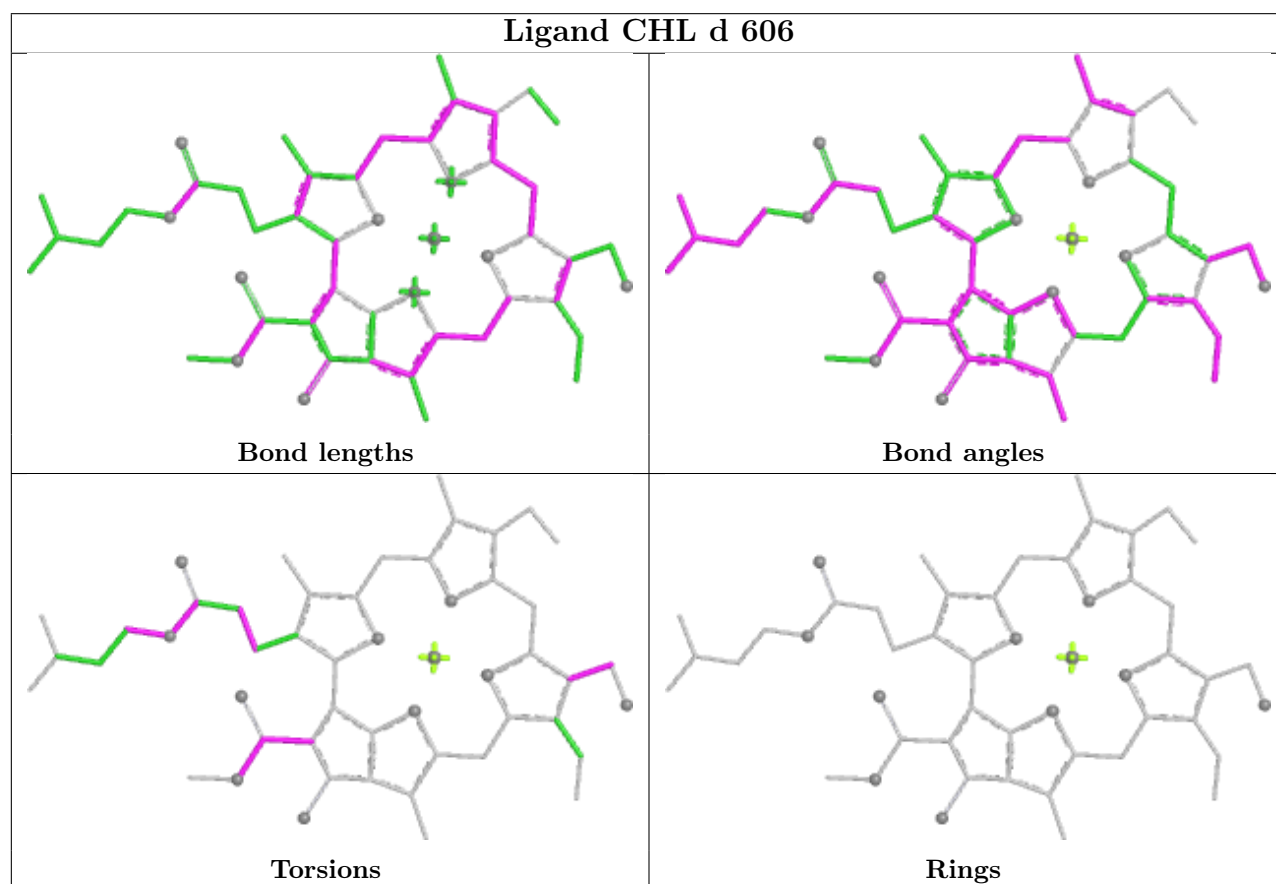
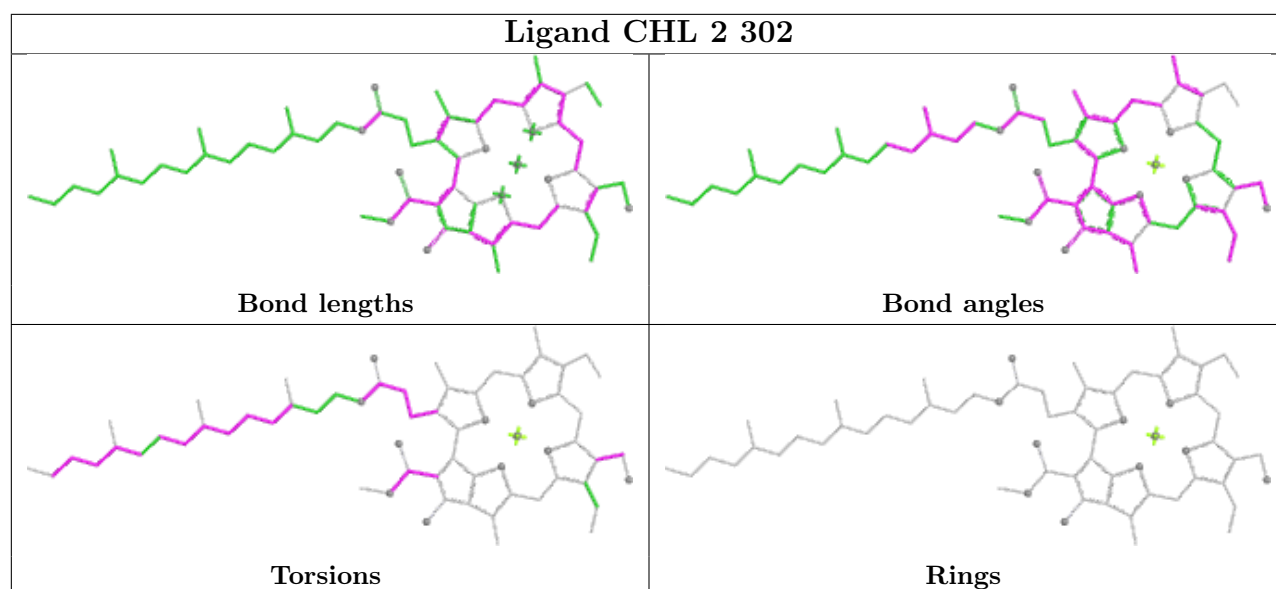
## Ligand 8CT K 107



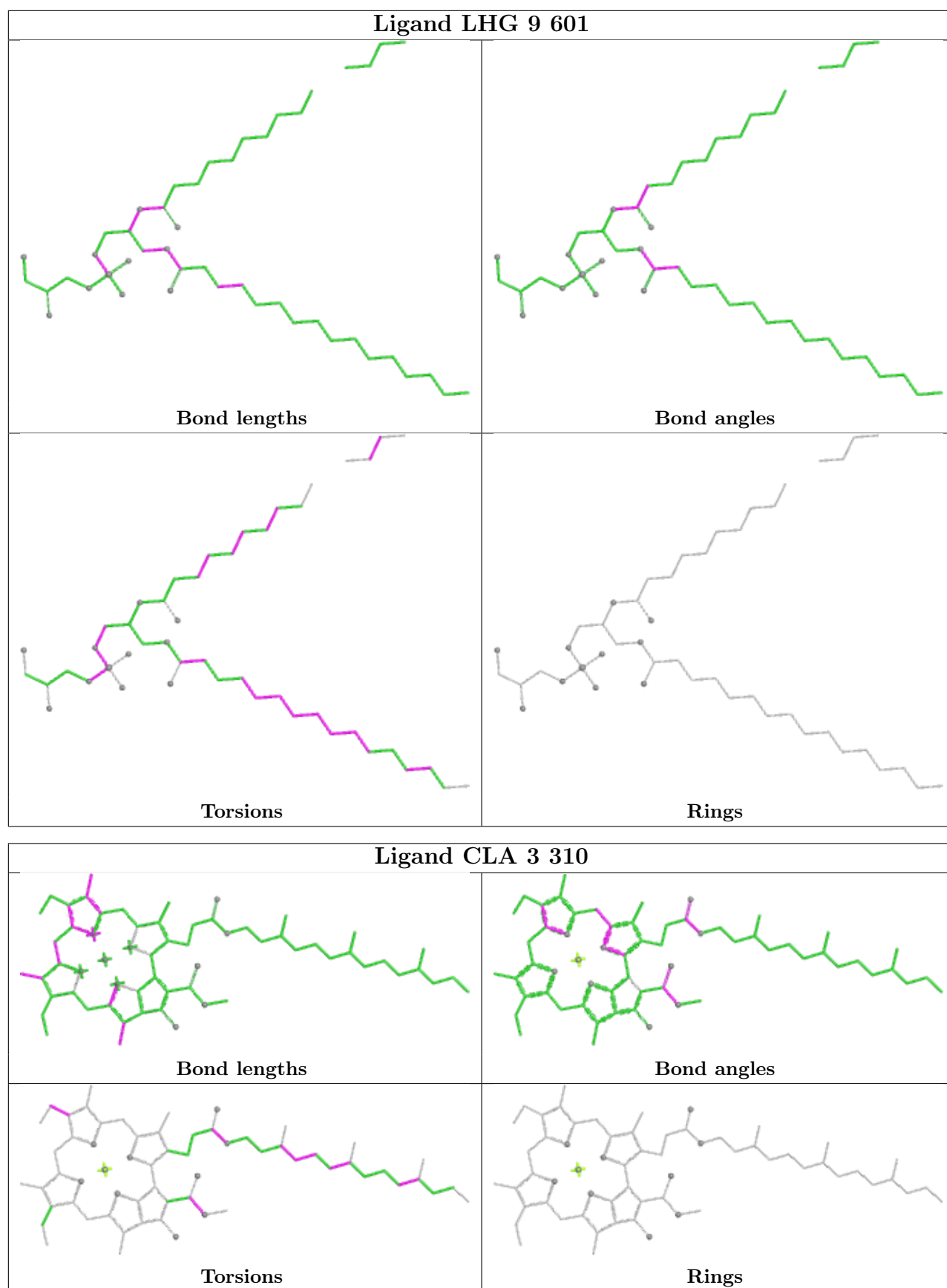
## Ligand CLA 7 315



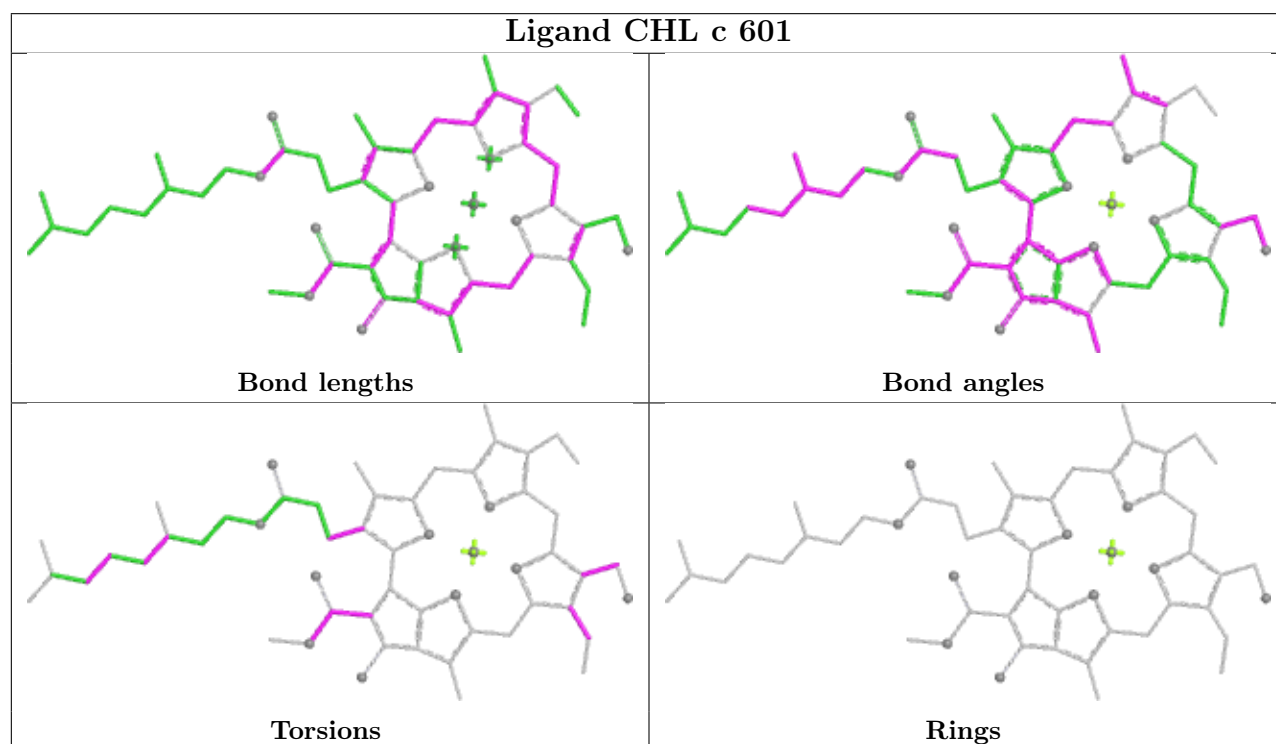
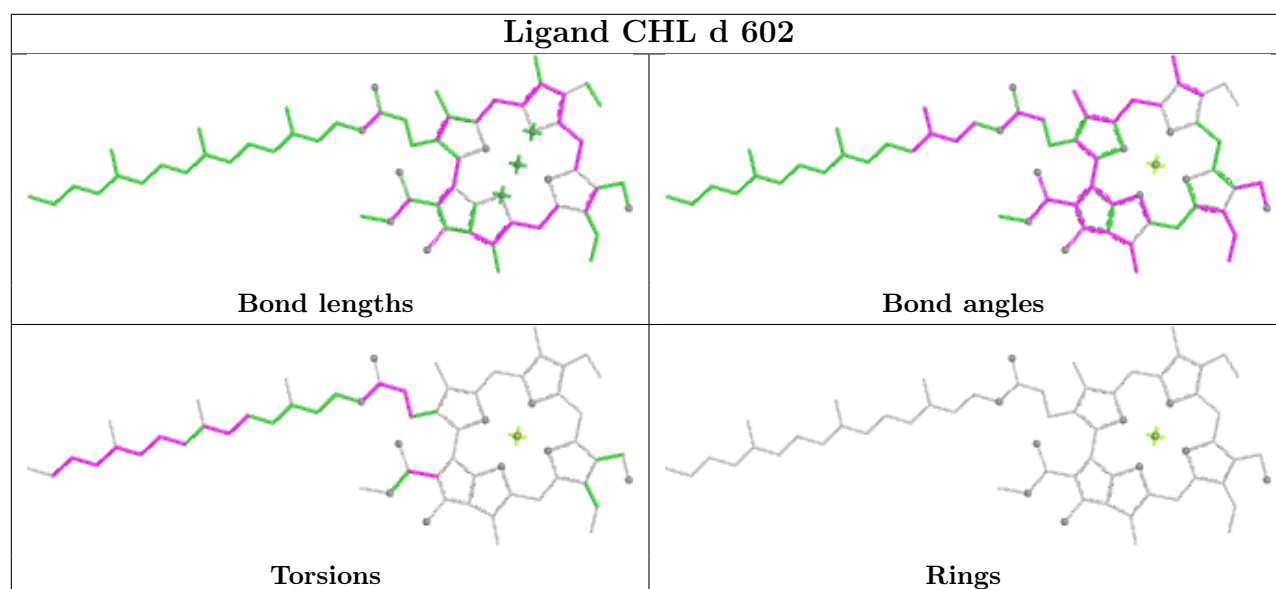




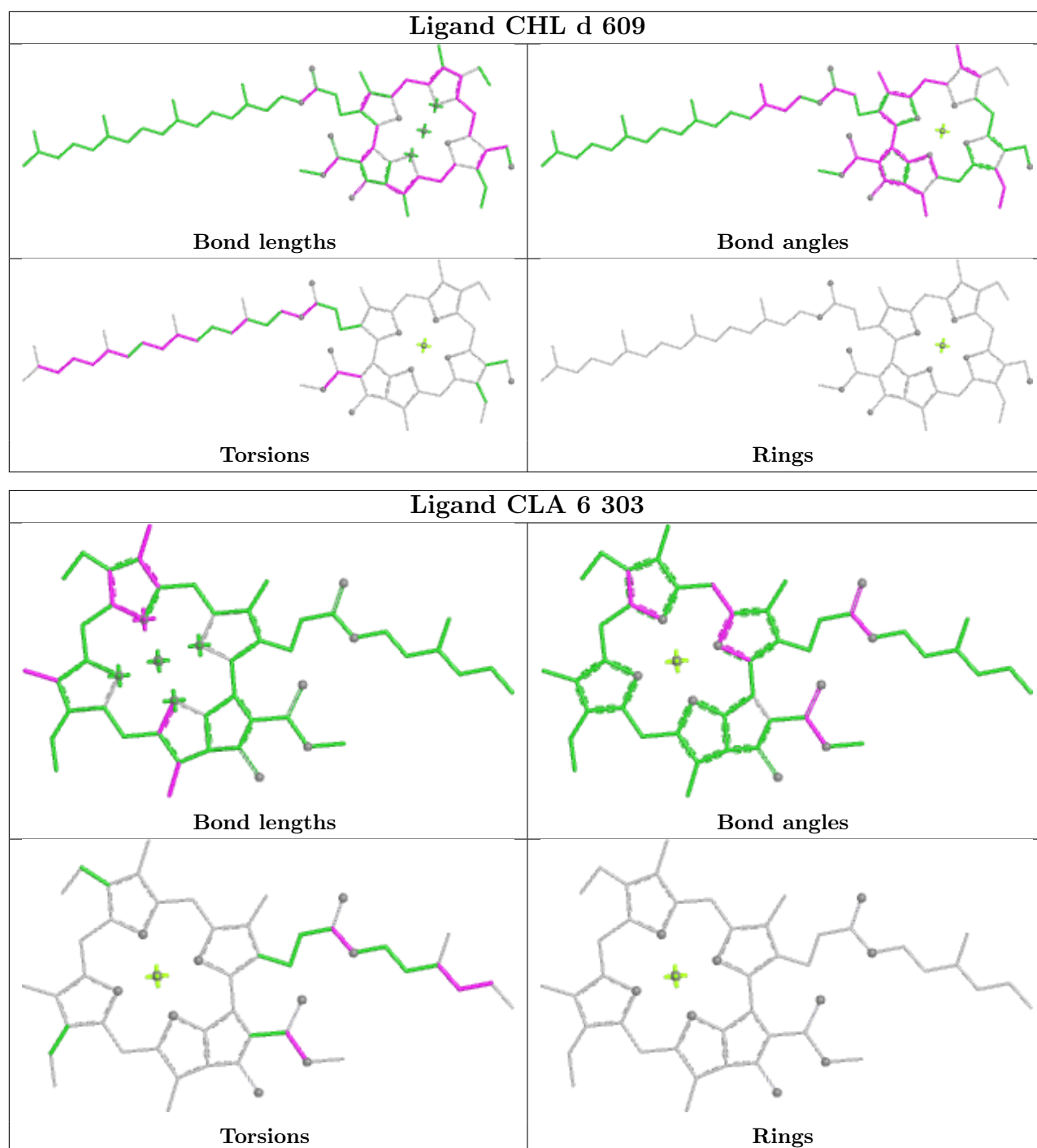




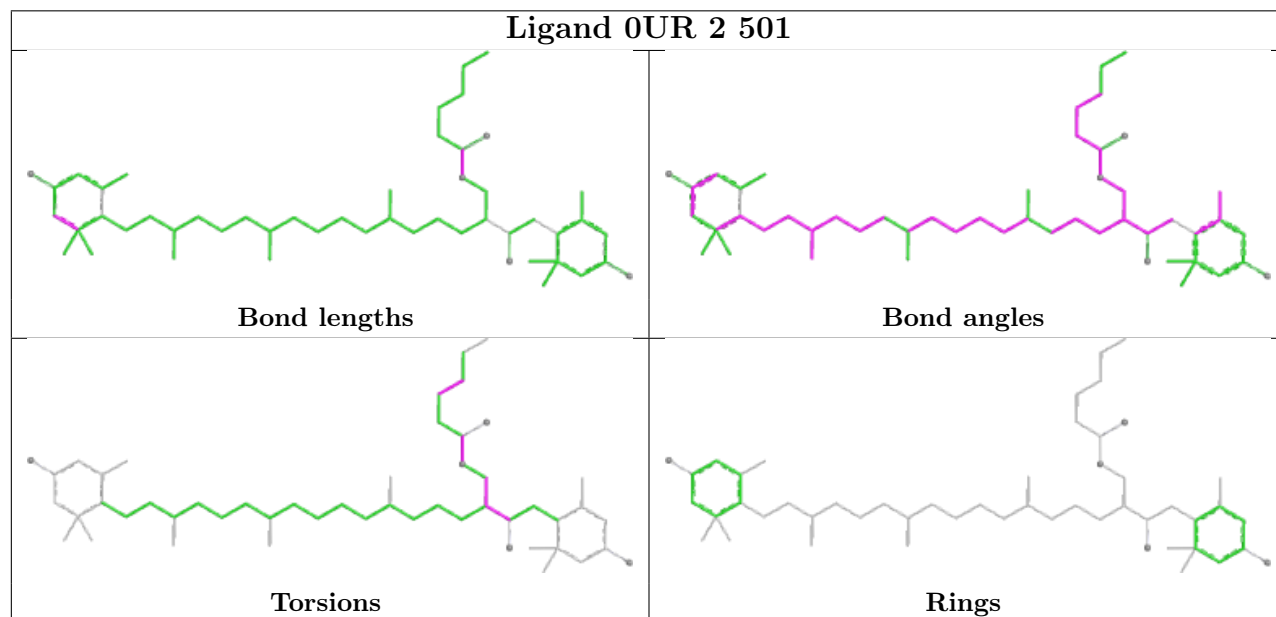
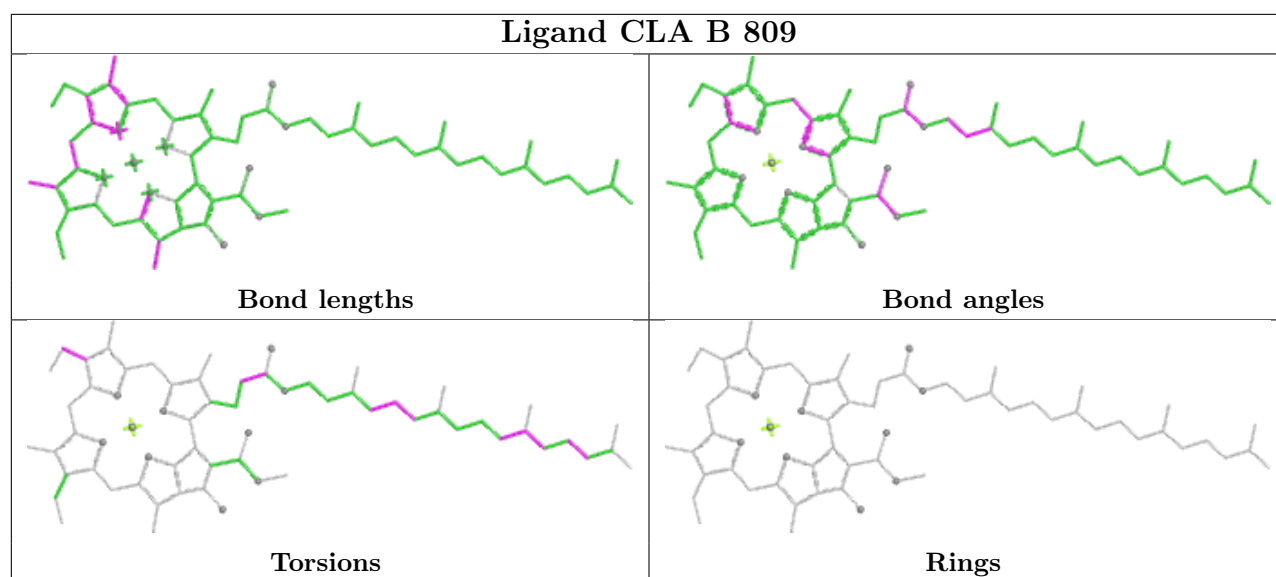






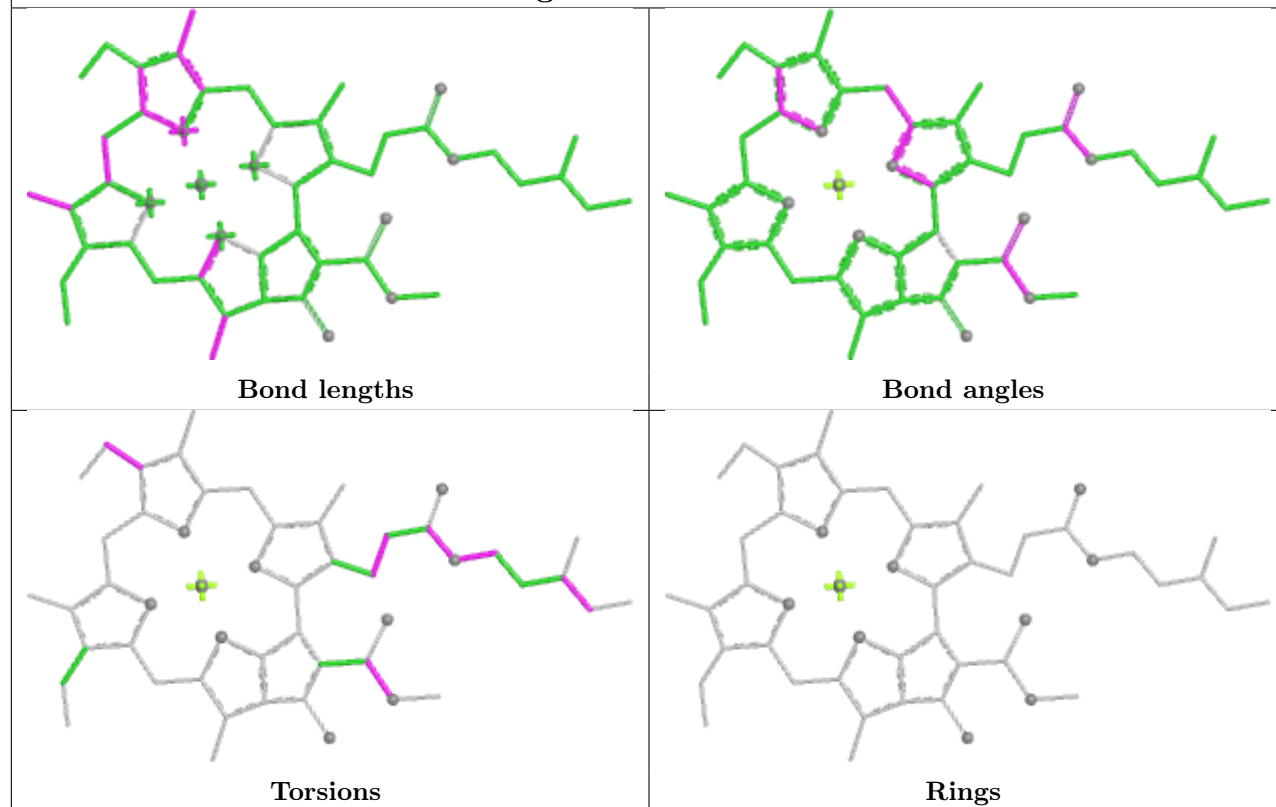




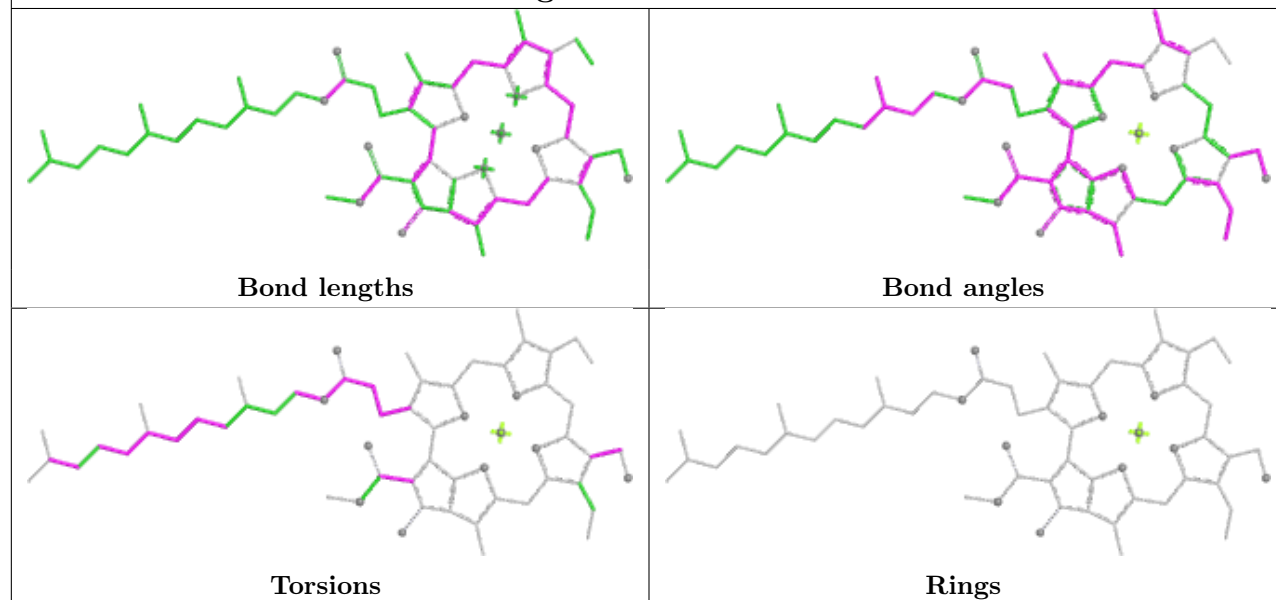




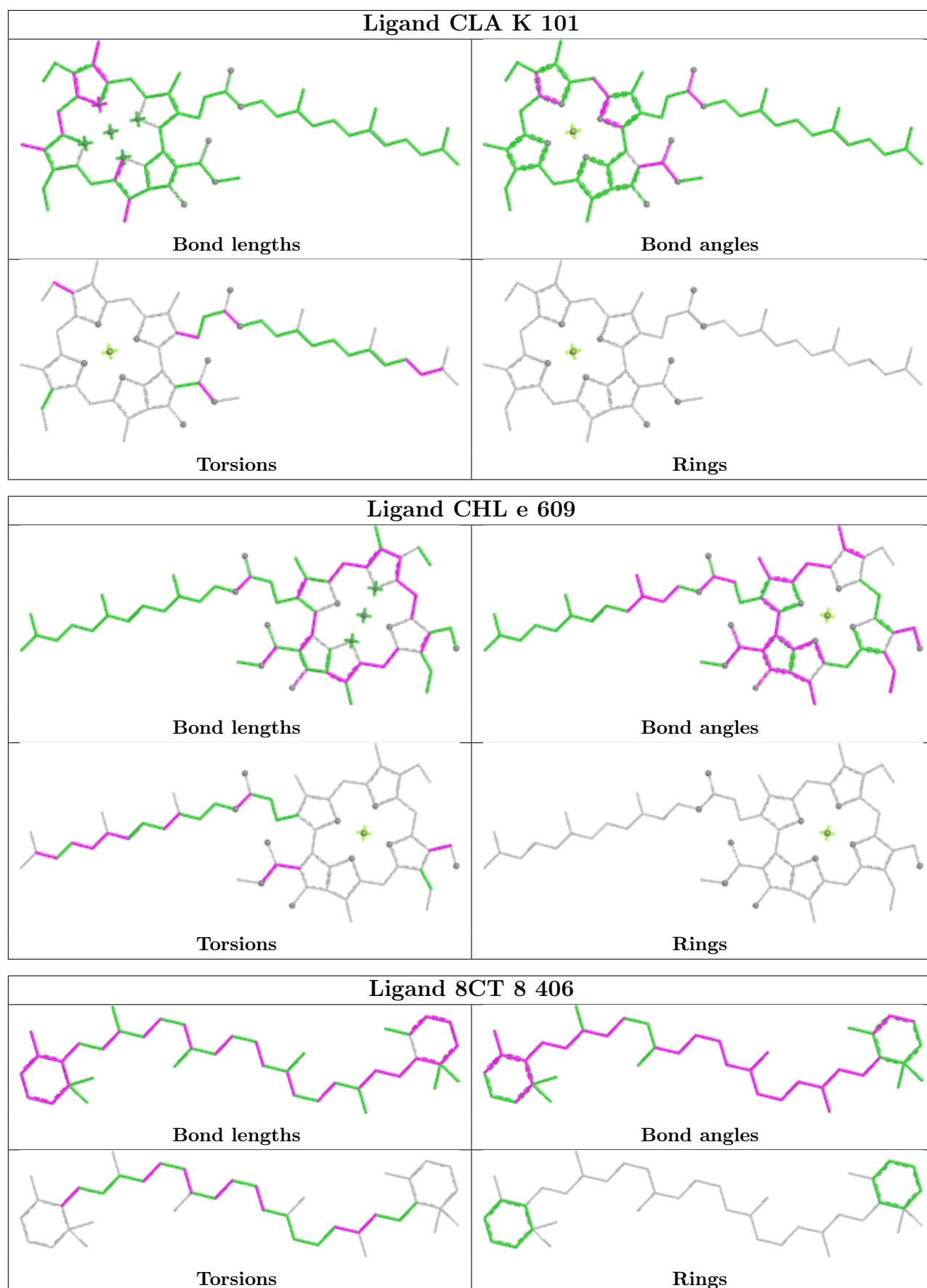
## Ligand CLA 6 320



## Ligand CHL e 602

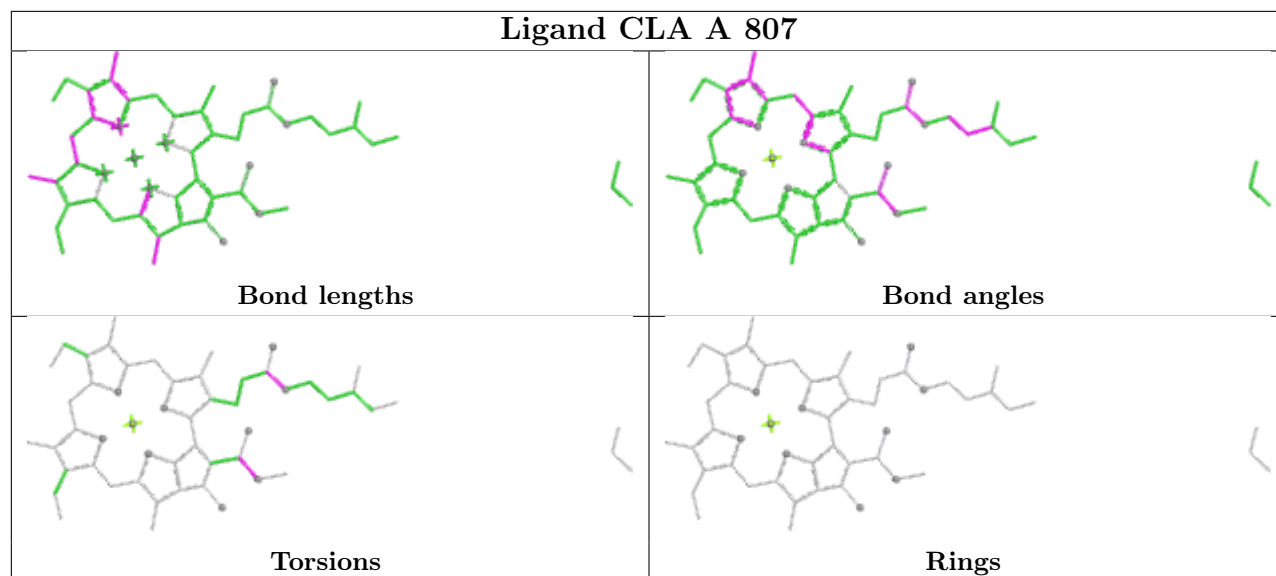




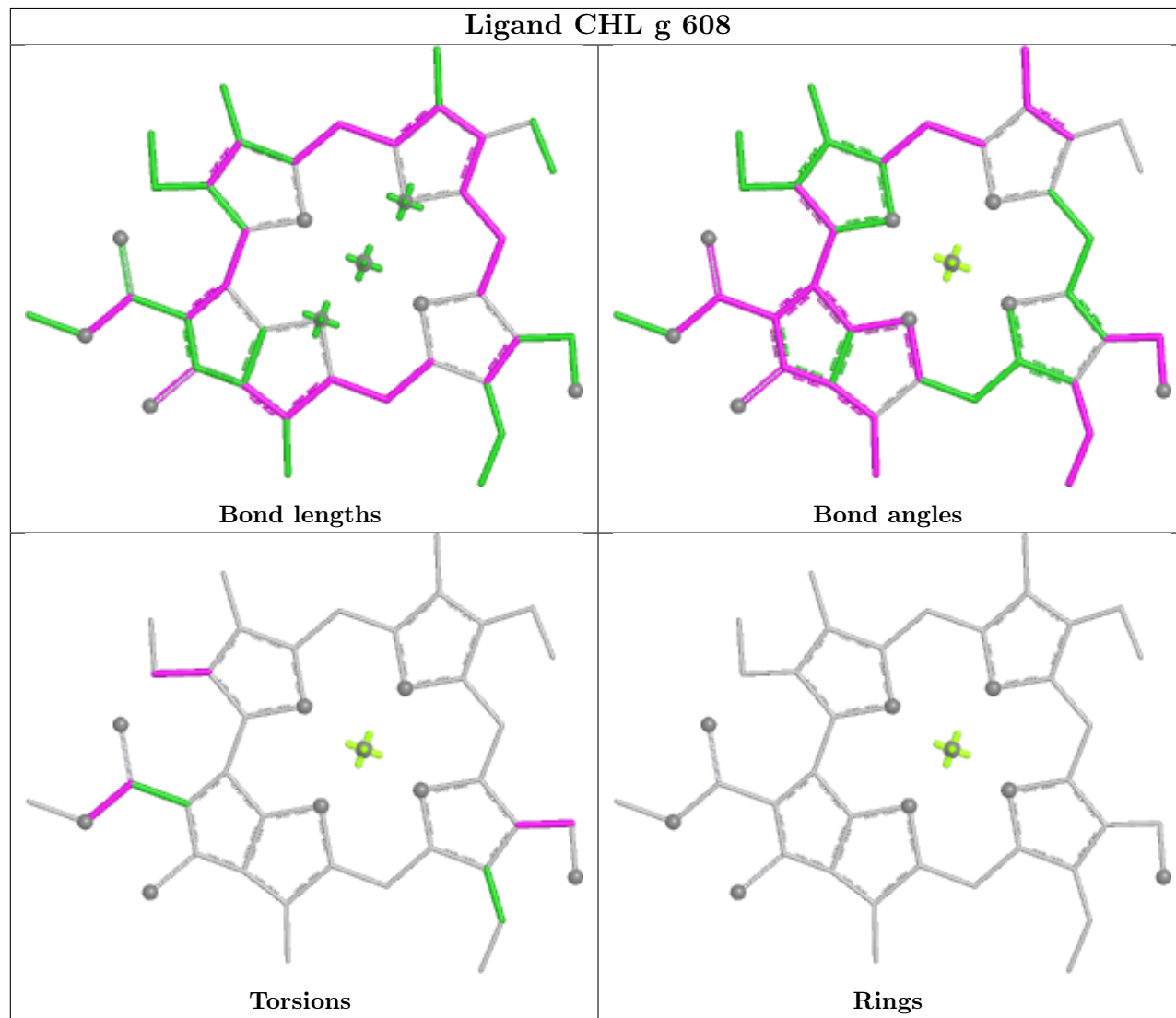




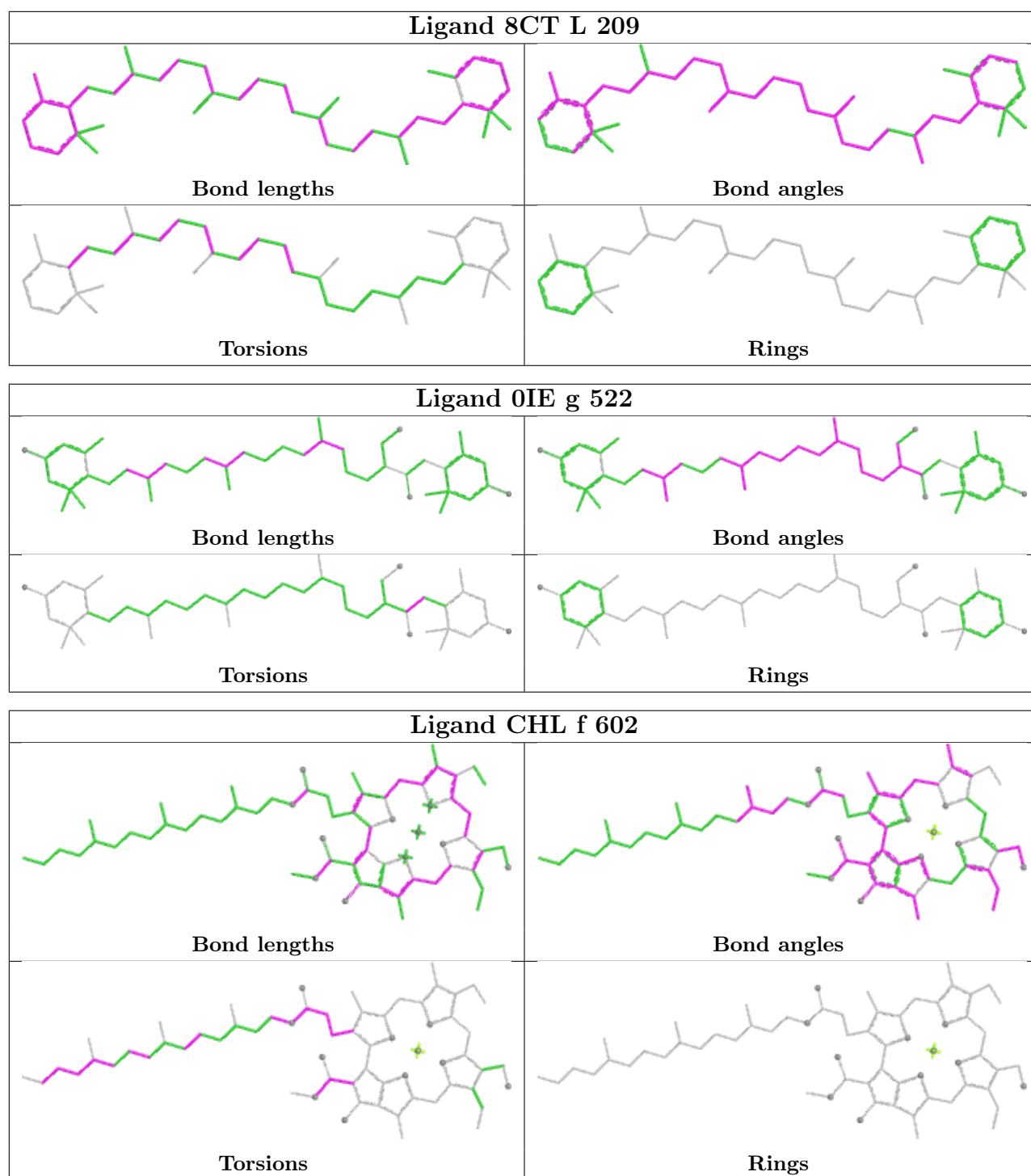
## Ligand CLA A 807



## Ligand CHL g 608

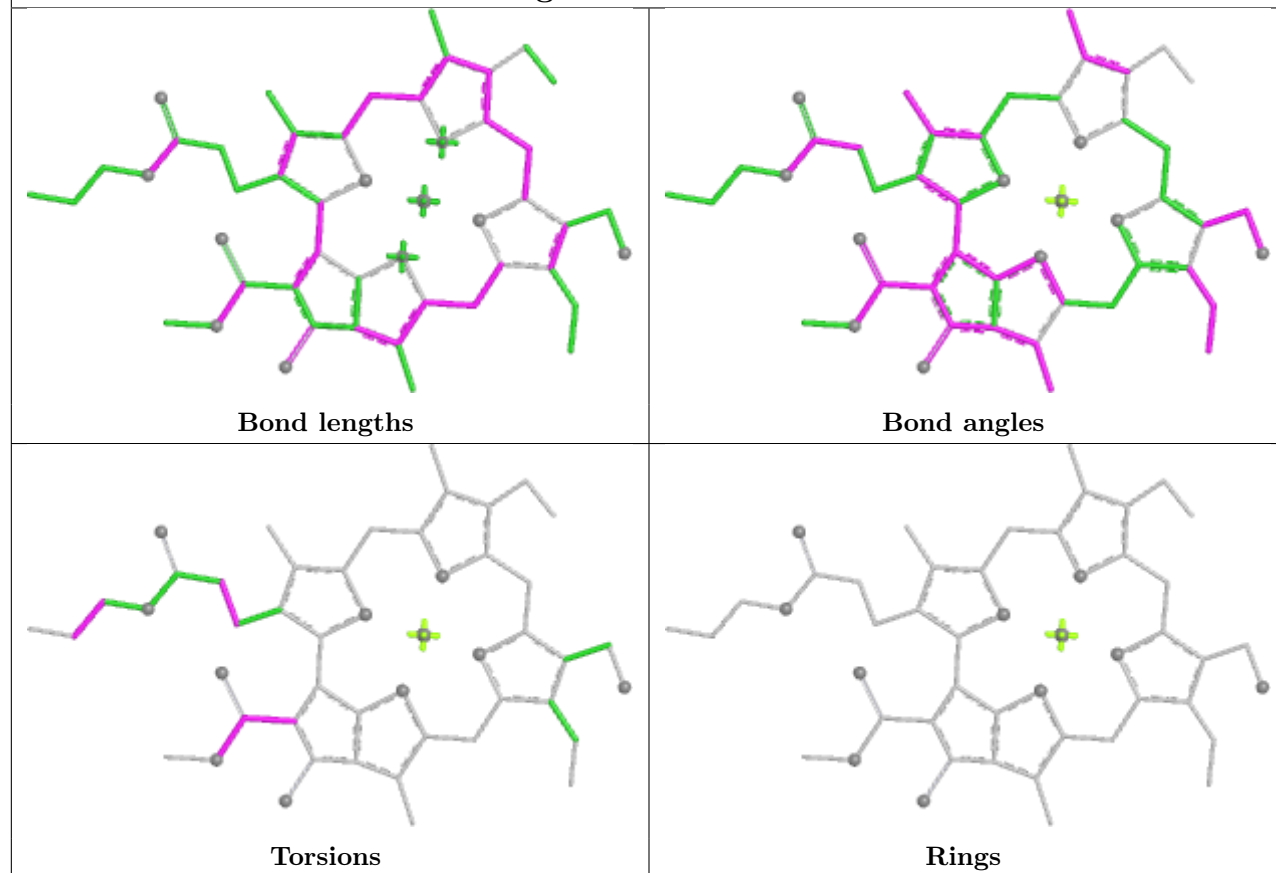




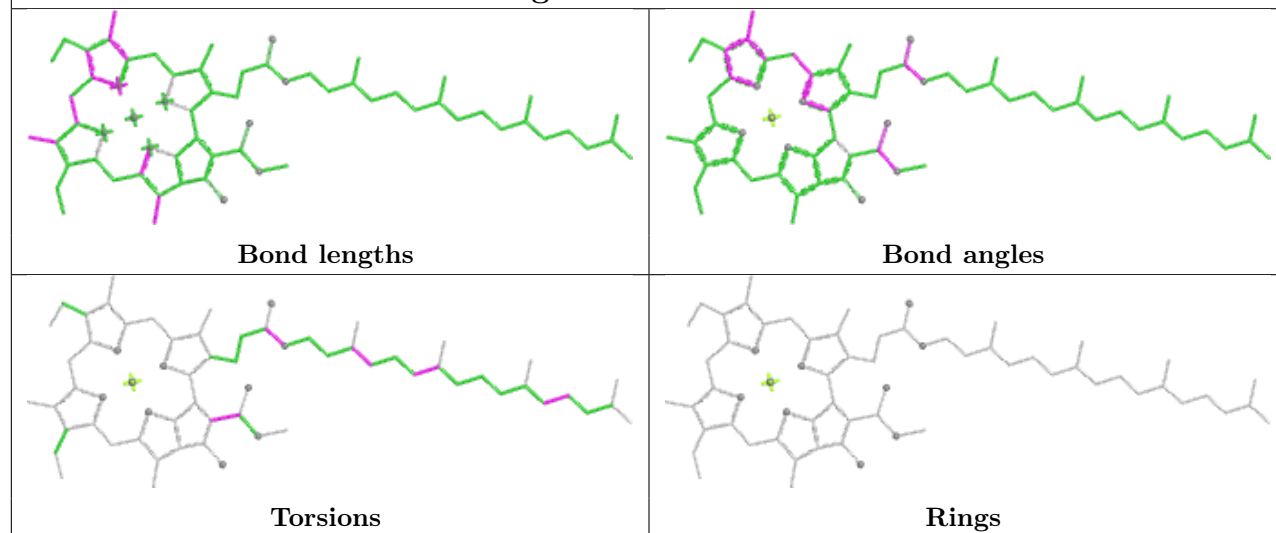




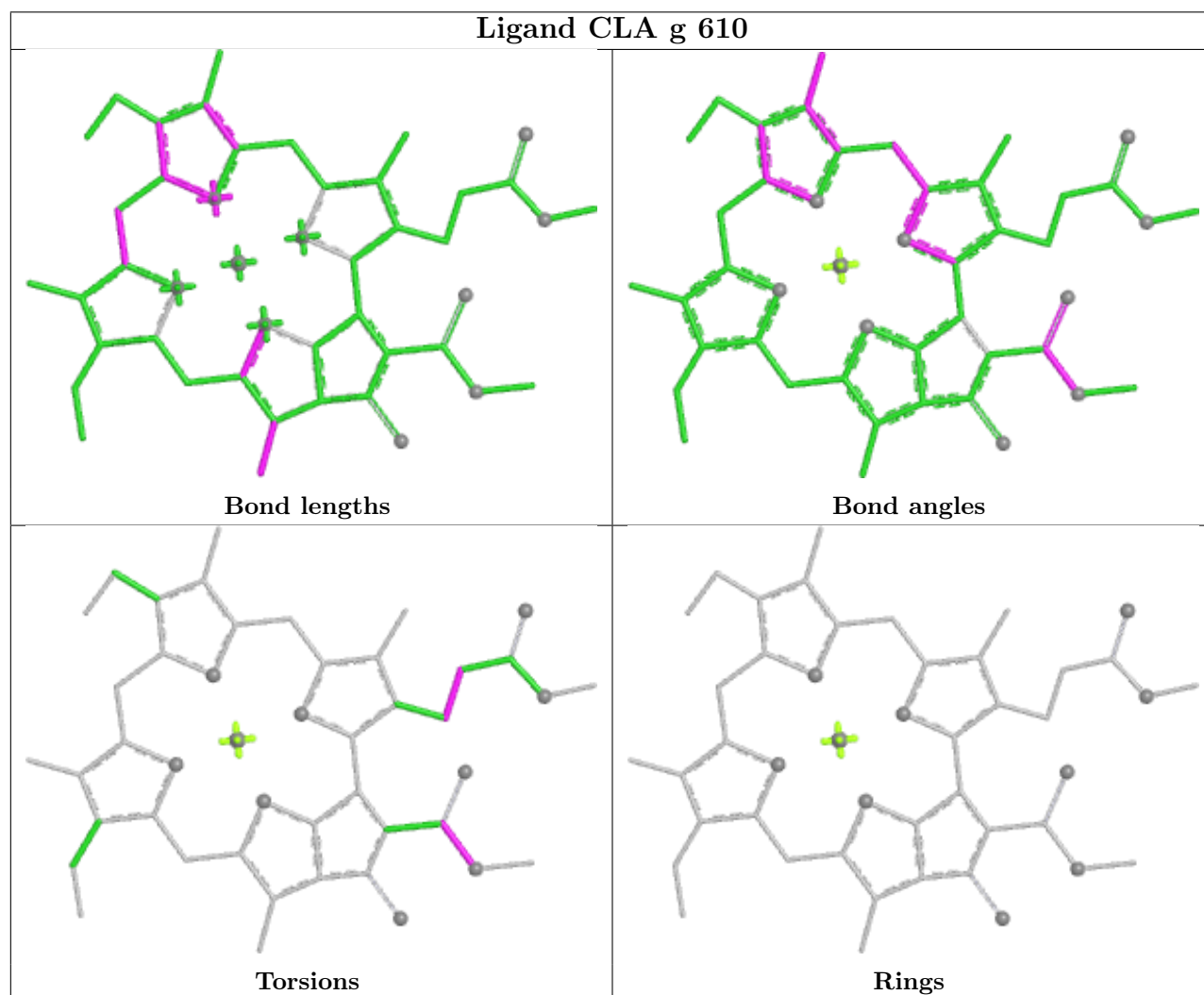
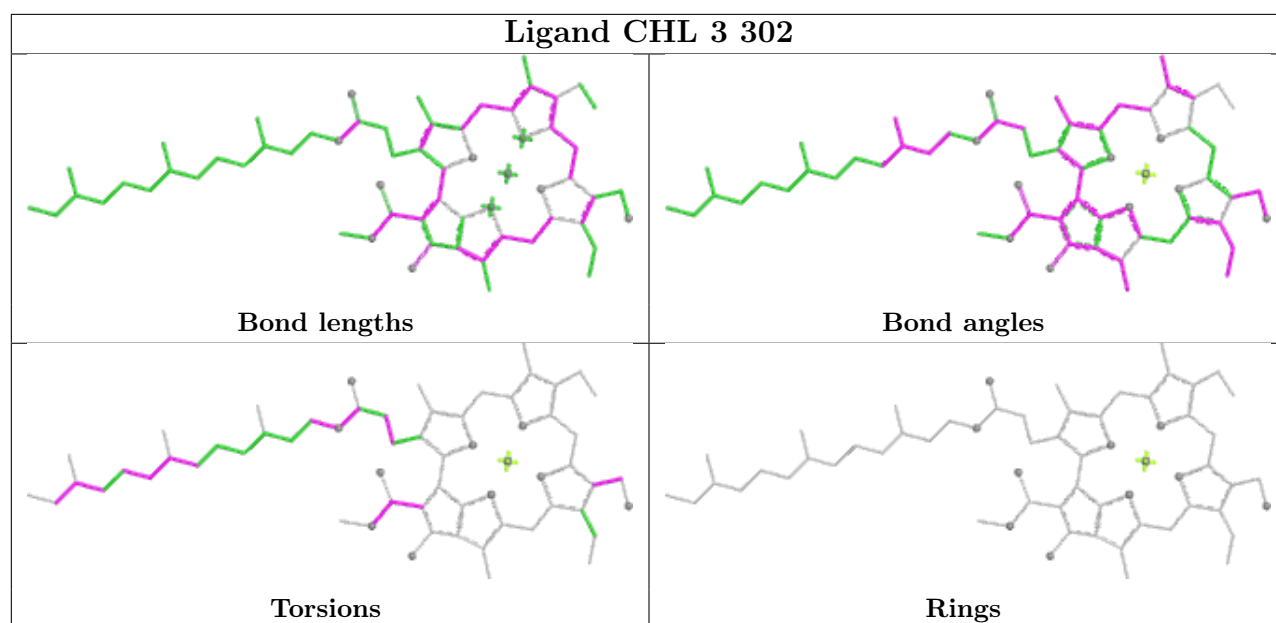
## Ligand CHL a 608



## Ligand CLA A 813

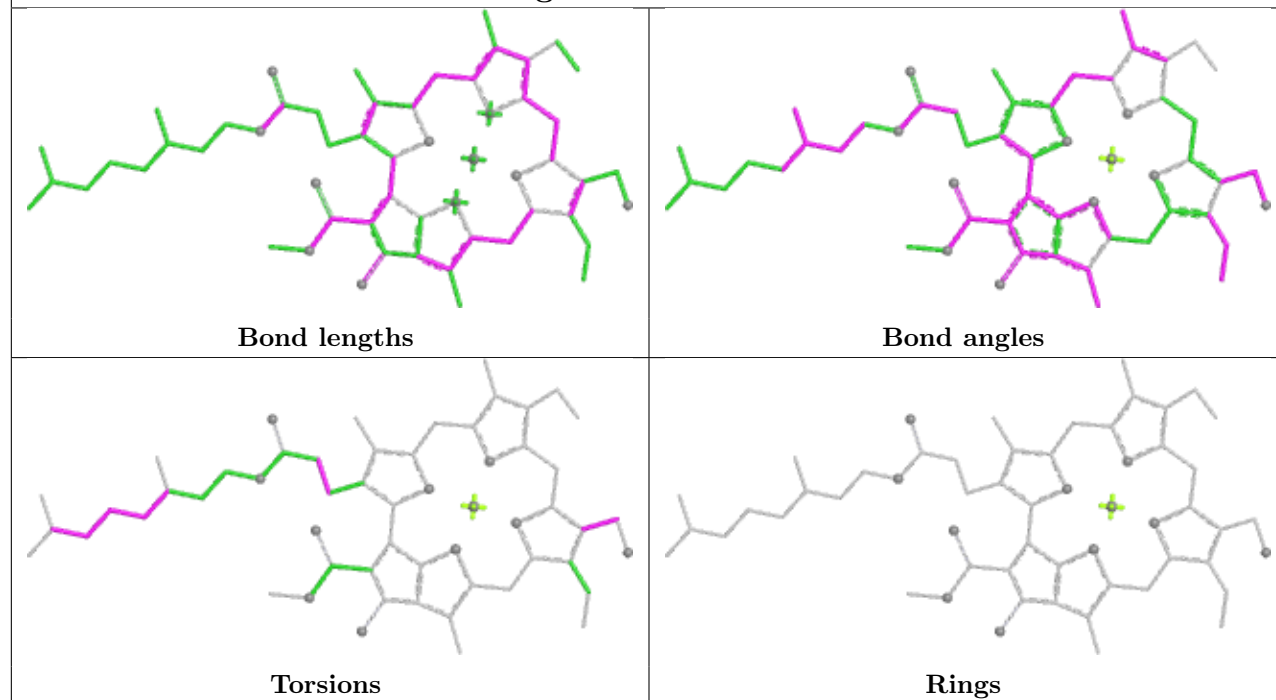




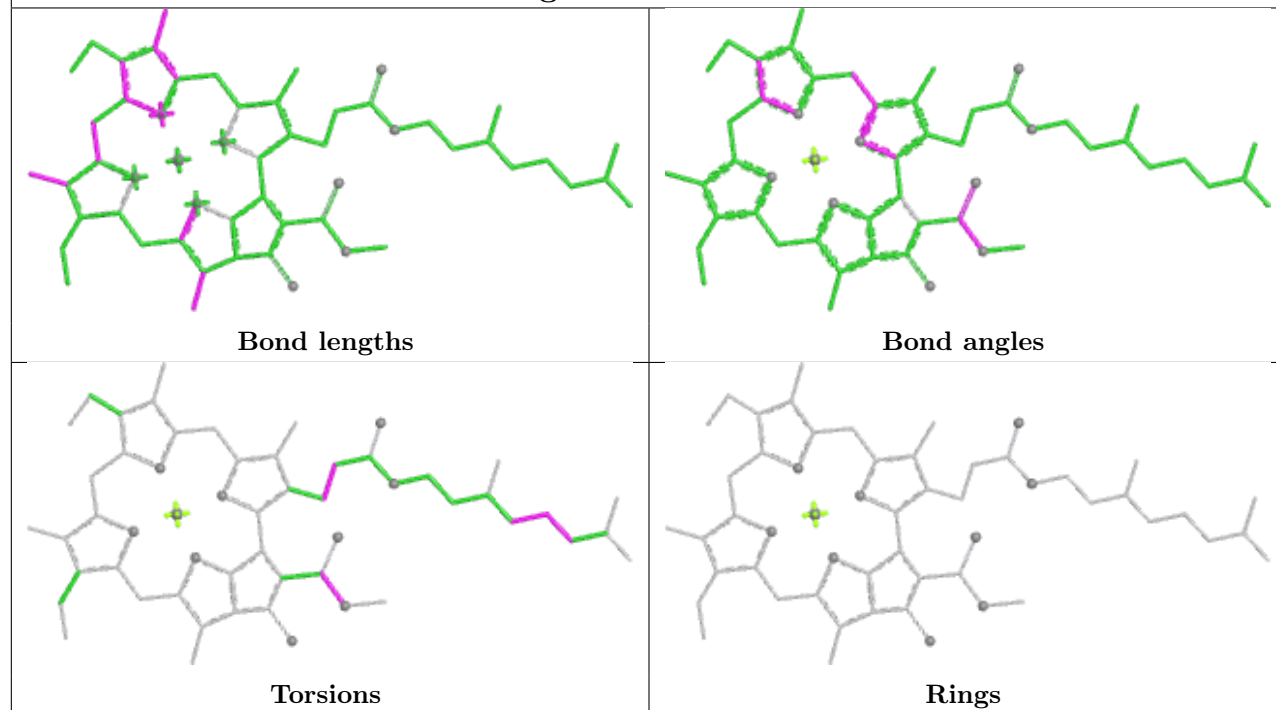




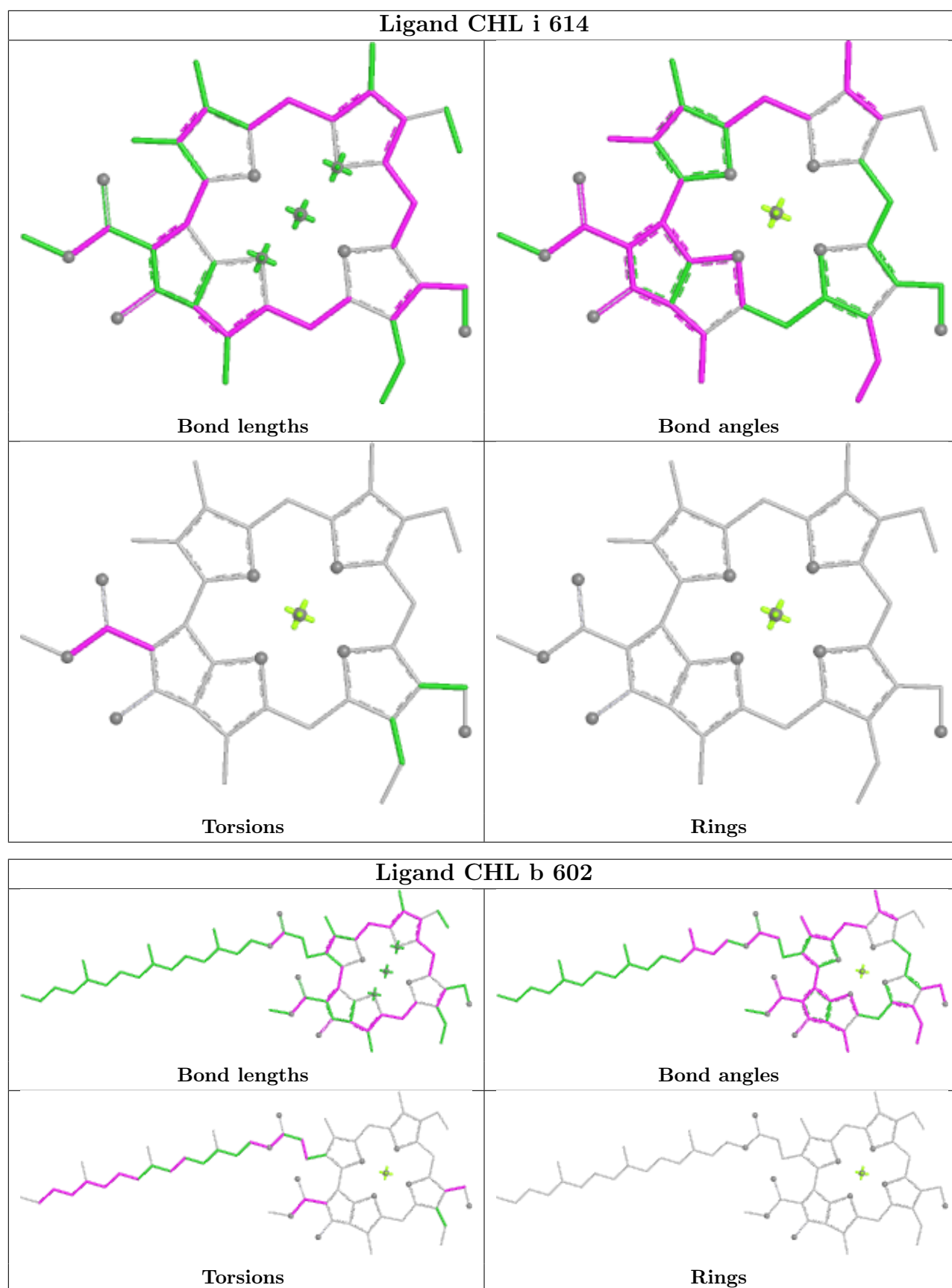
## Ligand CHL 8 313



## Ligand CLA f 611

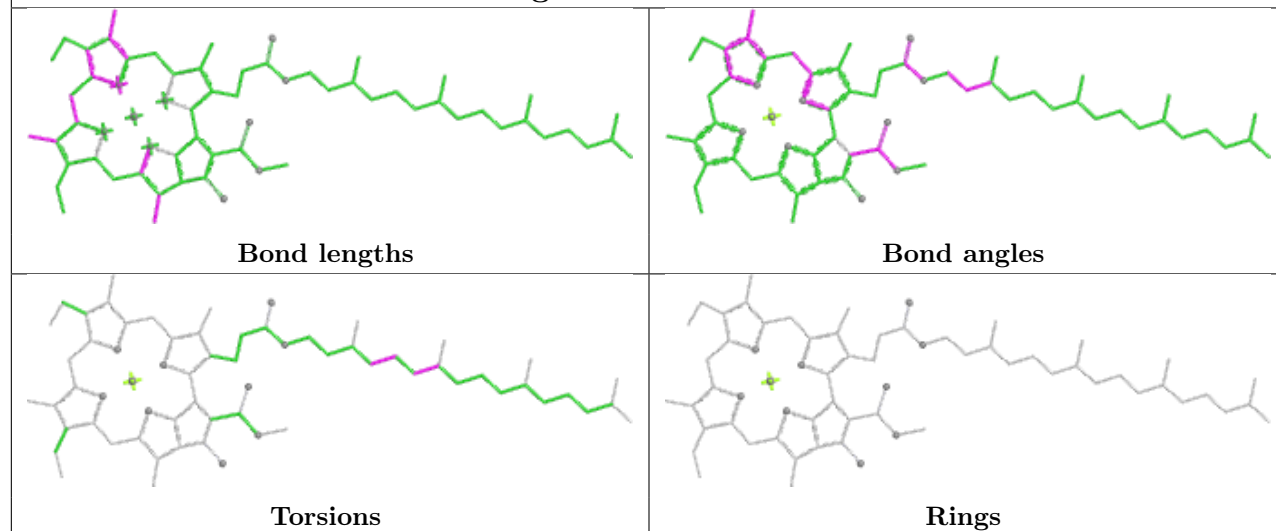




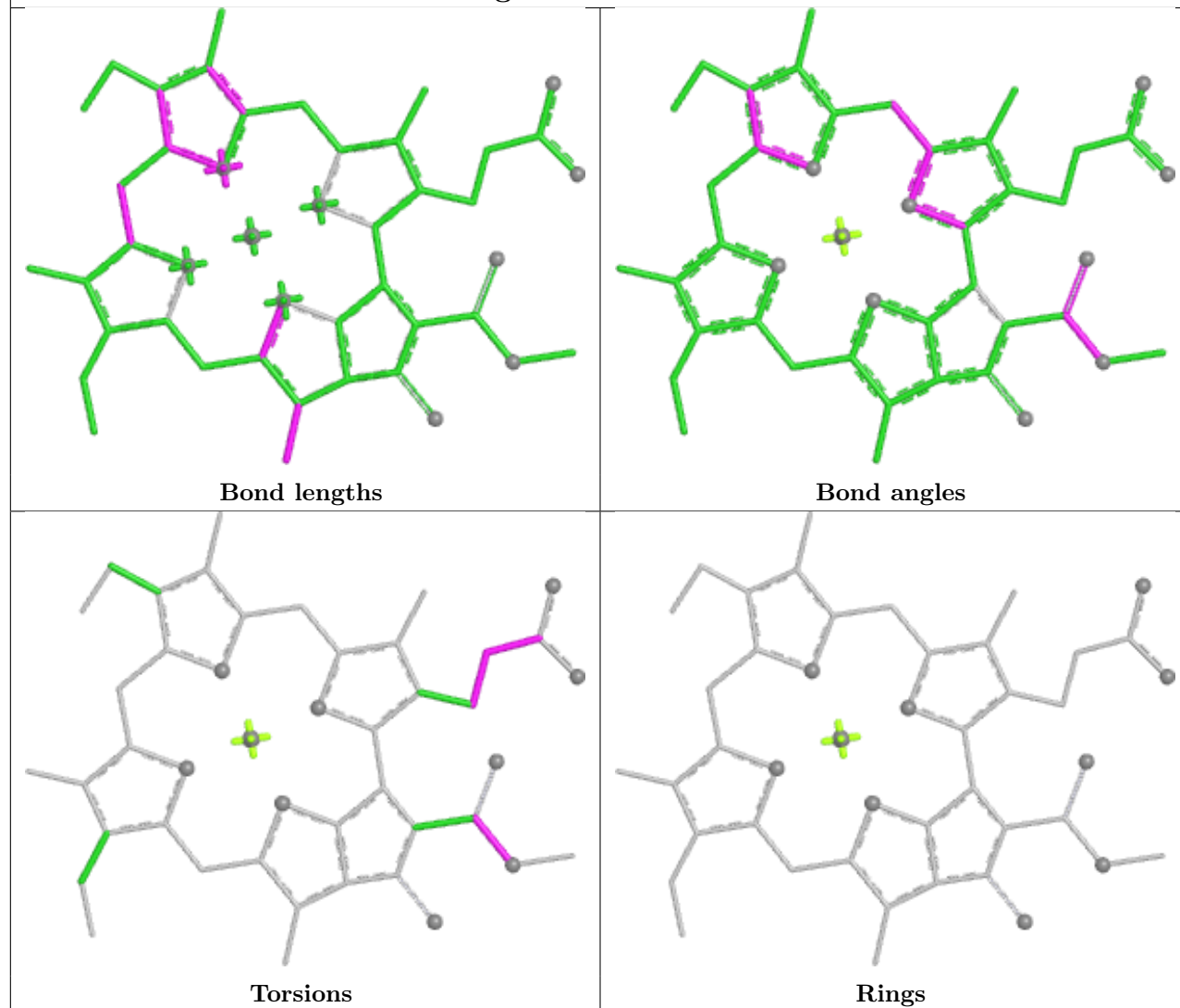




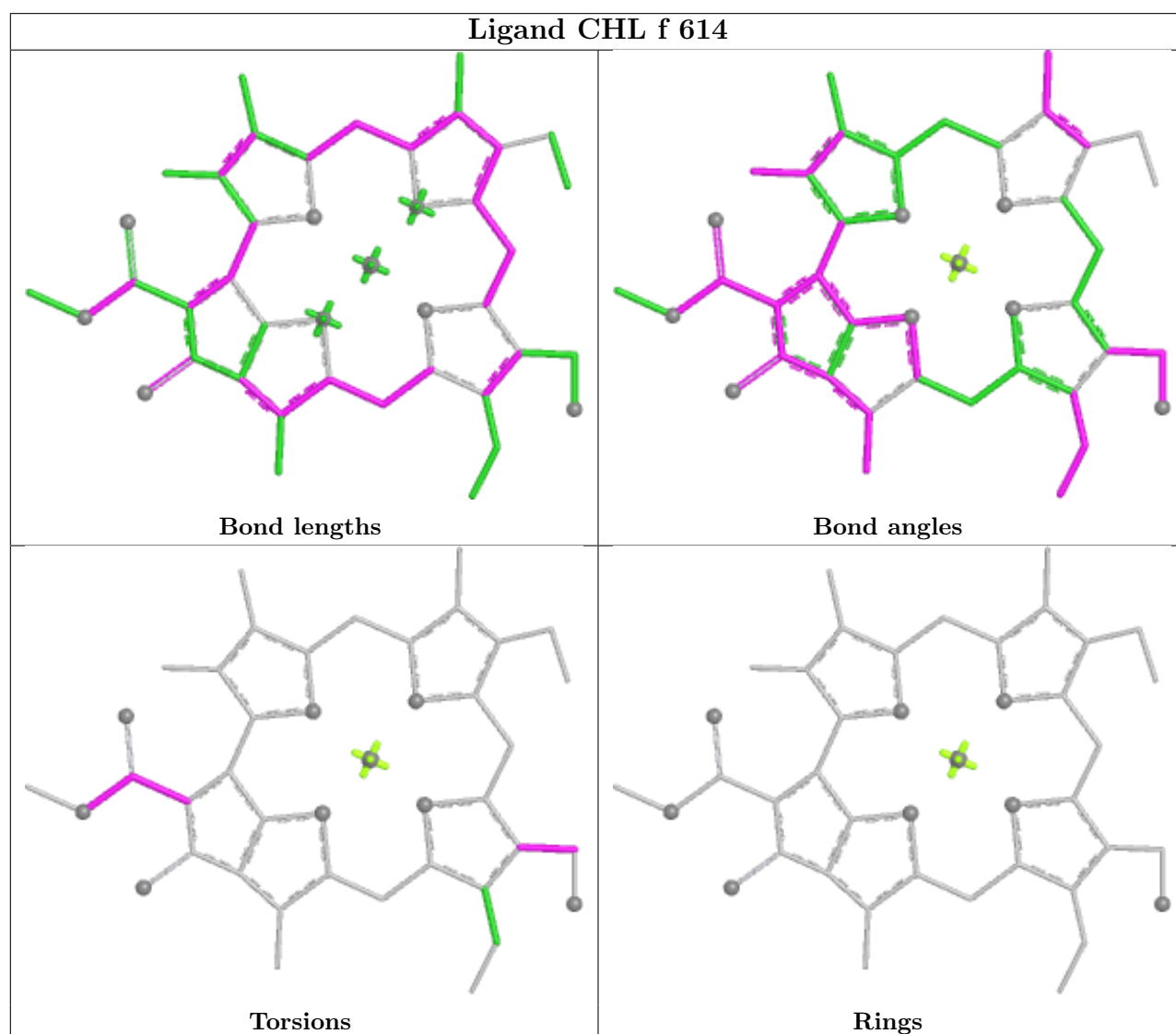
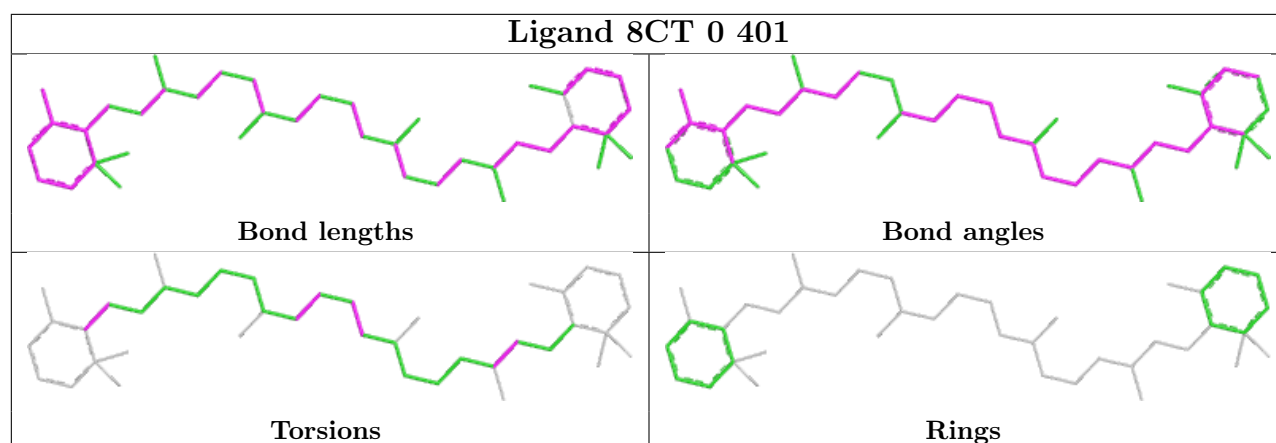
## Ligand CLA A 827



## Ligand CLA h 613

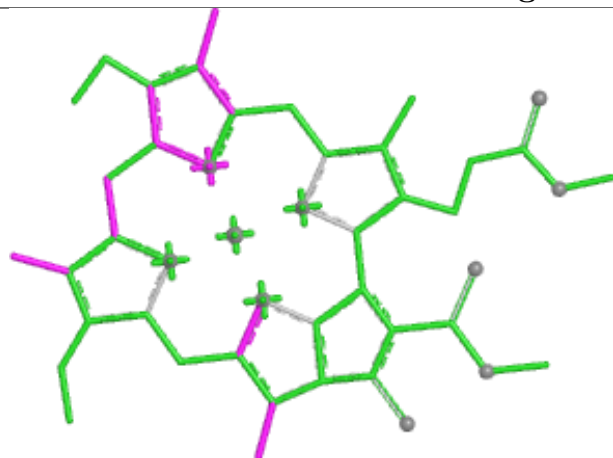




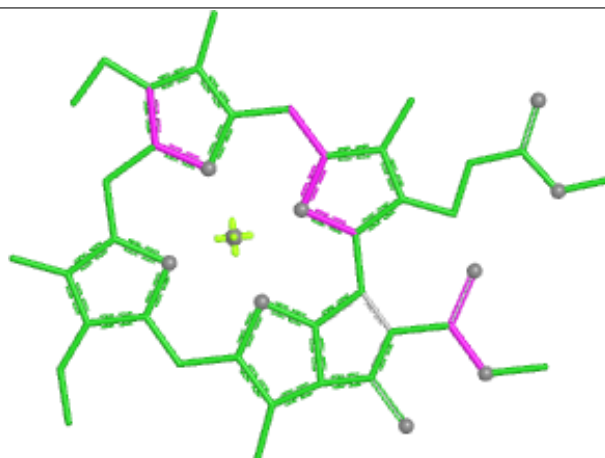




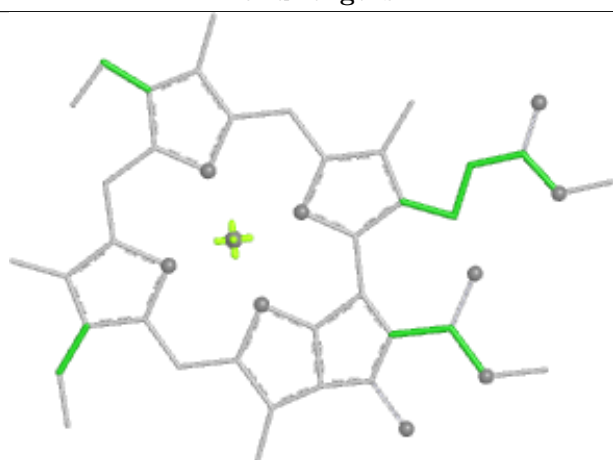
## Ligand CLA 3 318



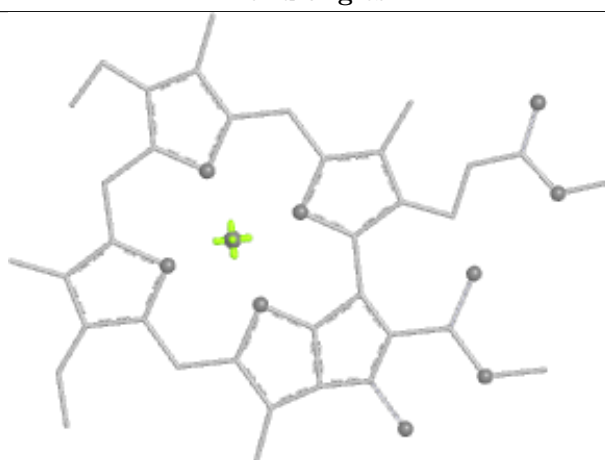
Bond lengths



Bond angles

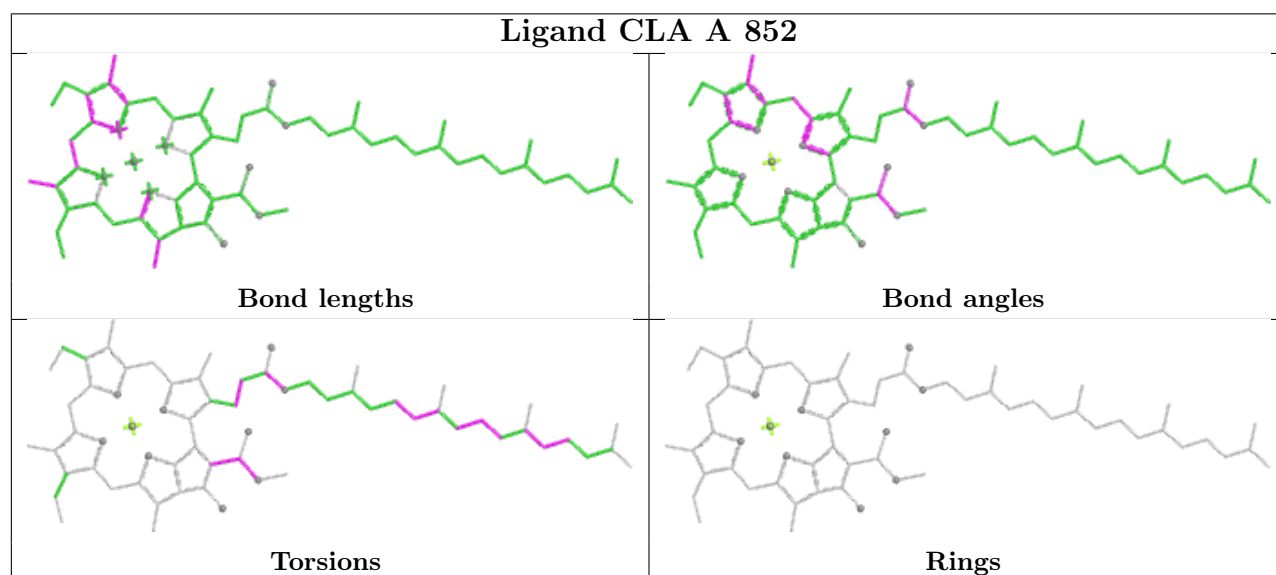
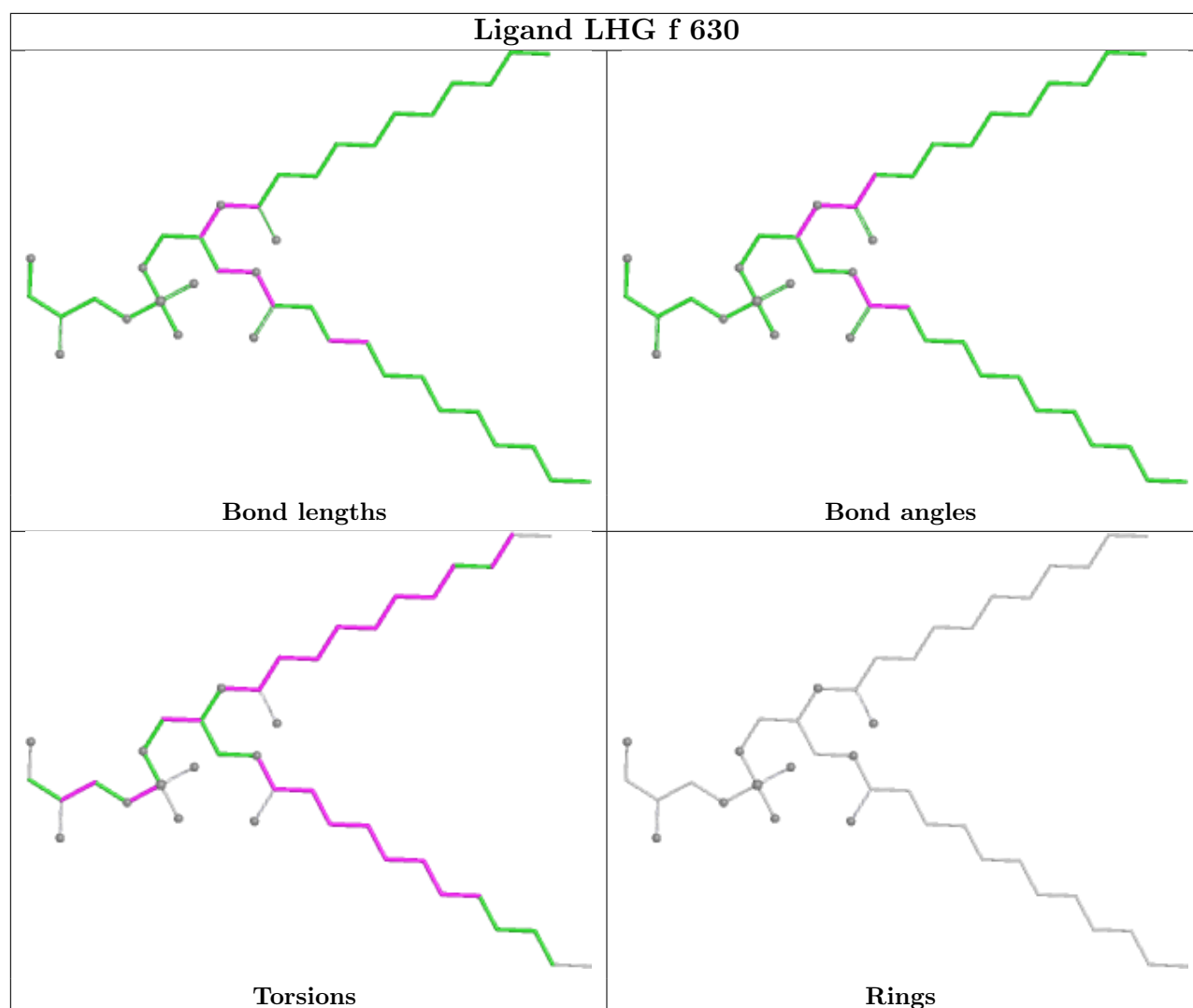


Torsions



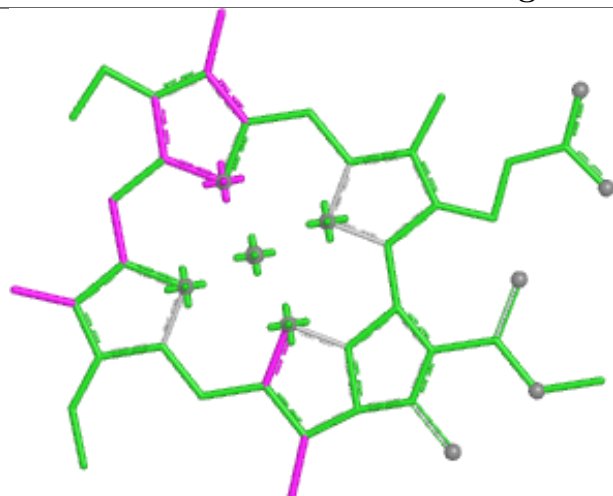
Rings



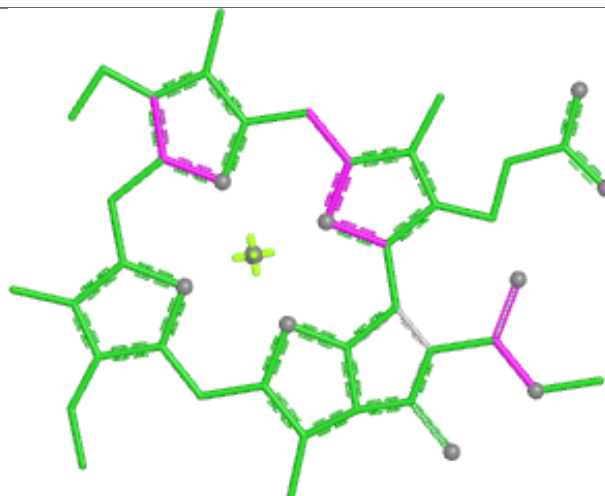




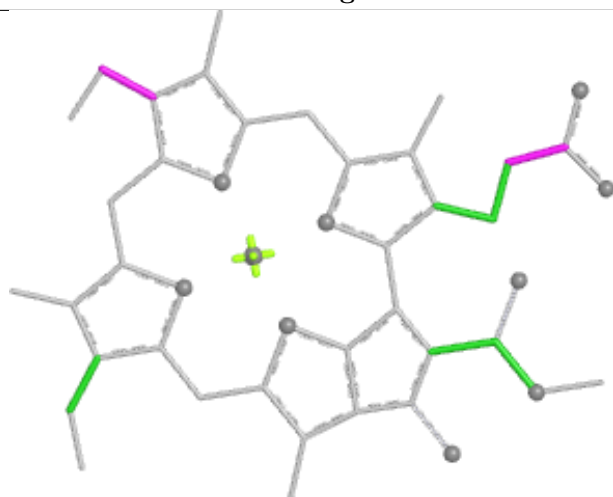
## Ligand CLA 4 303



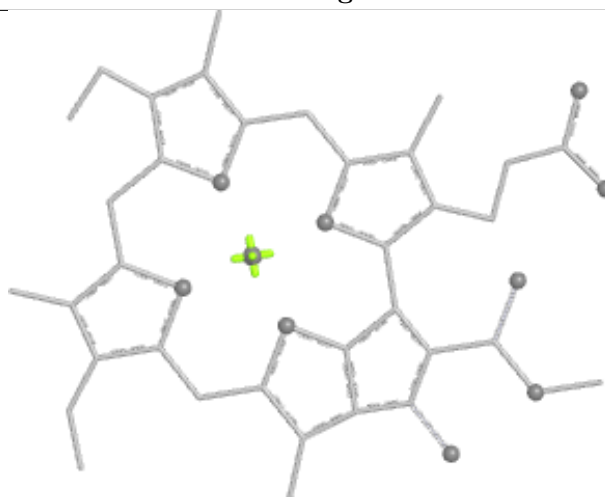
Bond lengths



Bond angles

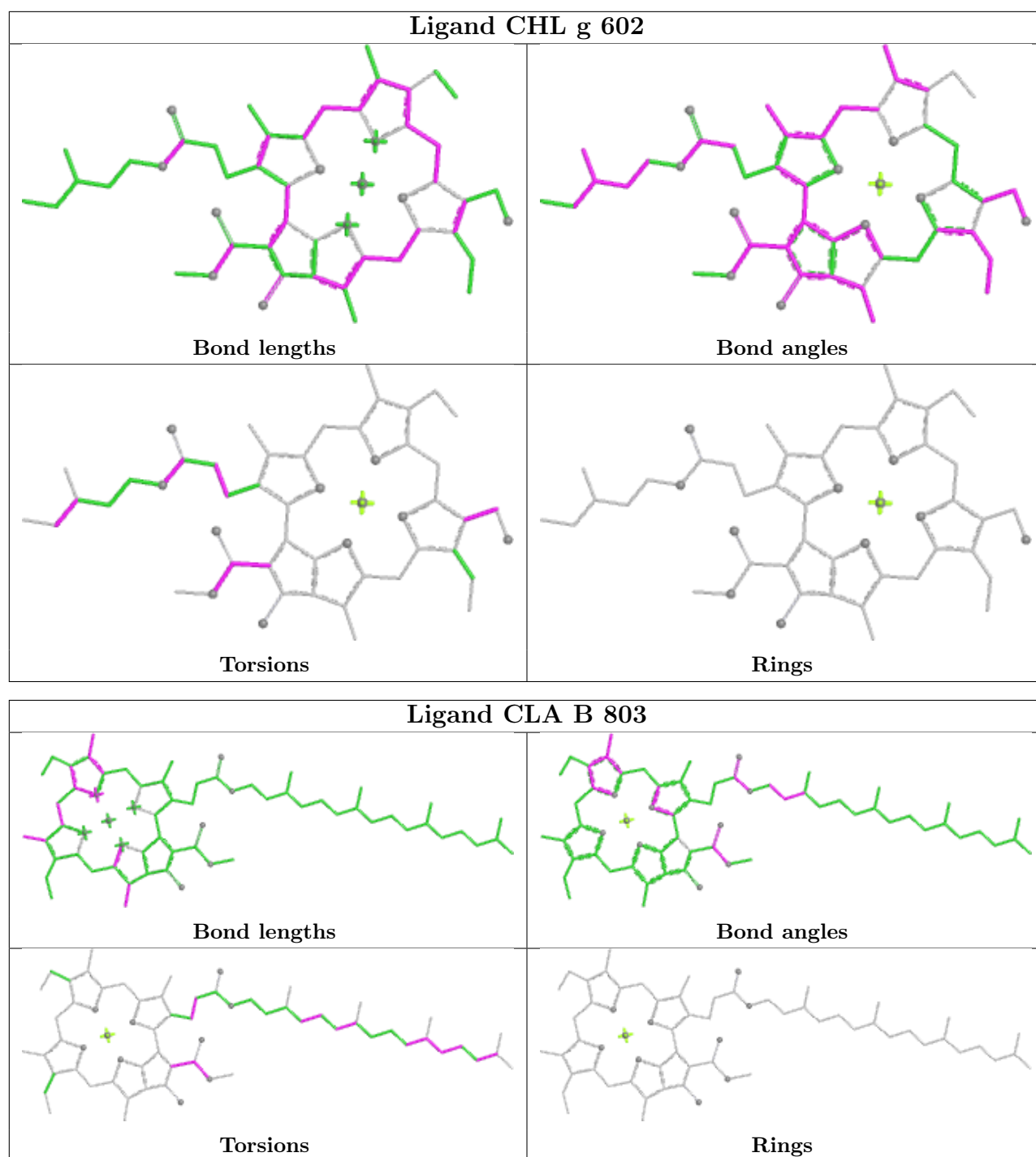


Torsions



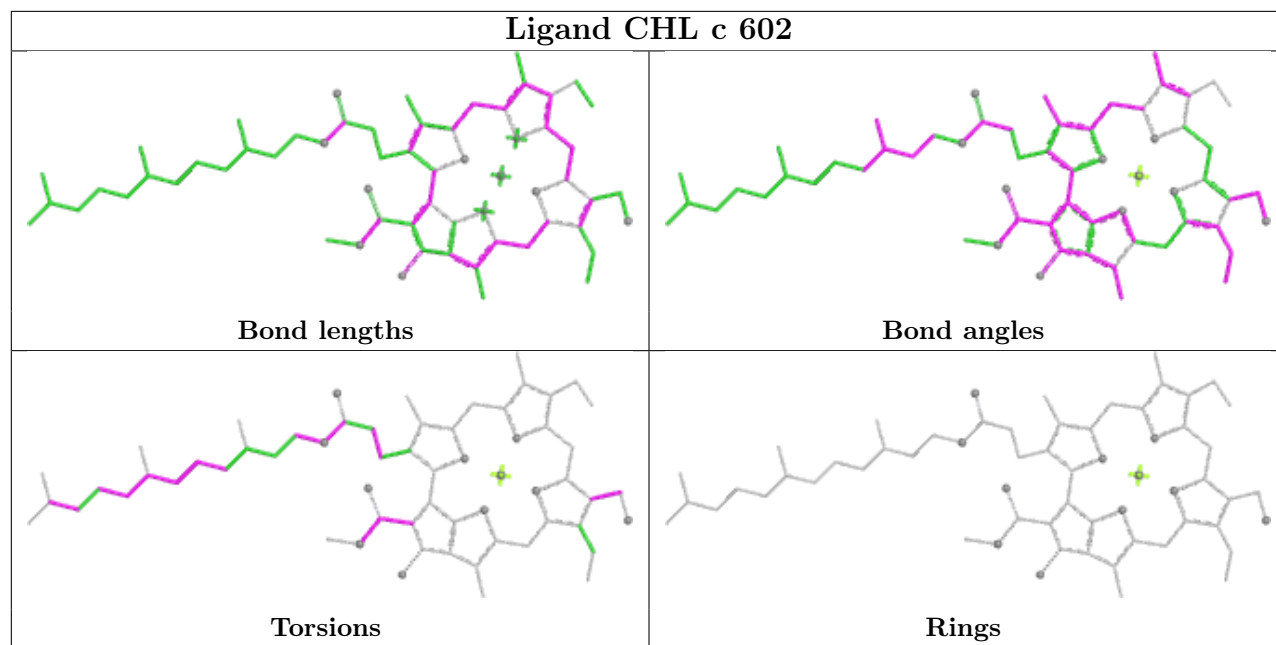
Rings



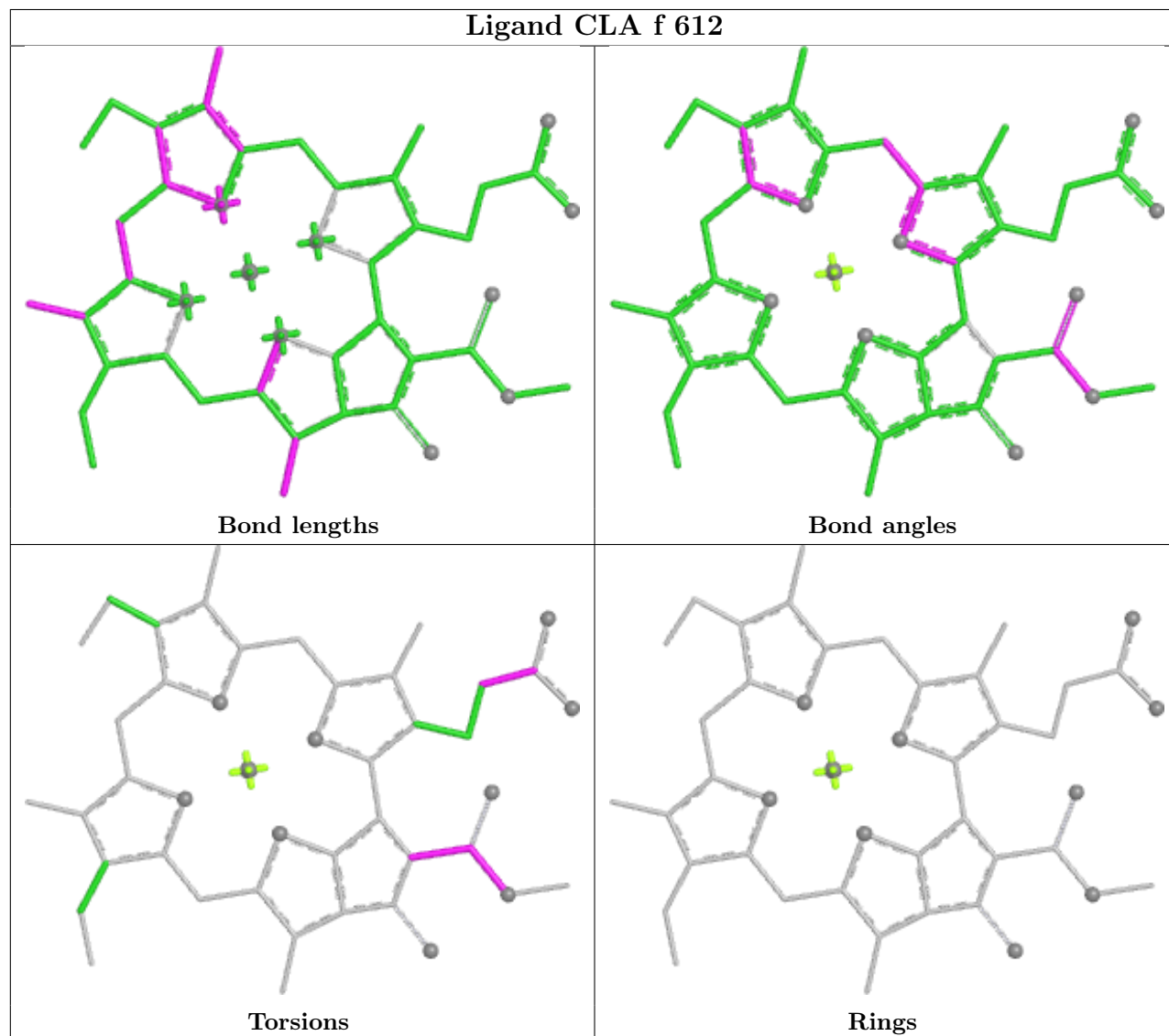




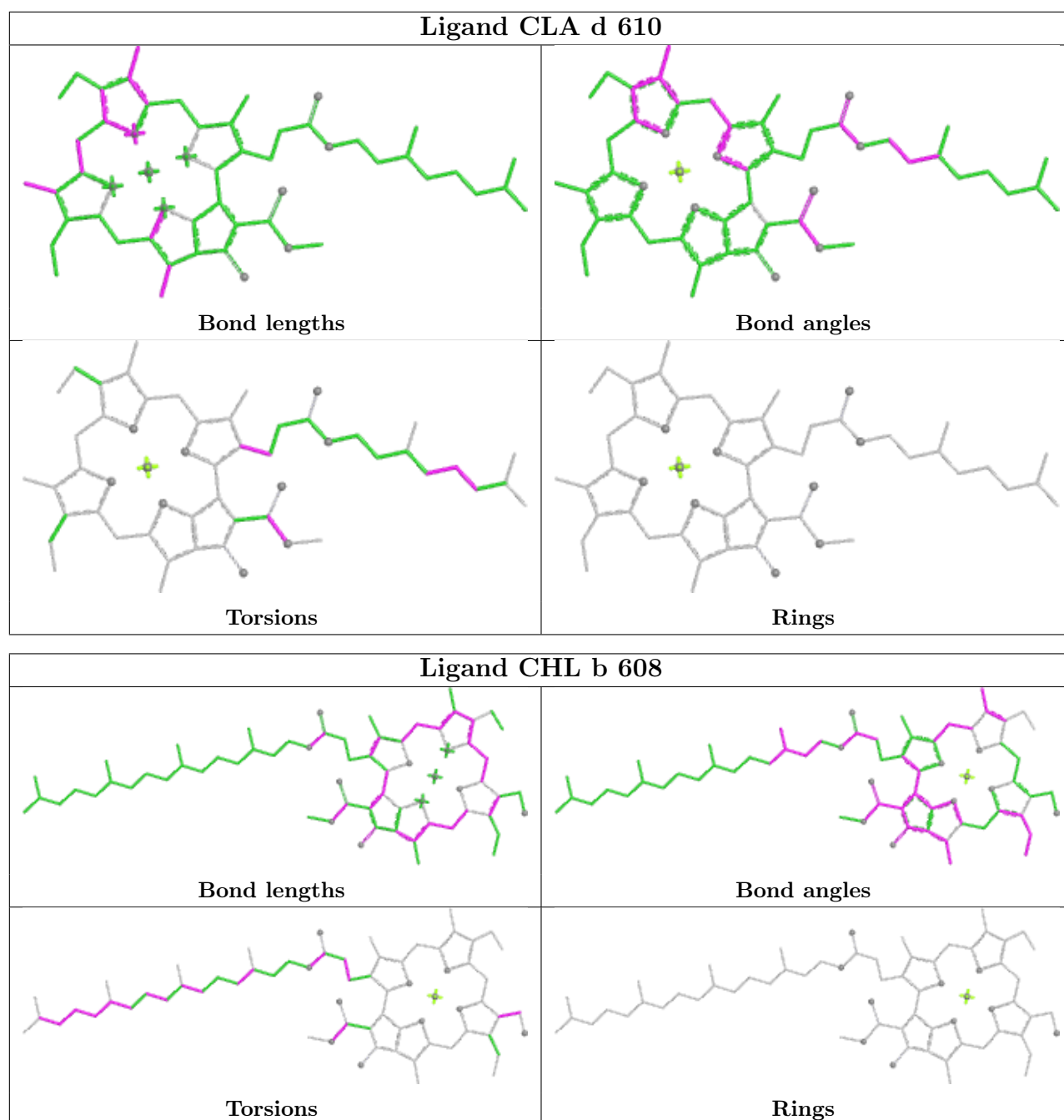
## Ligand CHL c 602



## Ligand CLA f 612

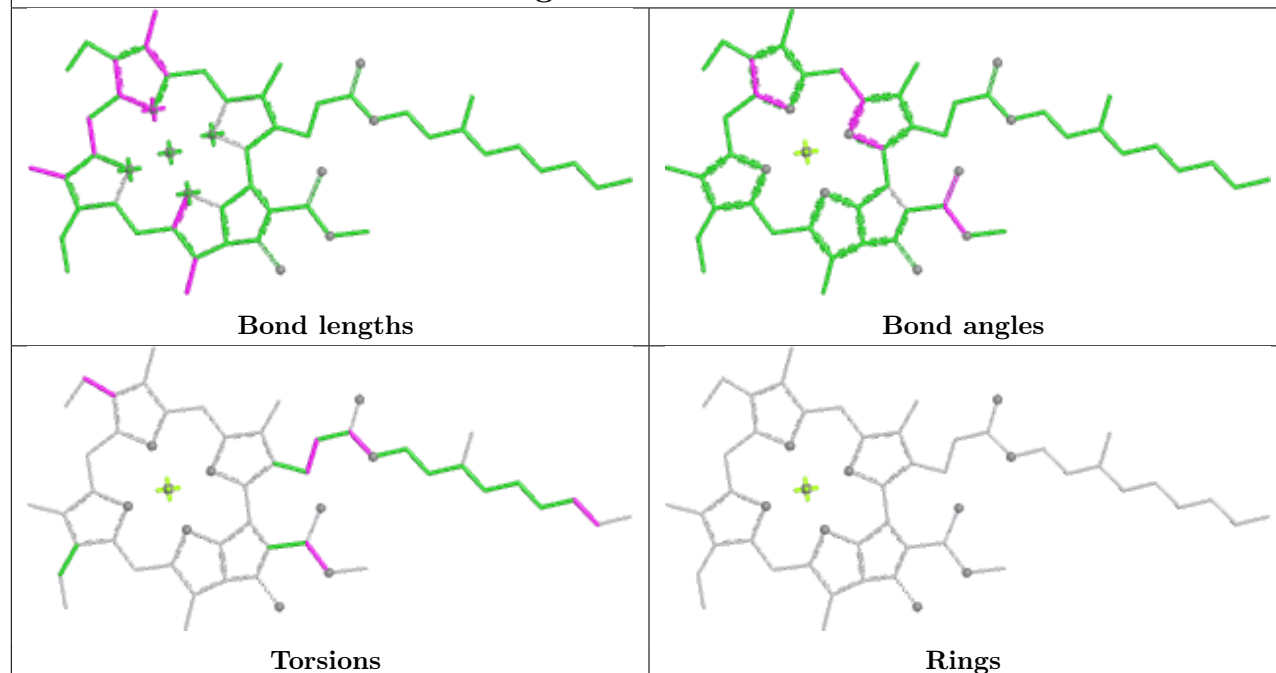




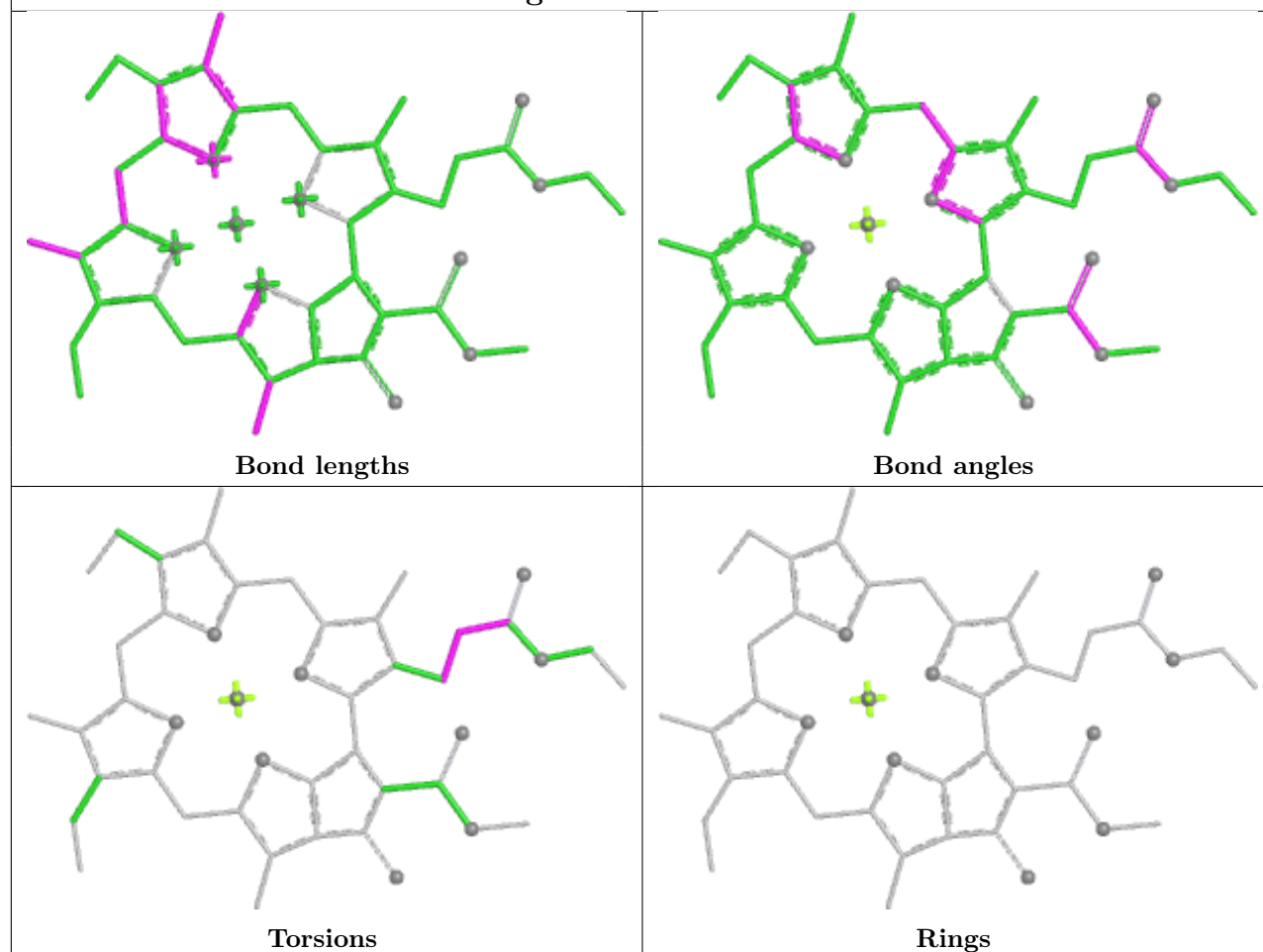




## Ligand CLA d 613

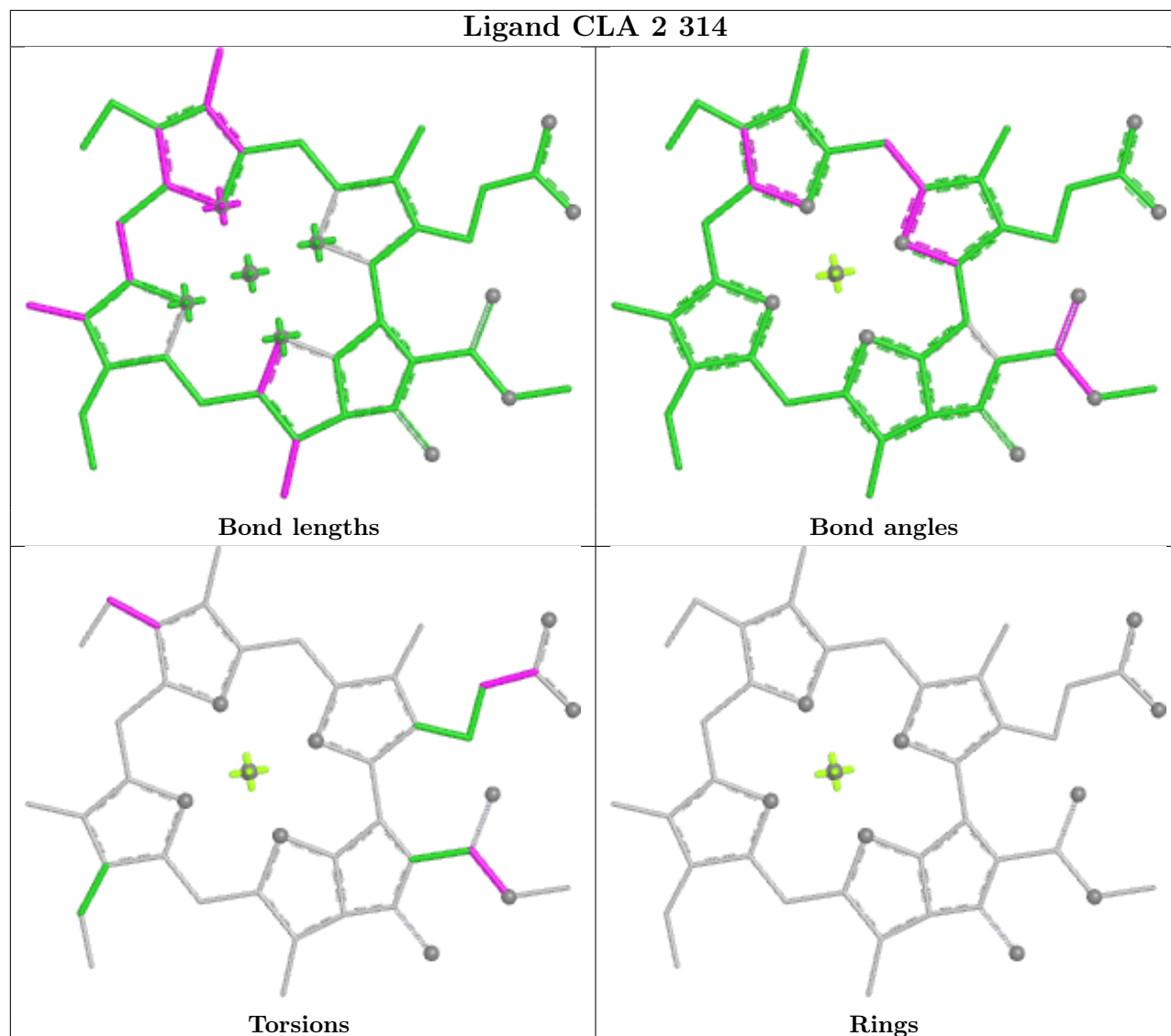


## Ligand CLA H 204

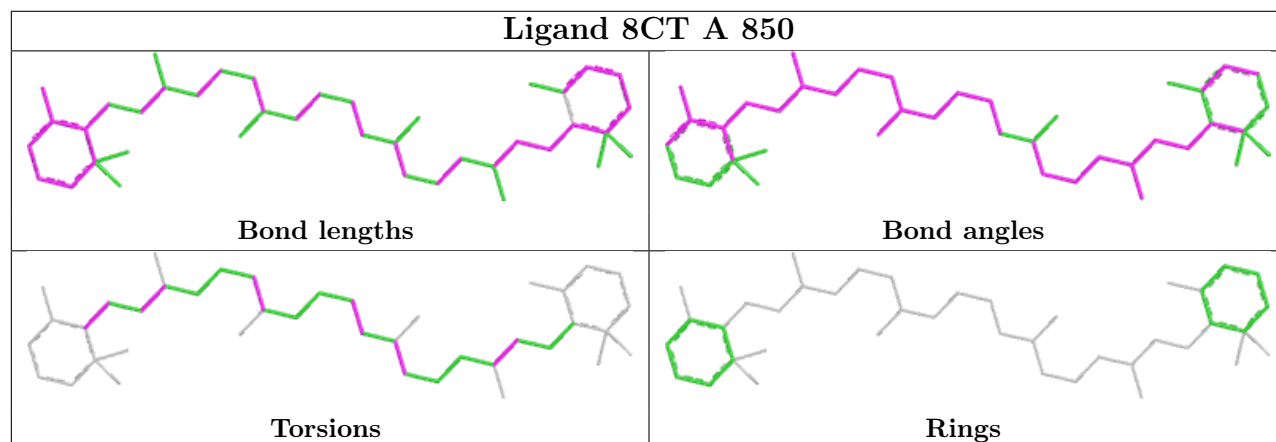




## Ligand CLA 2 314

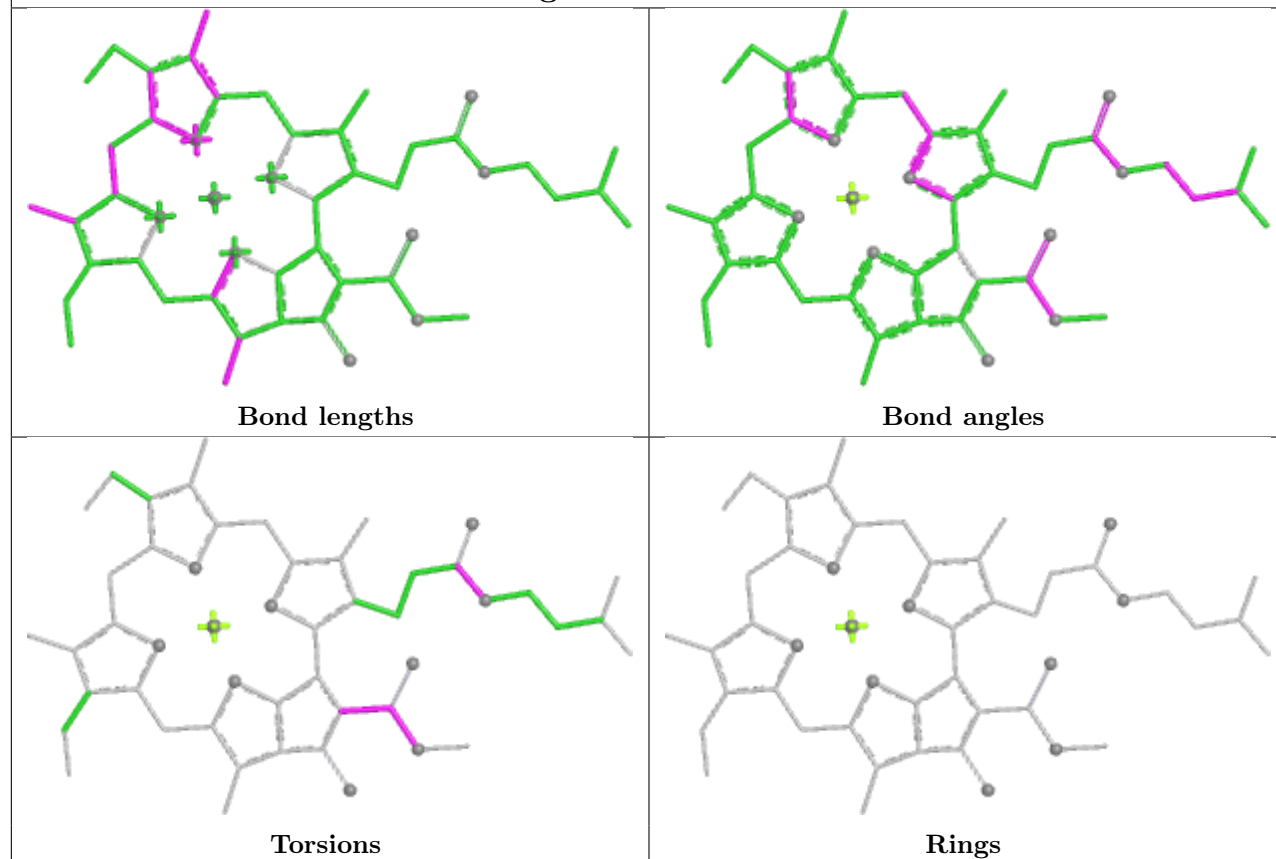


## Ligand 8CT A 850

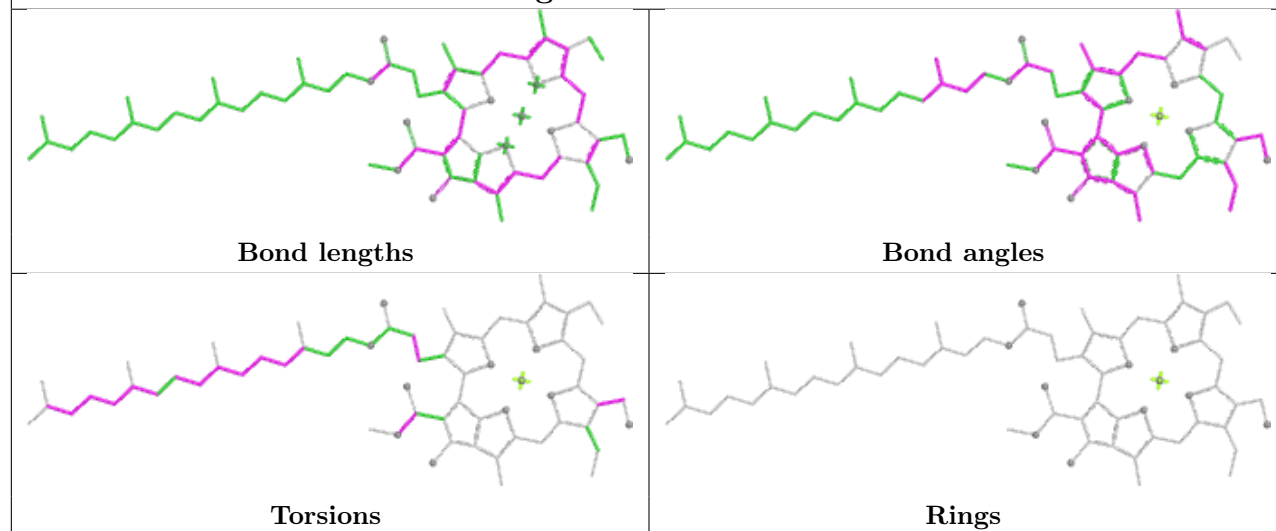




## Ligand CLA f 604

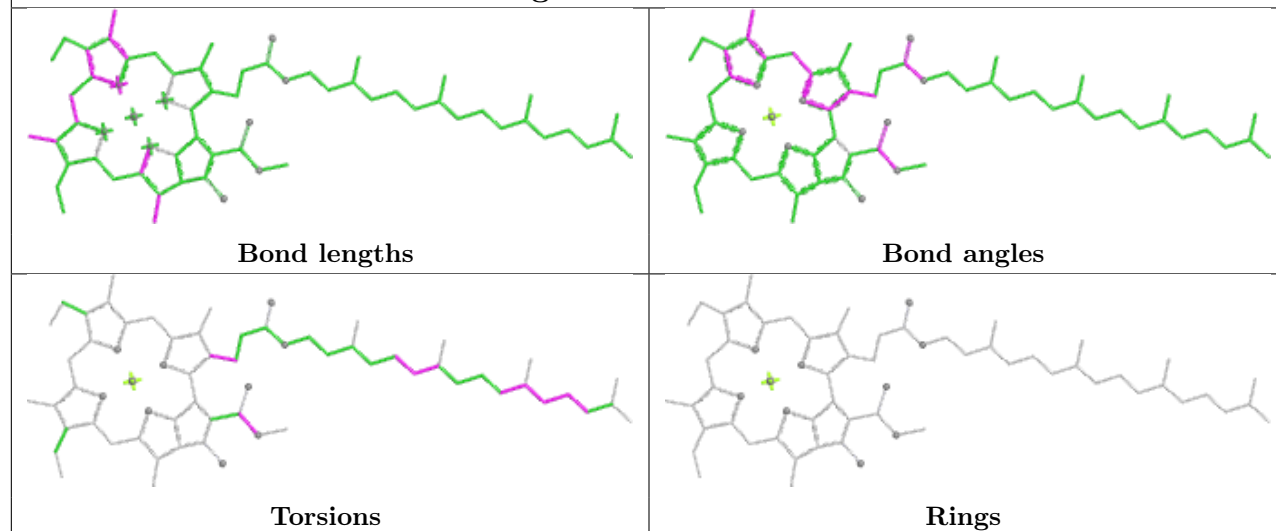


## Ligand CHL 1 307

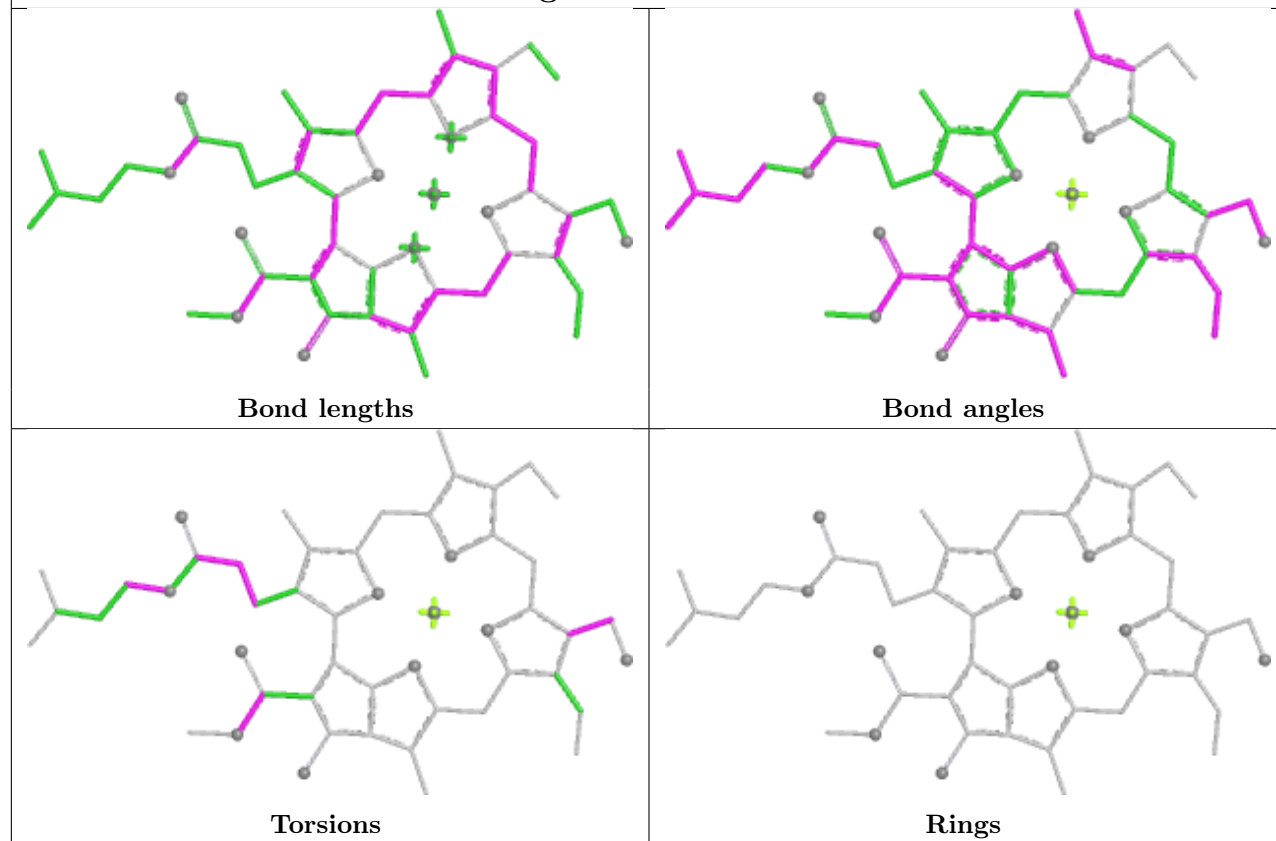




## Ligand CLA A 826

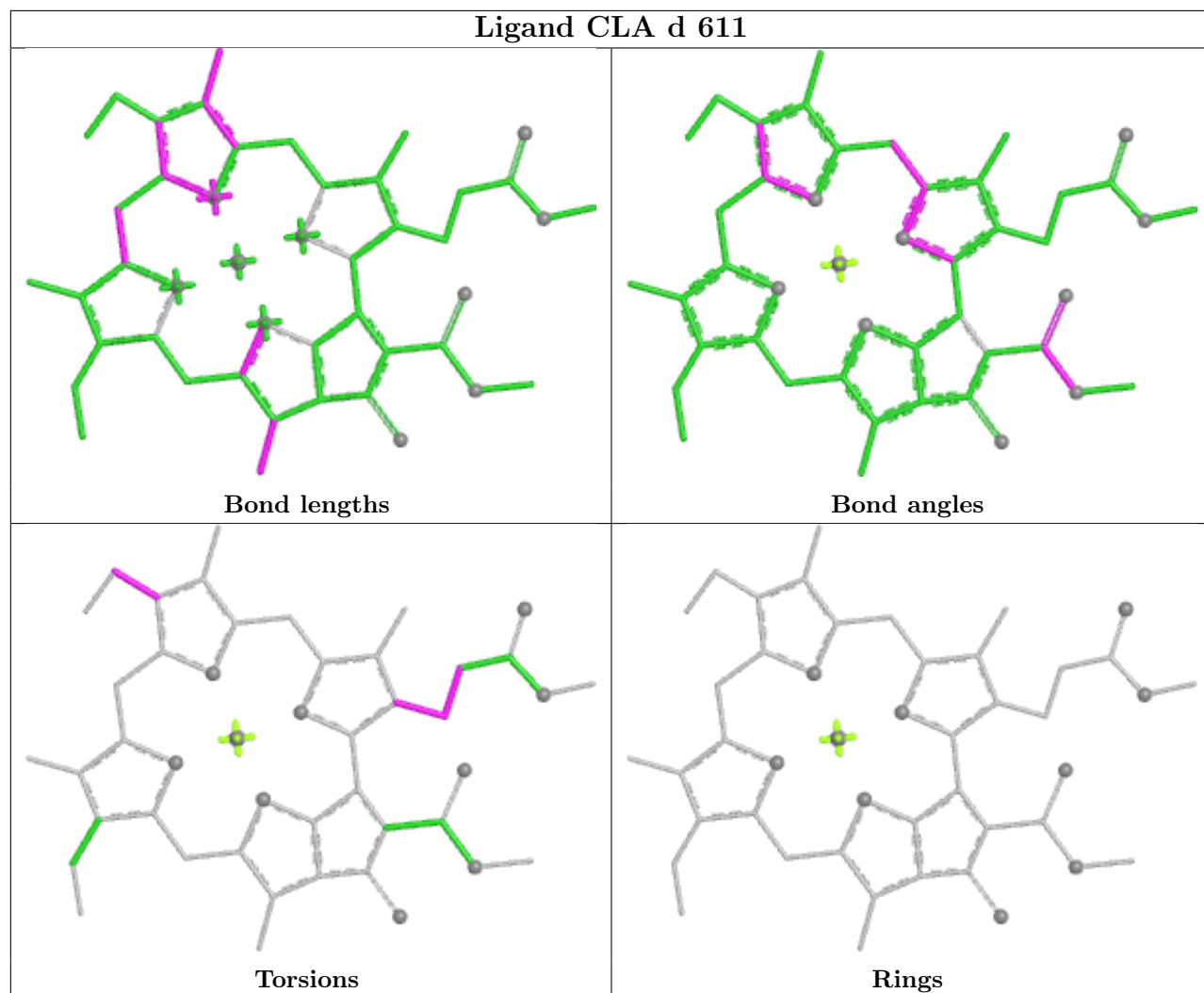


## Ligand CHL i 606

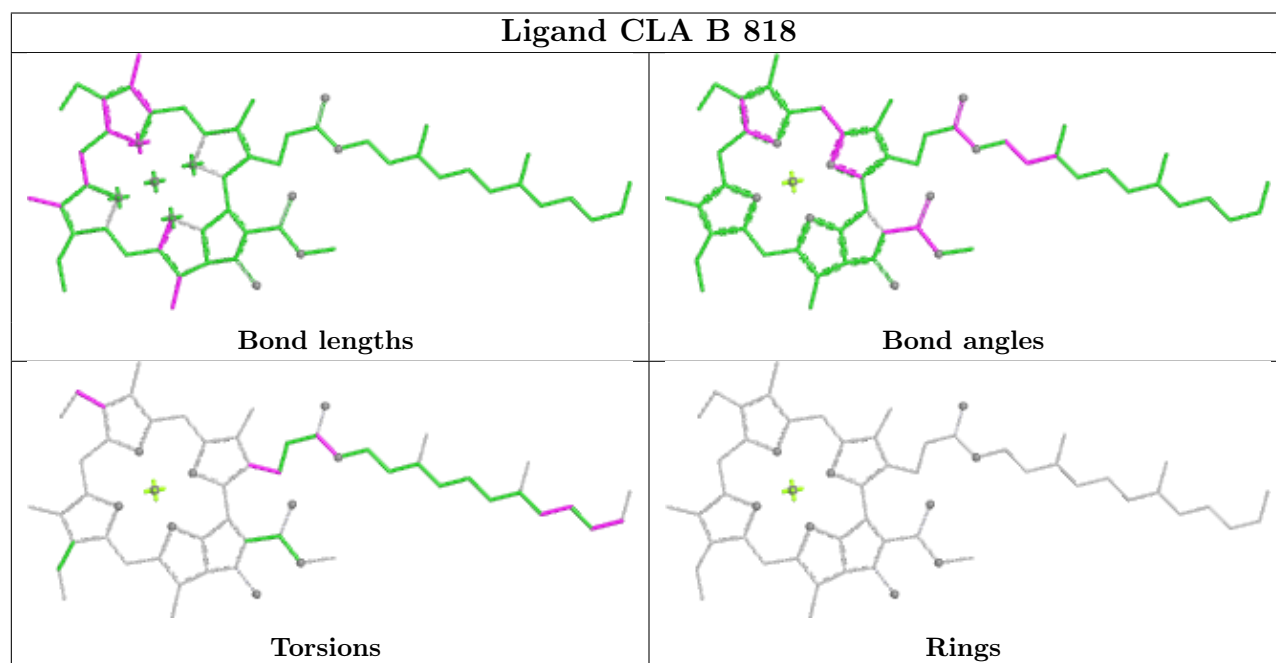
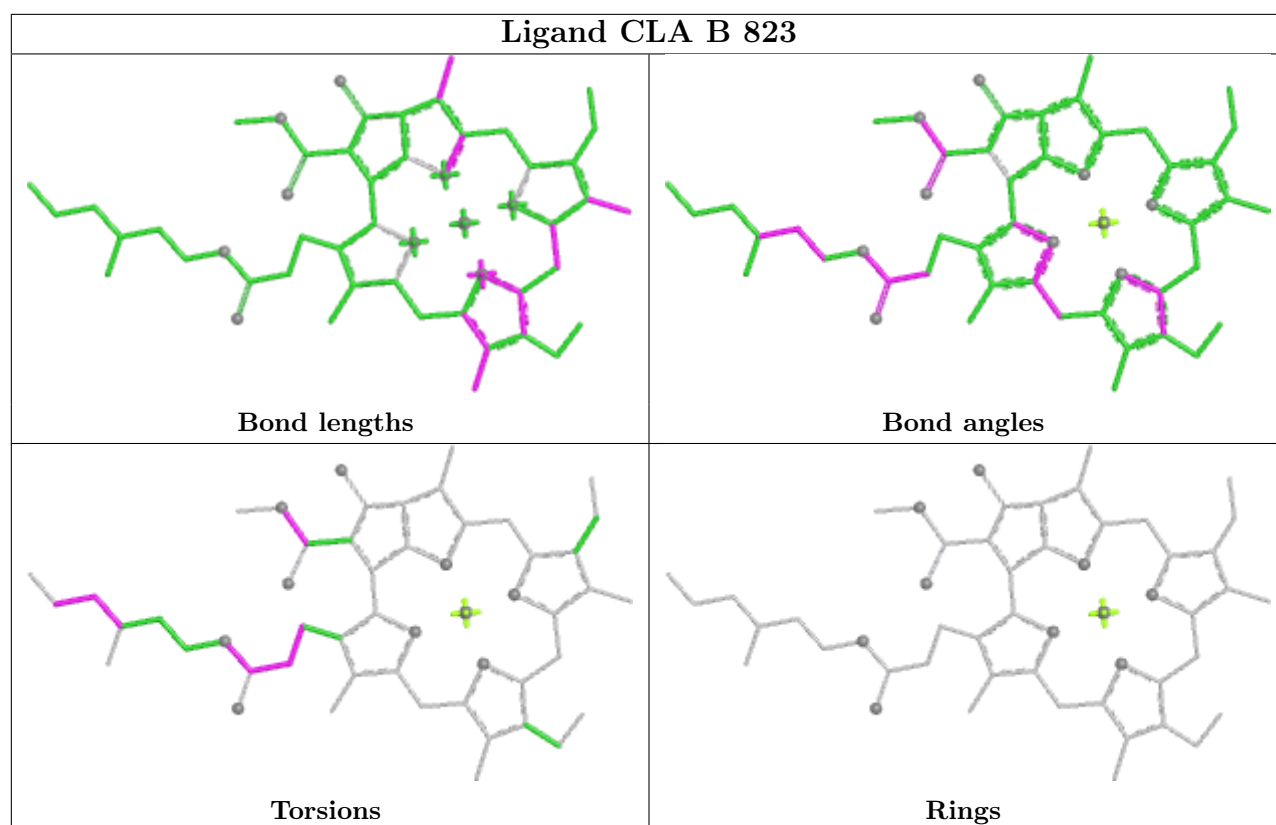




## Ligand CLA d 611

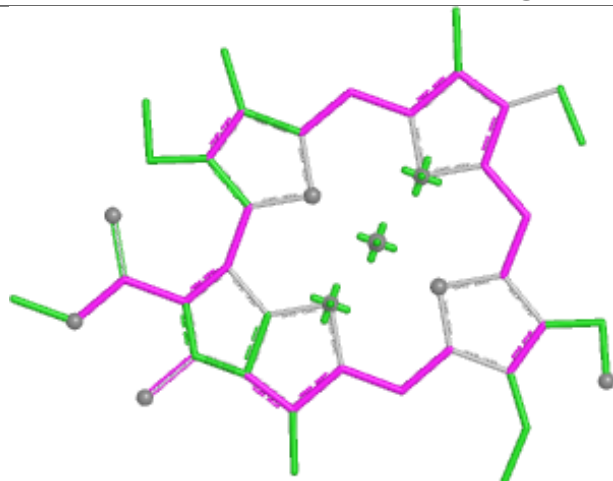




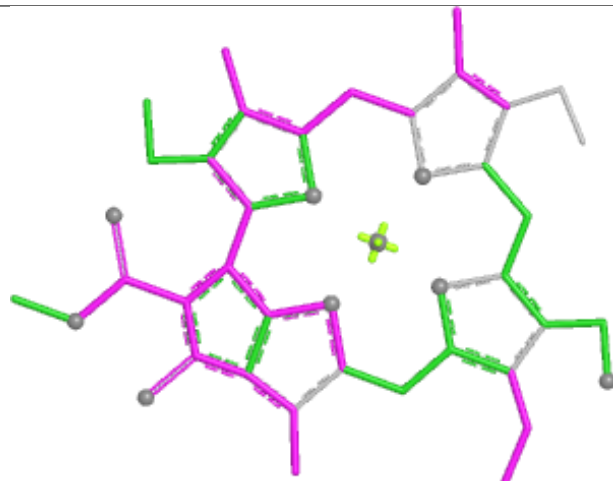




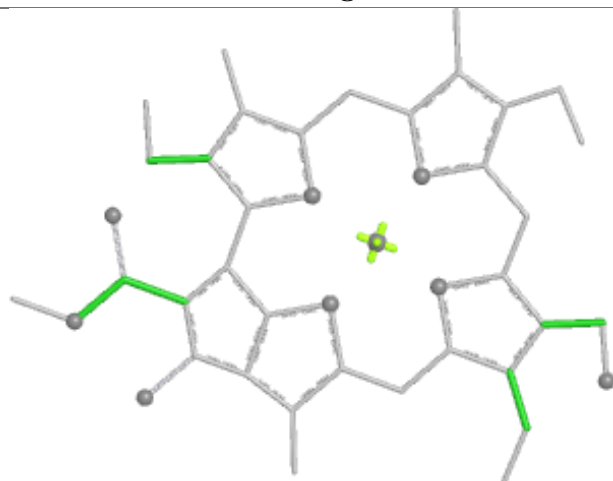
## Ligand CHL 6 305



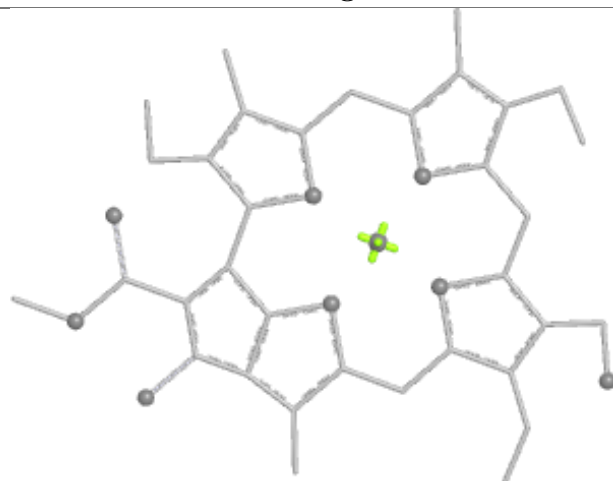
Bond lengths



Bond angles

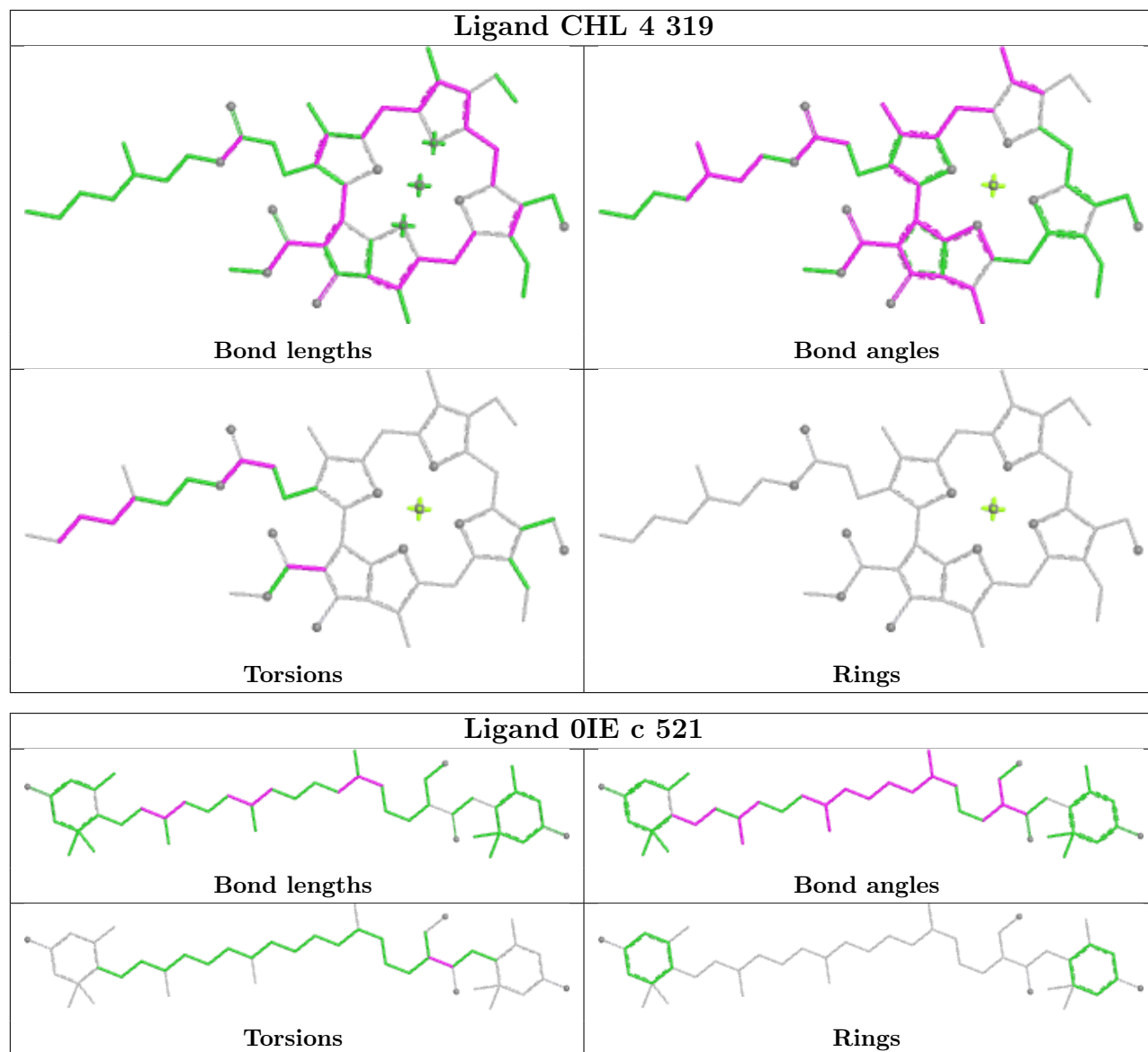


Torsions



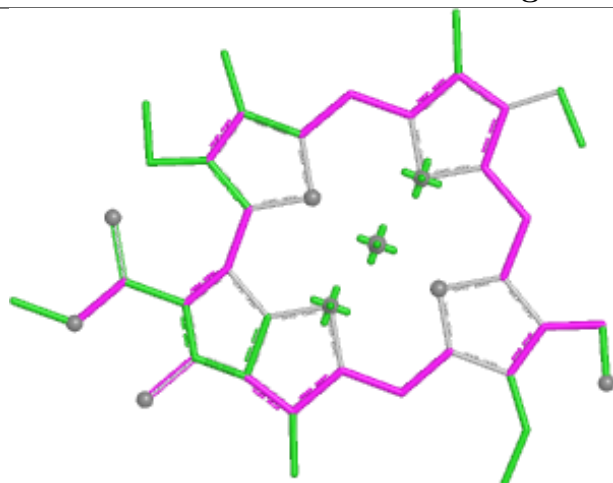
Rings



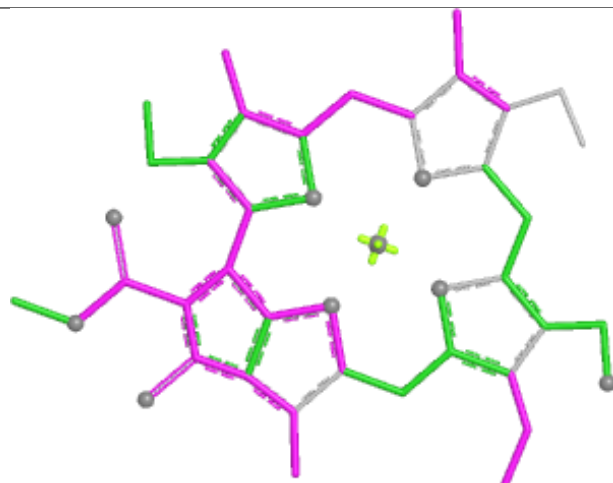




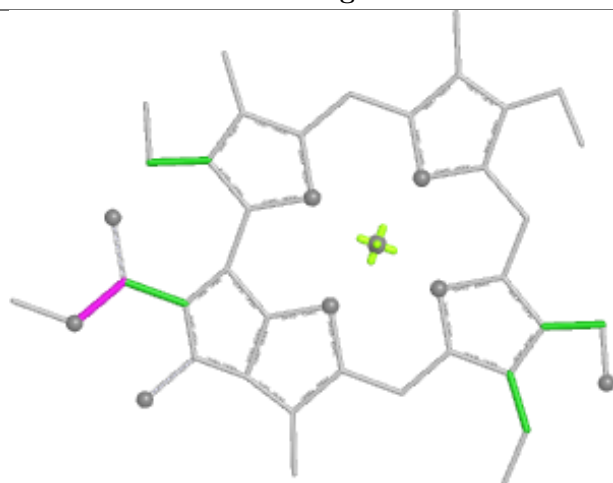
## Ligand CHL f 605



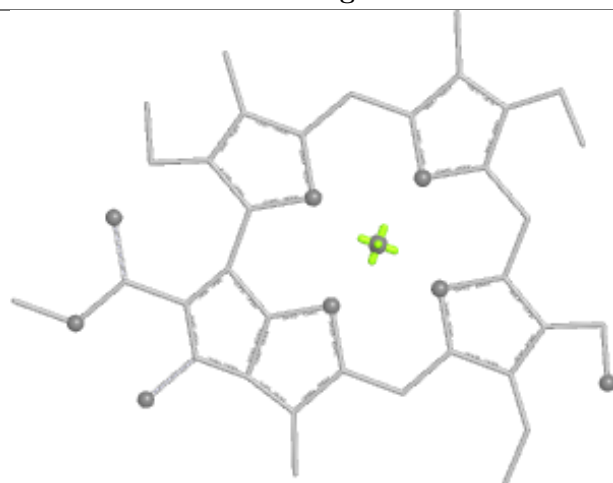
Bond lengths



Bond angles

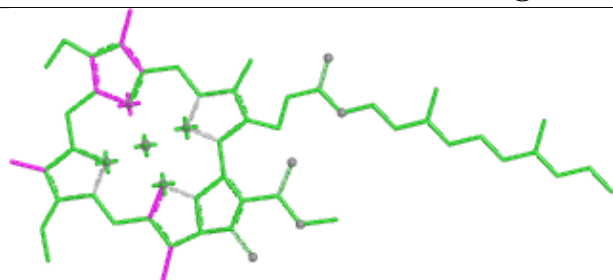


Torsions

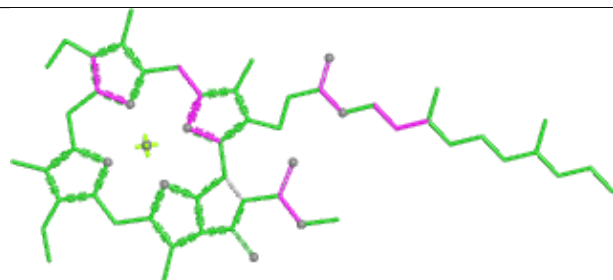


Rings

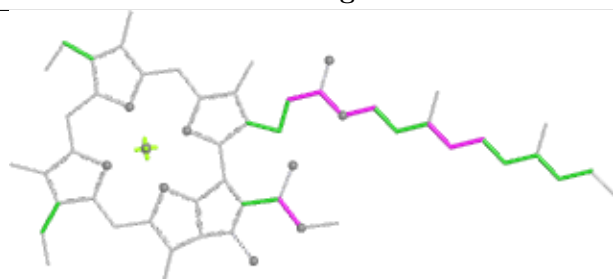
## Ligand CLA A 814



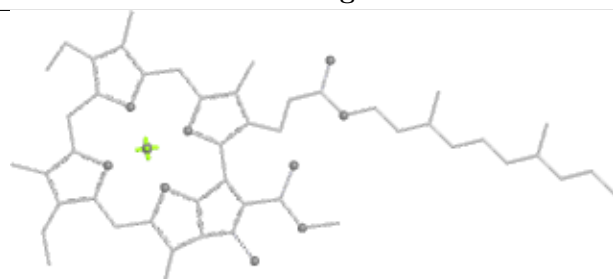
Bond lengths



Bond angles



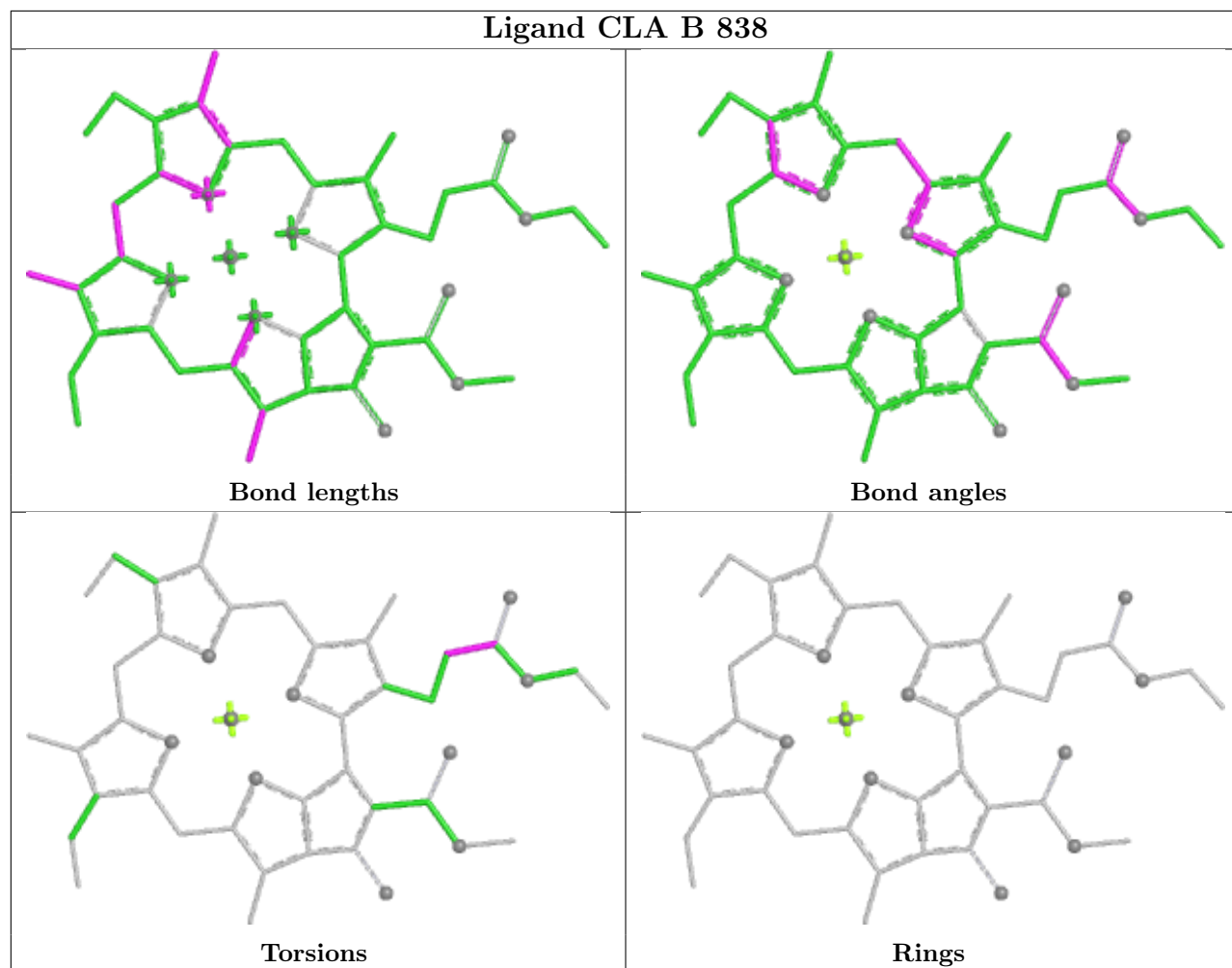
Torsions



Rings

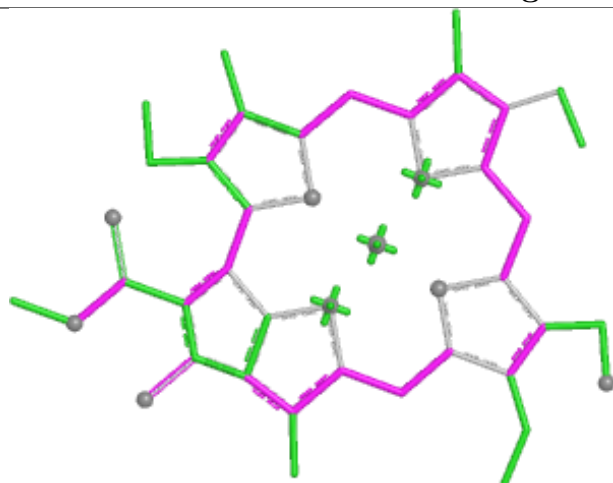


## Ligand CLA B 838

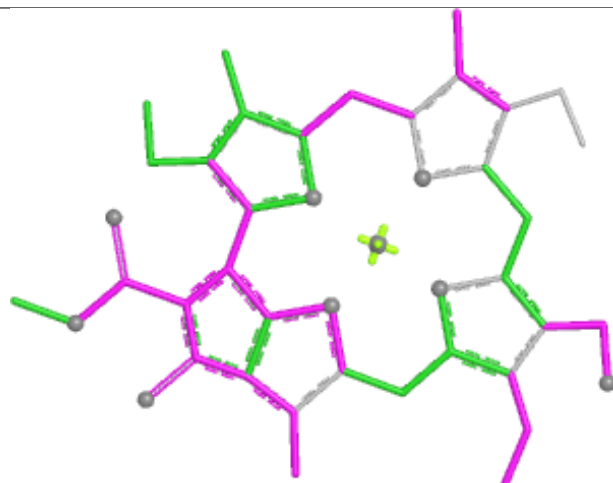




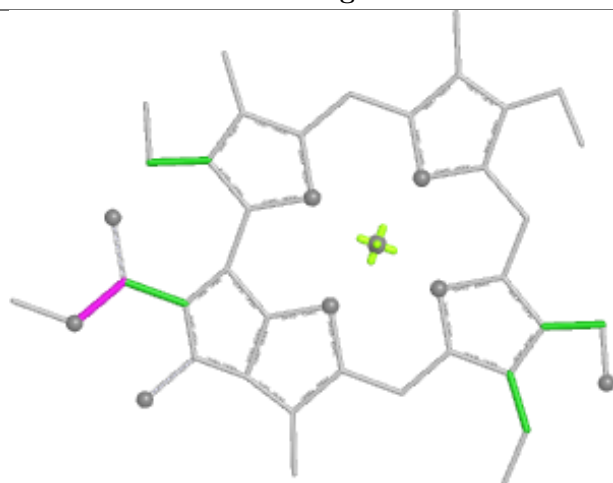
## Ligand CHL i 605



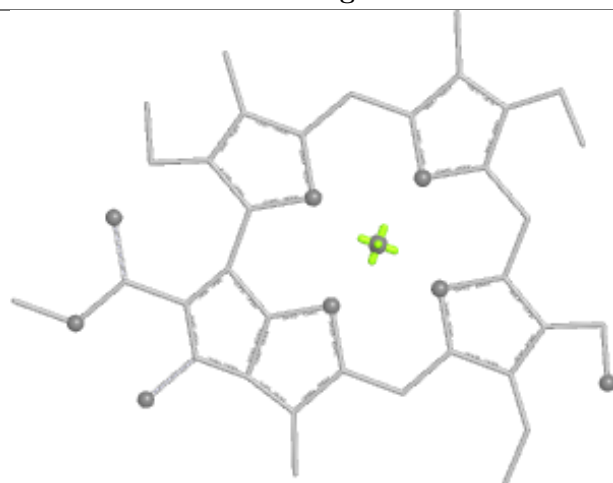
Bond lengths



Bond angles

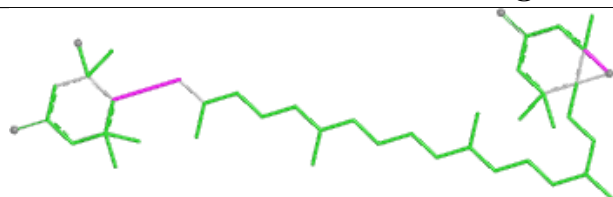


Torsions

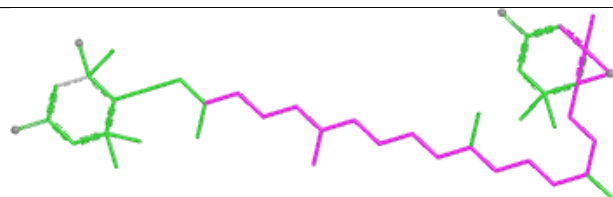


Rings

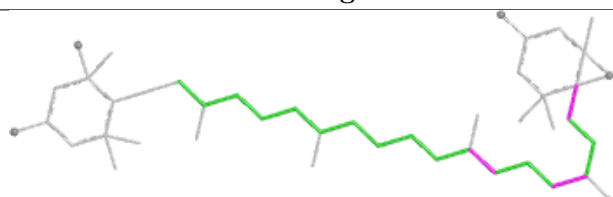
## Ligand NEX d 523



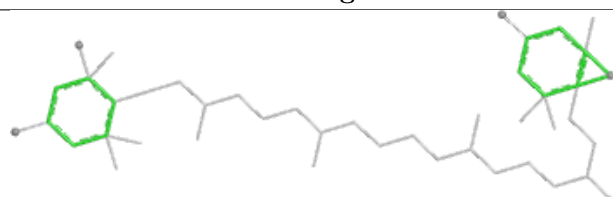
Bond lengths



Bond angles



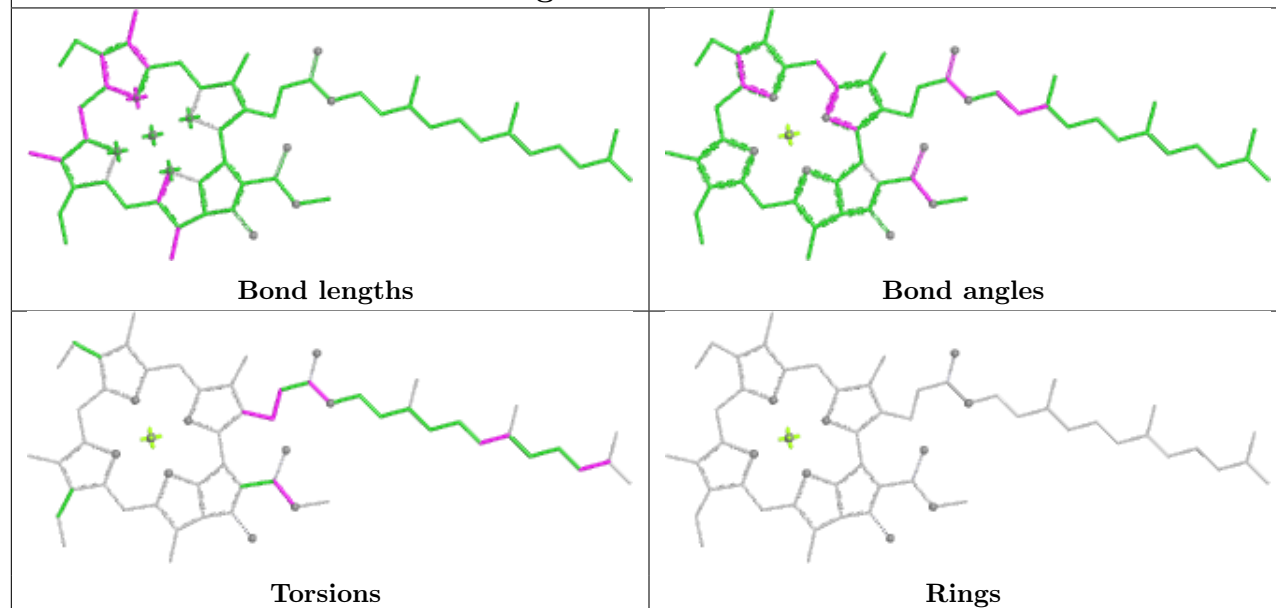
Torsions



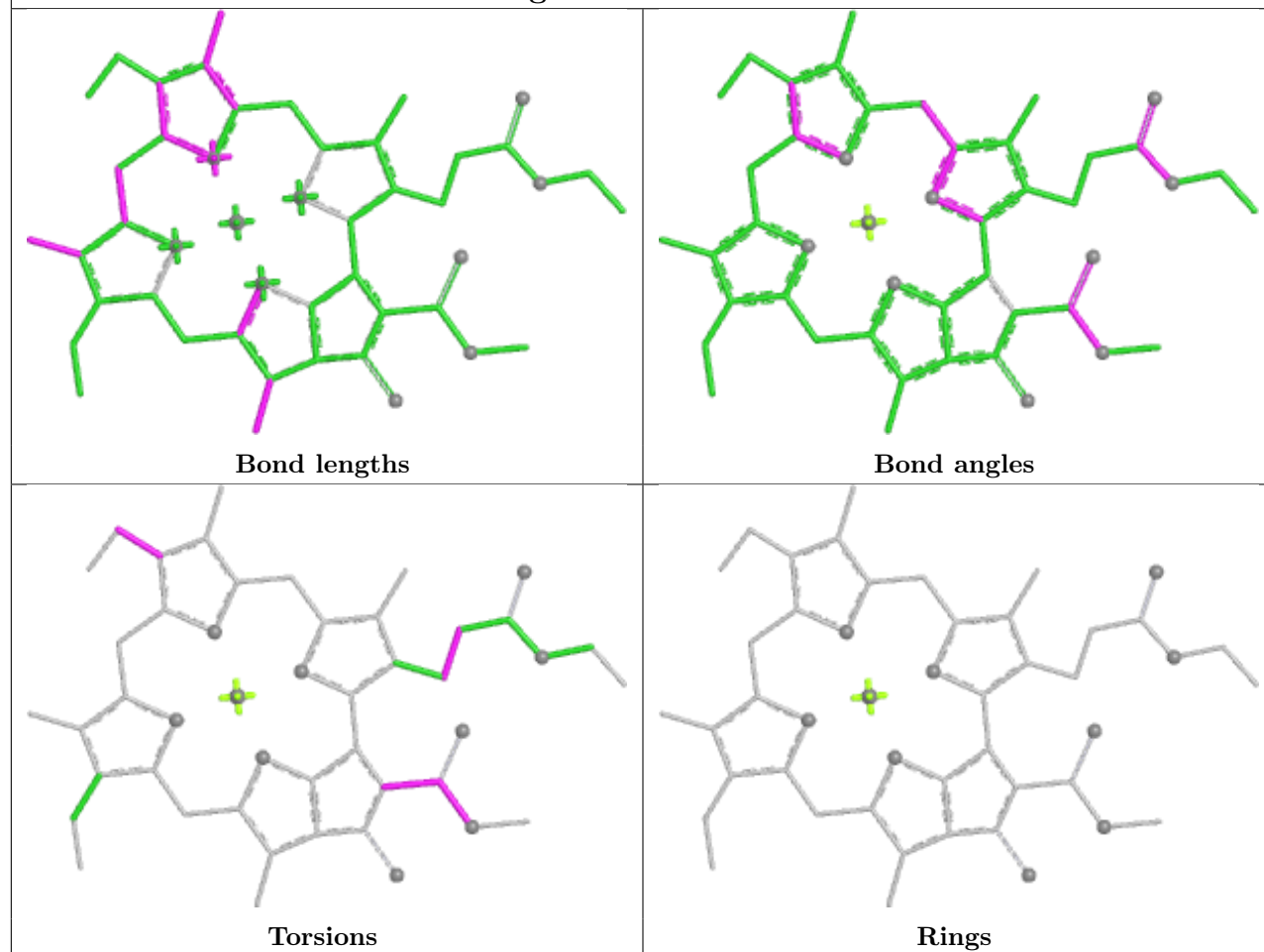
Rings



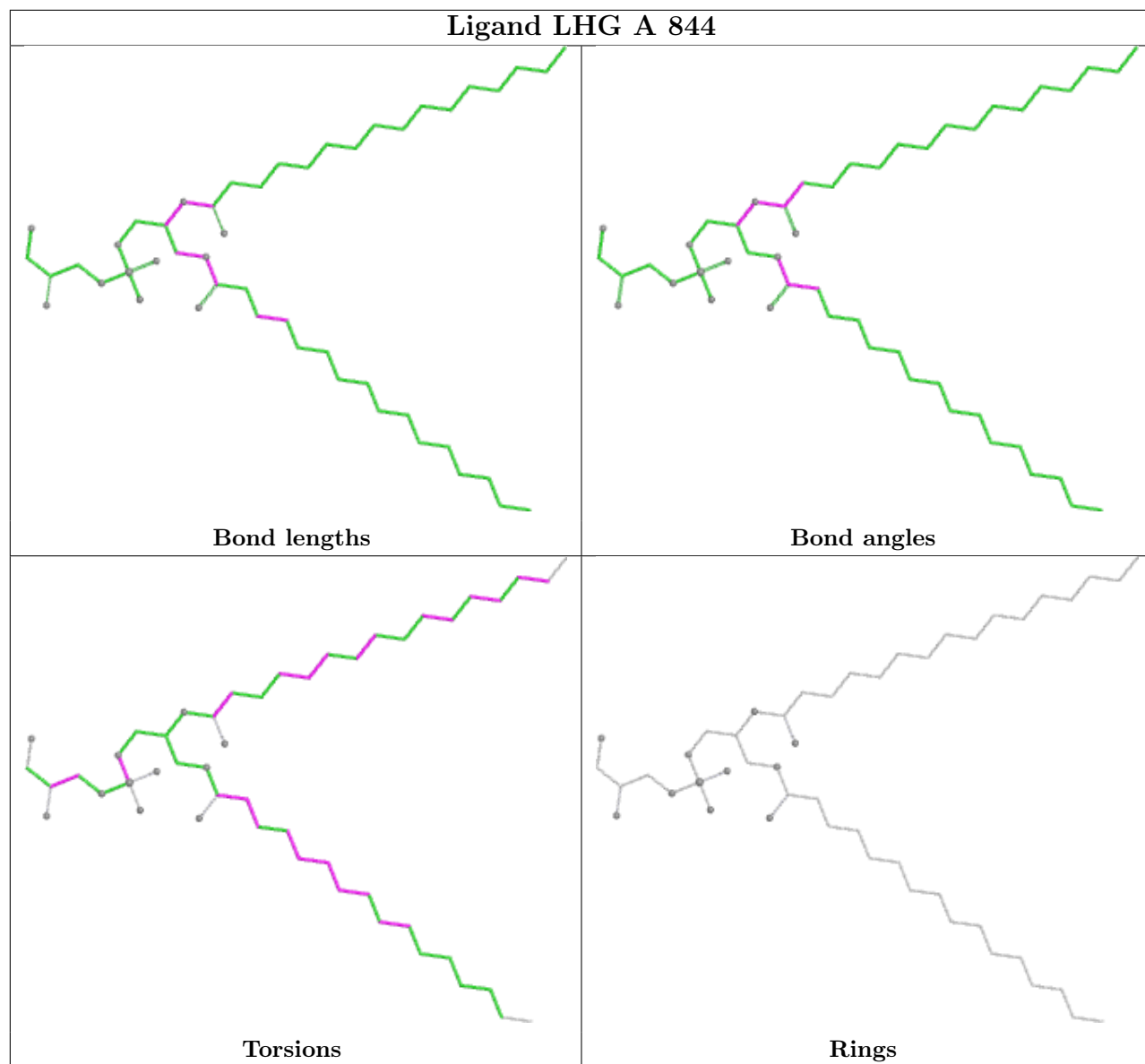
## Ligand CLA 7 318



## Ligand CLA L 207

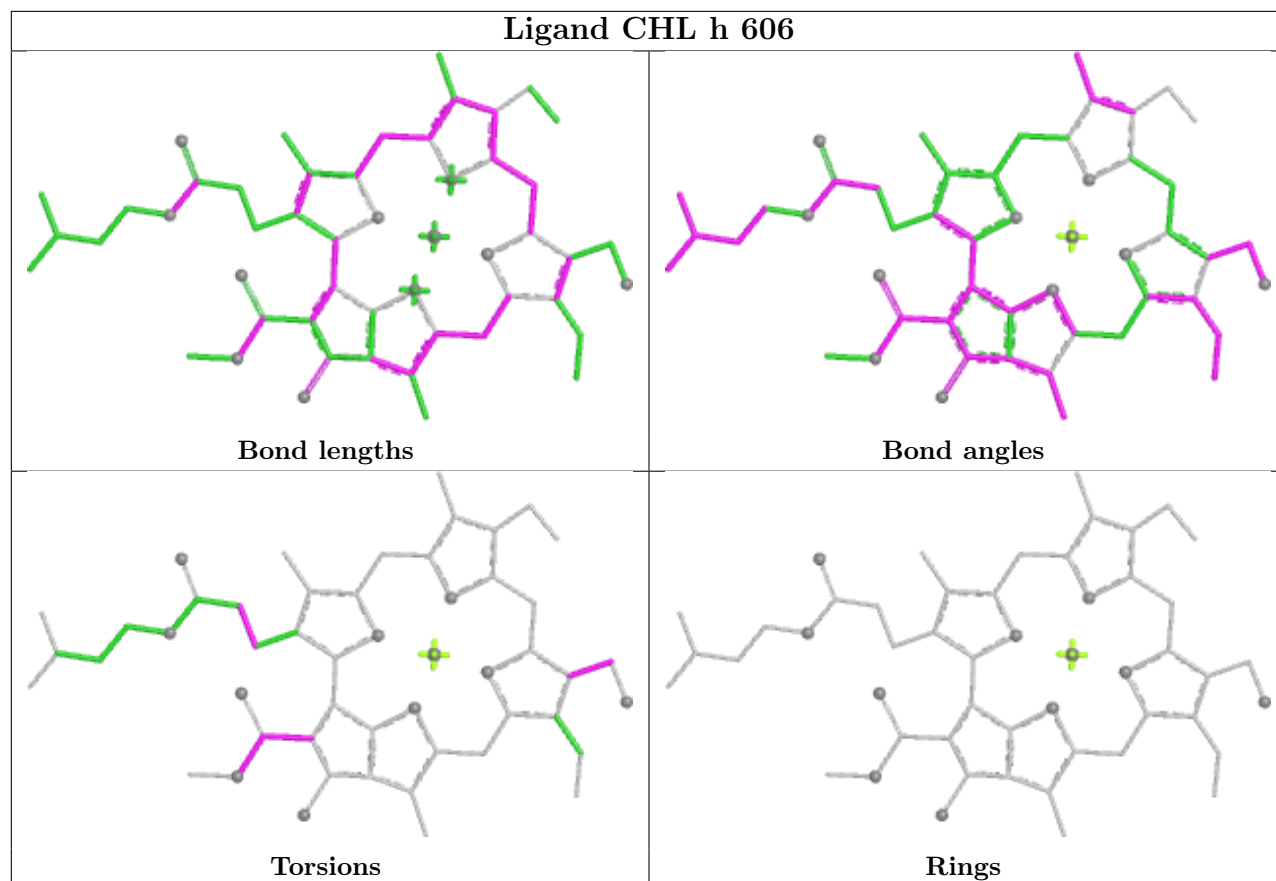




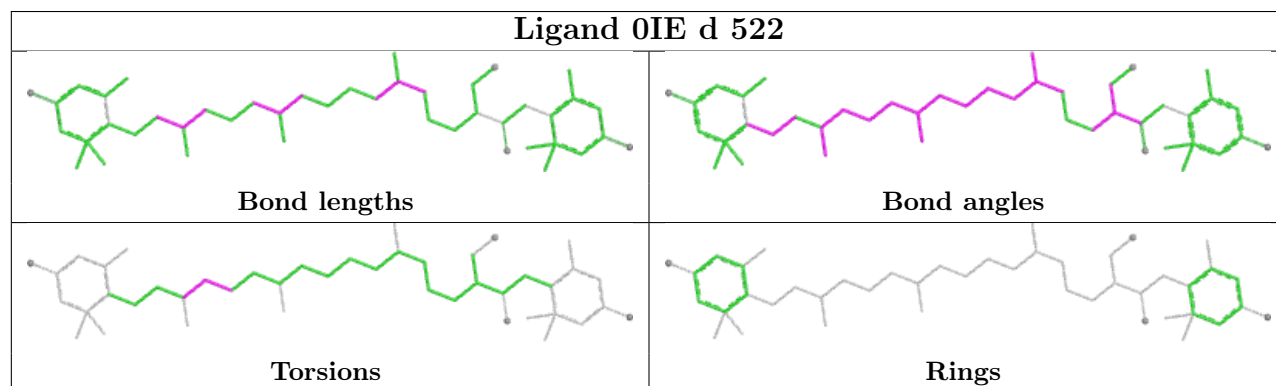




## Ligand CHL h 606

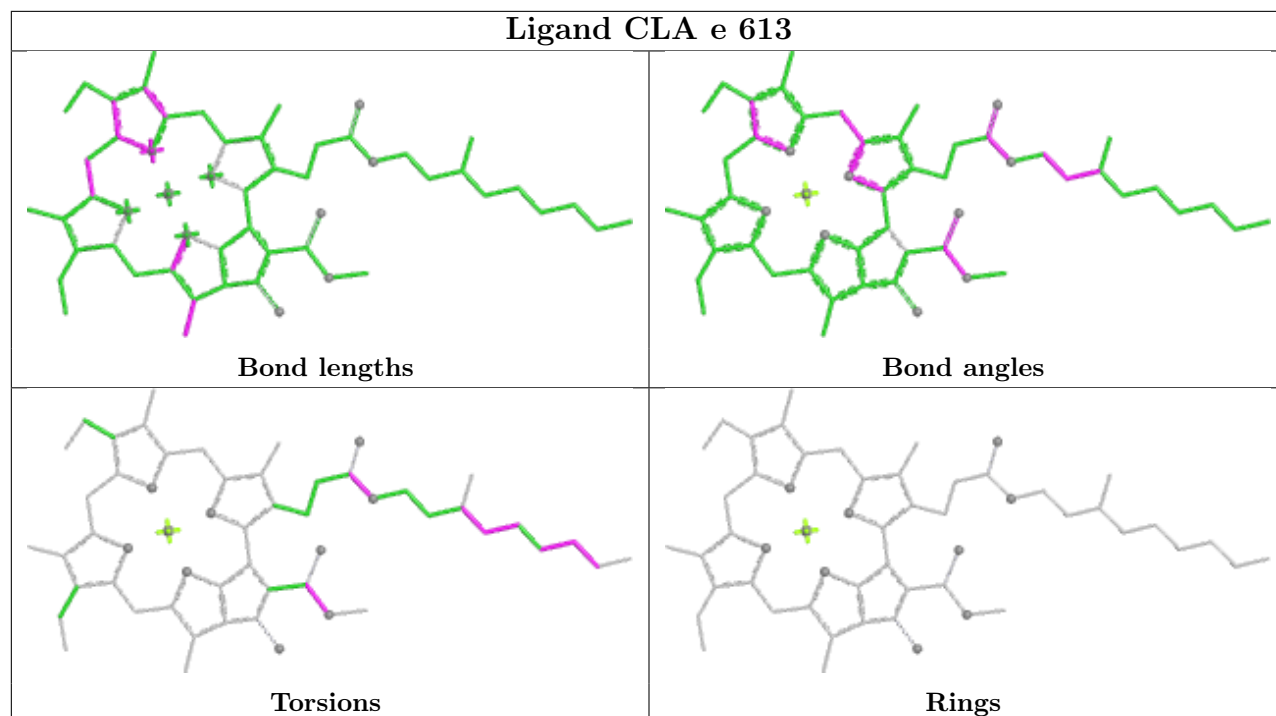


## Ligand OIE d 522

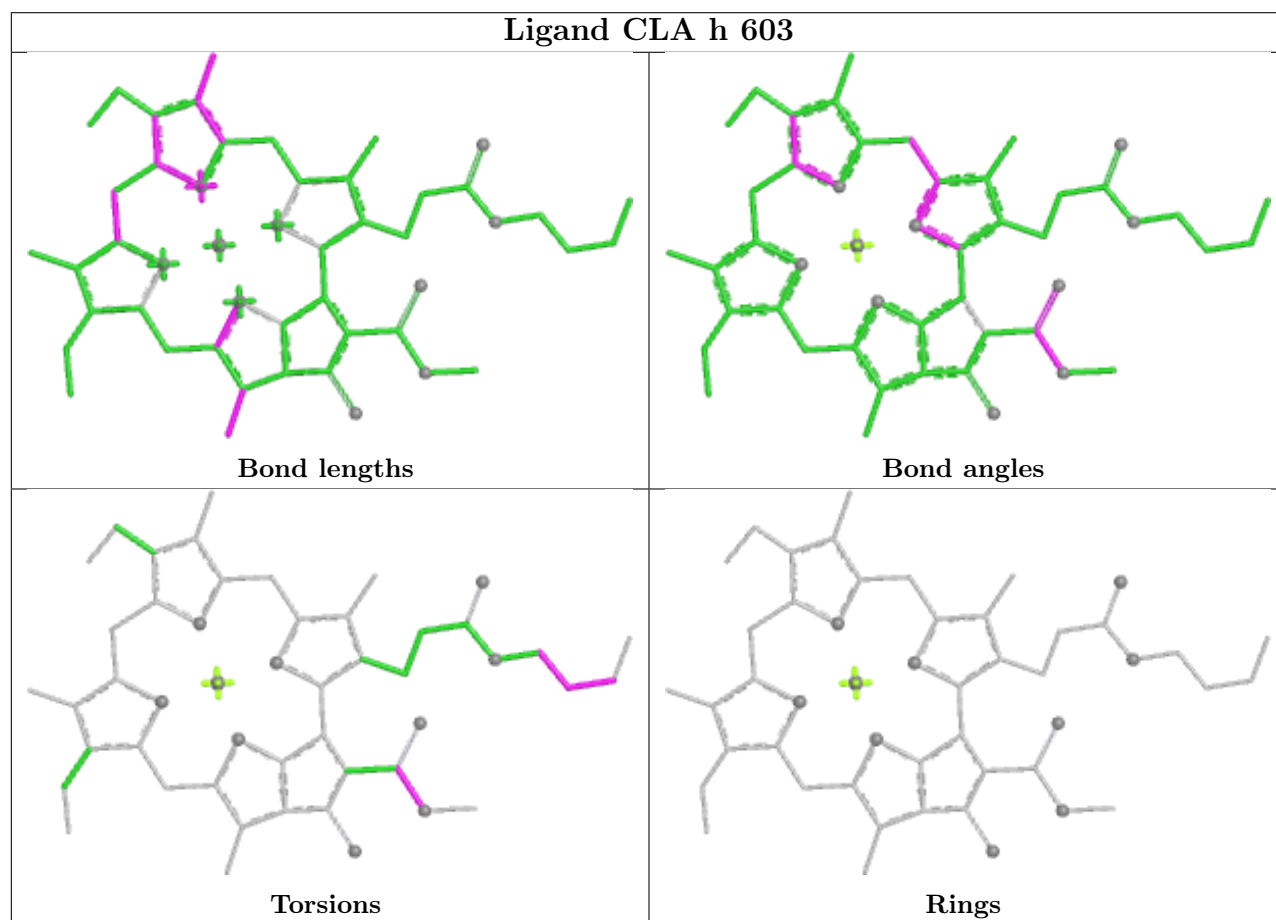




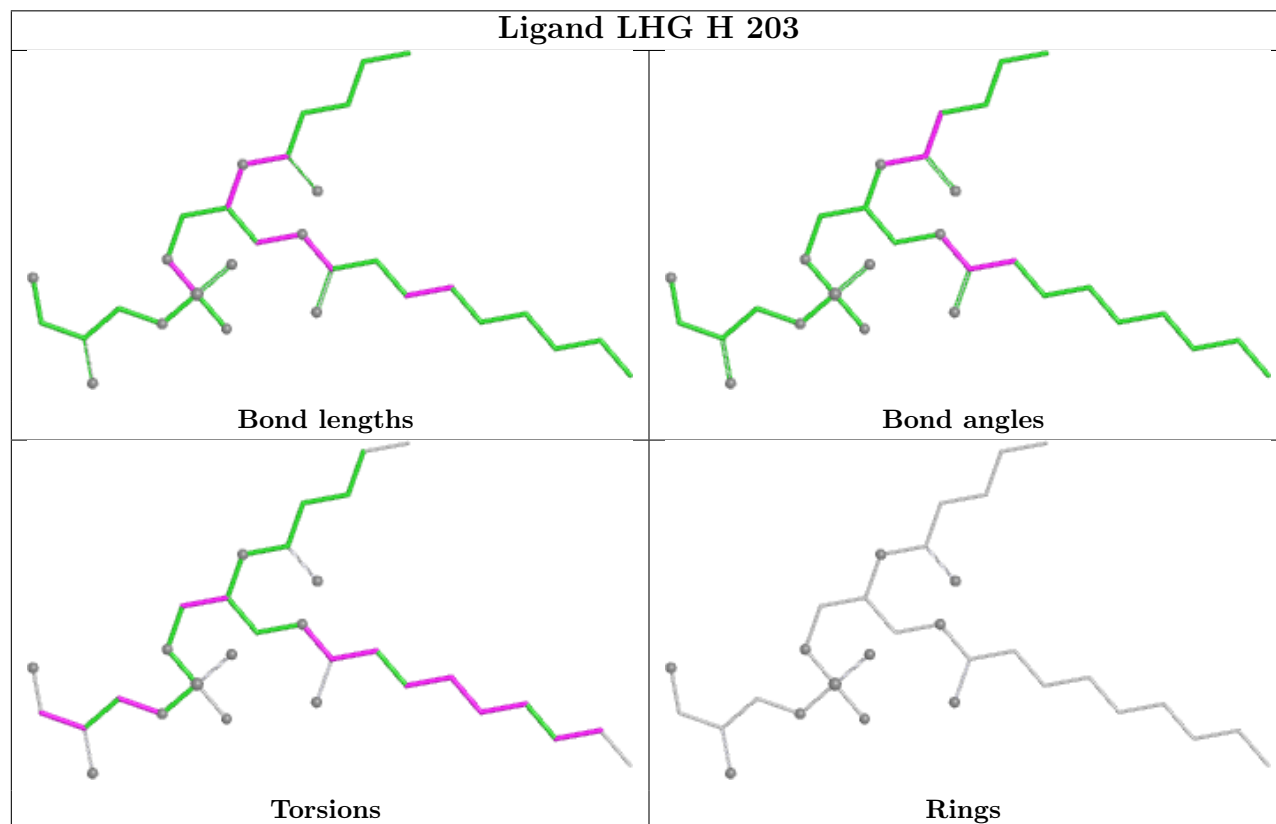
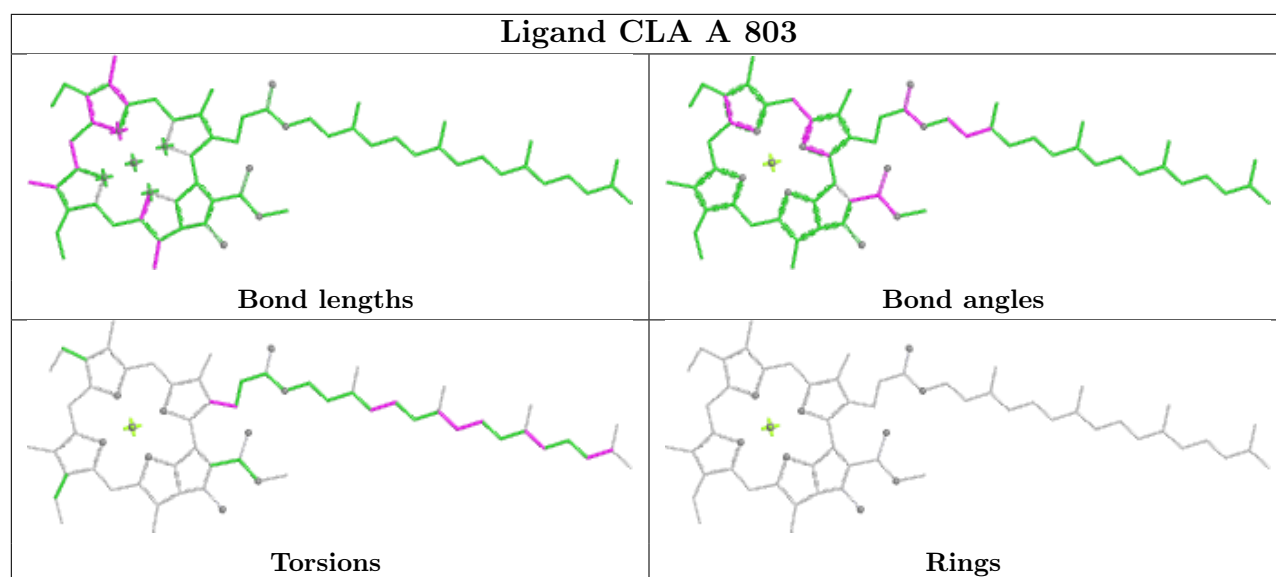
## Ligand CLA e 613



## Ligand CLA h 603

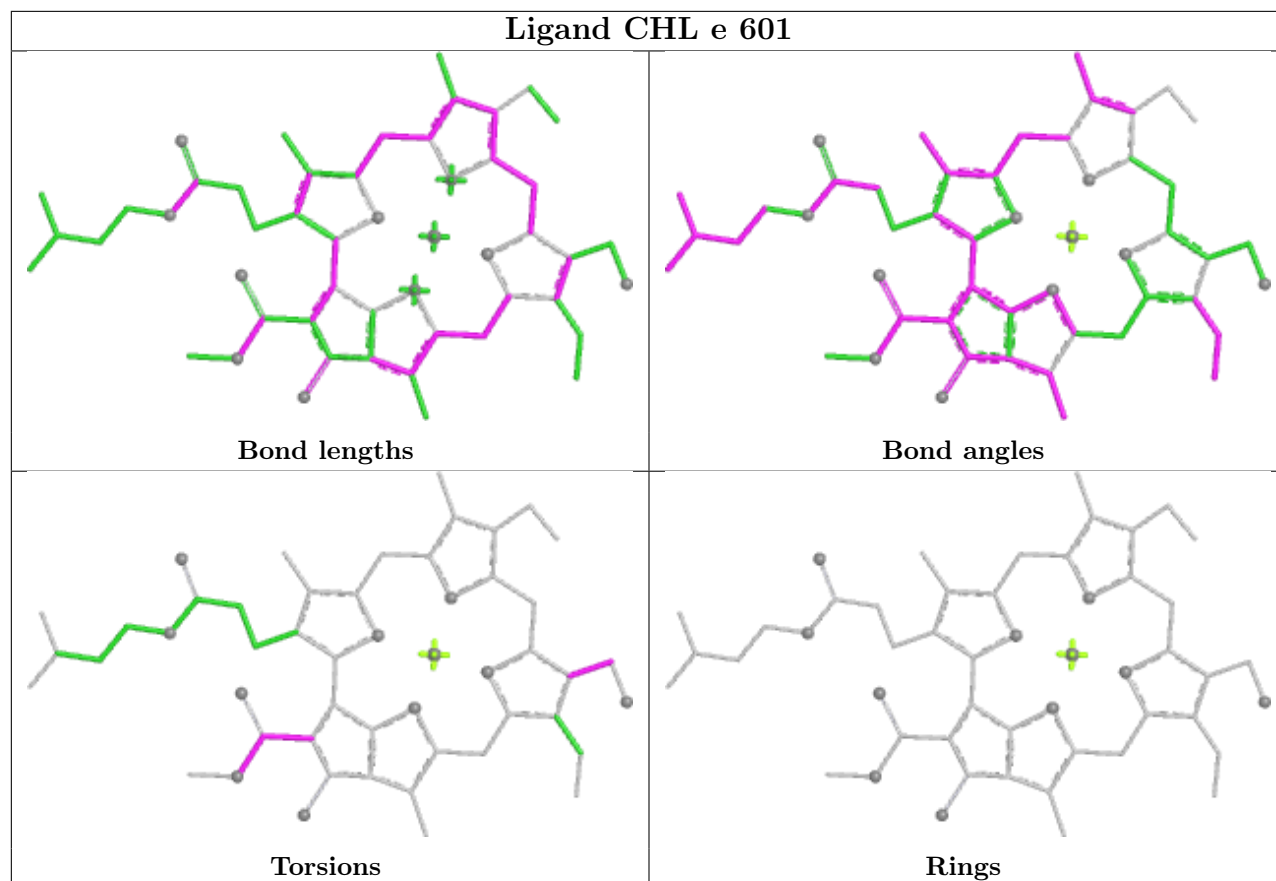




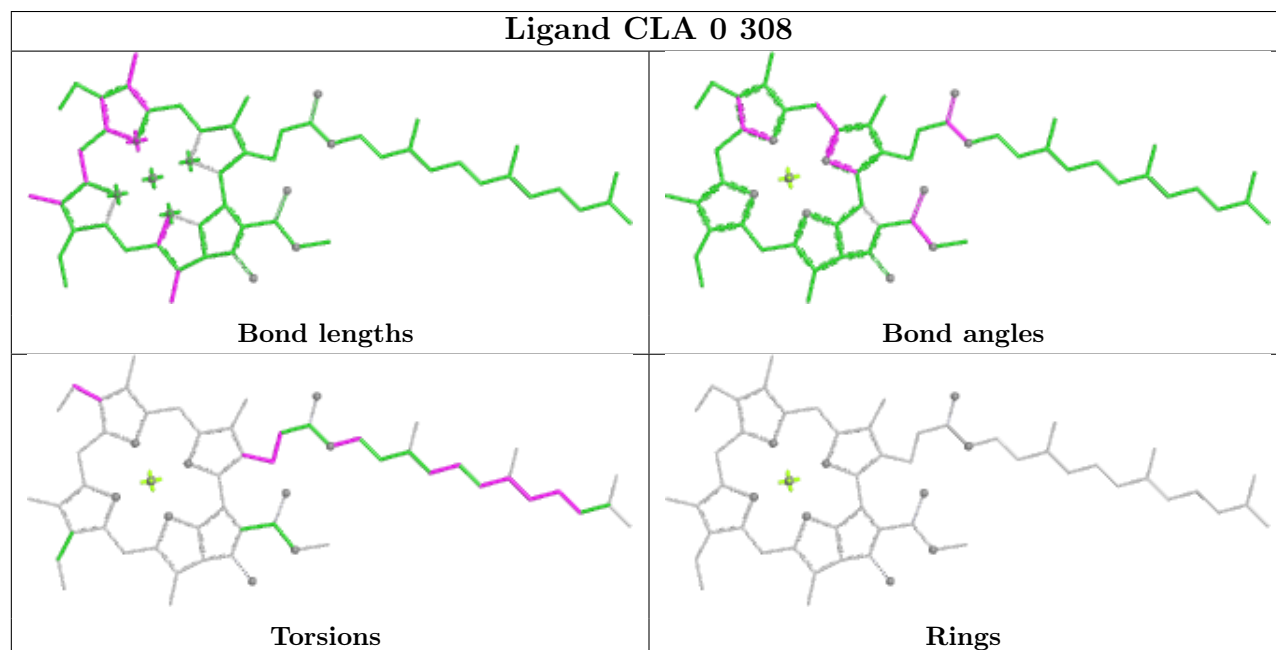




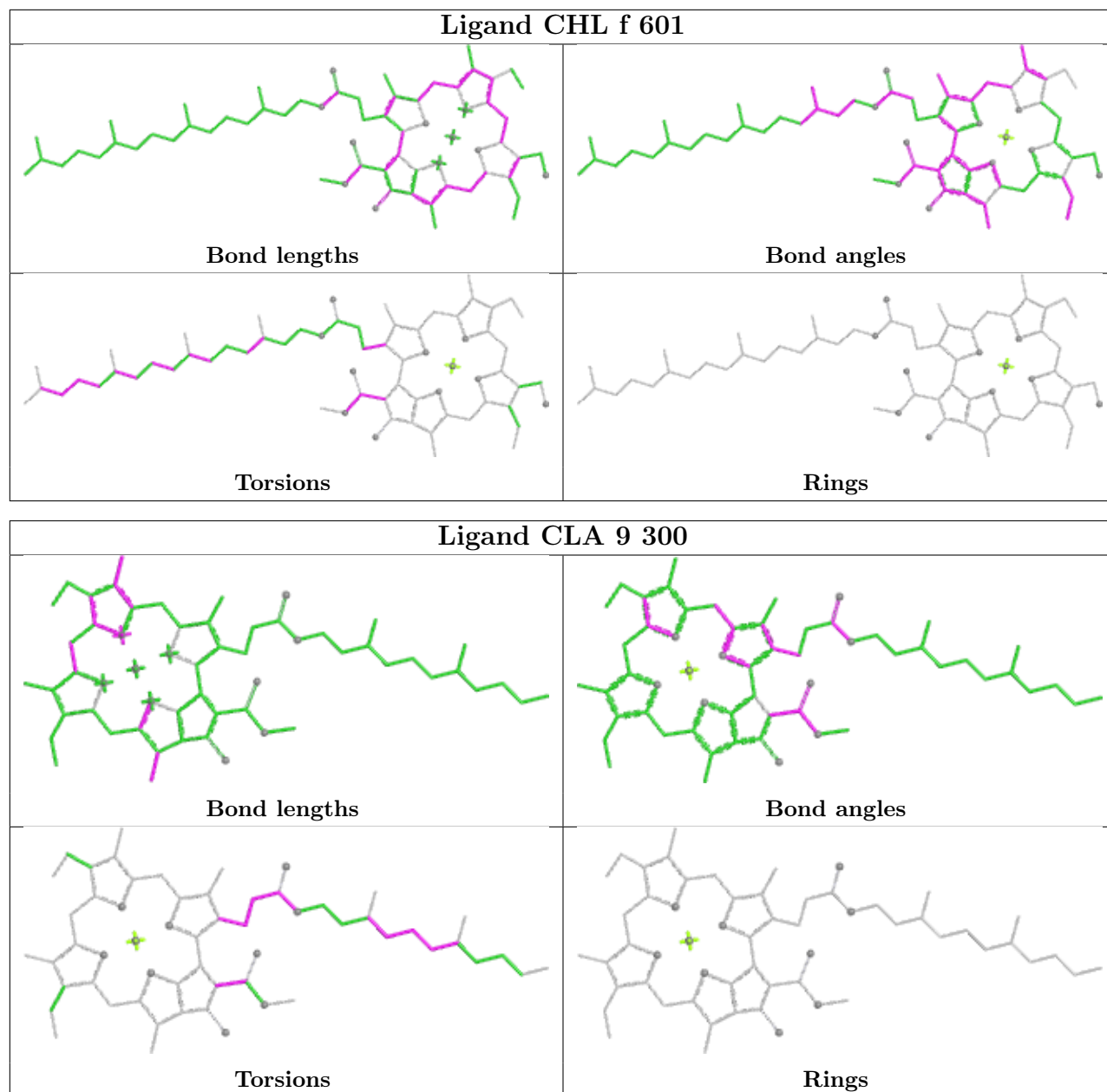
## Ligand CHL e 601



## Ligand CLA 0 308

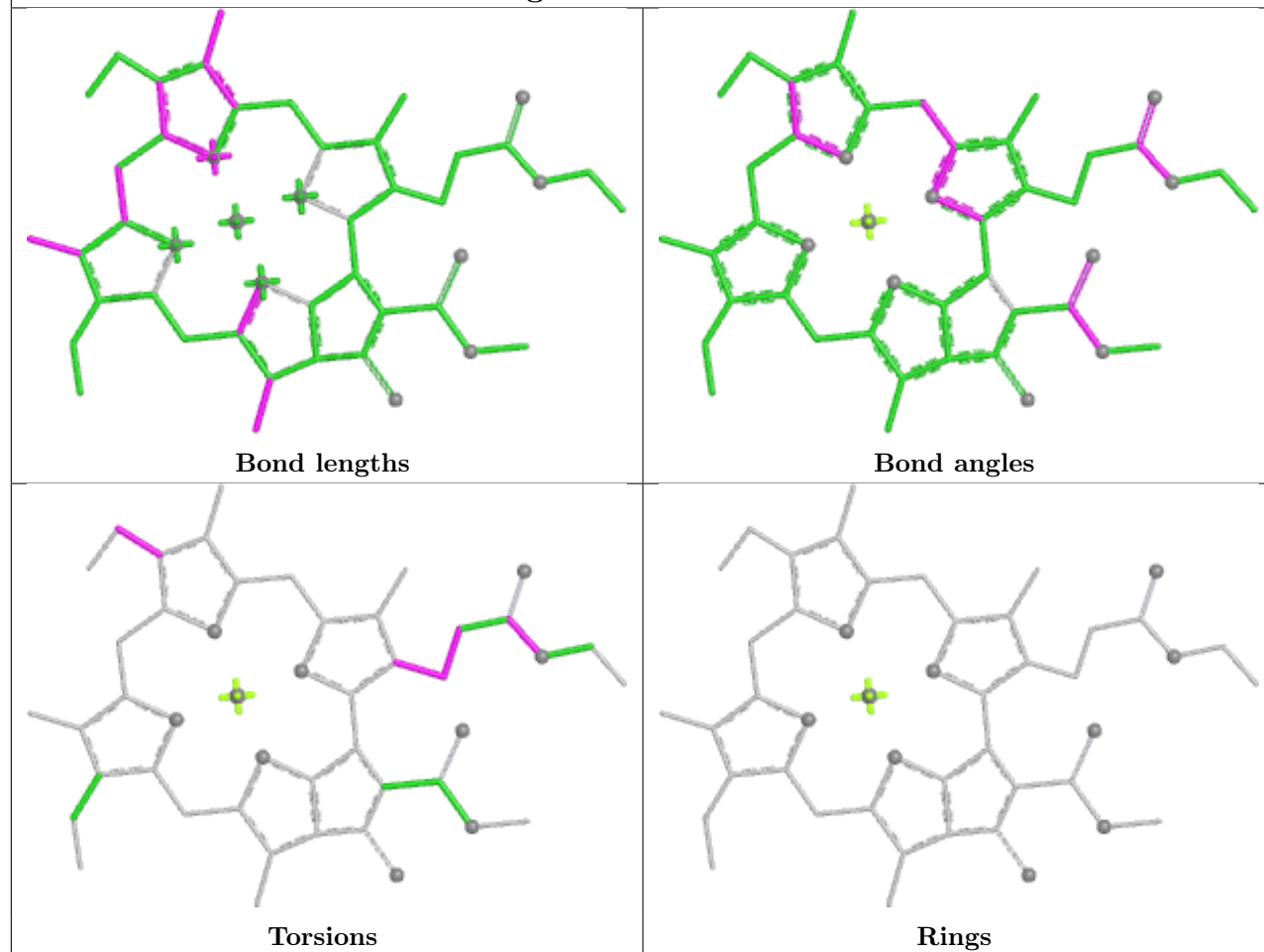




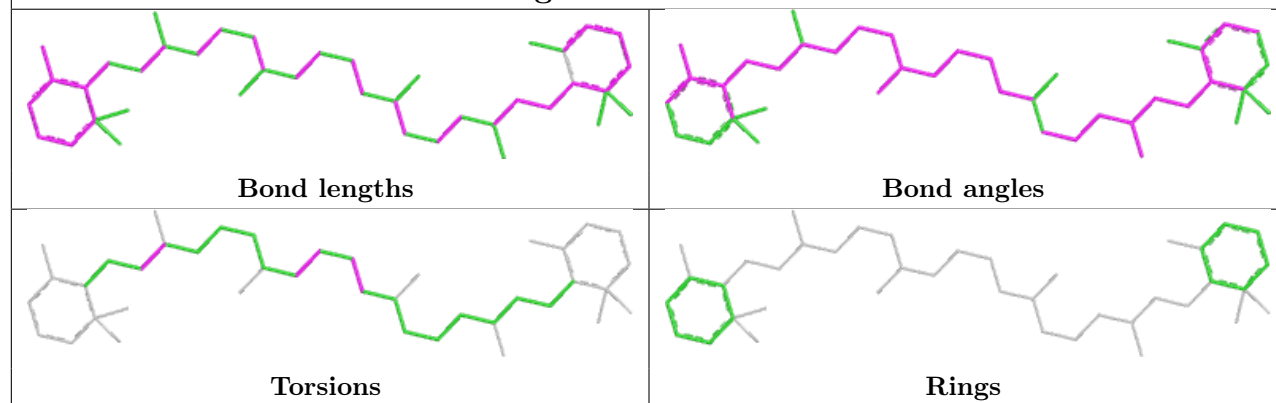




## Ligand CLA H 202

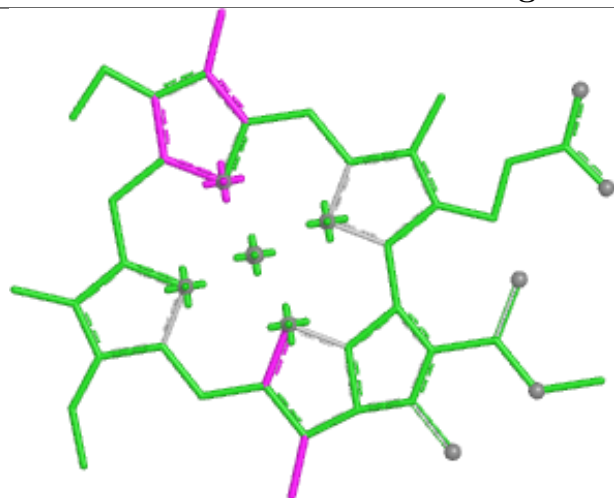


## Ligand 8CT A 846

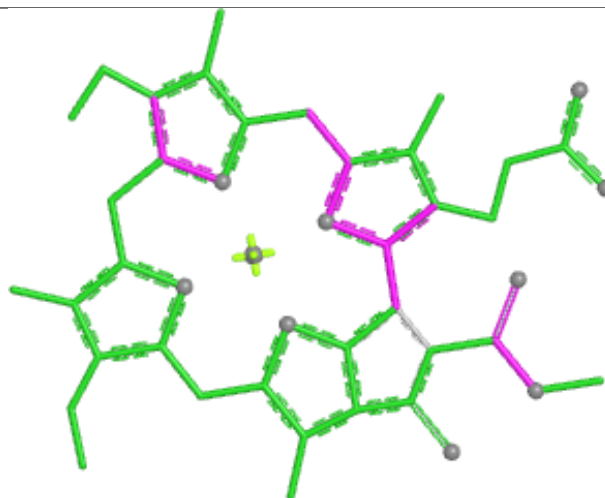




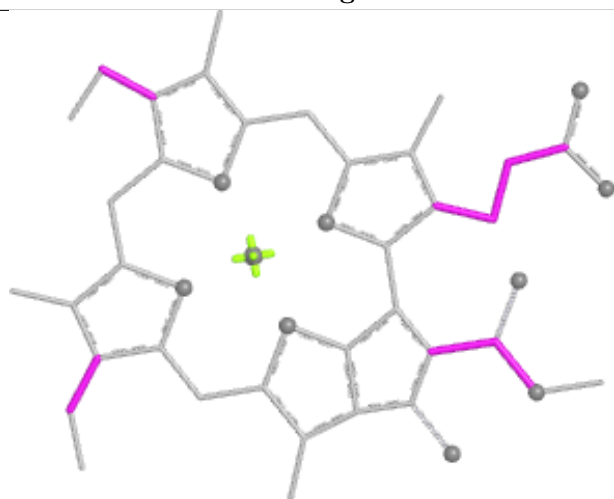
## Ligand CLA 7 317



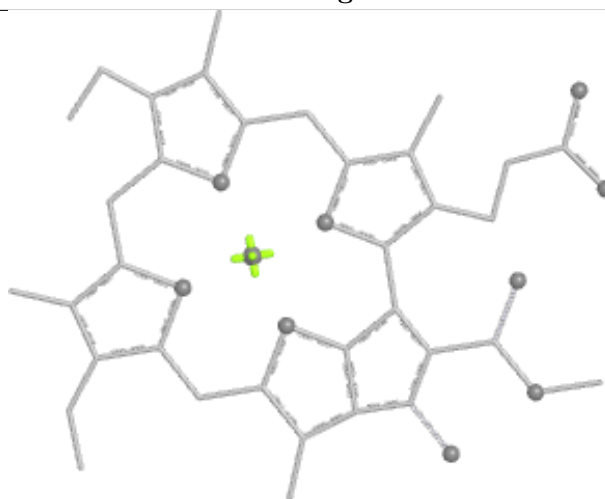
Bond lengths



Bond angles



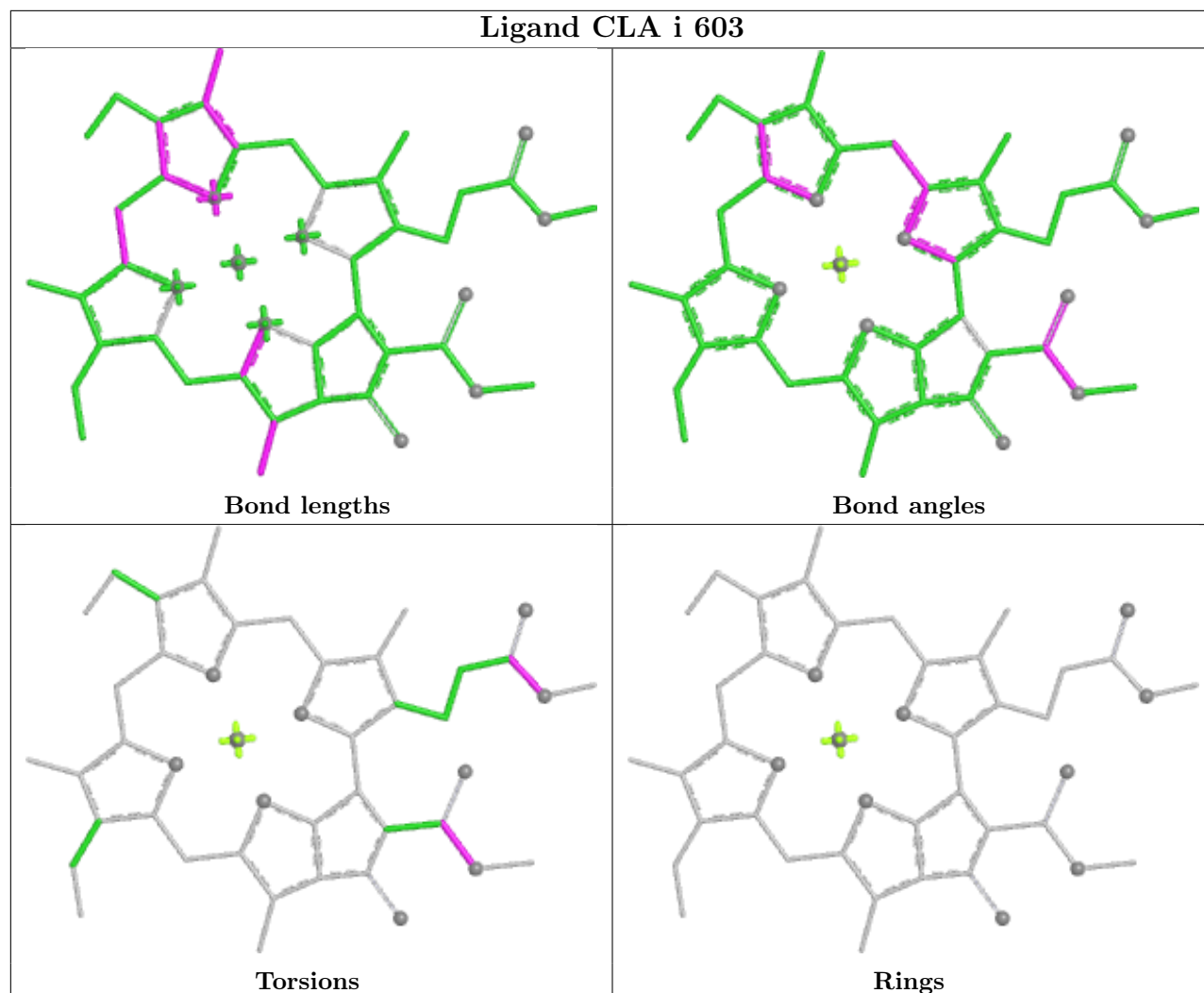
Torsions



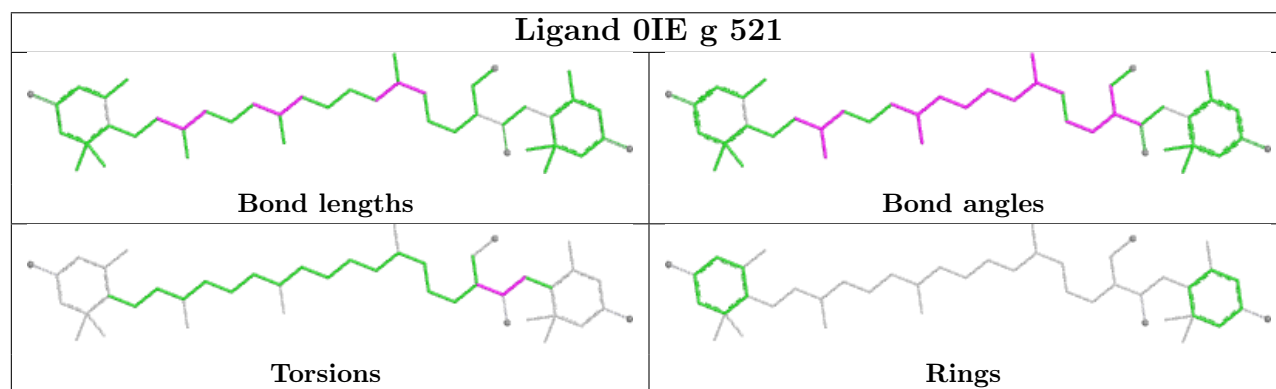
Rings



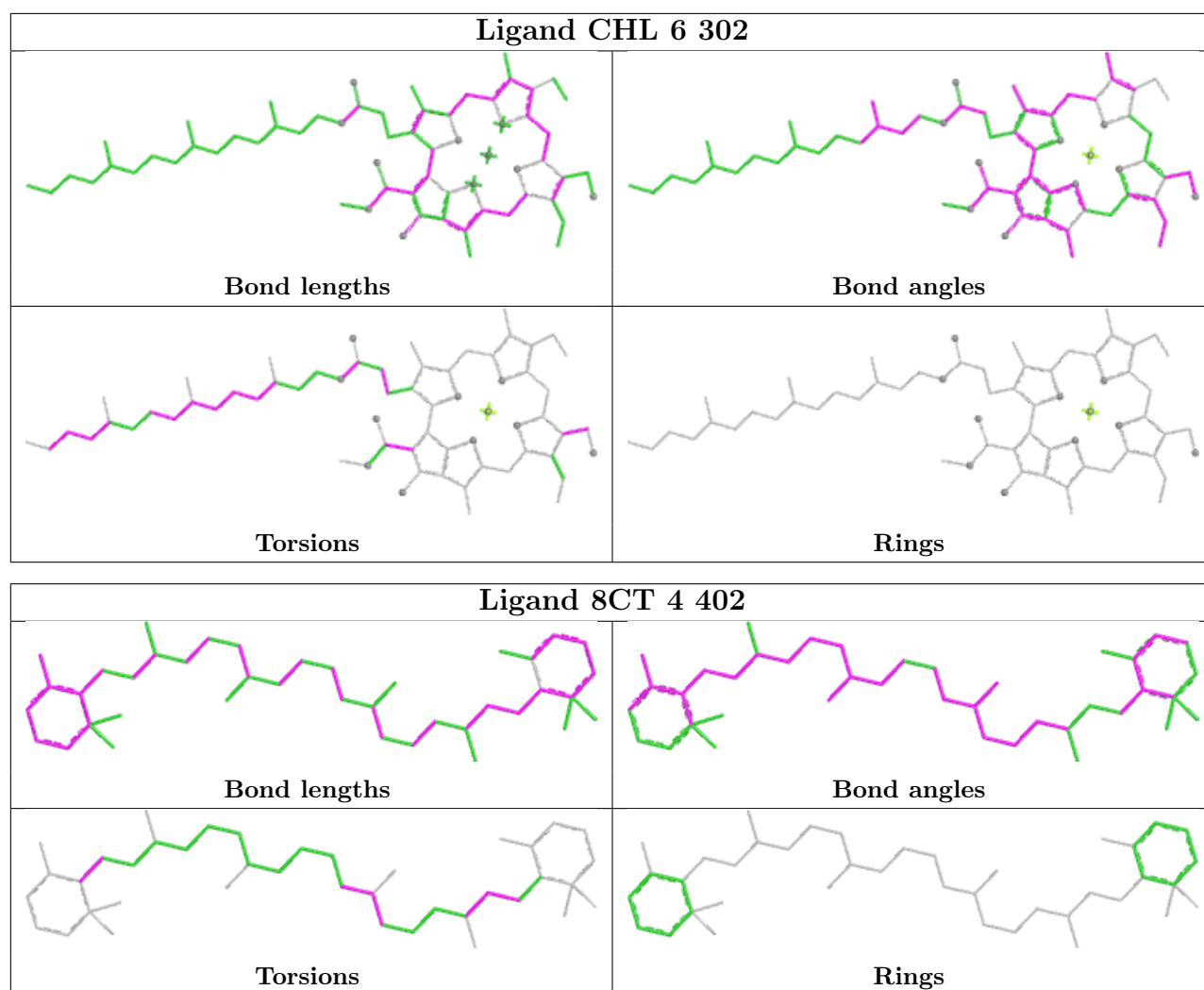
## Ligand CLA i 603



## Ligand OIE g 521

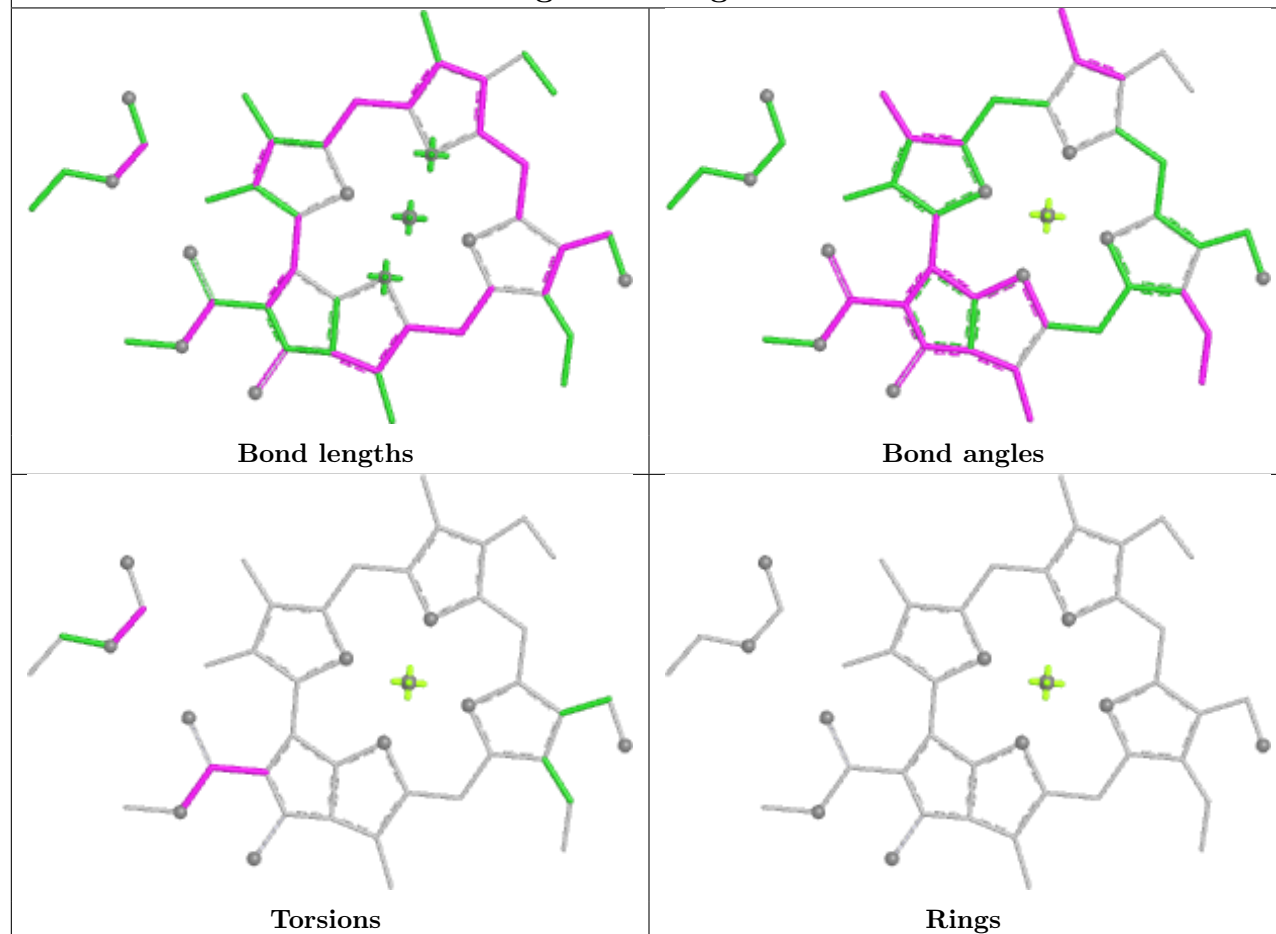




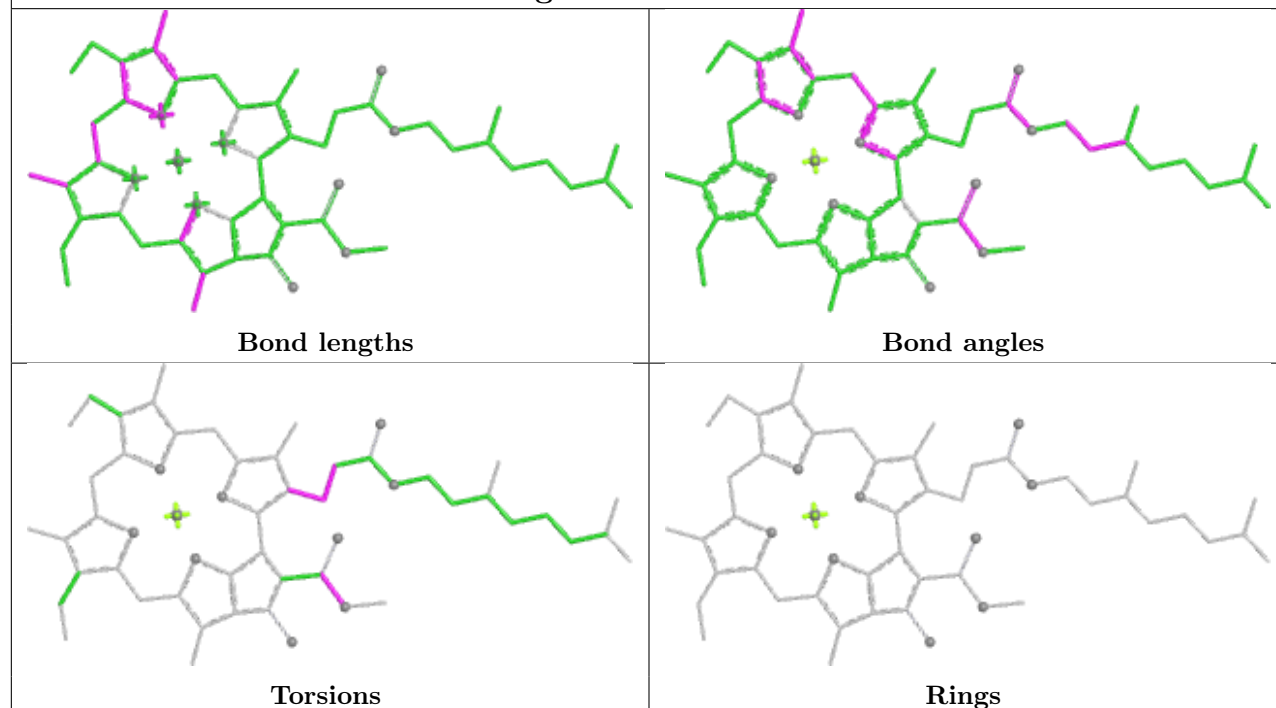




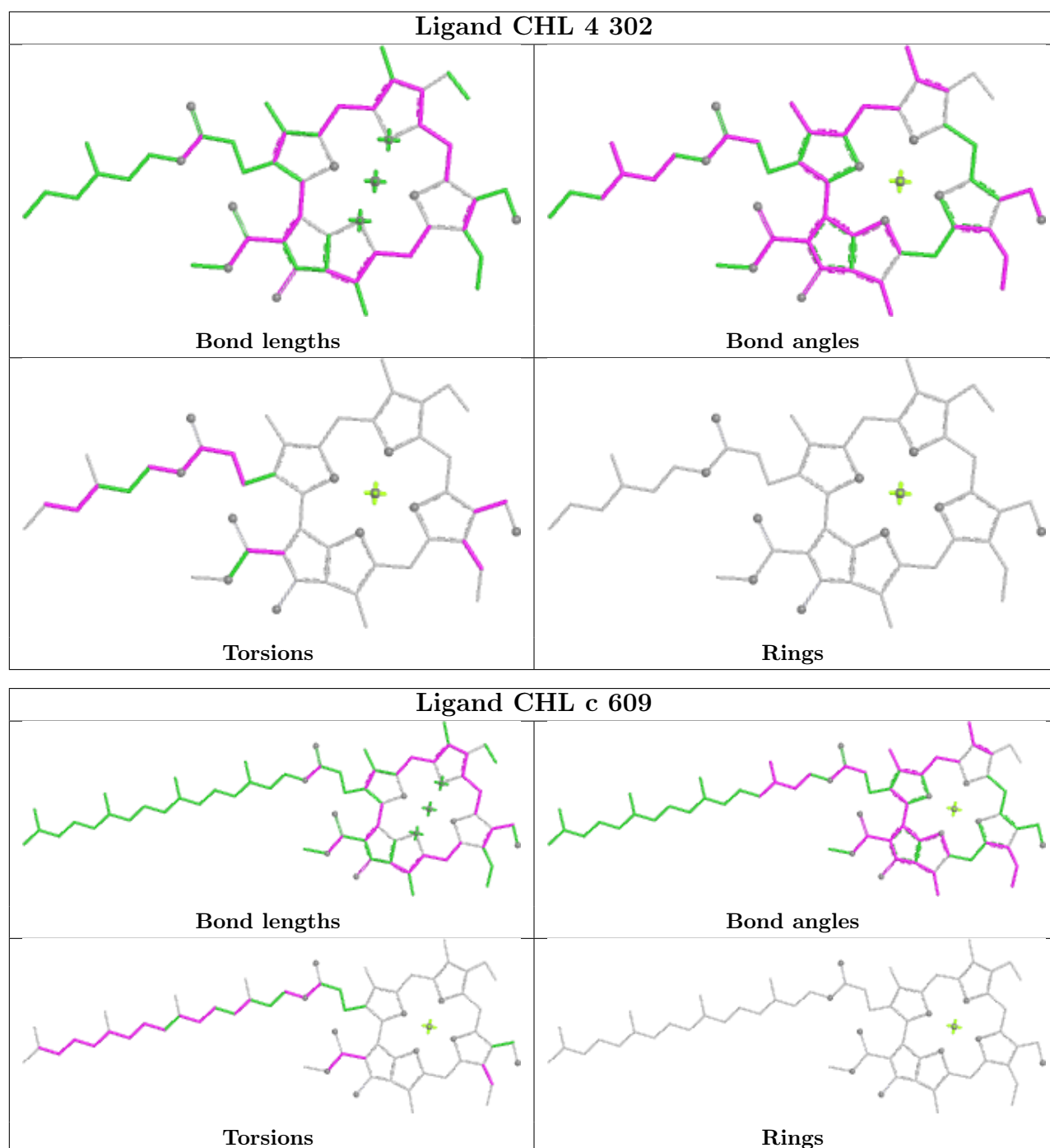
## Ligand CHL g 609



## Ligand CLA b 610

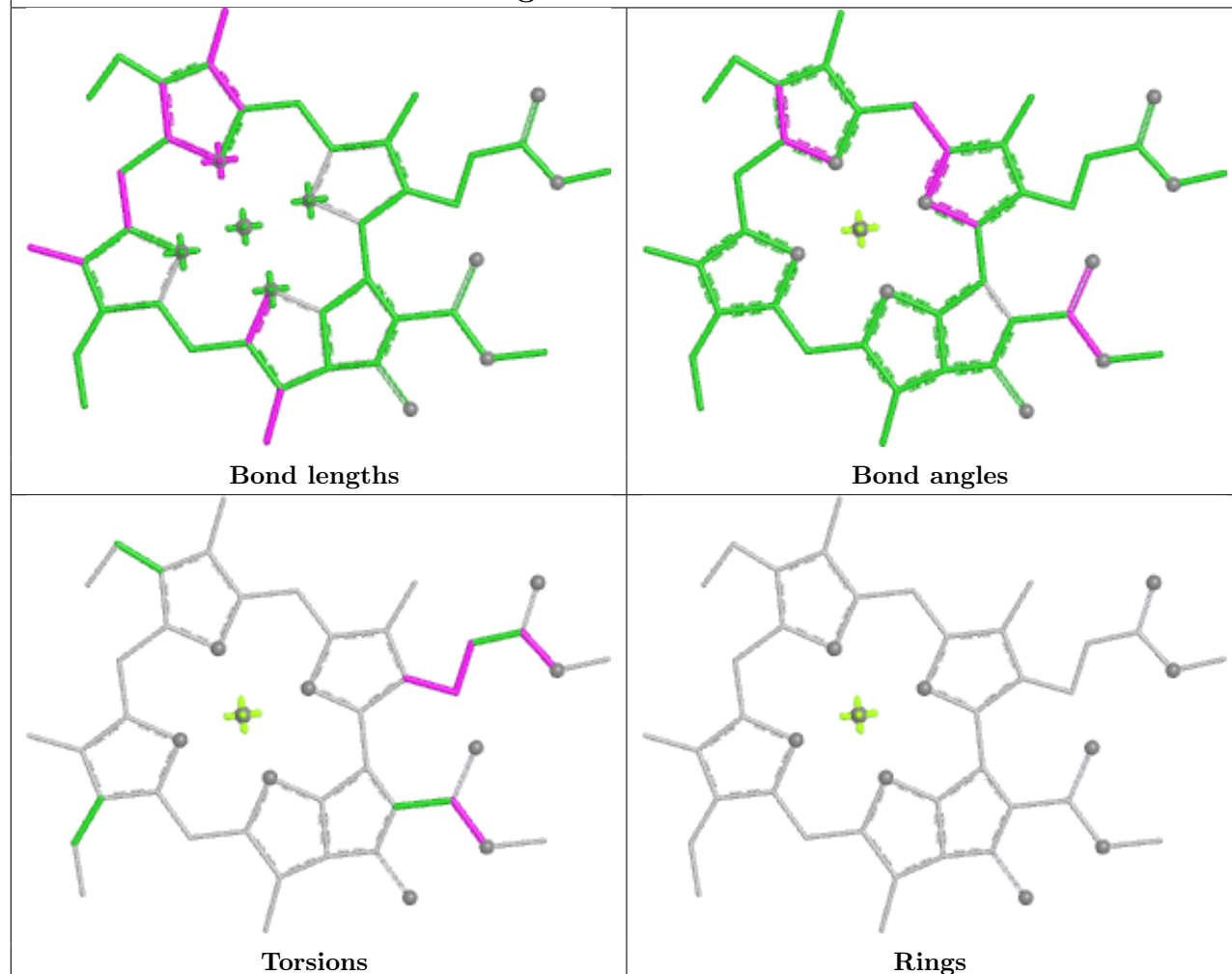




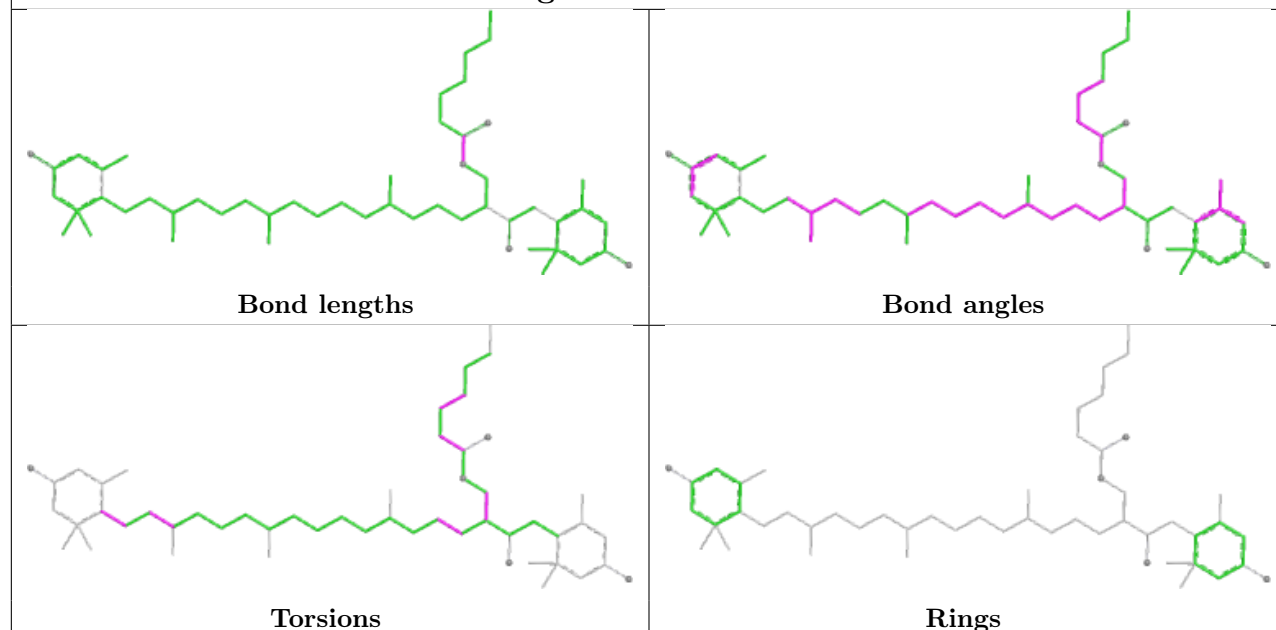




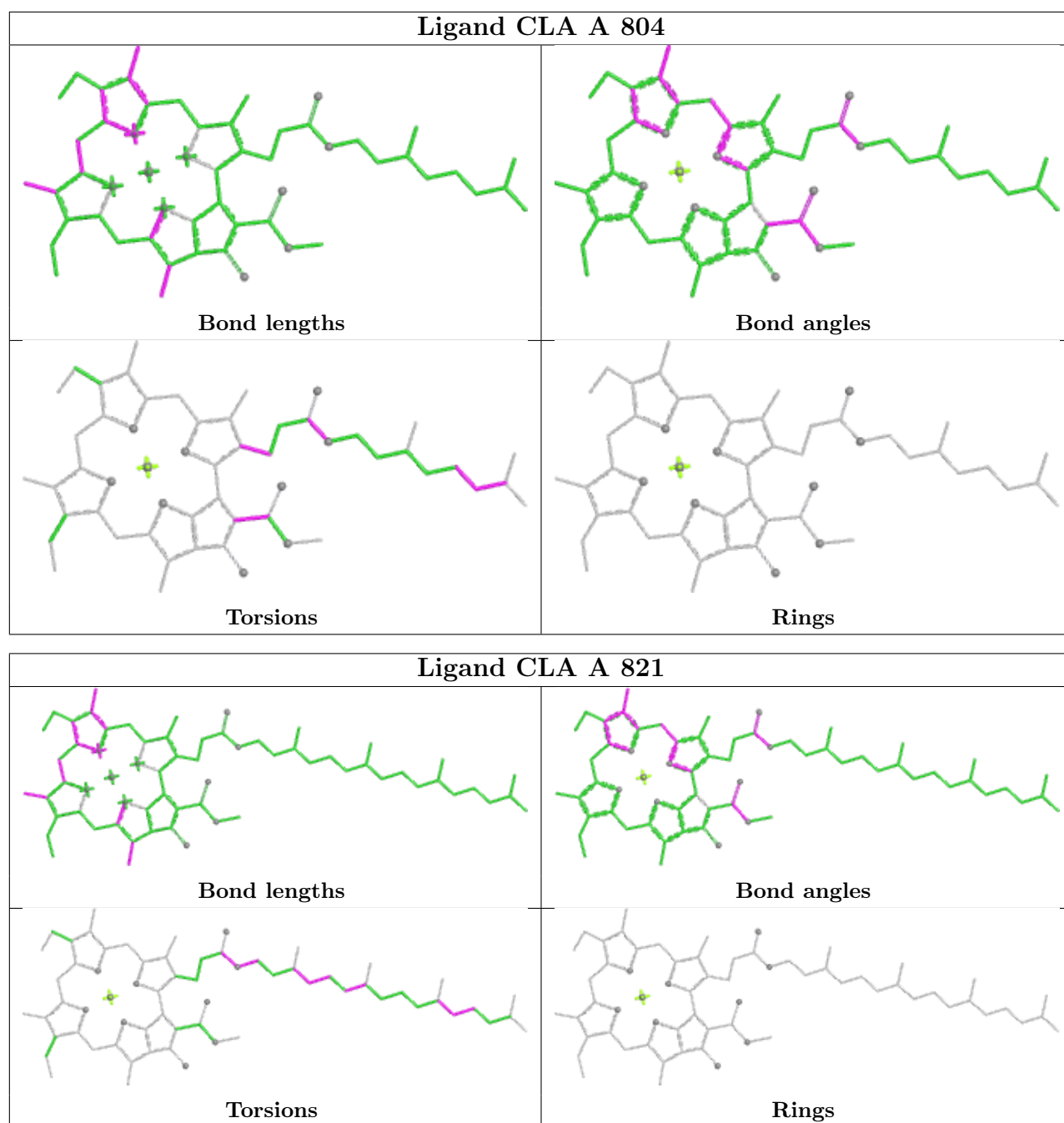
## Ligand CLA 5 308



## Ligand OUR 5 502

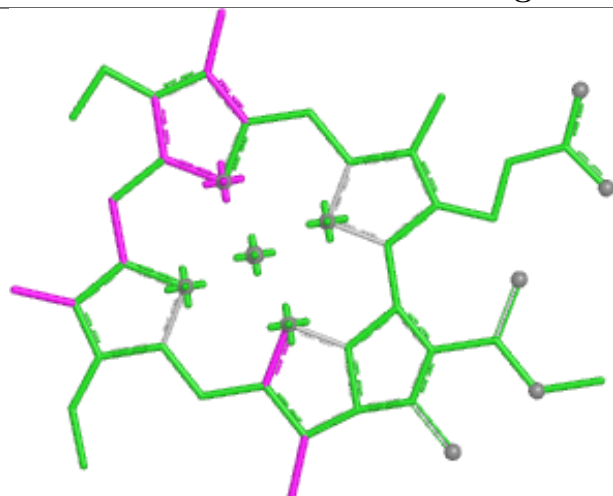




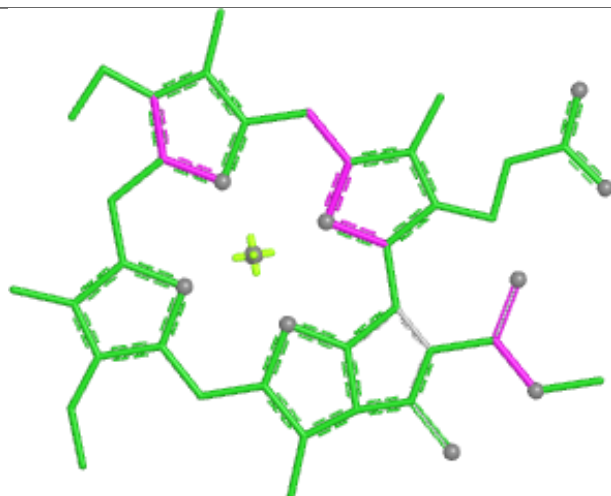




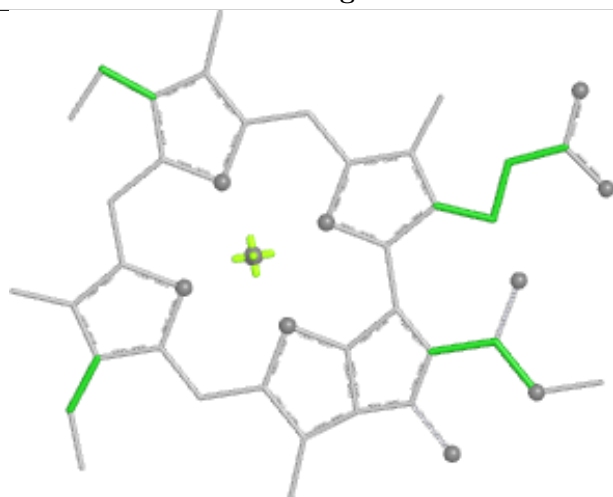
## Ligand CLA B 835



Bond lengths



Bond angles



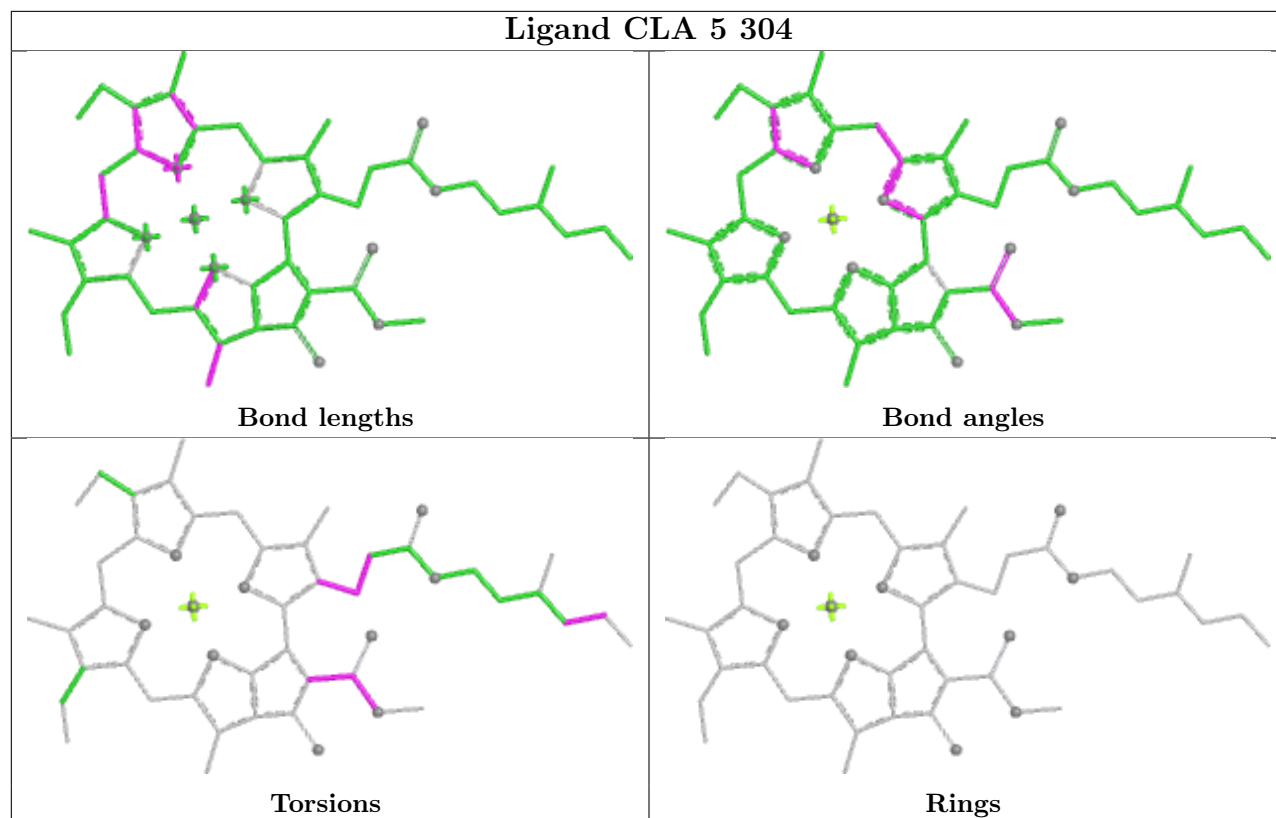
Torsions



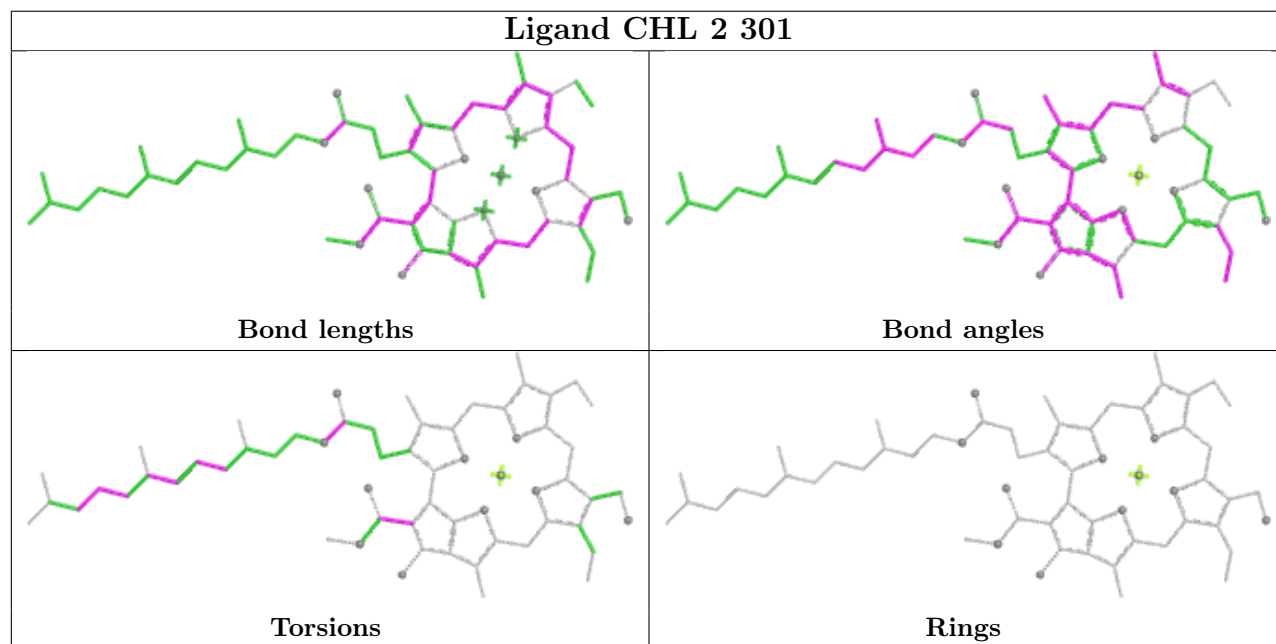
Rings



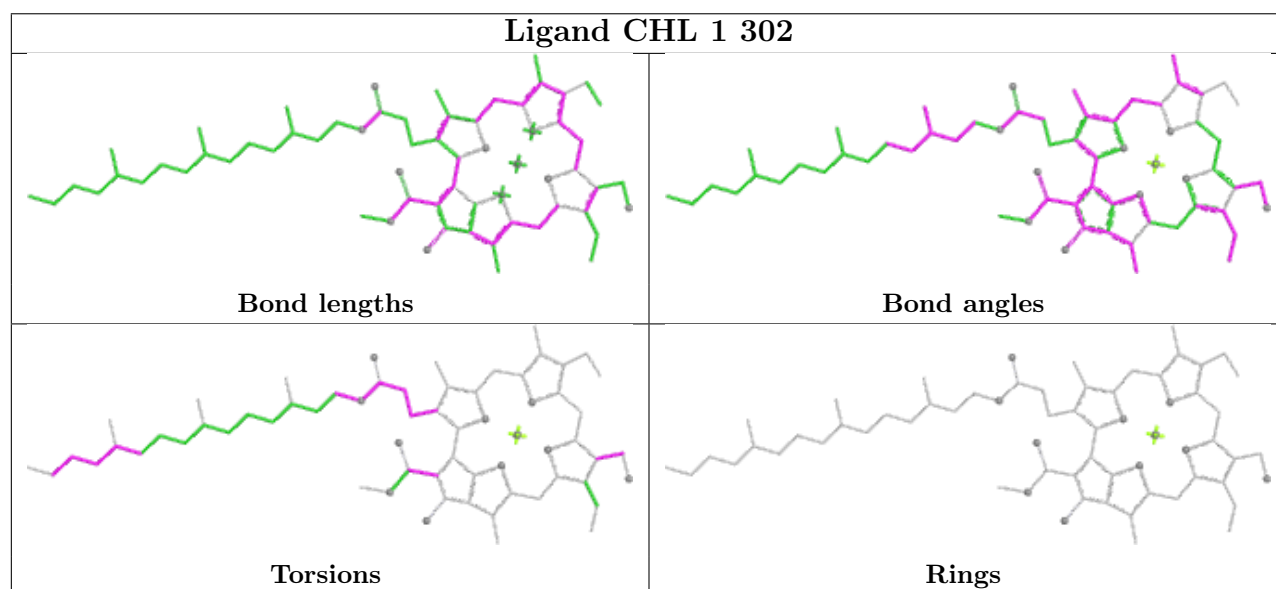
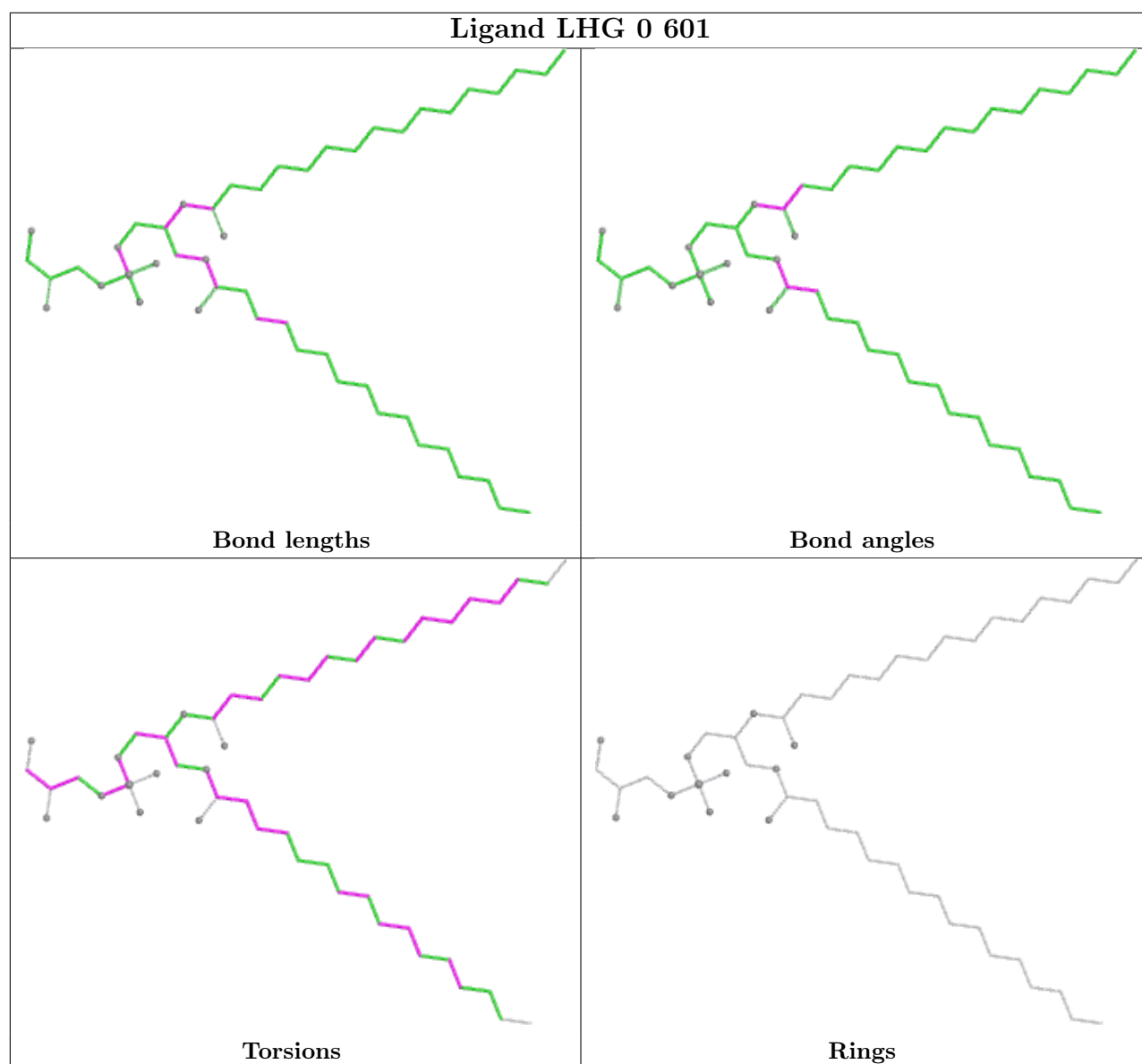
## Ligand CLA 5 304



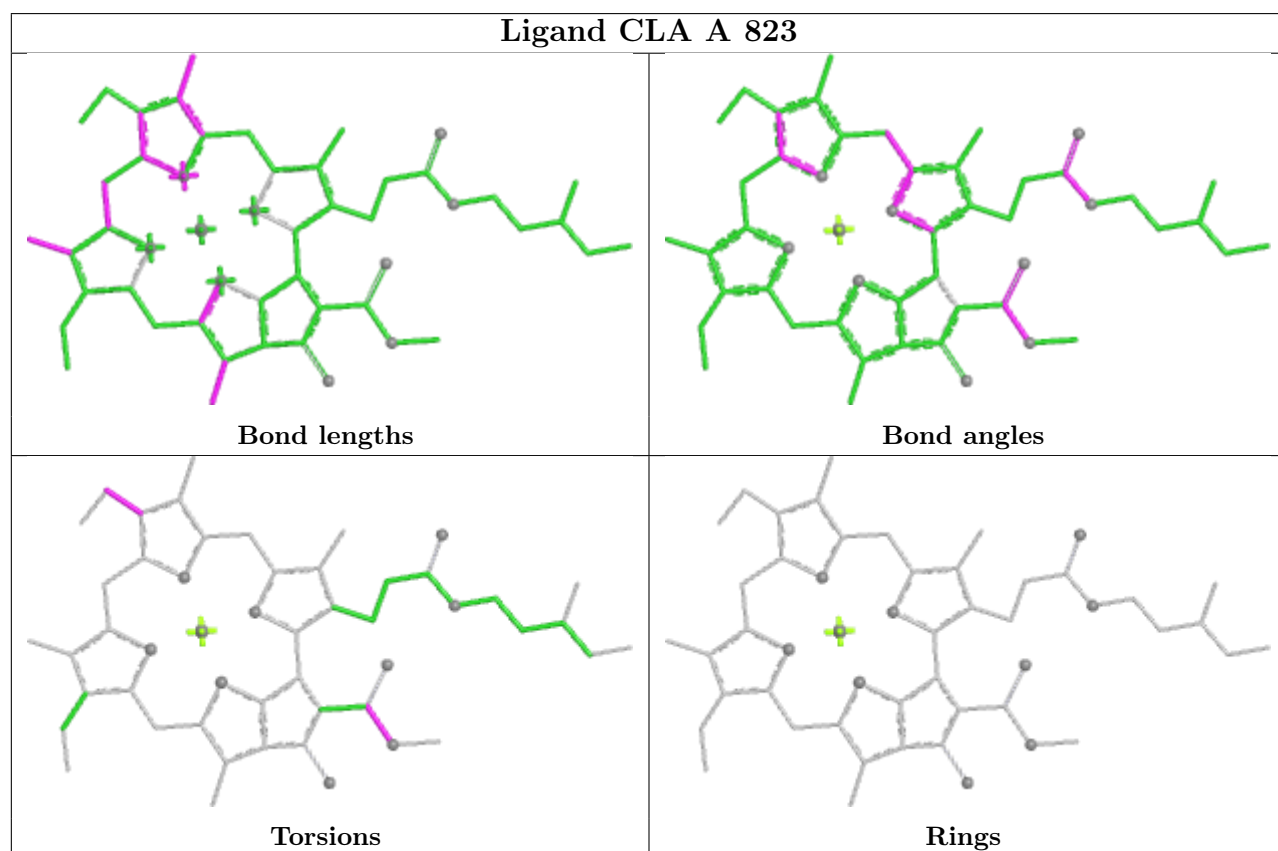
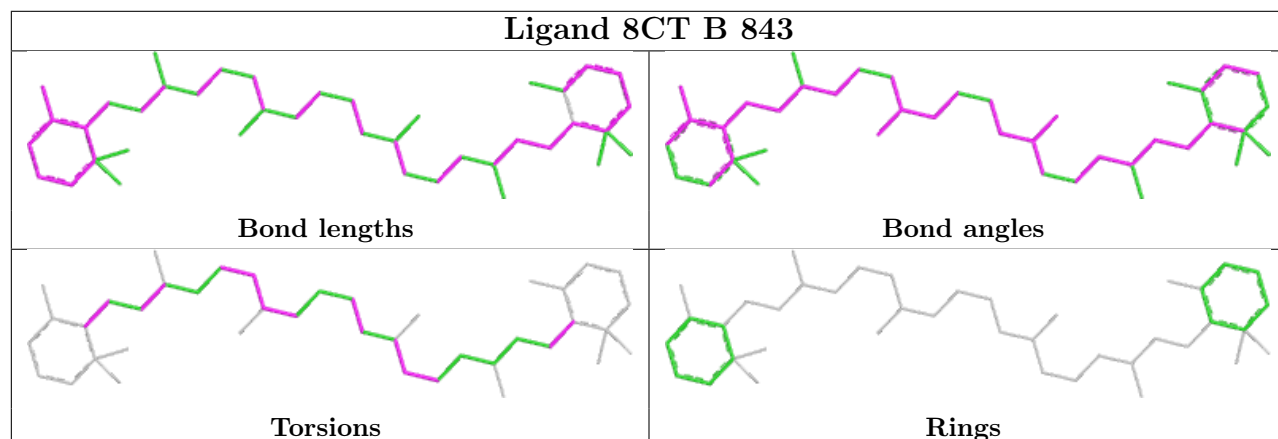
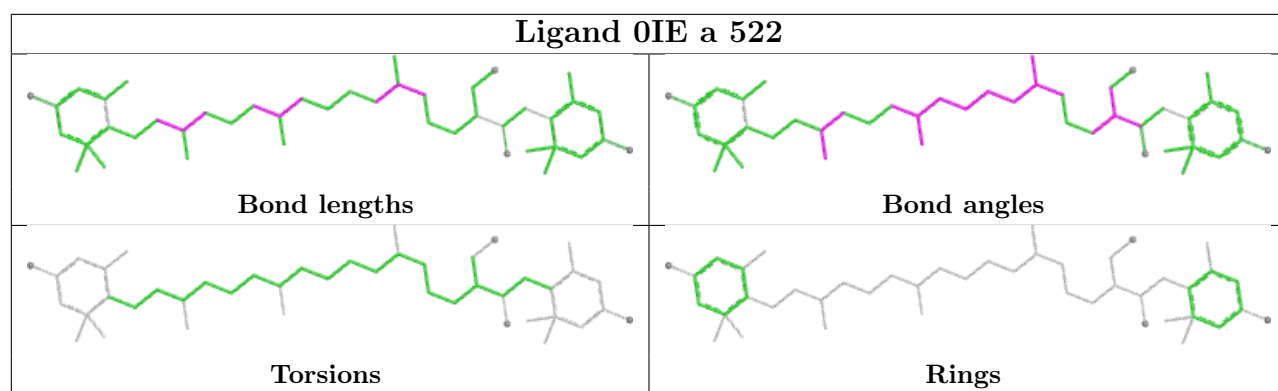
## Ligand CHL 2 301





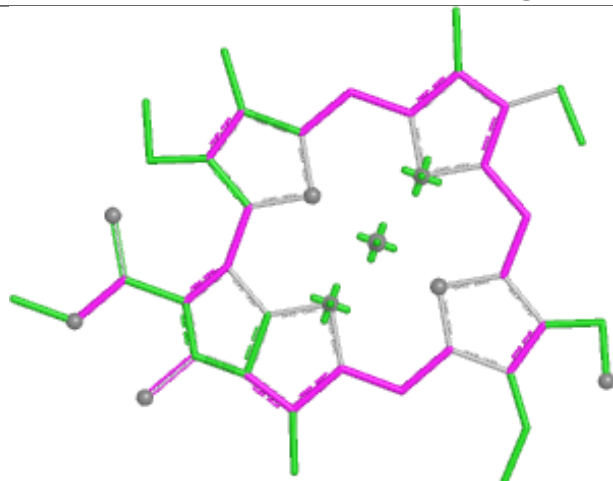




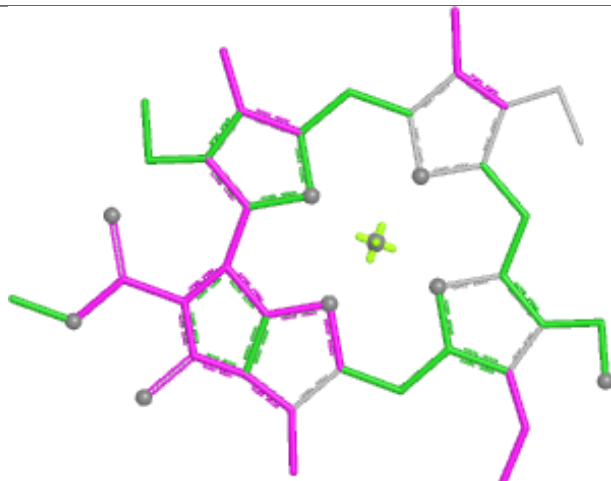




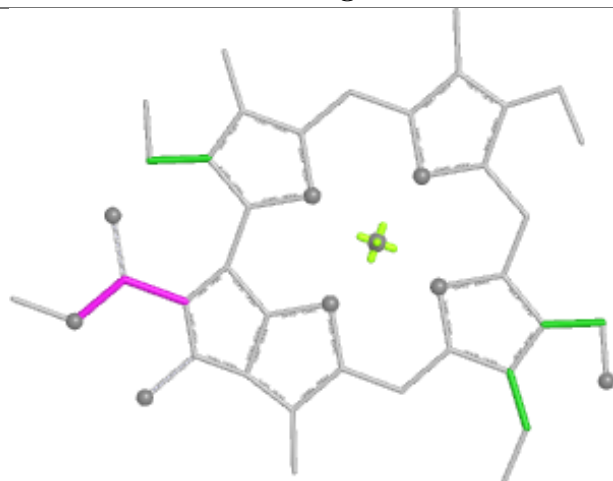
## Ligand CHL 8 315



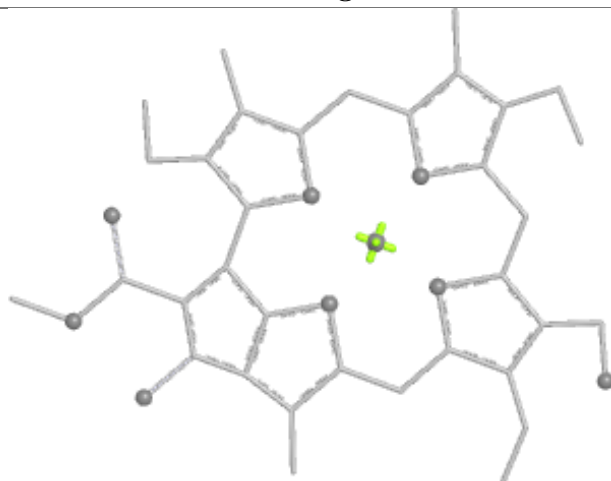
Bond lengths



Bond angles



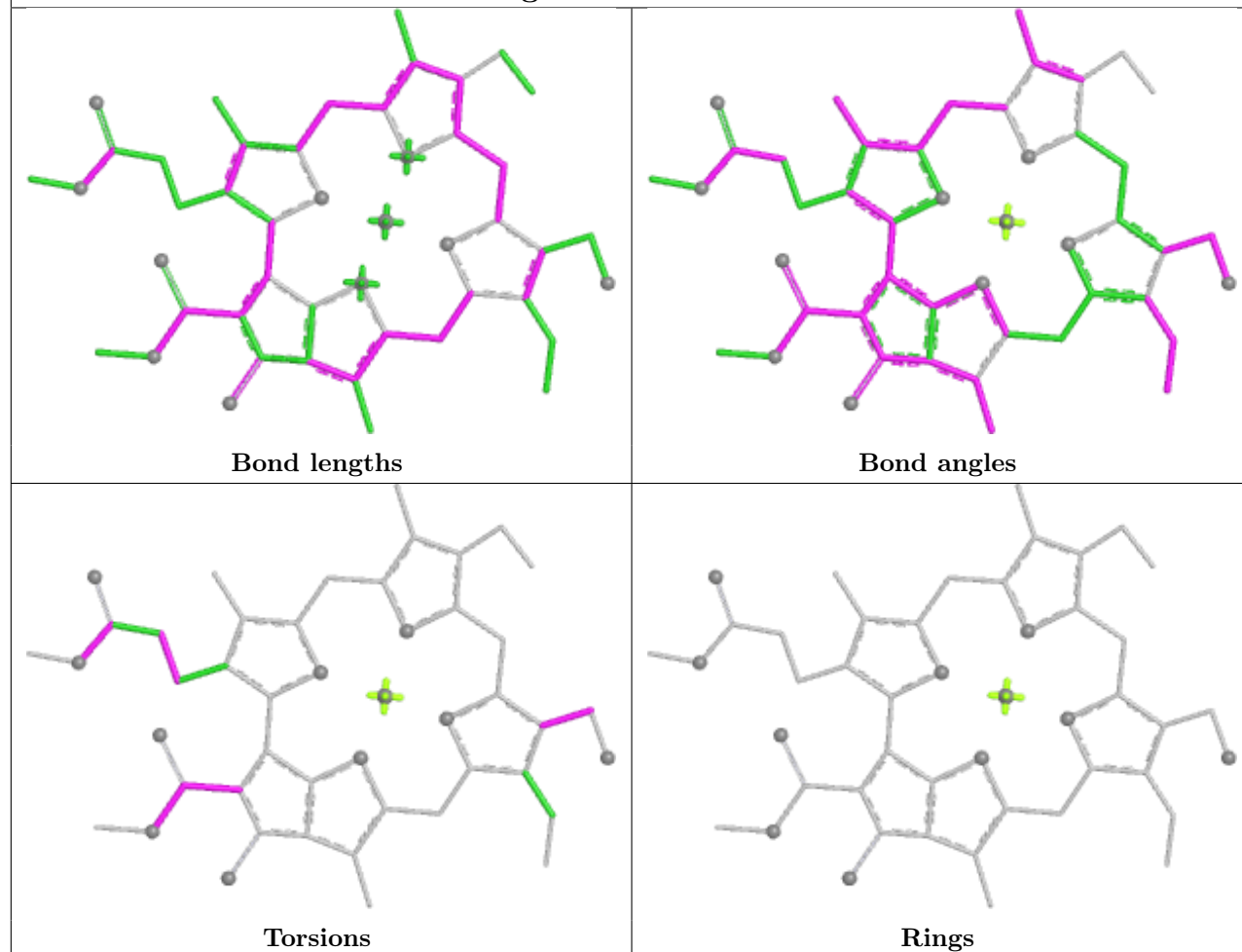
Torsions



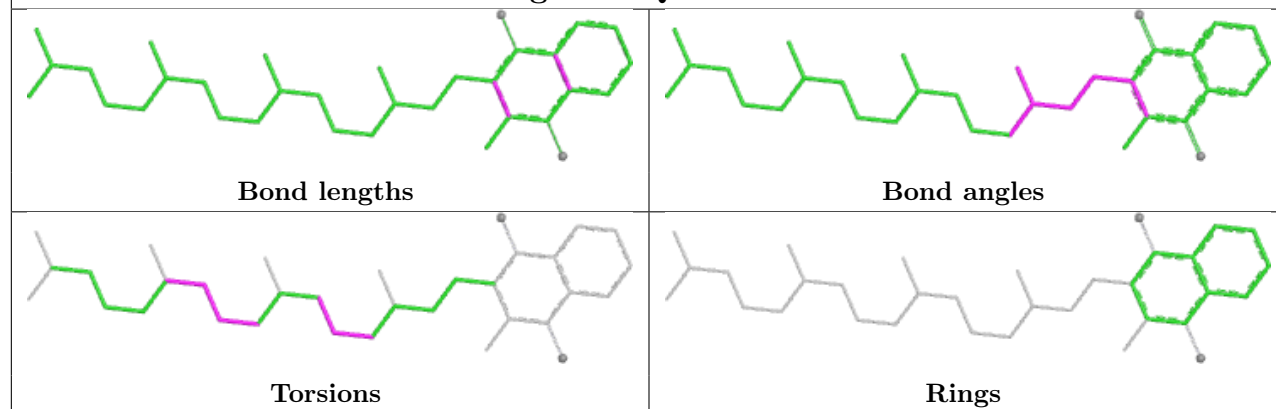
Rings



## Ligand CHL 7 313

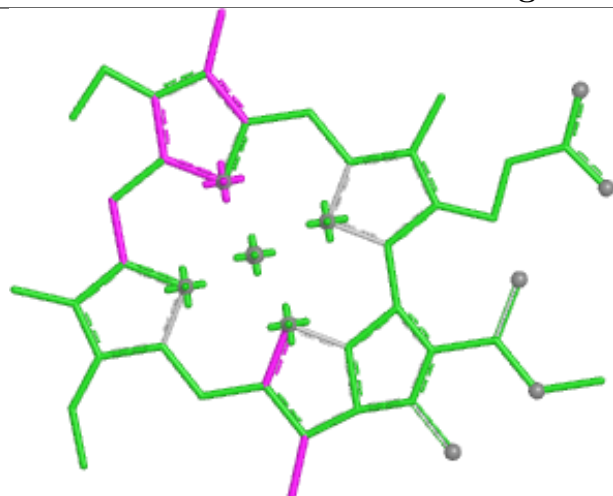


## Ligand PQN B 842

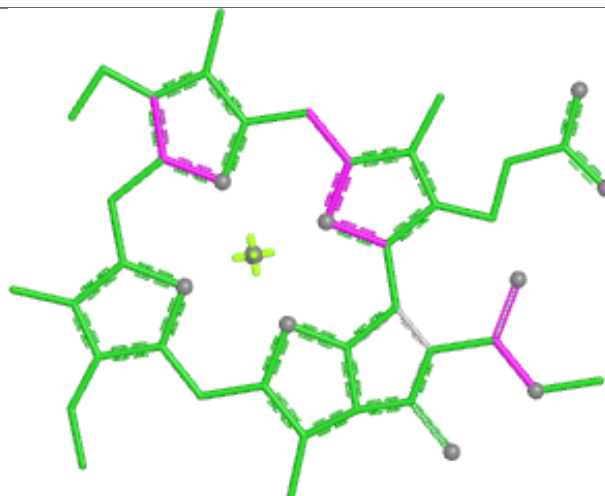




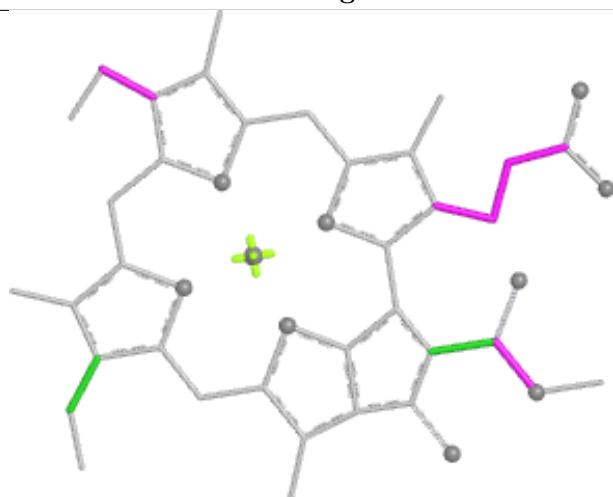
## Ligand CLA 5 311



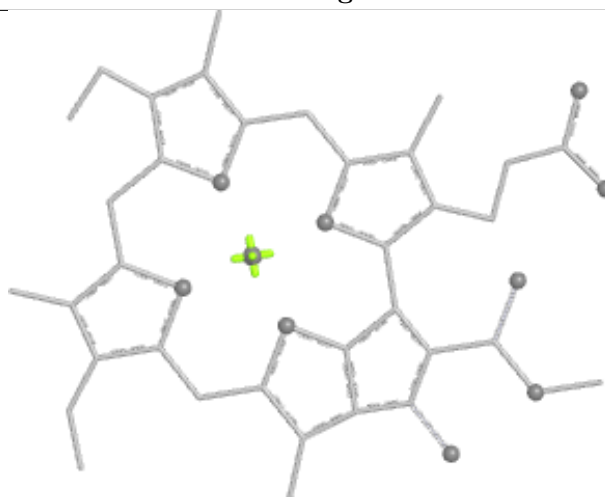
Bond lengths



Bond angles



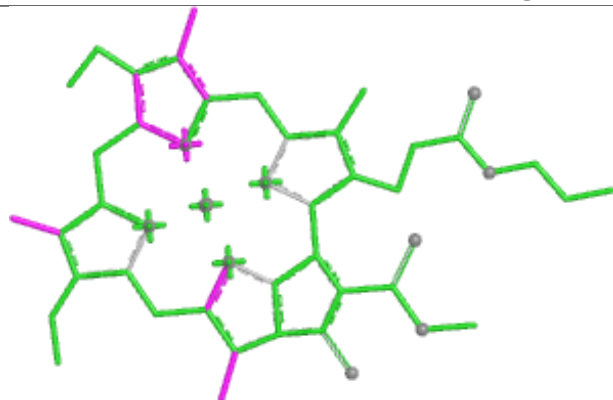
Torsions



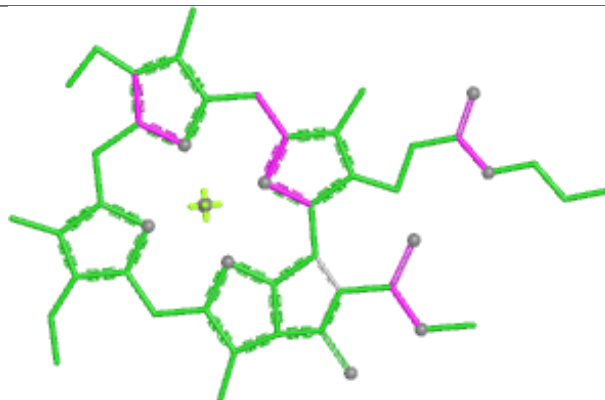
Rings



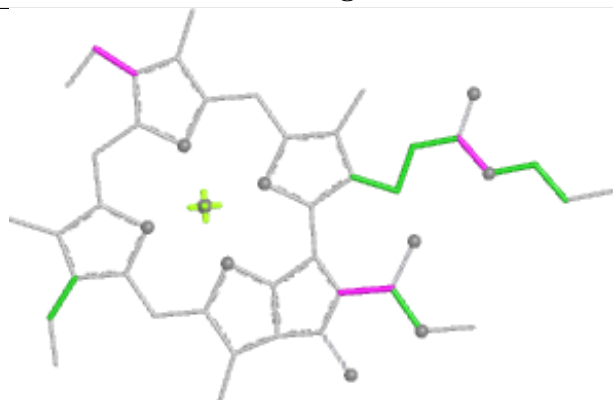
## Ligand CLA 9 303



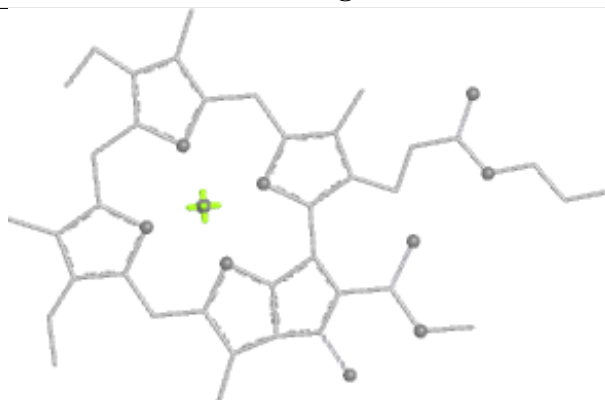
Bond lengths



Bond angles

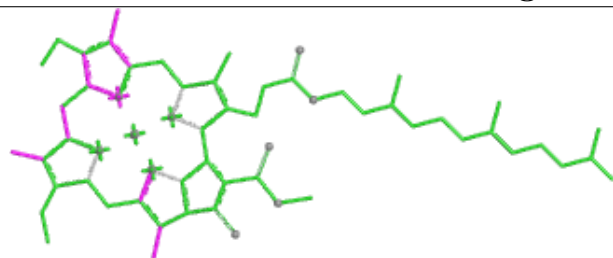


Torsions

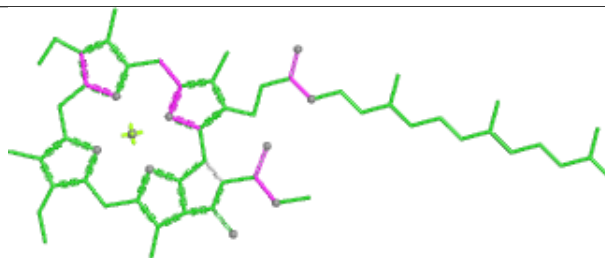


Rings

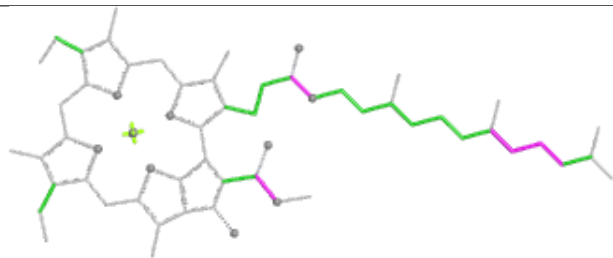
## Ligand CLA 4 304



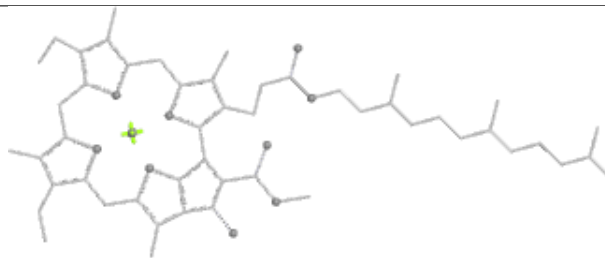
Bond lengths



Bond angles

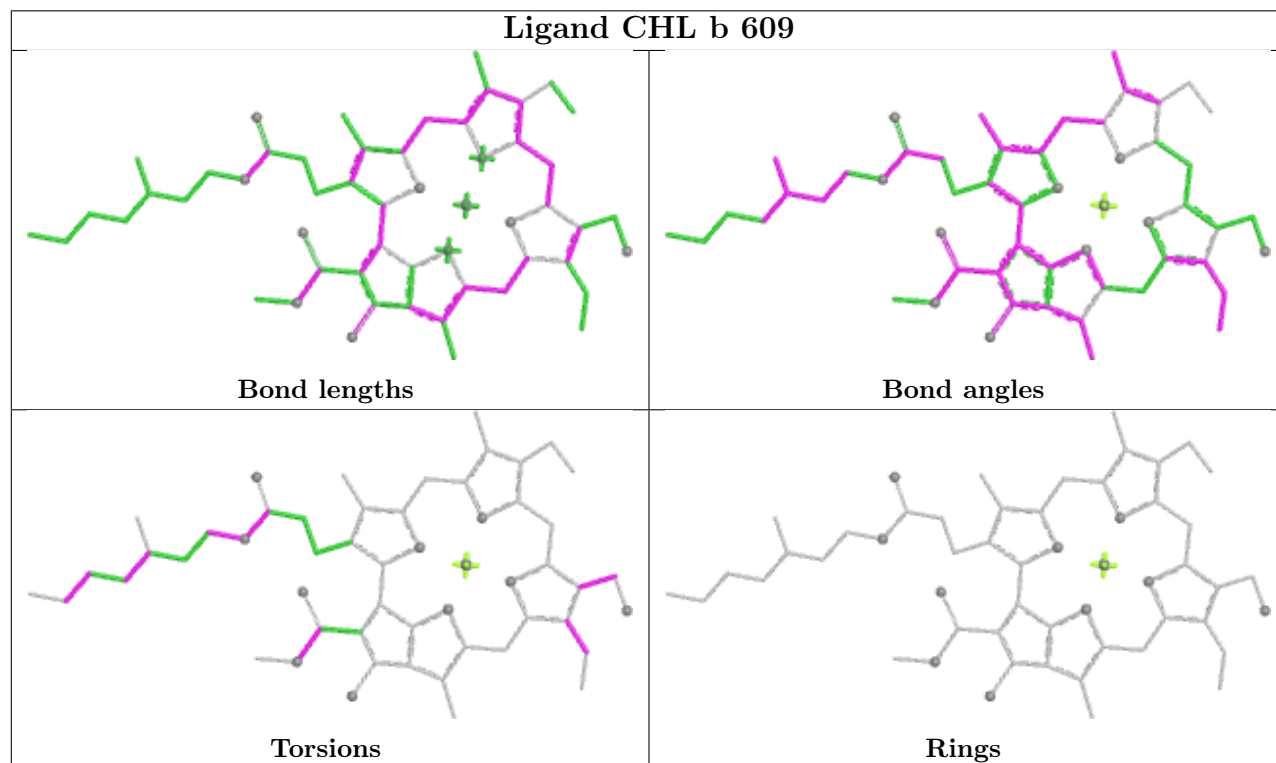
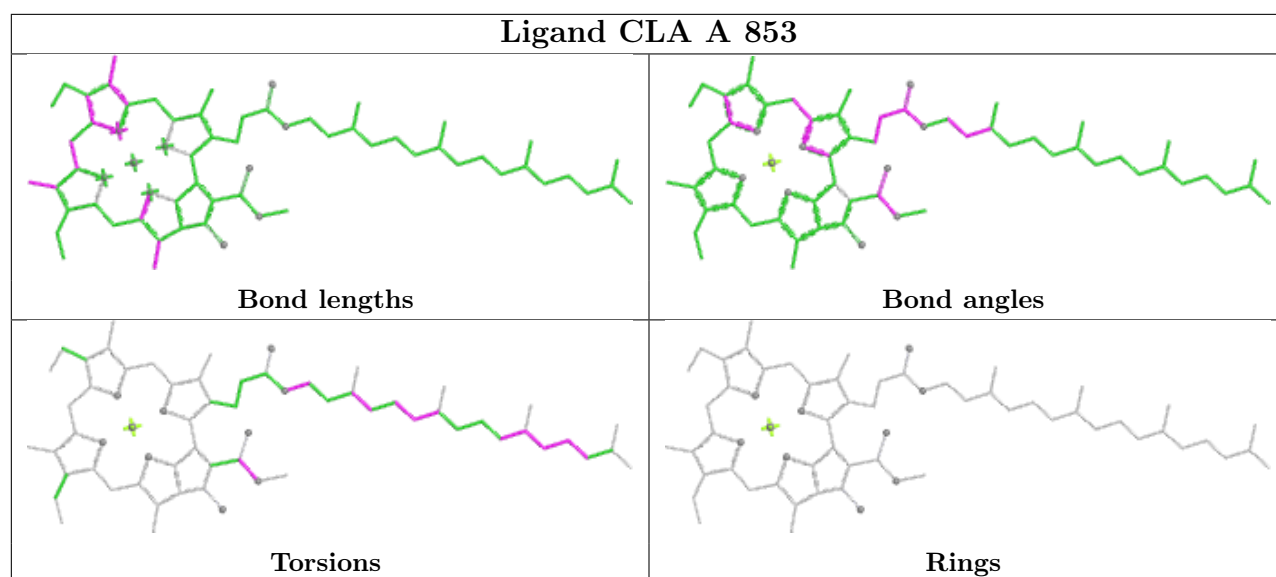


Torsions



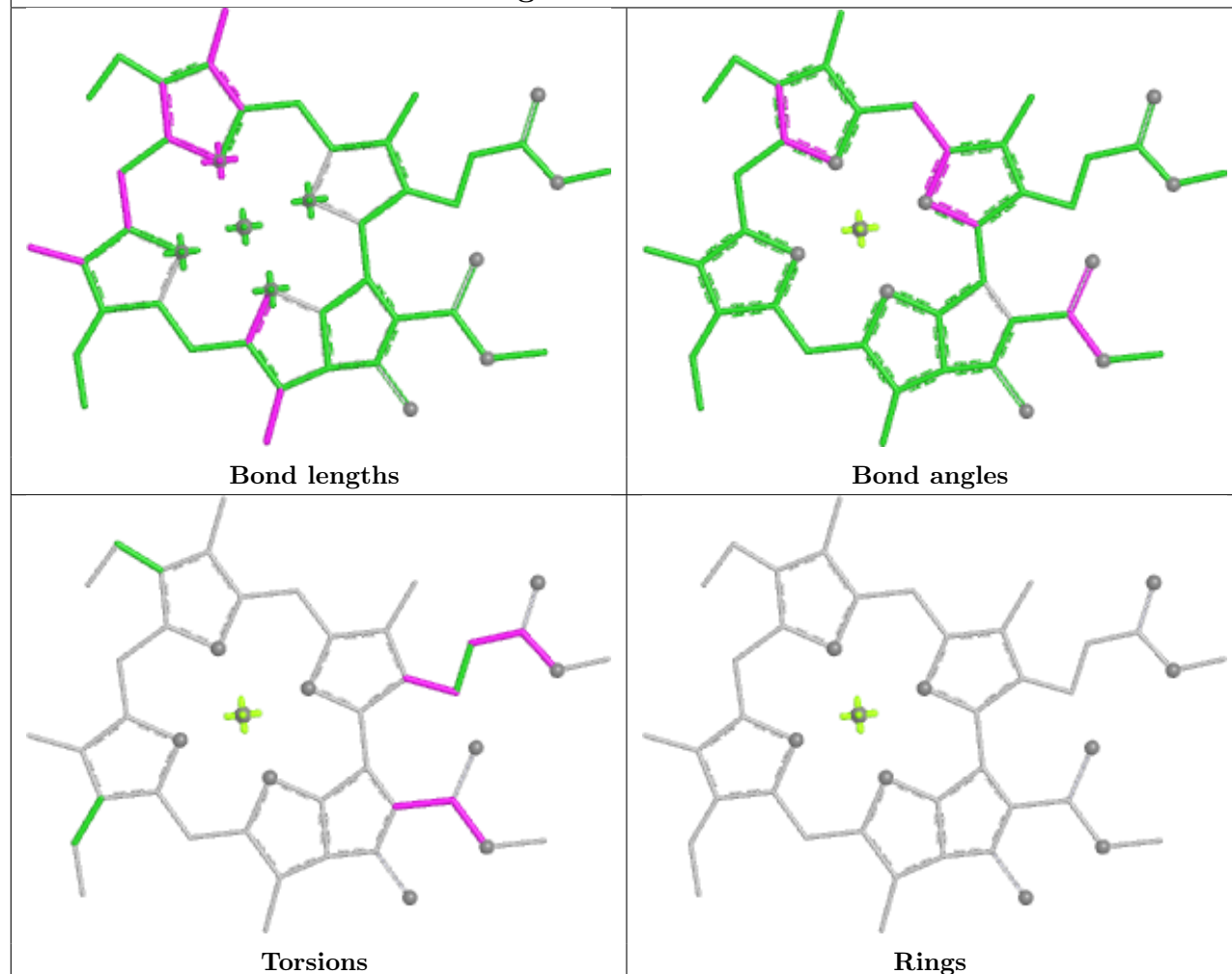
Rings



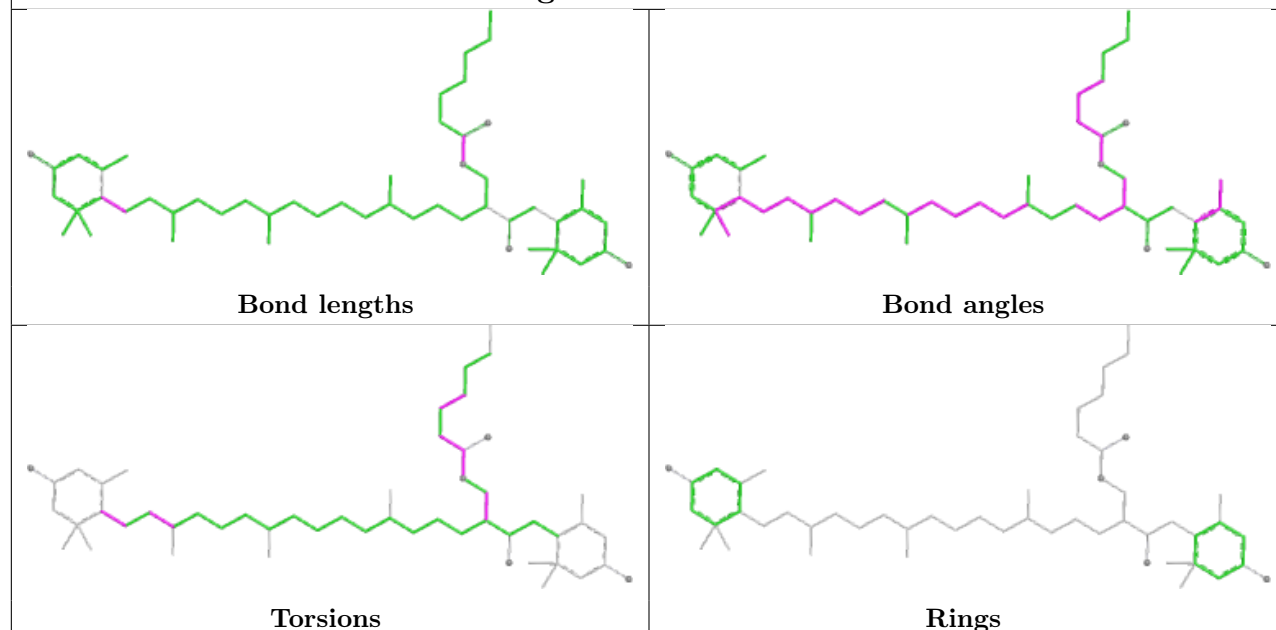




## Ligand CLA 0 313

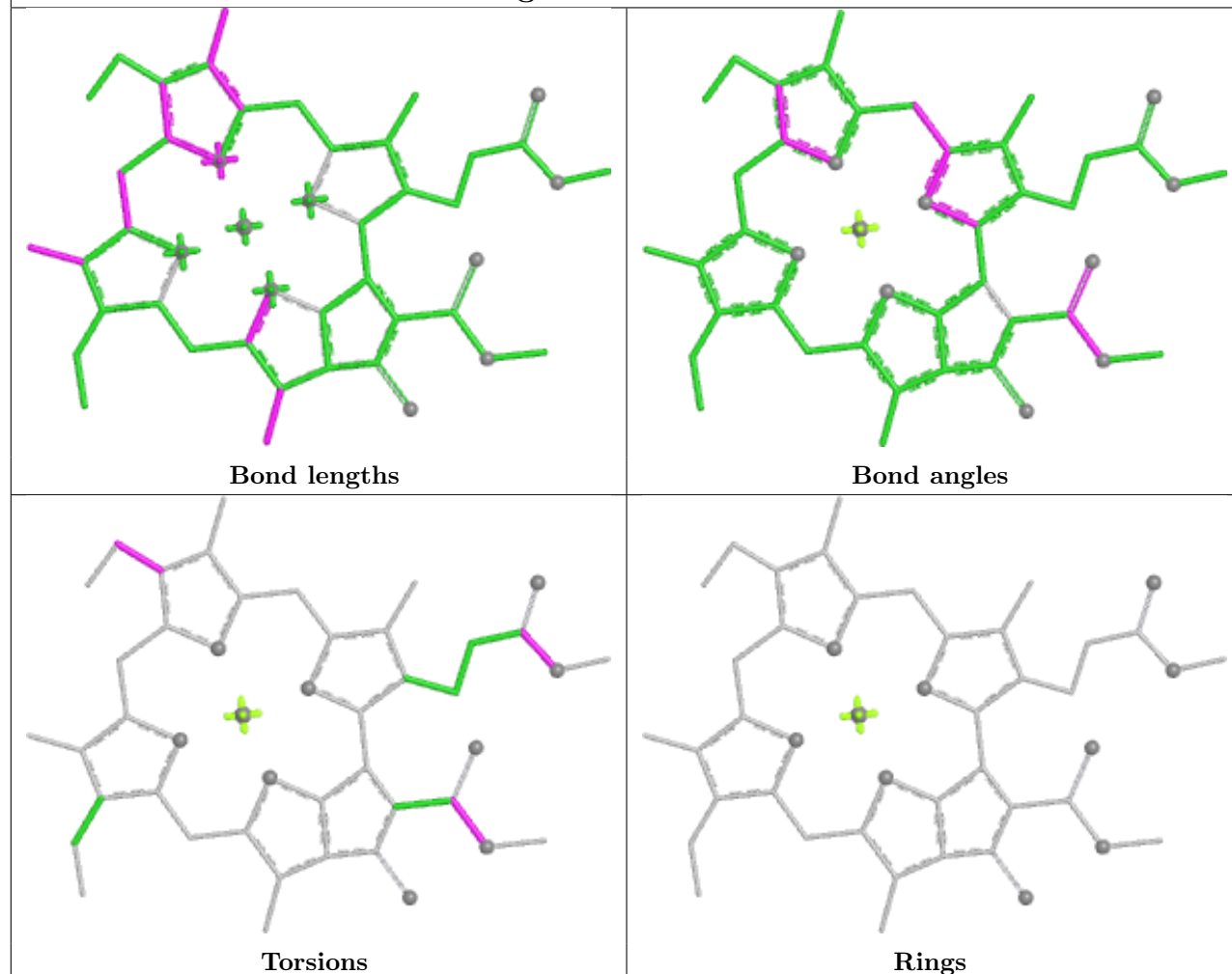


## Ligand OUR 6 502

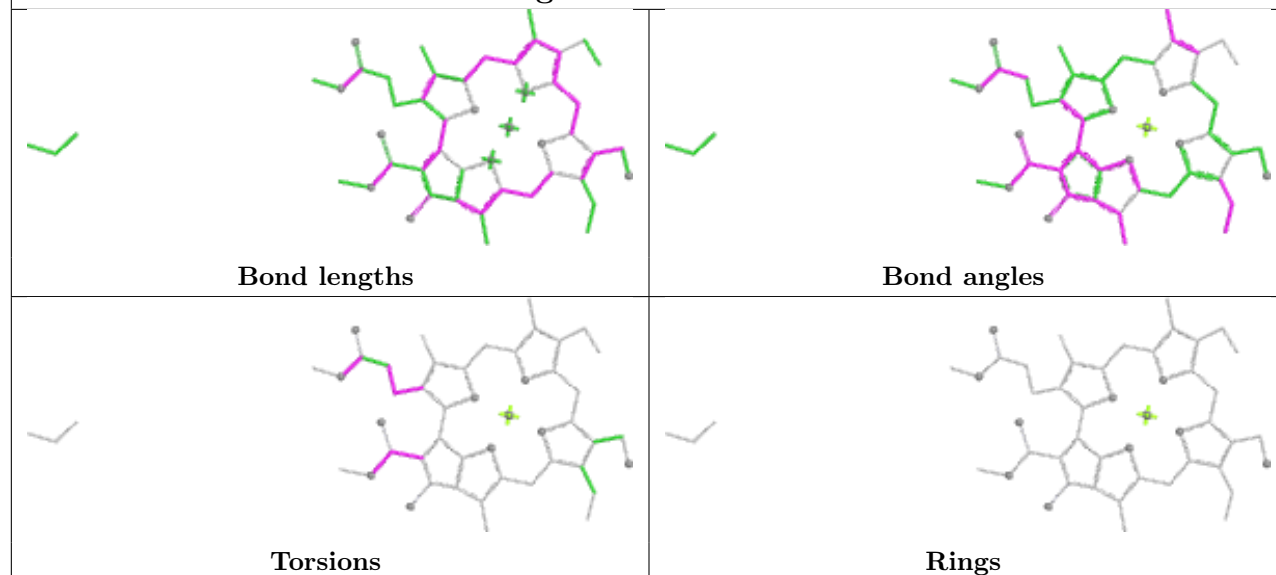




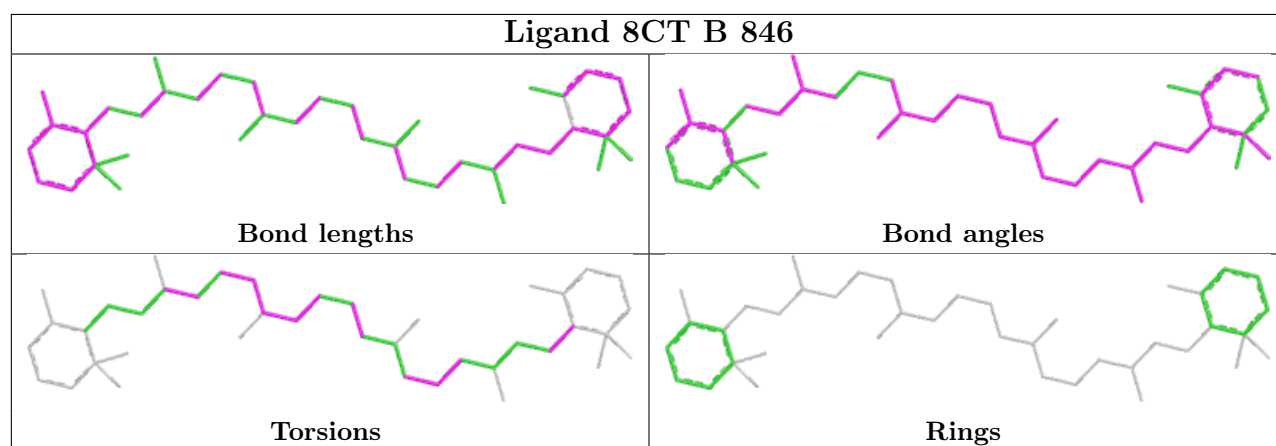
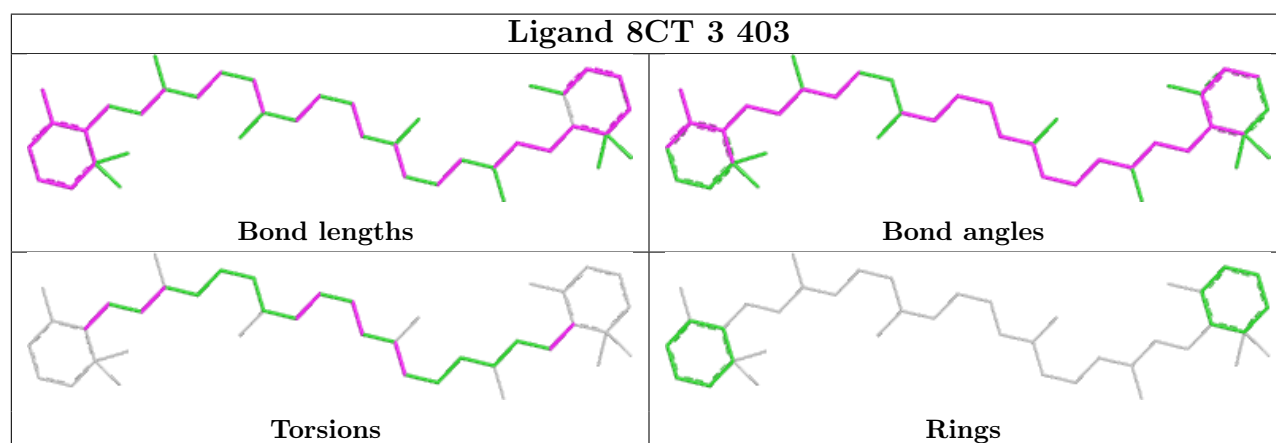
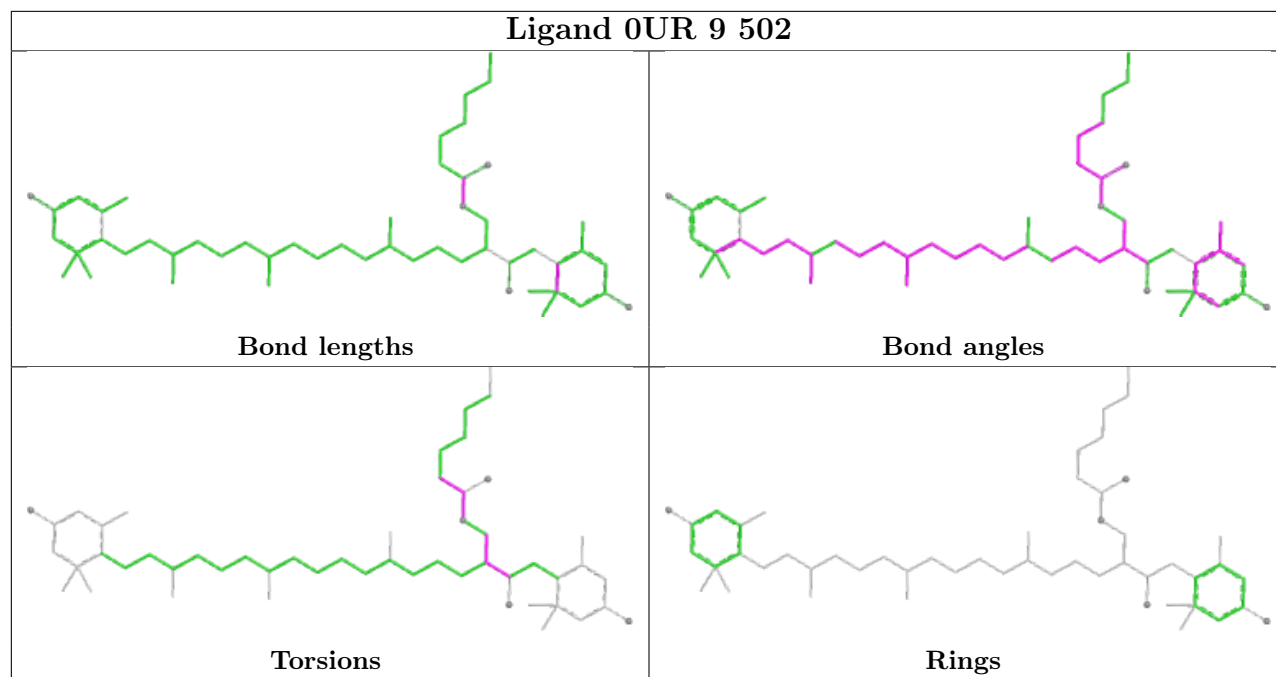
## Ligand CLA 8 303



## Ligand CHL a 607

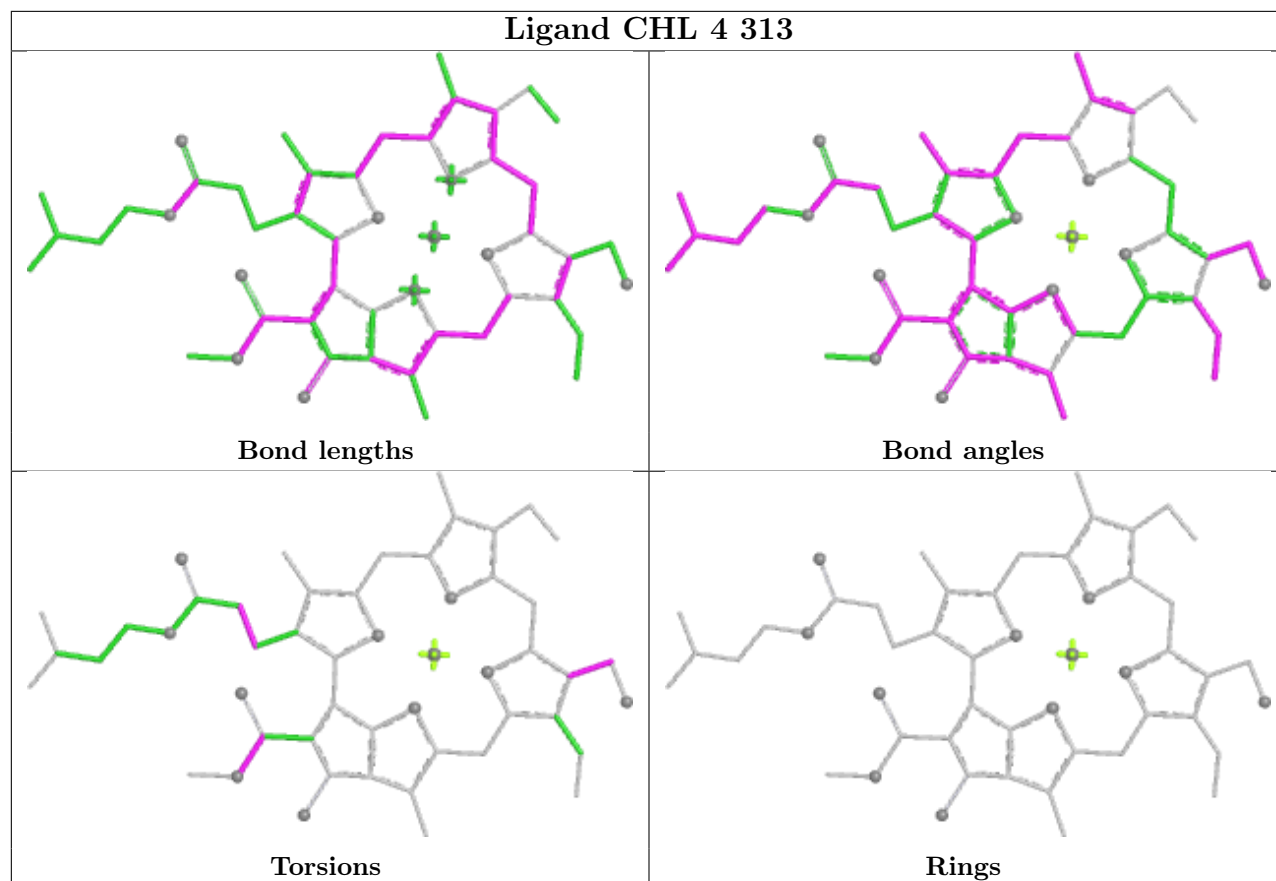




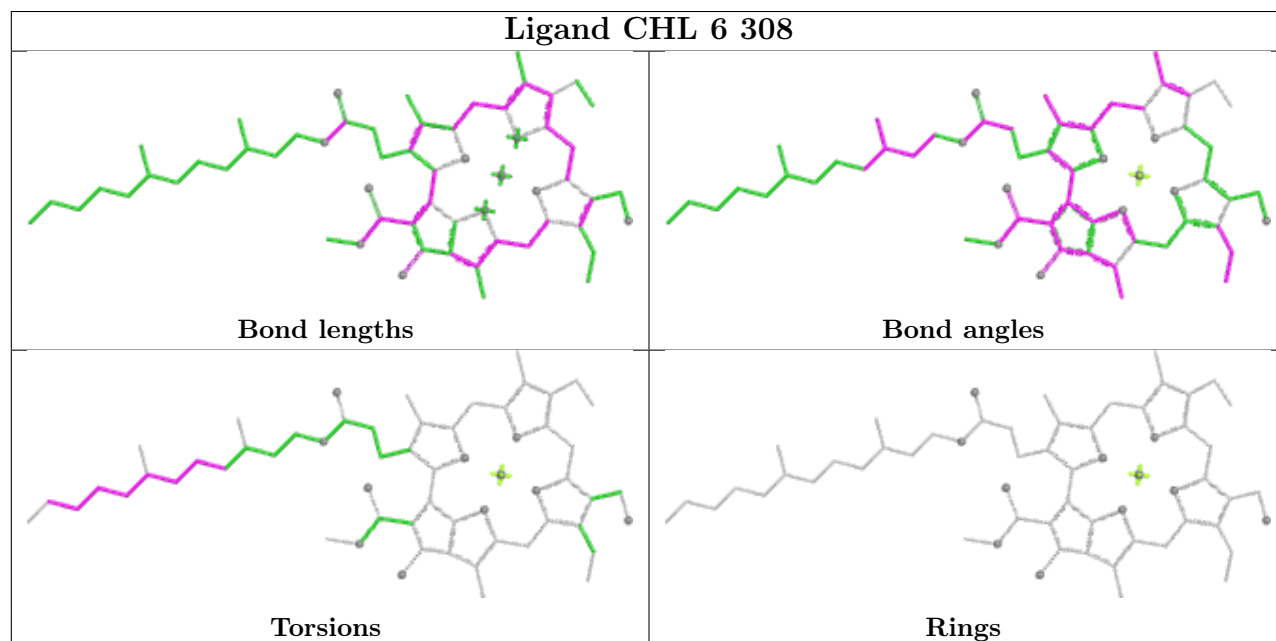




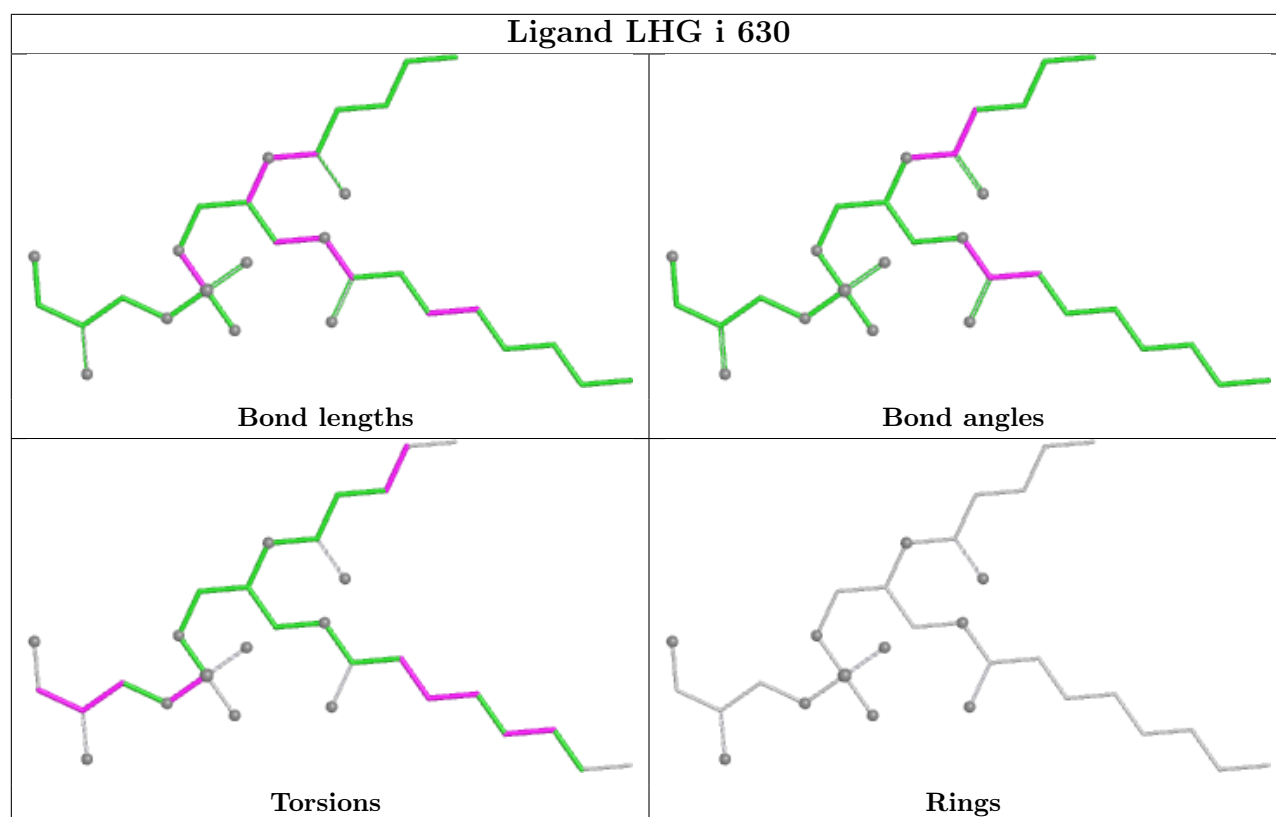
## Ligand CHL 4 313



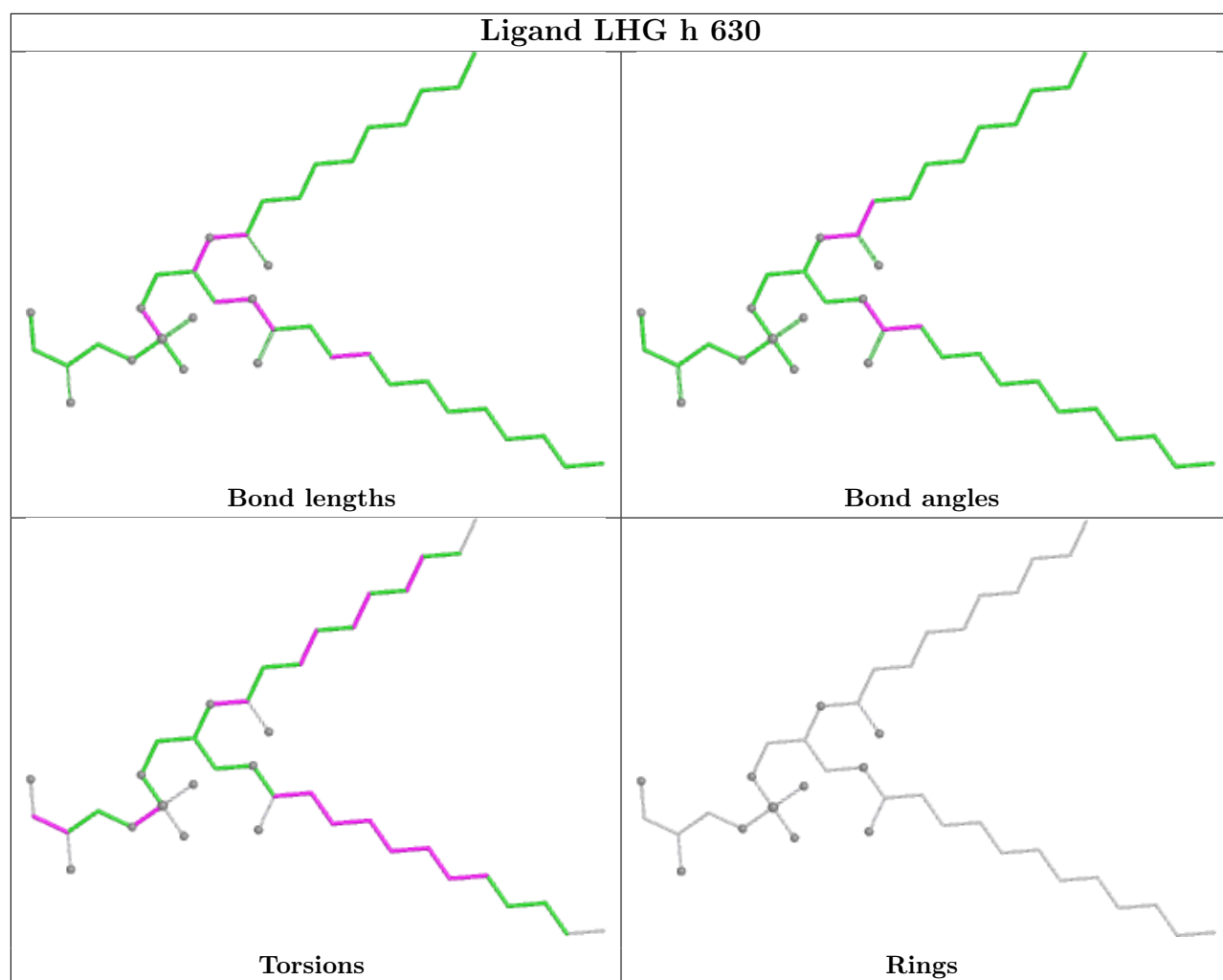
## Ligand CHL 6 308





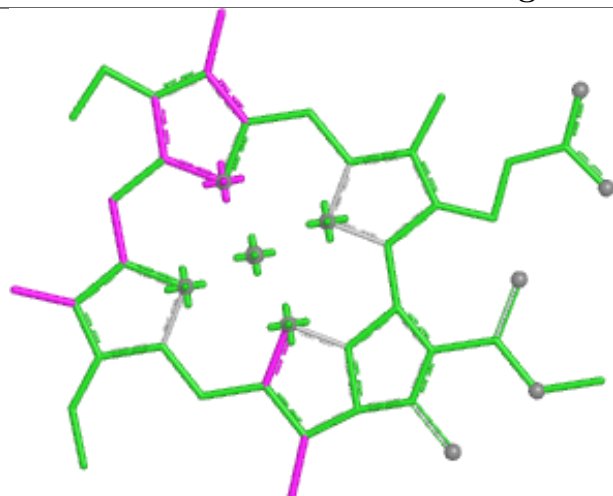




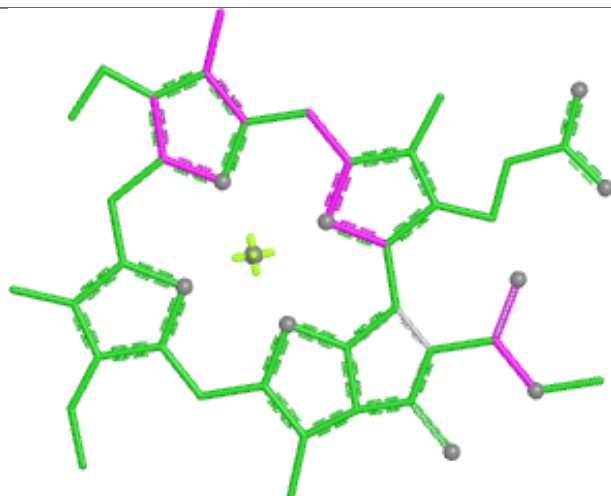




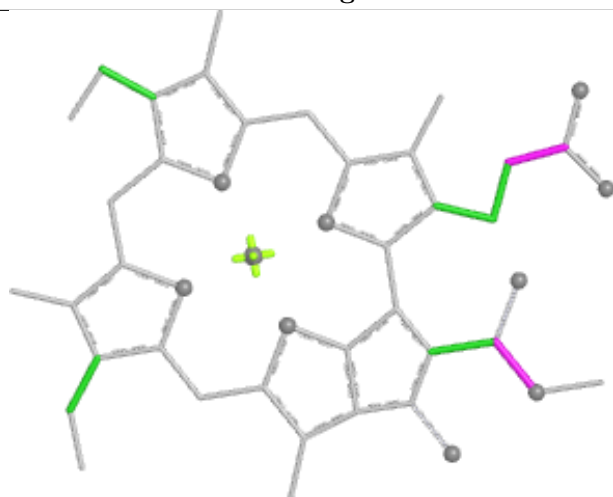
## Ligand CLA 4 314



Bond lengths



Bond angles

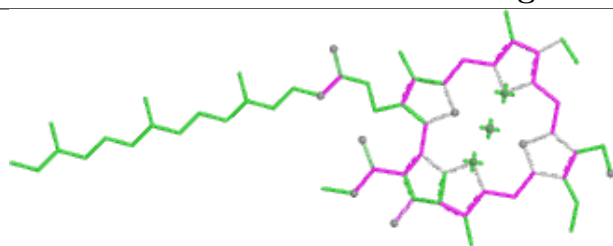


Torsions

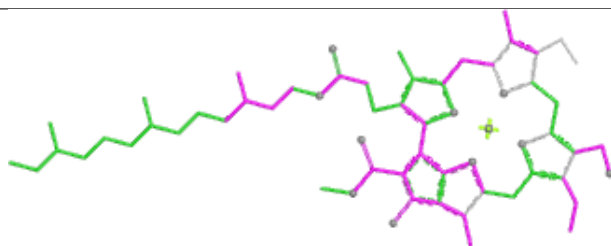


Rings

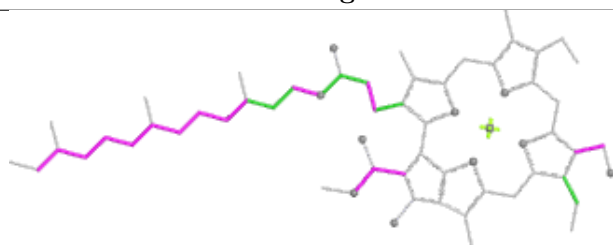
## Ligand CHL 1 313



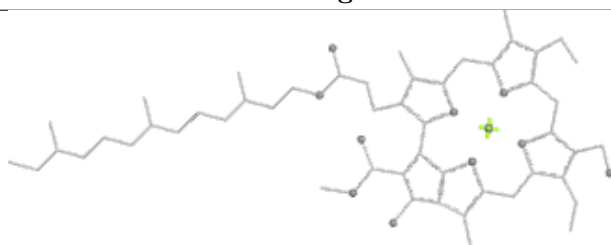
Bond lengths



Bond angles

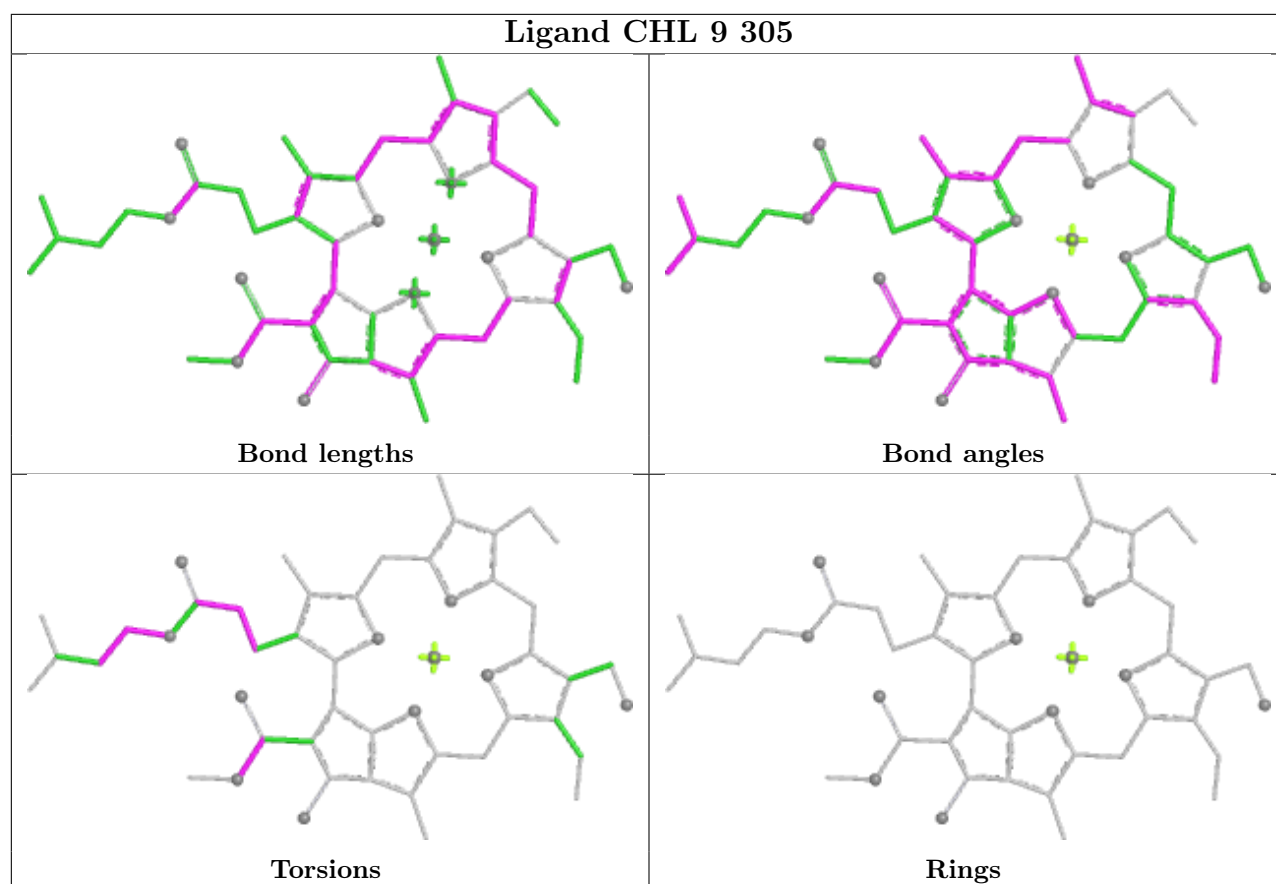


Torsions



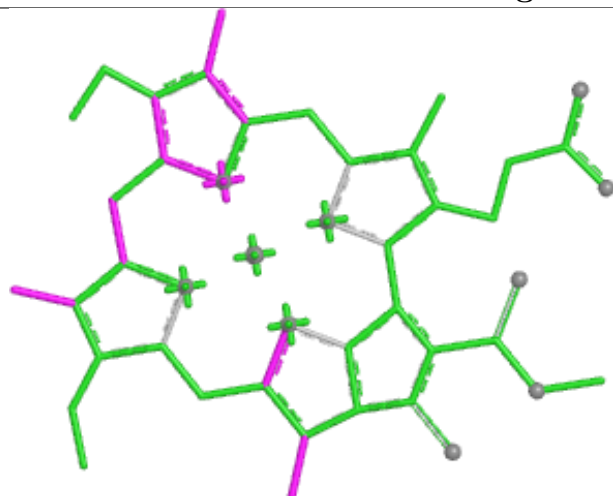
Rings



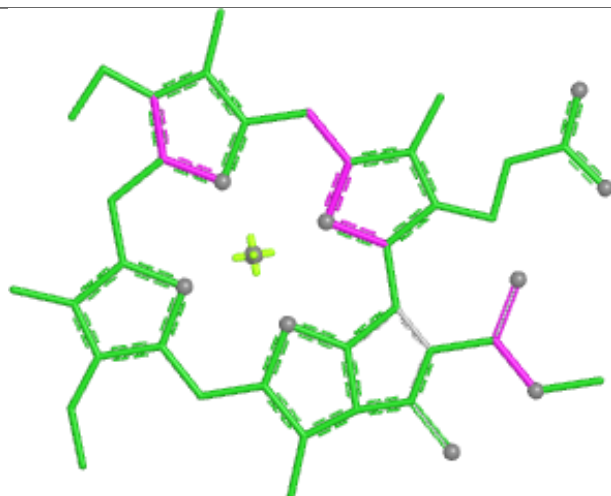




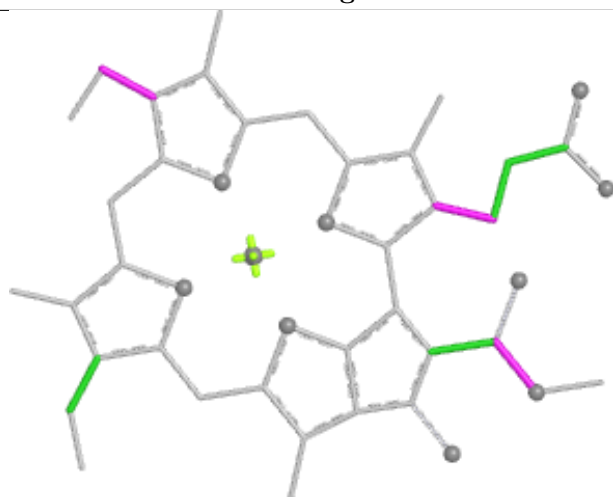
## Ligand CLA F 301



Bond lengths



Bond angles



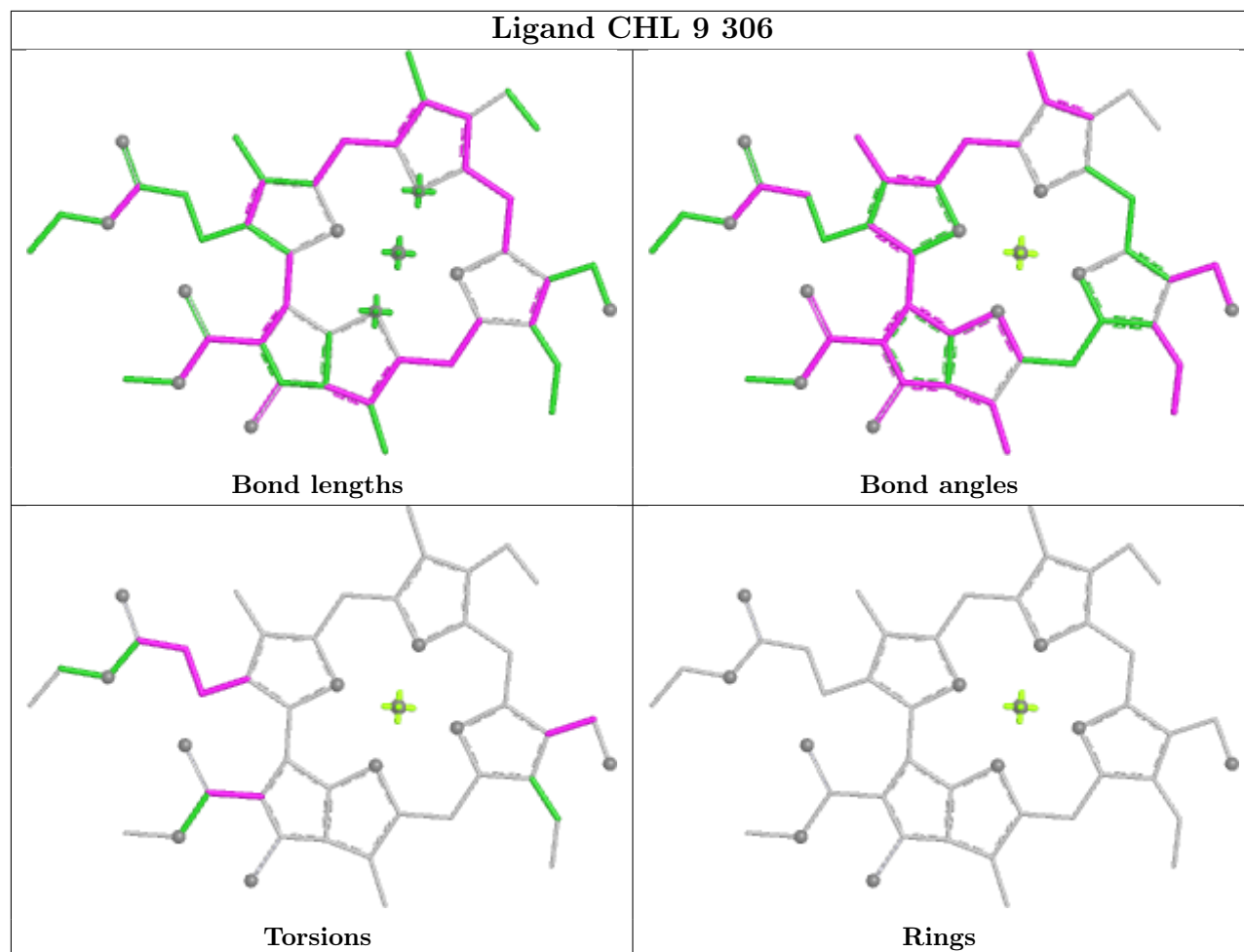
Torsions



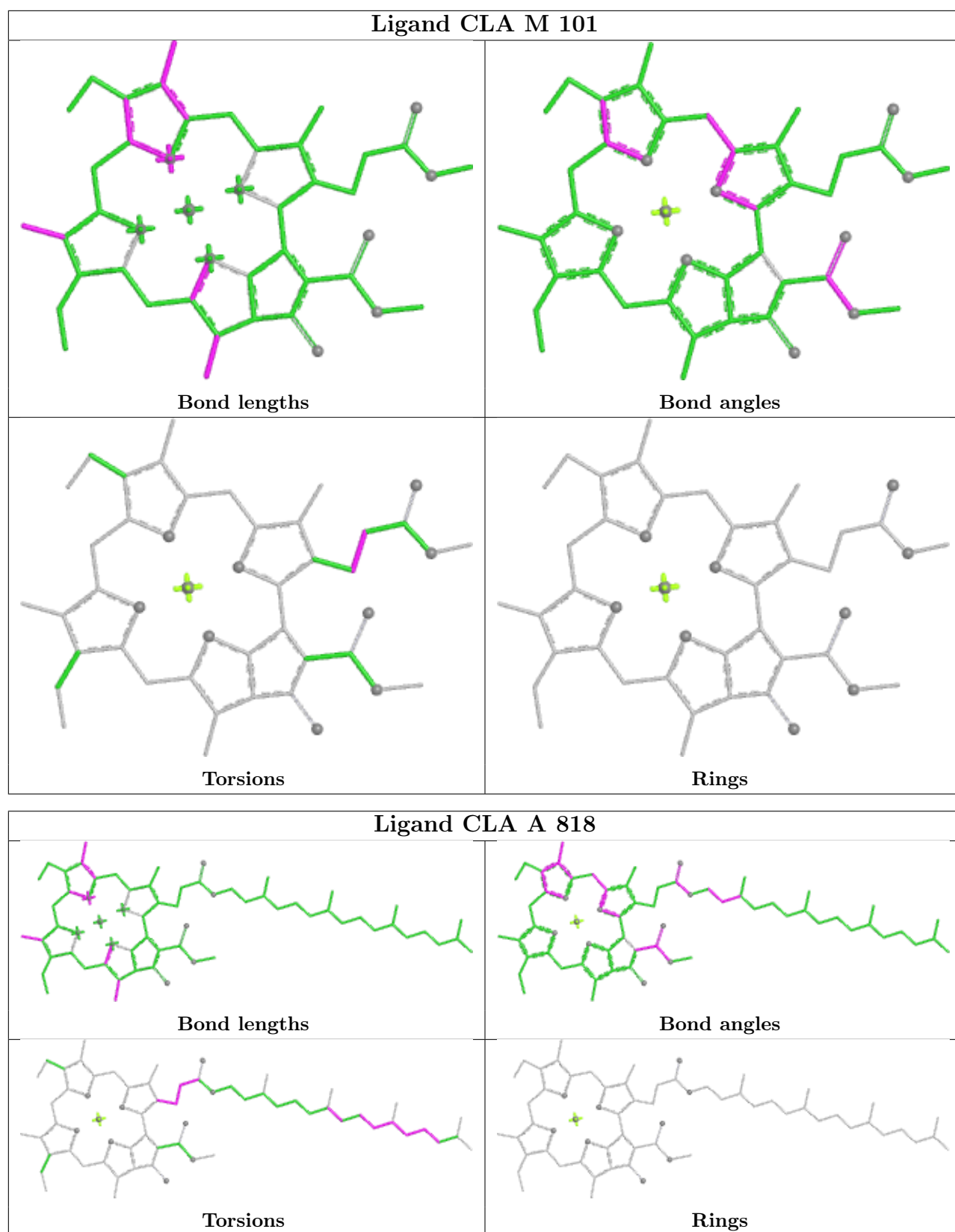
Rings



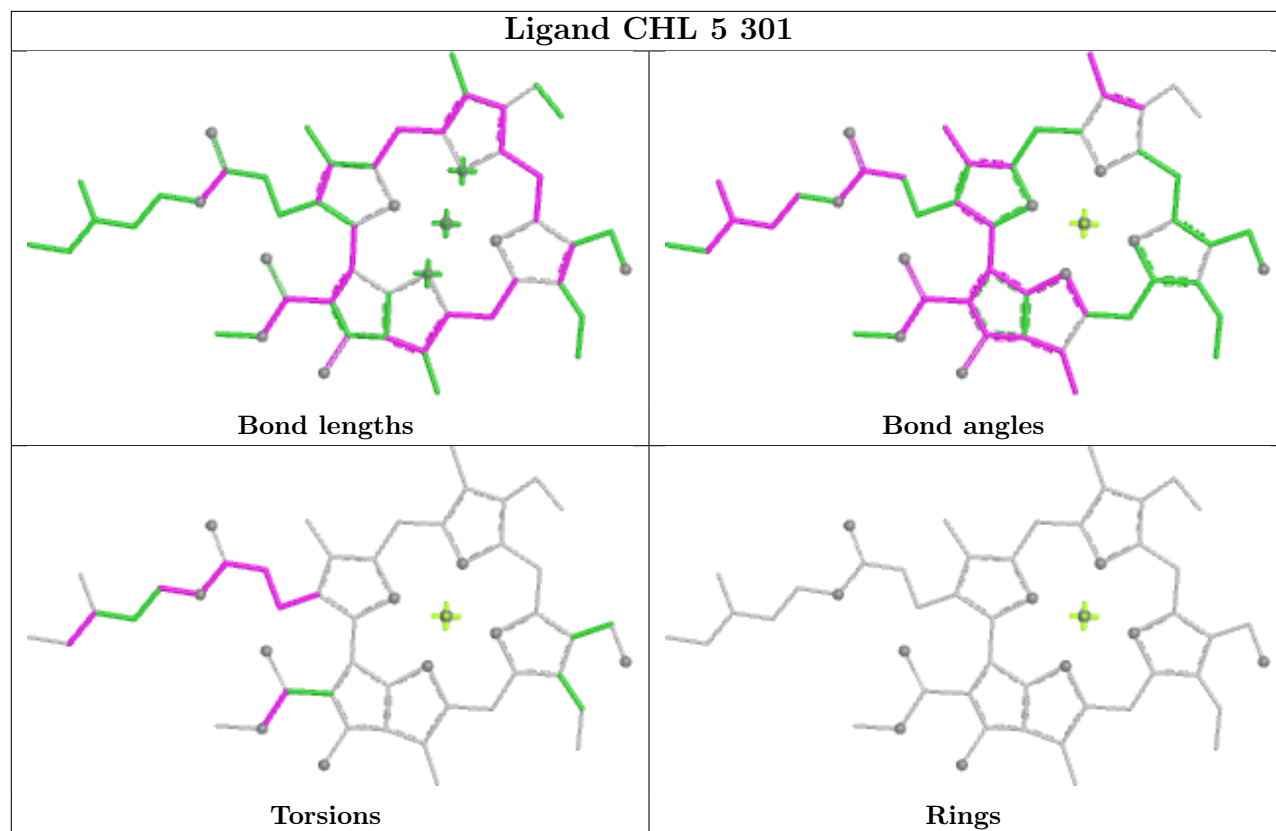
## Ligand CHL 9 306





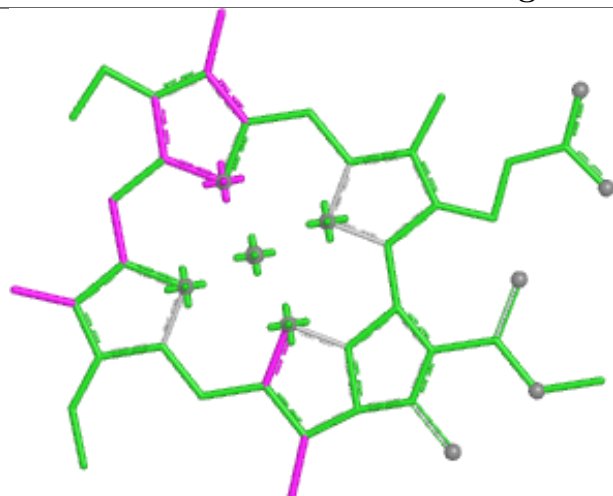




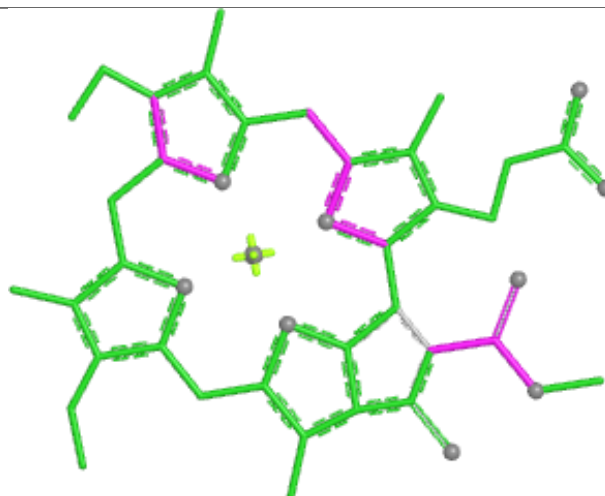




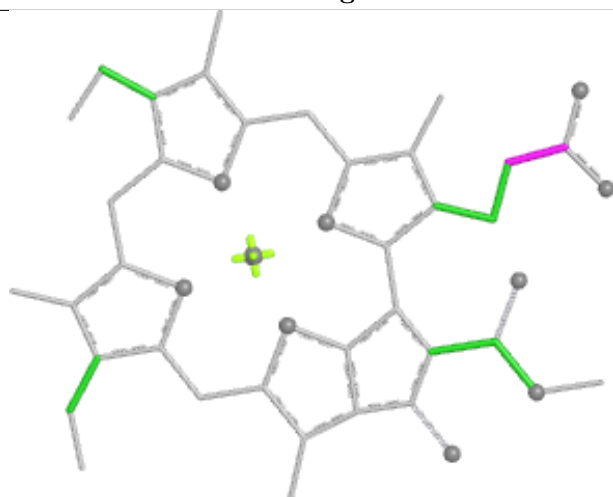
## Ligand CLA 6 314



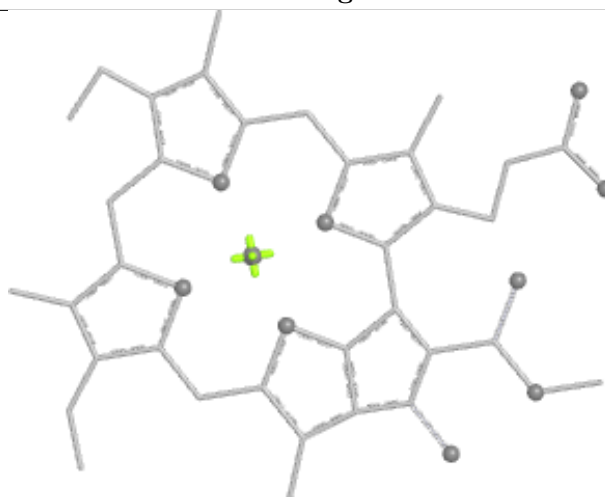
Bond lengths



Bond angles

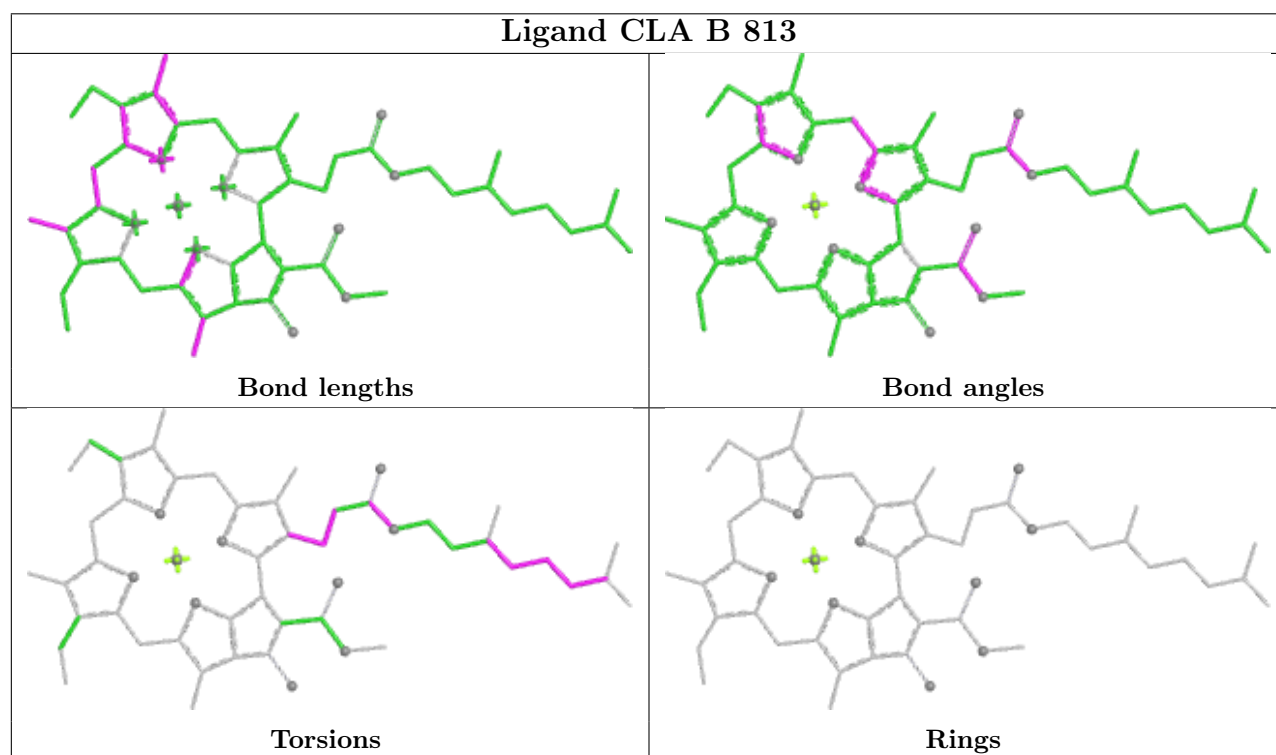
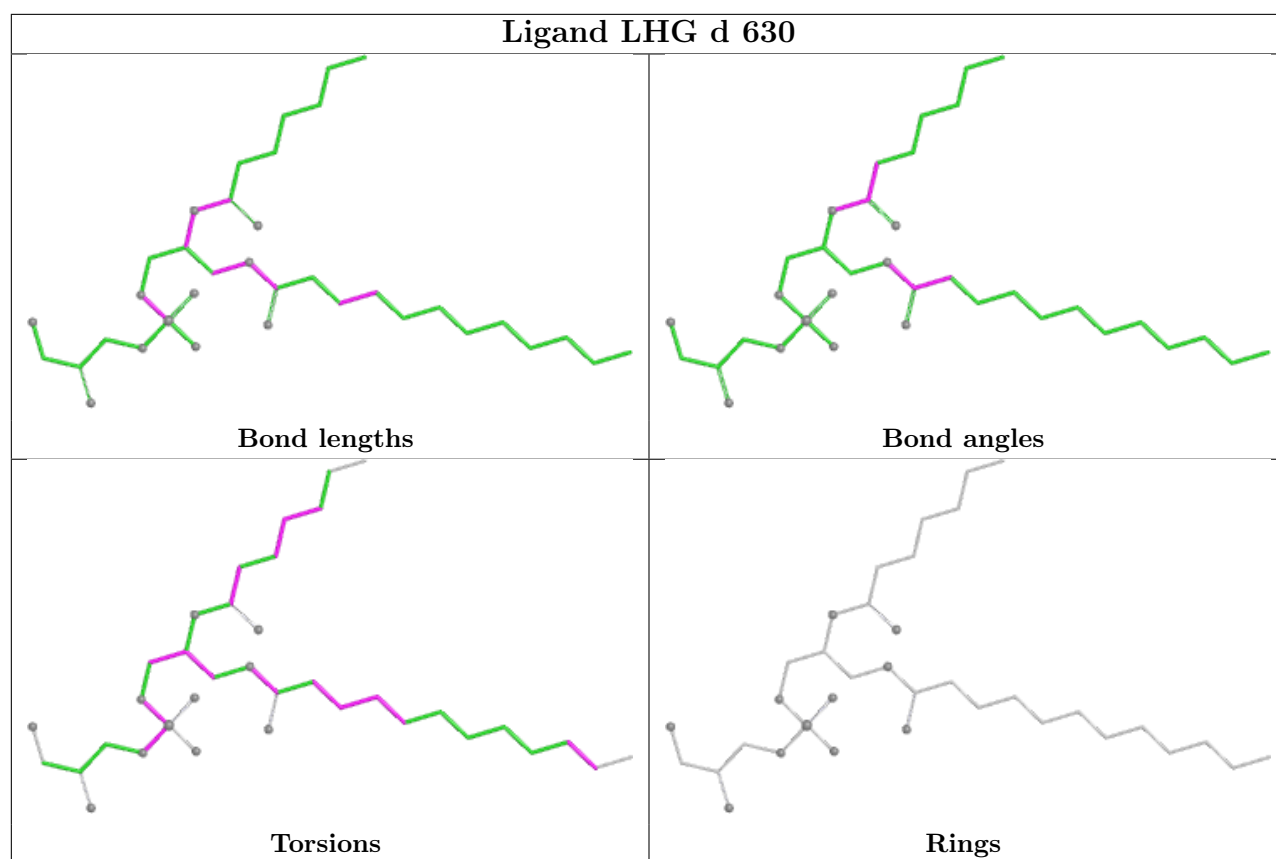


Torsions

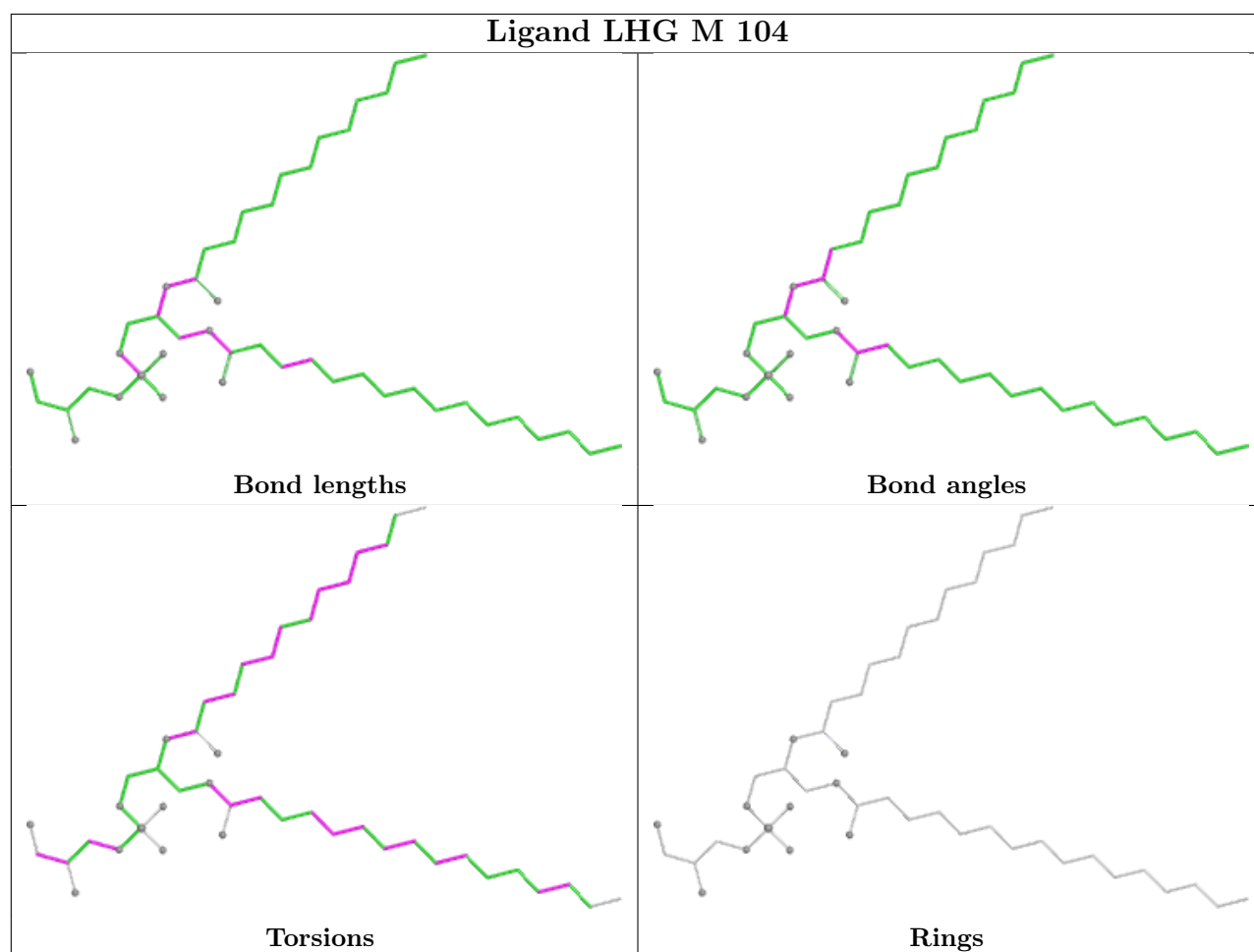


Rings



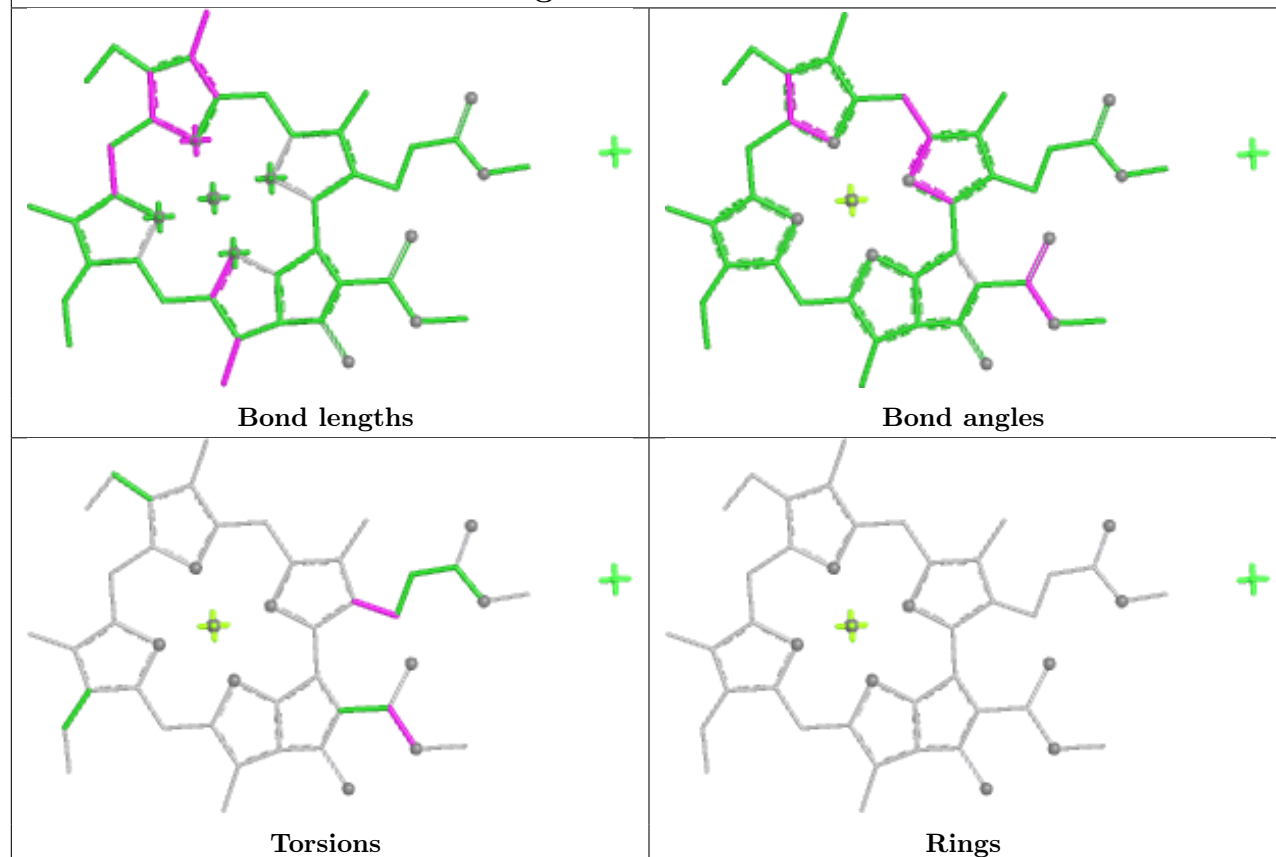




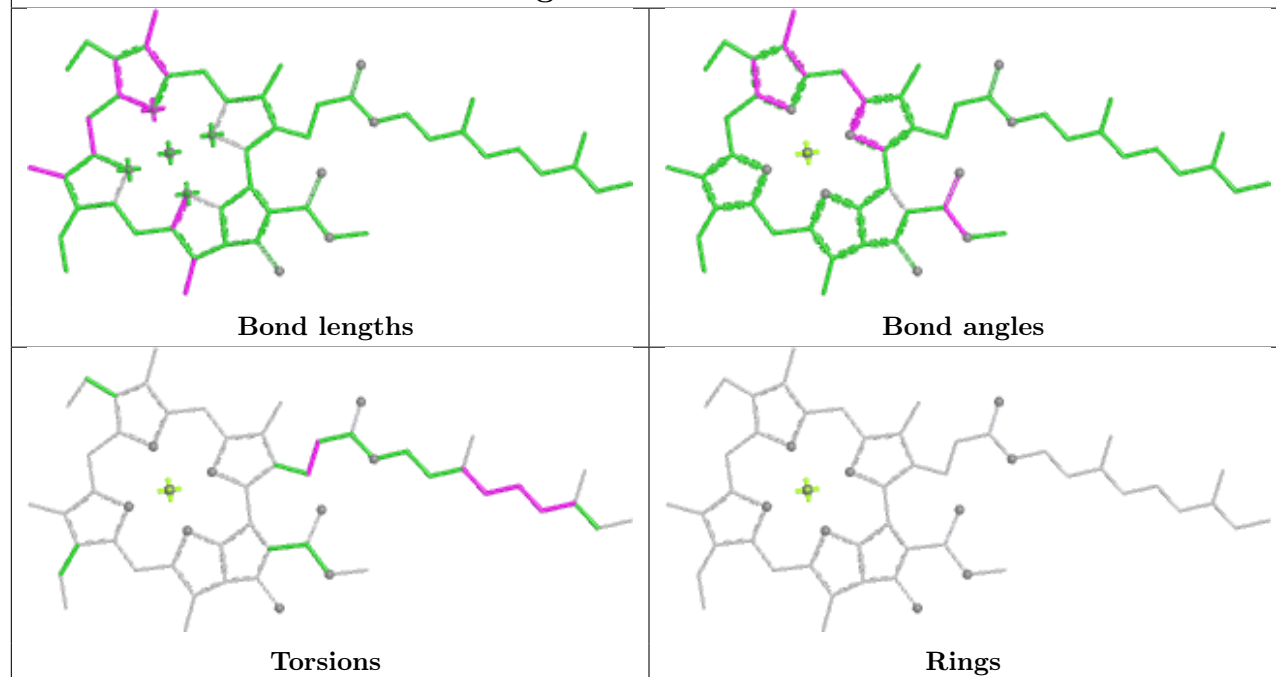




## Ligand CLA h 610

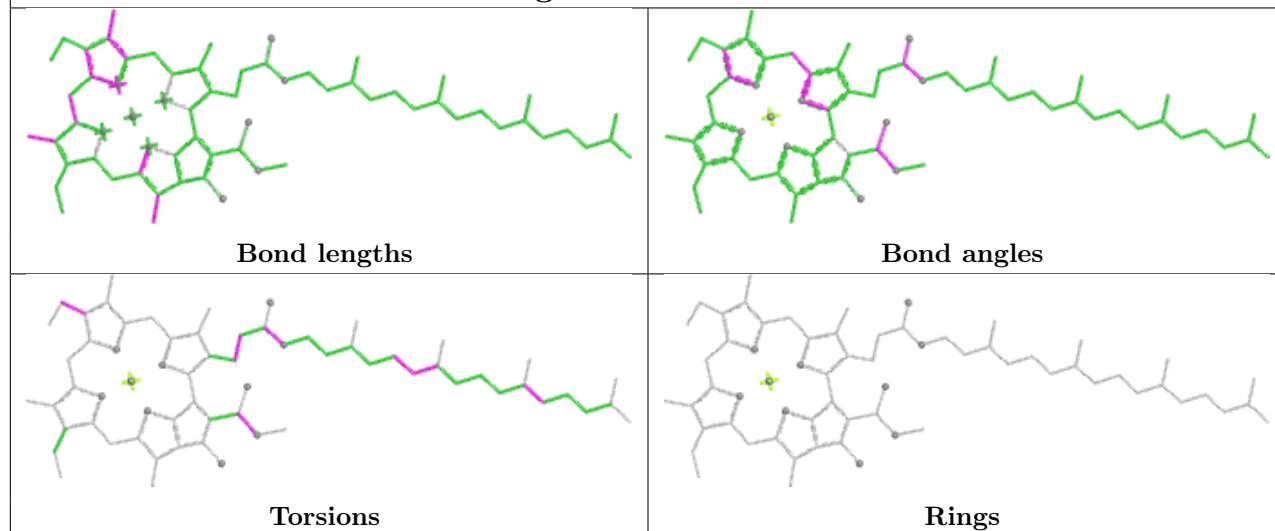


## Ligand CLA 9 312

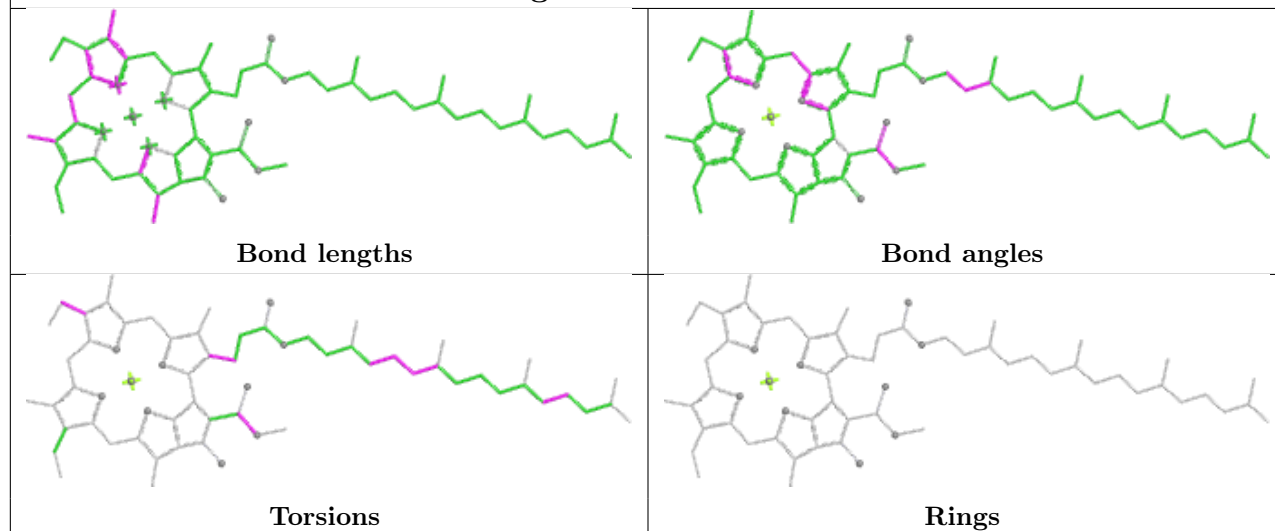




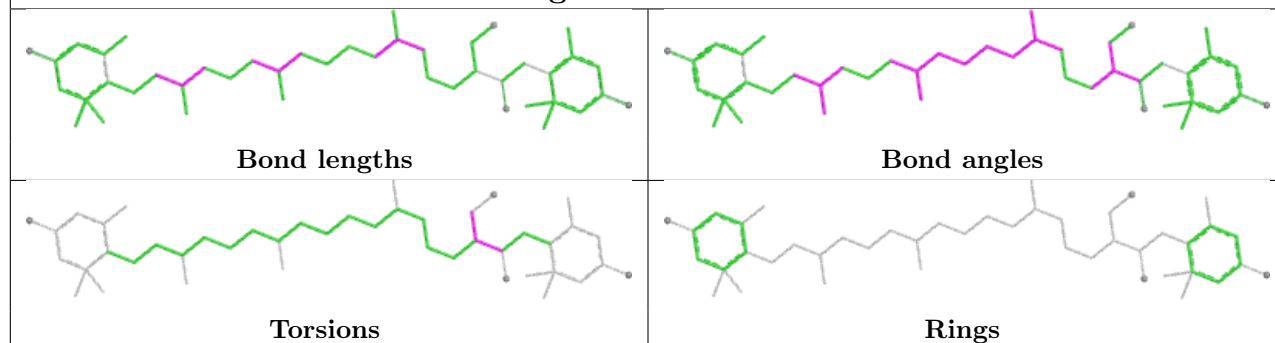
## Ligand CLA 0 312



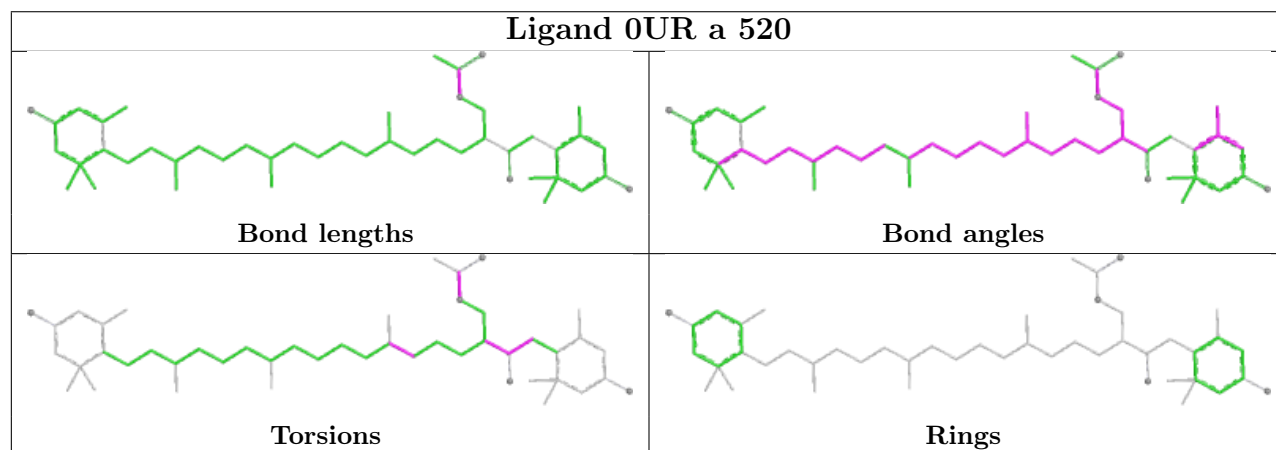
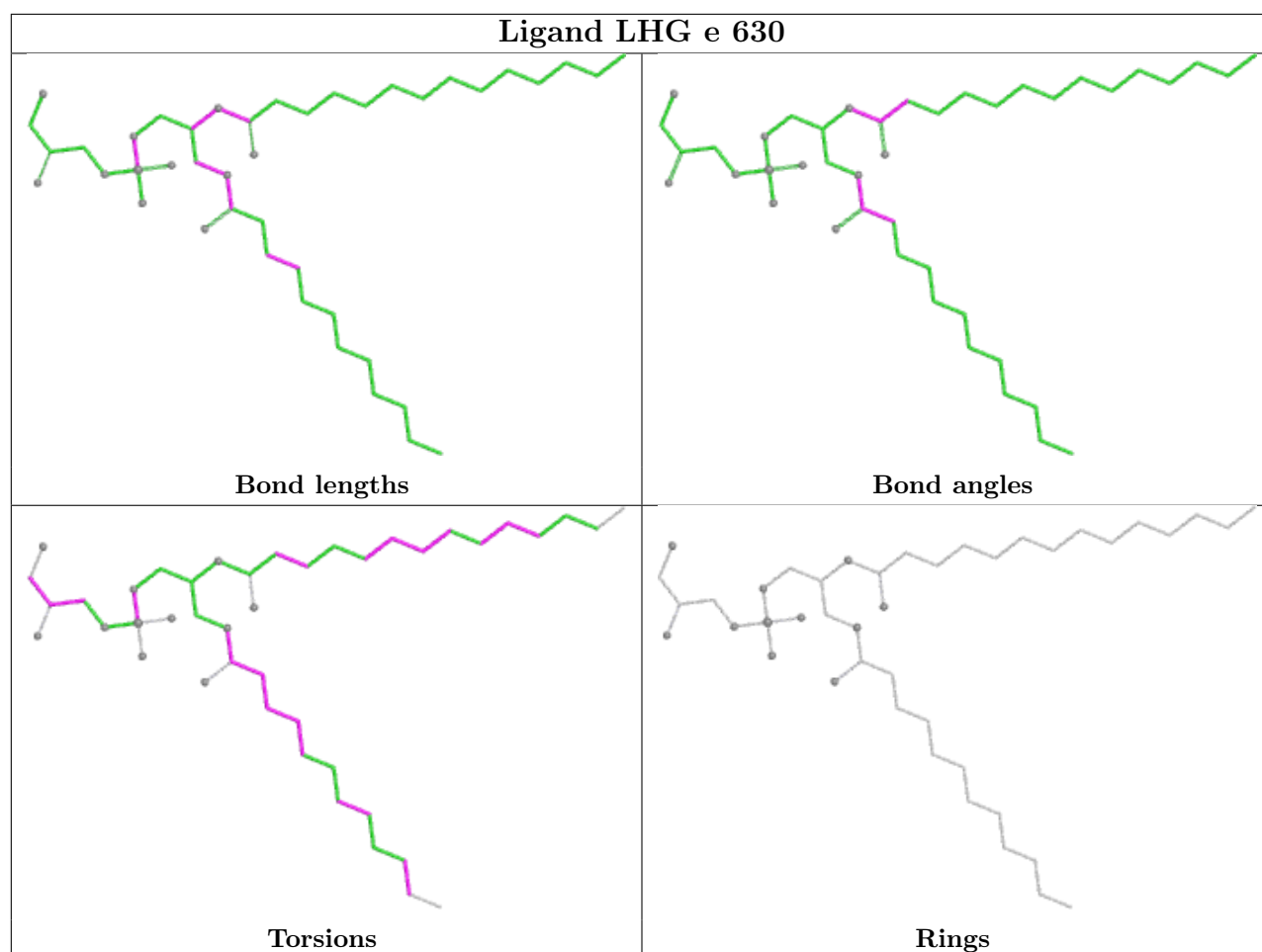
## Ligand CLA A 832



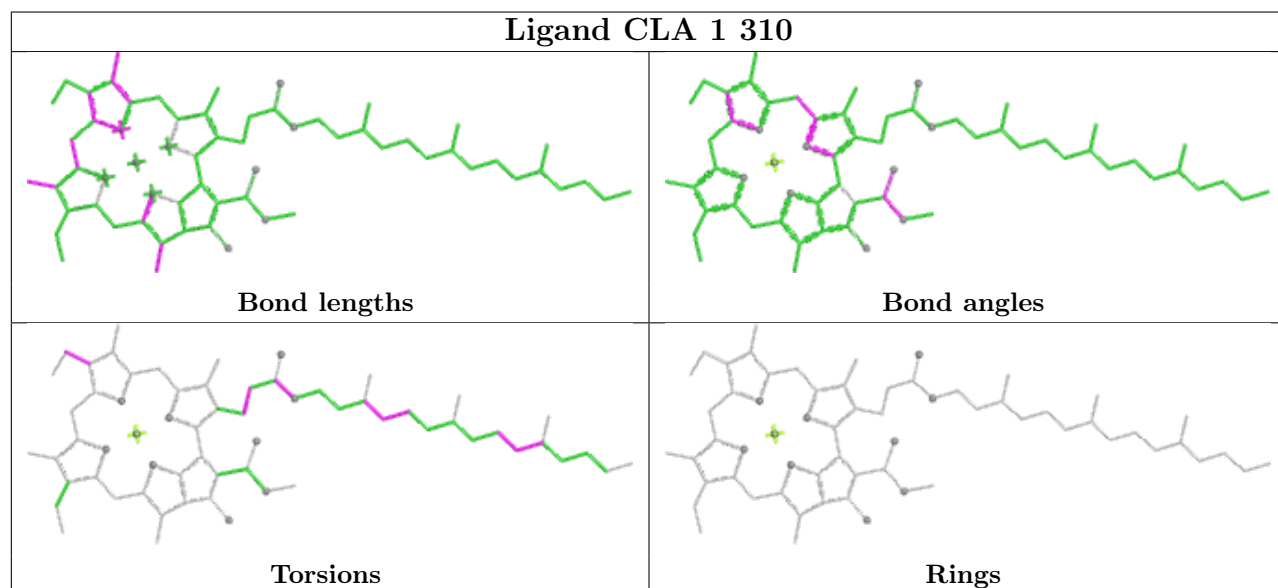
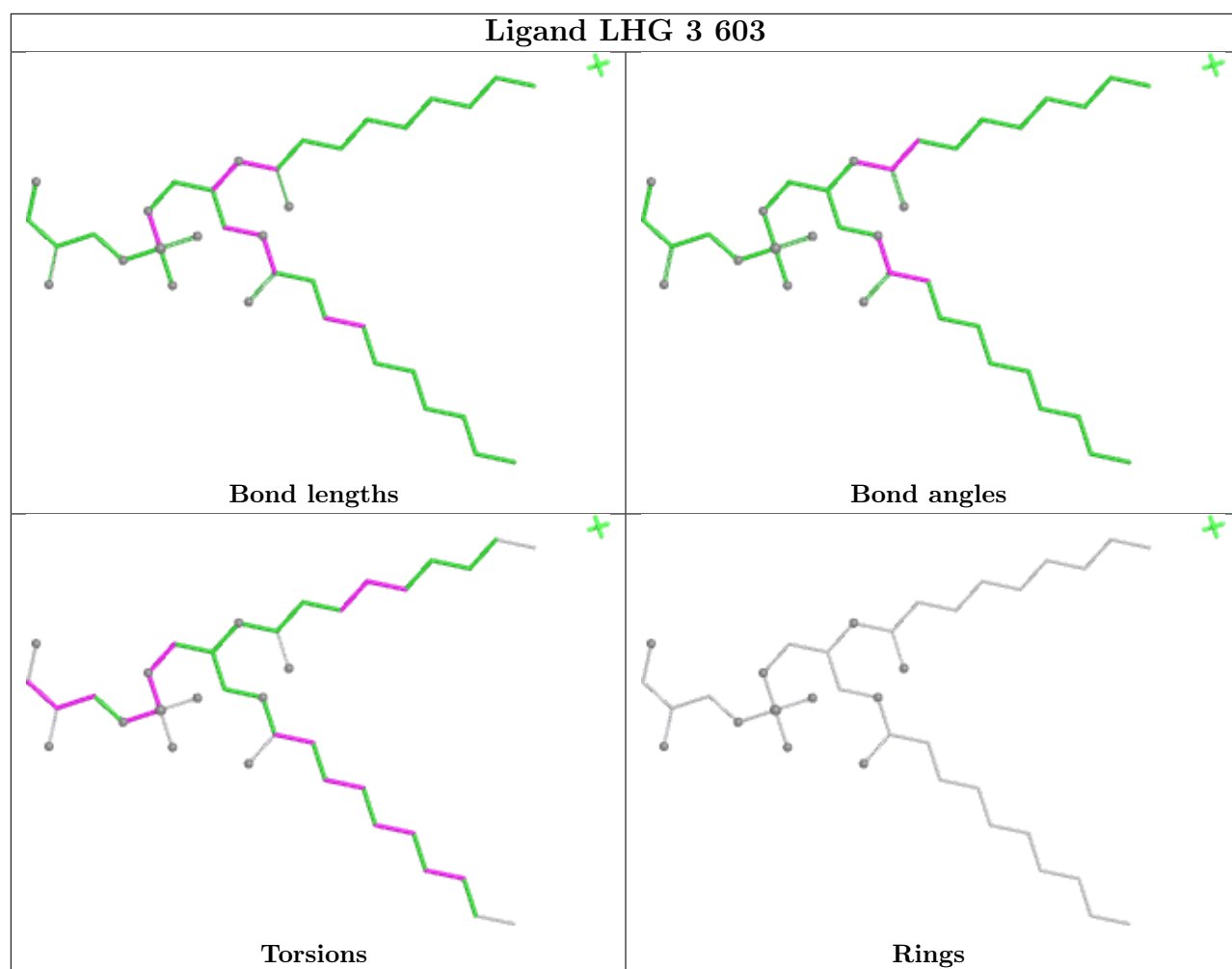
## Ligand OIE i 521





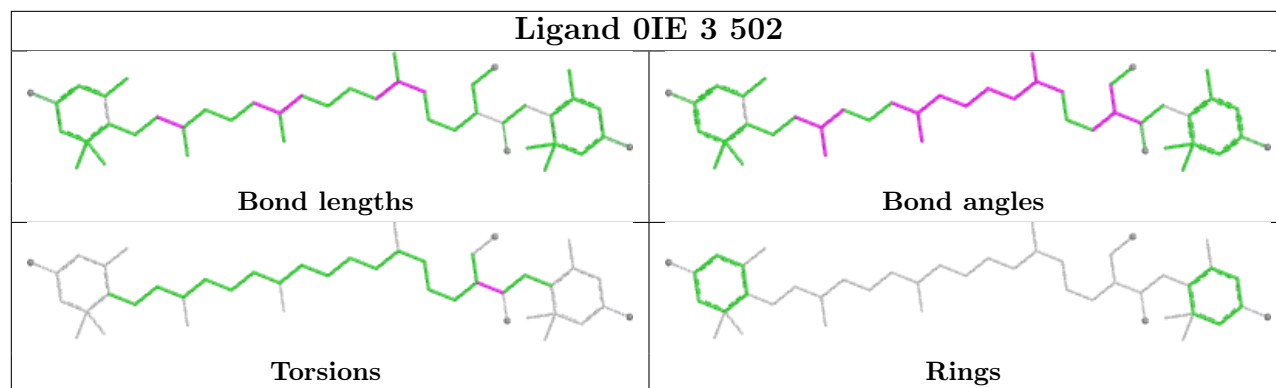




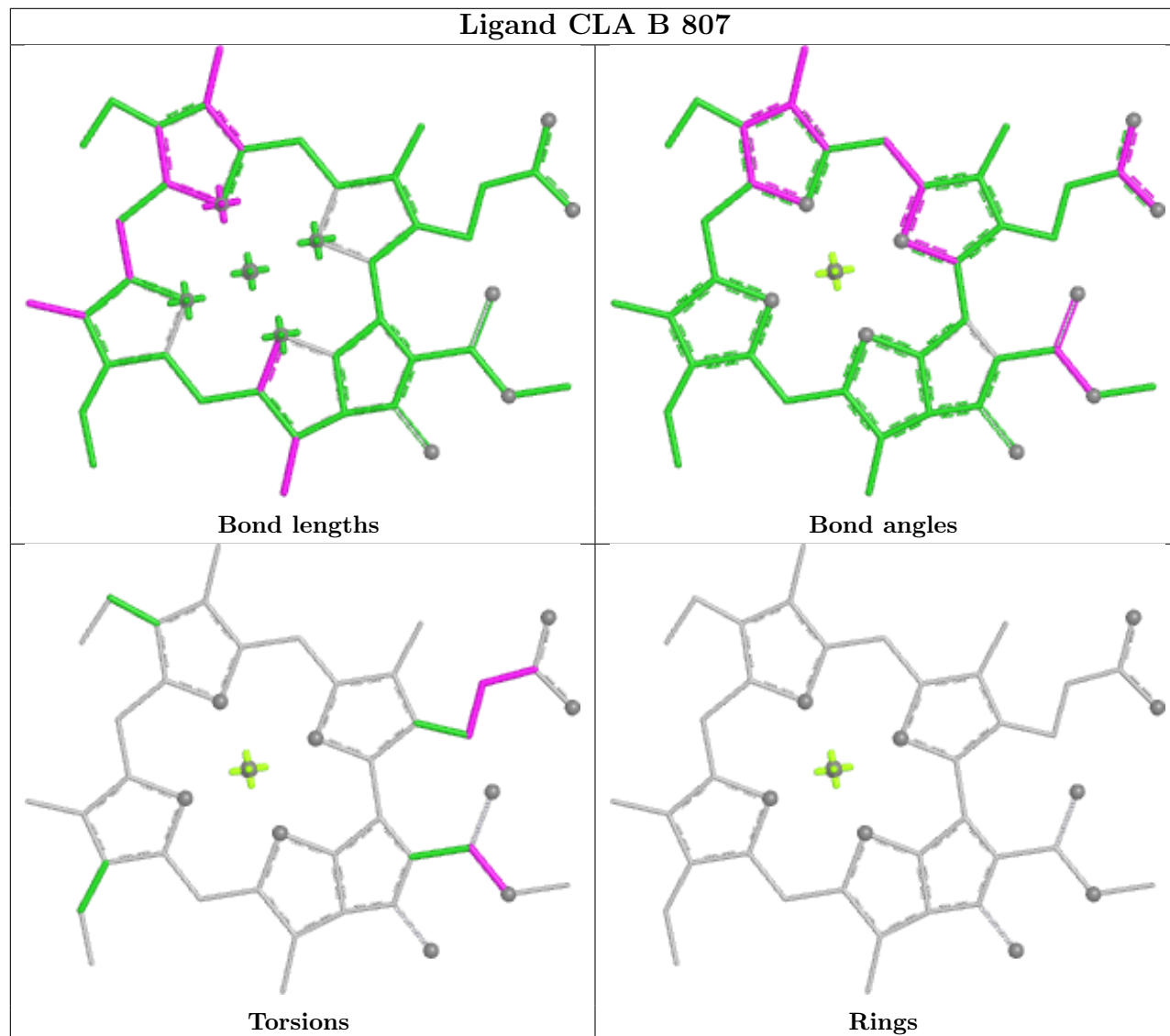




## Ligand OIE 3 502

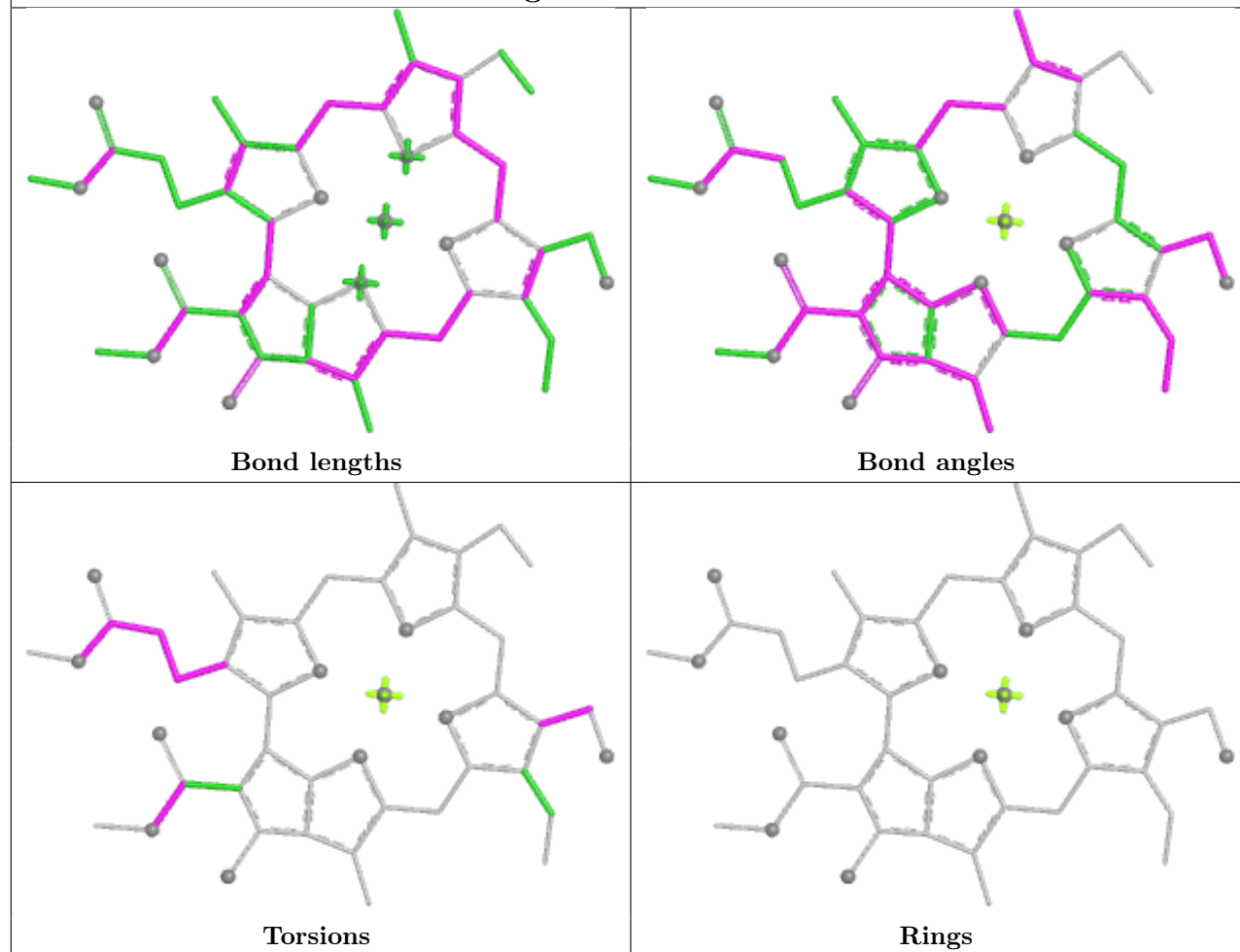


## Ligand CLA B 807

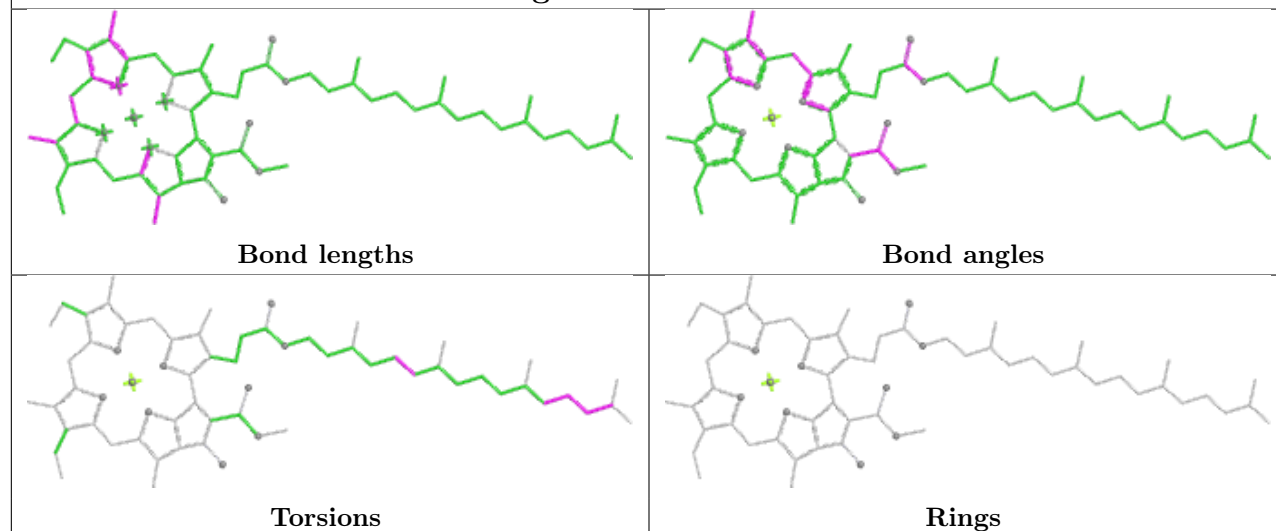




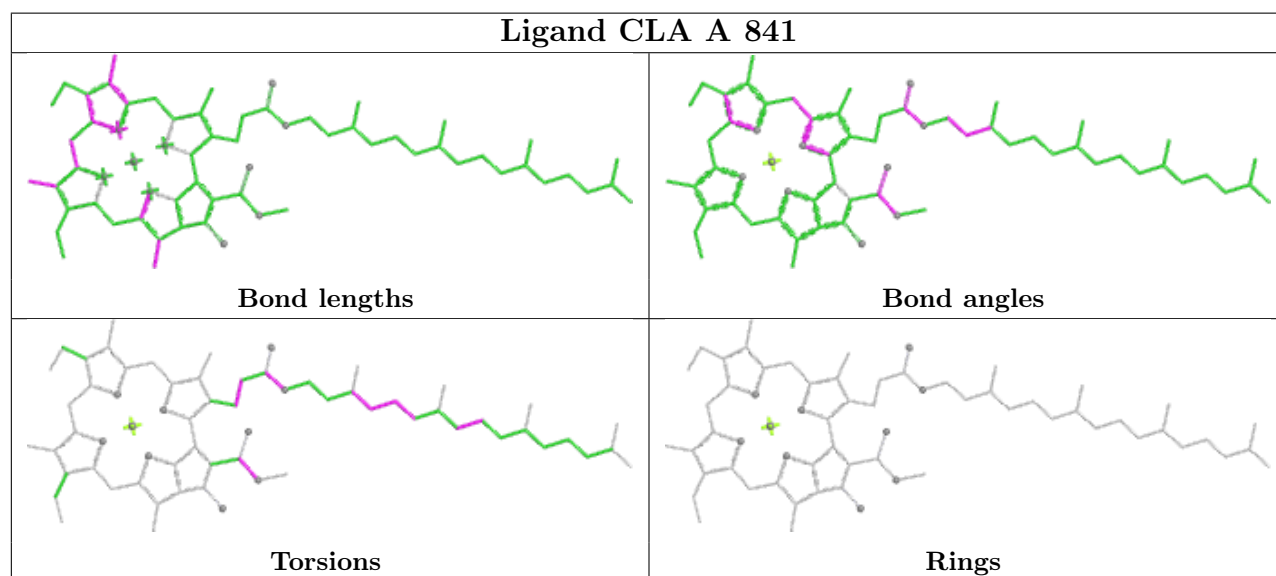
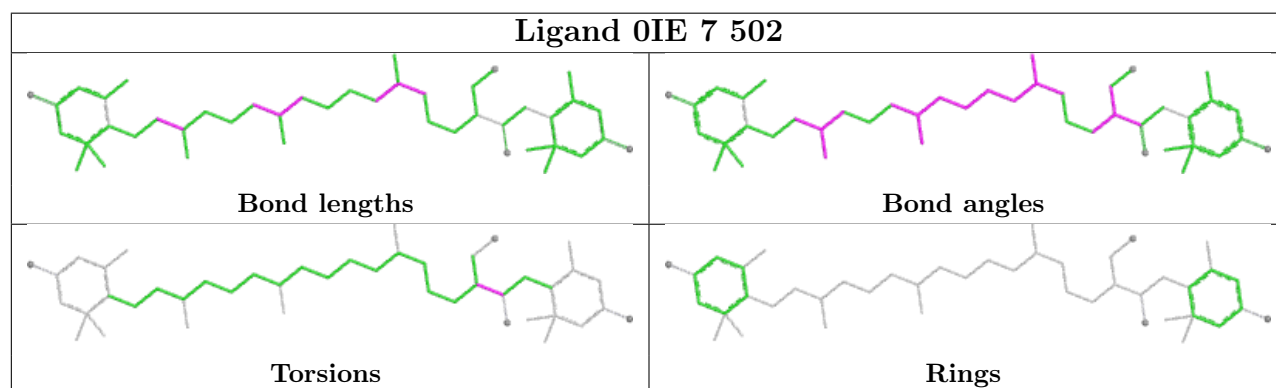
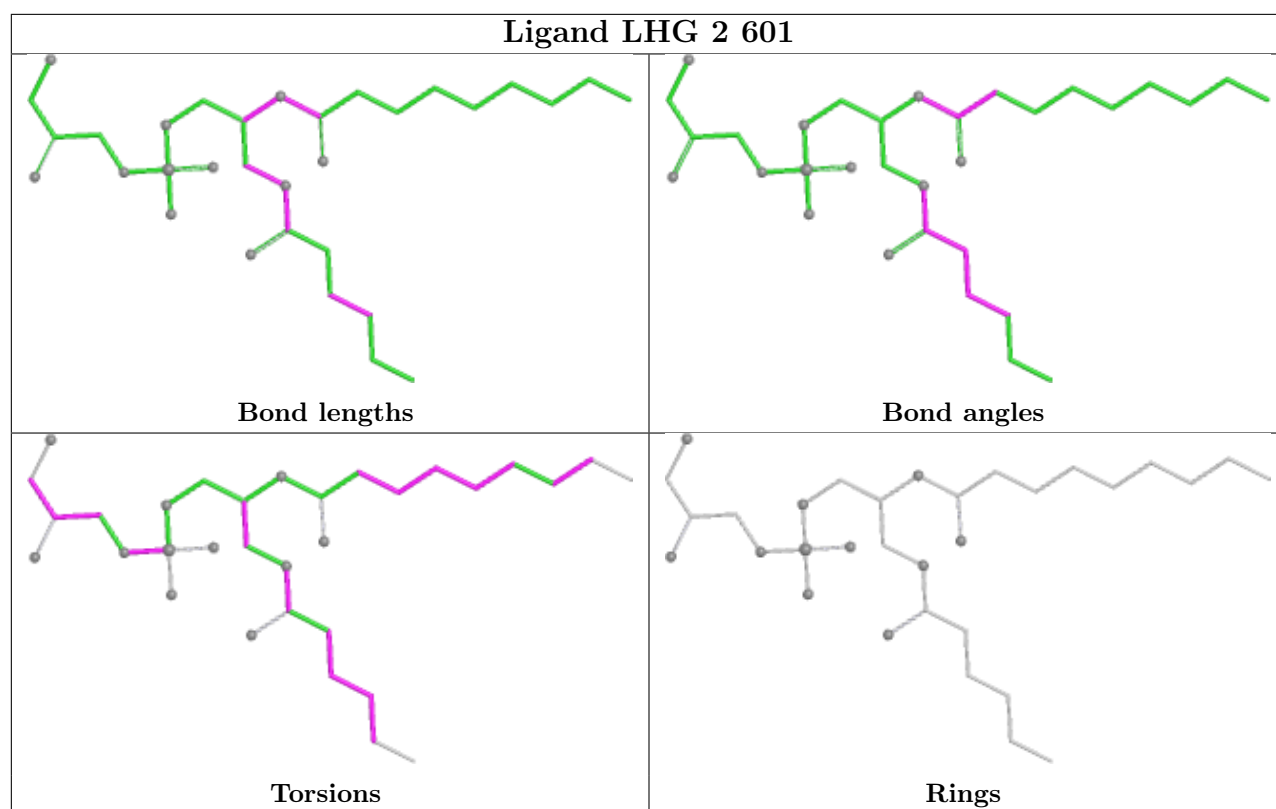
## Ligand CHL i 607



## Ligand CLA B 837

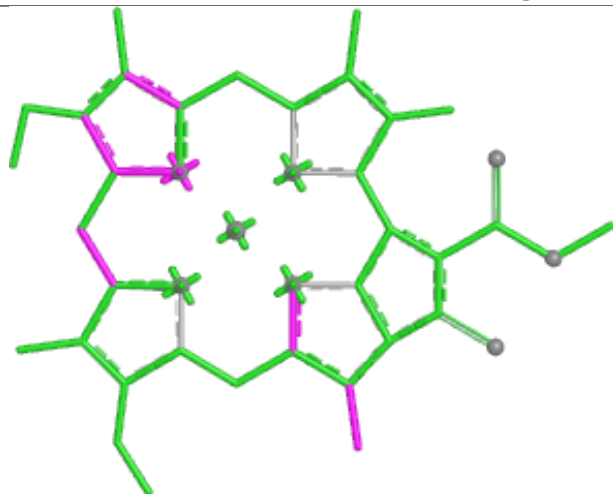




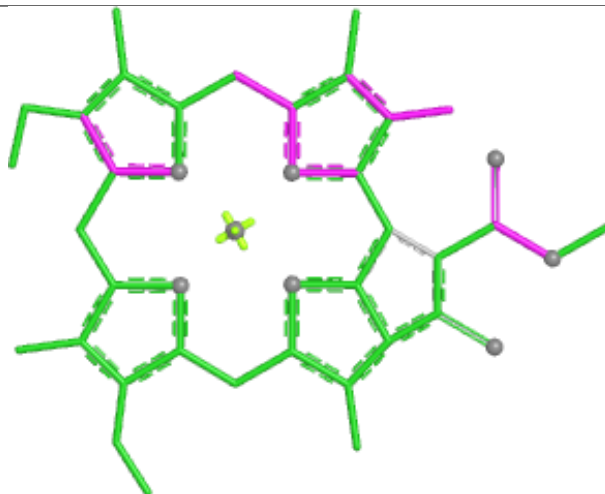




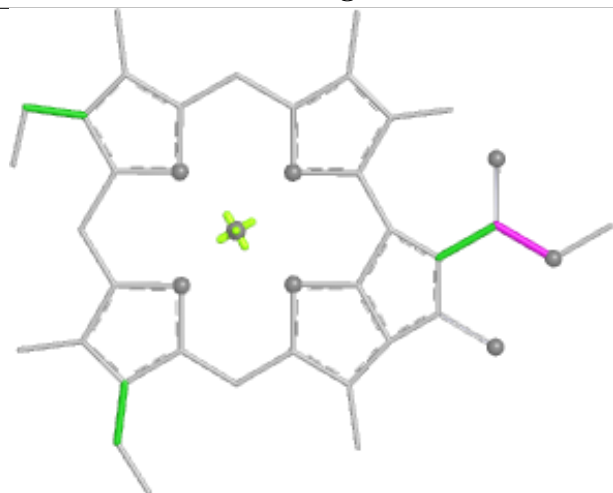
## Ligand CLA h 611



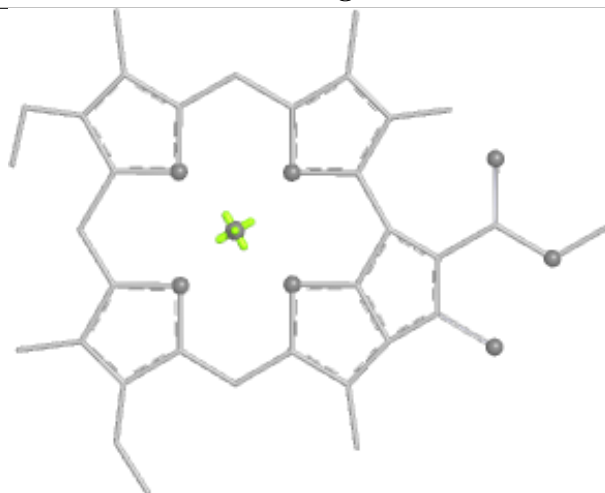
Bond lengths



Bond angles

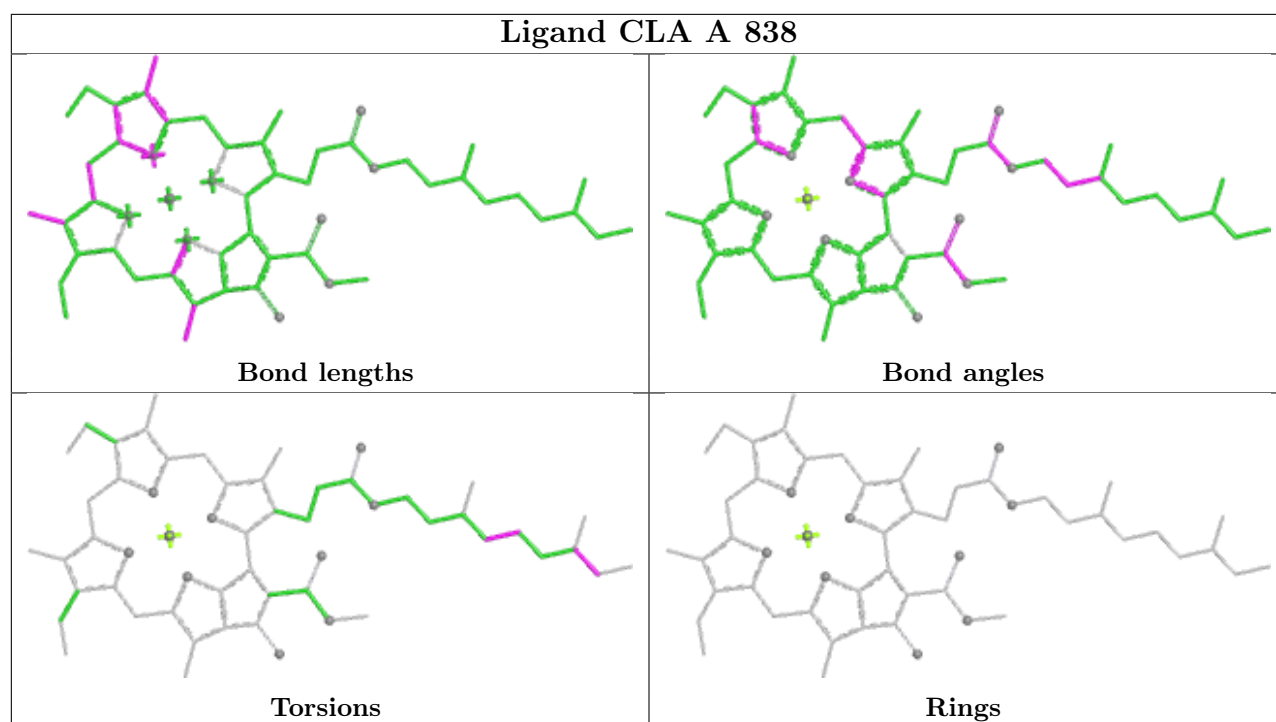


Torsions



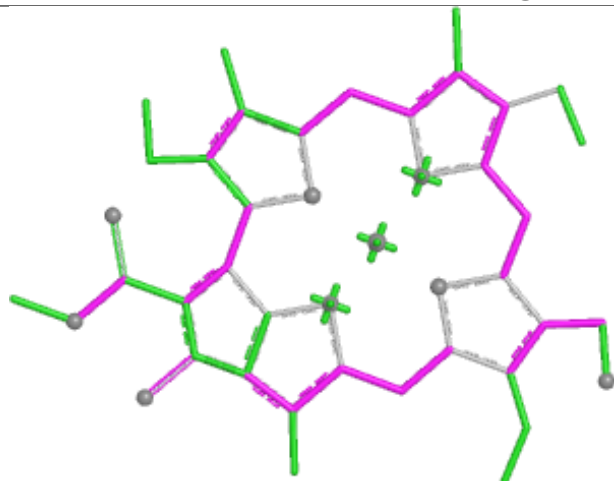
Rings



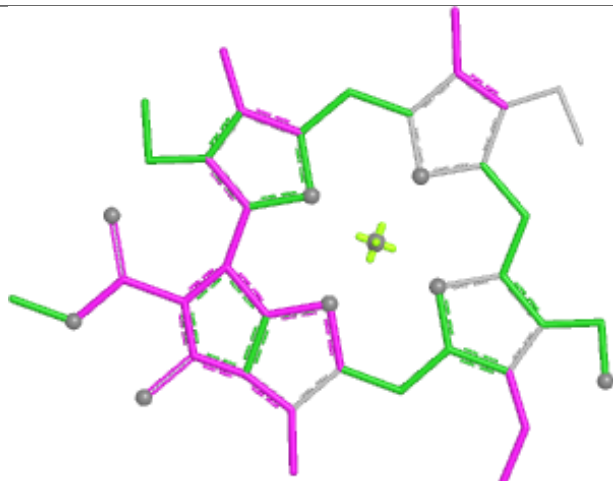




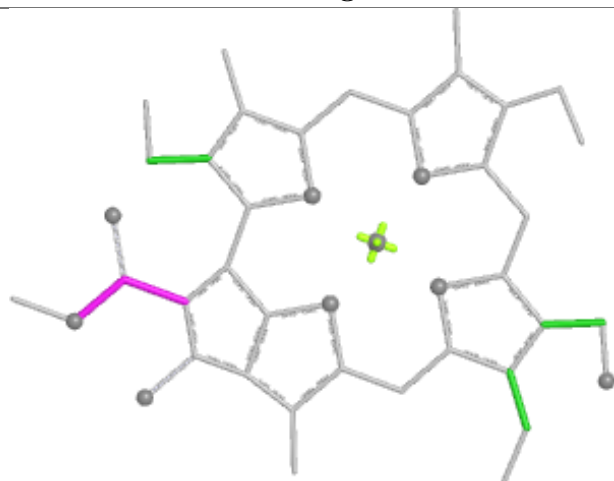
## Ligand CHL h 605



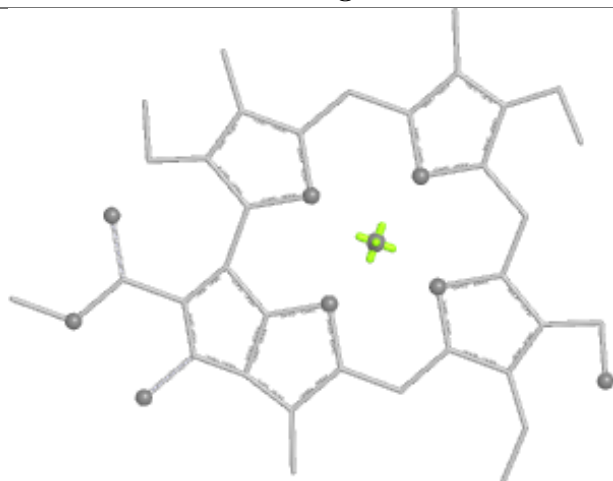
Bond lengths



Bond angles



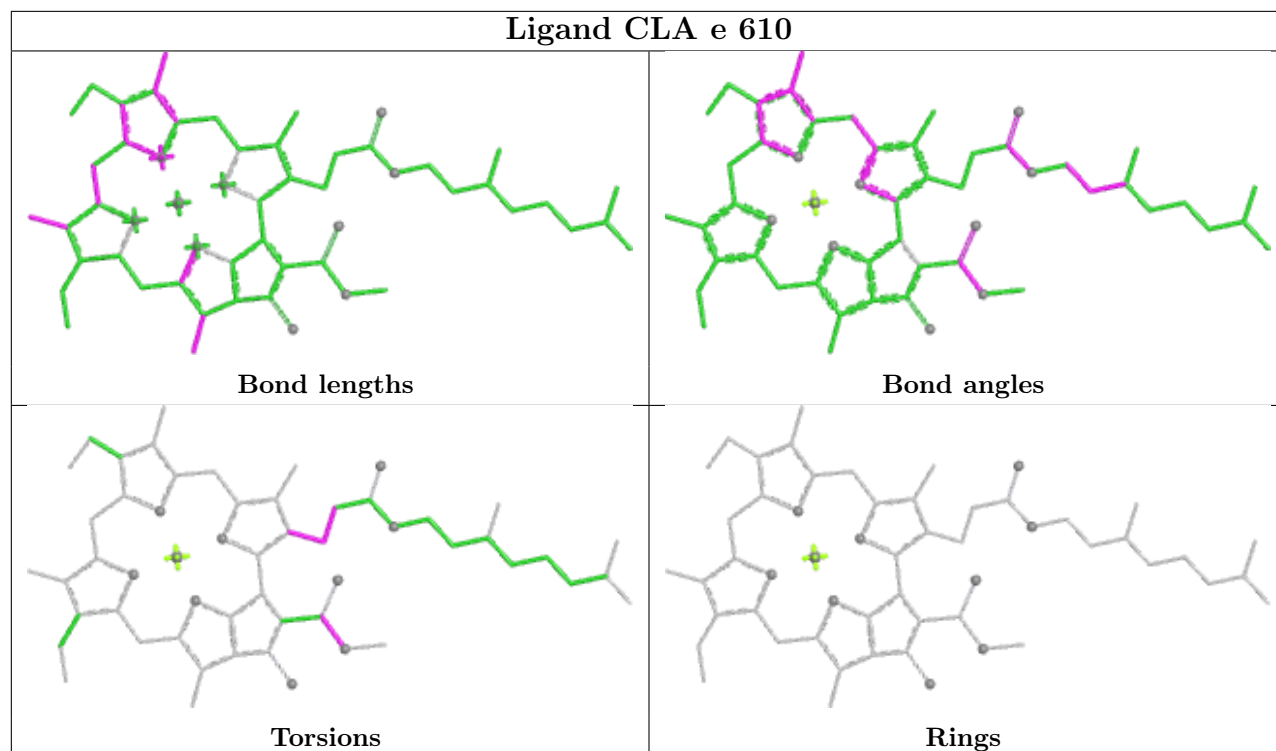
Torsions



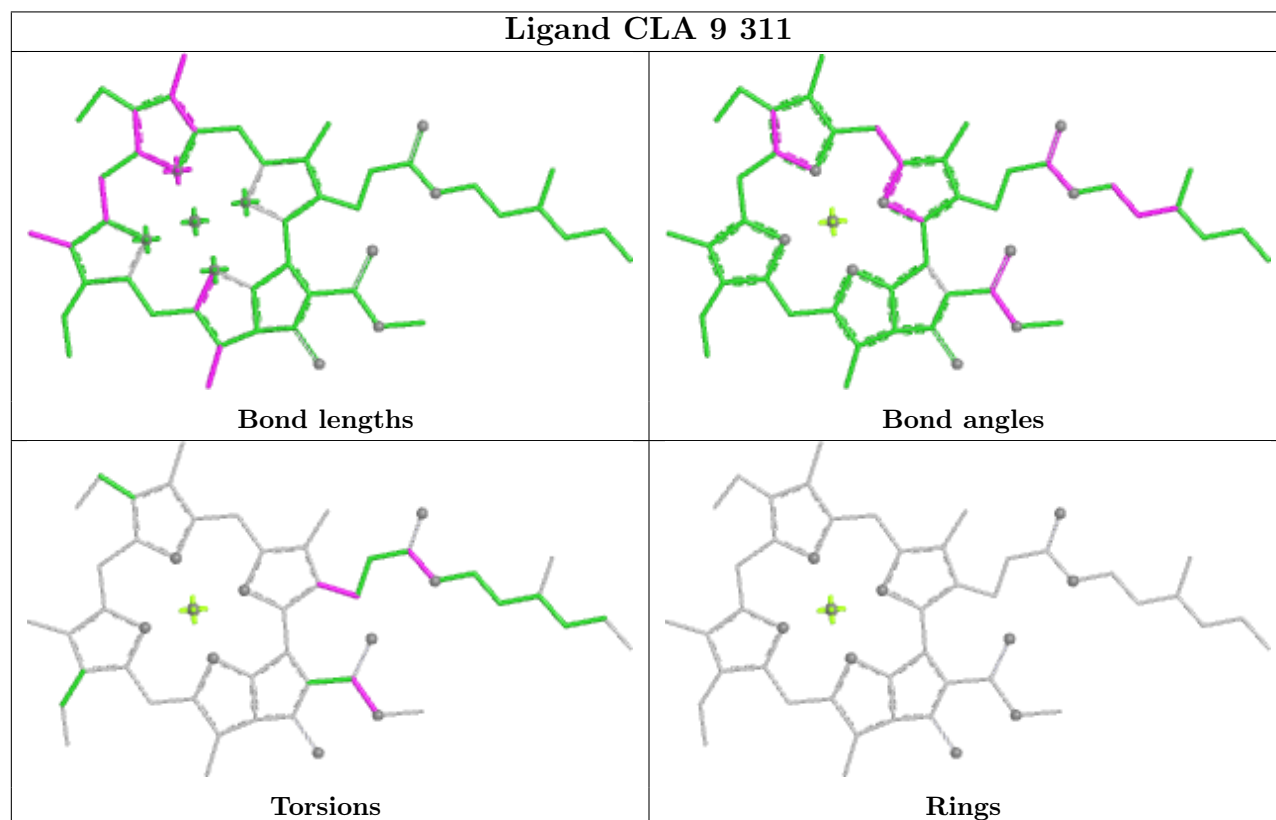
Rings



## Ligand CLA e 610

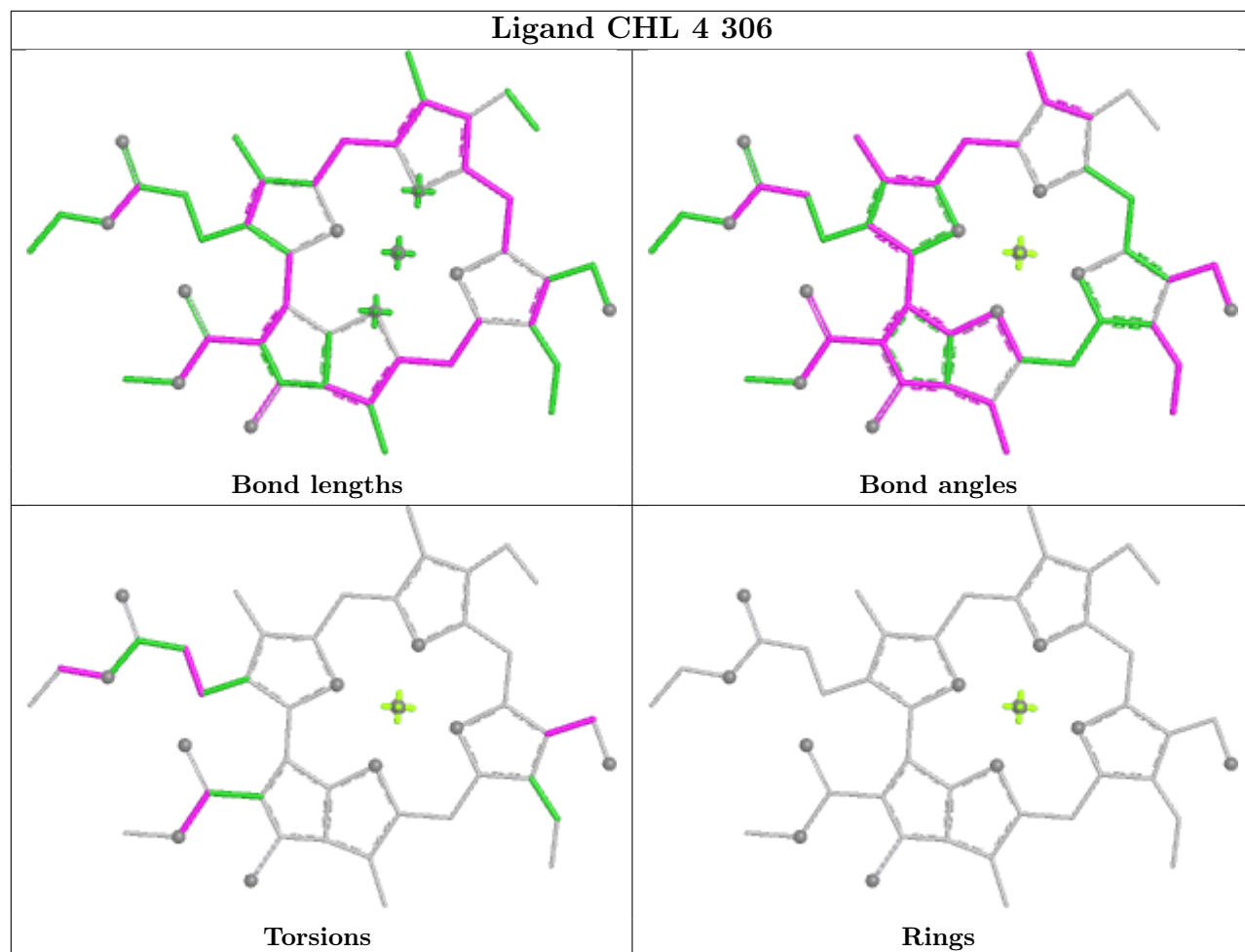


## Ligand CLA 9 311



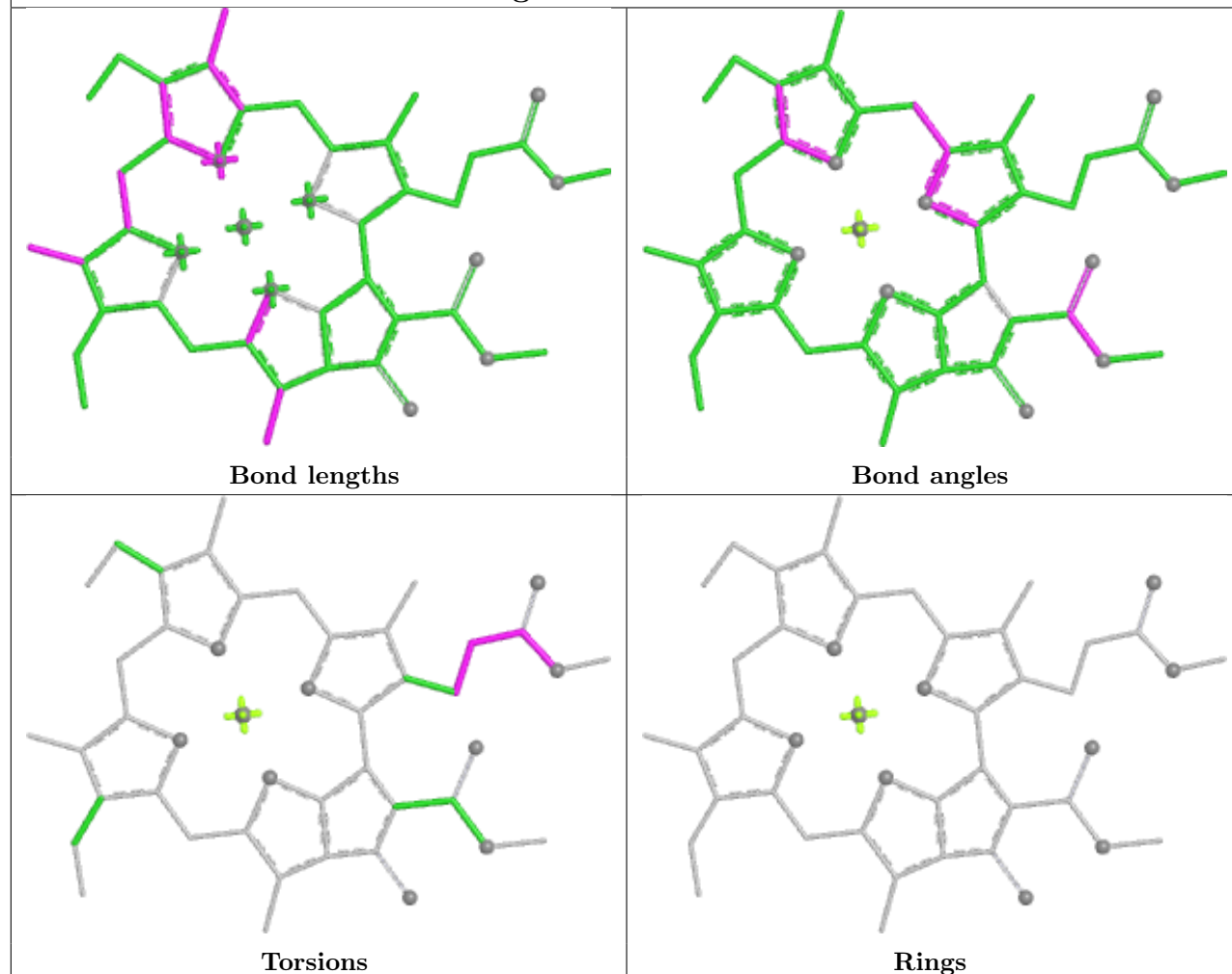


## Ligand CHL 4 306

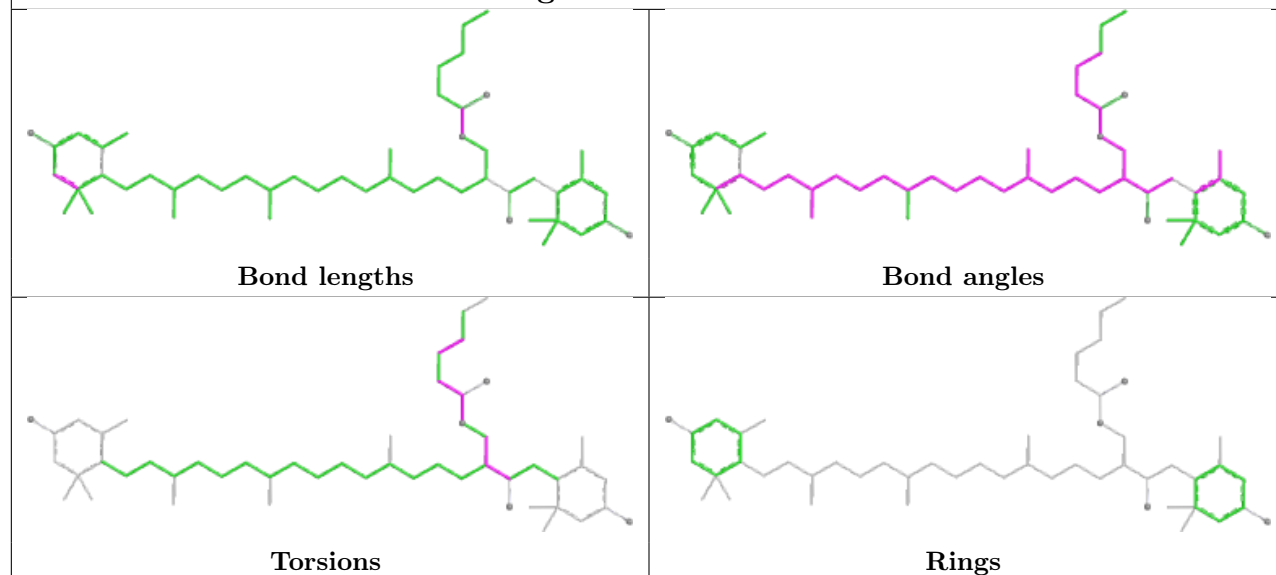




## Ligand CLA K 104

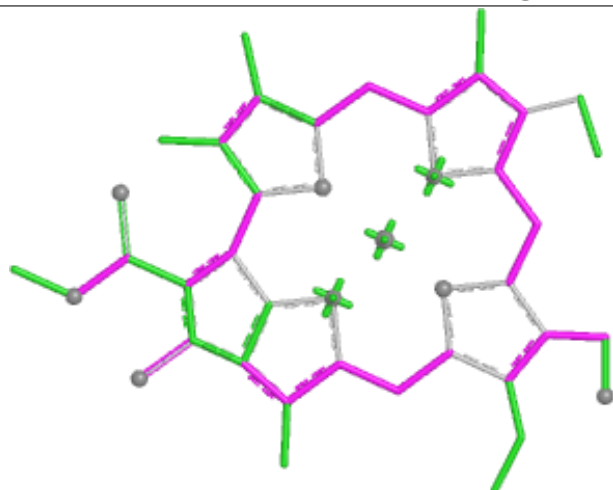


## Ligand OUR 4 501





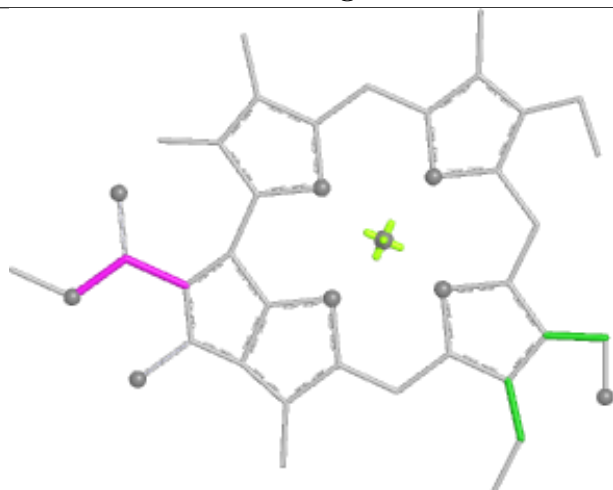
## Ligand CHL h 614



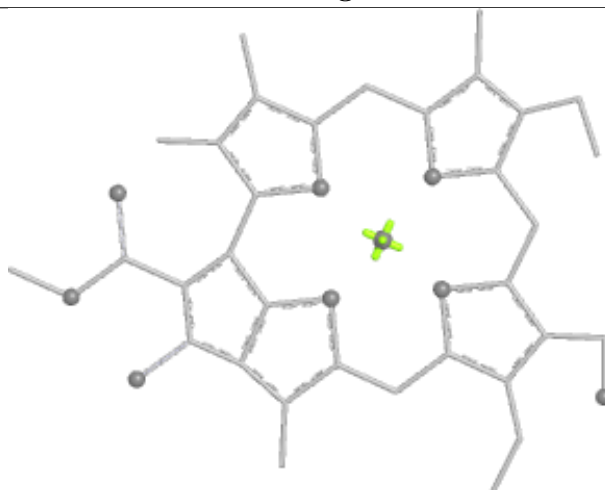
Bond lengths



Bond angles

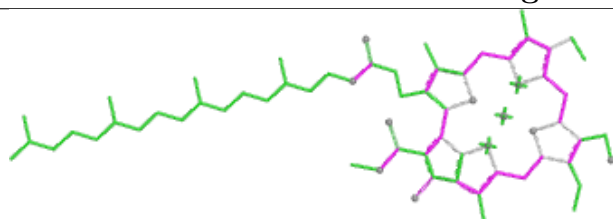


Torsions

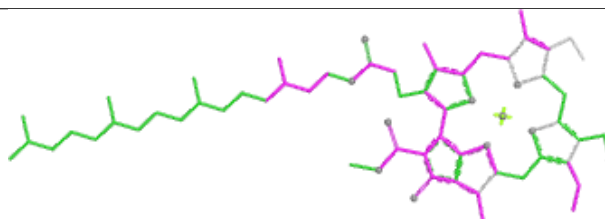


Rings

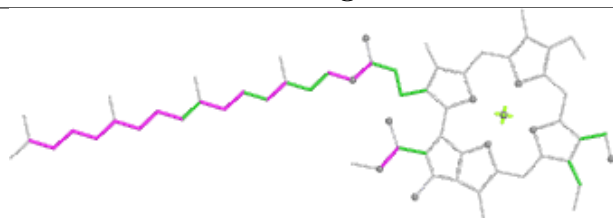
## Ligand CHL f 609



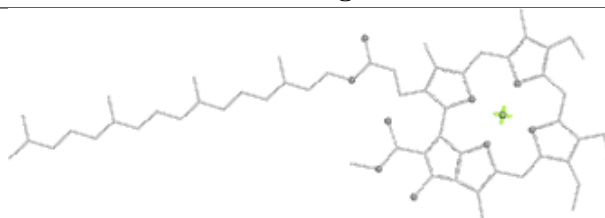
Bond lengths



Bond angles

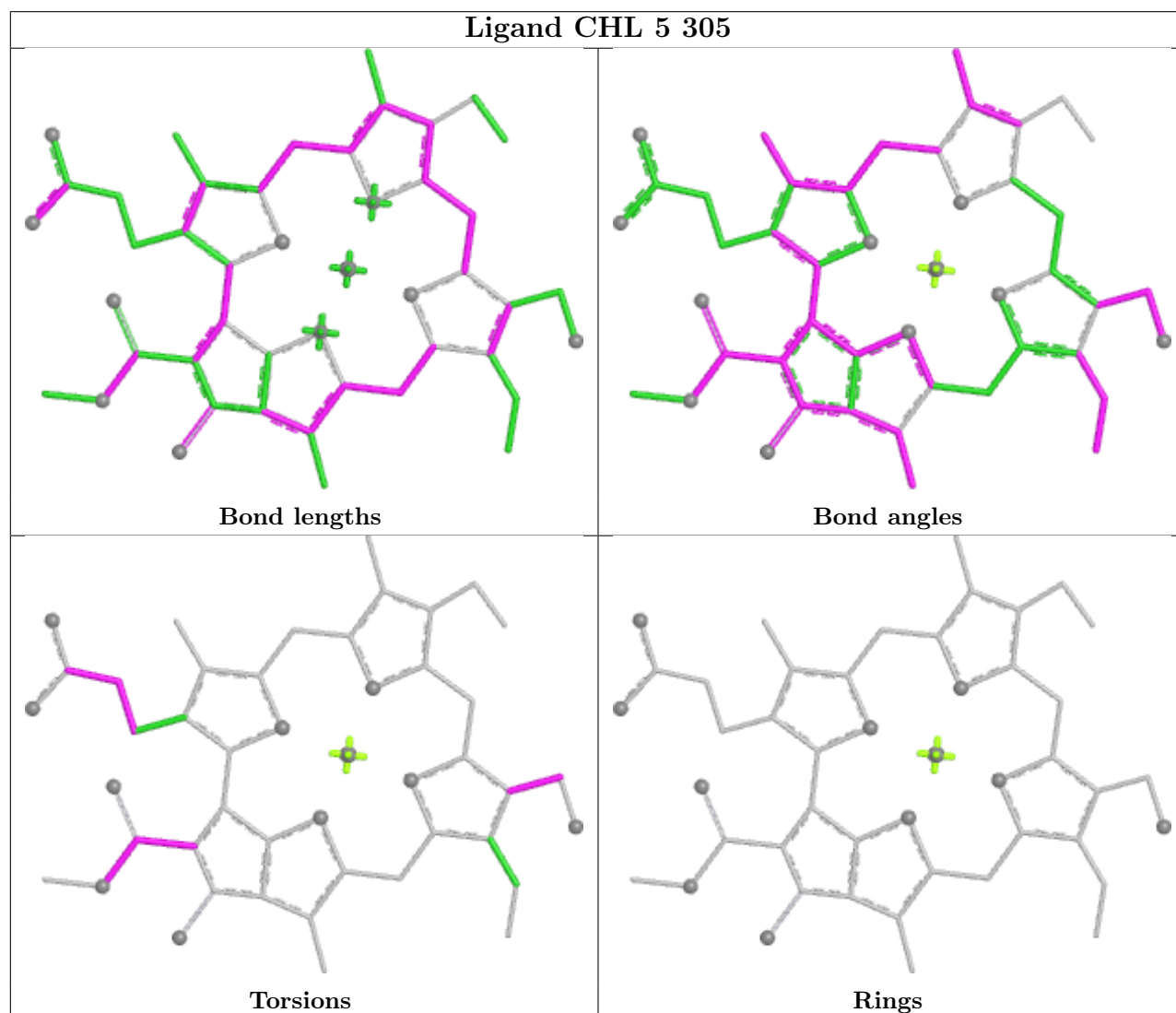
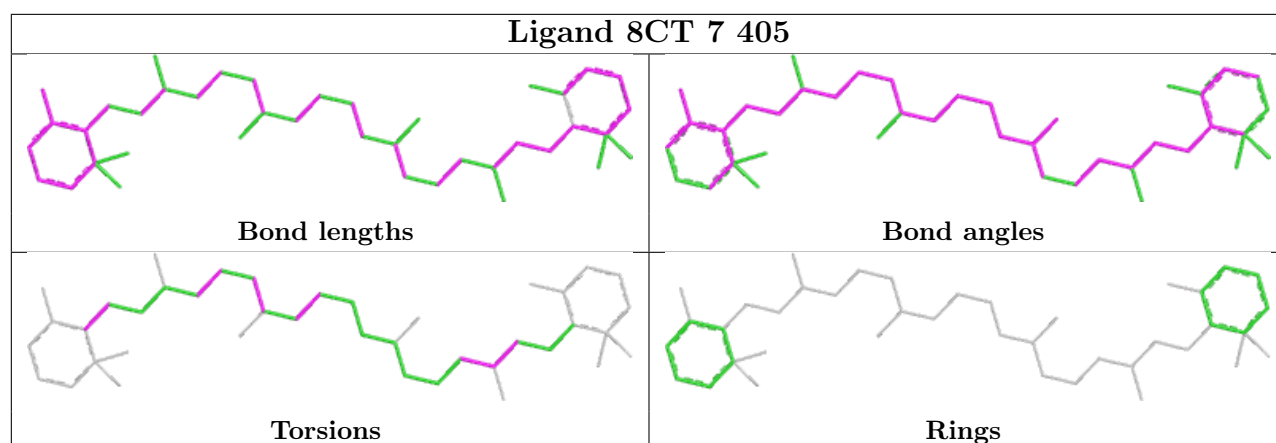


Torsions



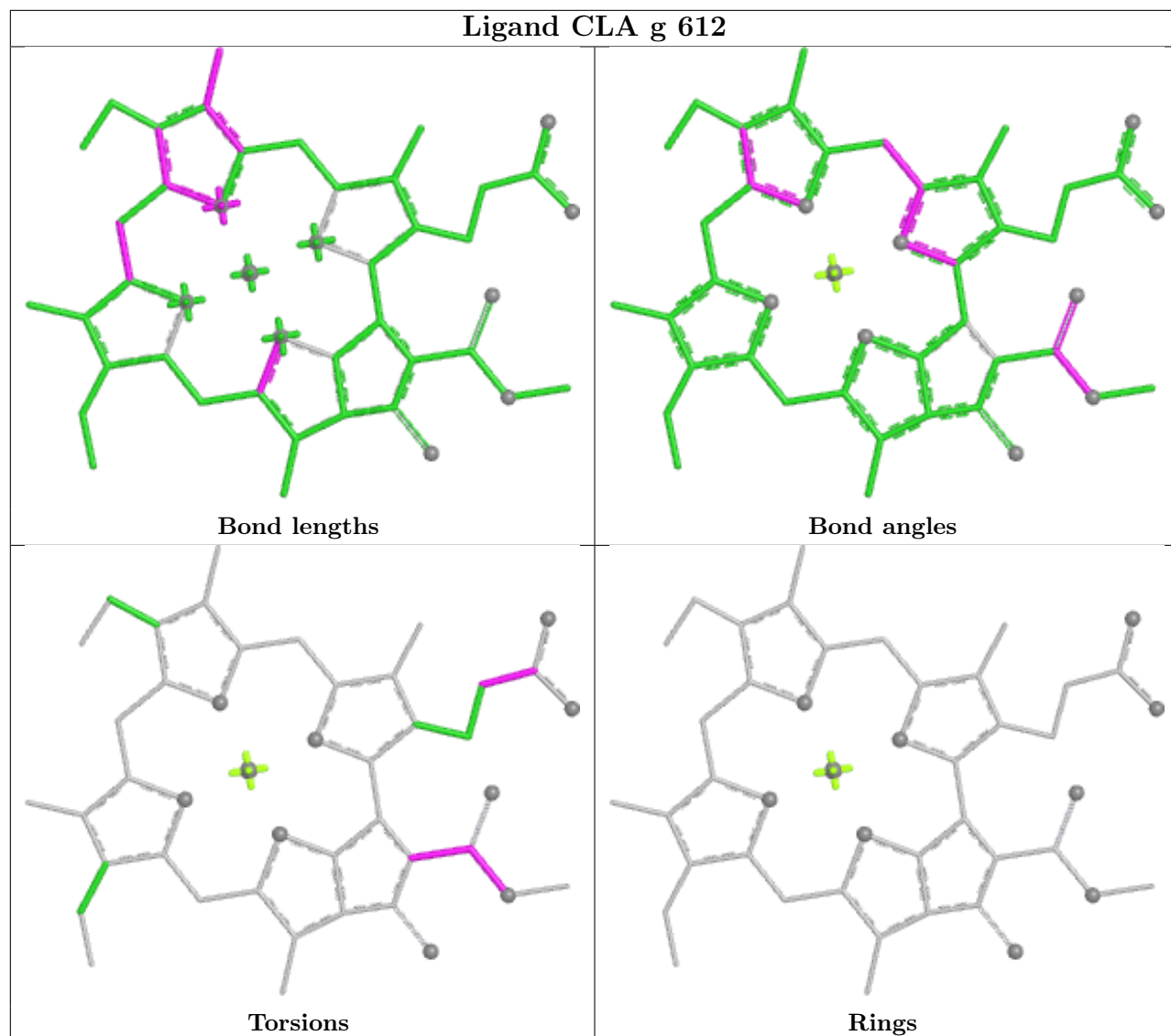
Rings



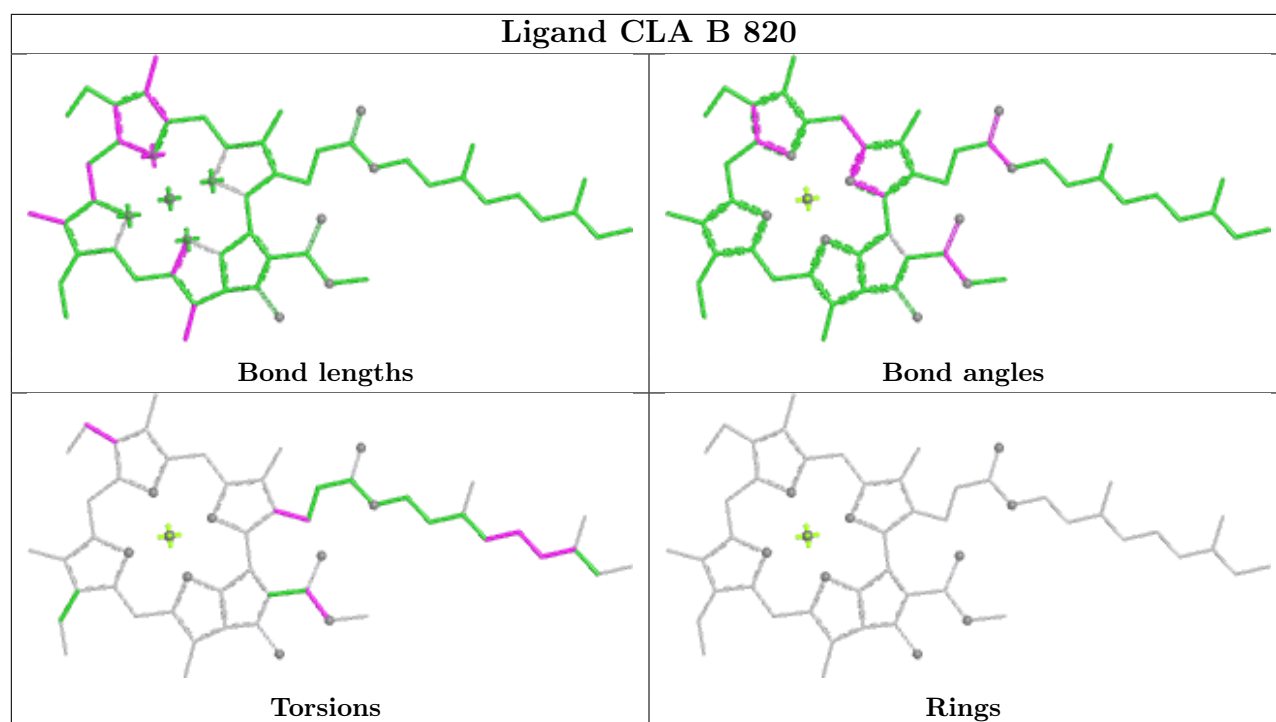




## Ligand CLA g 612

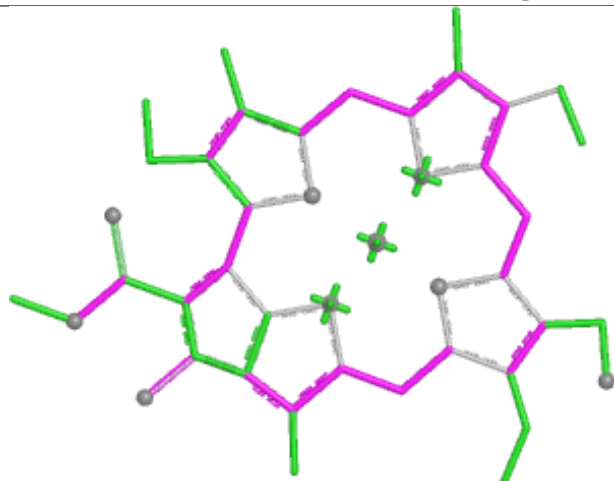




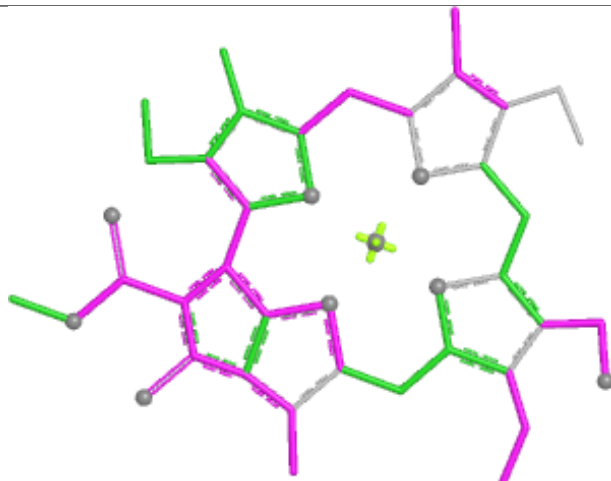




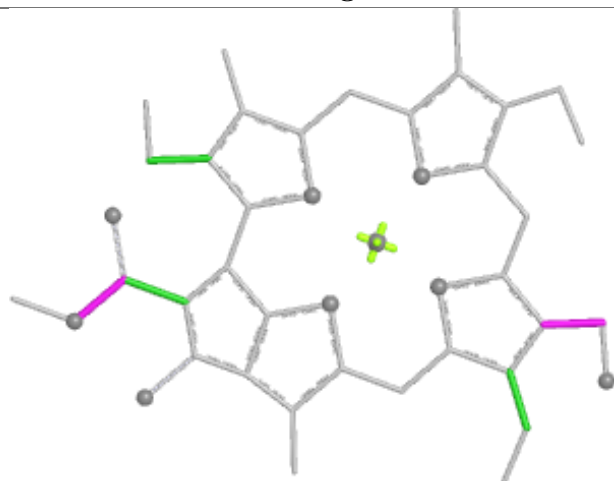
## Ligand CHL d 605



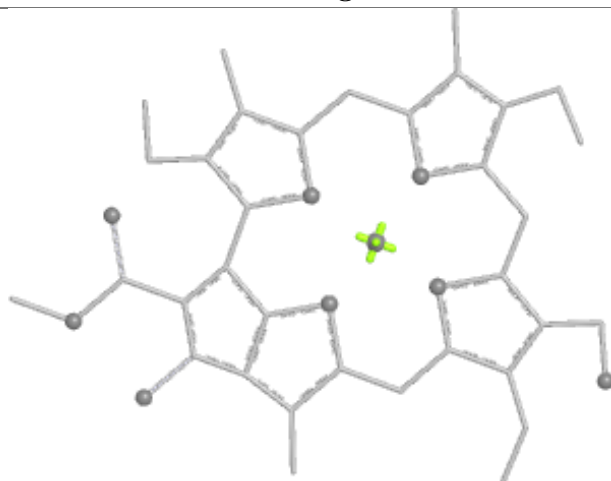
Bond lengths



Bond angles

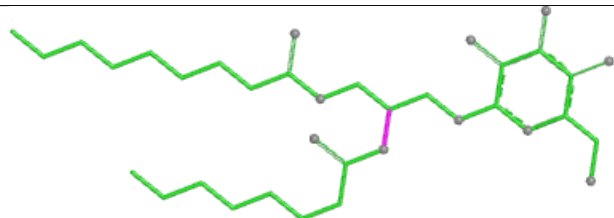


Torsions

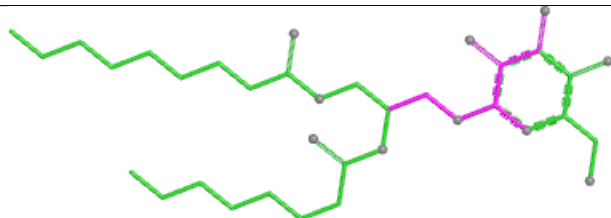


Rings

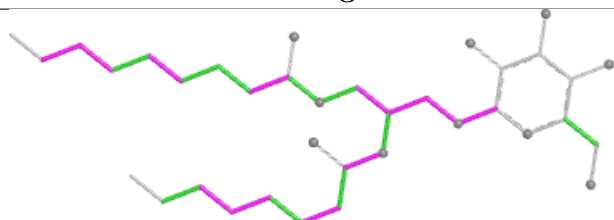
## Ligand LMG 2 602



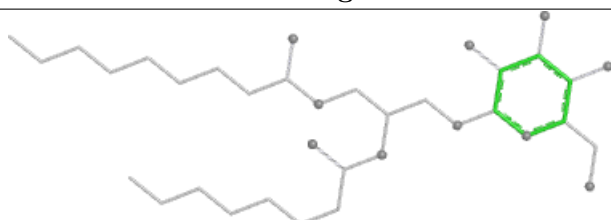
Bond lengths



Bond angles

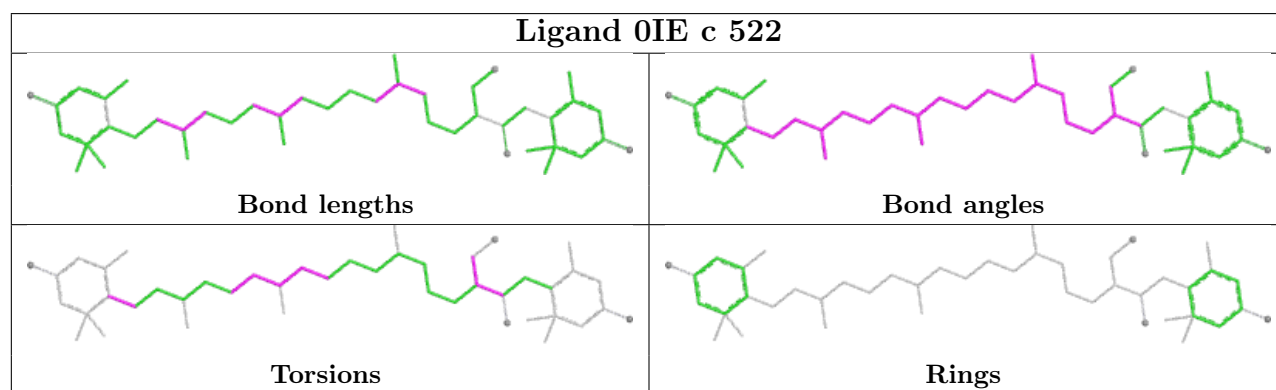
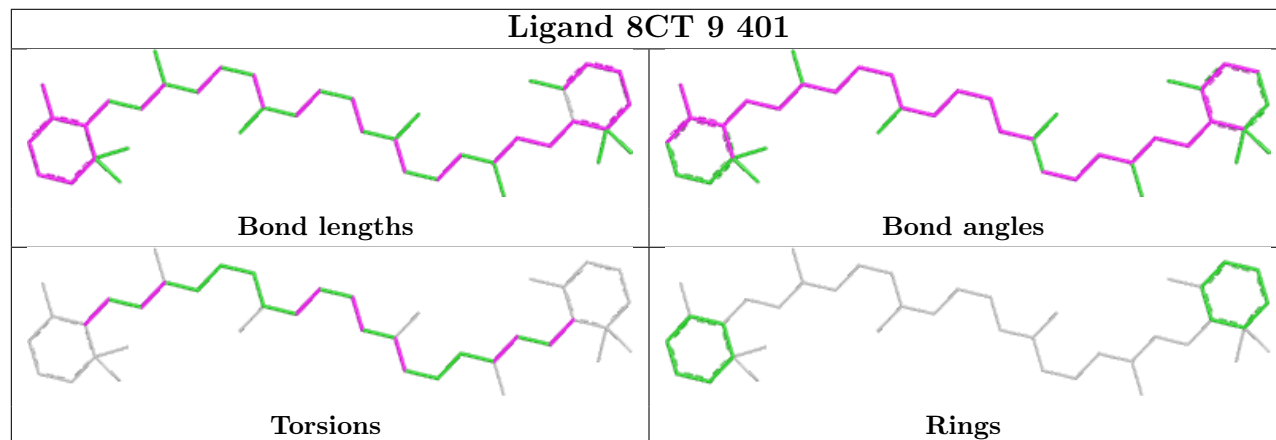
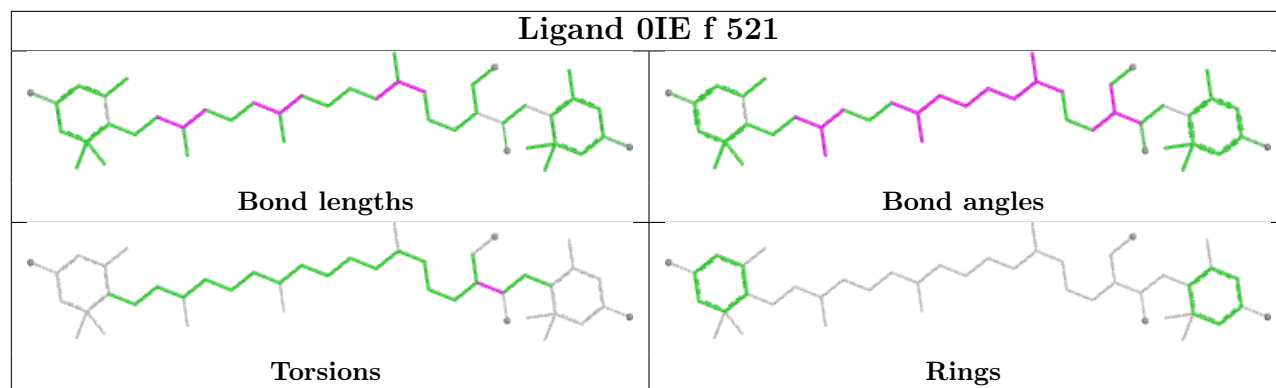


Torsions

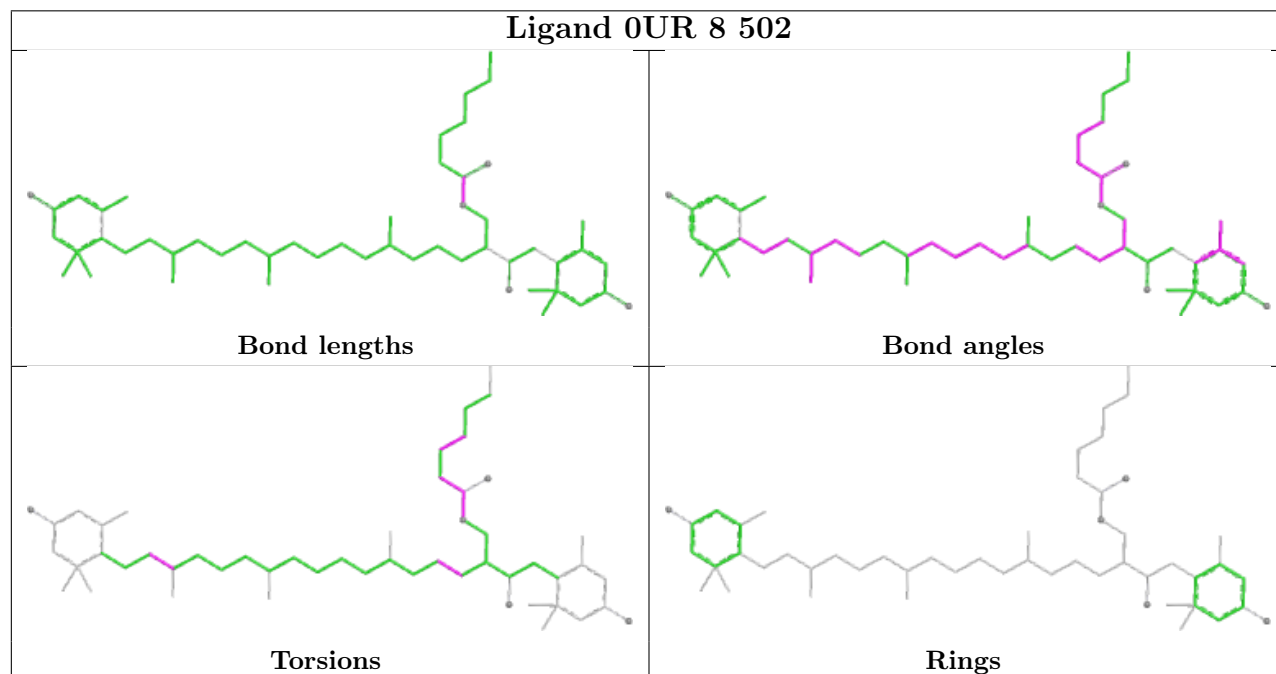
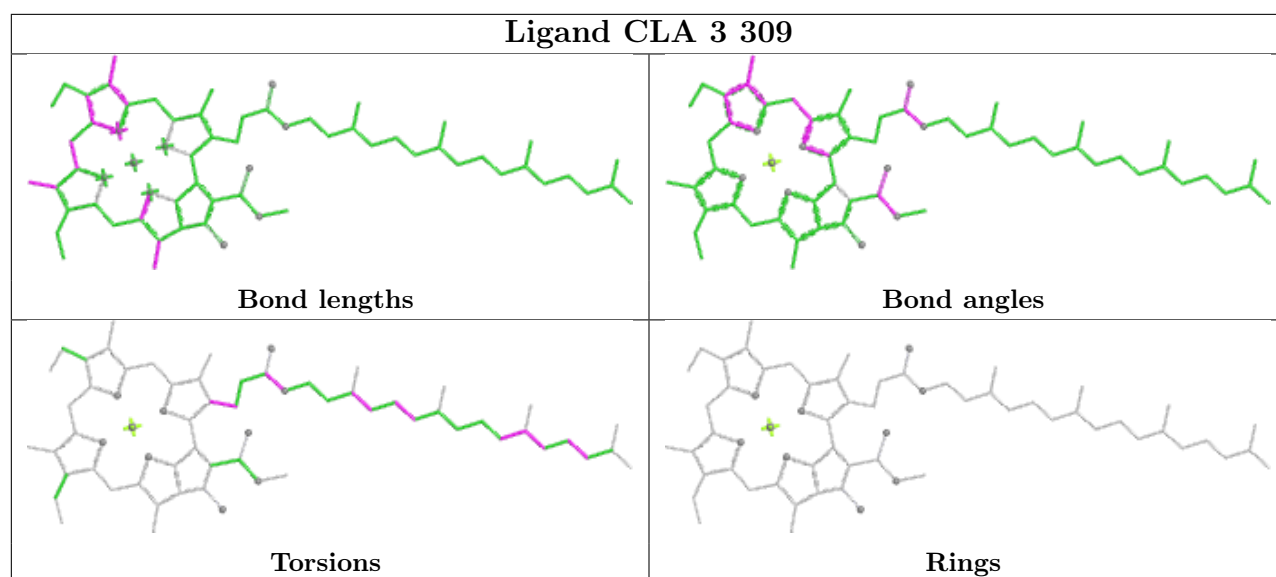


Rings



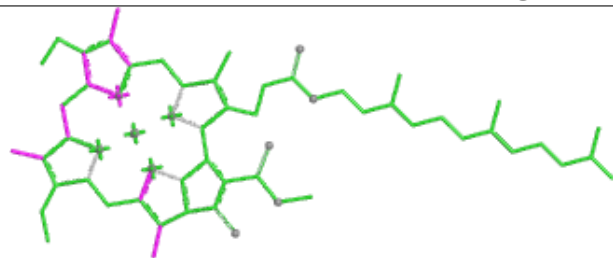




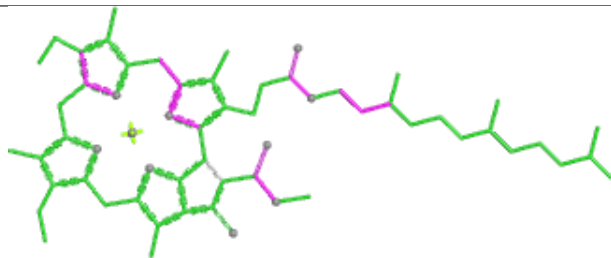




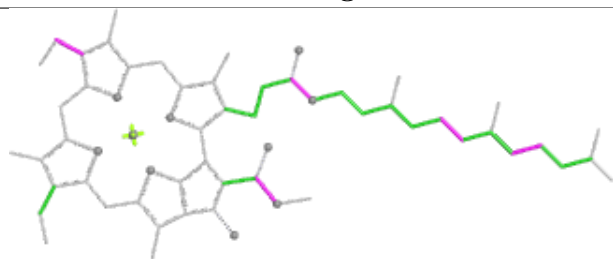
## Ligand CLA B 824



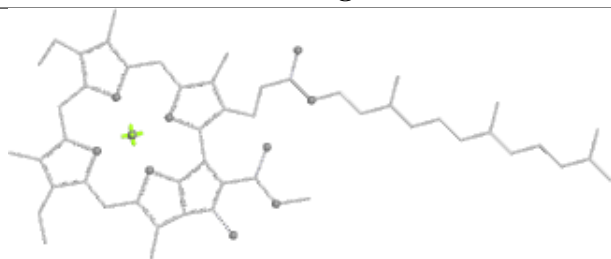
Bond lengths



Bond angles

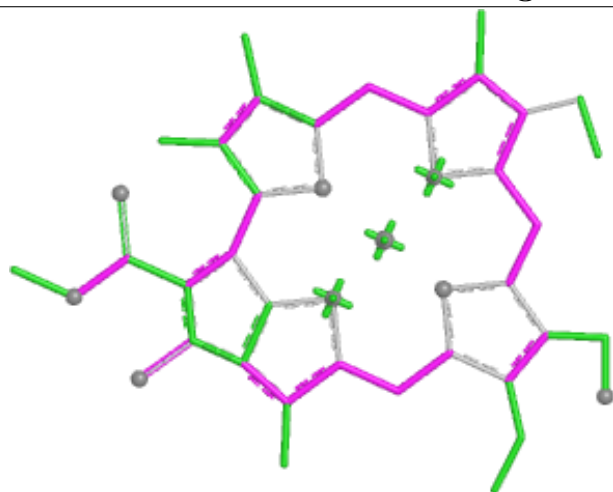


Torsions

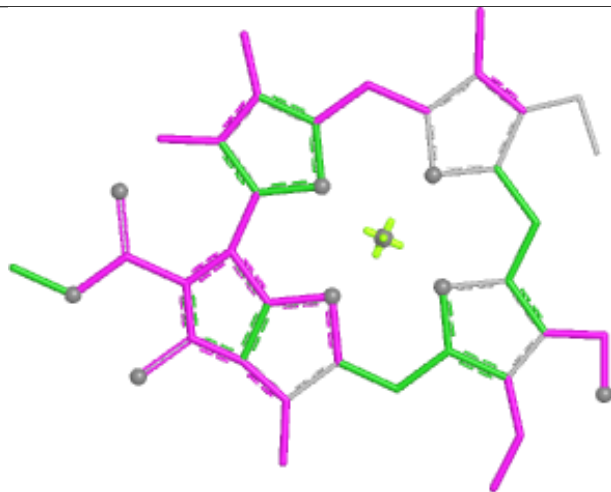


Rings

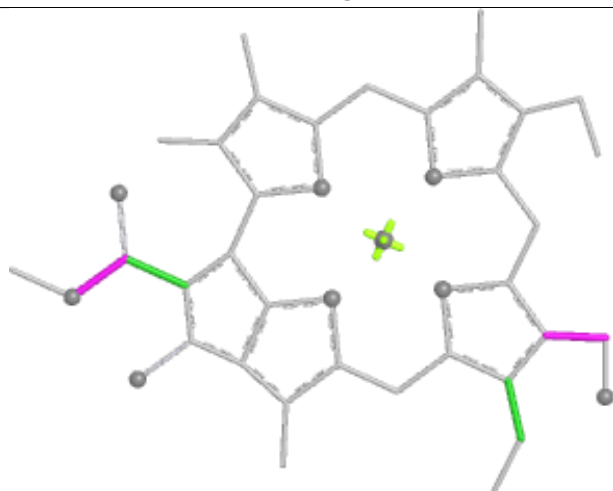
## Ligand CHL b 614



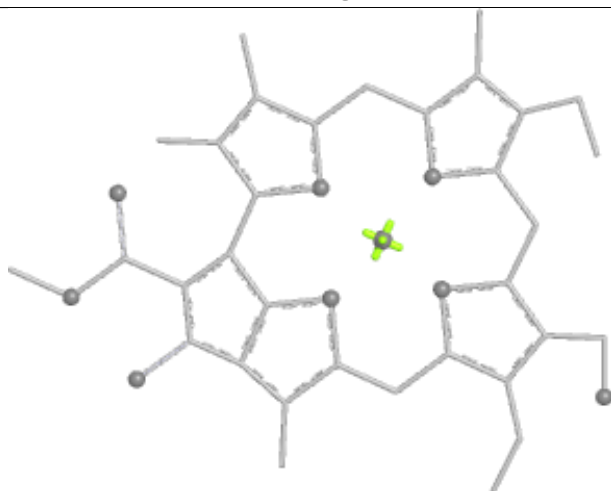
Bond lengths



Bond angles

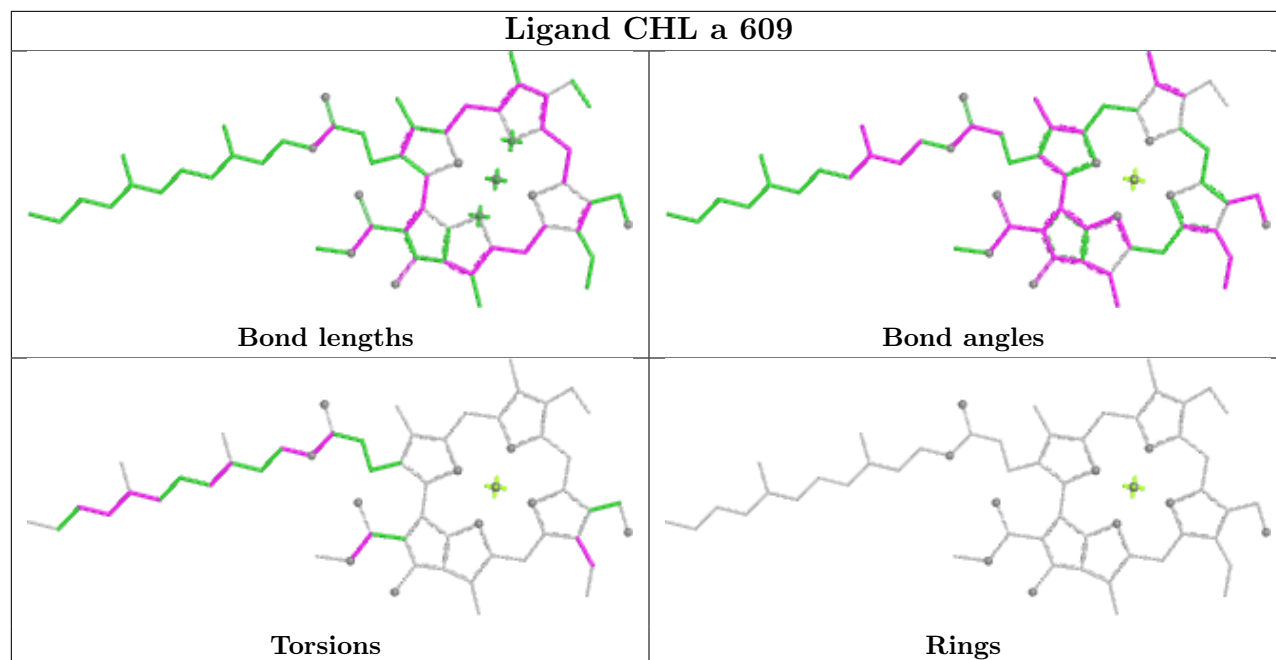
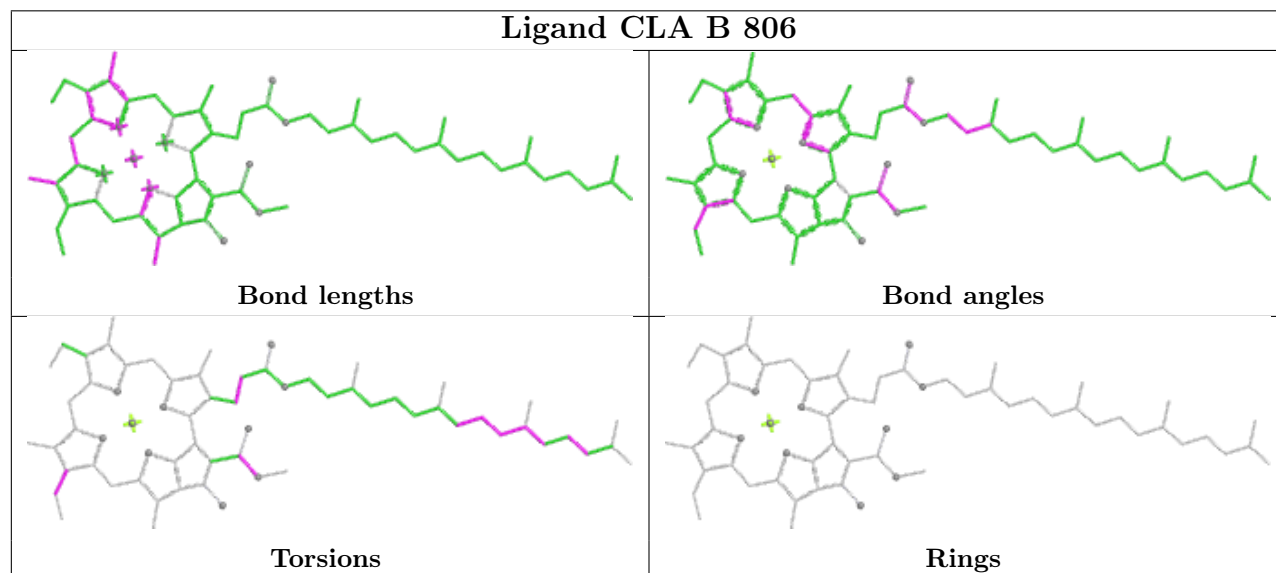


Torsions

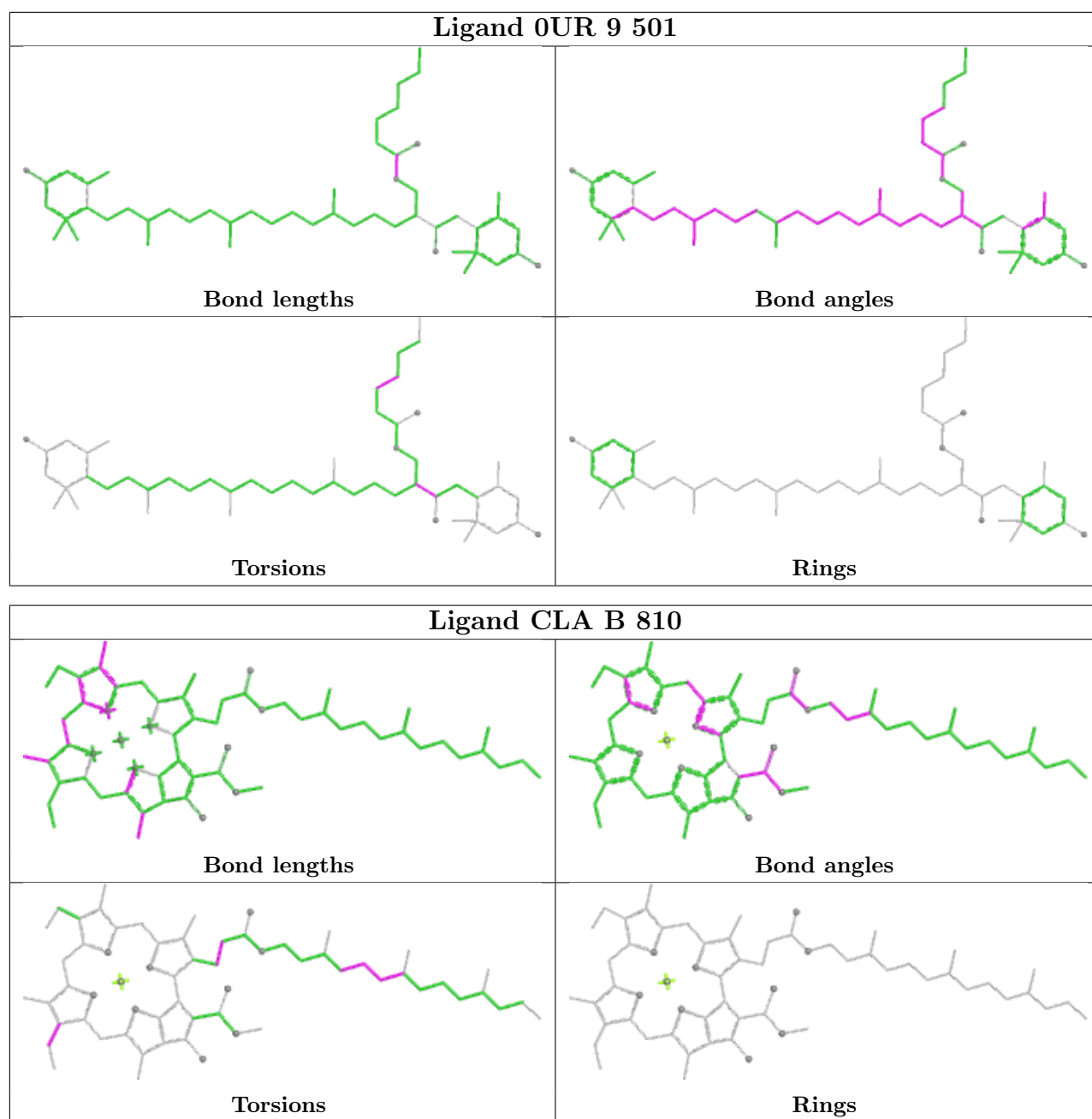


Rings

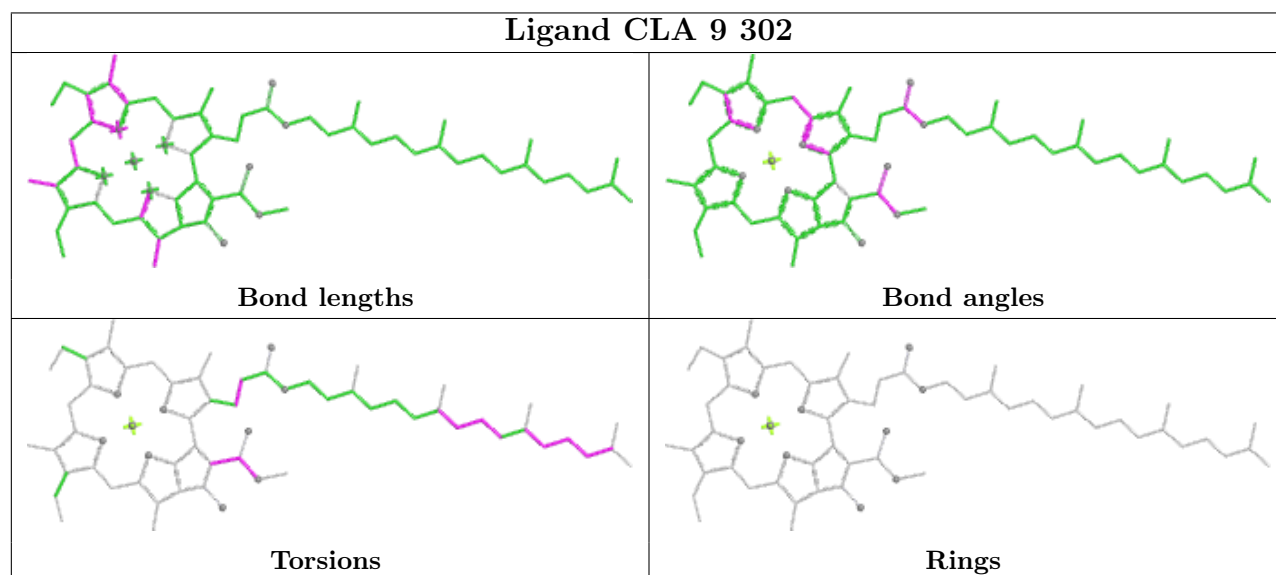
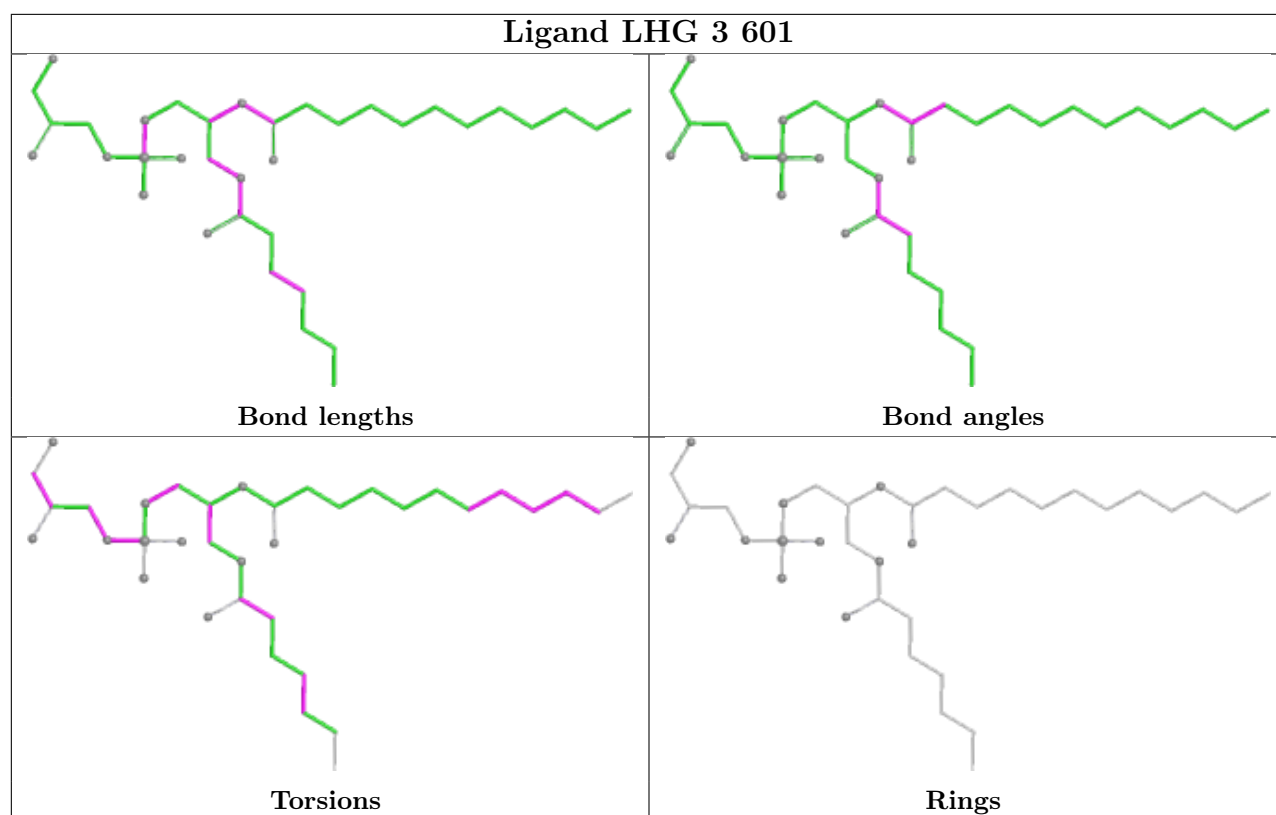


**Ligand CHL a 609****Ligand CLA B 806**

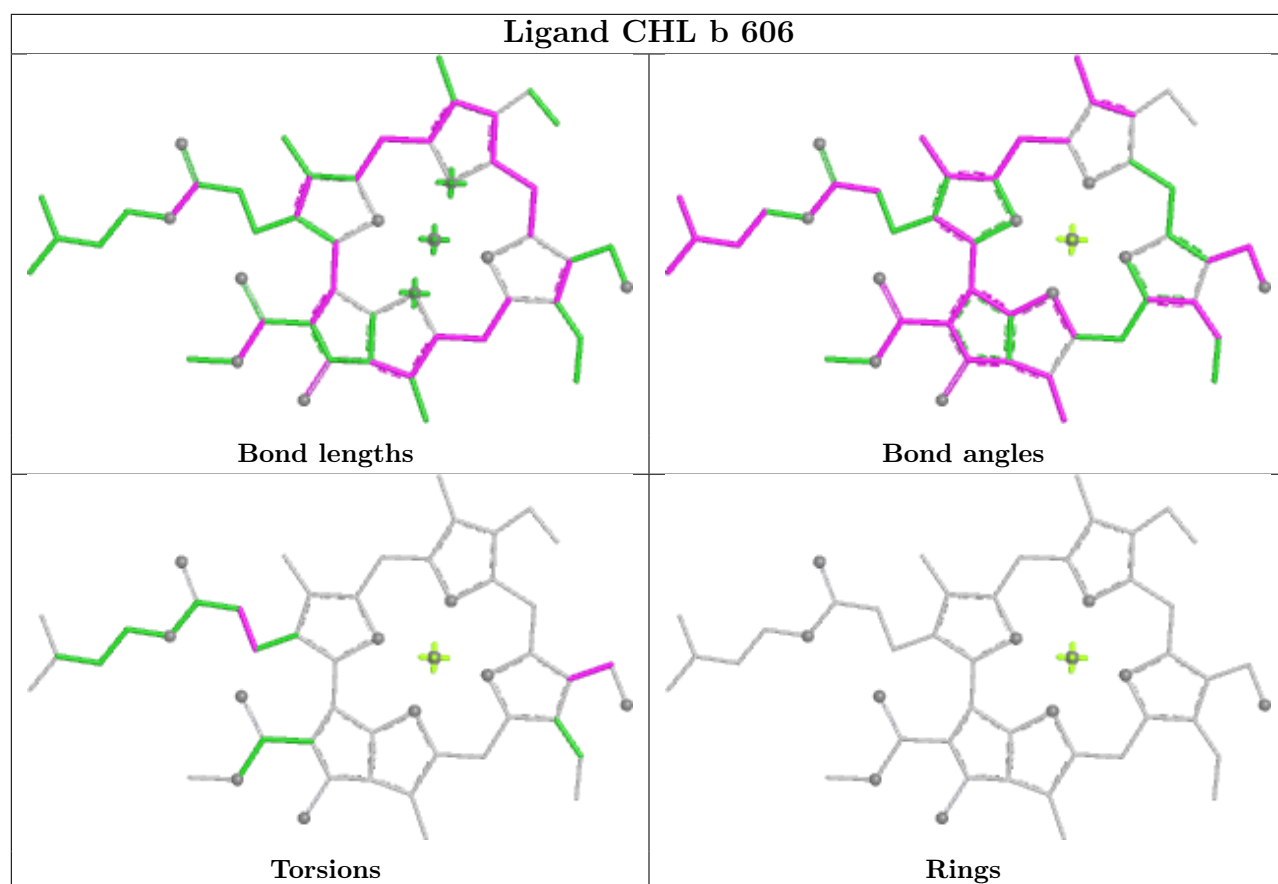






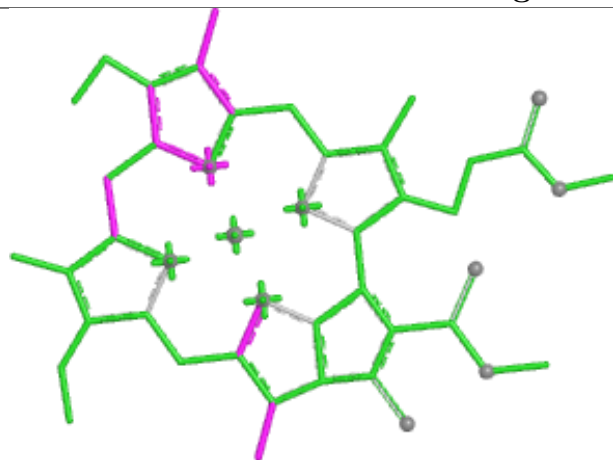




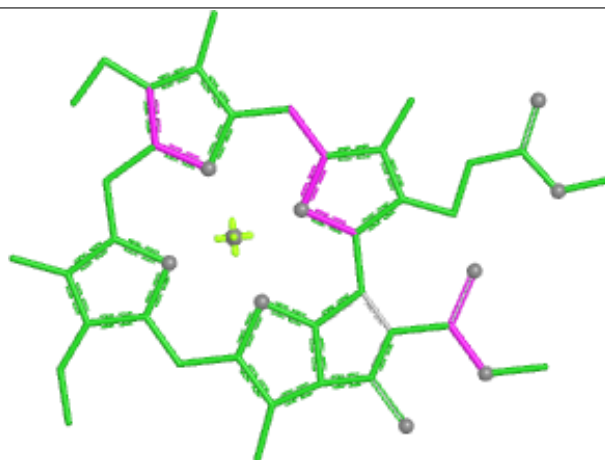




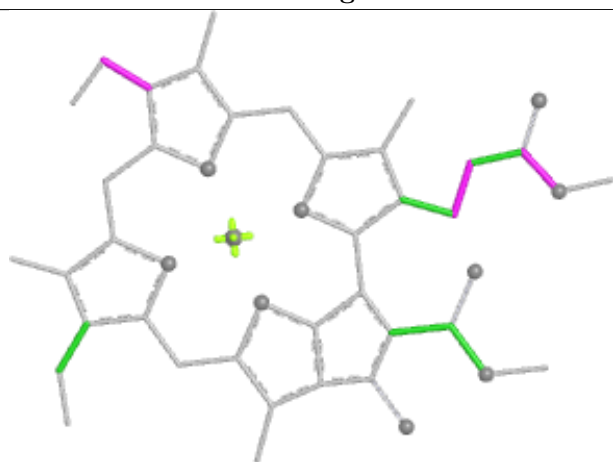
## Ligand CLA G 103



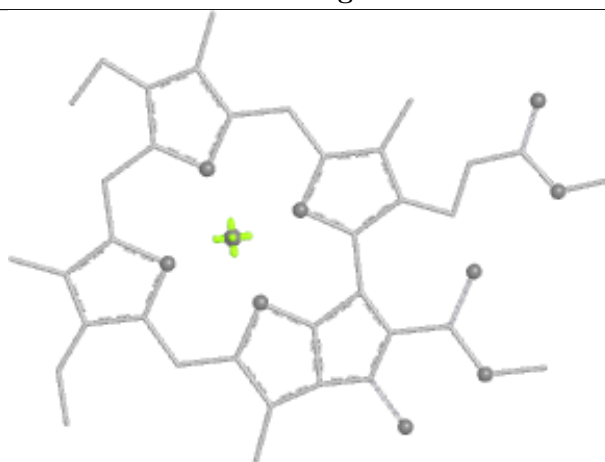
Bond lengths



Bond angles

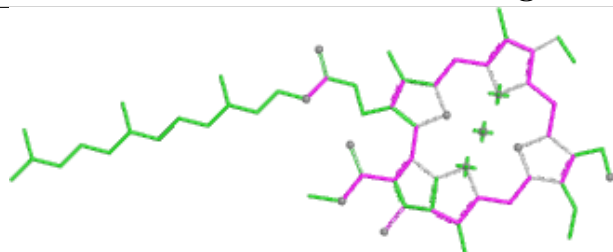


Torsions

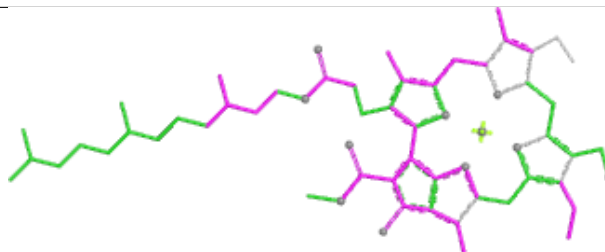


Rings

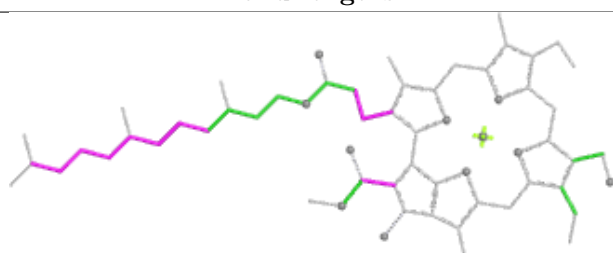
## Ligand CHL 6 301



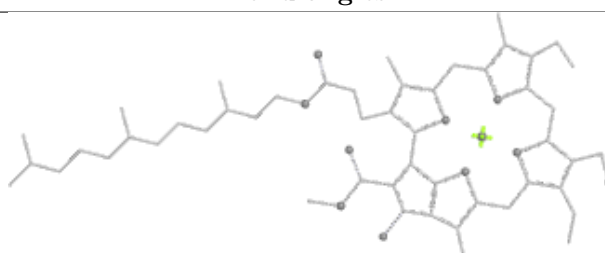
Bond lengths



Bond angles



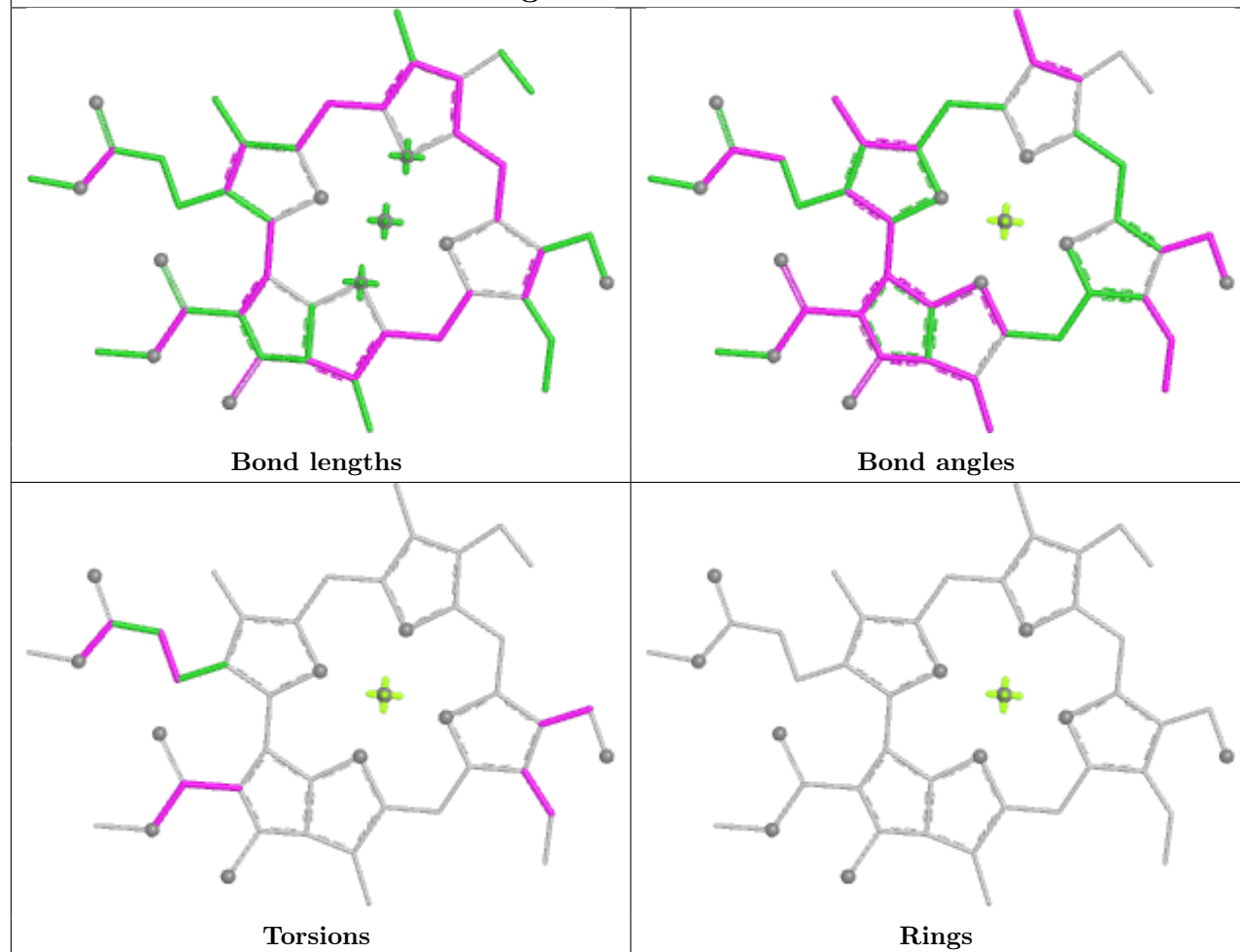
Torsions



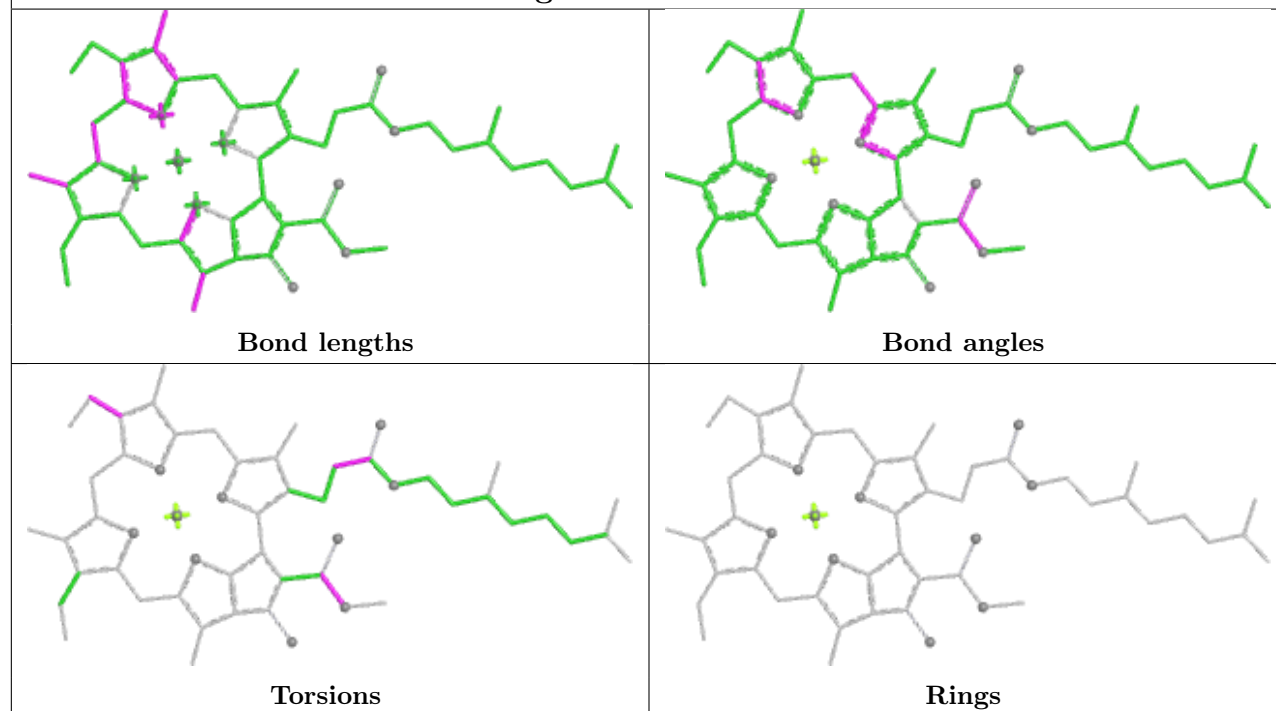
Rings



## Ligand CHL c 607

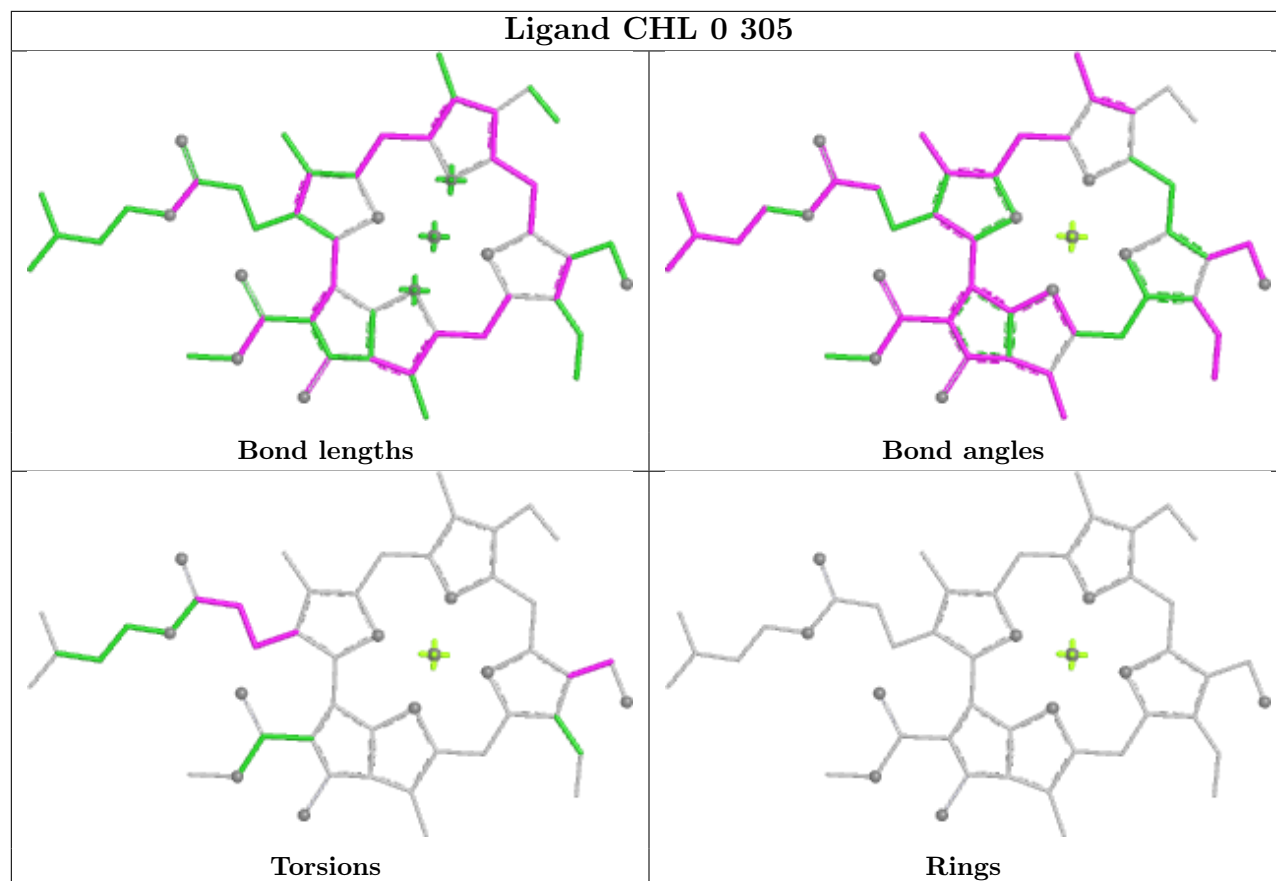


## Ligand CLA b 603

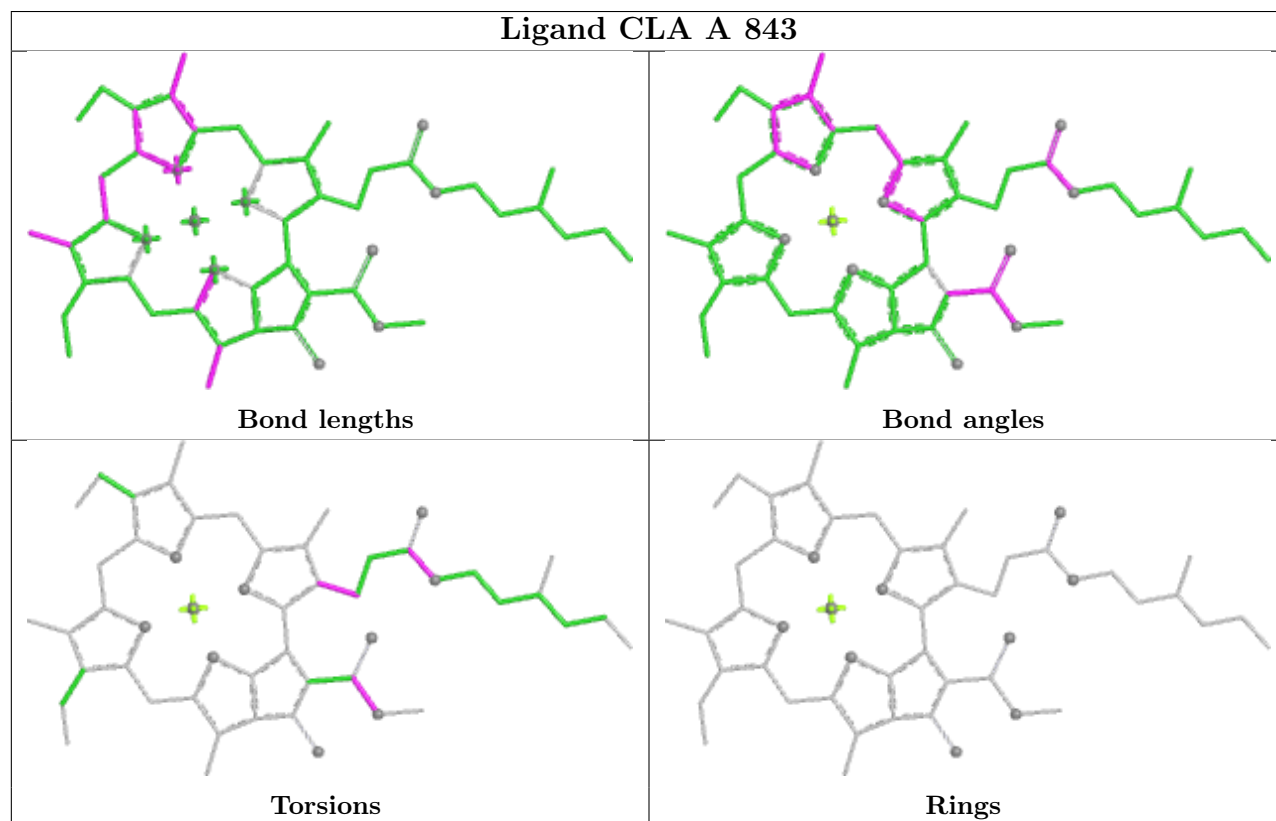




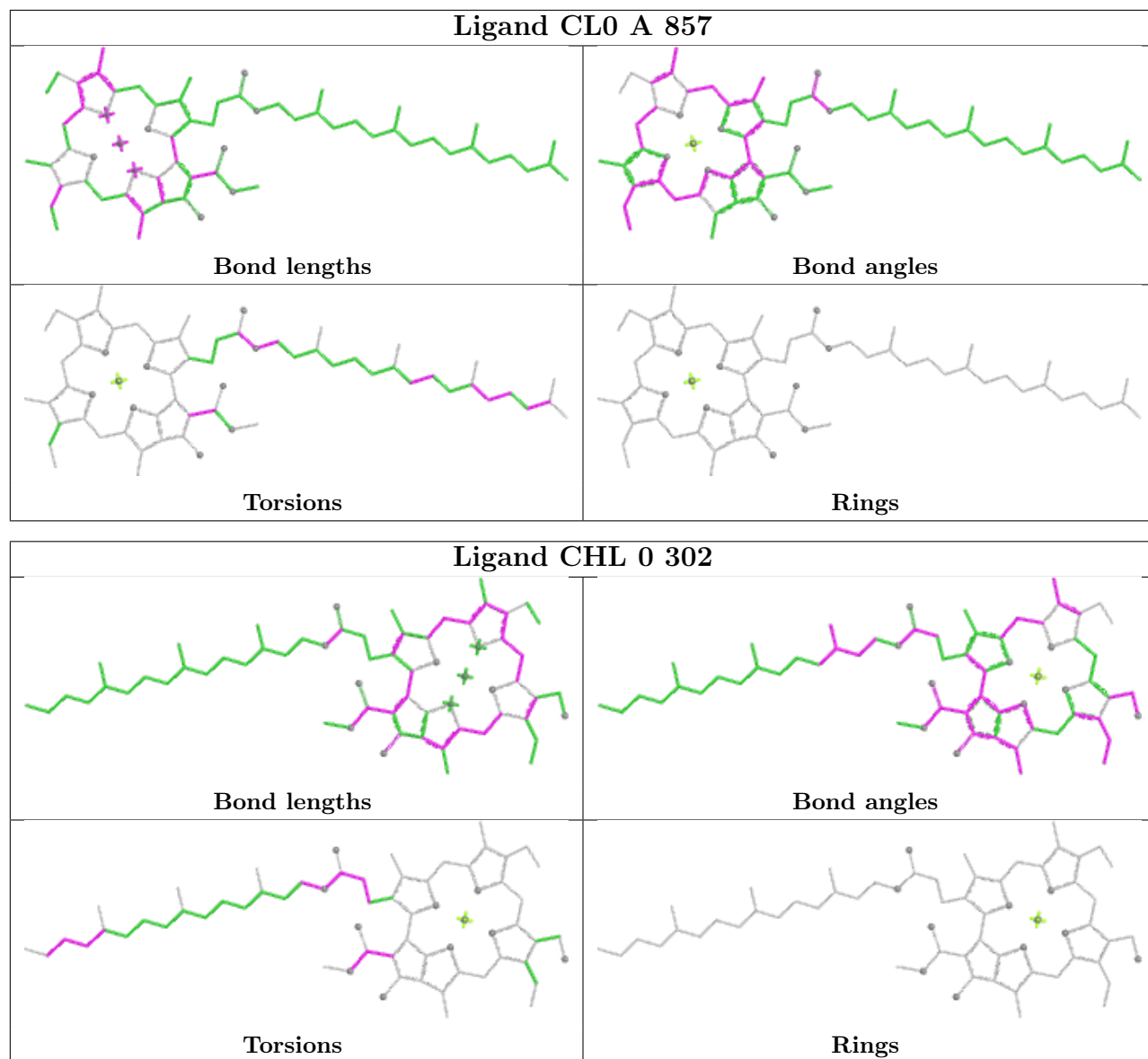
## Ligand CHL 0 305



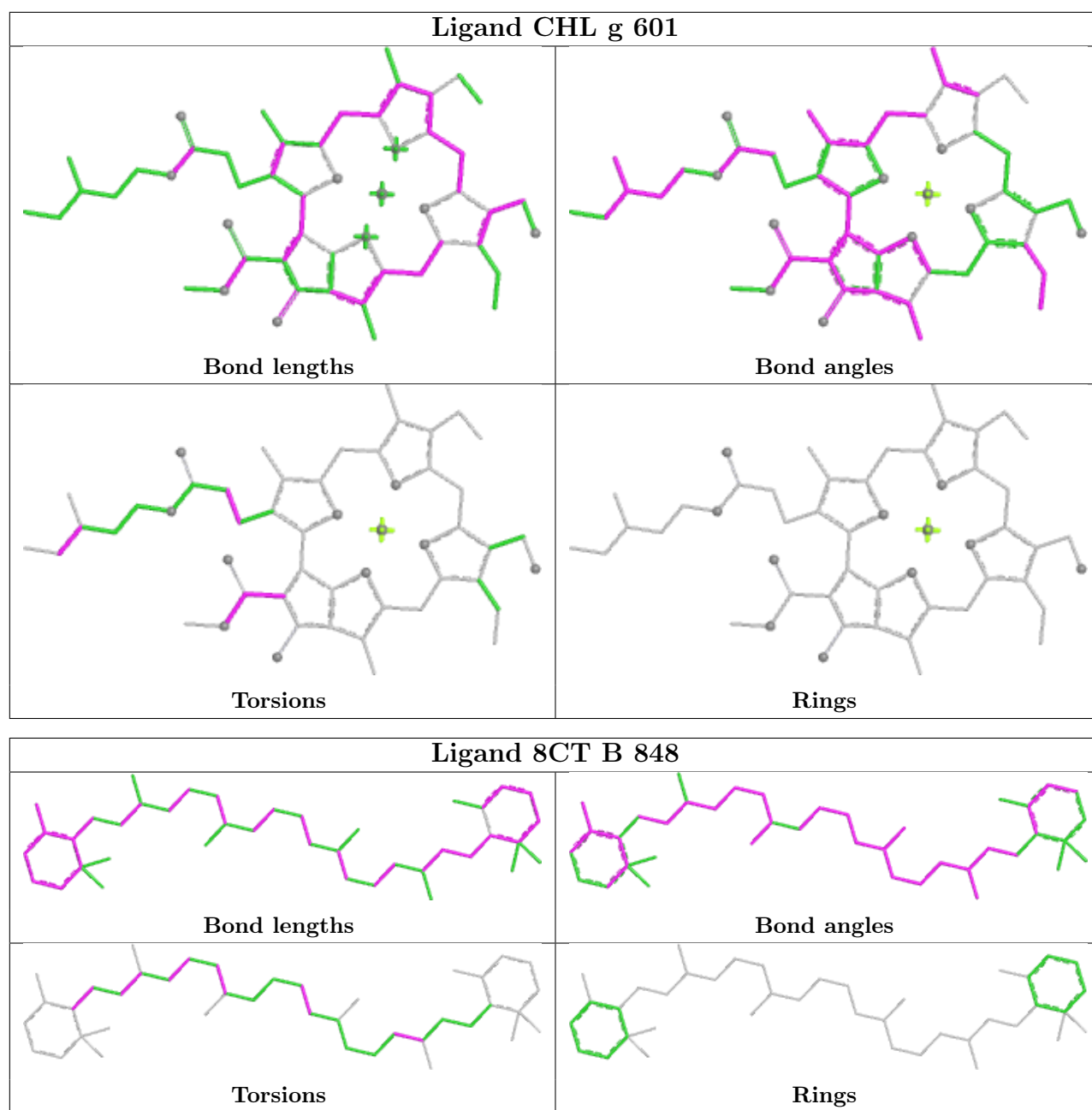
## Ligand CLA A 843





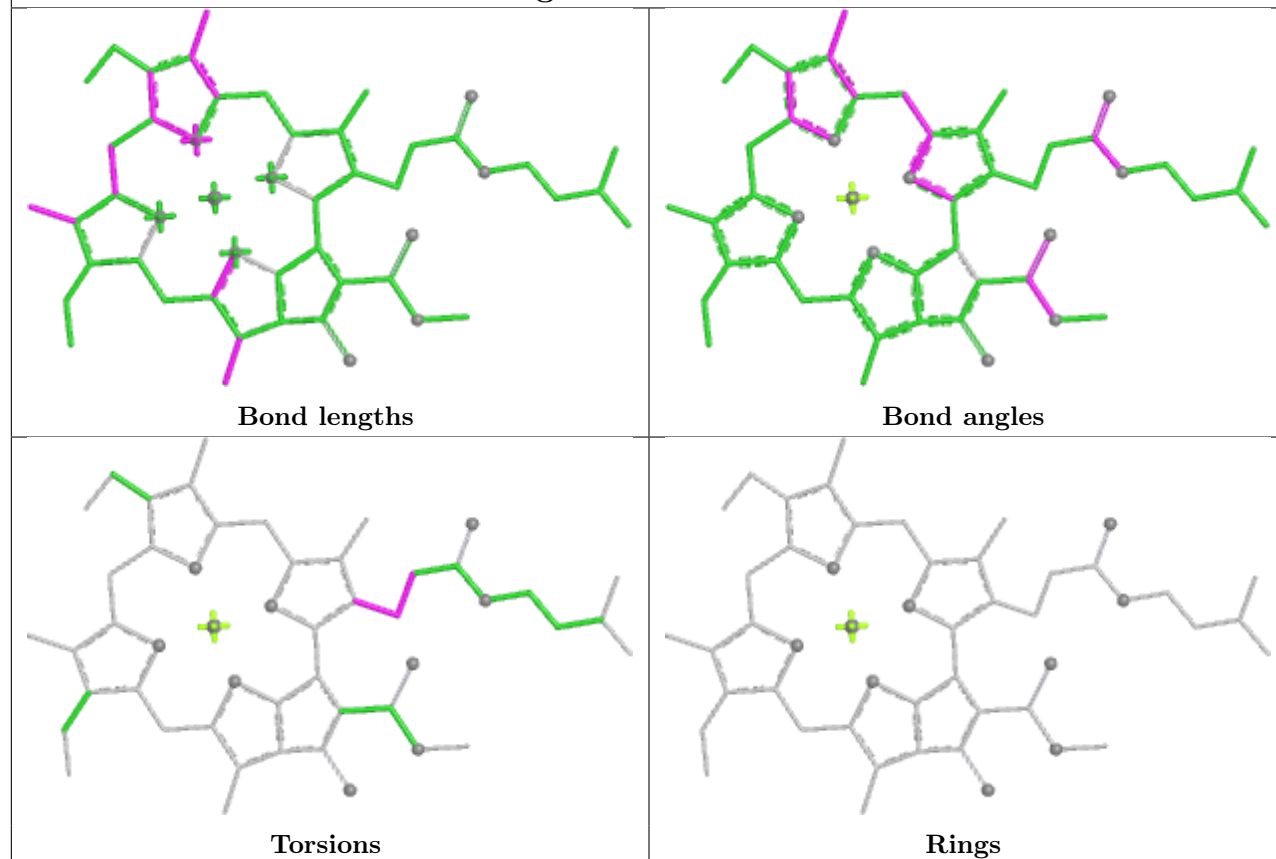




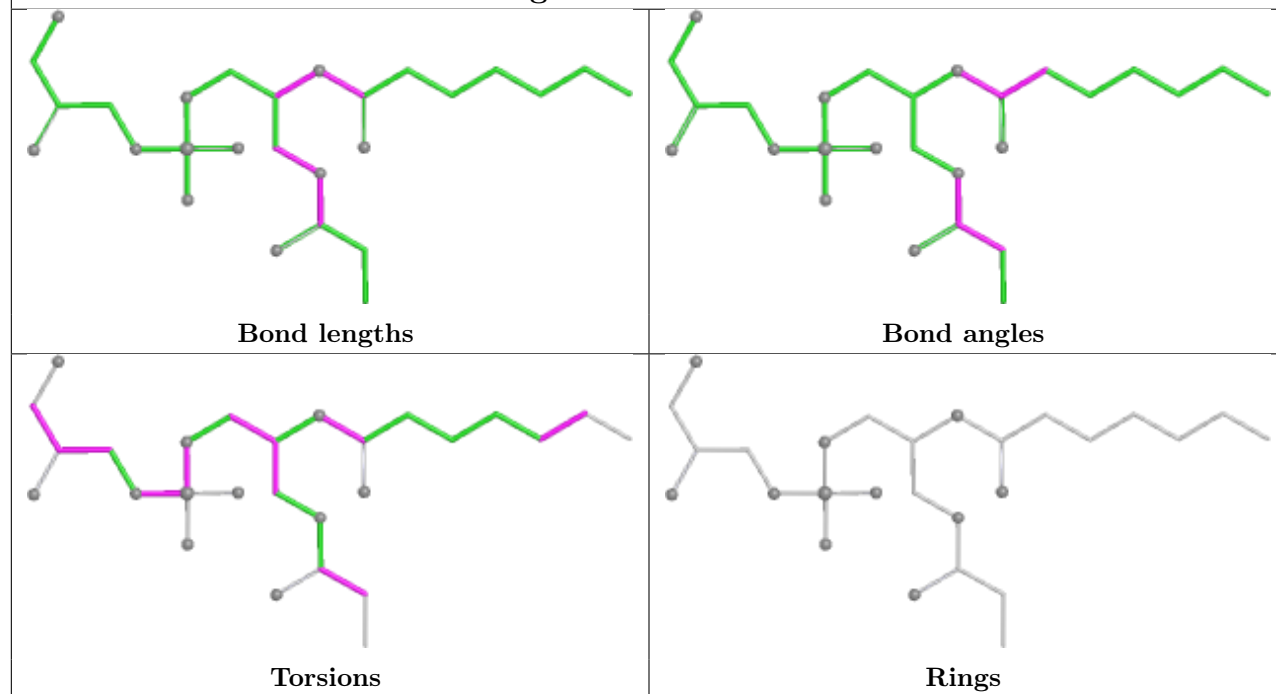




## Ligand CLA a 604

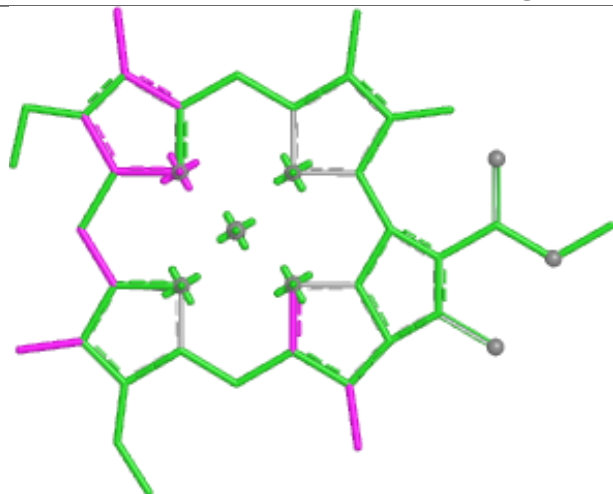


## Ligand LHG A 845

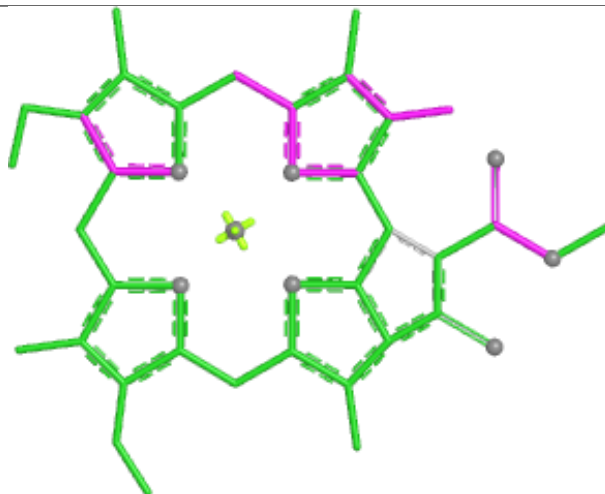




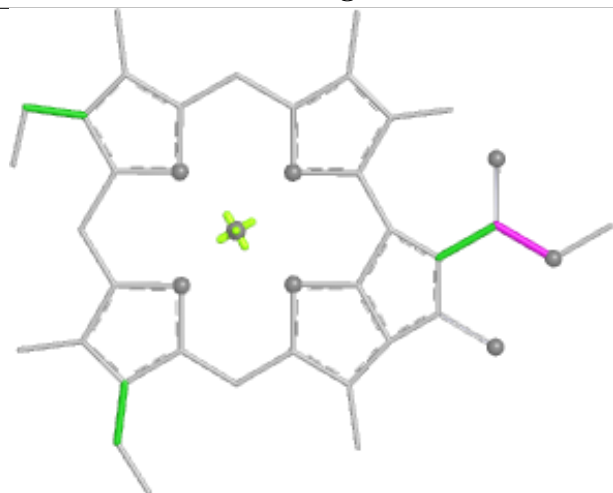
## Ligand CLA 0 310



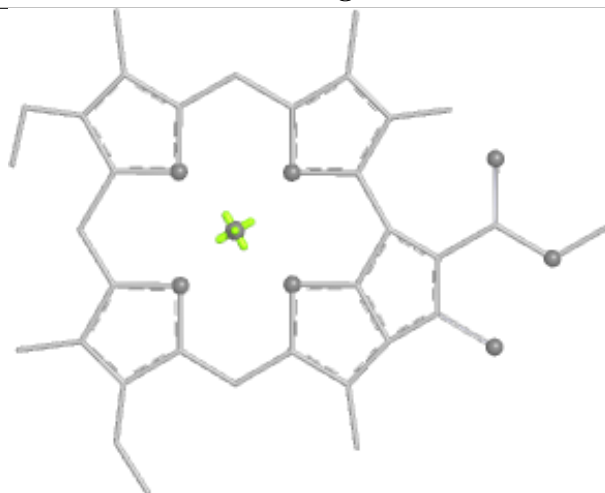
Bond lengths



Bond angles

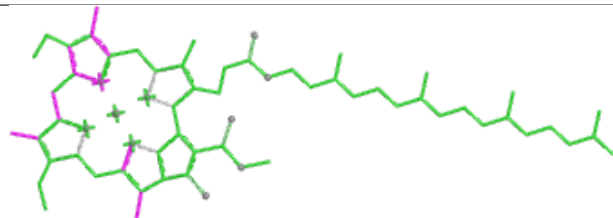


Torsions

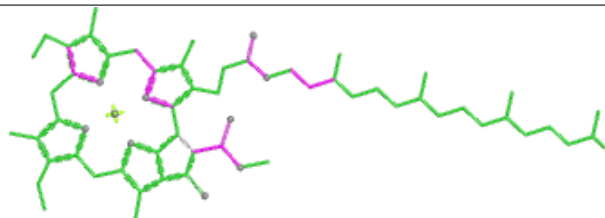


Rings

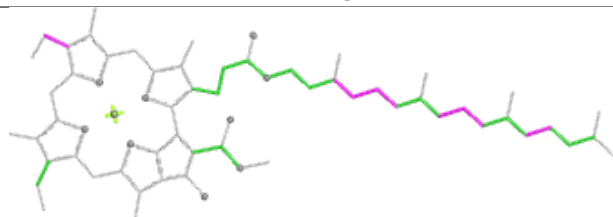
## Ligand CLA B 811



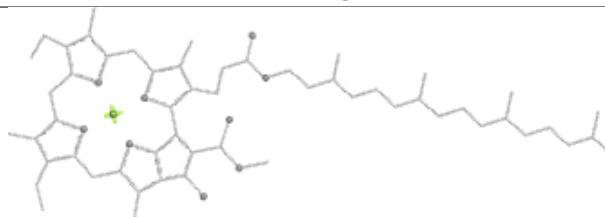
Bond lengths



Bond angles

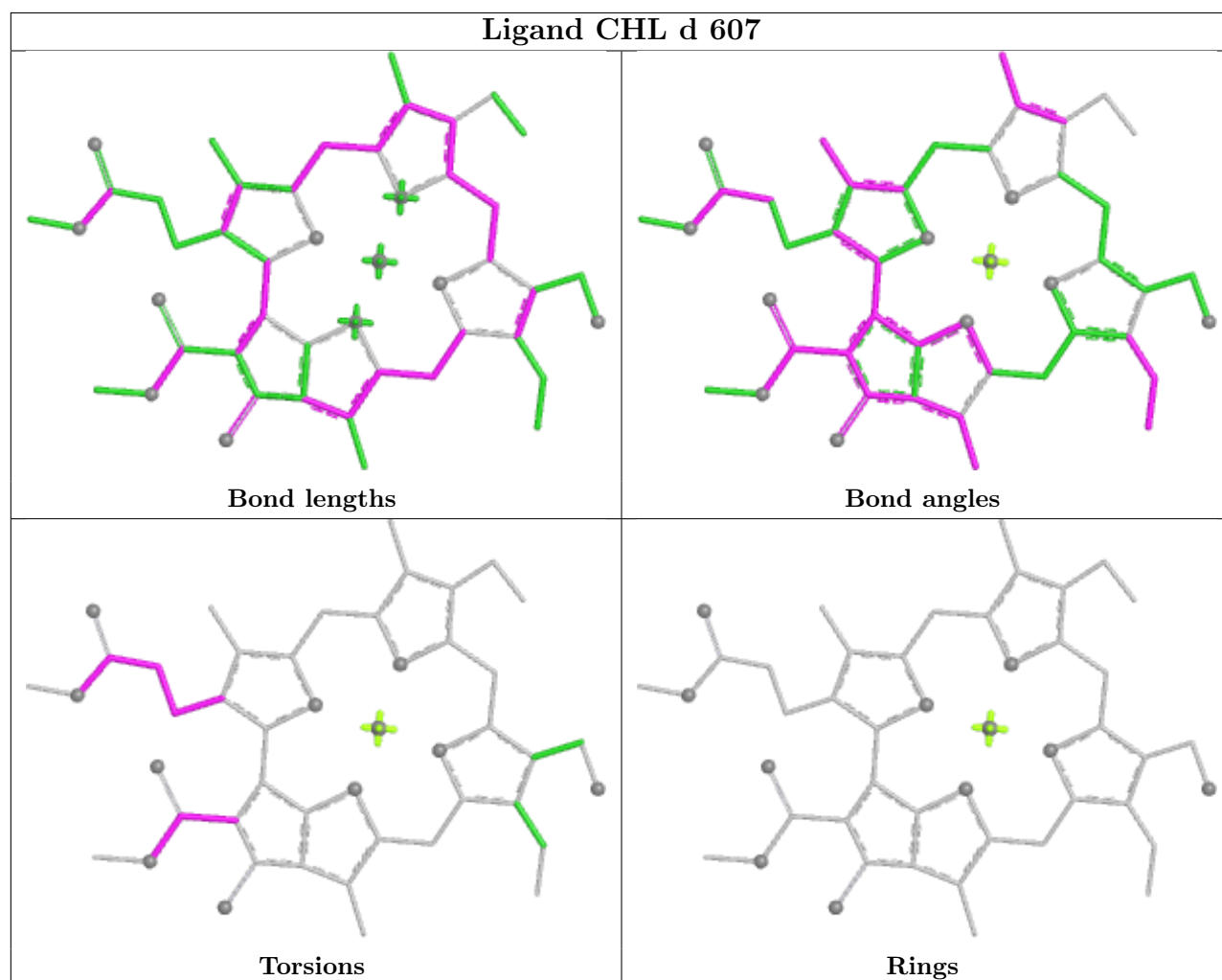
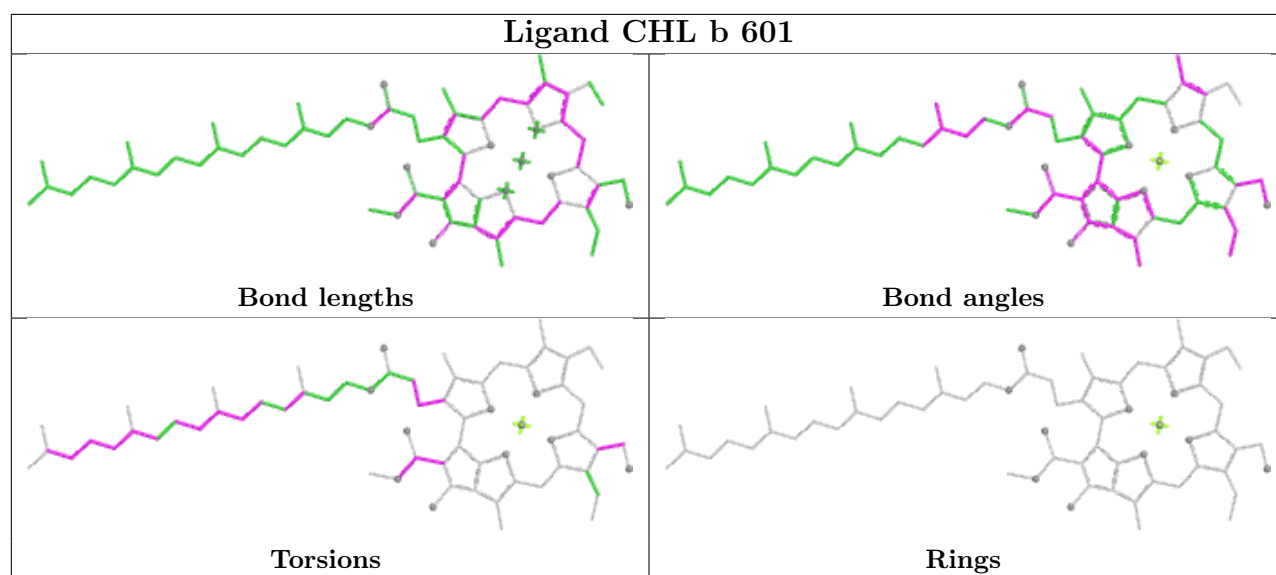


Torsions

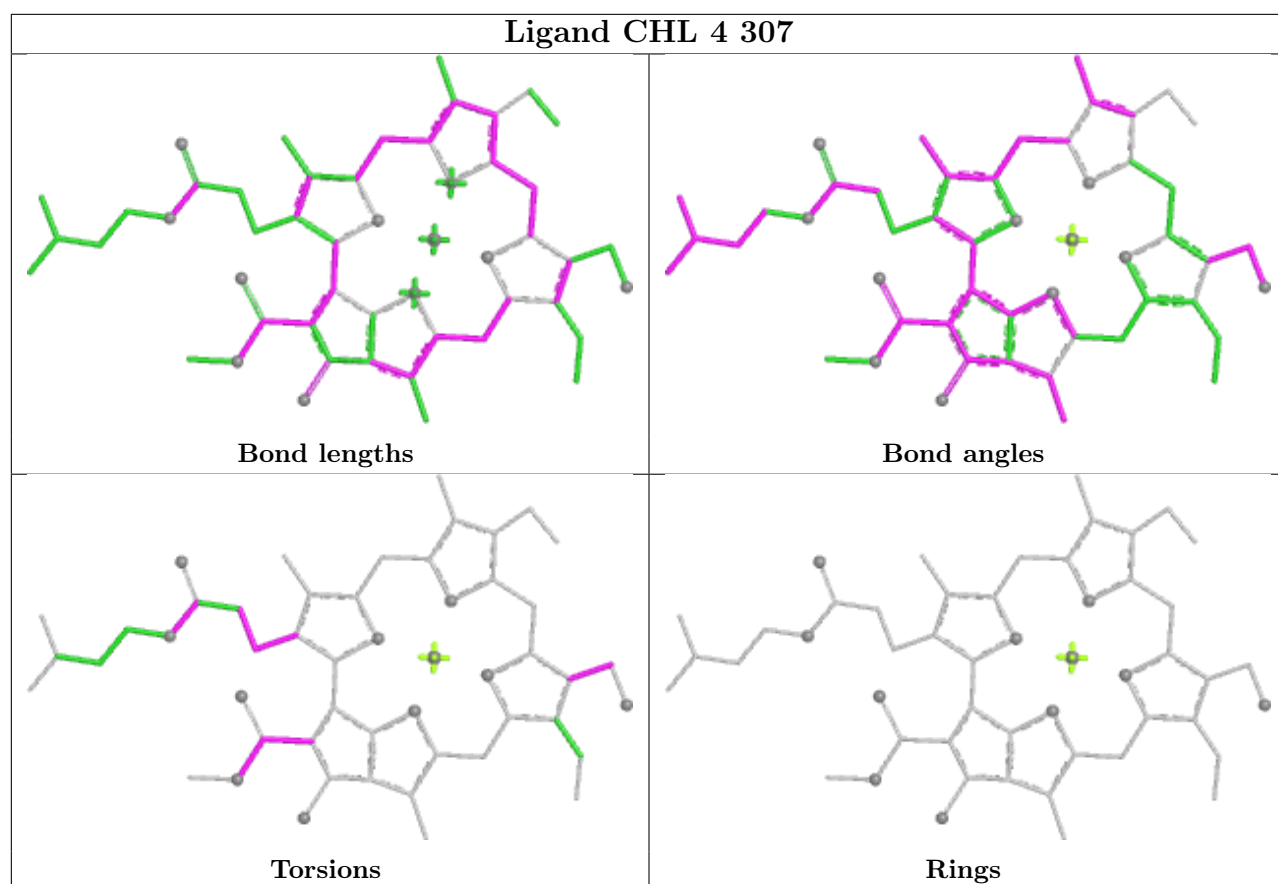


Rings



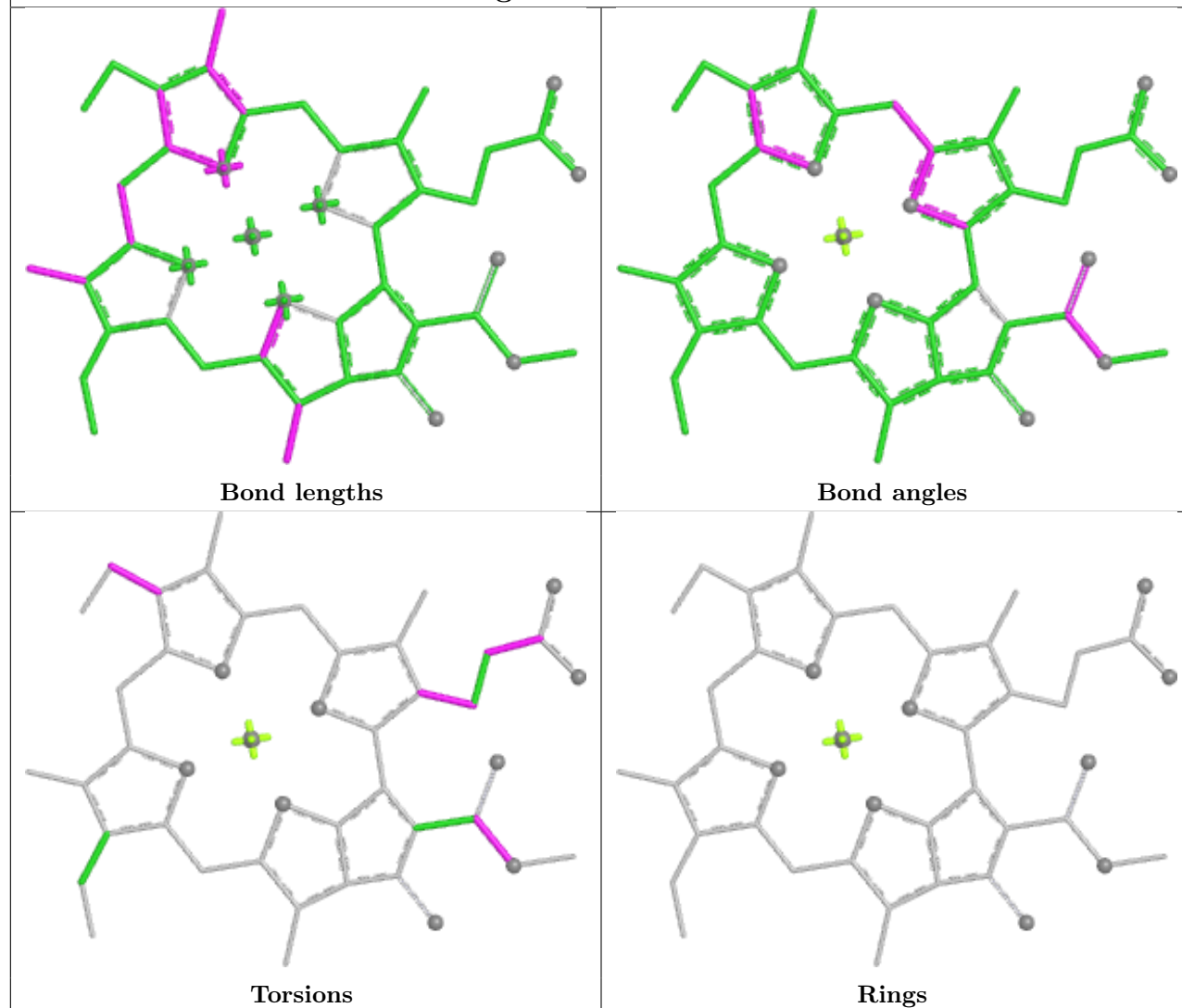




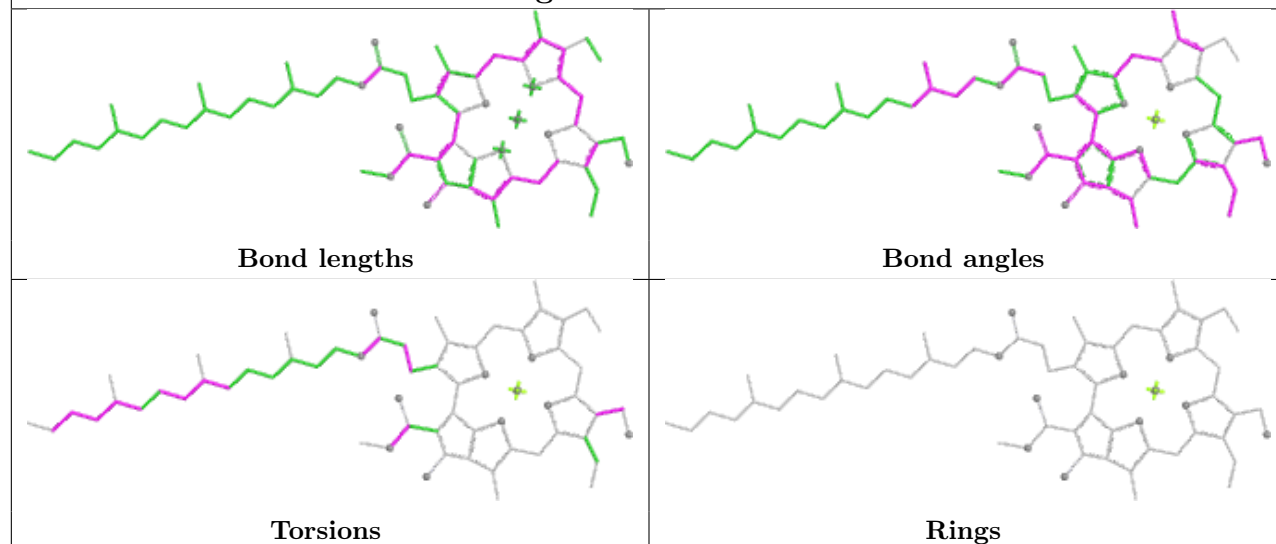




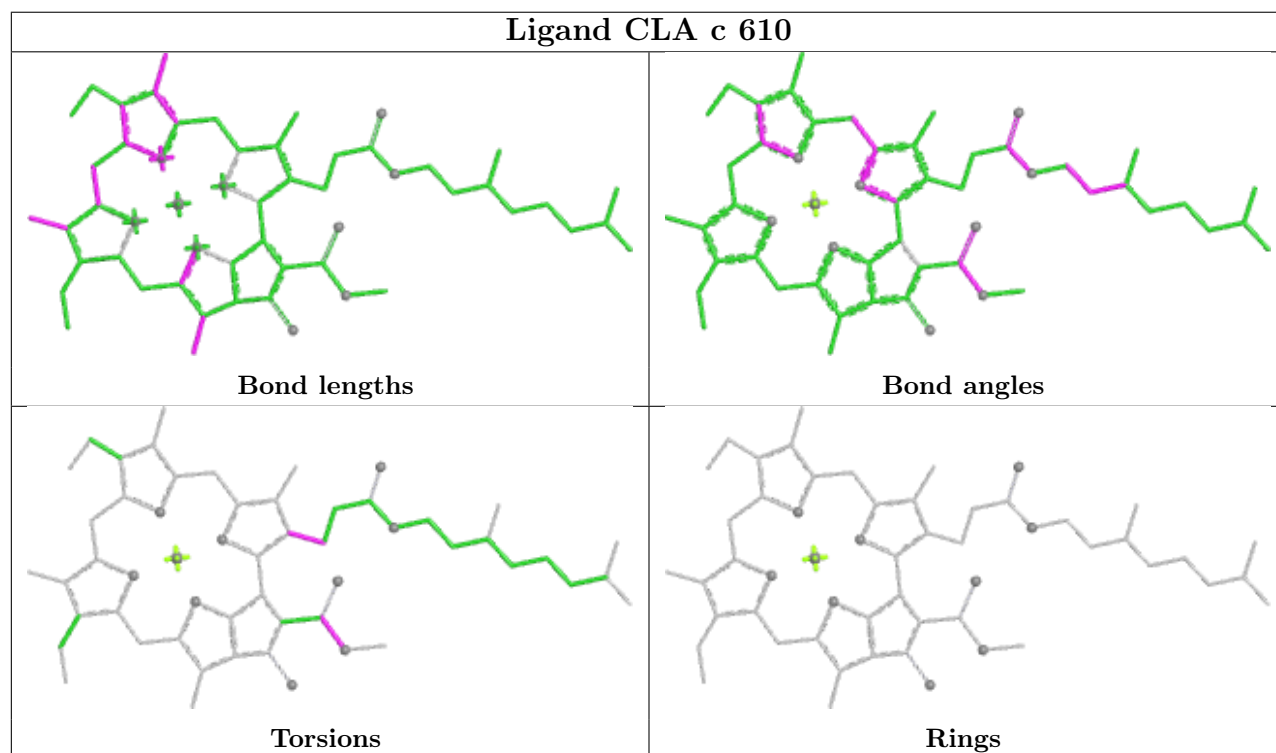
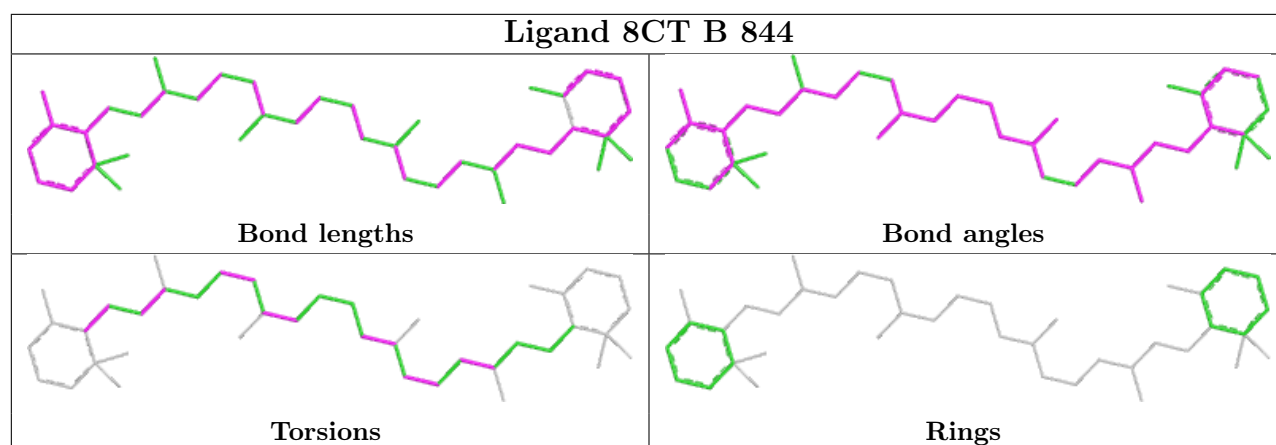
## Ligand CLA d 612



## Ligand CHL 5 302

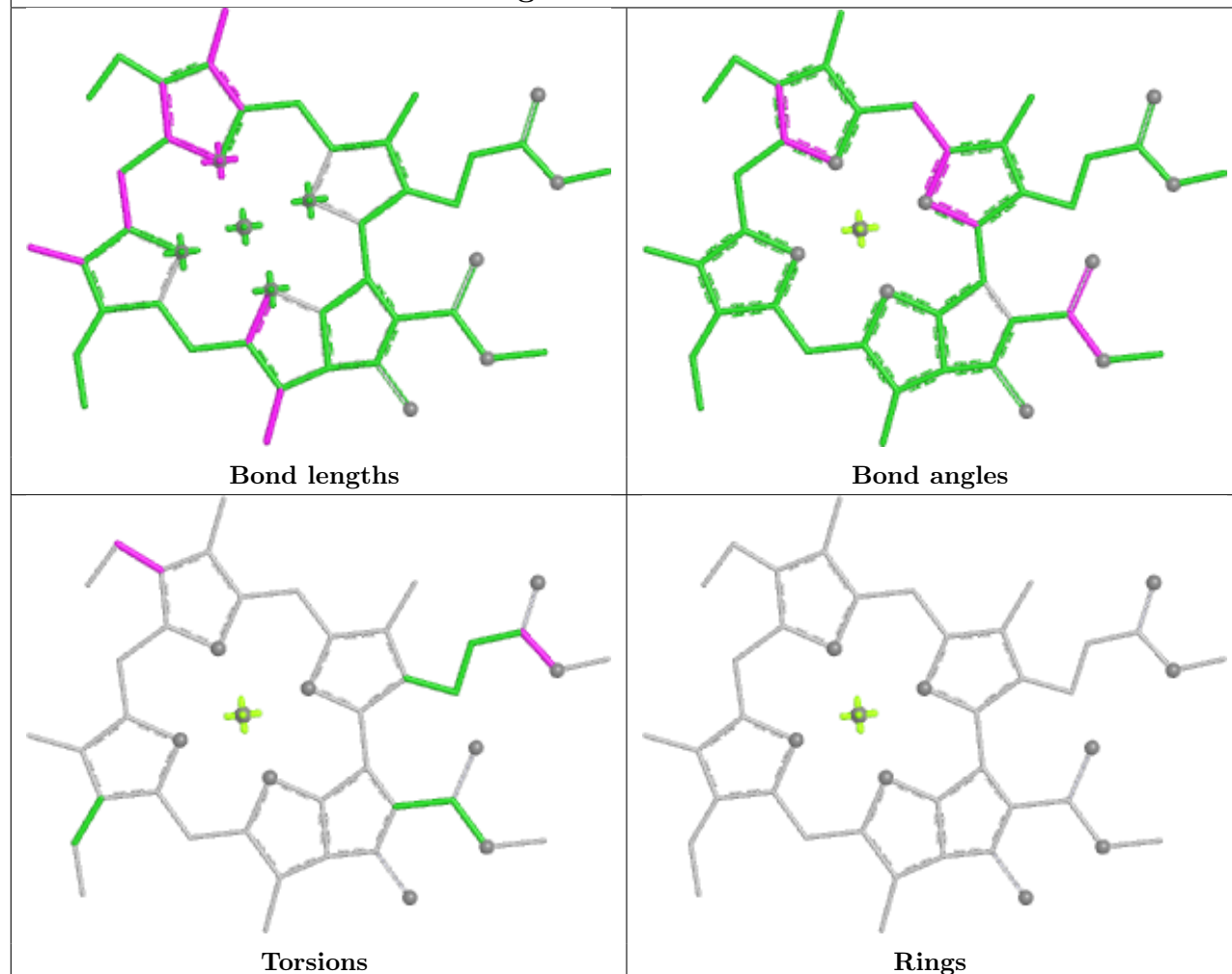




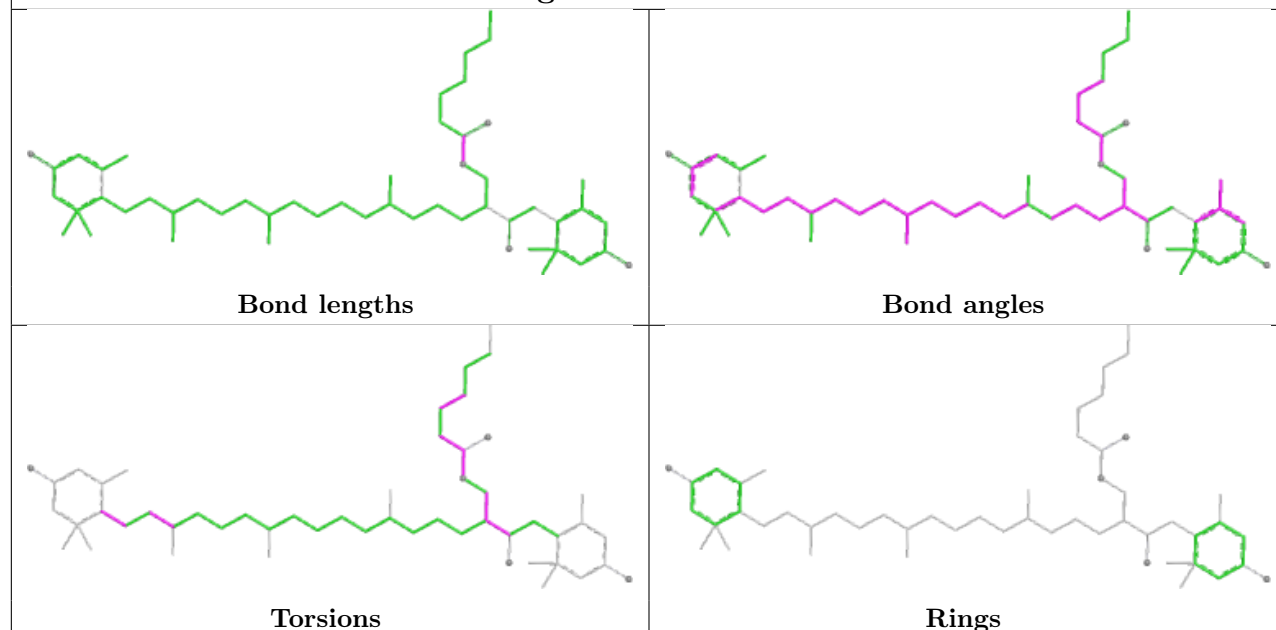




## Ligand CLA 8 310

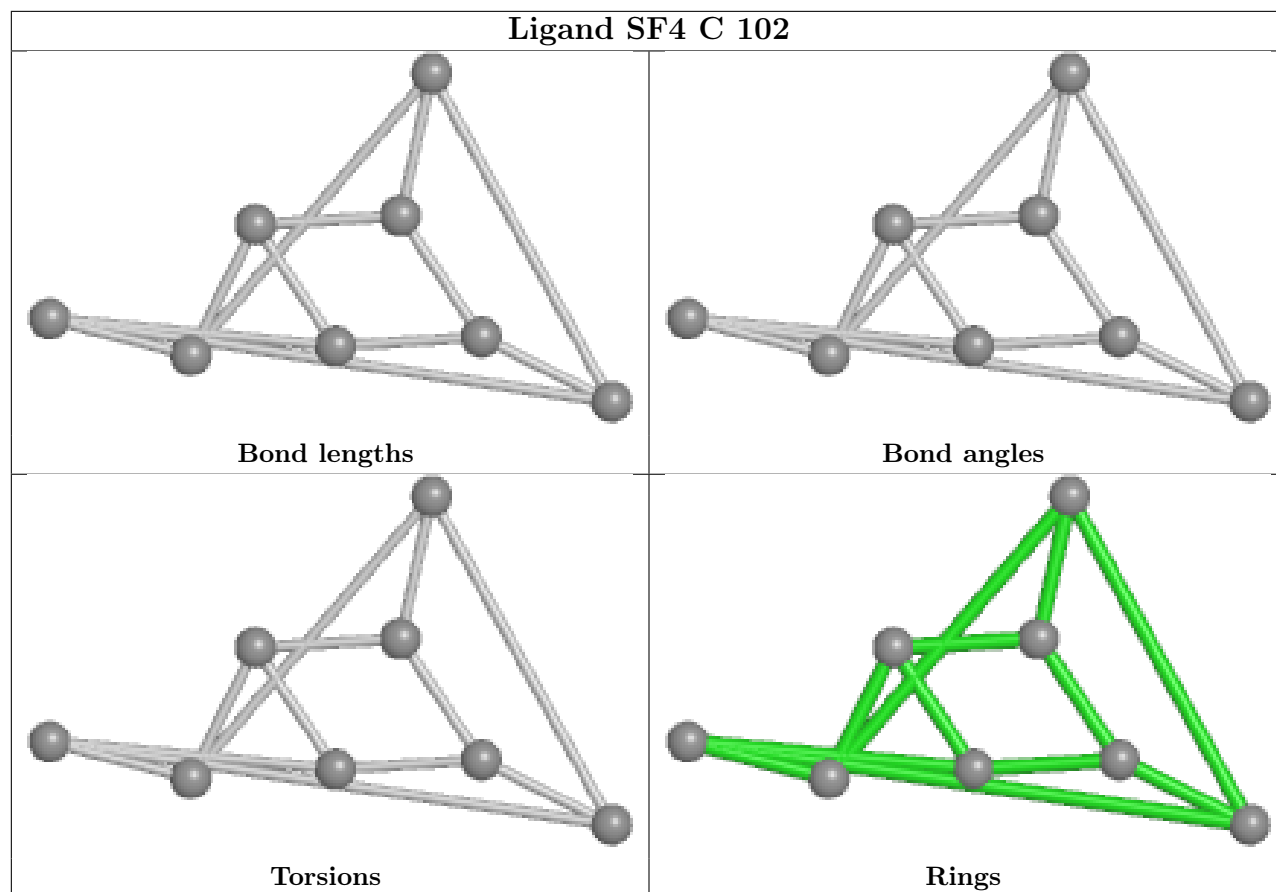


## Ligand OUR 0 502

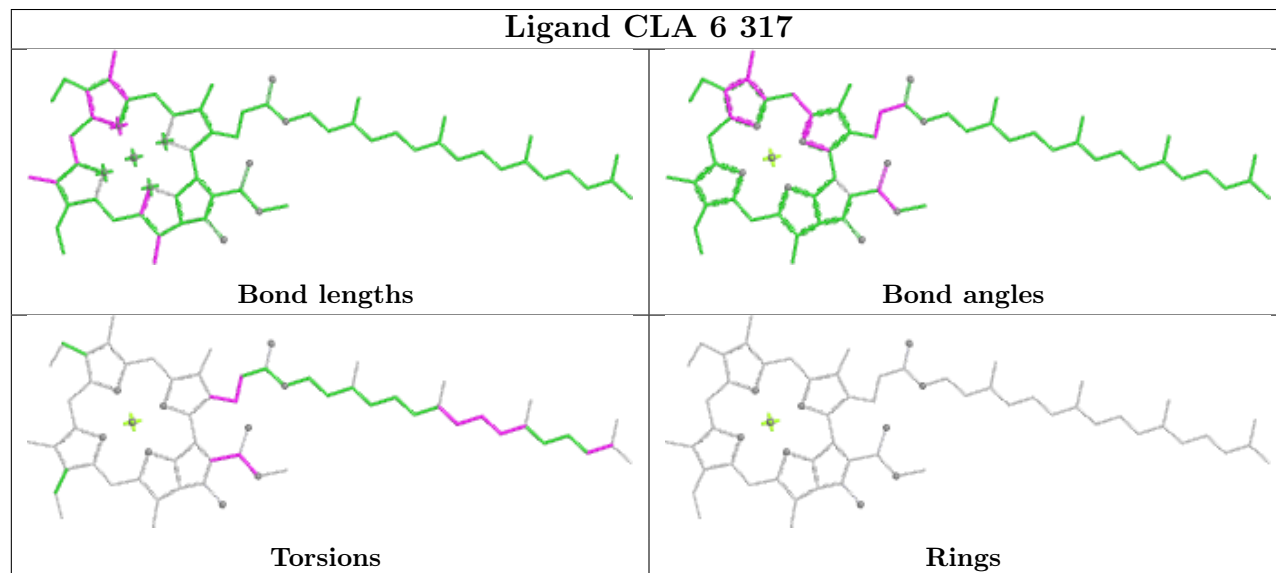




## Ligand SF4 C 102

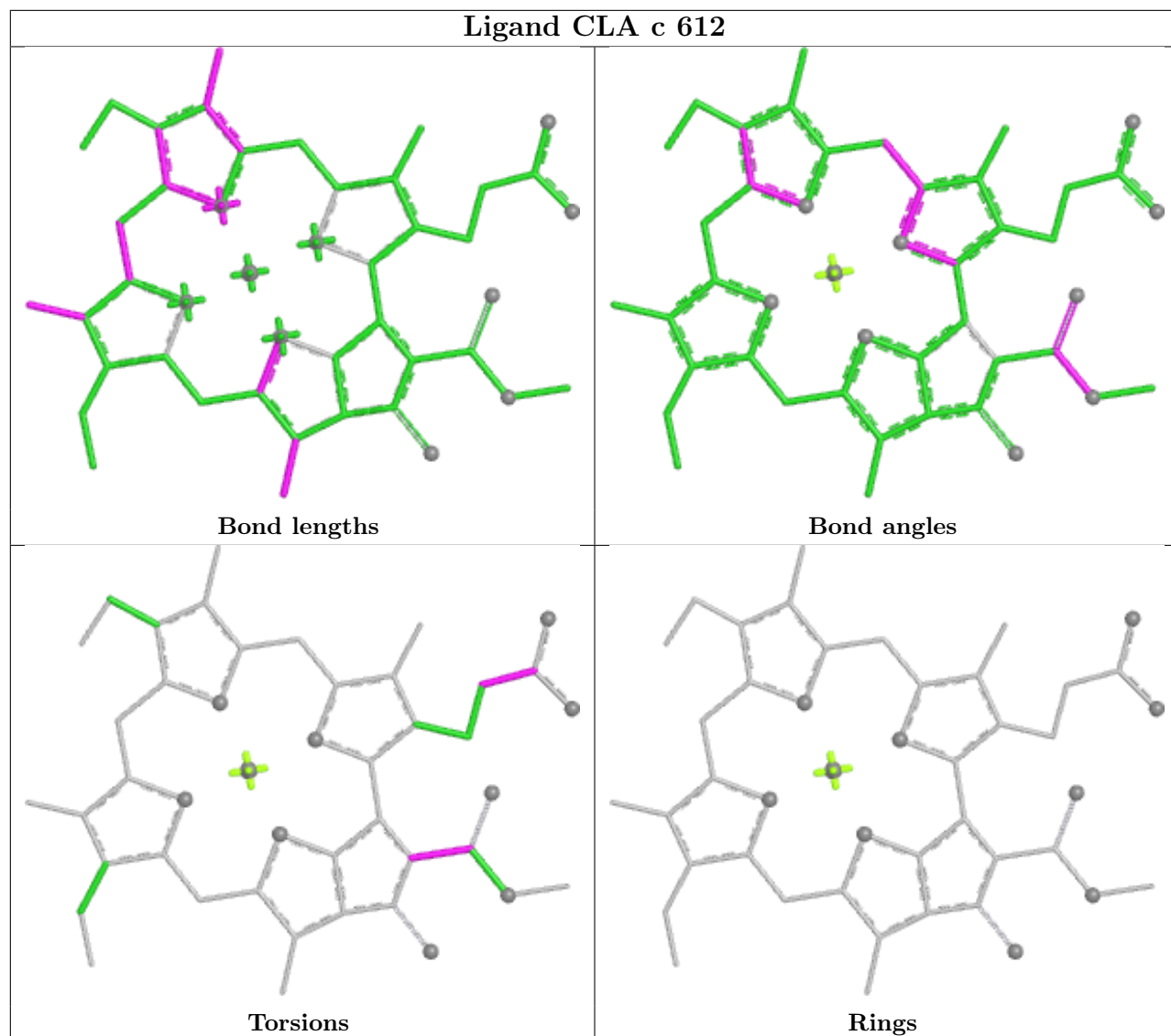


## Ligand CLA 6 317



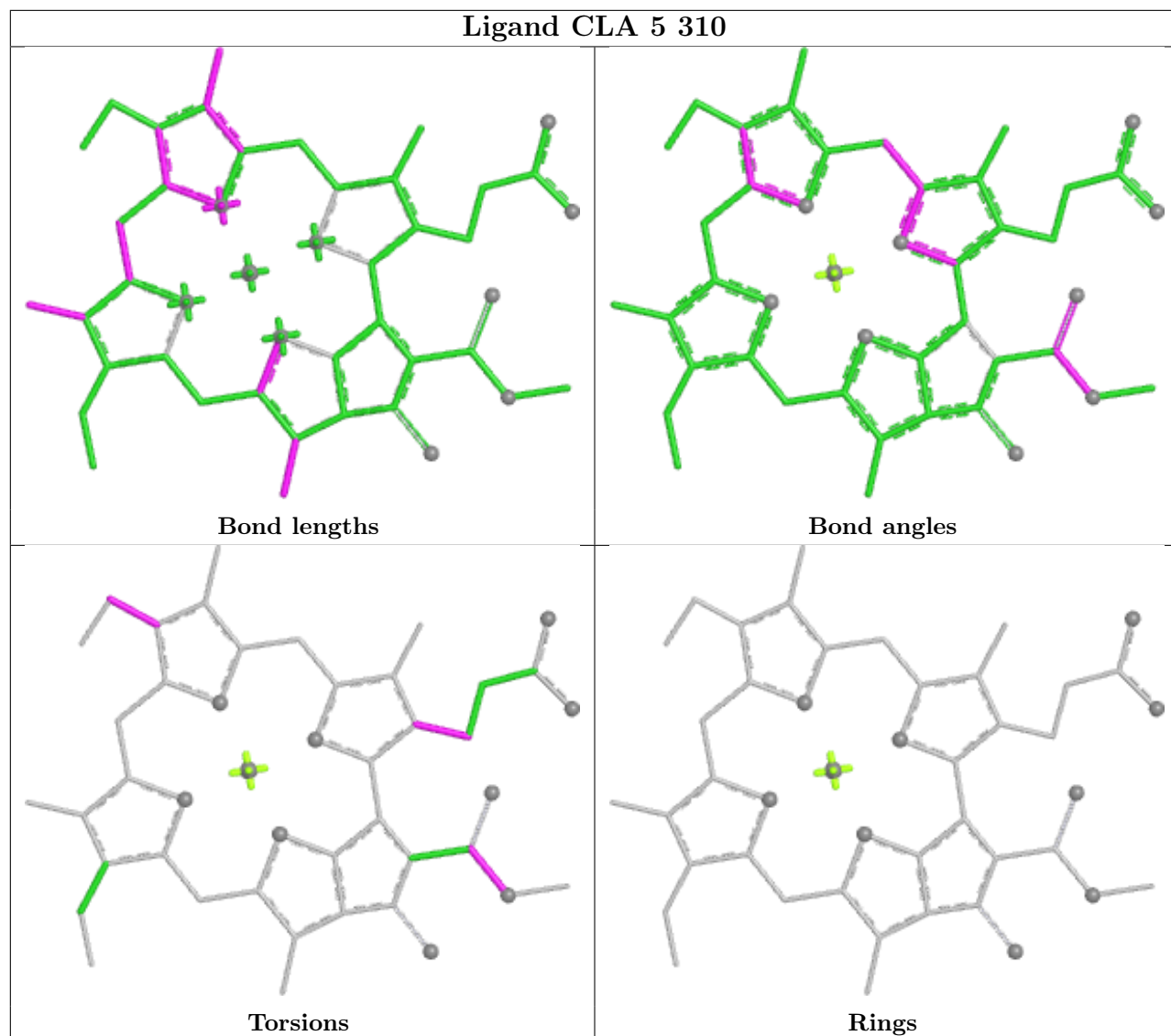


## Ligand CLA c 612

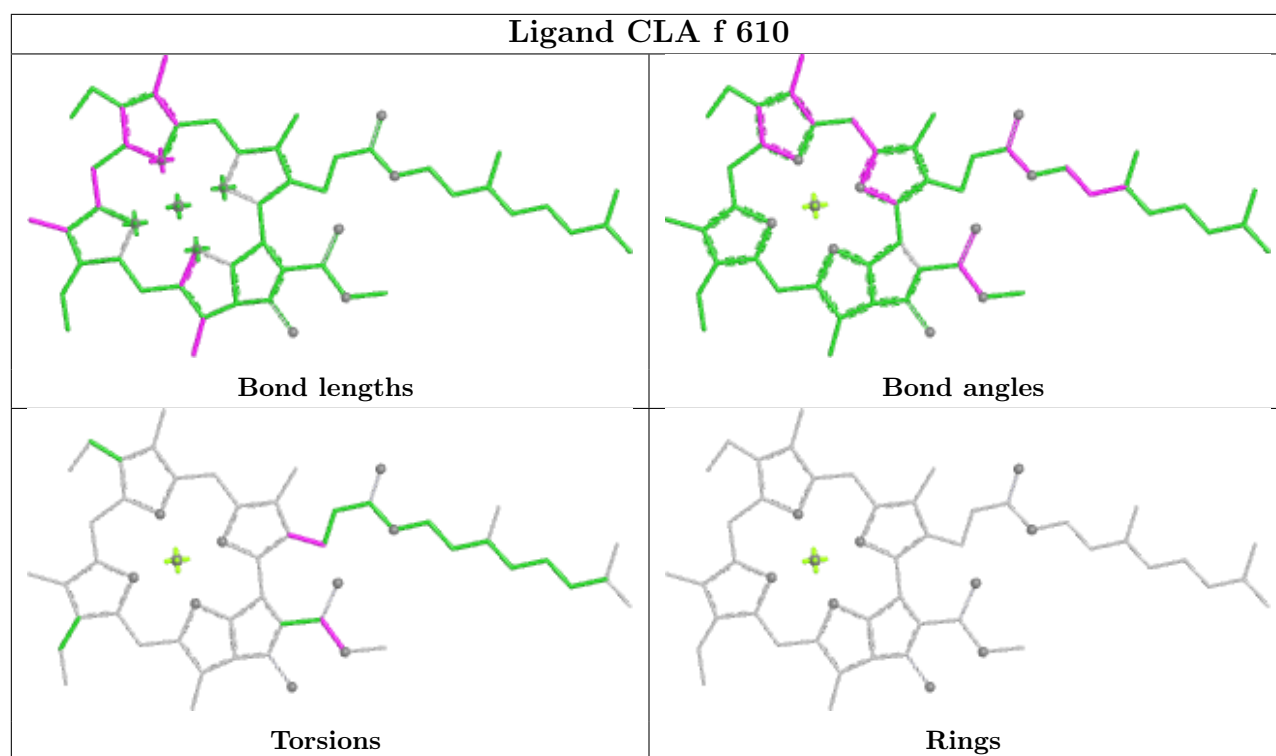




## Ligand CLA 5 310

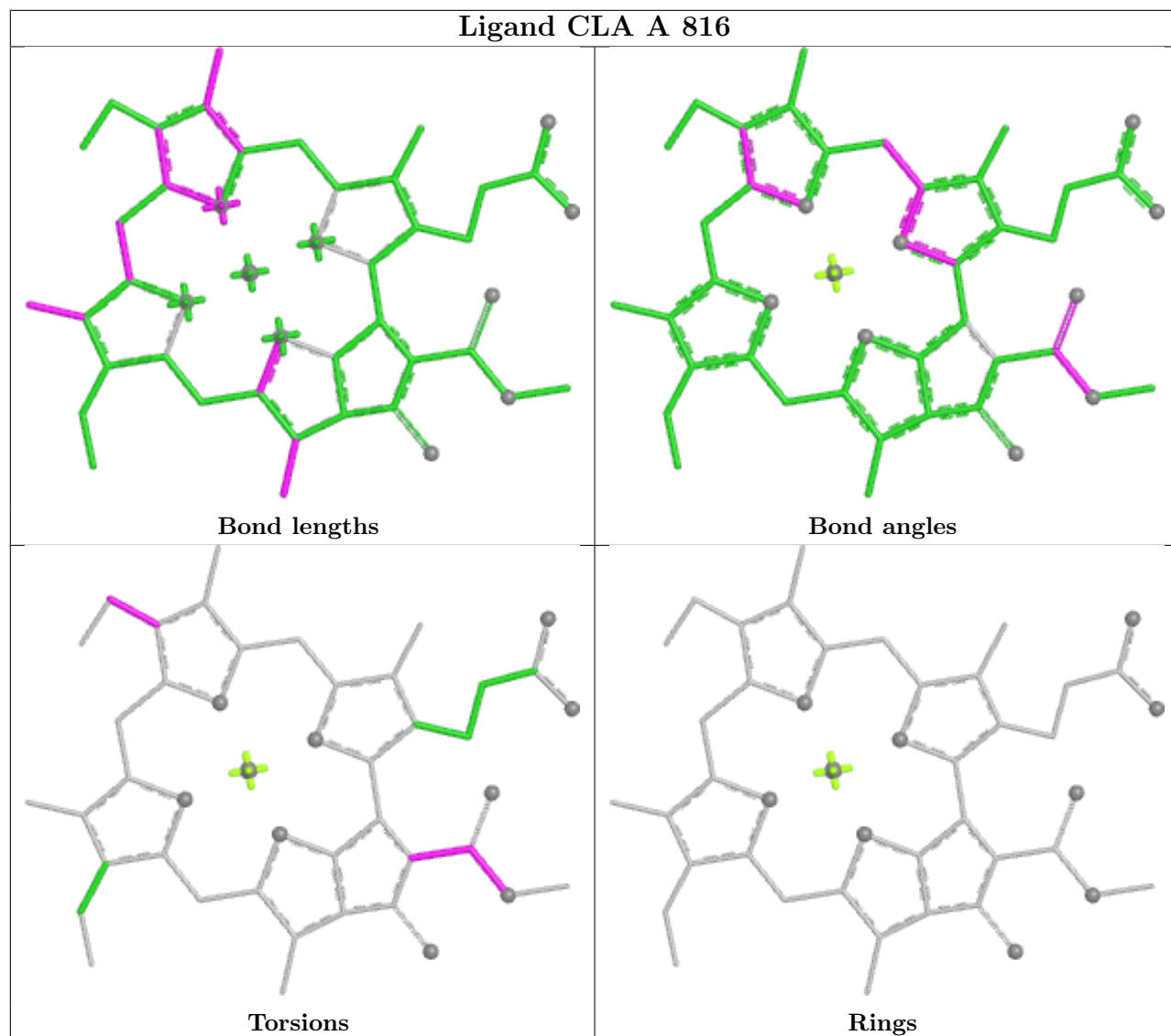




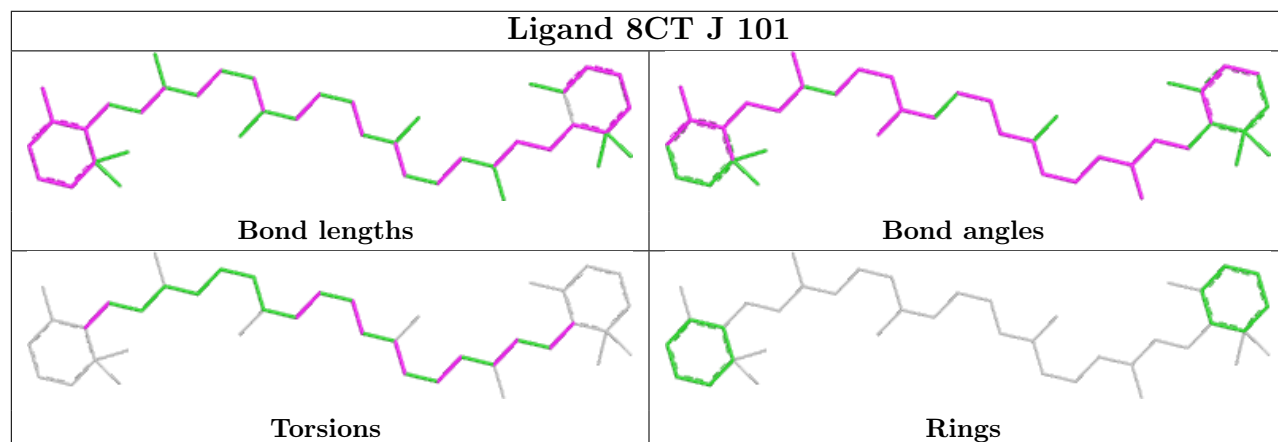




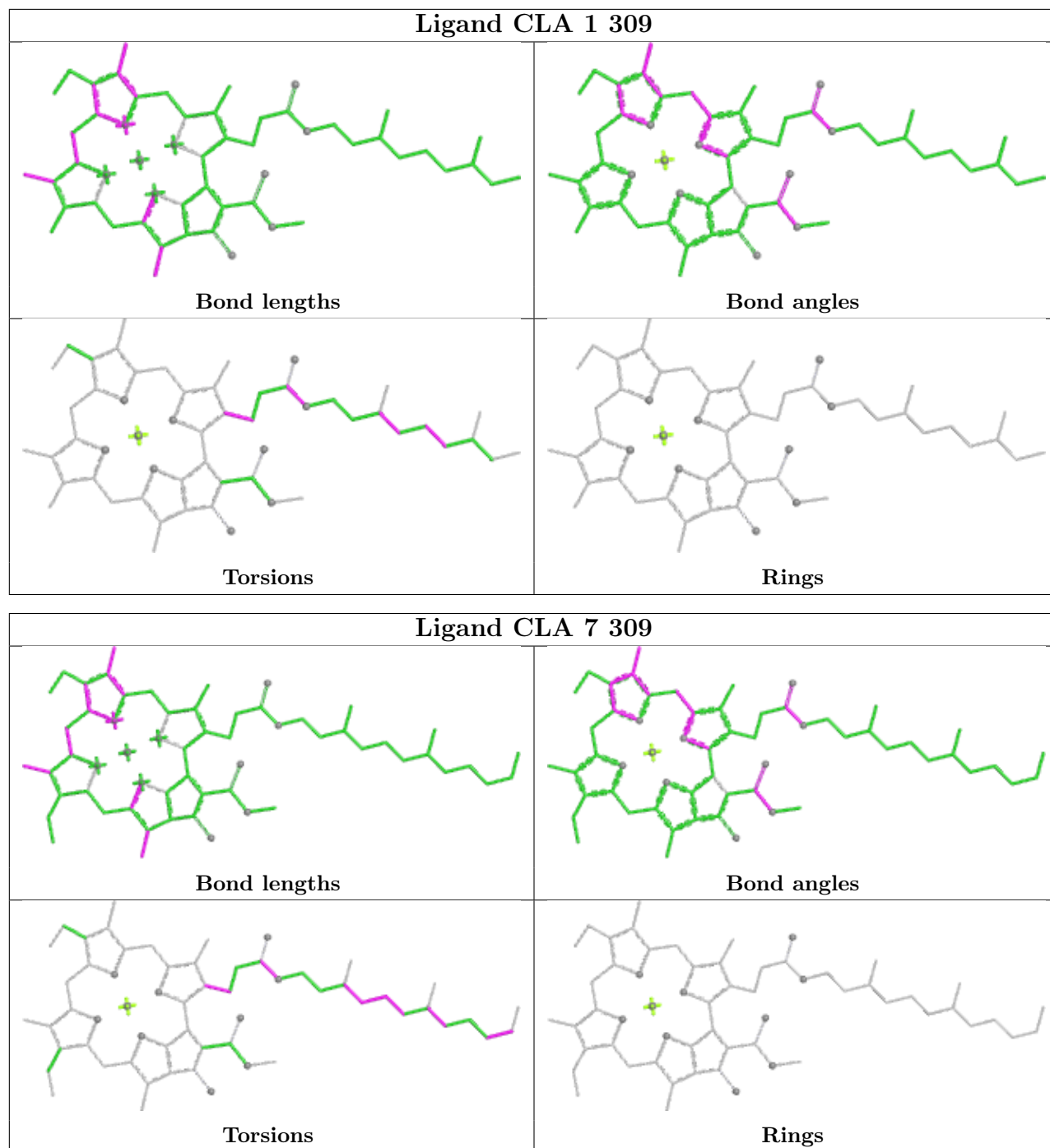
## Ligand CLA A 816



## Ligand 8CT J 101

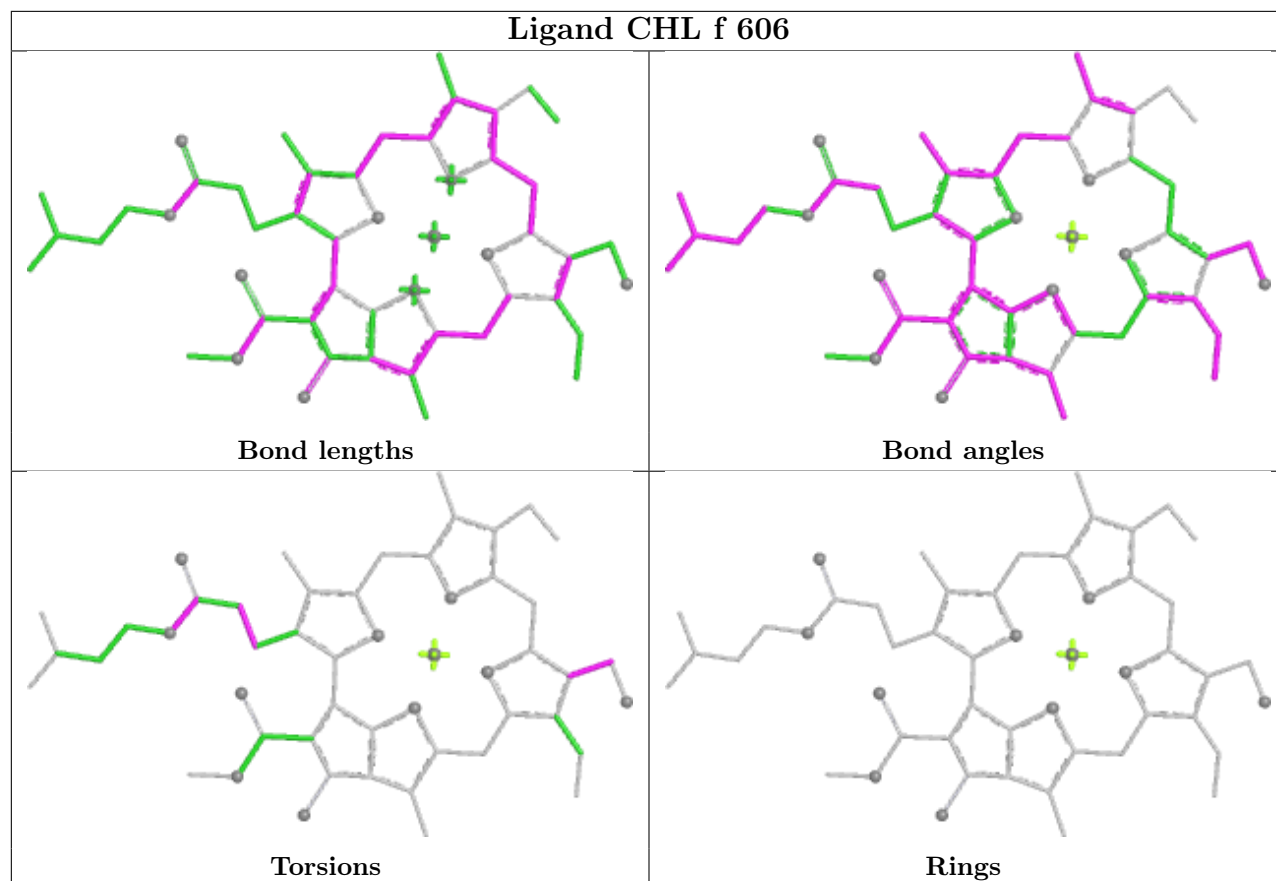




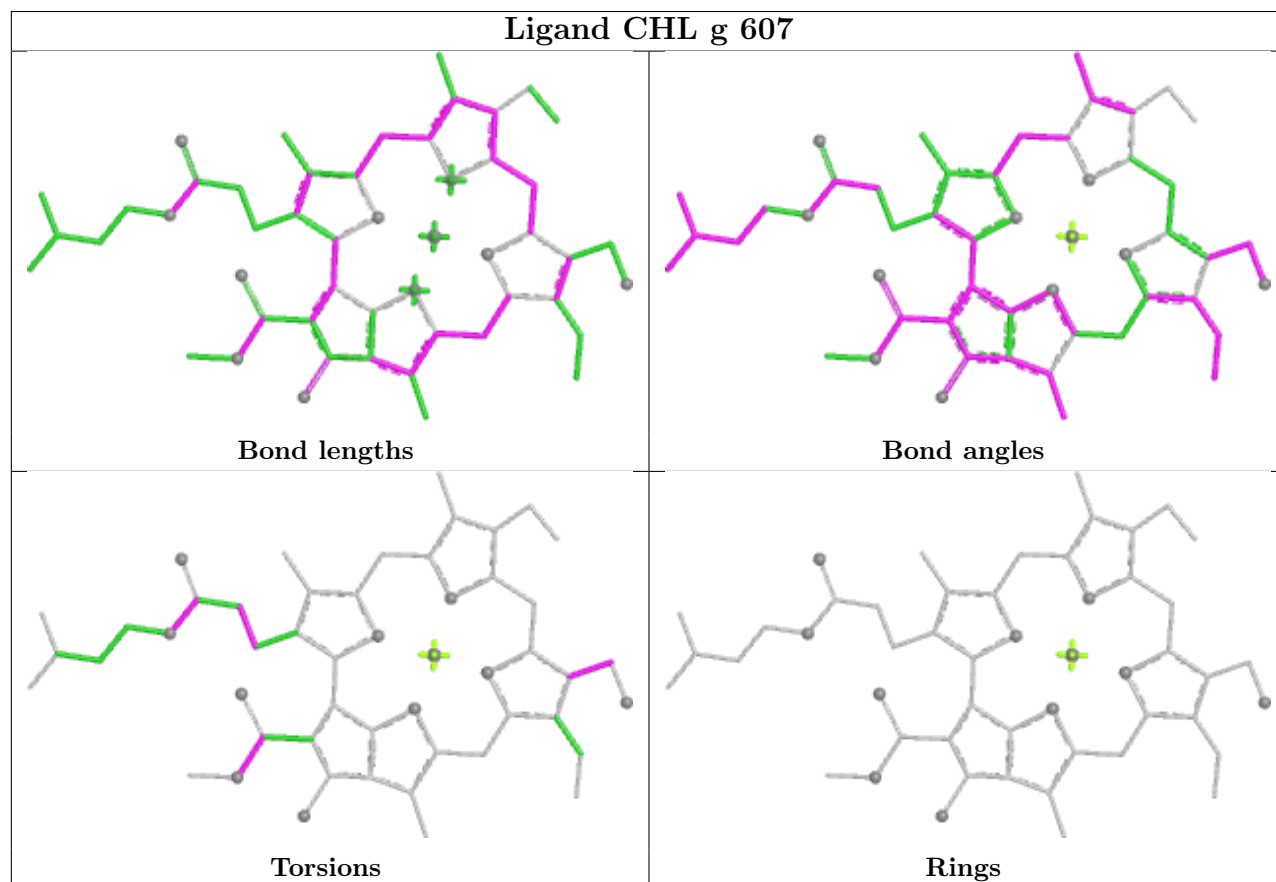




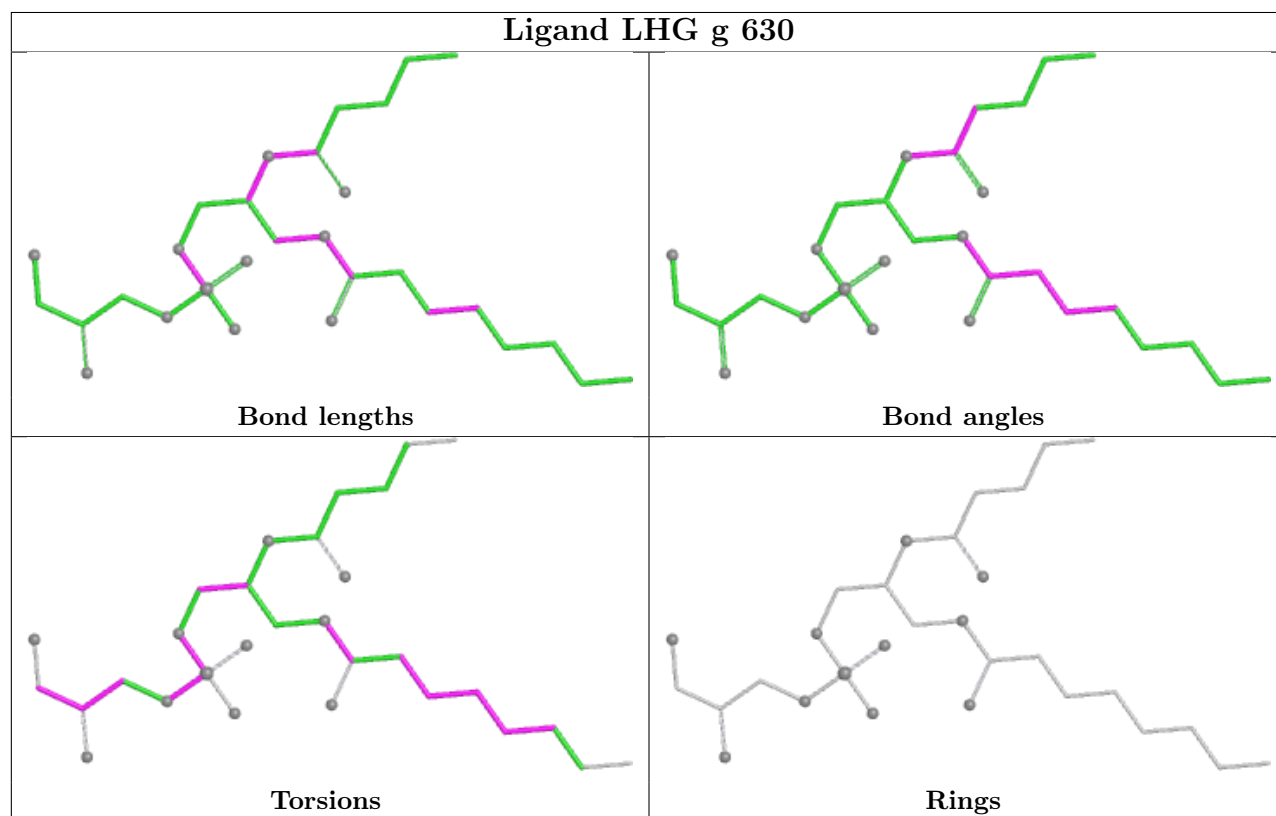
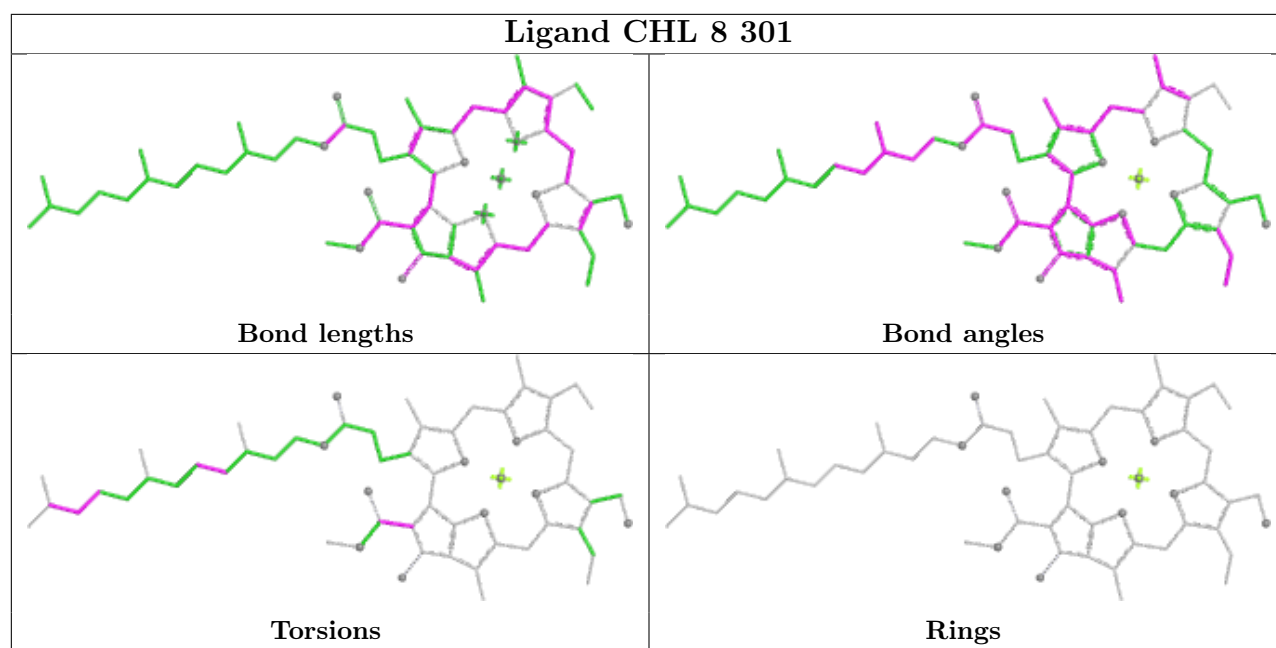
## Ligand CHL f 606



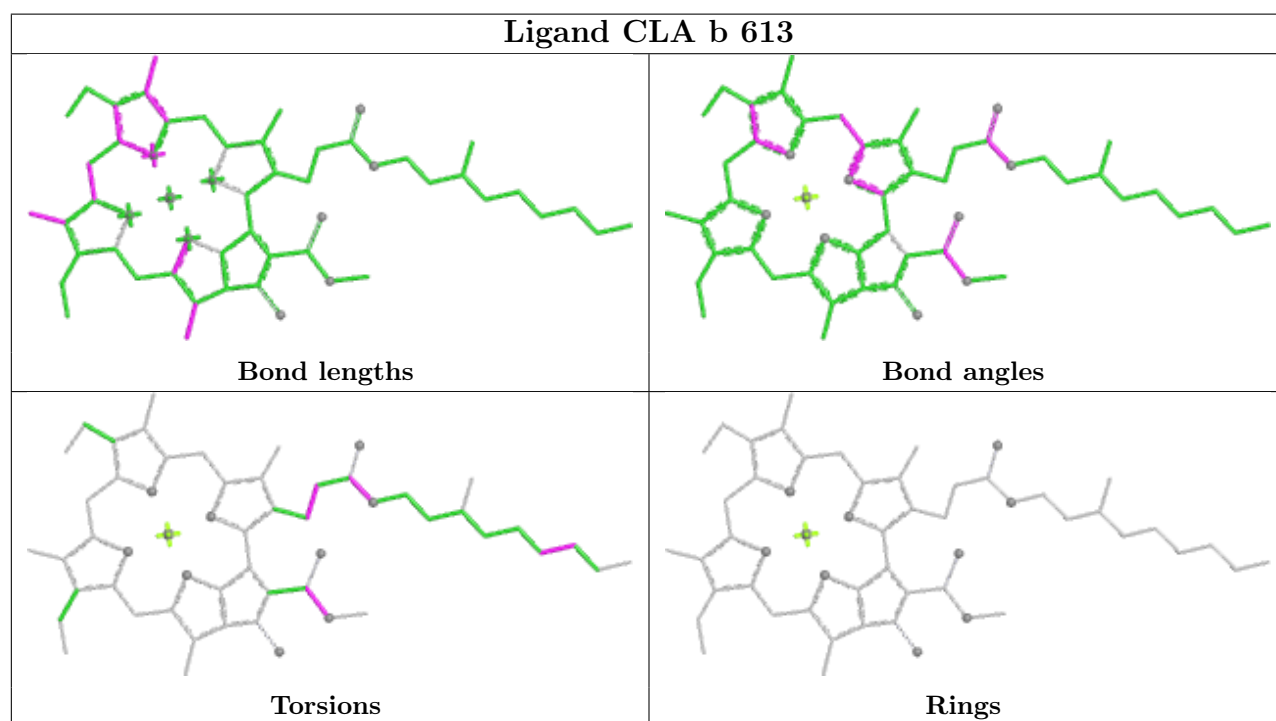
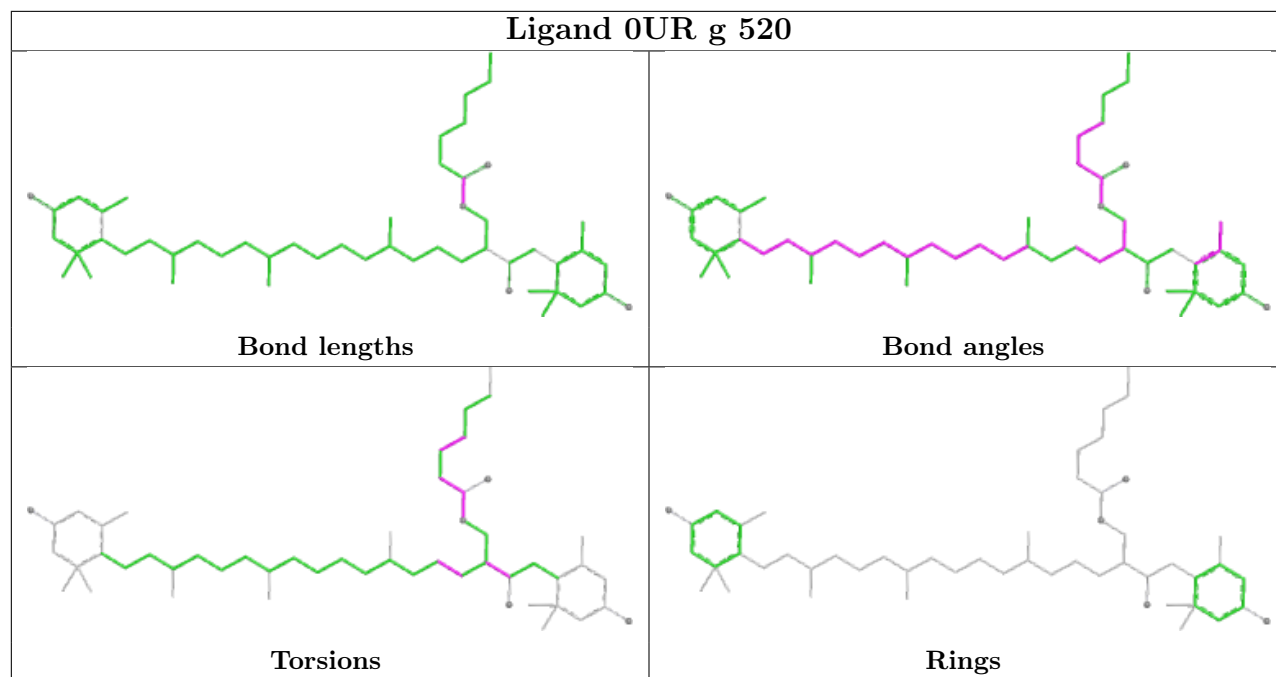
## Ligand CHL g 607



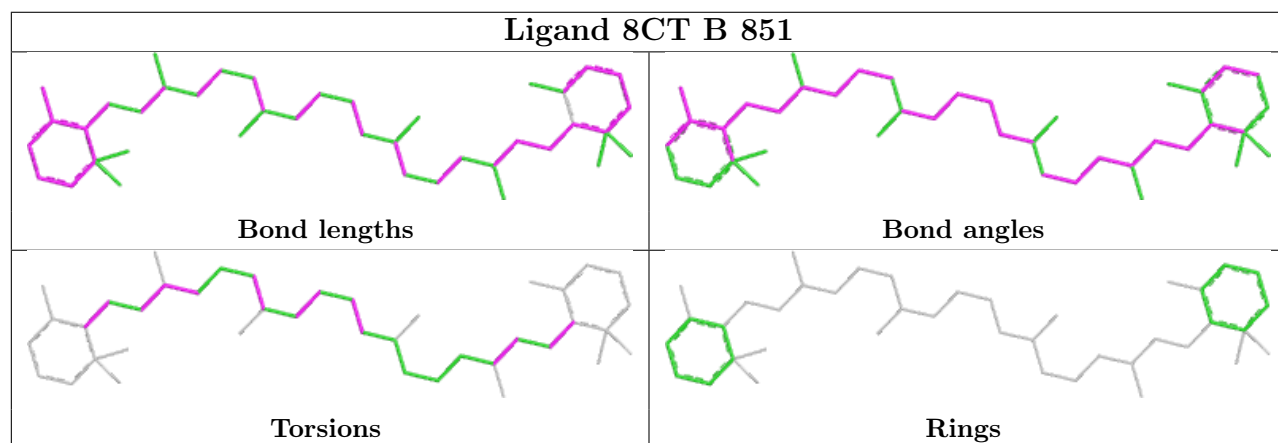
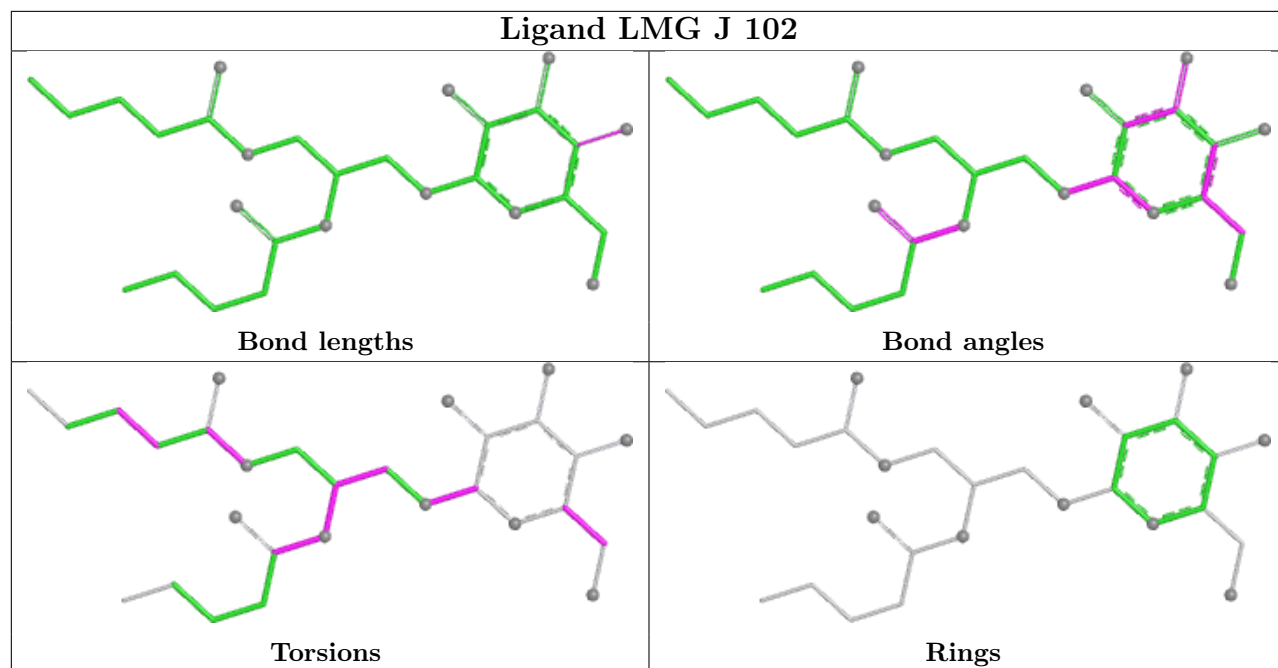






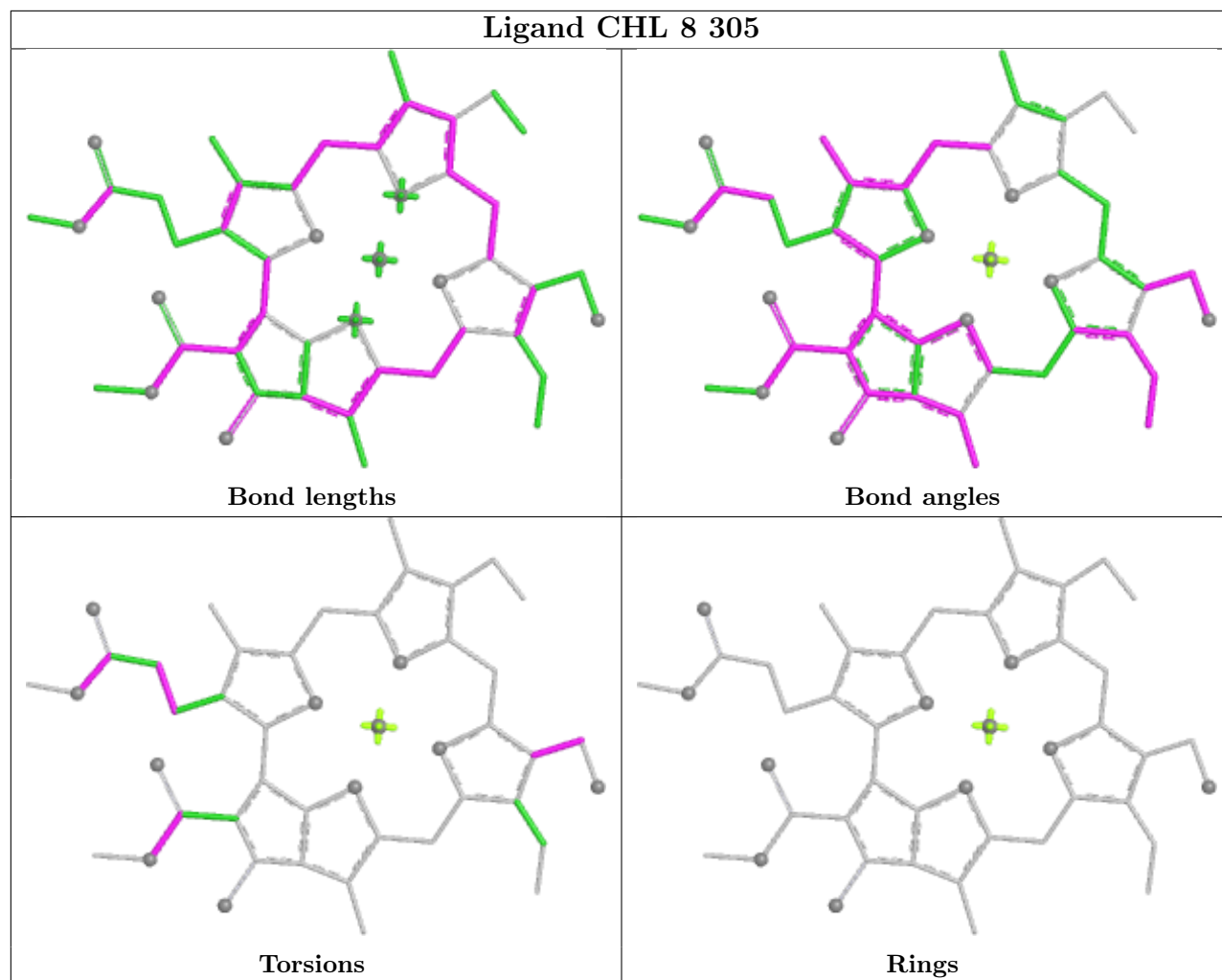






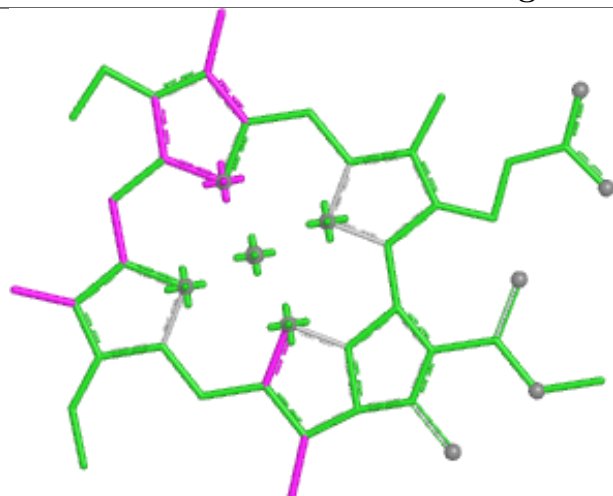


## Ligand CHL 8 305

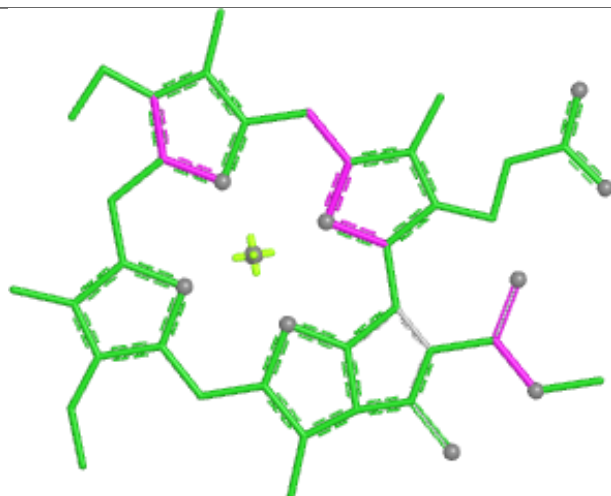




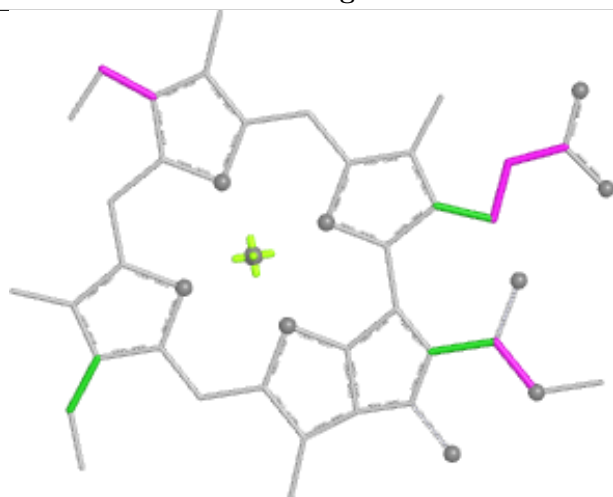
## Ligand CLA 7 303



Bond lengths



Bond angles



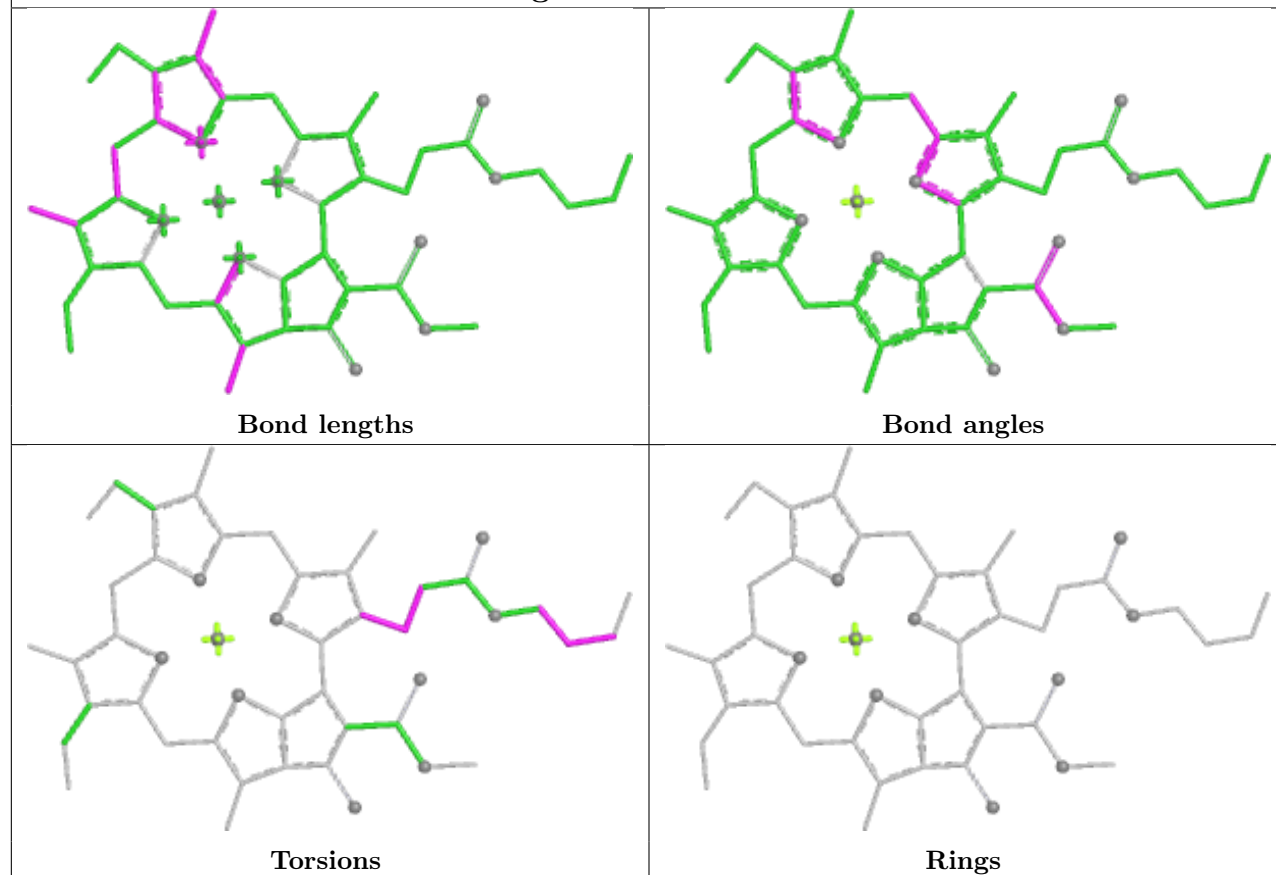
Torsions



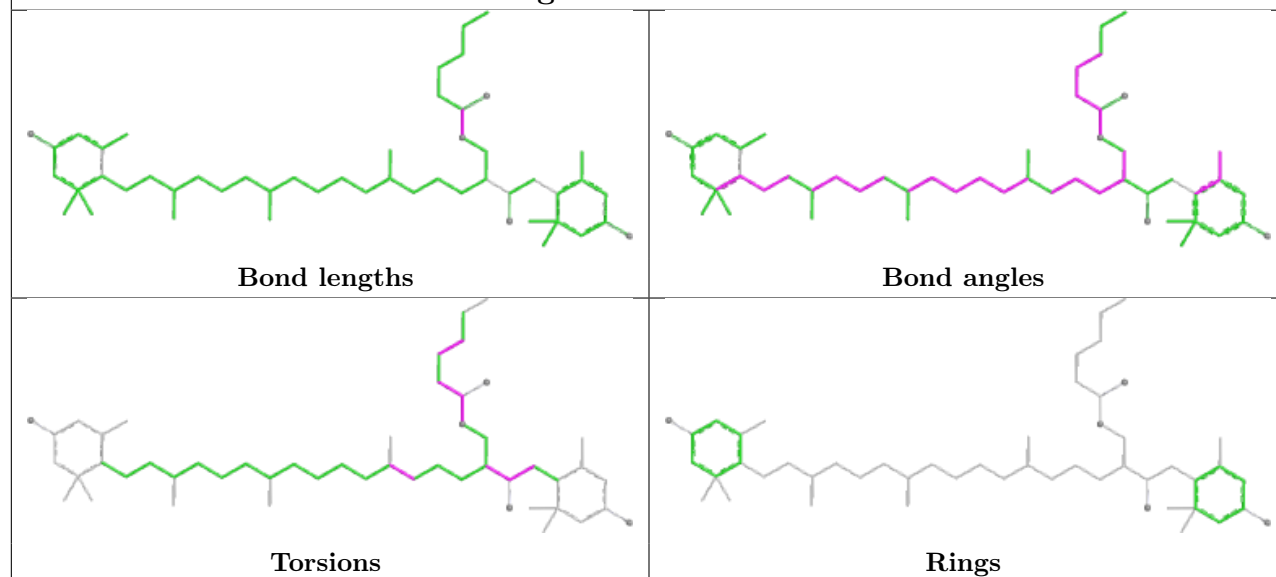
Rings



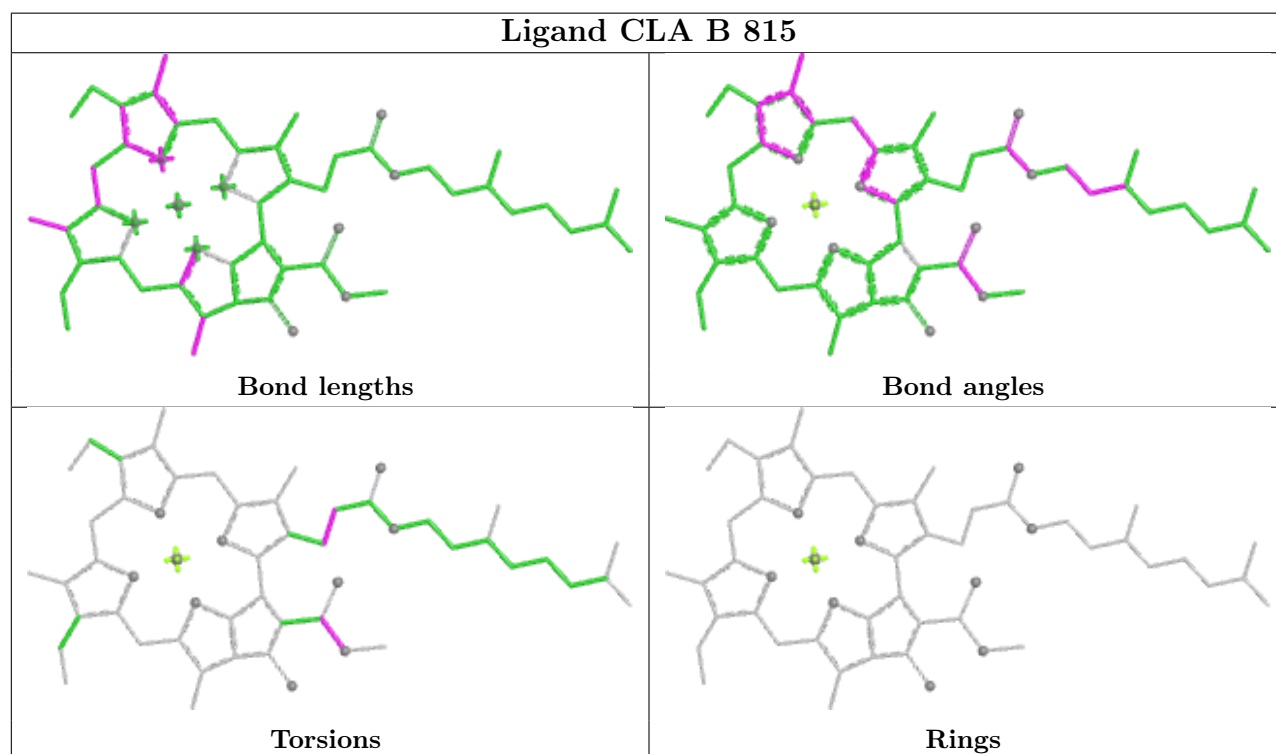
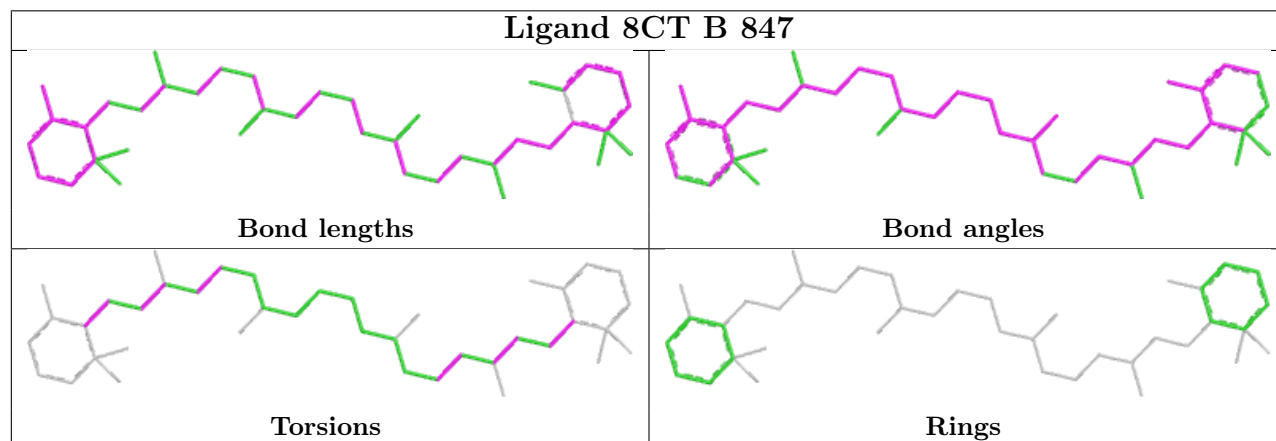
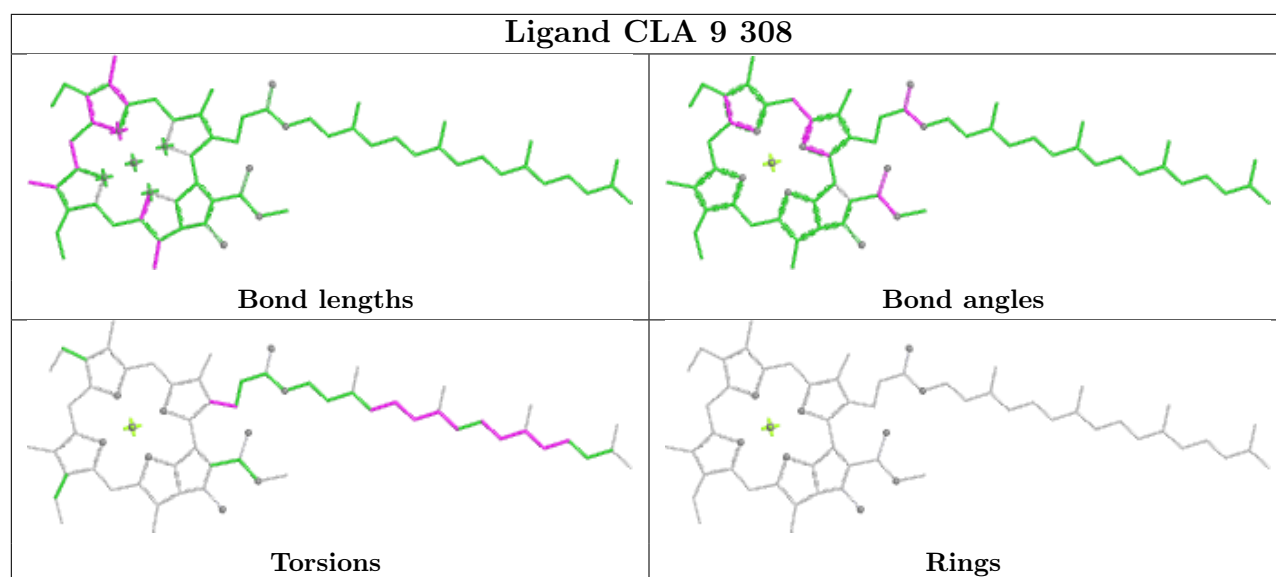
## Ligand CLA A 822



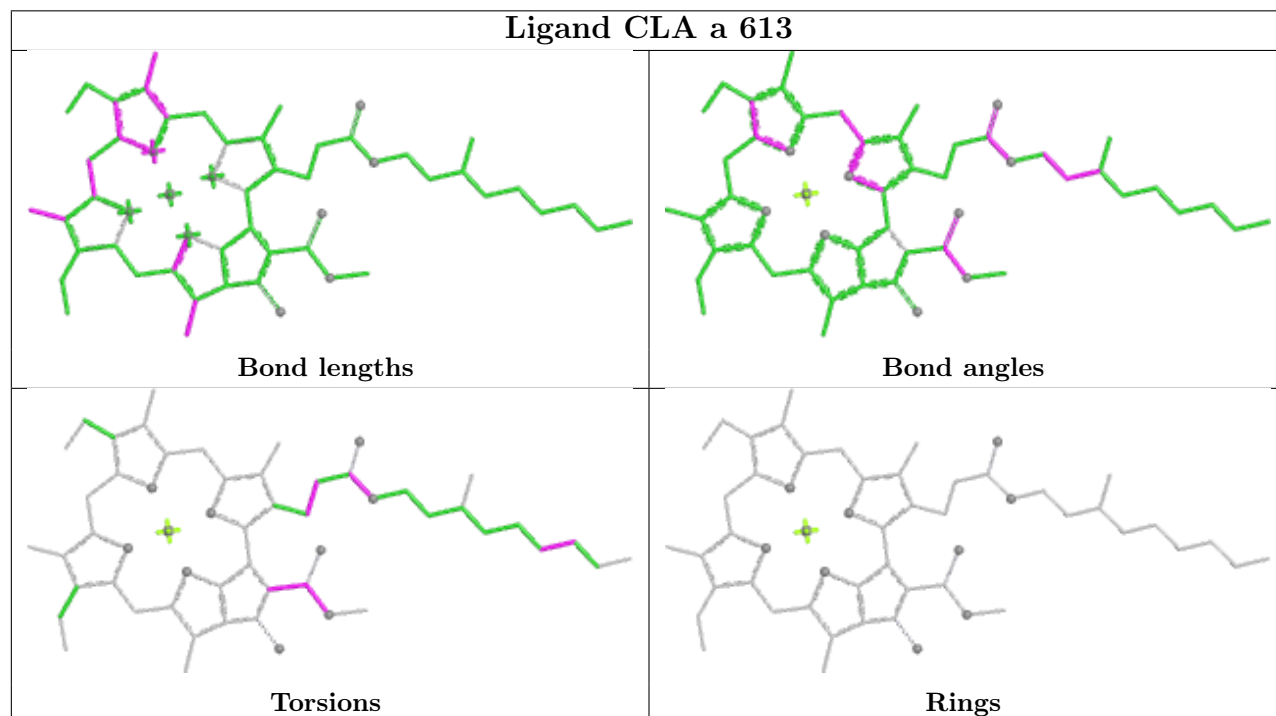
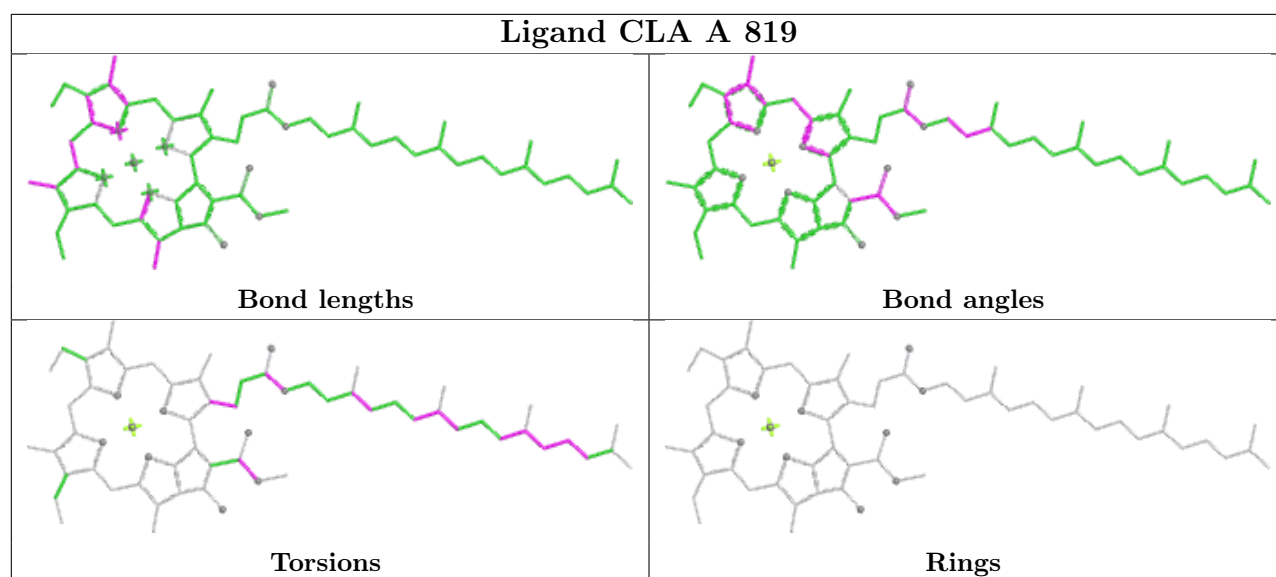
## Ligand 0UR 5 501





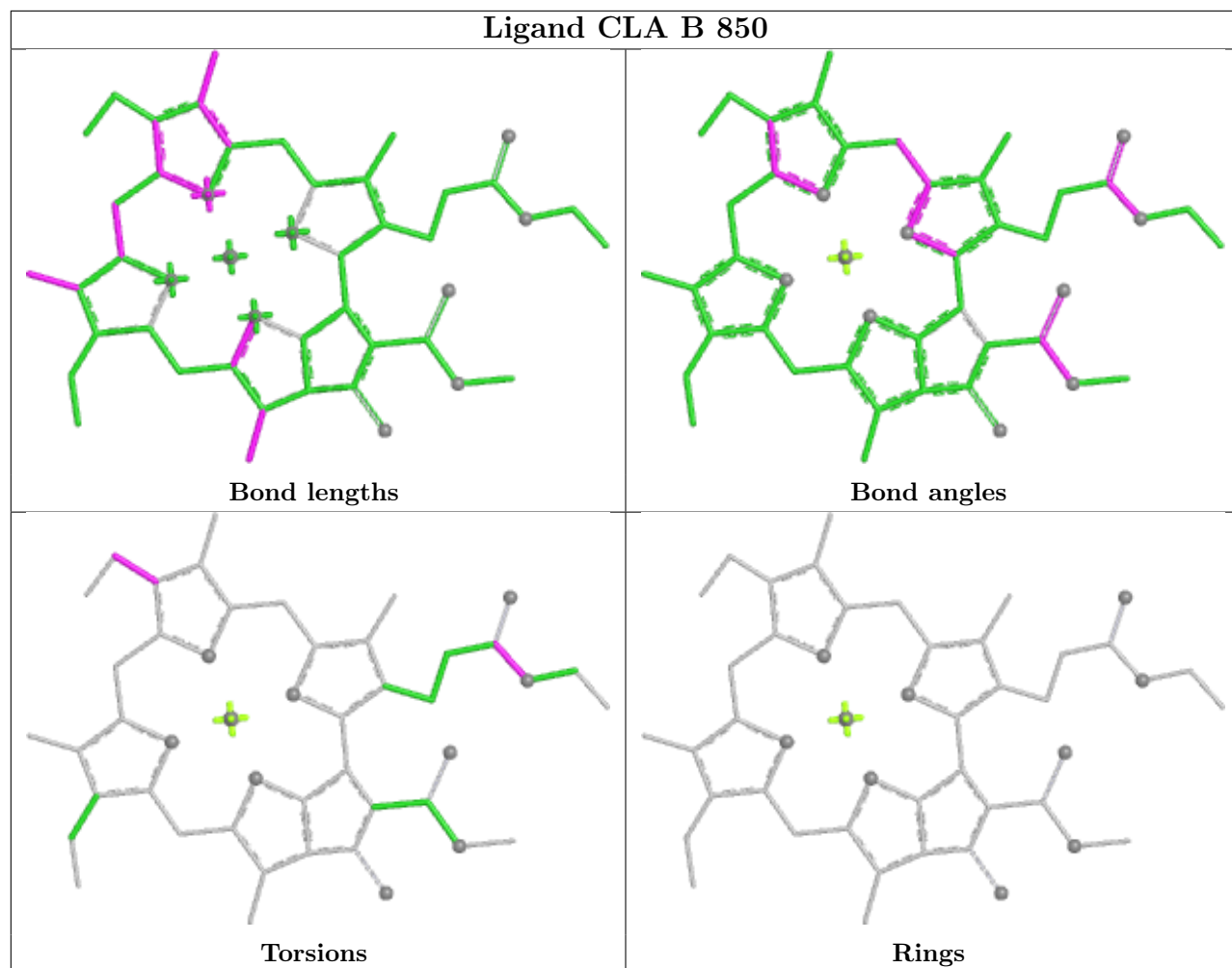






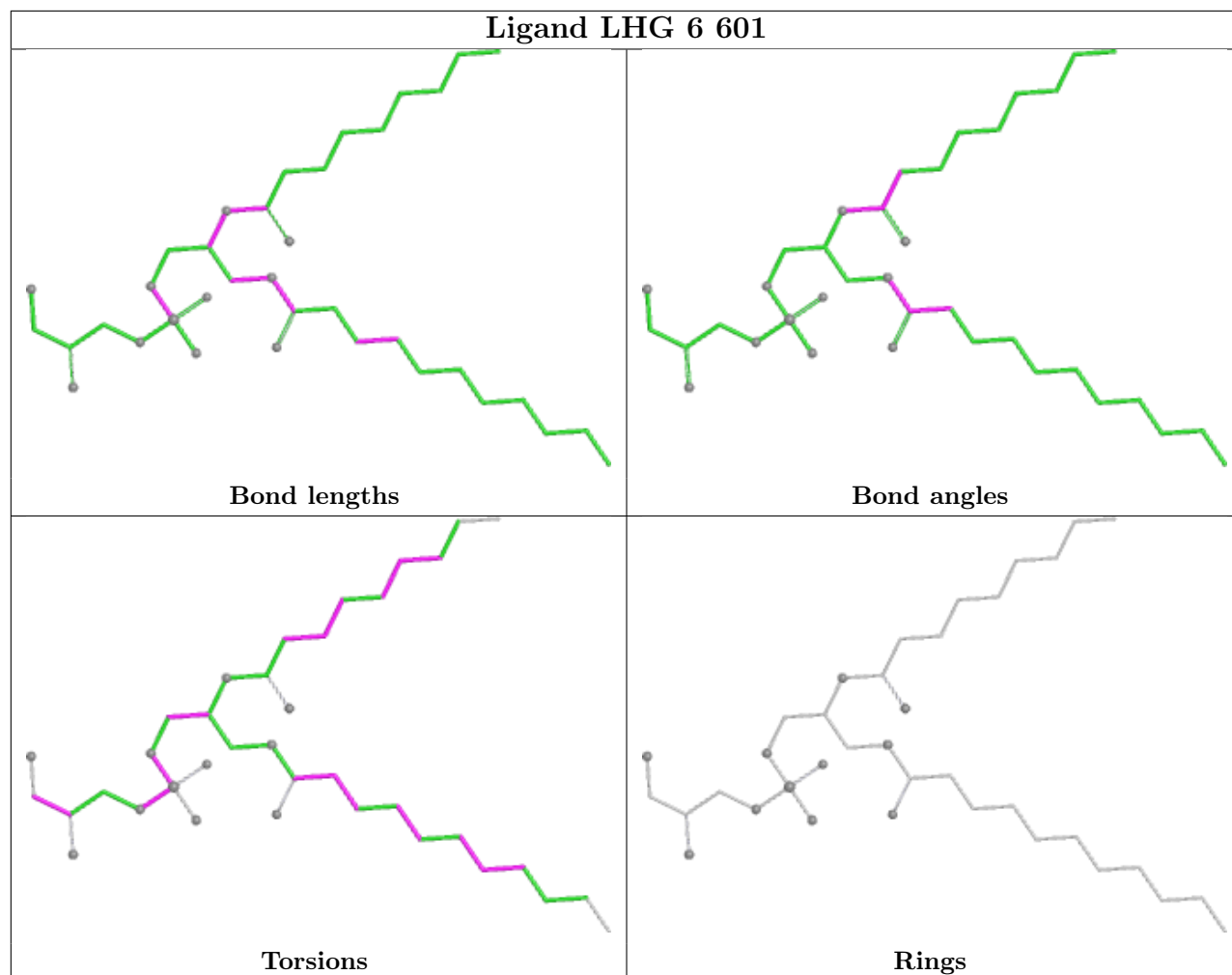


## Ligand CLA B 850

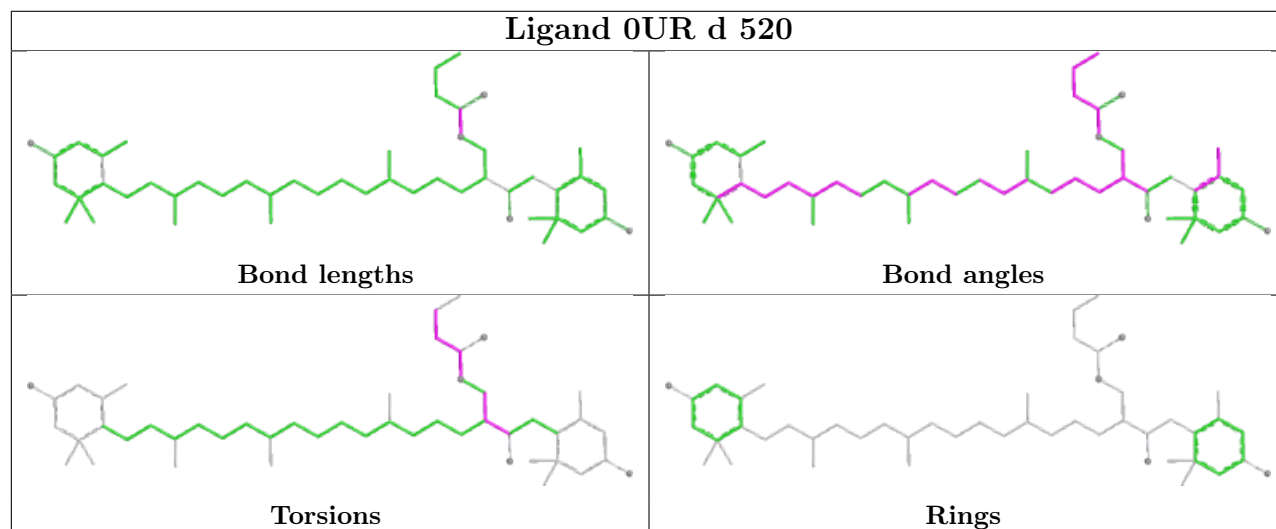




## Ligand LHG 6 601

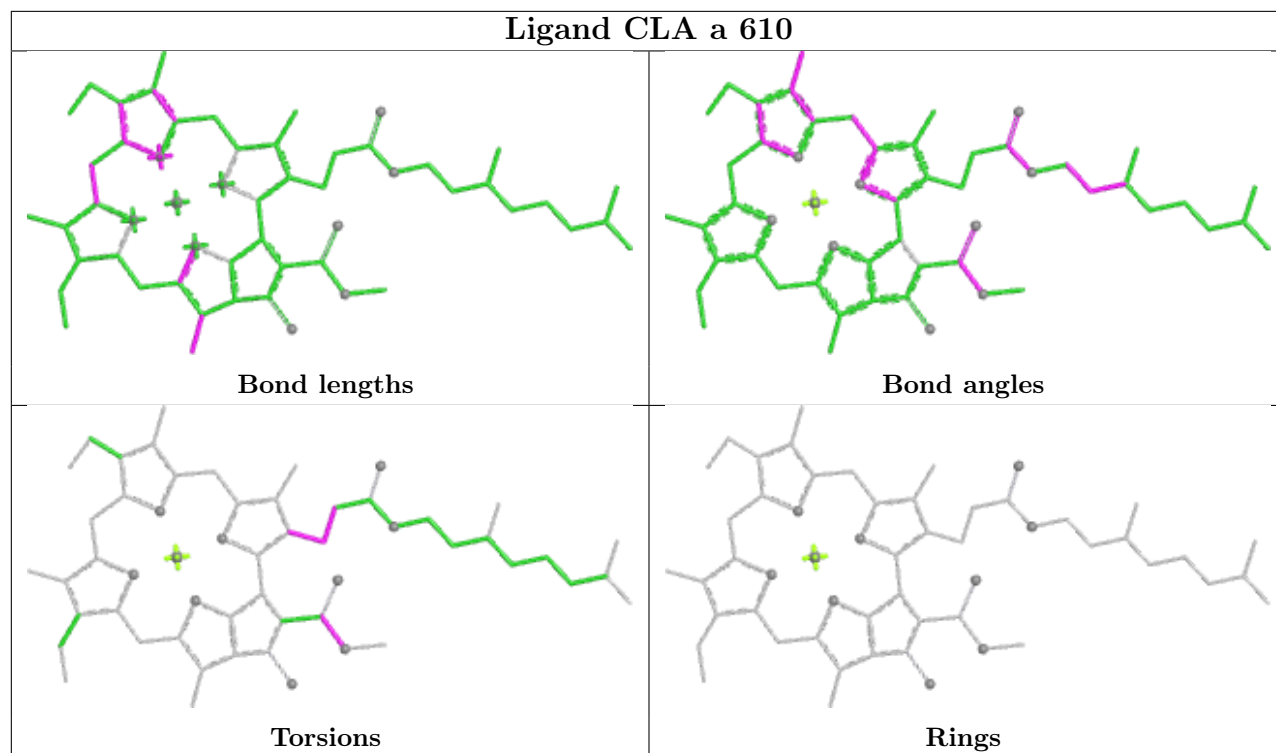


## Ligand OUR d 520

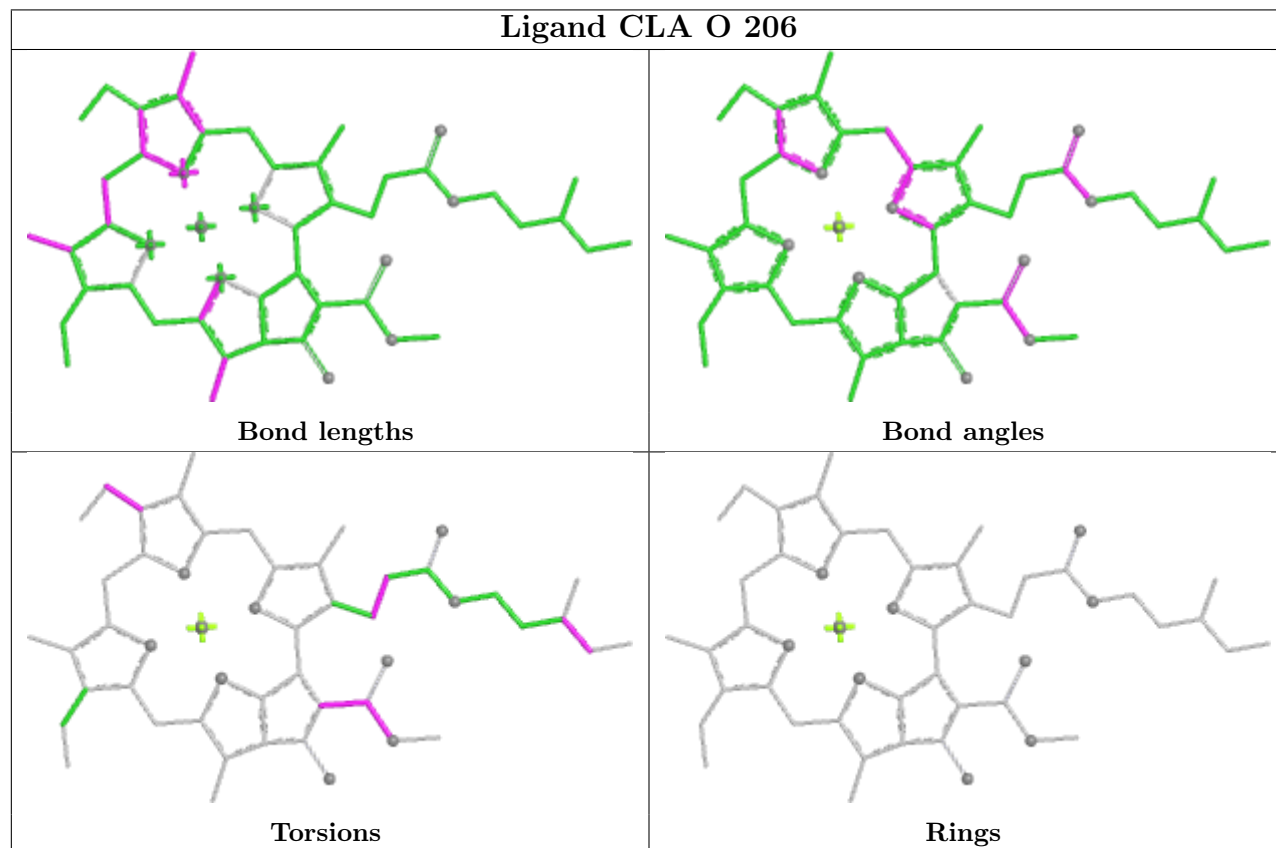




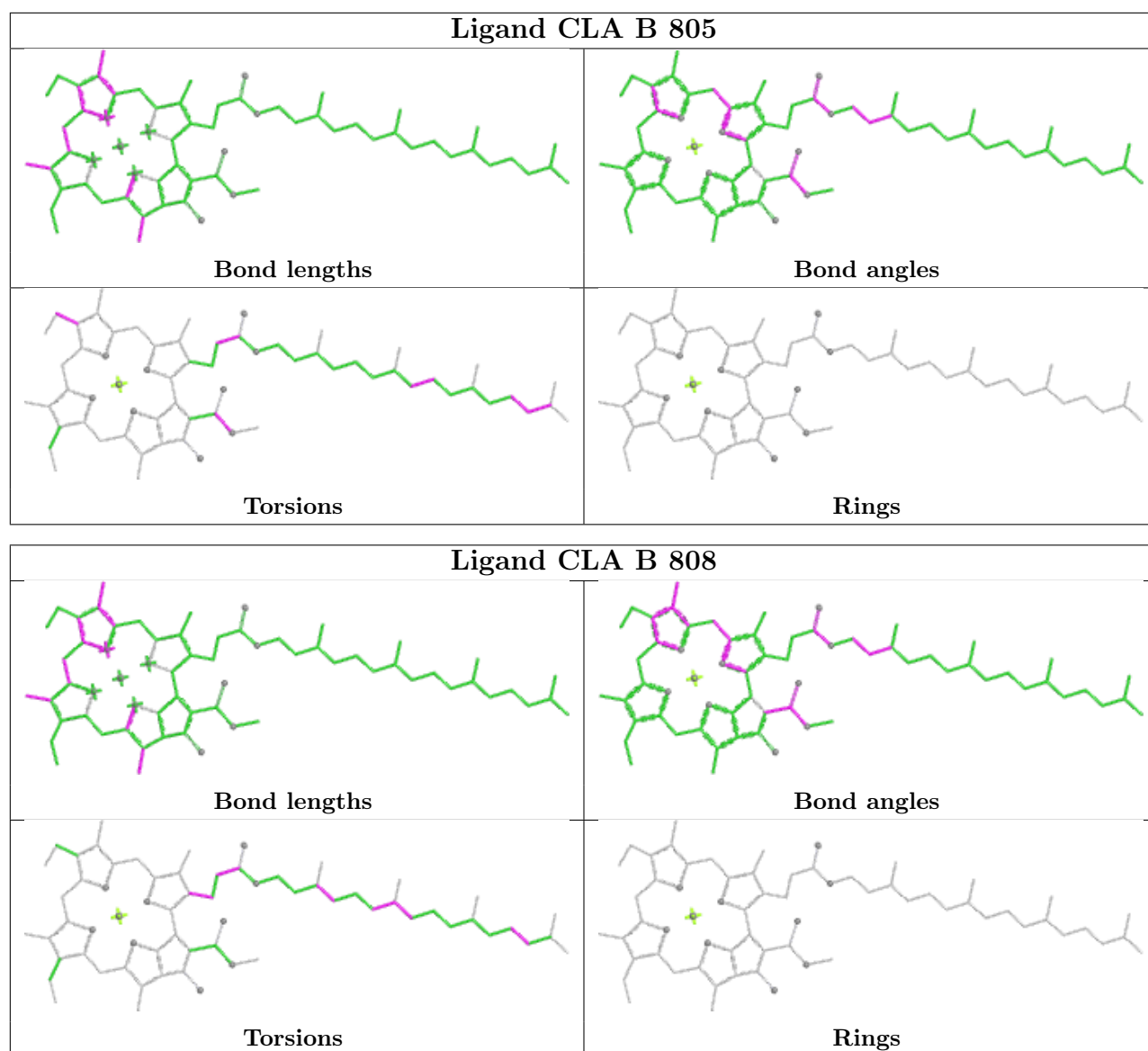
## Ligand CLA a 610



## Ligand CLA O 206

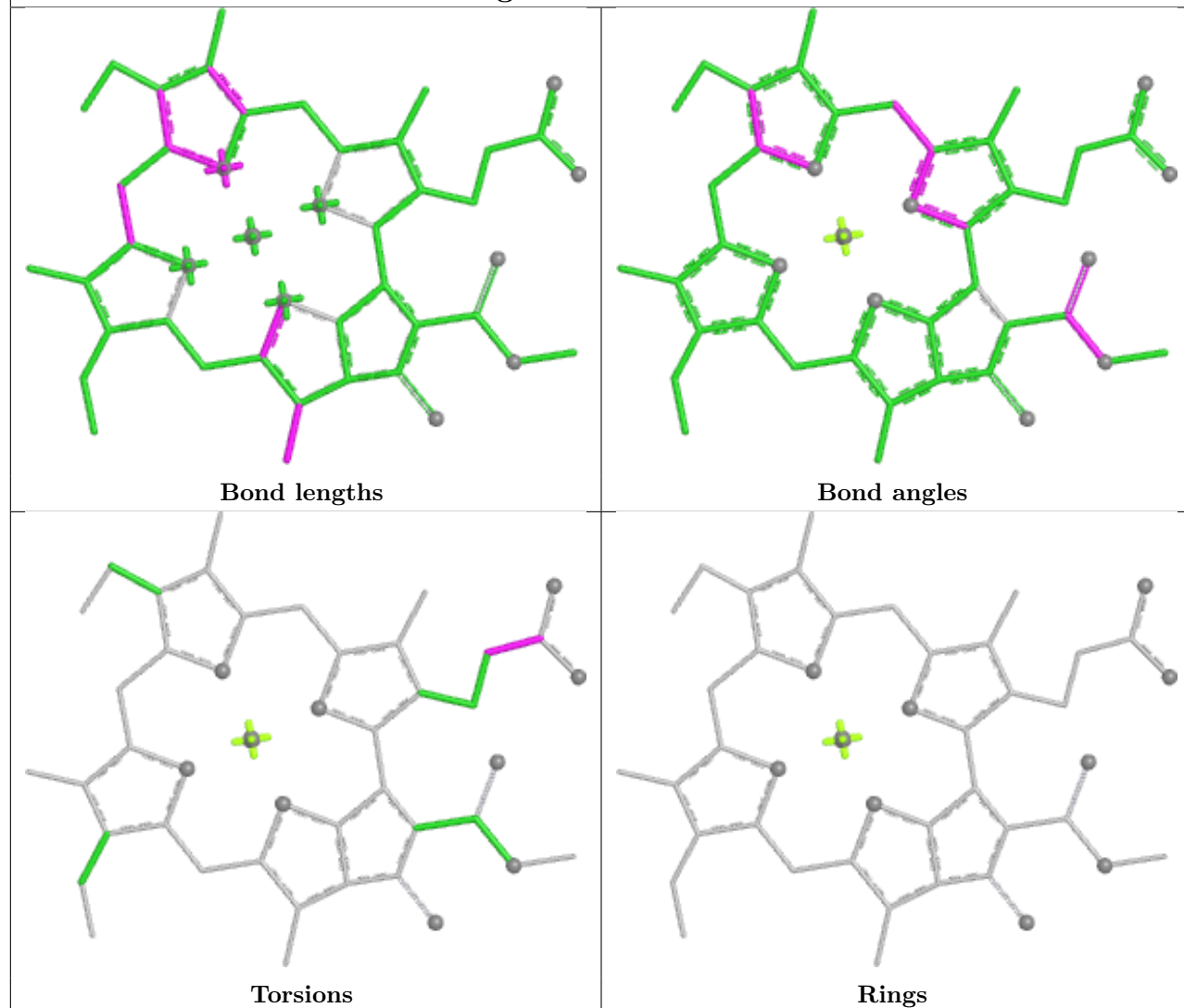




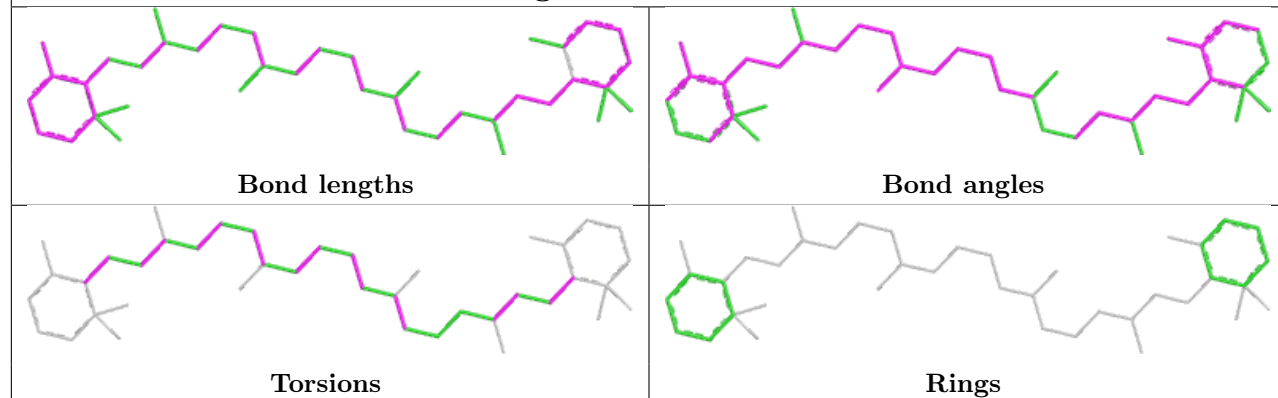




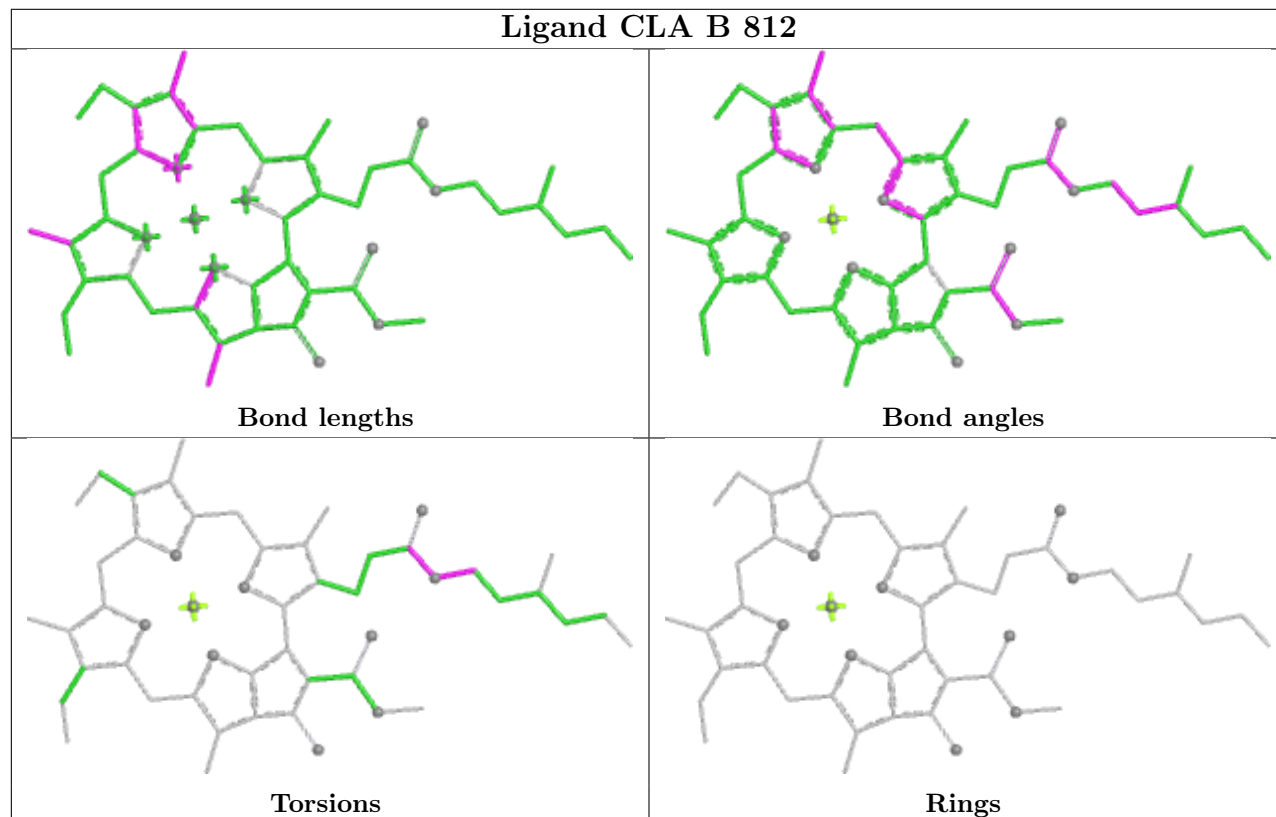
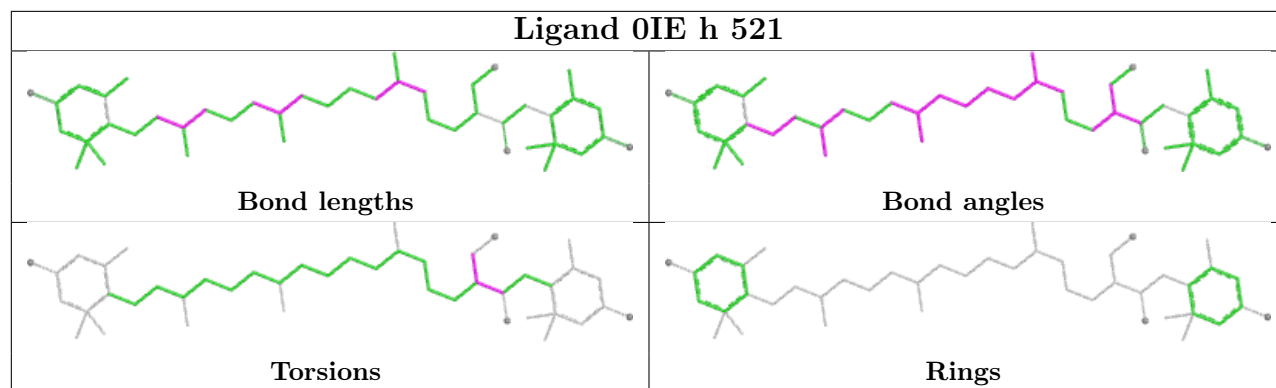
## Ligand CLA a 612



## Ligand 8CT G 104

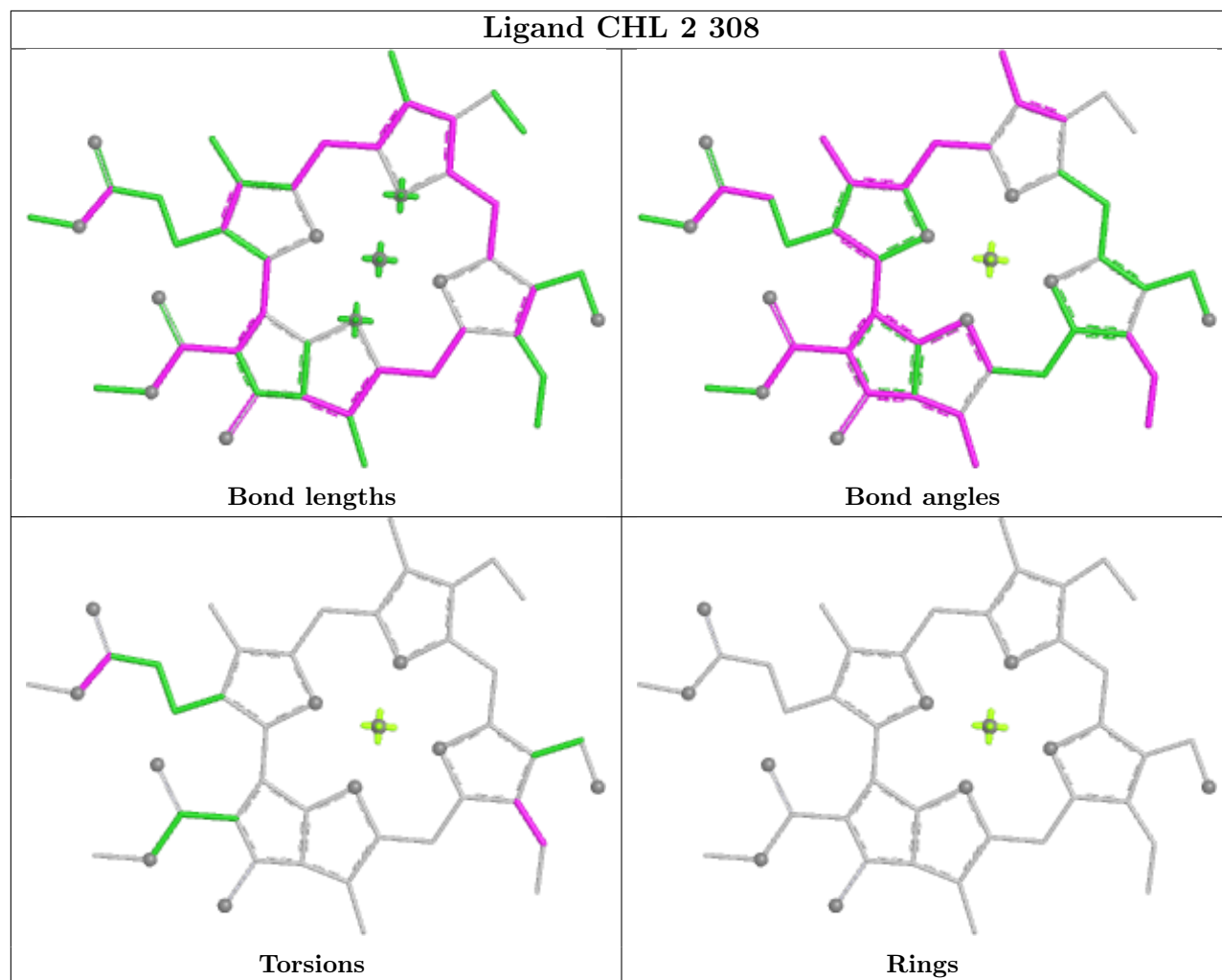






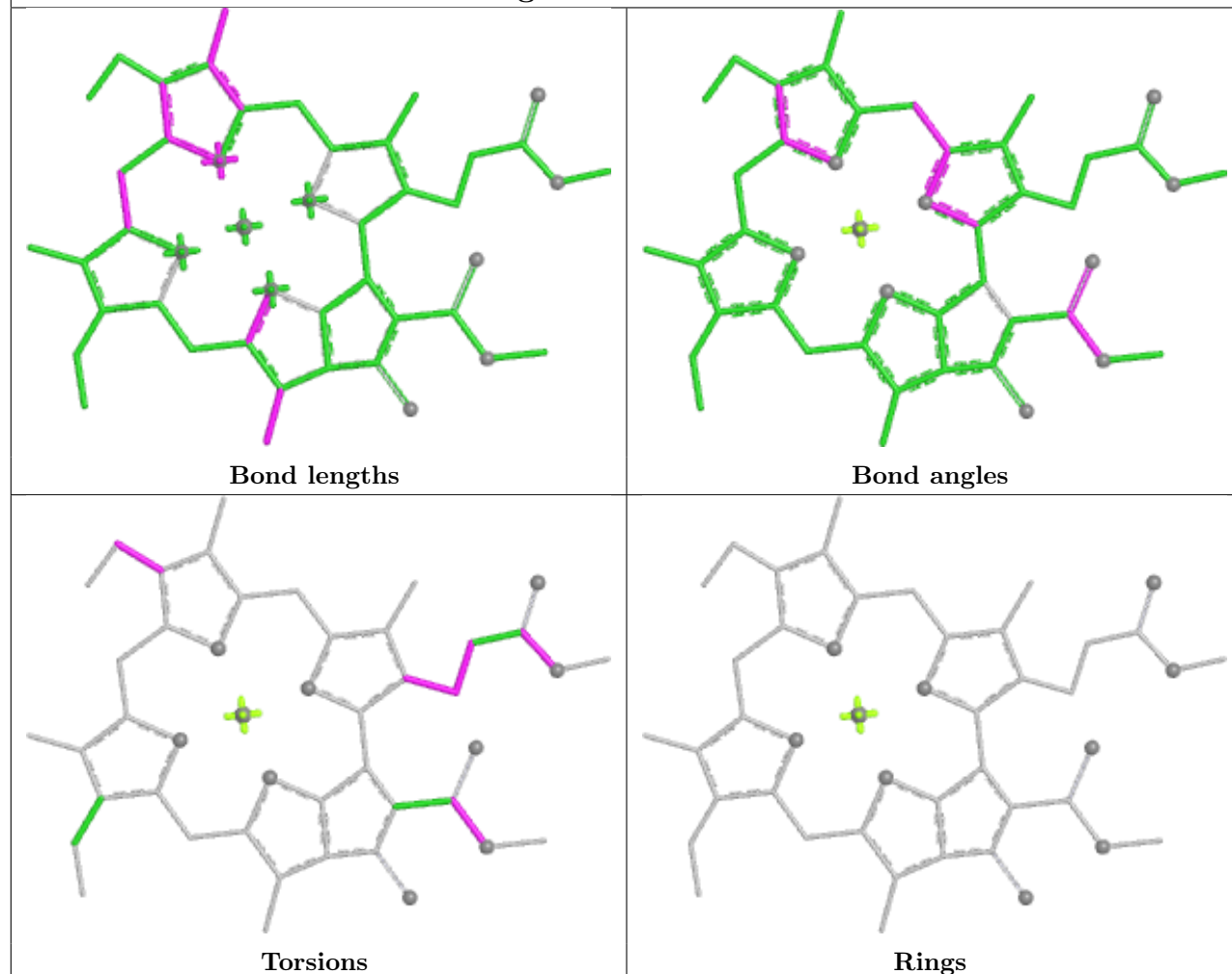


## Ligand CHL 2 308

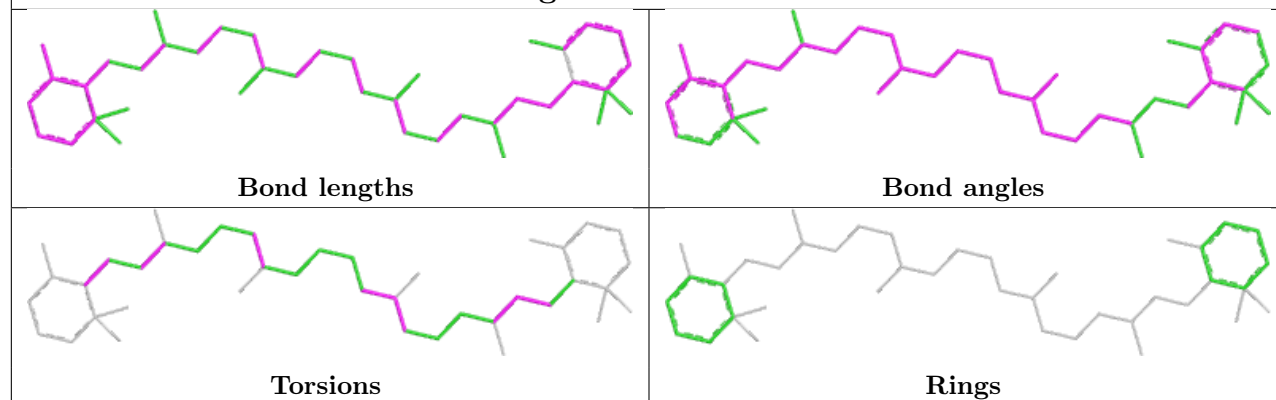




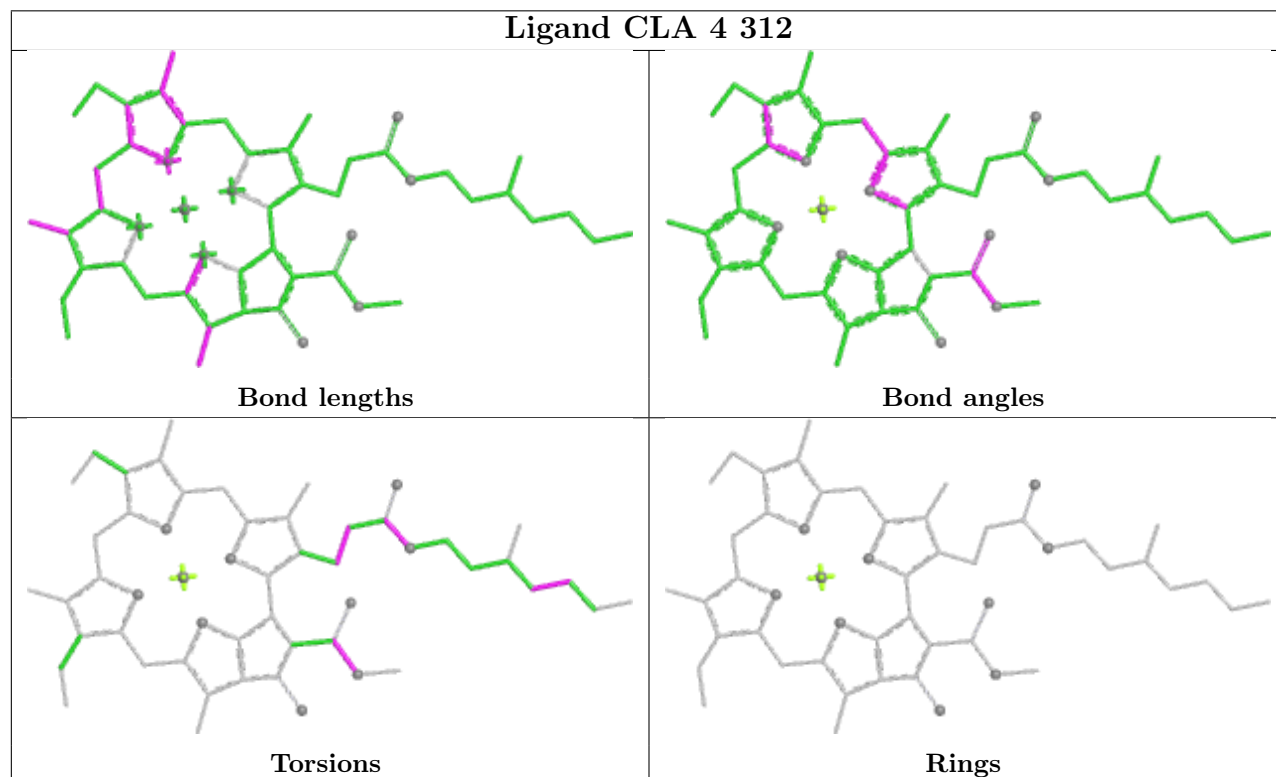
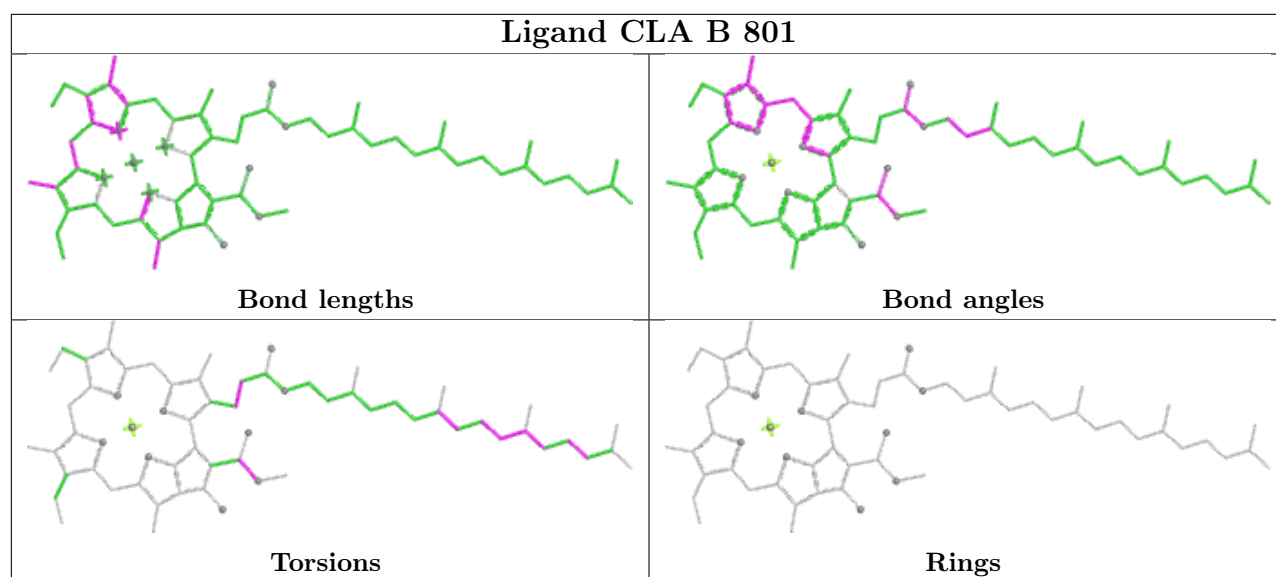
## Ligand CLA 5 314



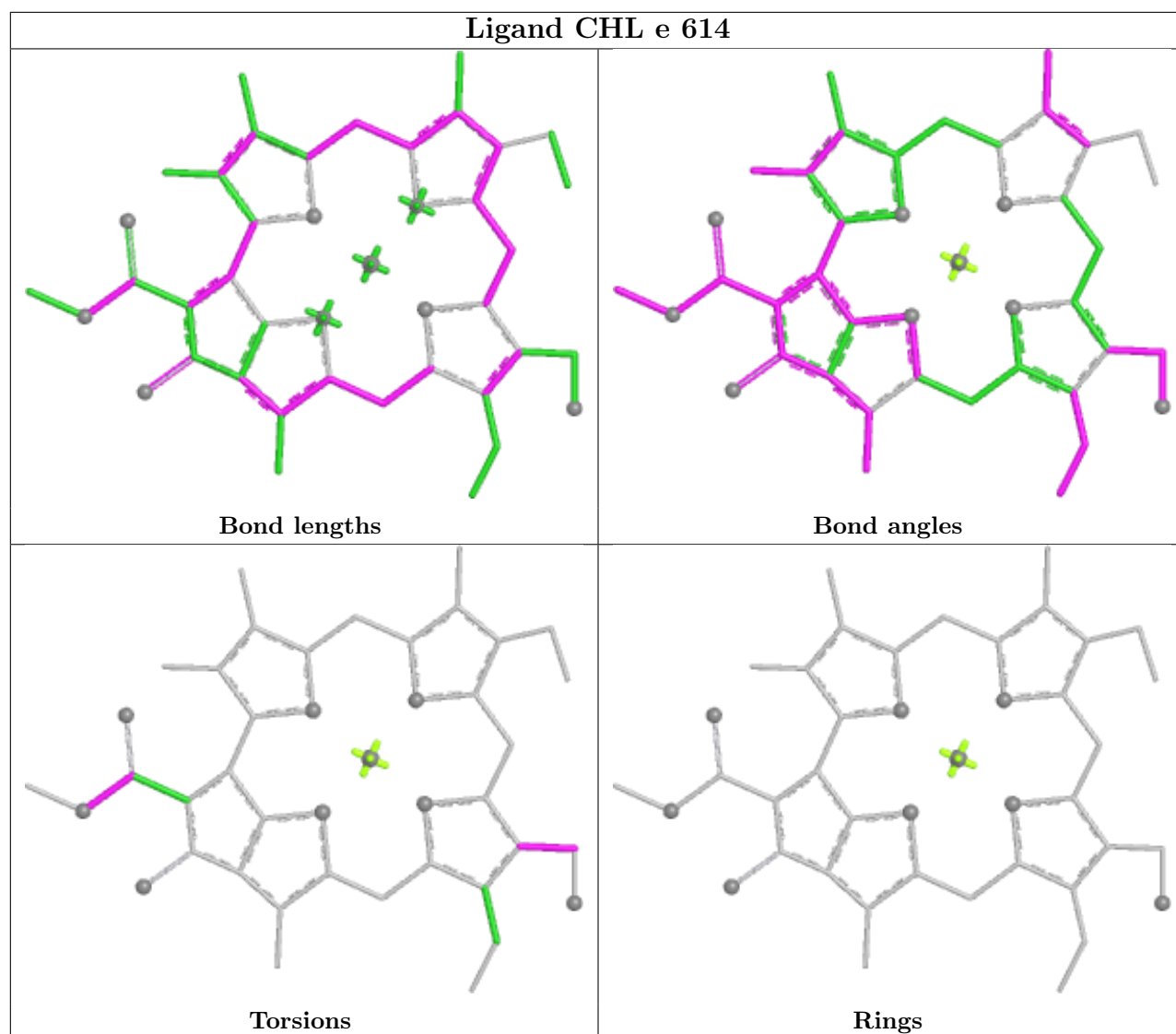
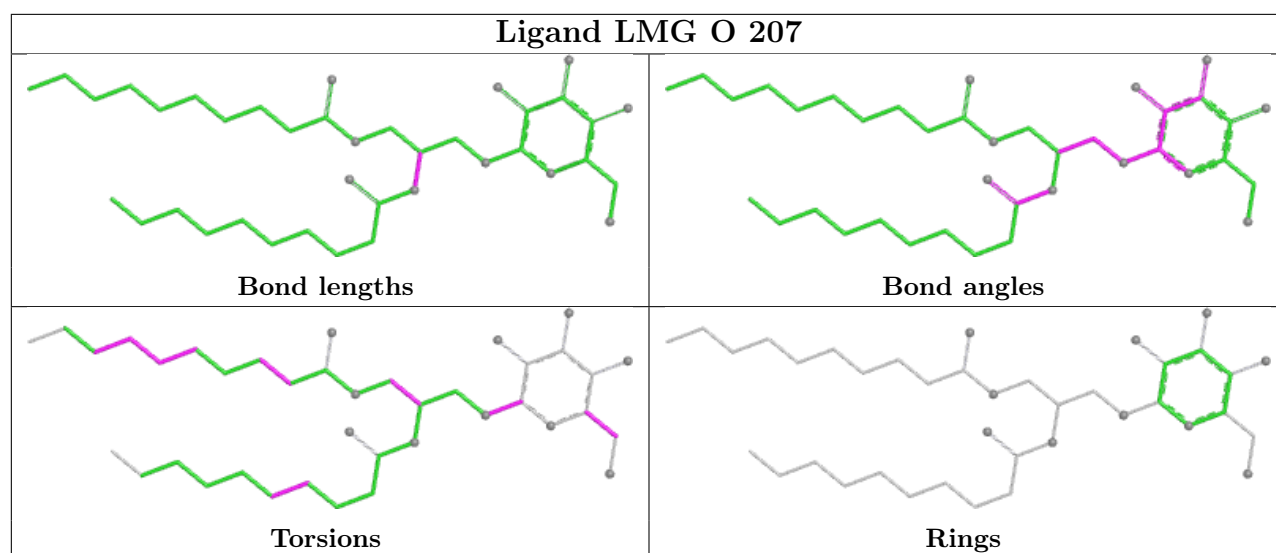
## Ligand 8CT 2 402



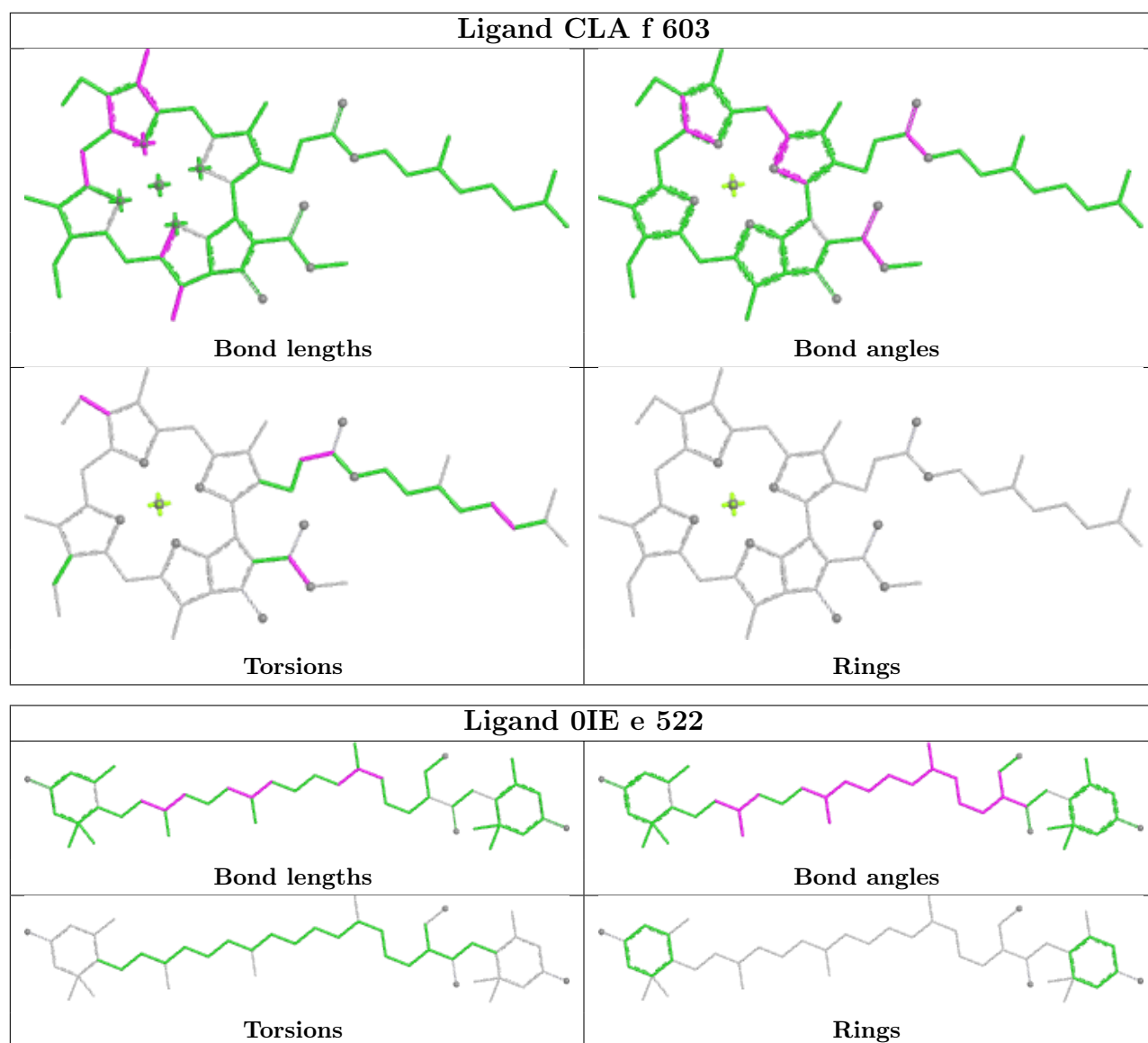






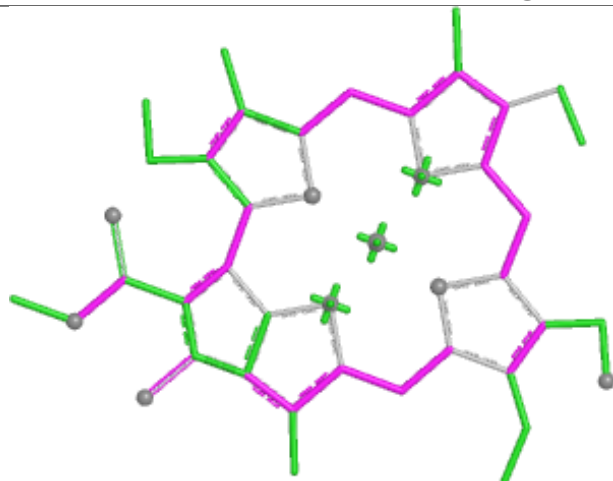




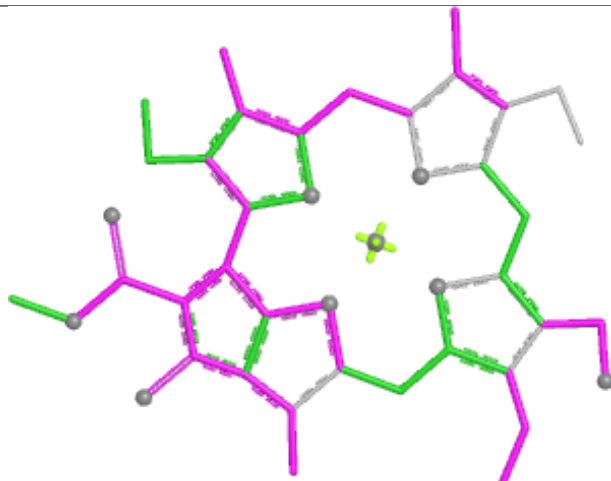




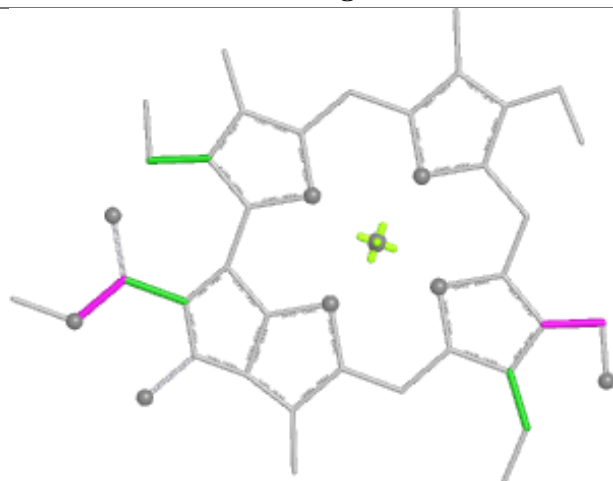
## Ligand CHL e 605



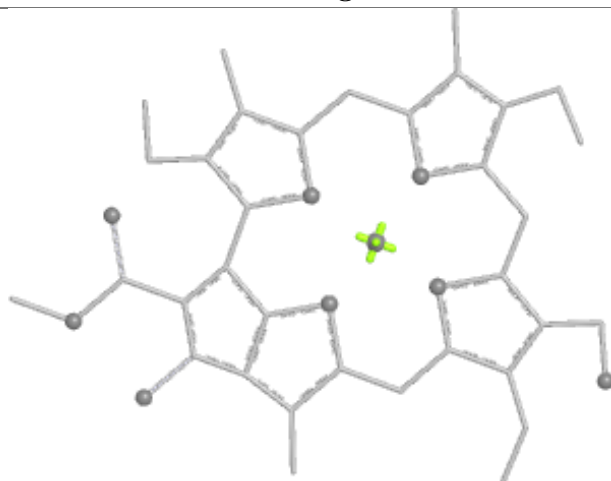
Bond lengths



Bond angles

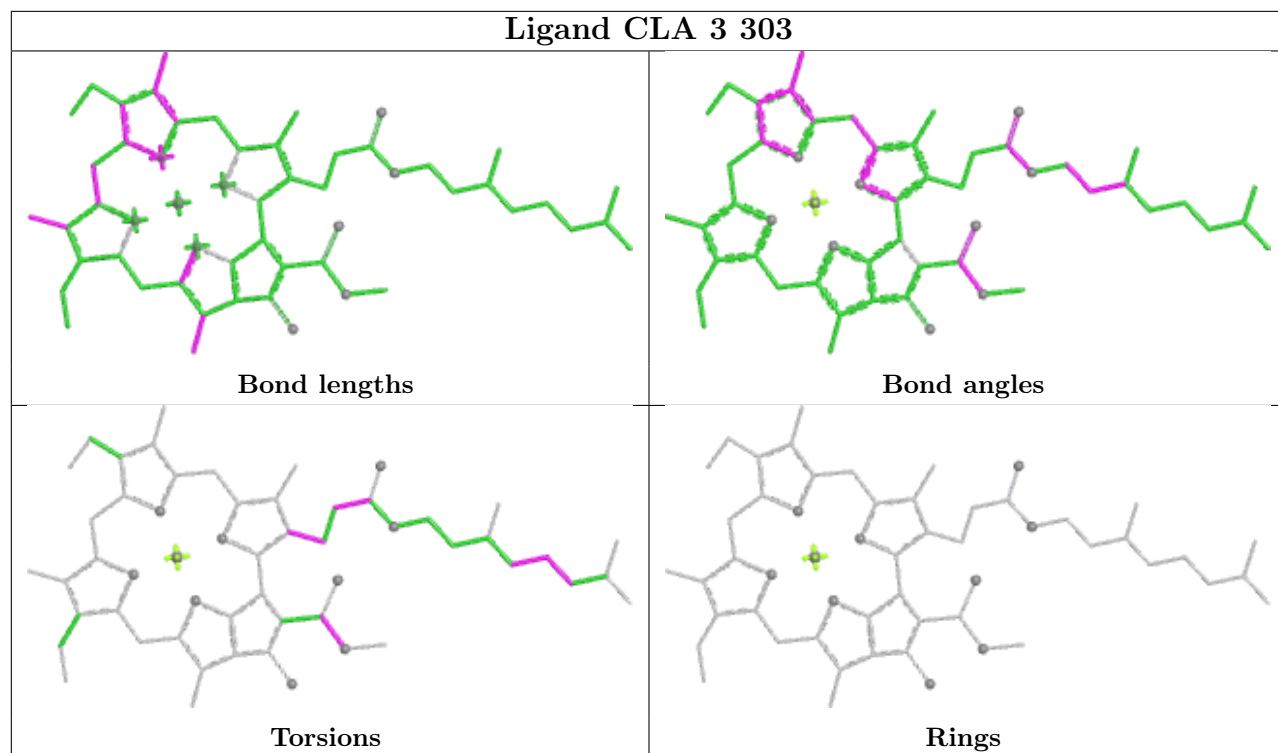
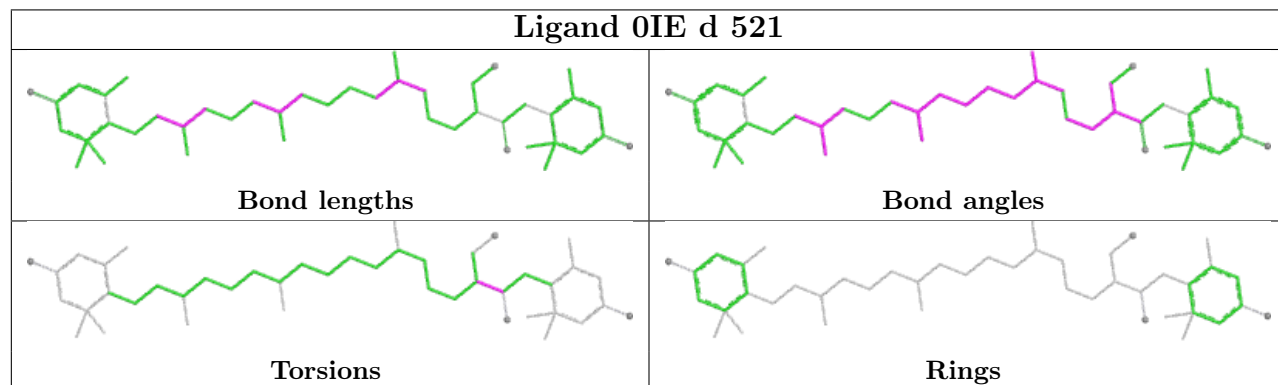


Torsions



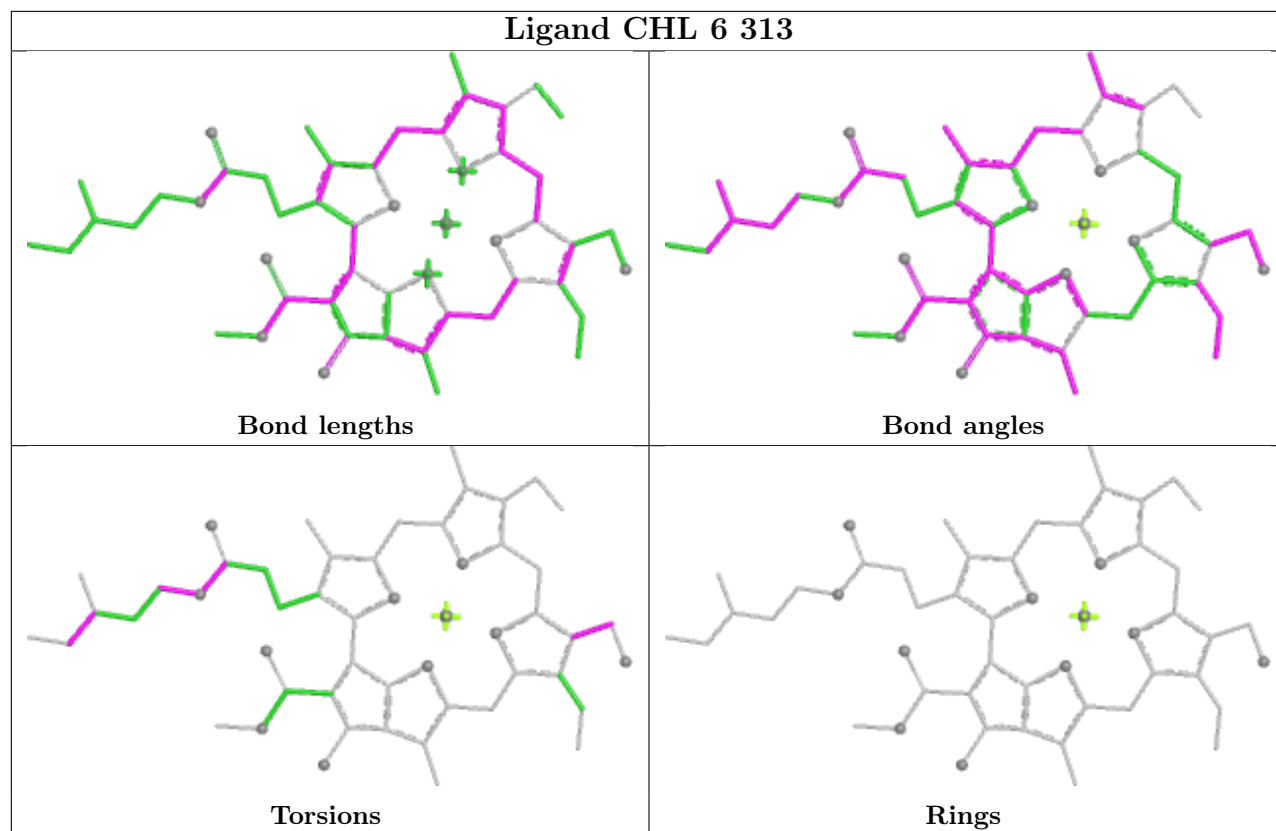
Rings



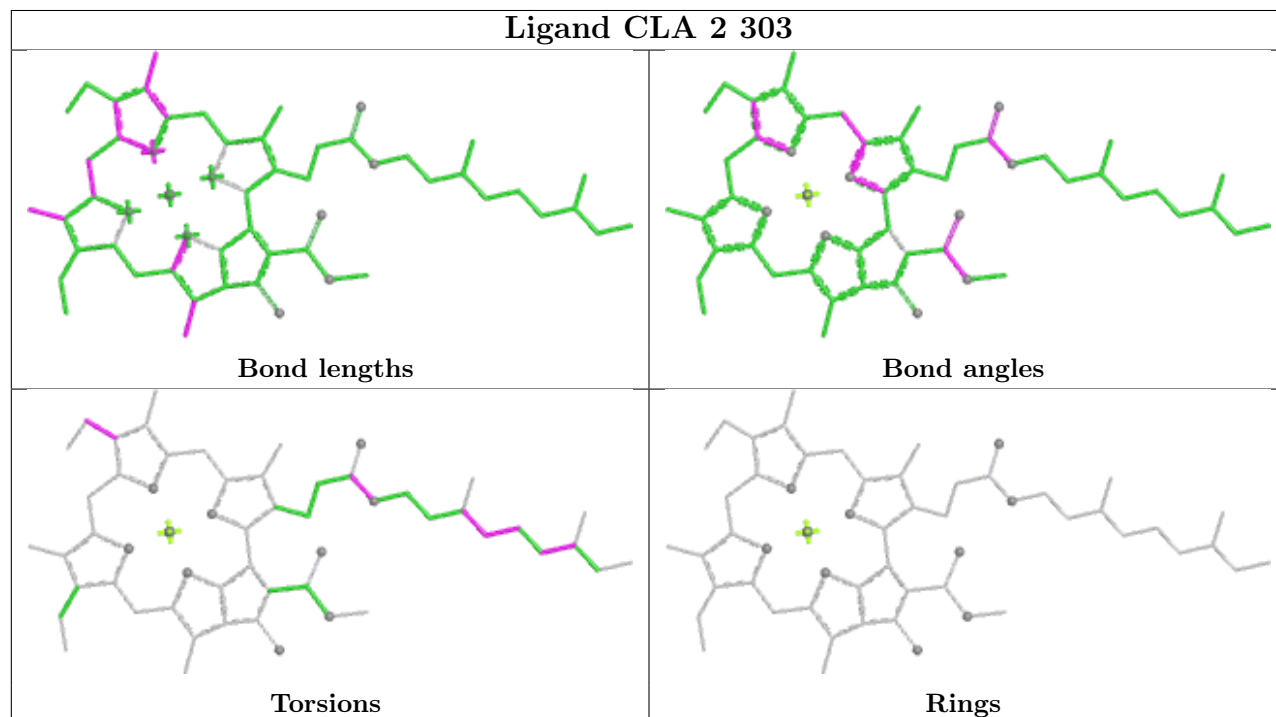
**Ligand CLA 3 303****Ligand OIE d 521**



## Ligand CHL 6 313

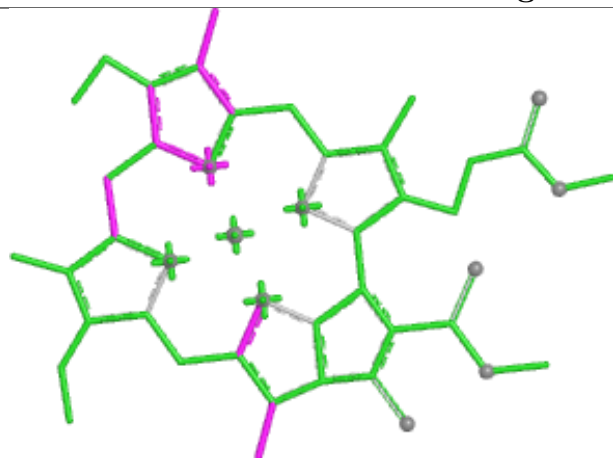


## Ligand CLA 2 303

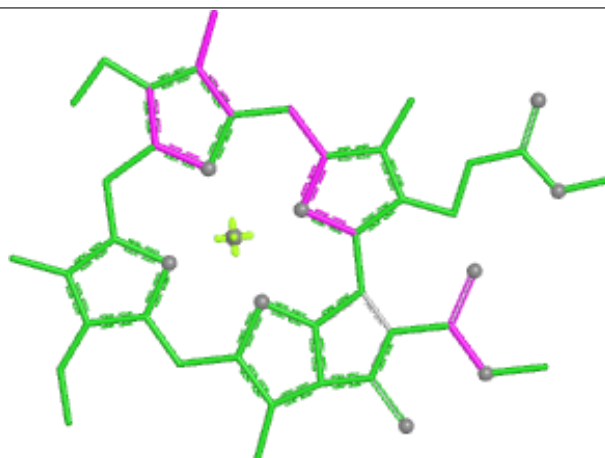




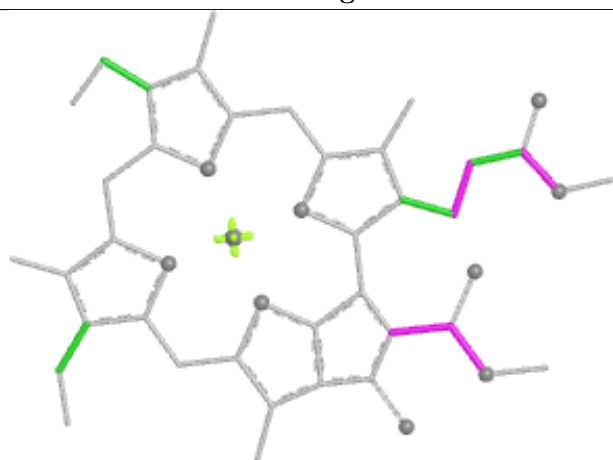
## Ligand CLA h 604



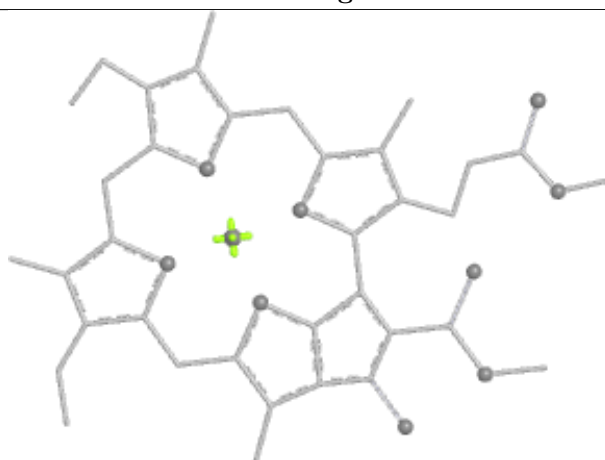
Bond lengths



Bond angles

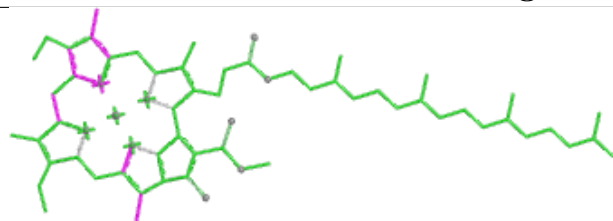


Torsions

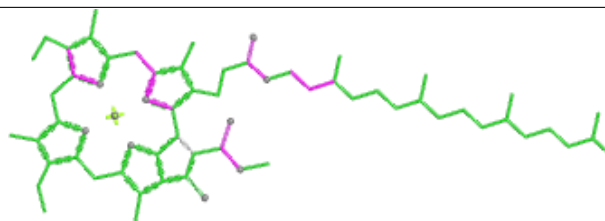


Rings

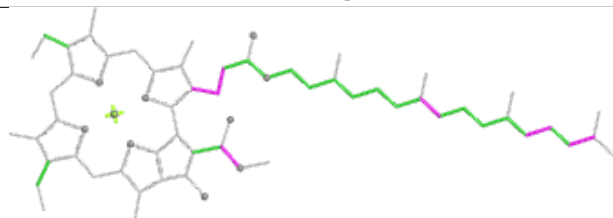
## Ligand CLA 8 304



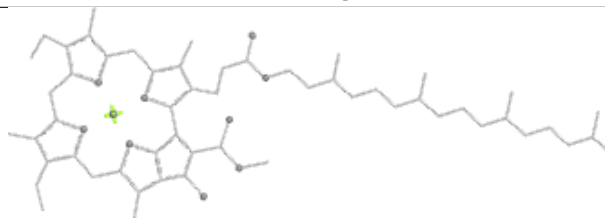
Bond lengths



Bond angles

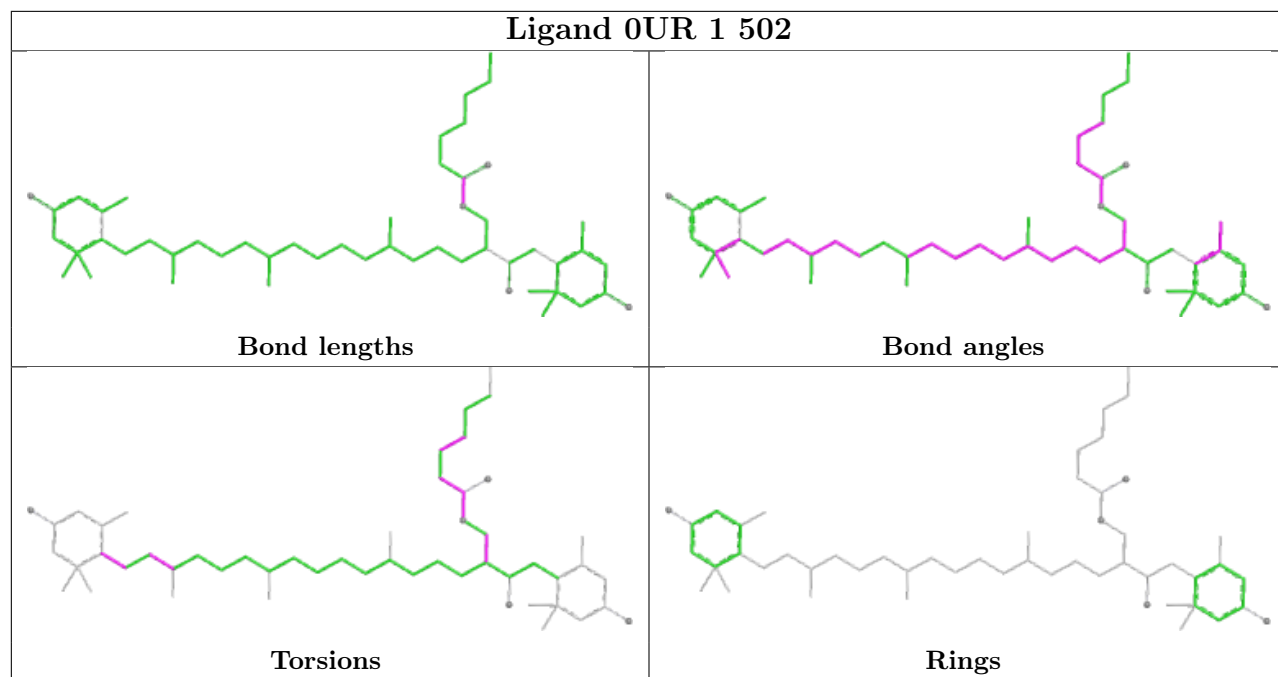


Torsions



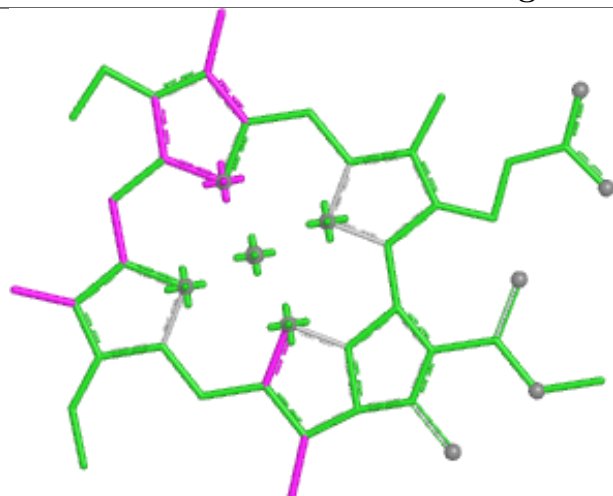
Rings



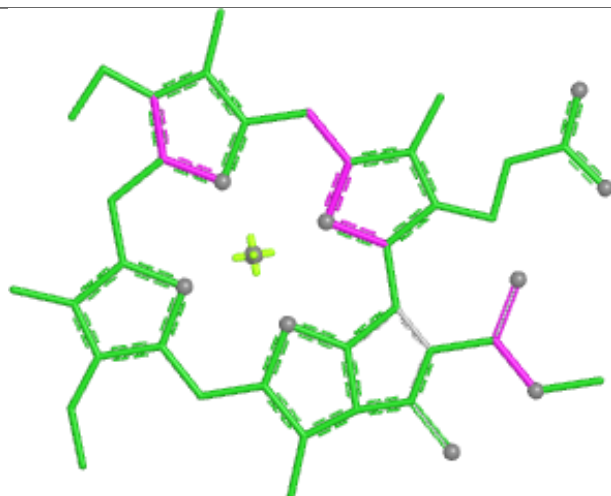




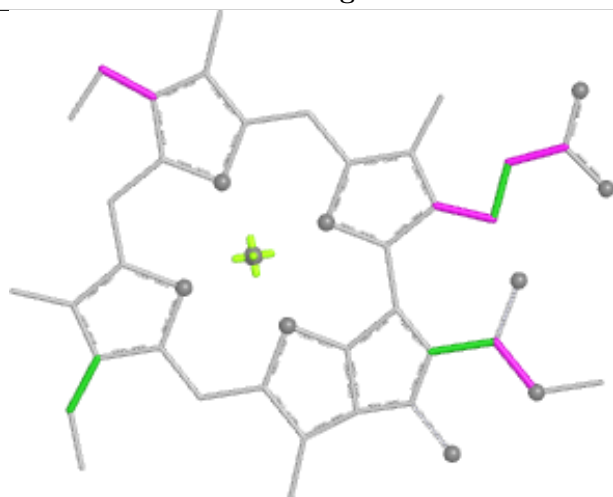
## Ligand CLA 3 313



Bond lengths



Bond angles

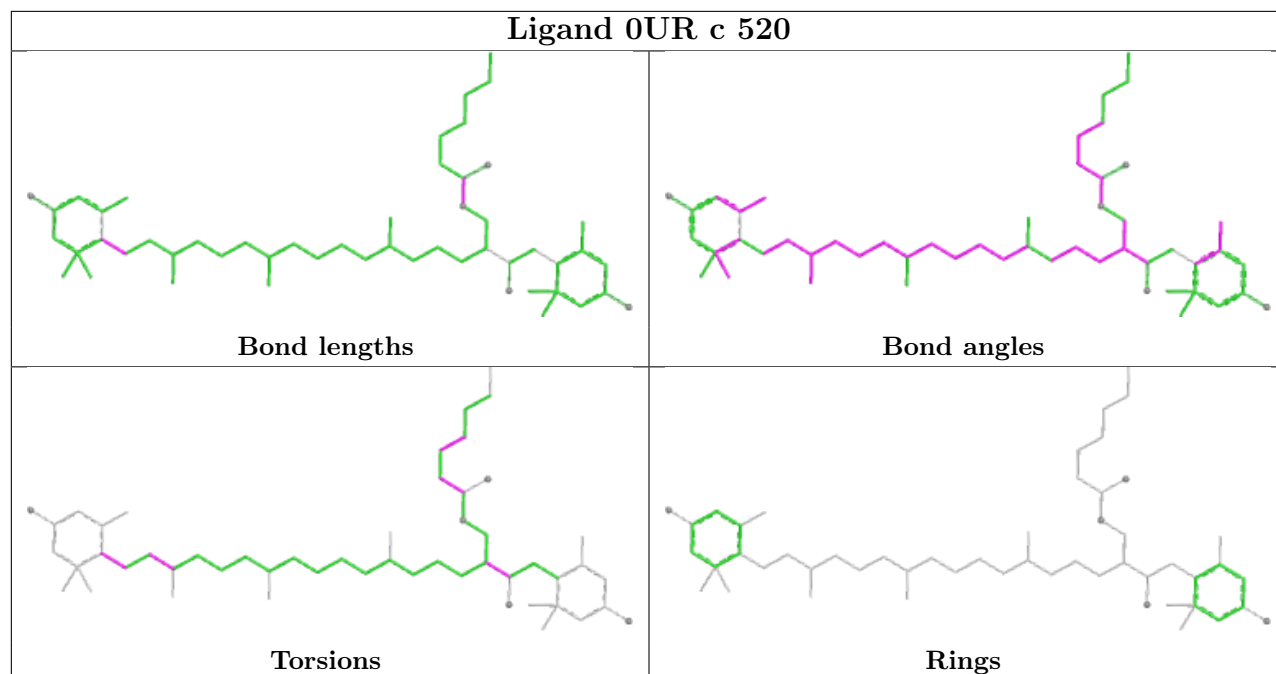
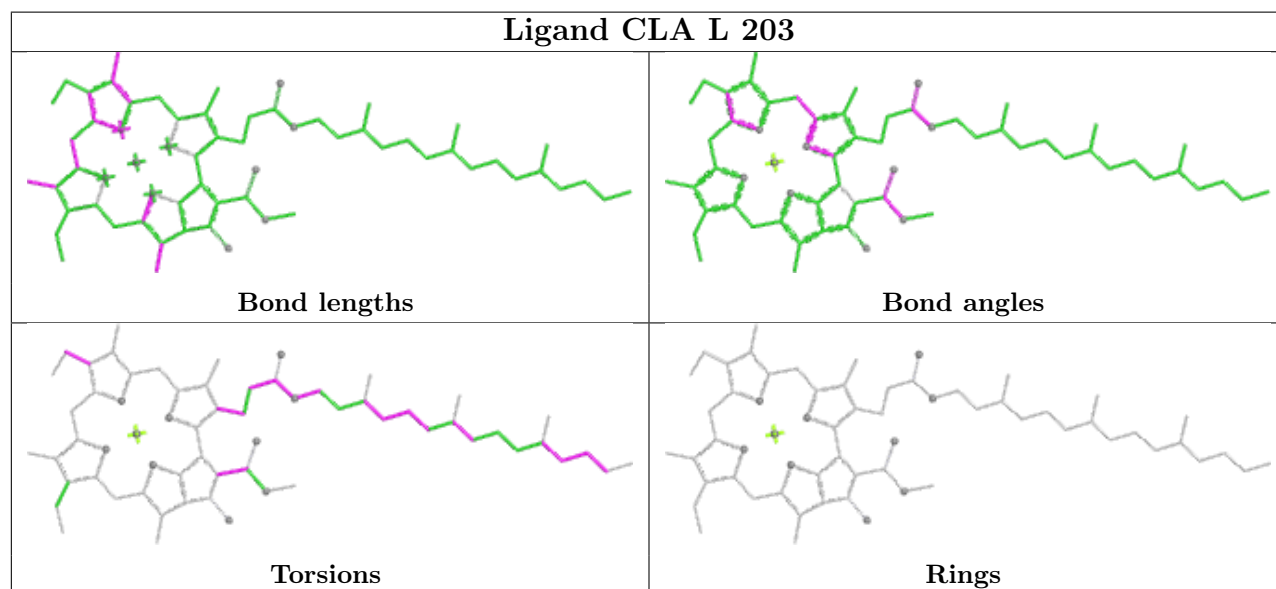


Torsions

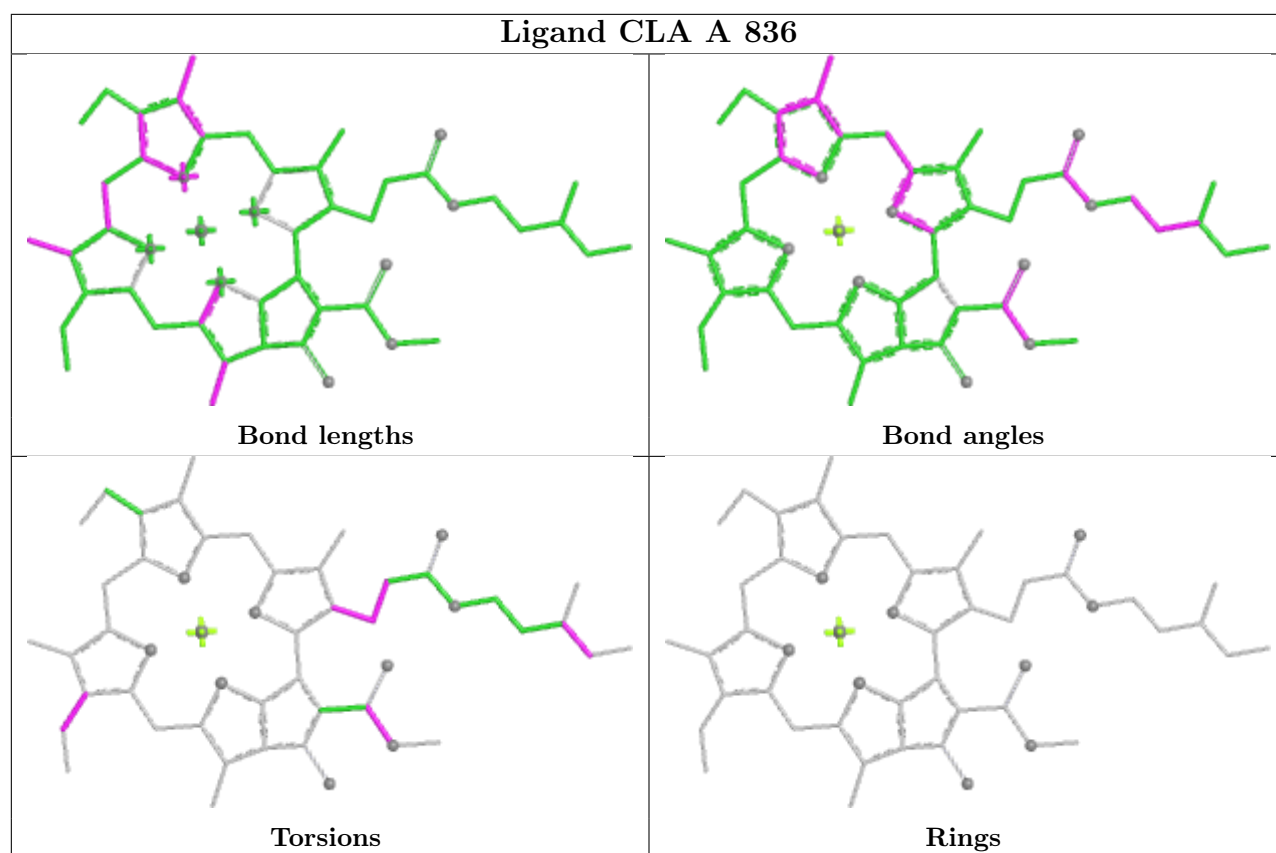


Rings



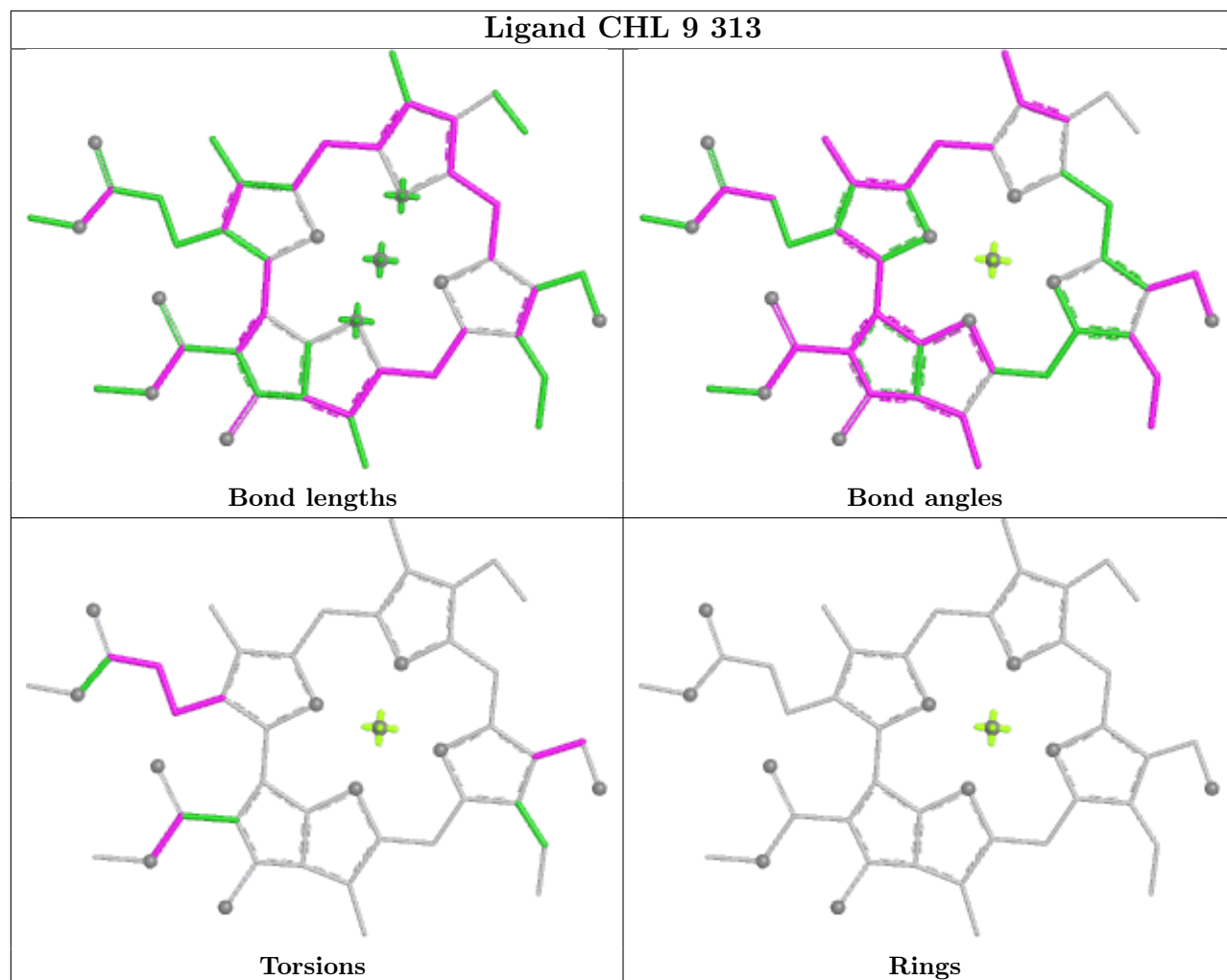
**Ligand OUR c 520****Ligand CLA L 203**



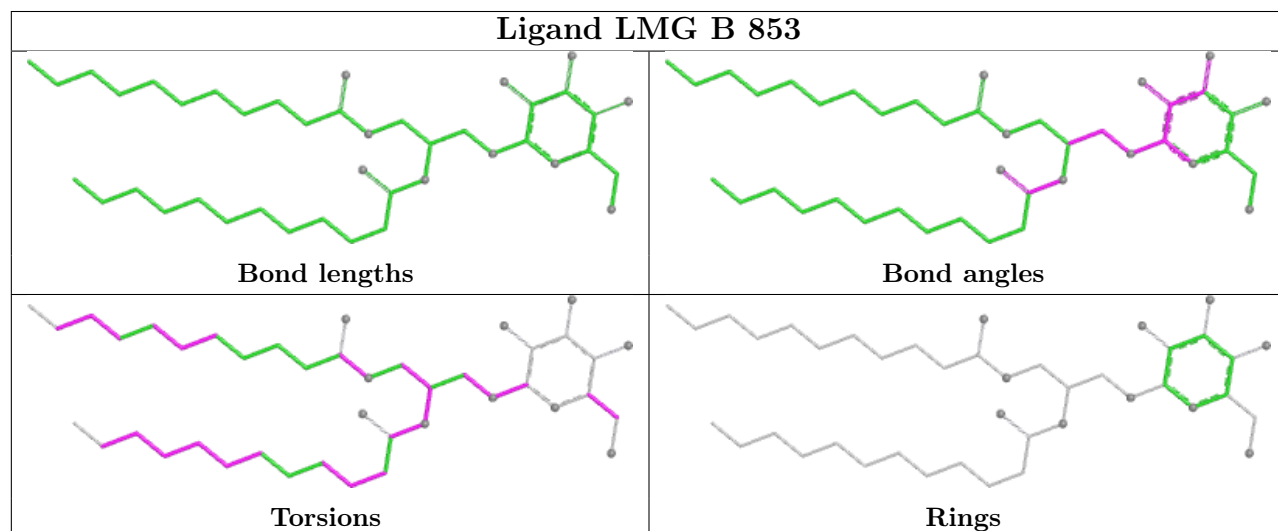




## Ligand CHL 9 313

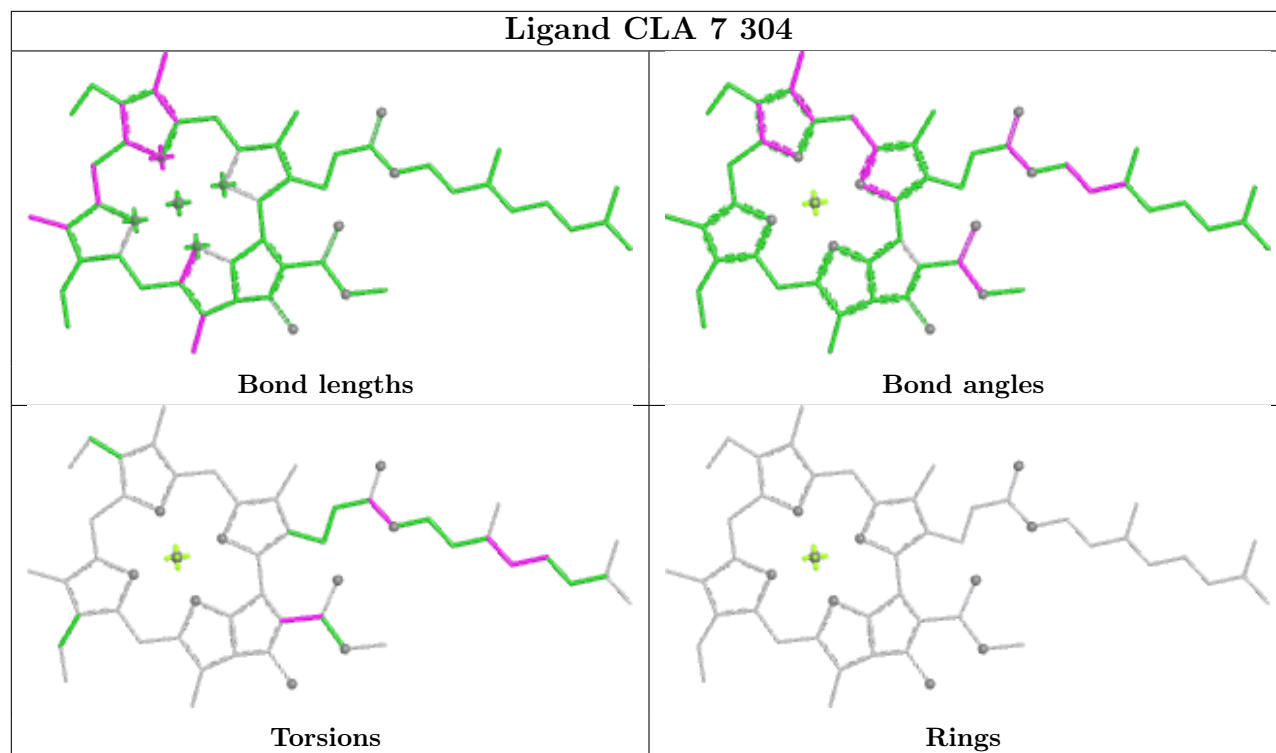


## Ligand LMG B 853

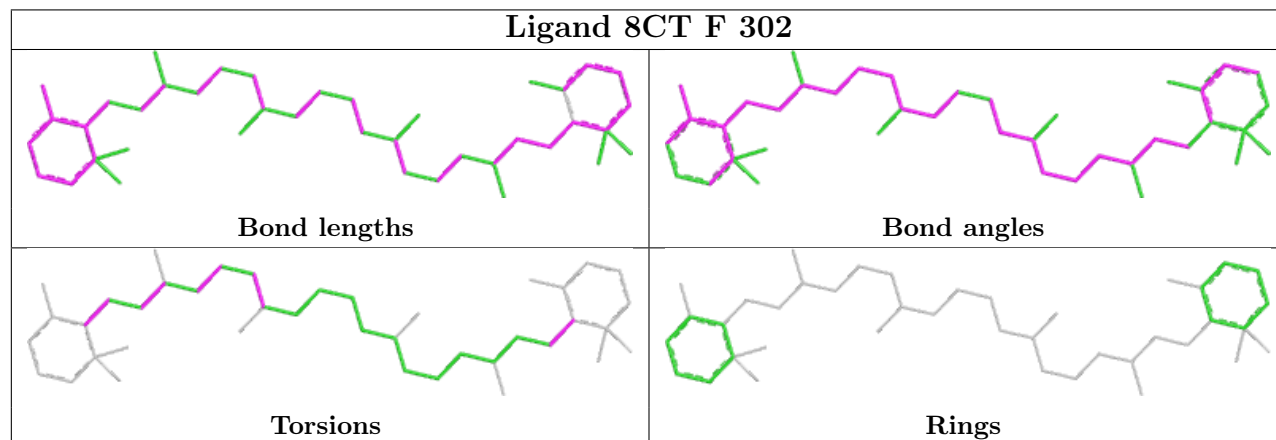




## Ligand CLA 7 304

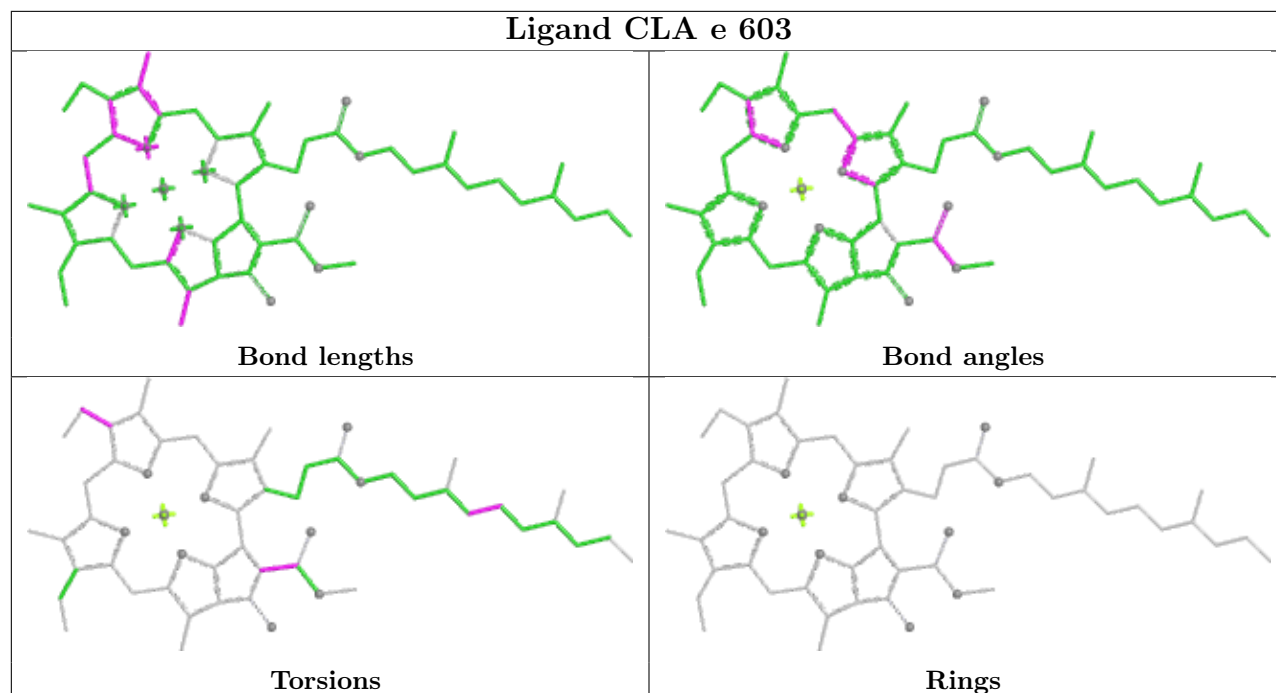


## Ligand 8CT F 302

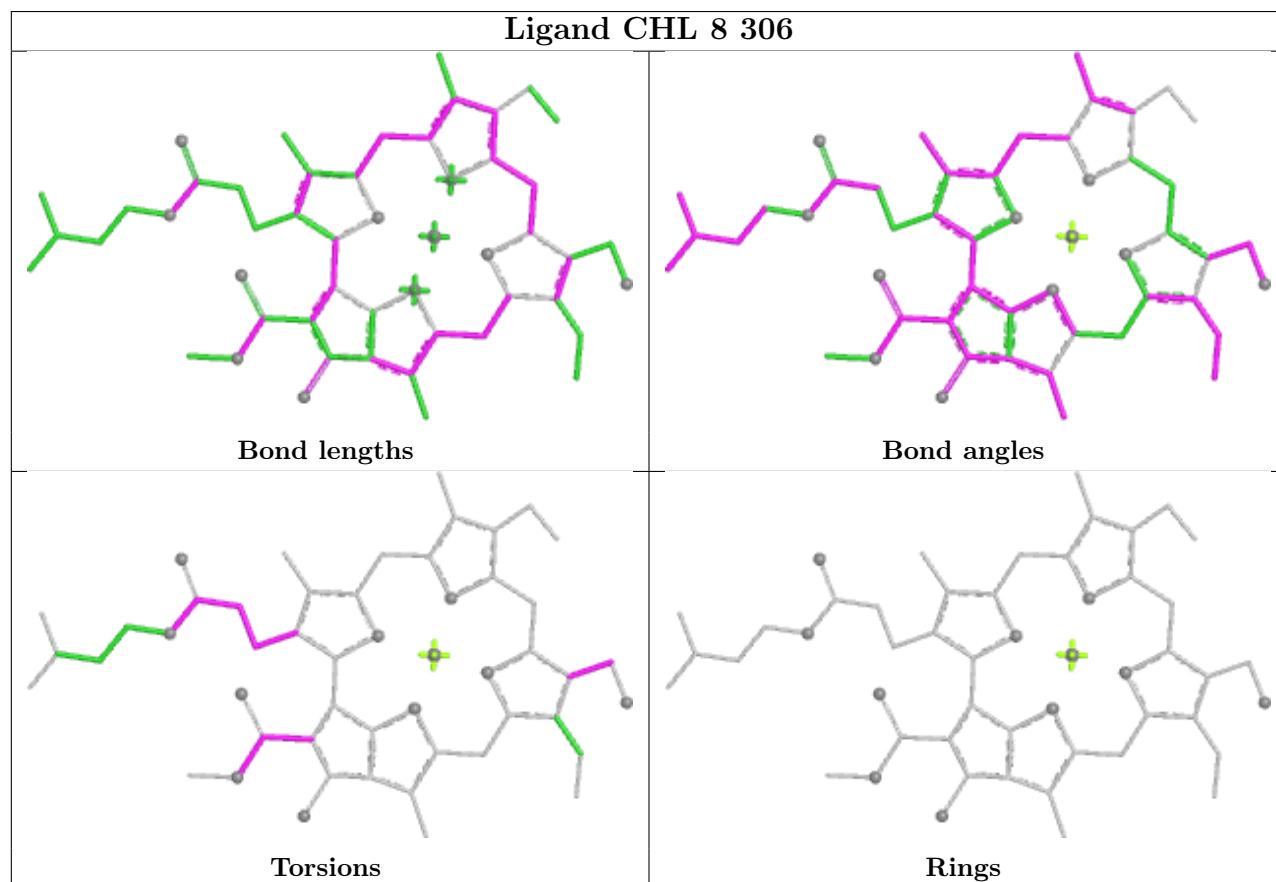




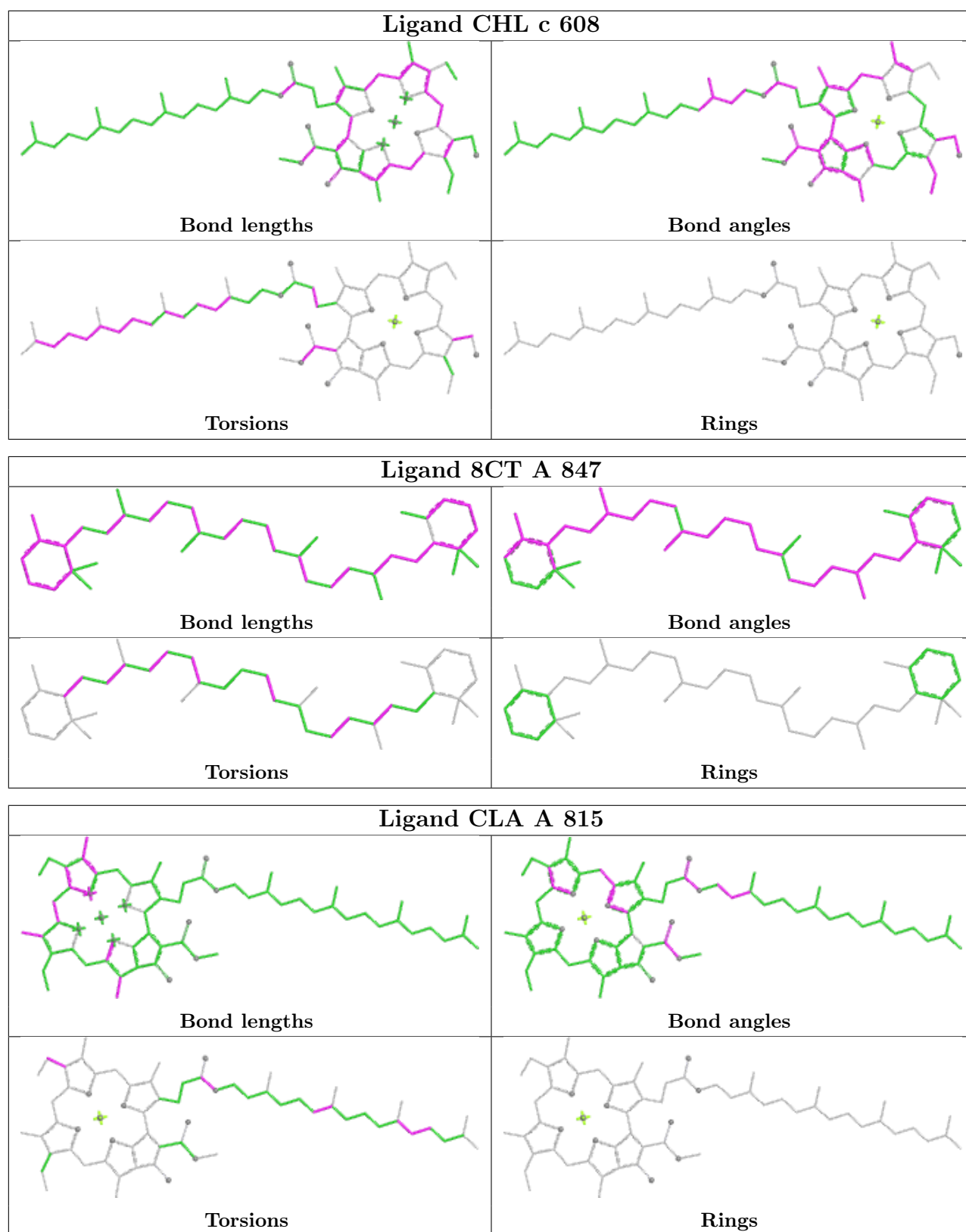
## Ligand CLA e 603



## Ligand CHL 8 306

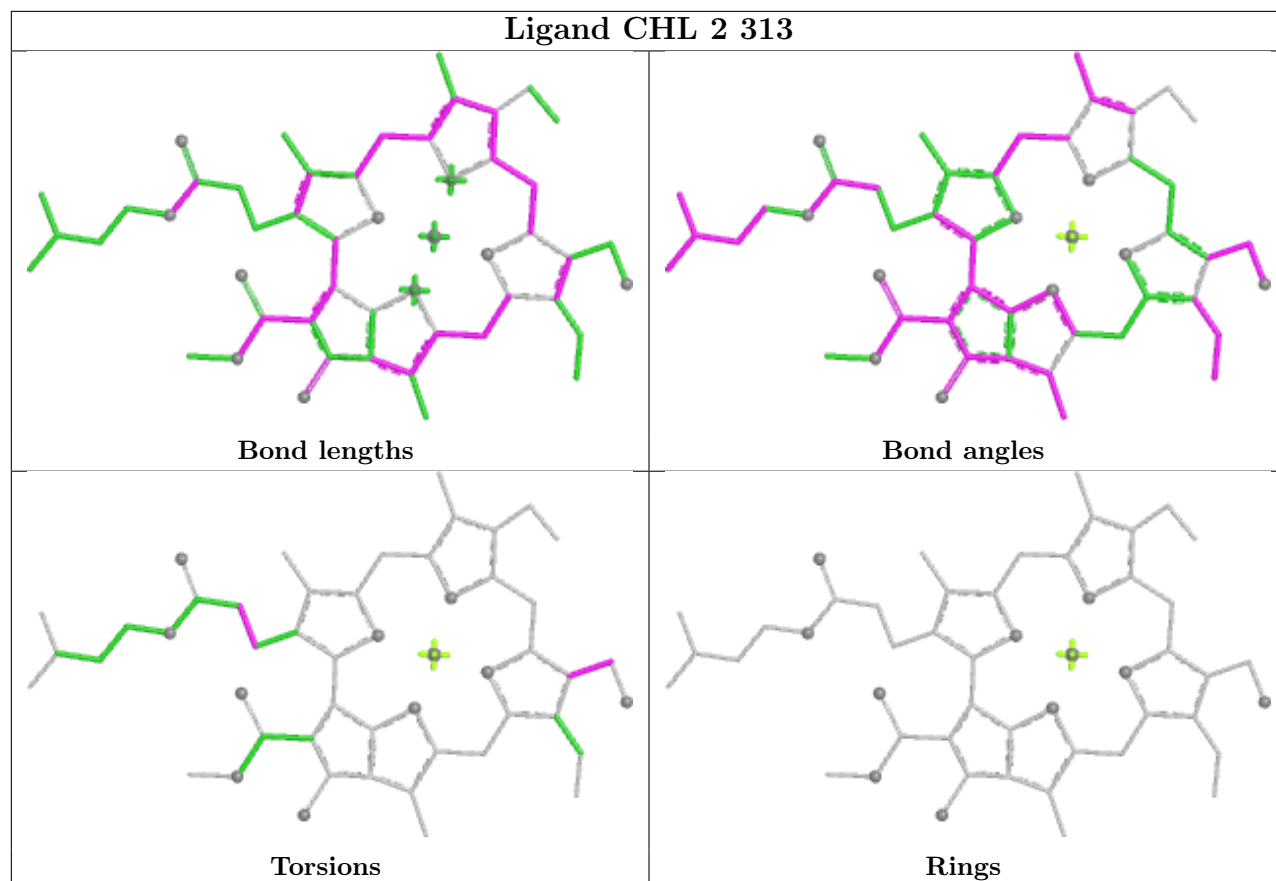




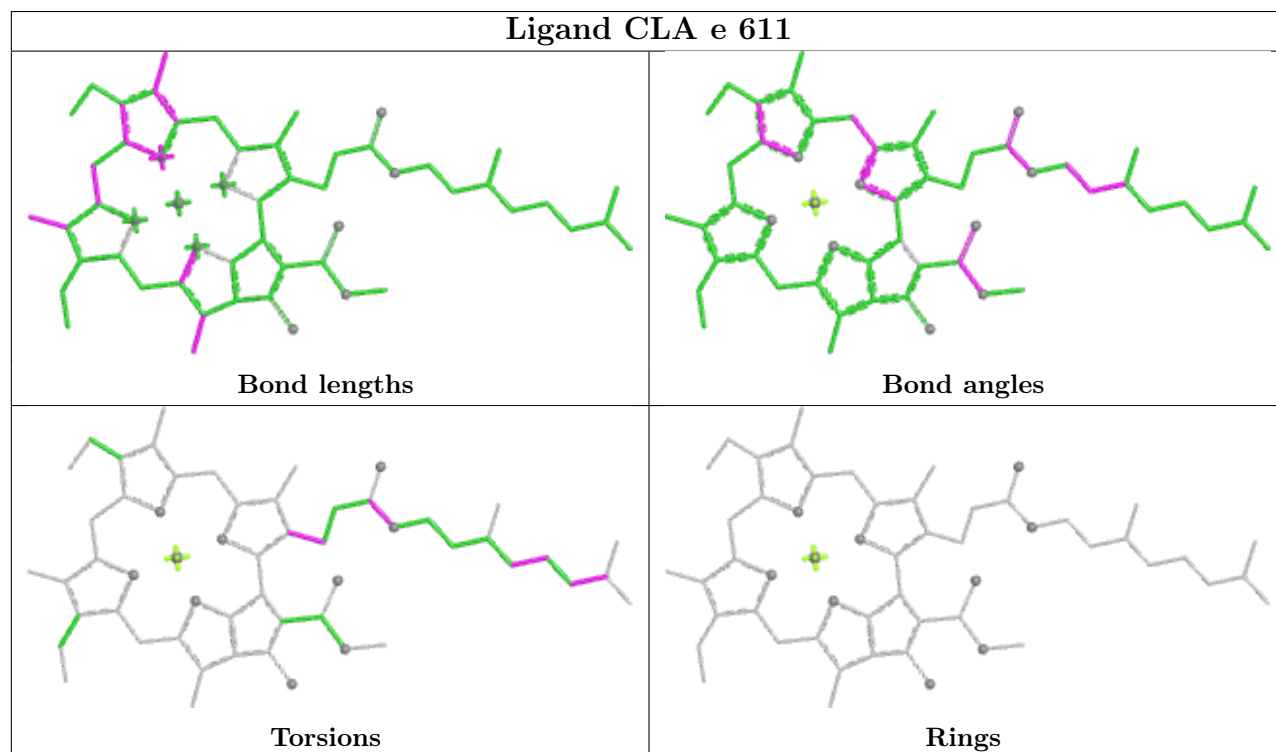




## Ligand CHL 2 313

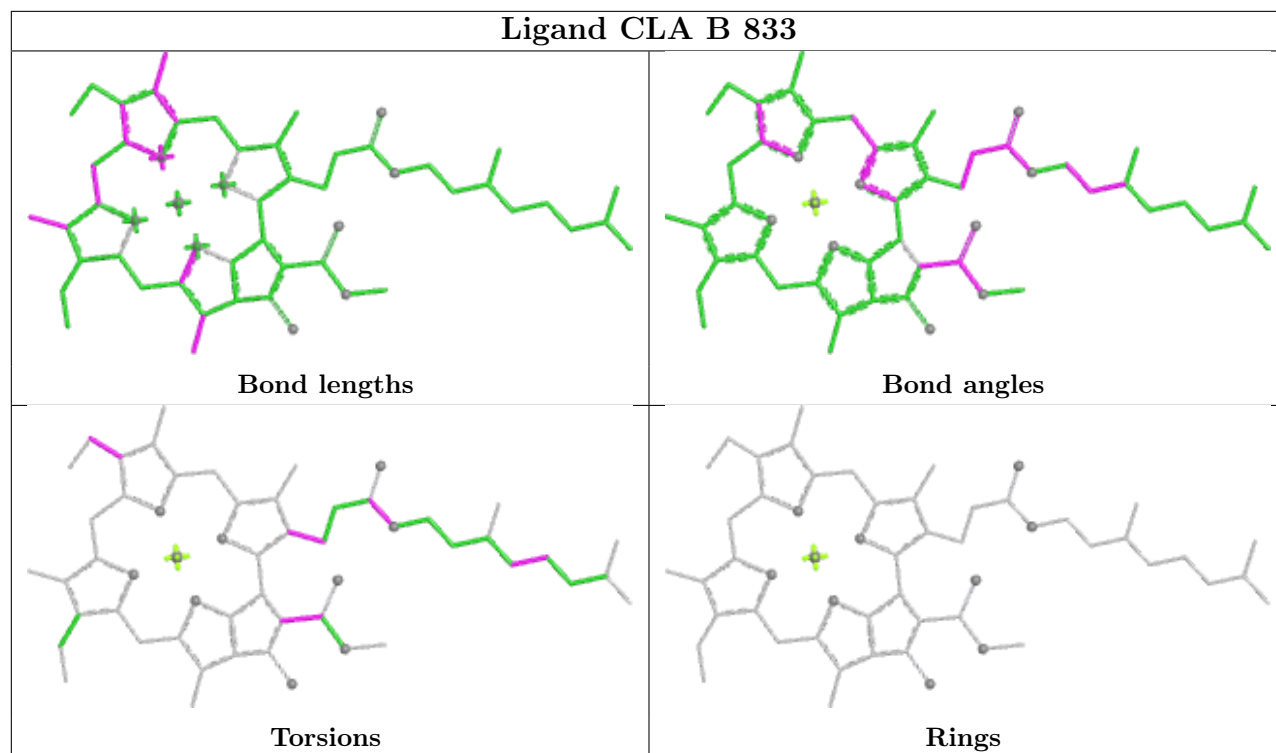


## Ligand CLA e 611

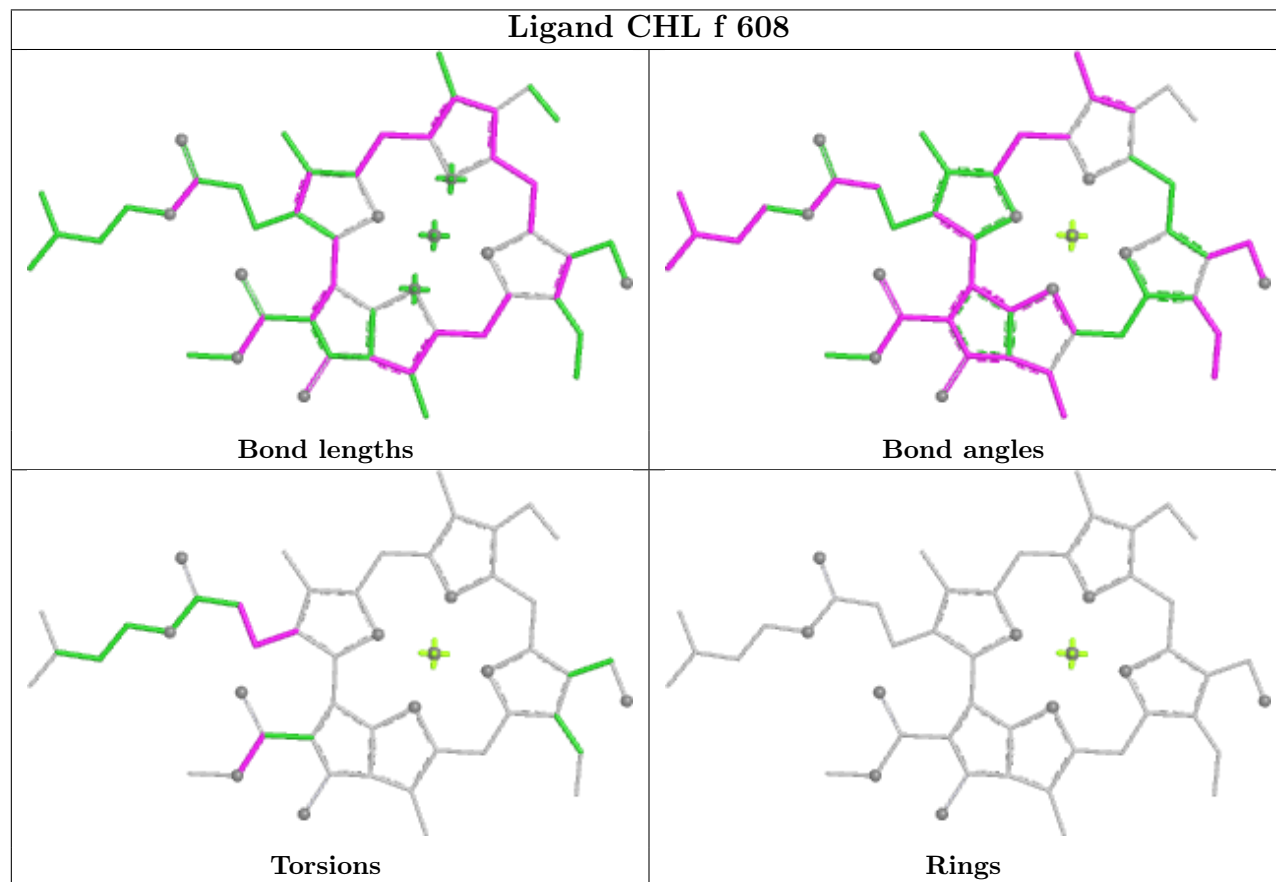




## Ligand CLA B 833

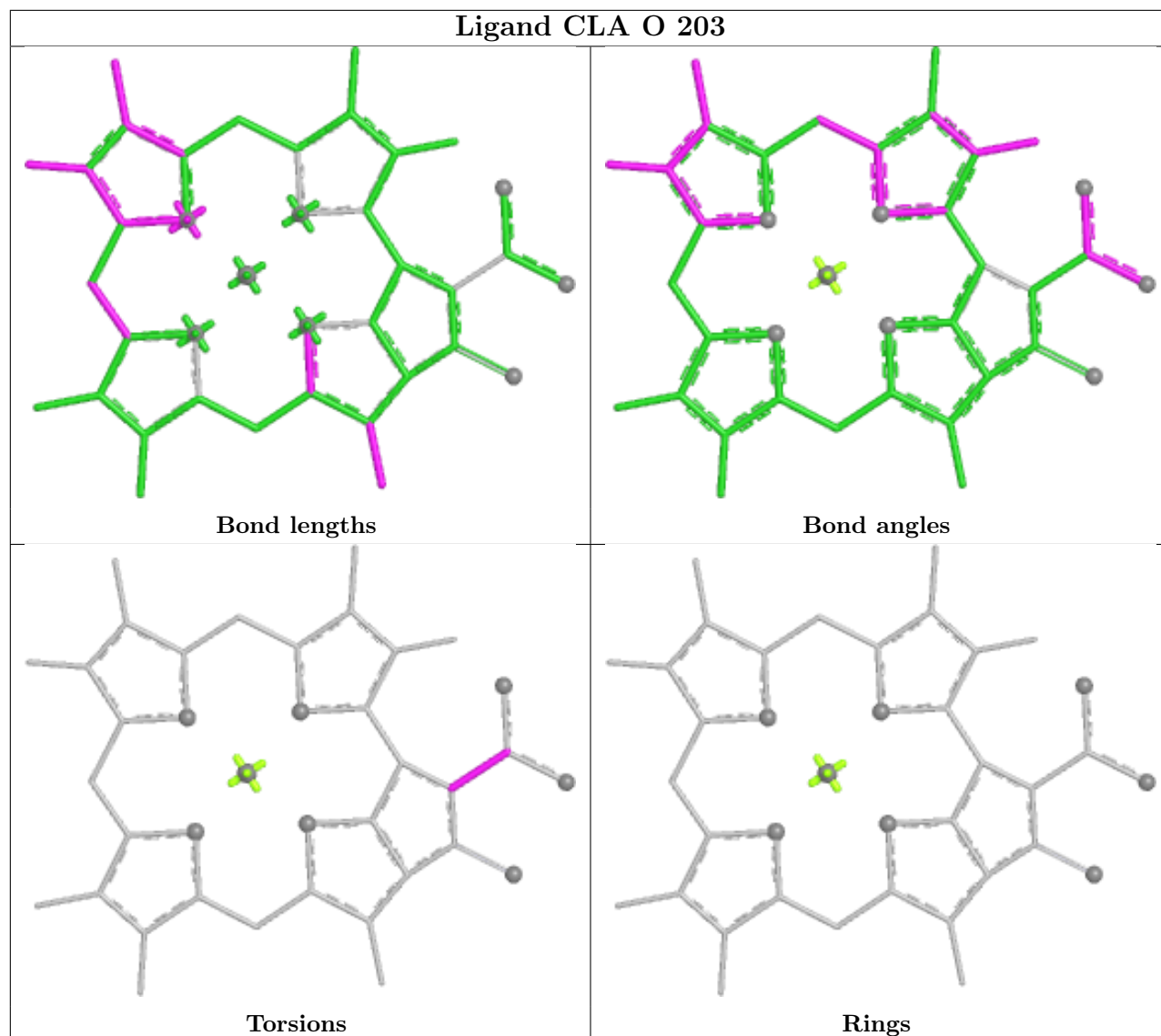


## Ligand CHL f 608

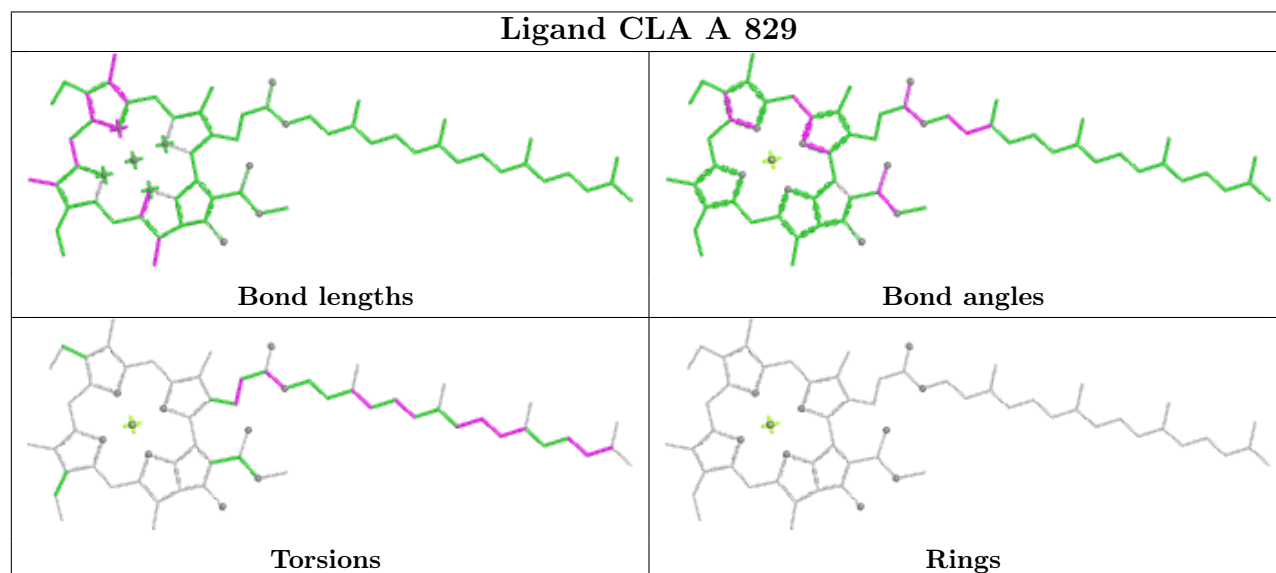




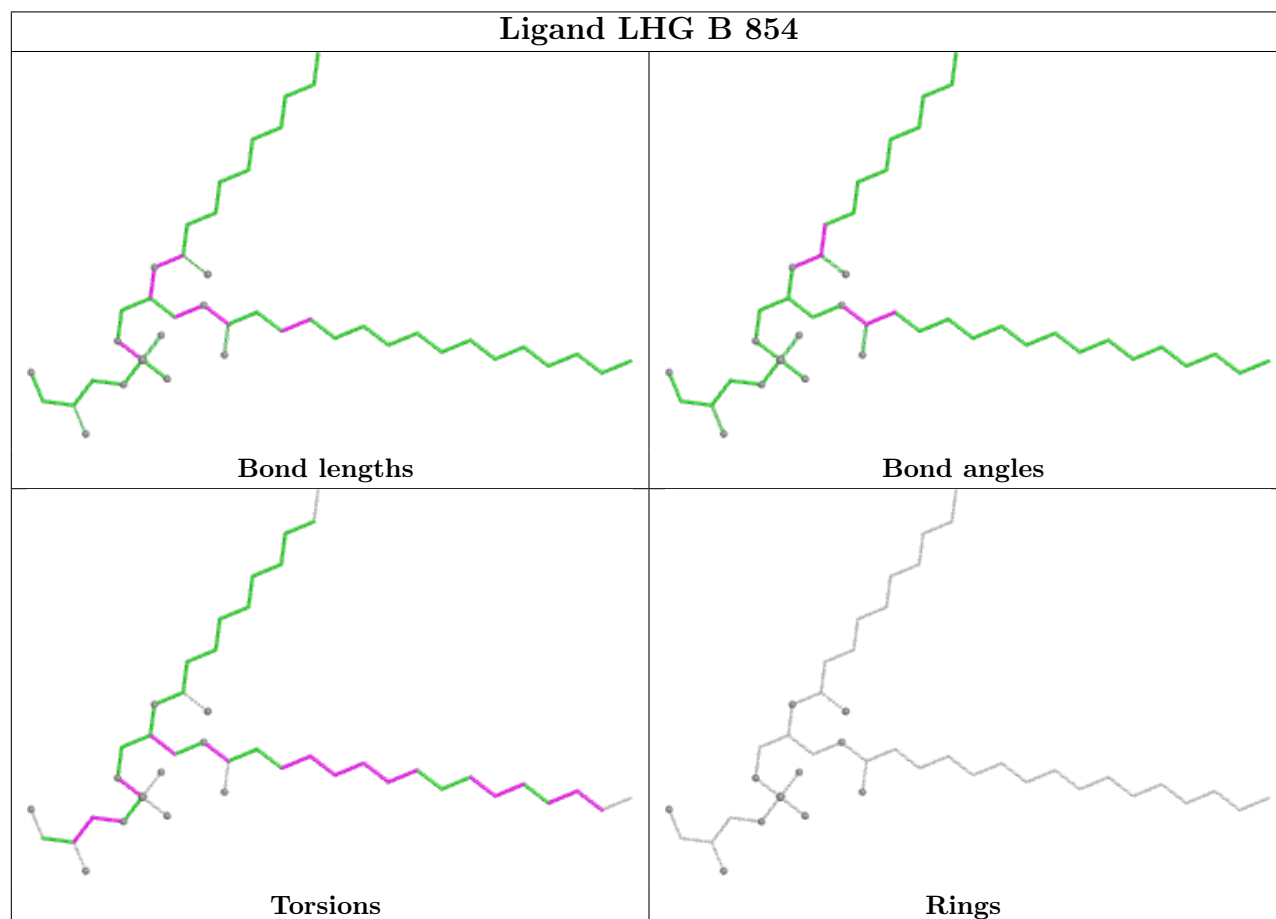
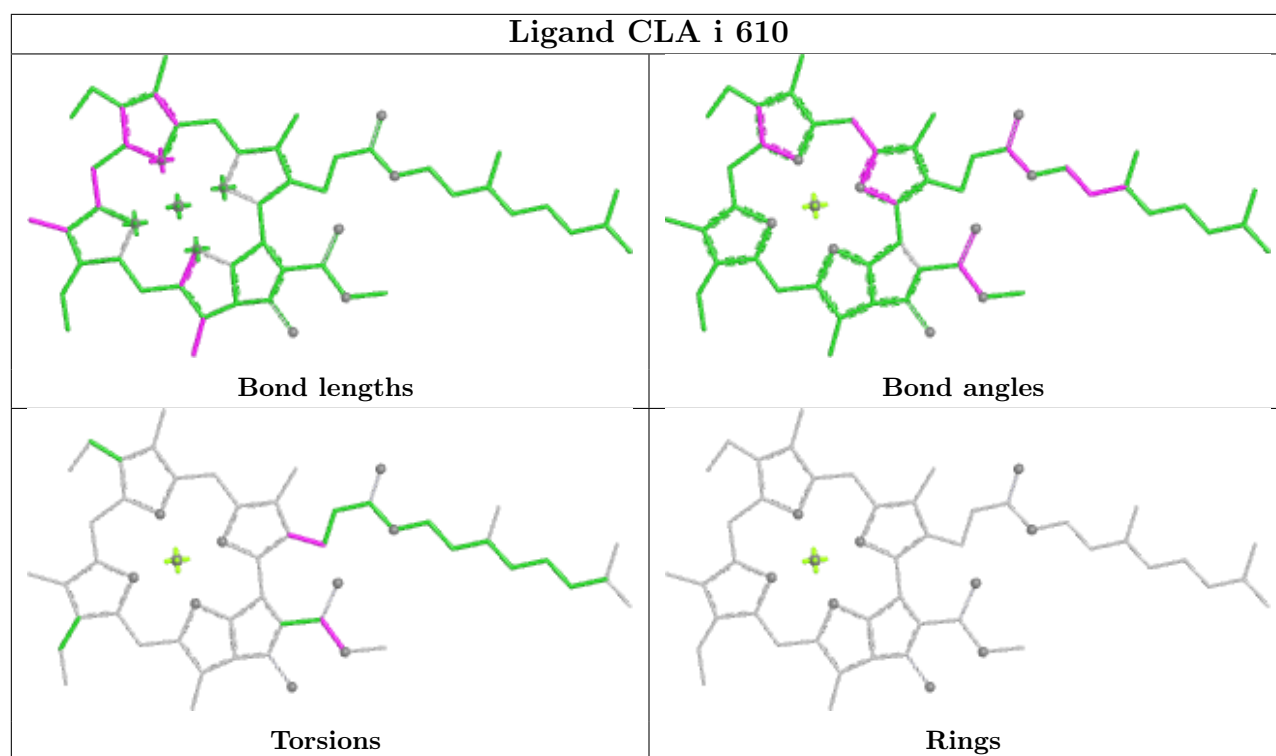
## Ligand CLA O 203



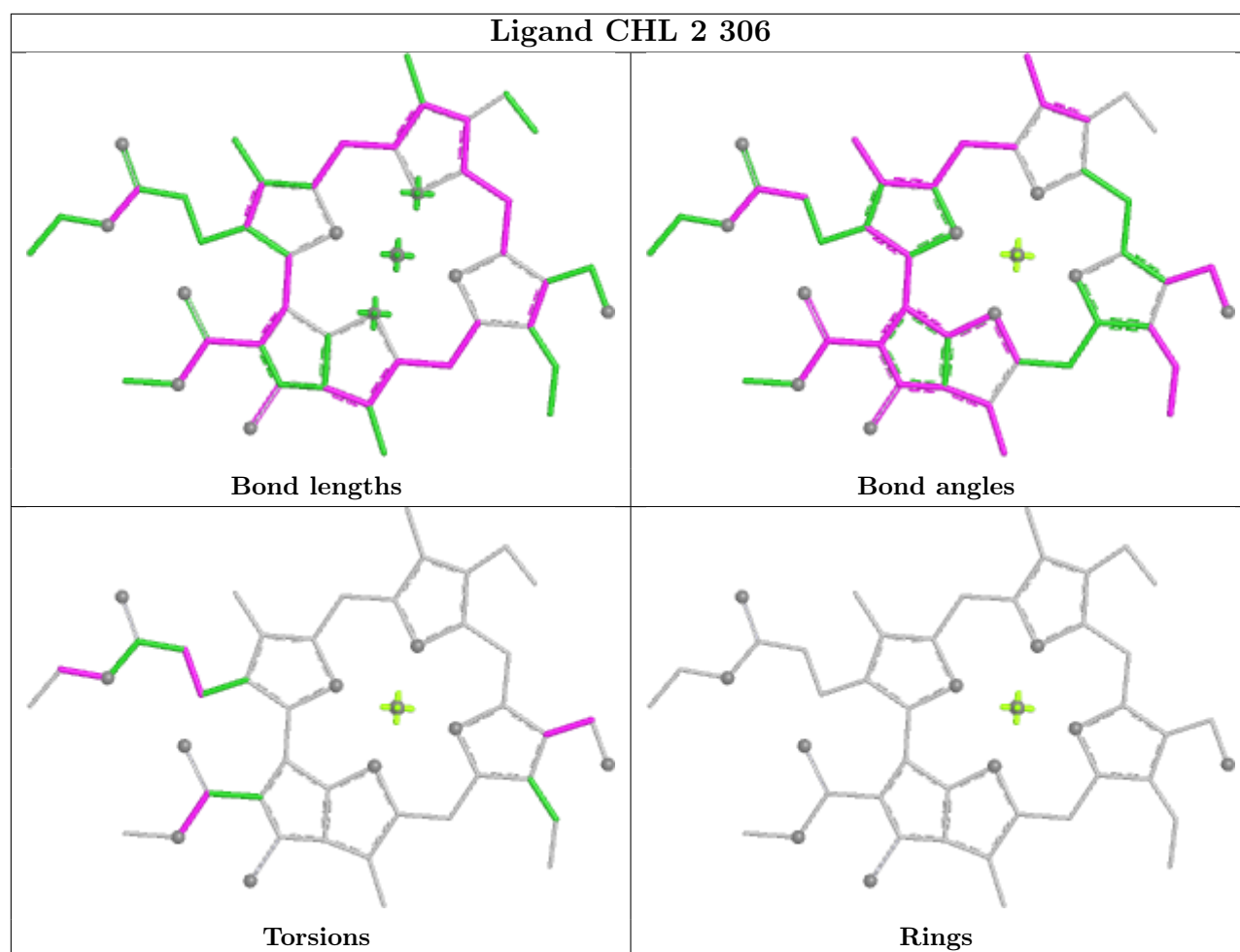
## Ligand CLA A 829





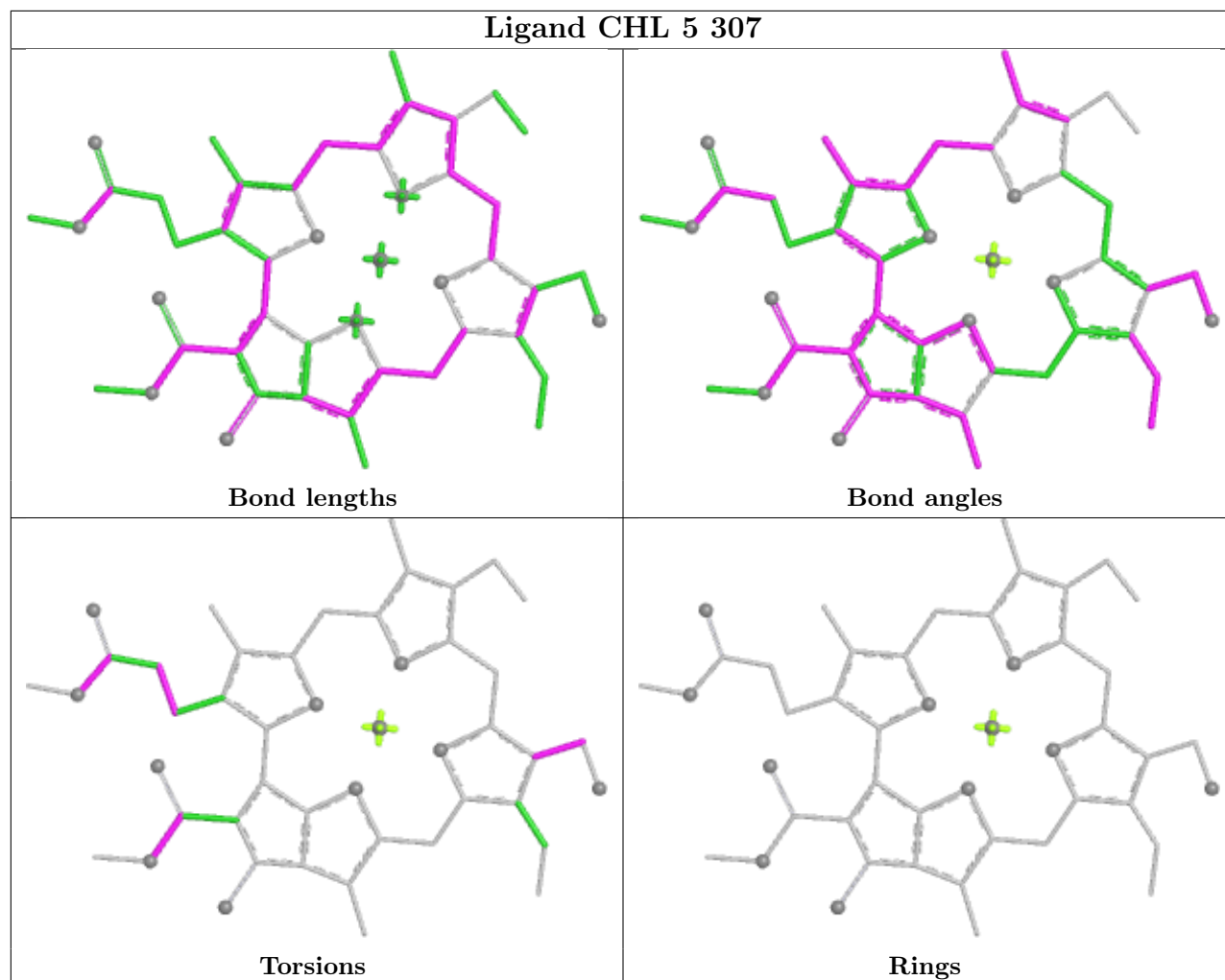




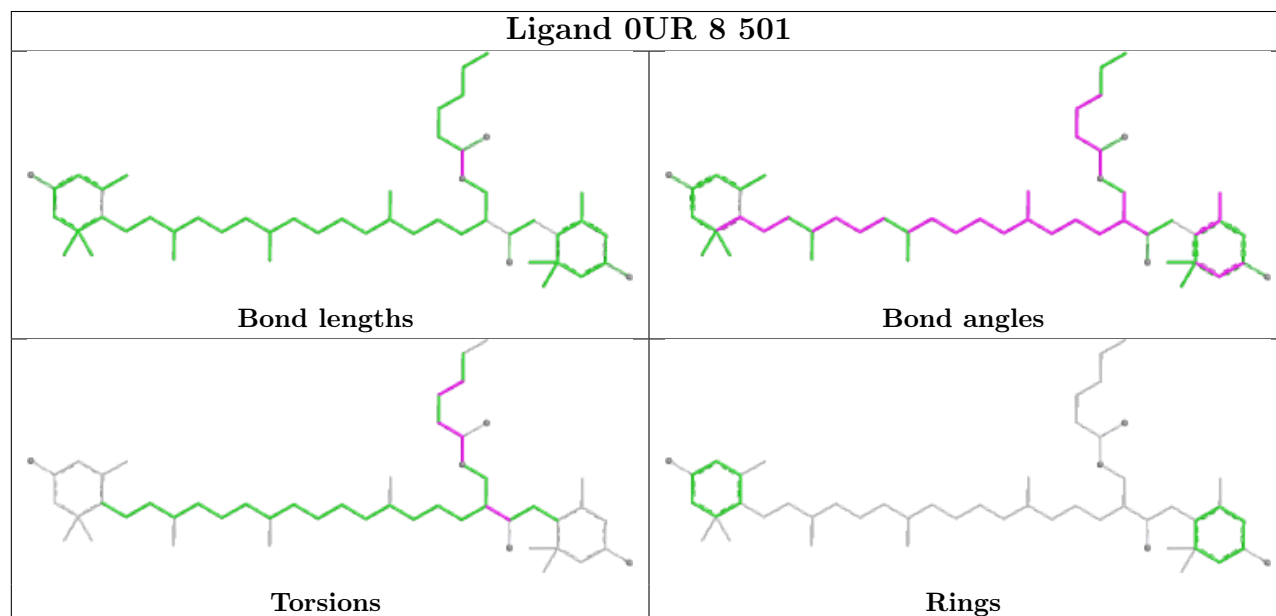




## Ligand CHL 5 307

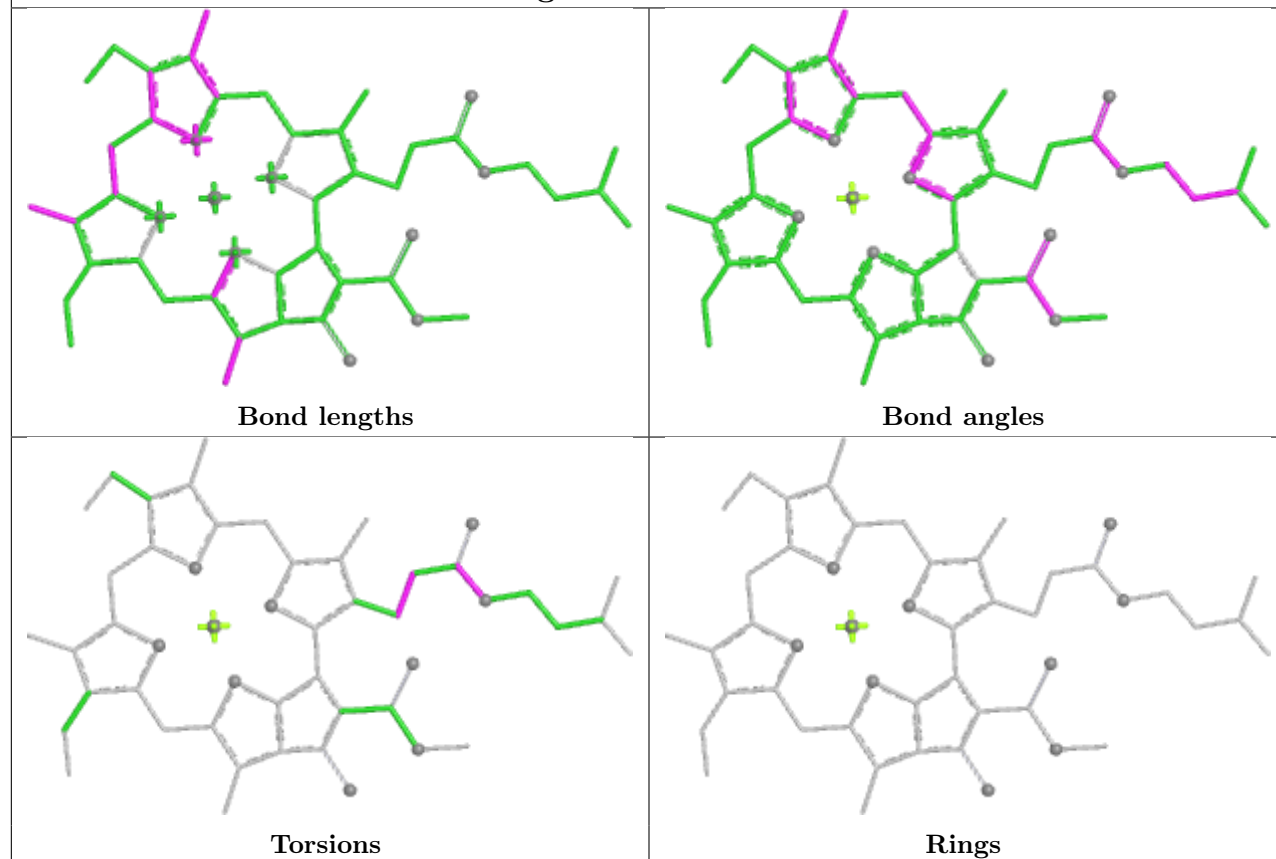


## Ligand OUR 8 501

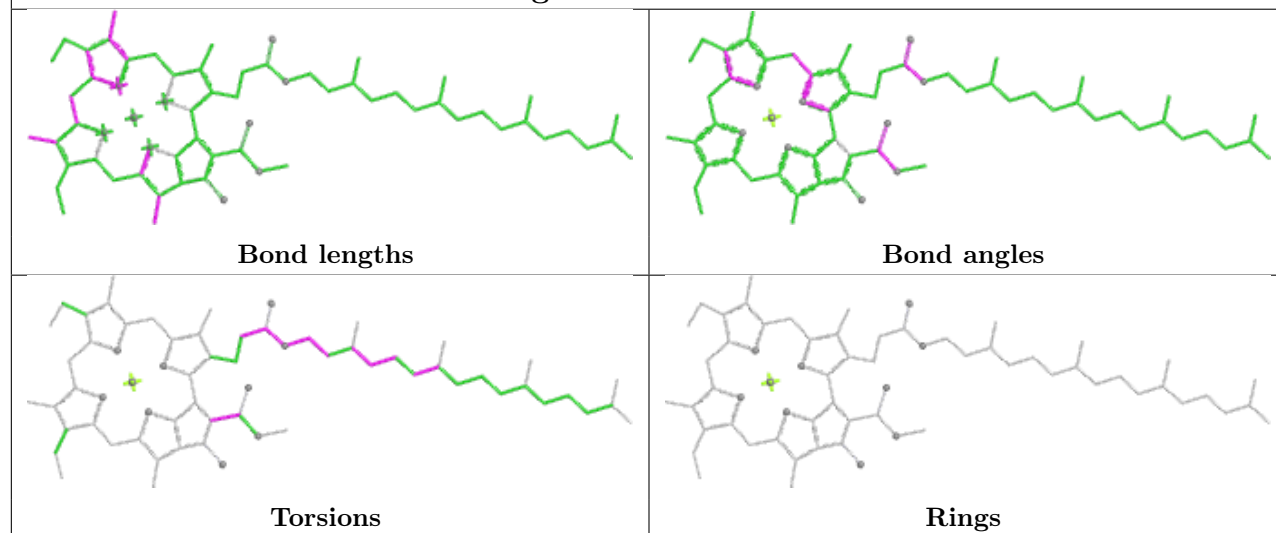




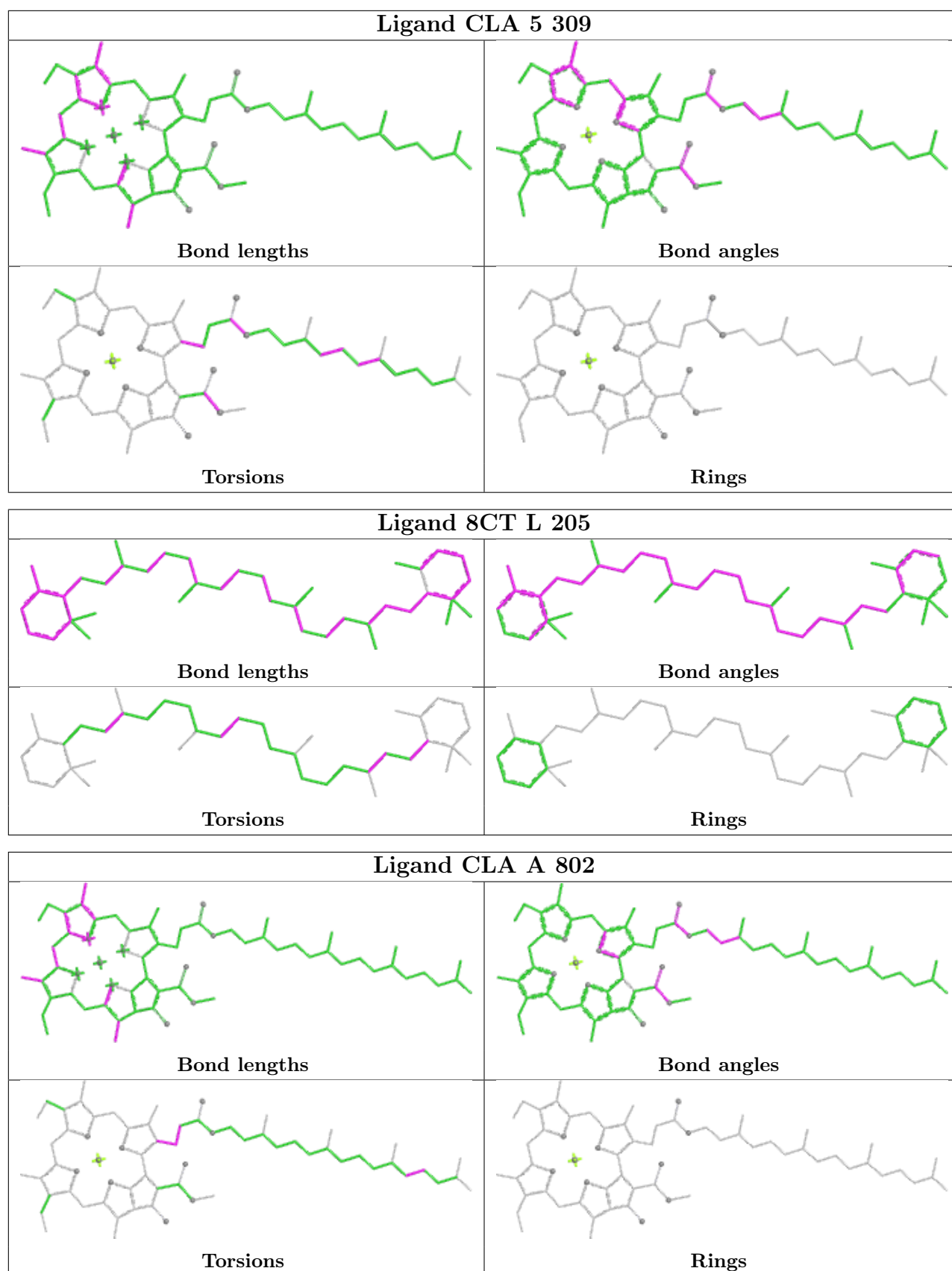
## Ligand CLA c 604



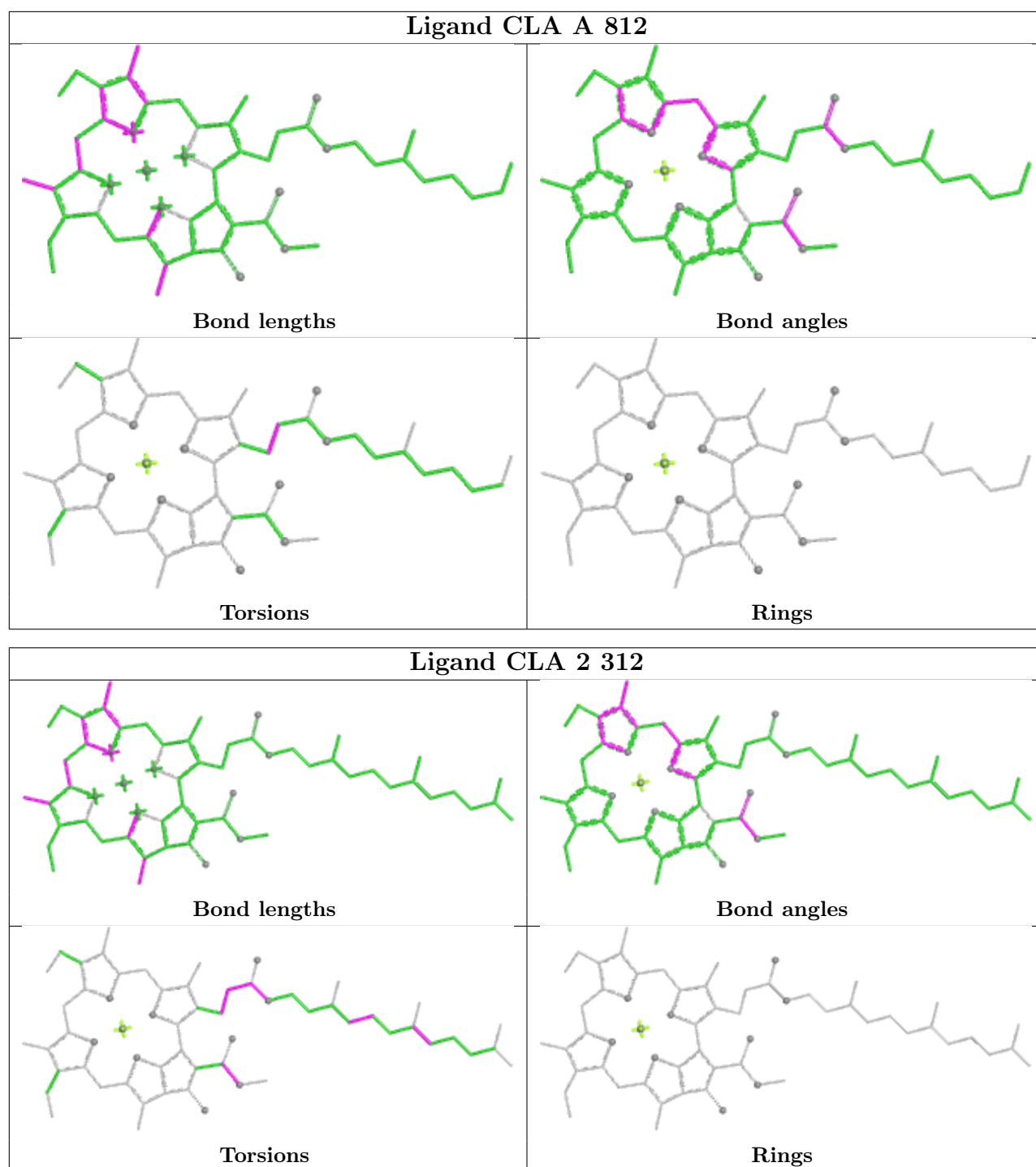
## Ligand CLA A 805



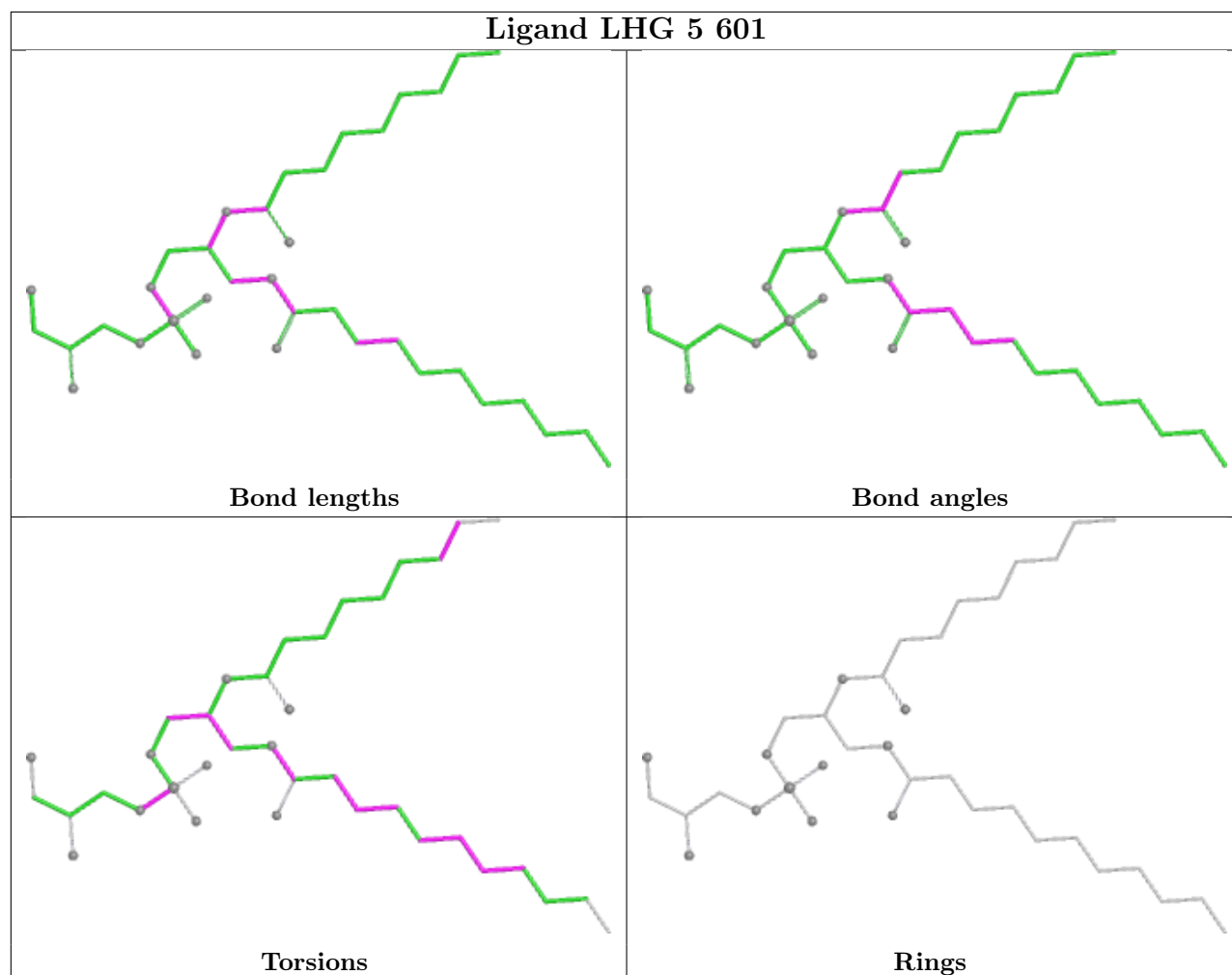
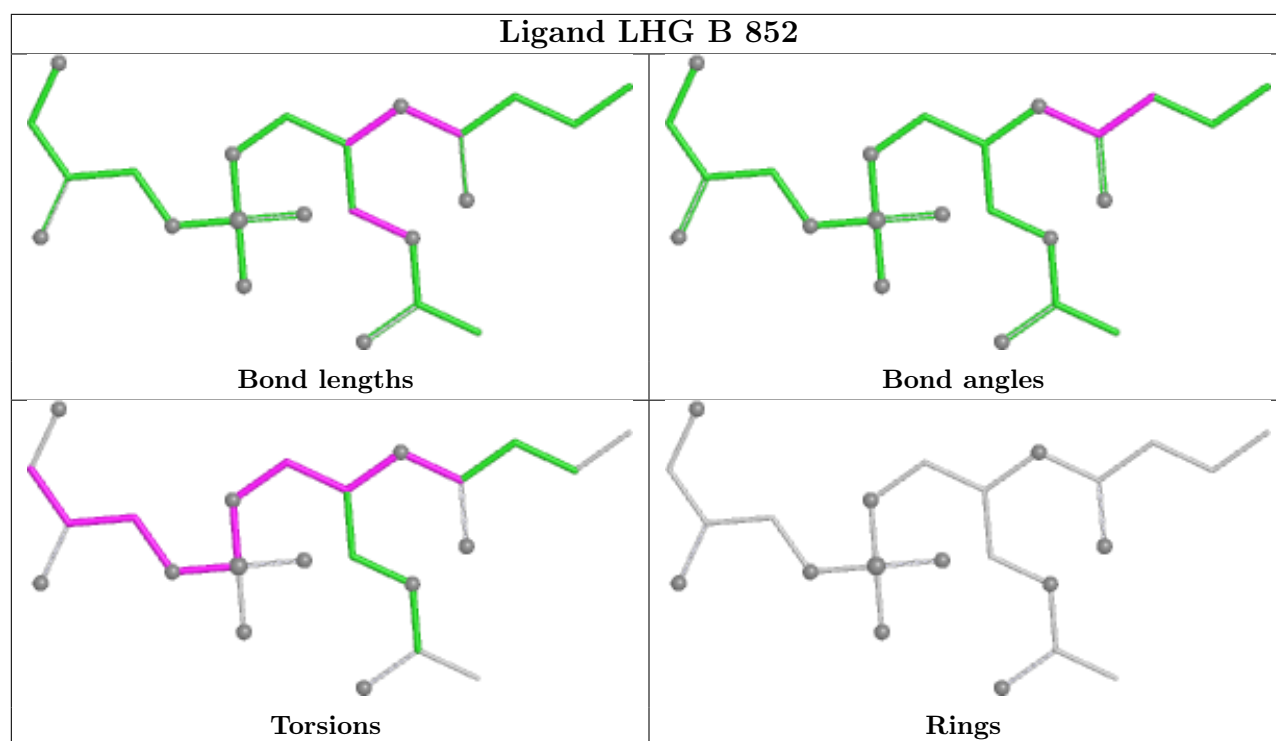




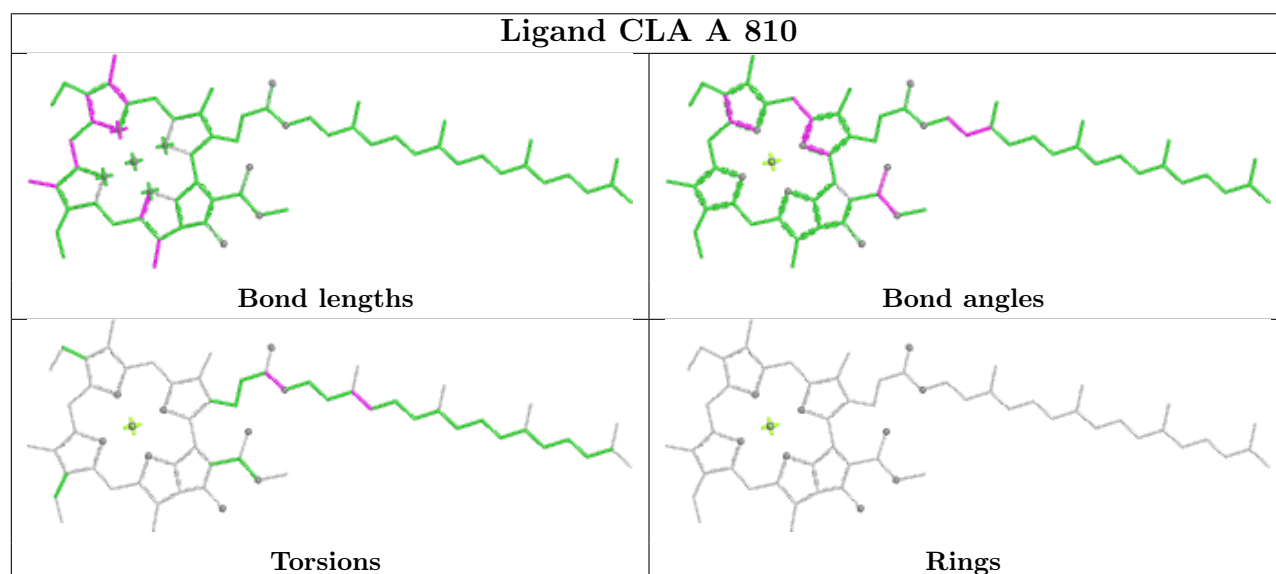
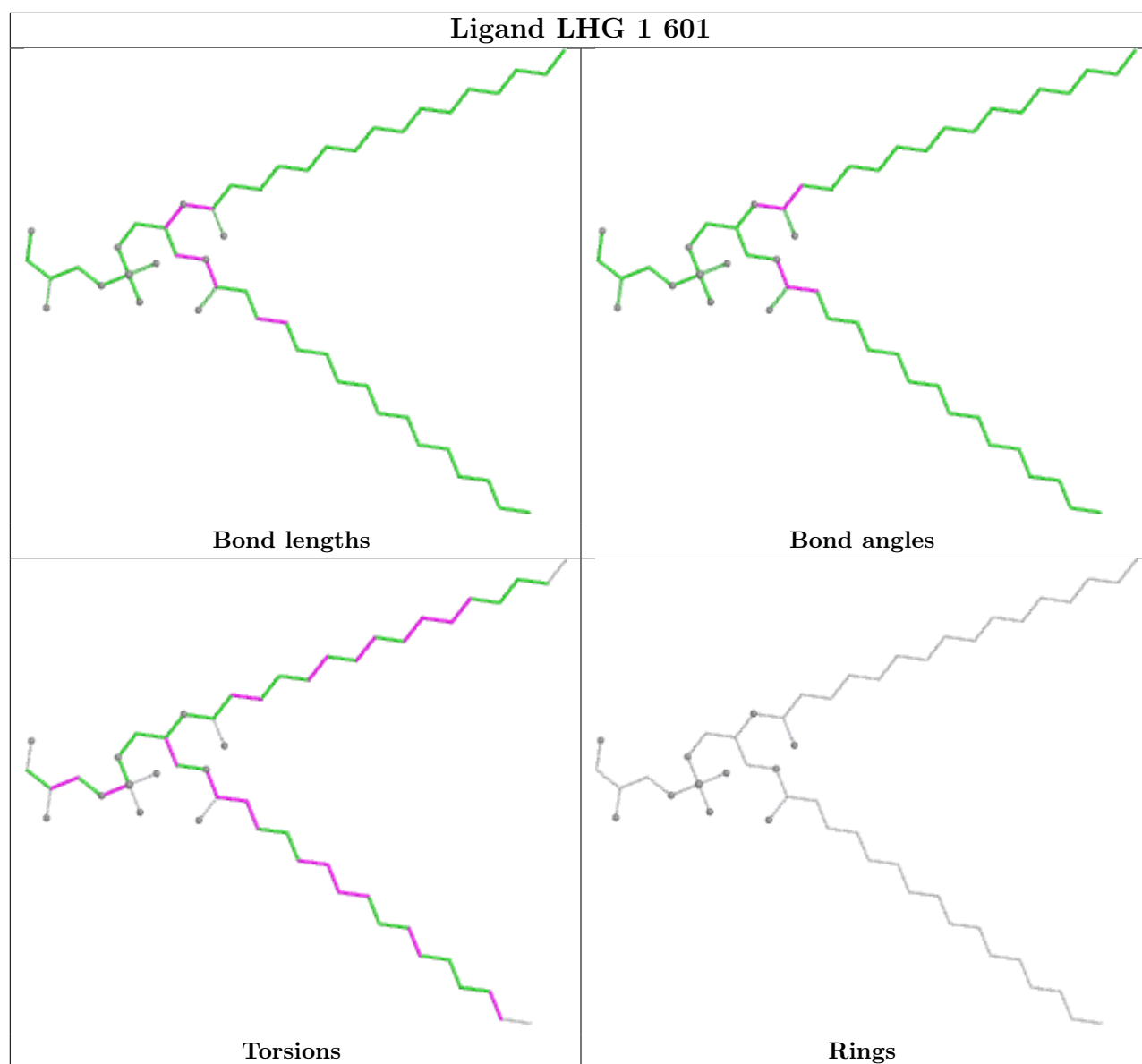




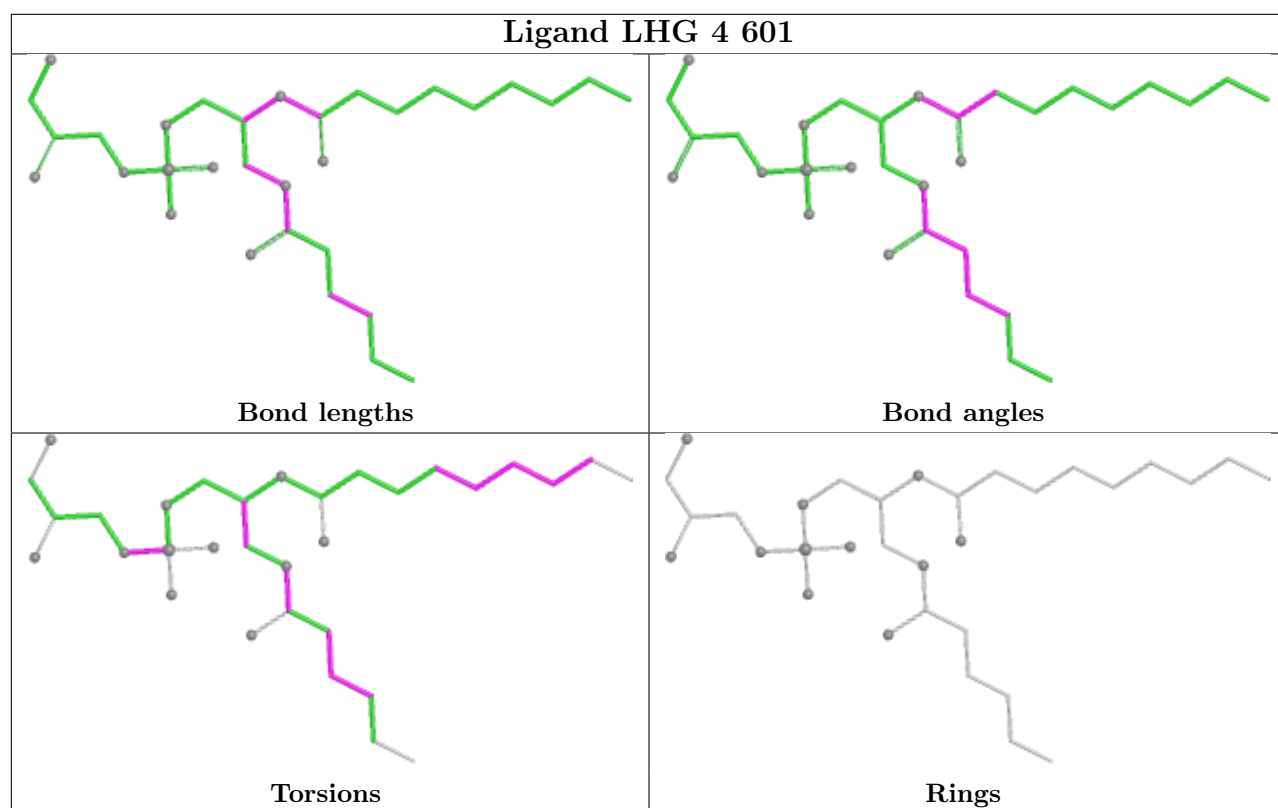
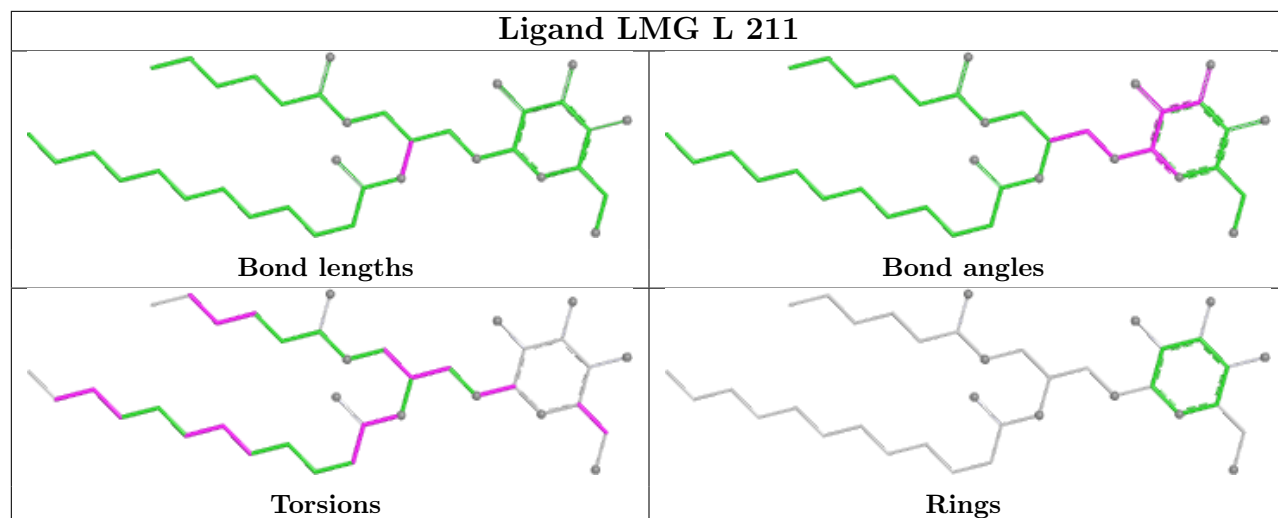






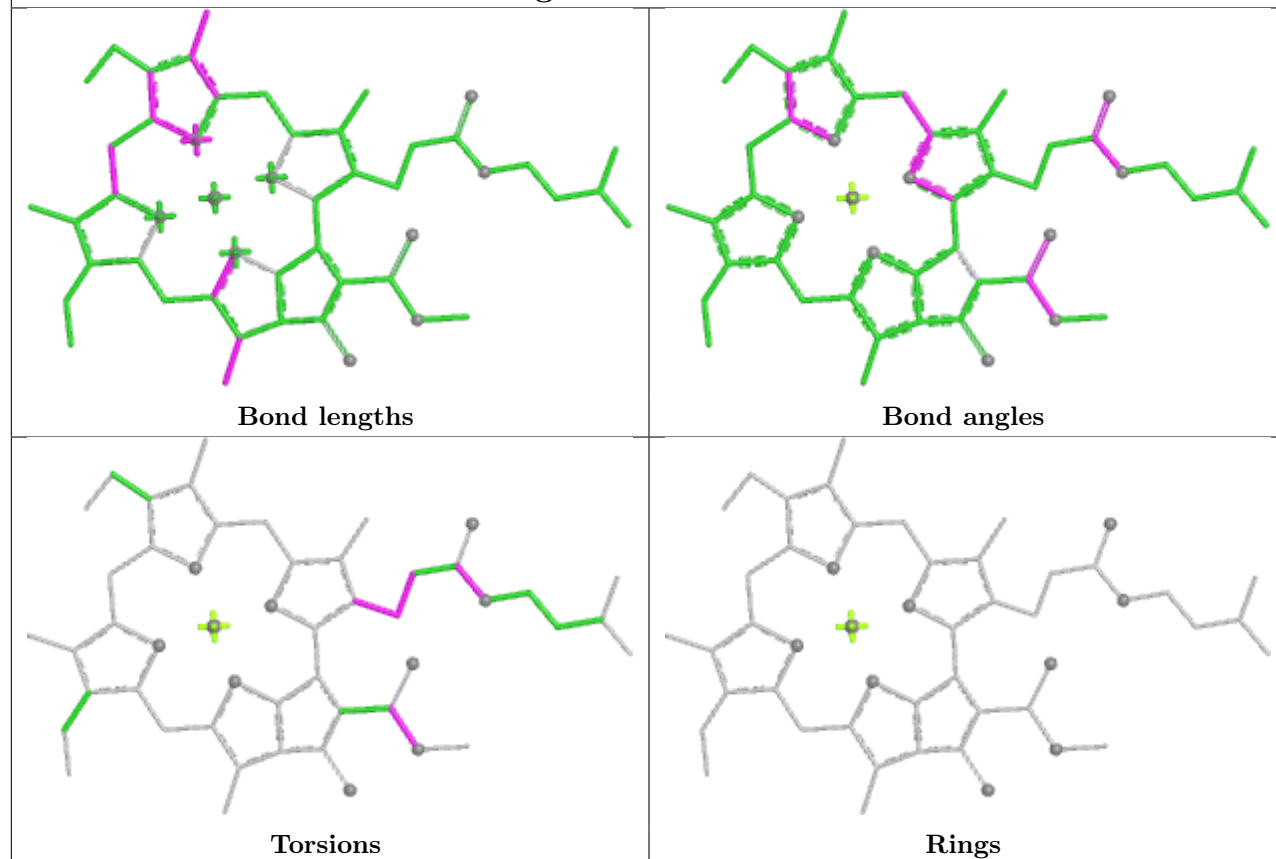




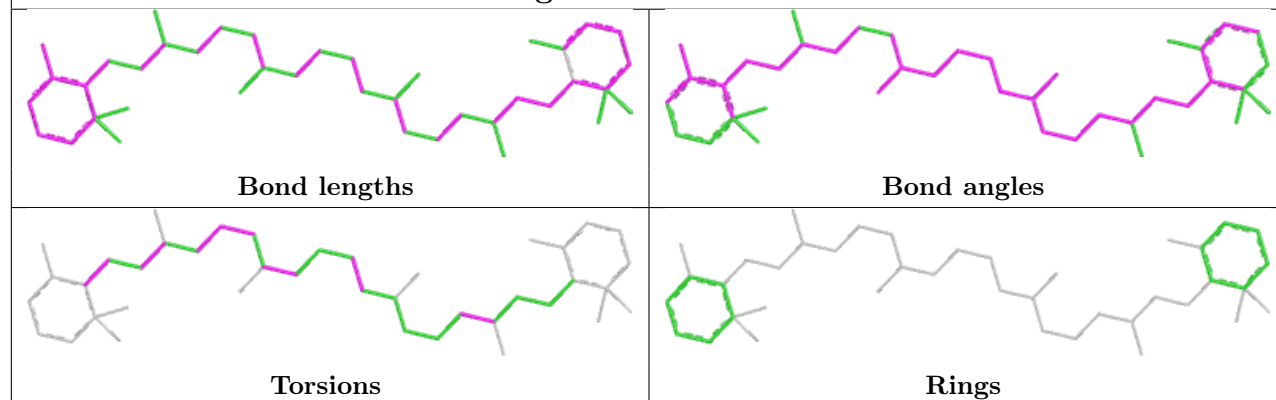




## Ligand CLA b 604

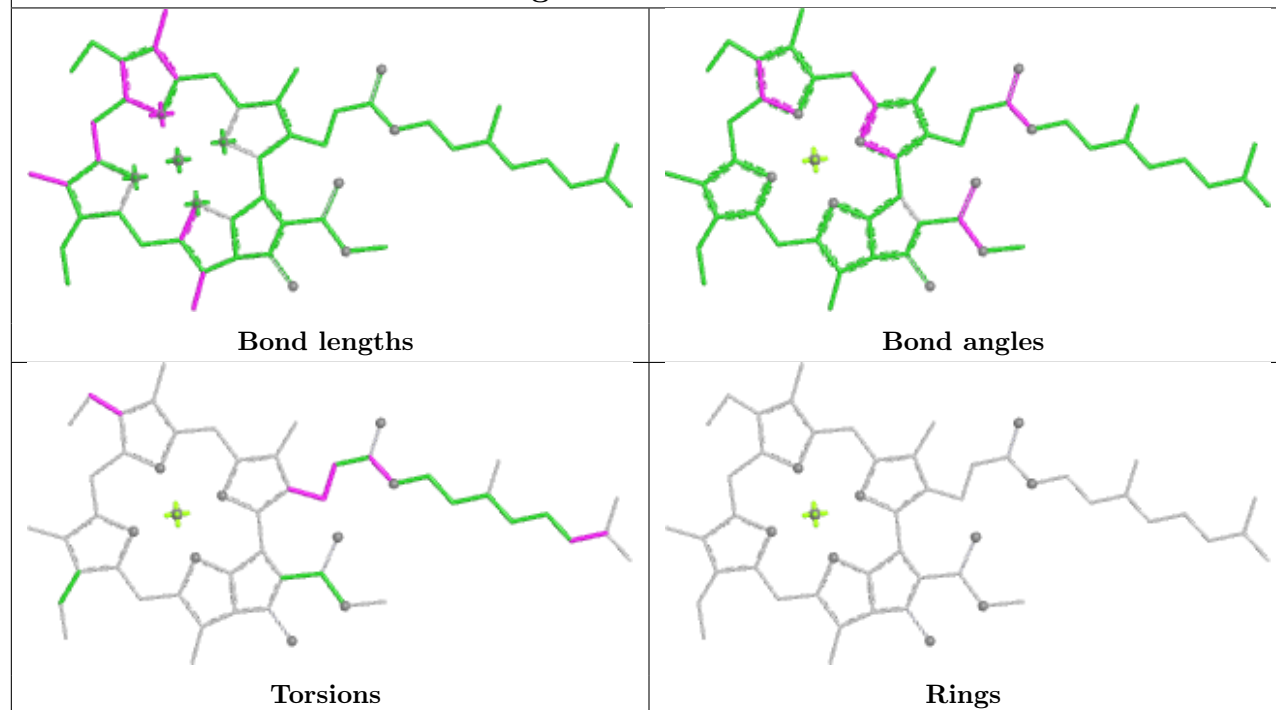


## Ligand 8CT B 845

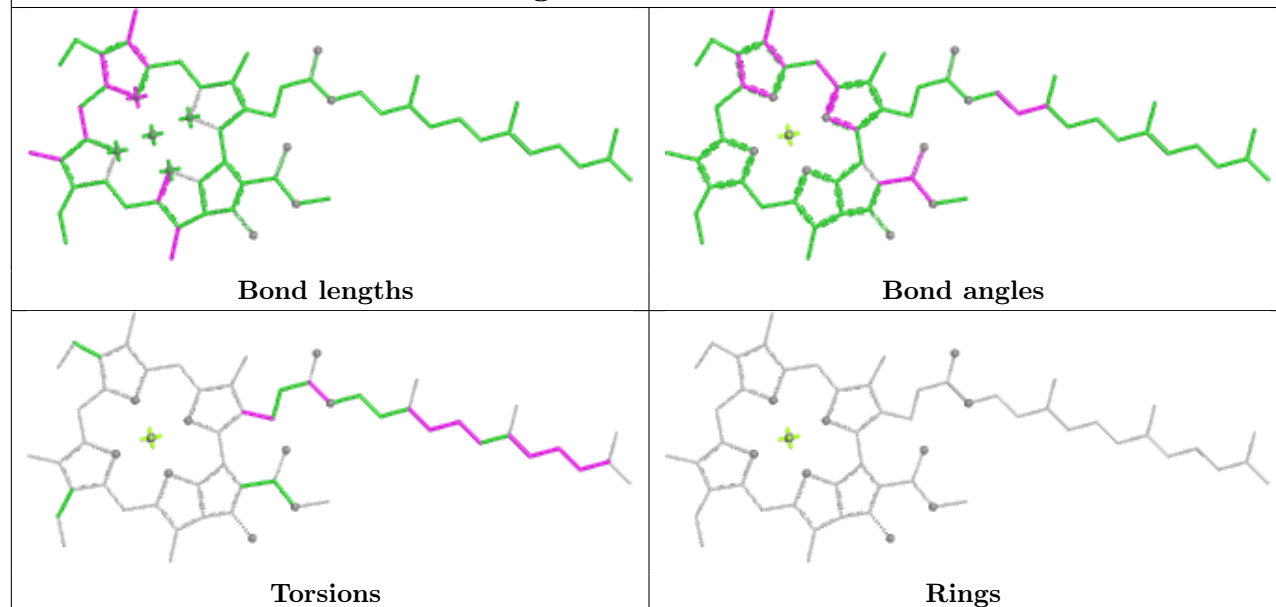




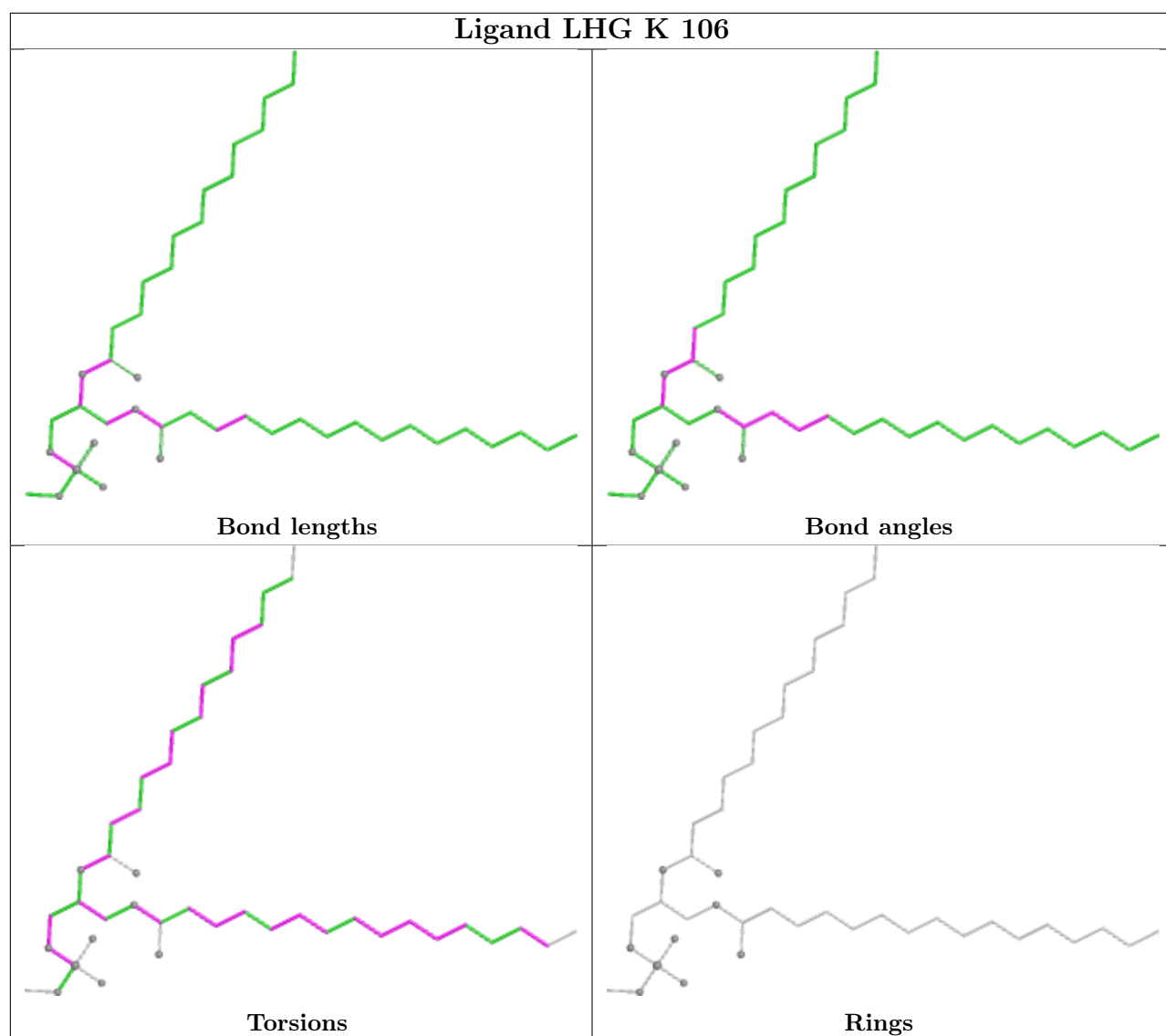
## Ligand CLA A 824



## Ligand CLA B 819

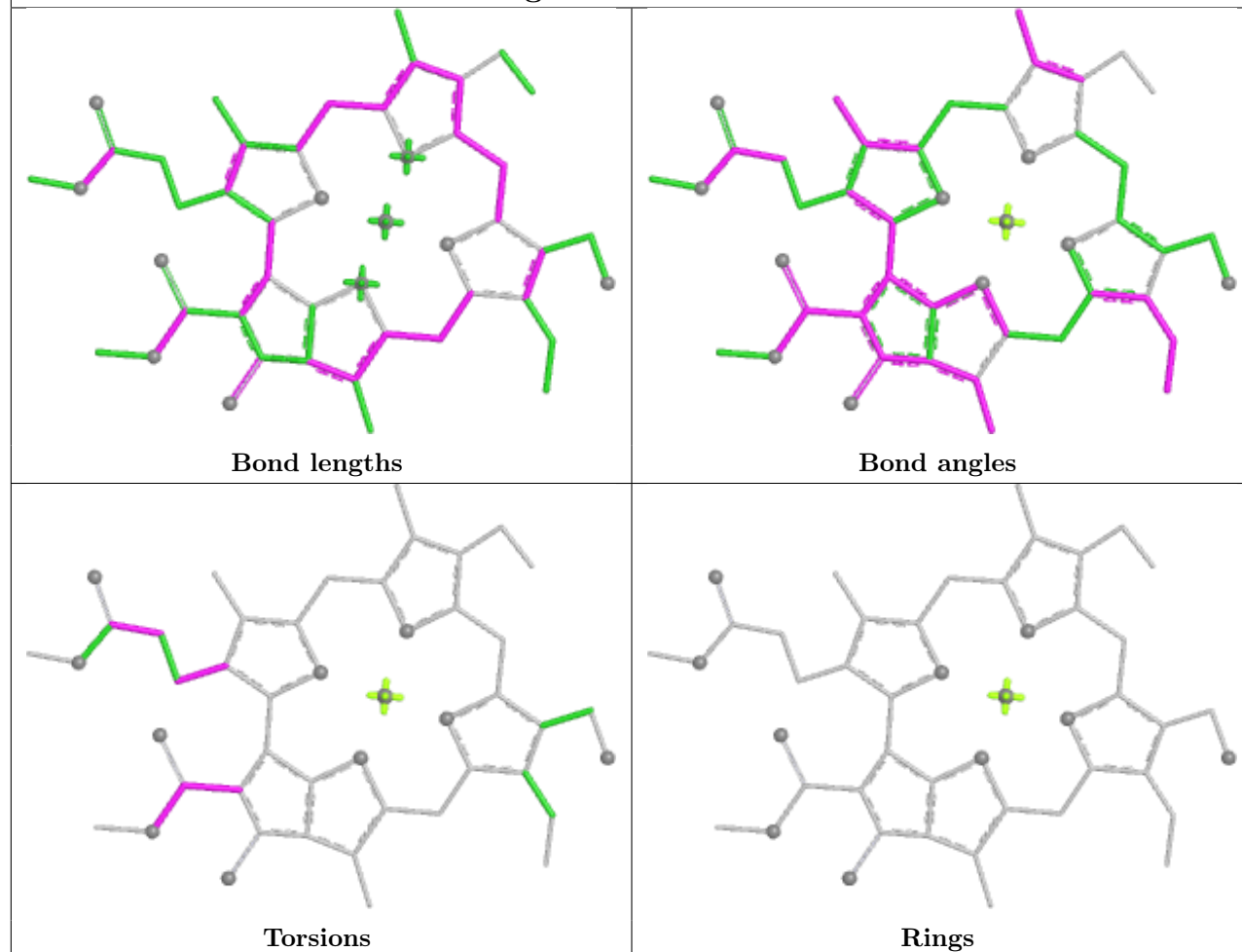




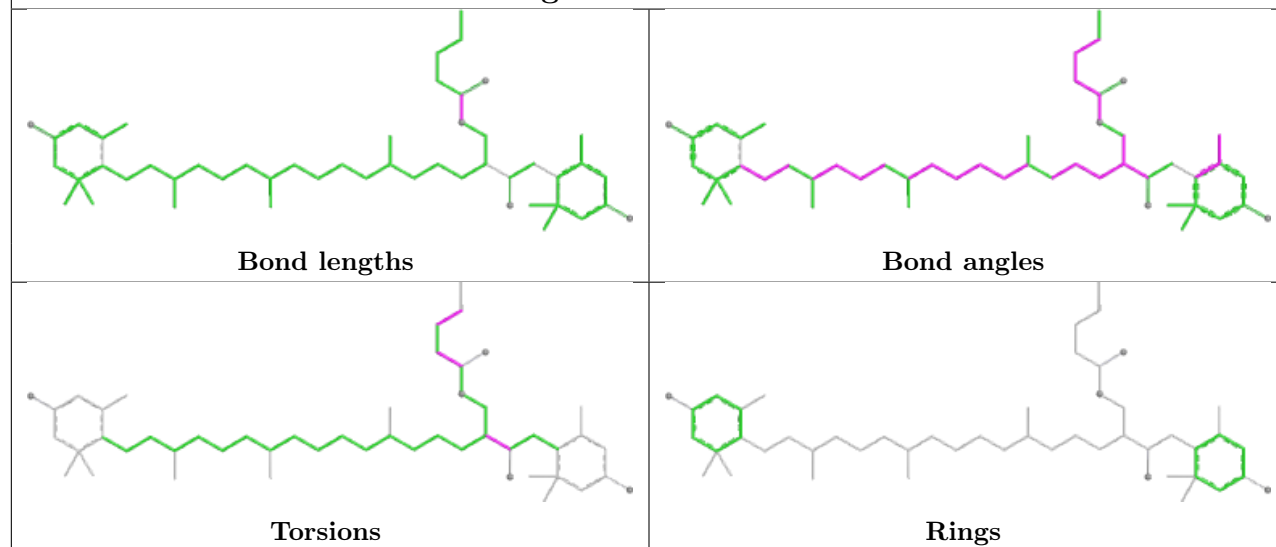




## Ligand CHL f 607

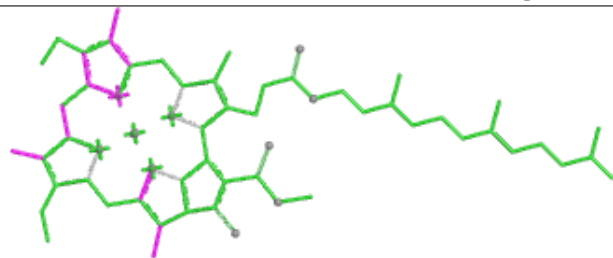


## Ligand OUR i 520

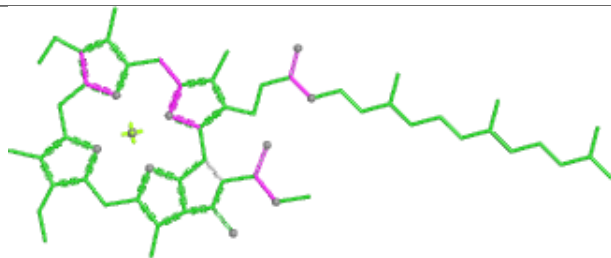




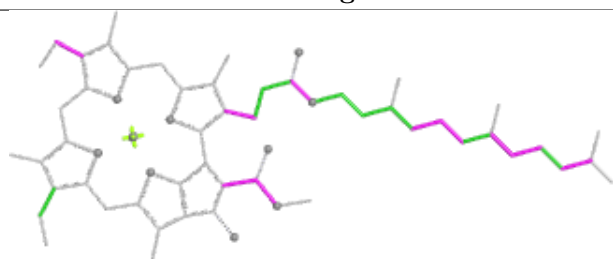
## Ligand CLA 4 310



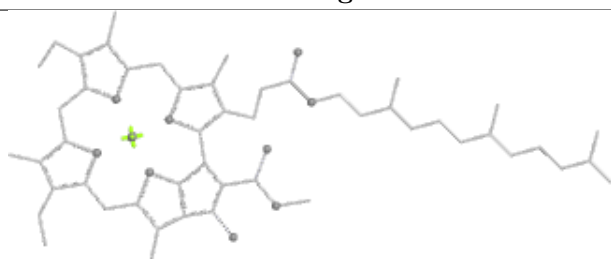
Bond lengths



Bond angles

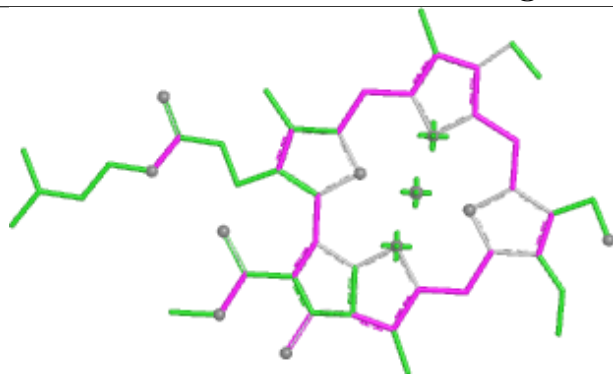


Torsions

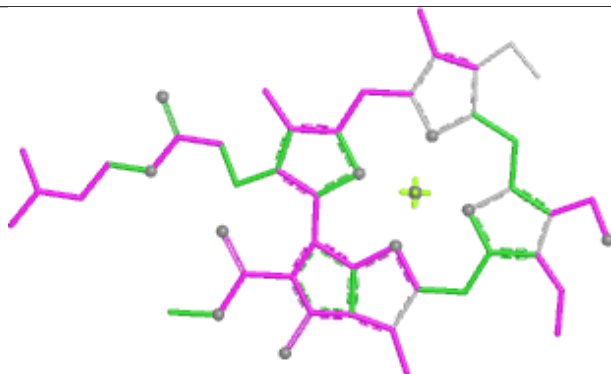


Rings

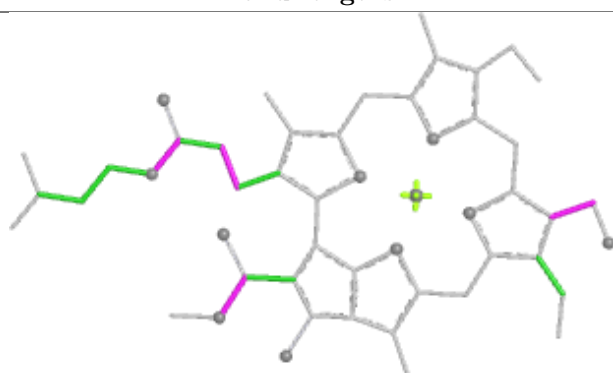
## Ligand CHL e 606



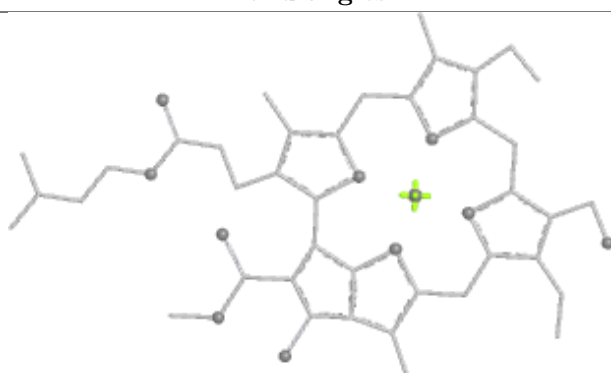
Bond lengths



Bond angles



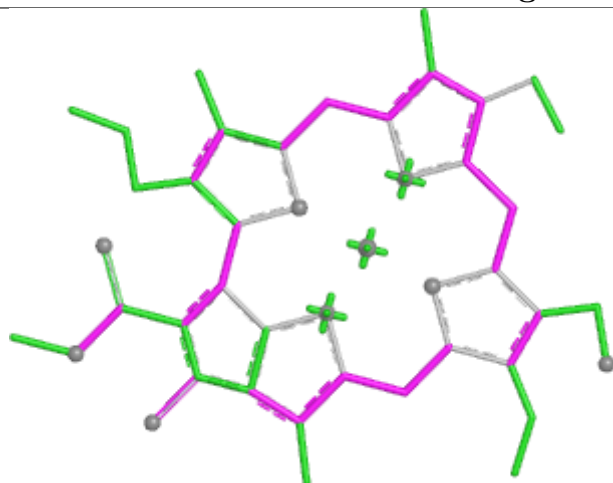
Torsions



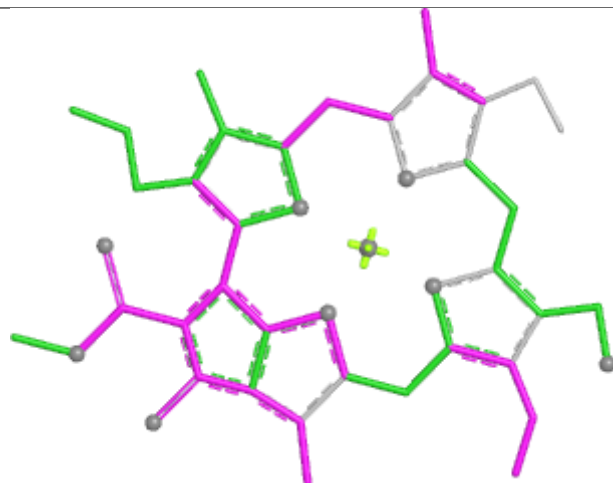
Rings



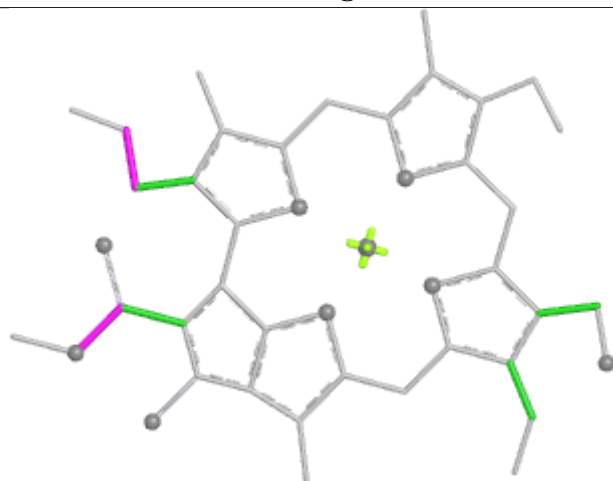
## Ligand CHL c 606



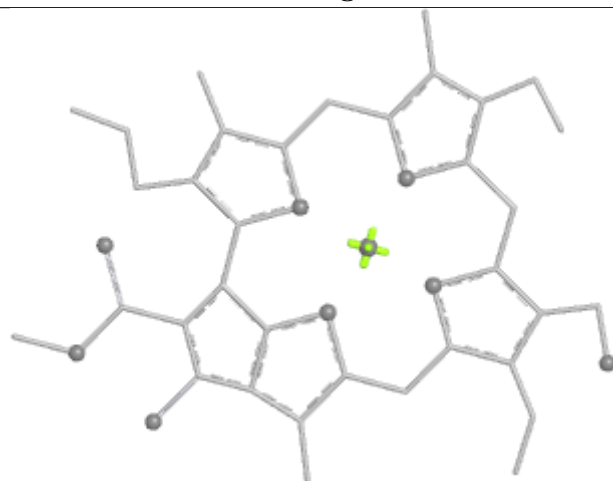
Bond lengths



Bond angles

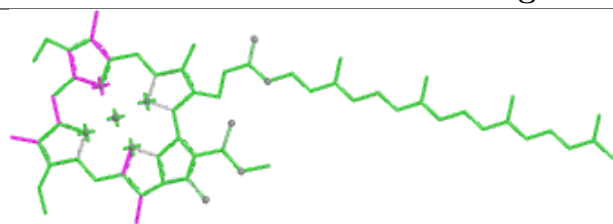


Torsions

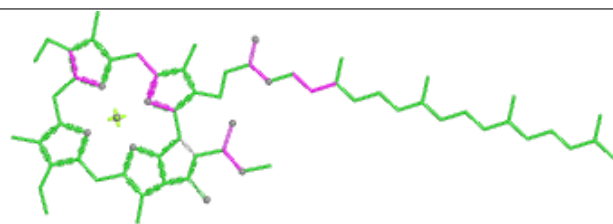


Rings

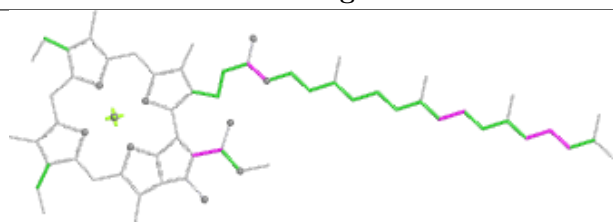
## Ligand CLA 3 304



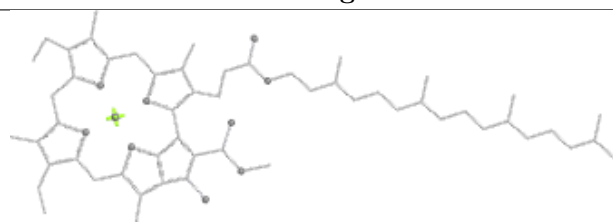
Bond lengths



Bond angles

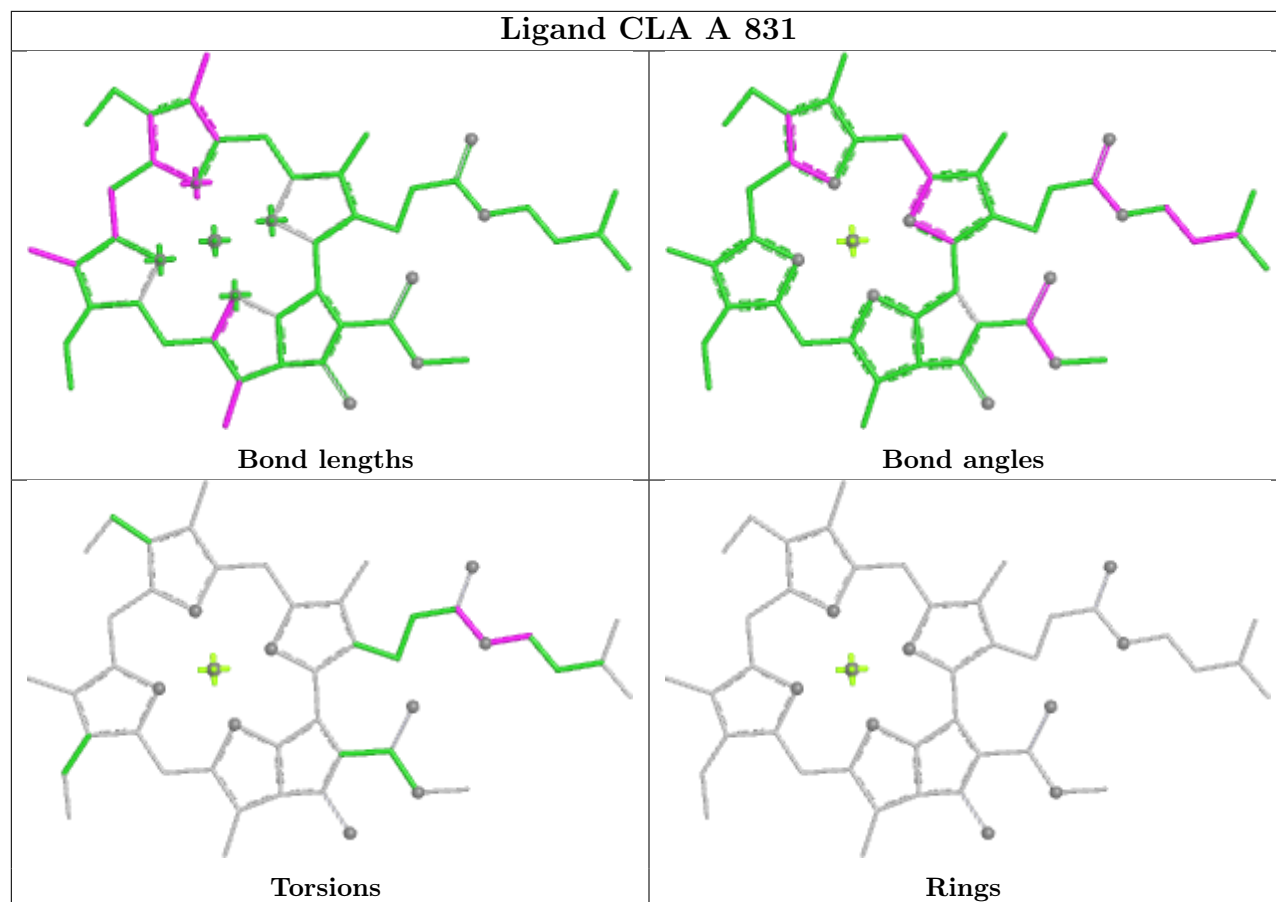


Torsions



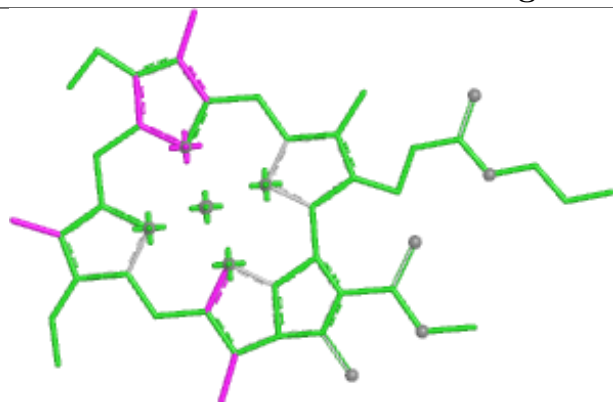
Rings



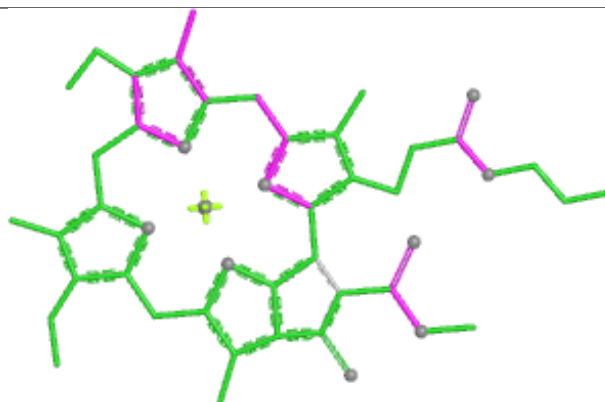




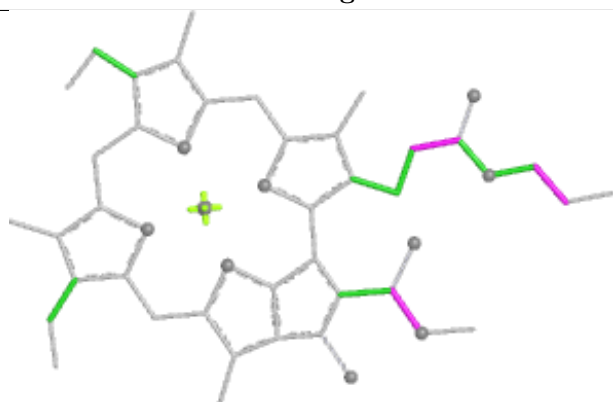
## Ligand CLA 2 311



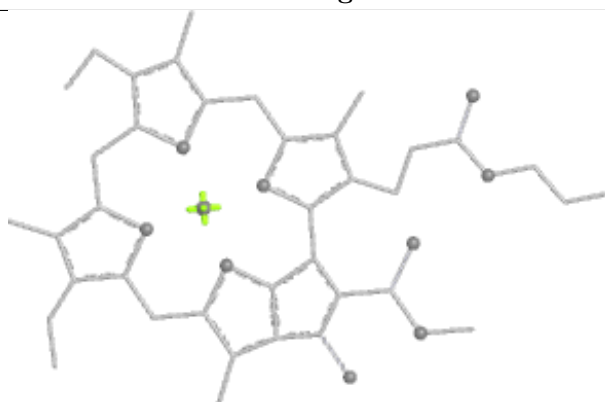
Bond lengths



Bond angles

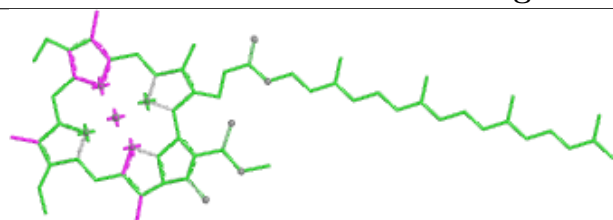


Torsions

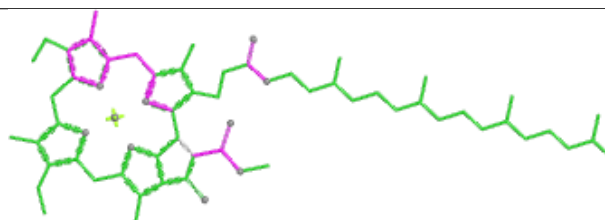


Rings

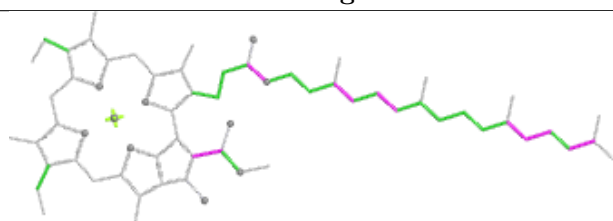
## Ligand CLA A 830



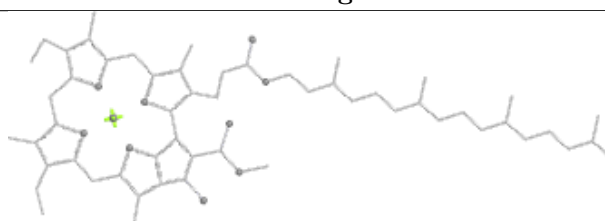
Bond lengths



Bond angles

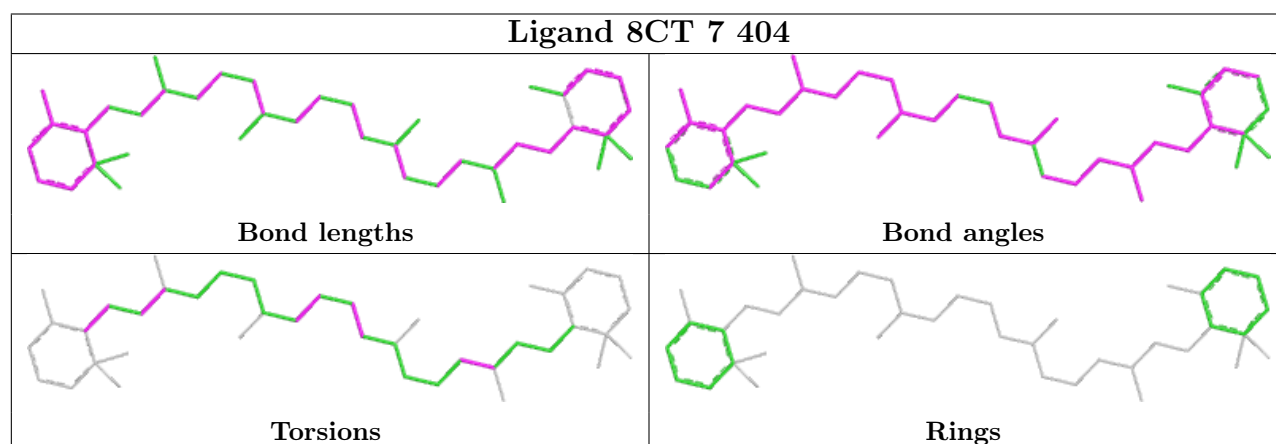
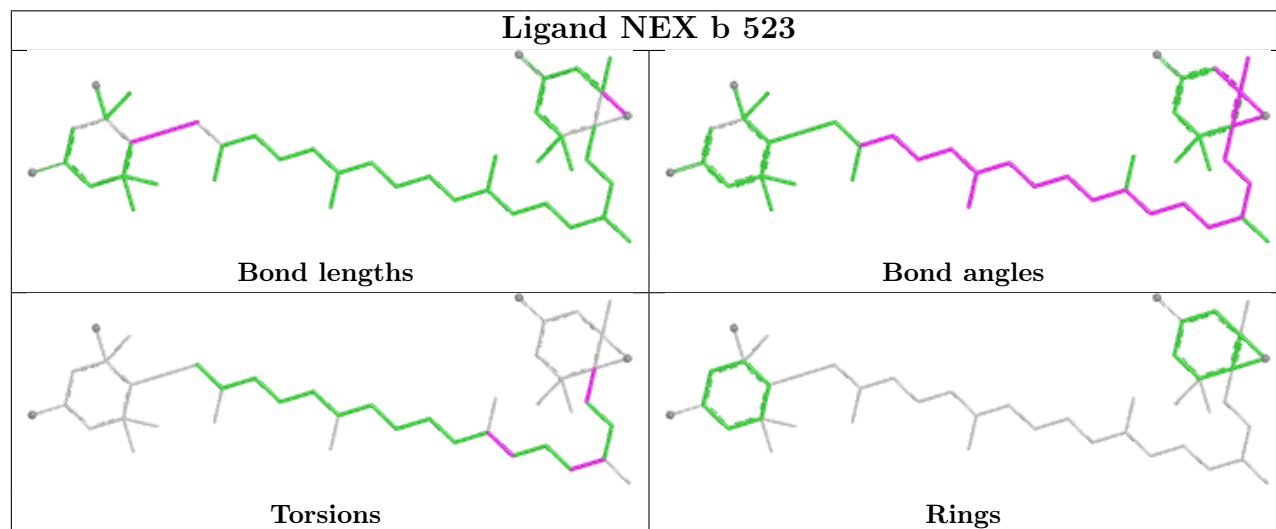
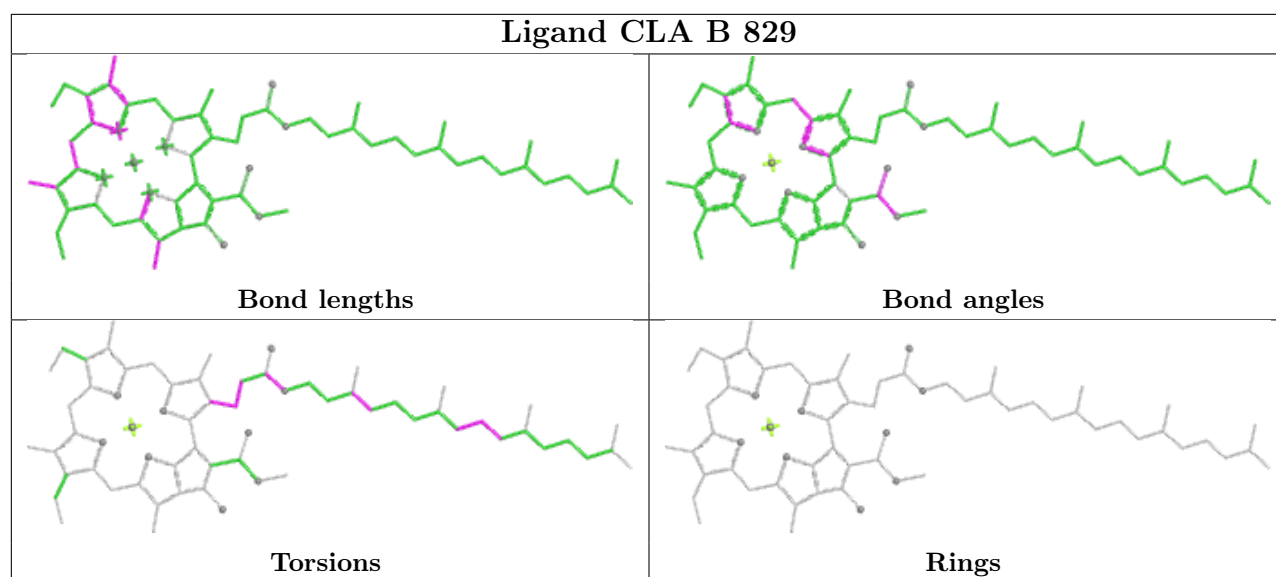


Torsions

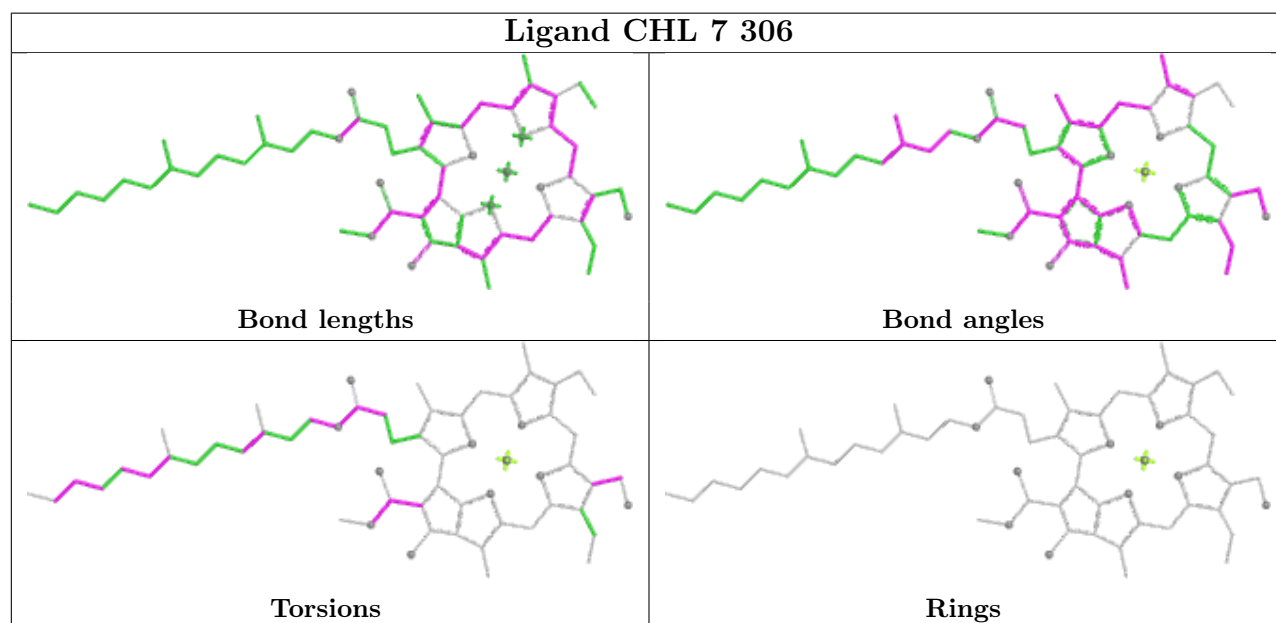
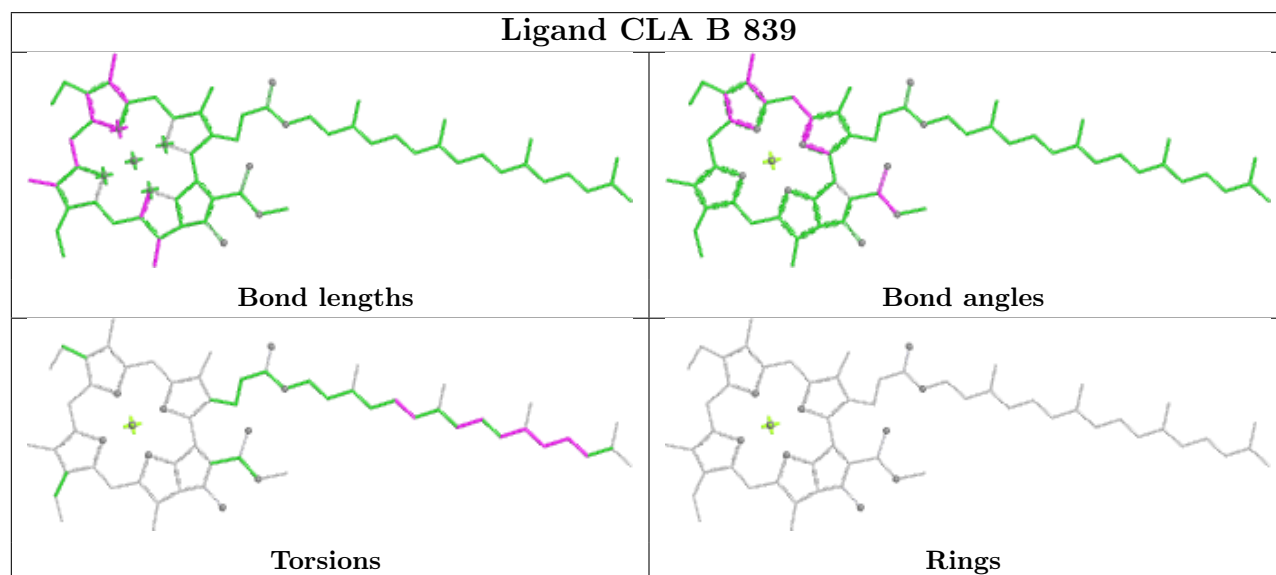
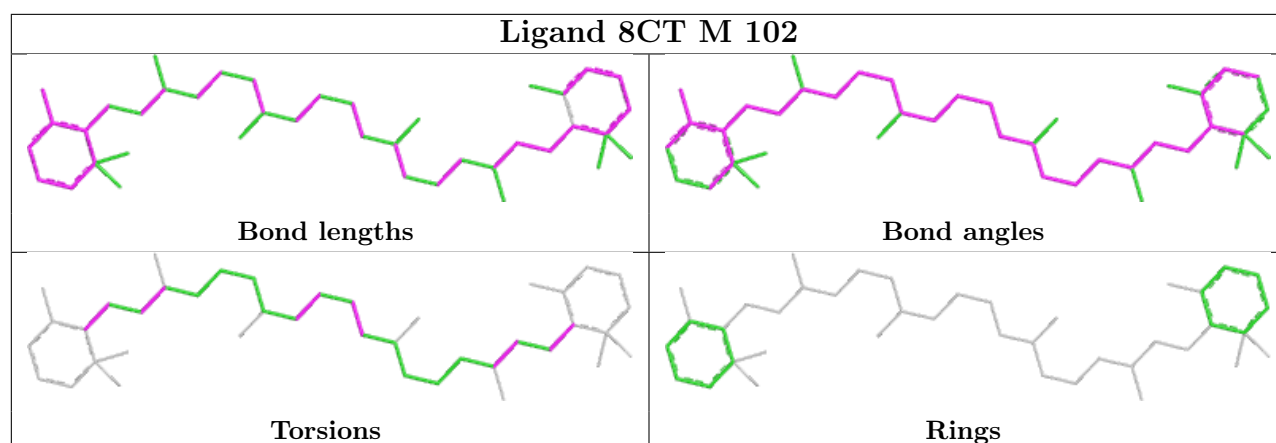


Rings

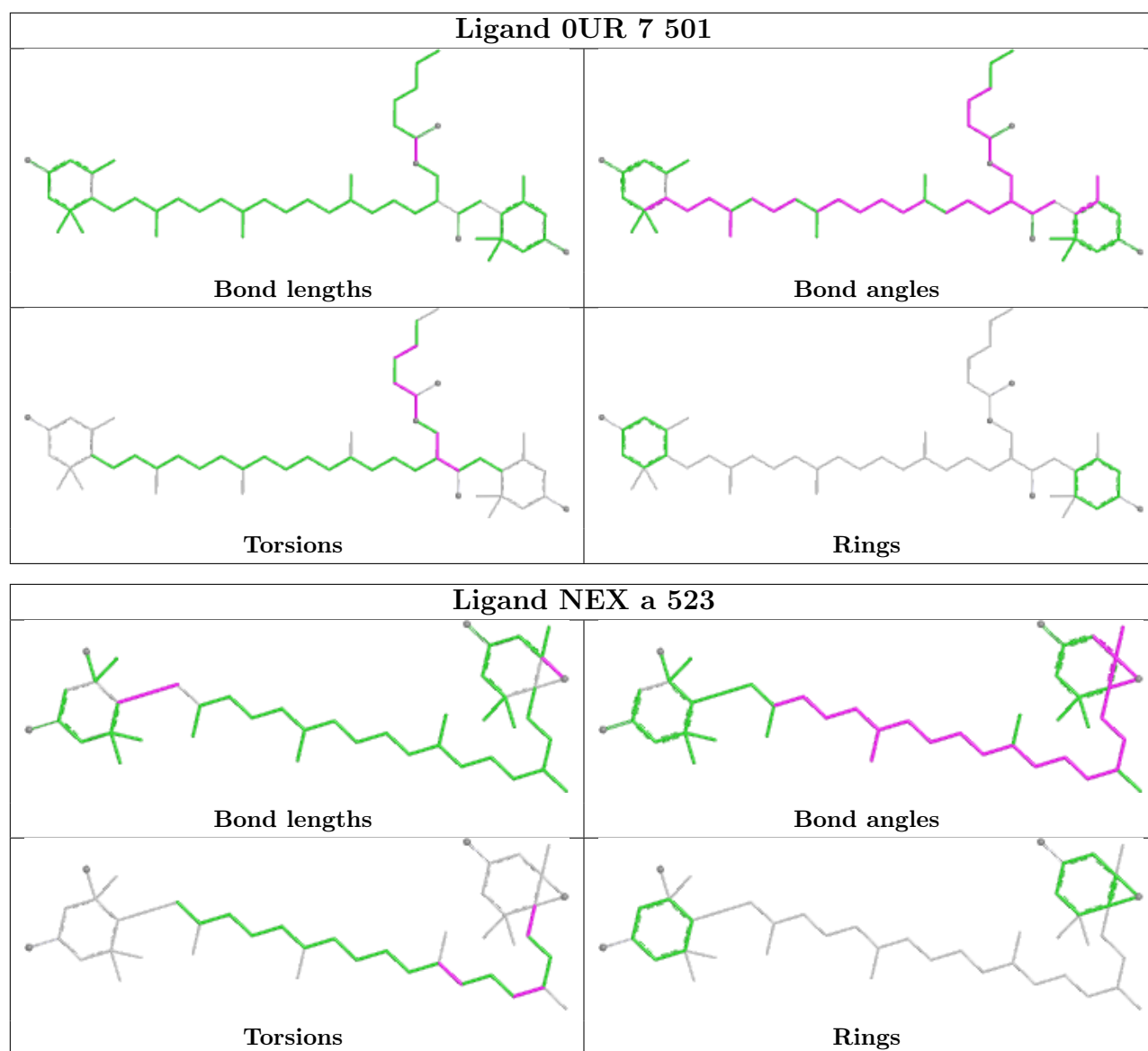




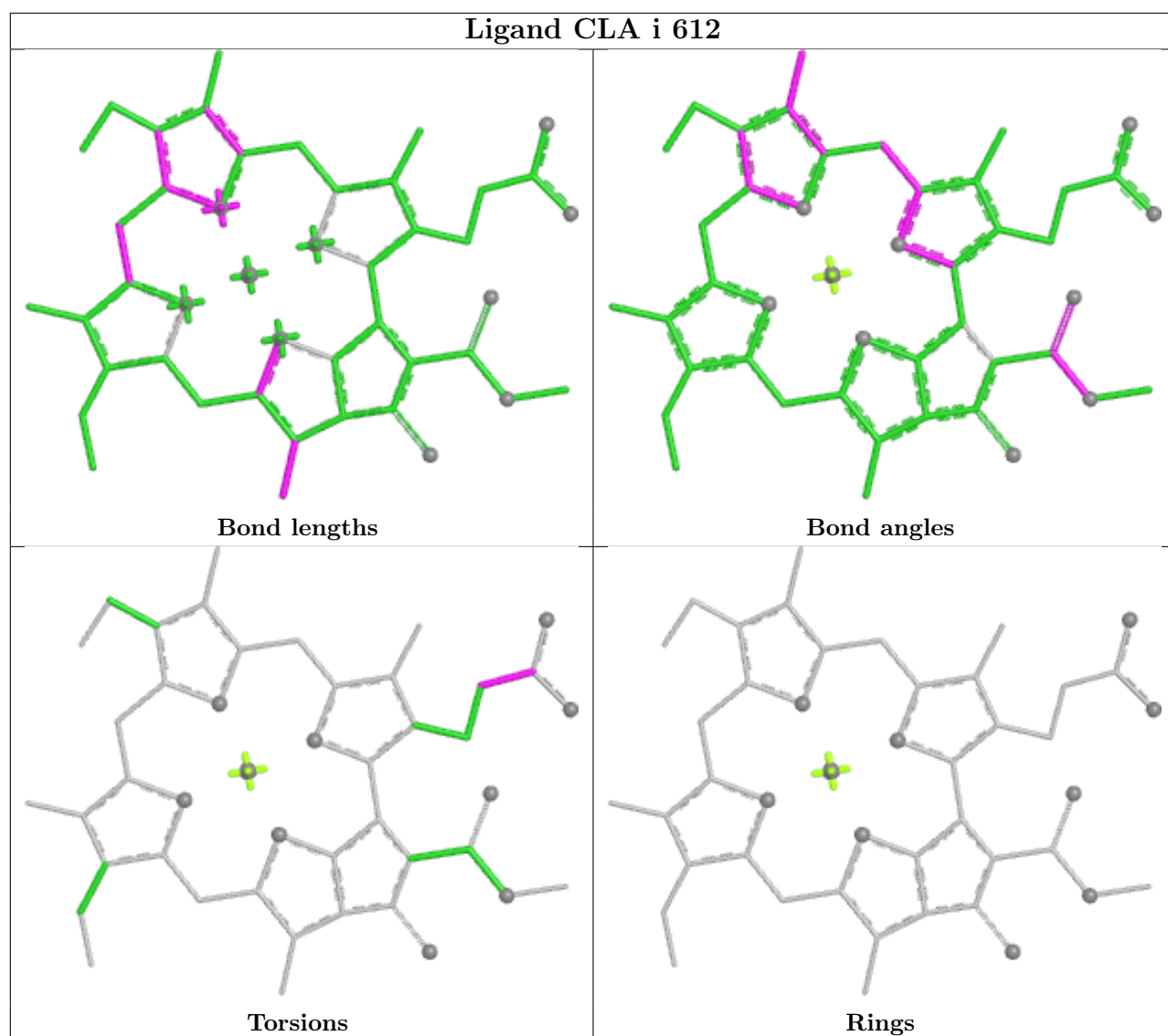






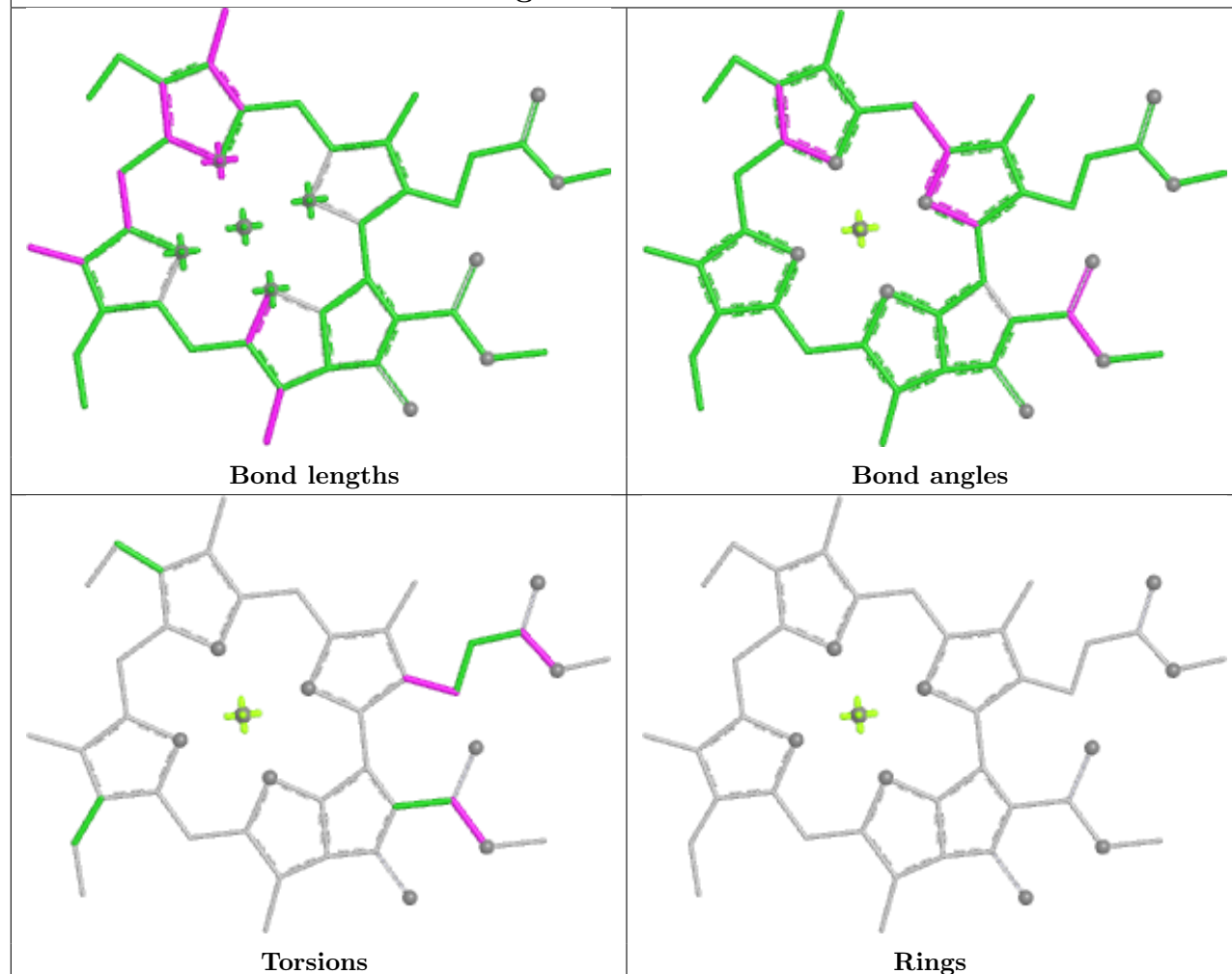




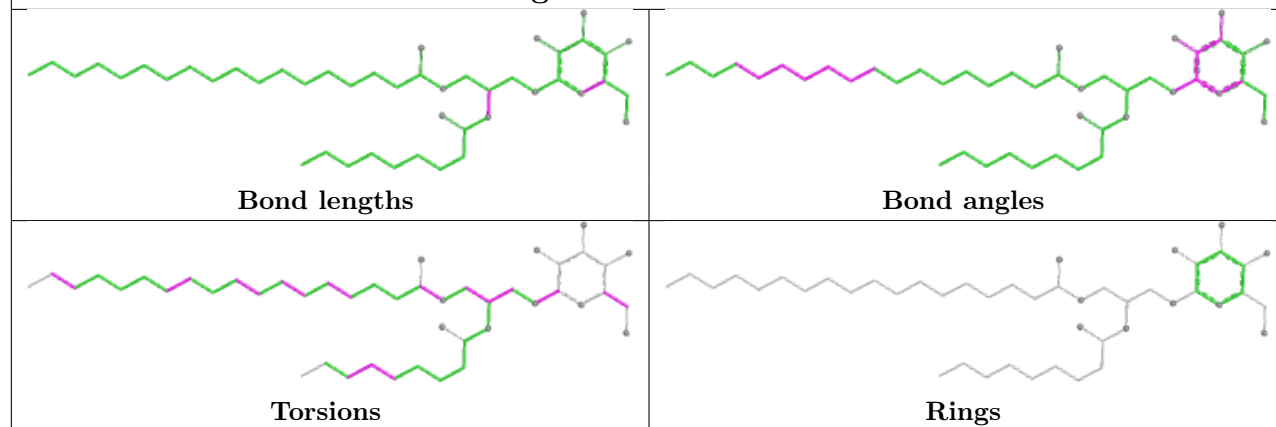




## Ligand CLA L 204

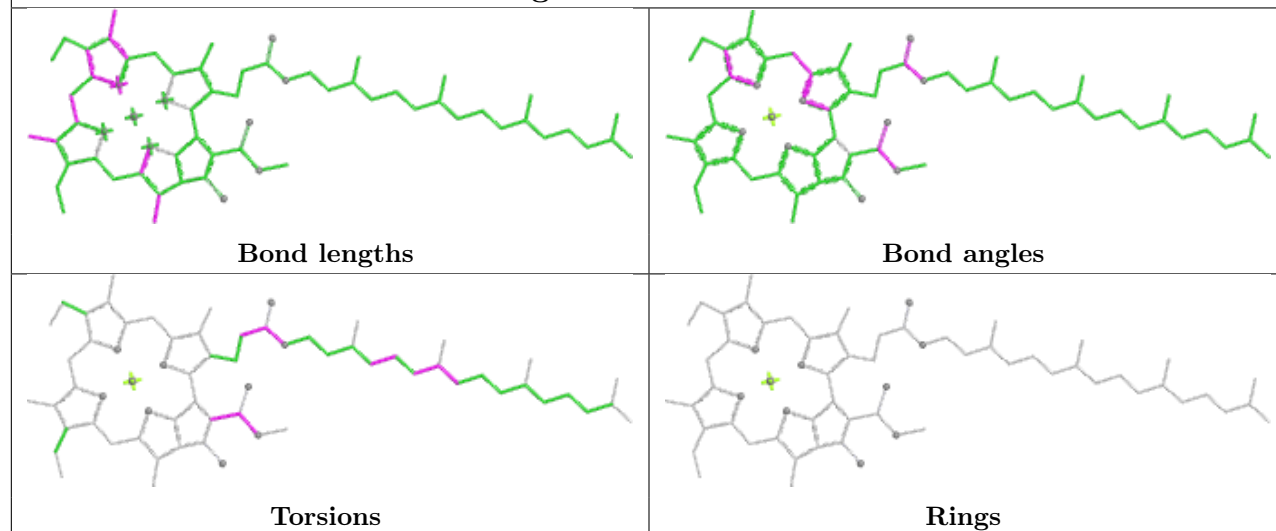


## Ligand LMG J 105

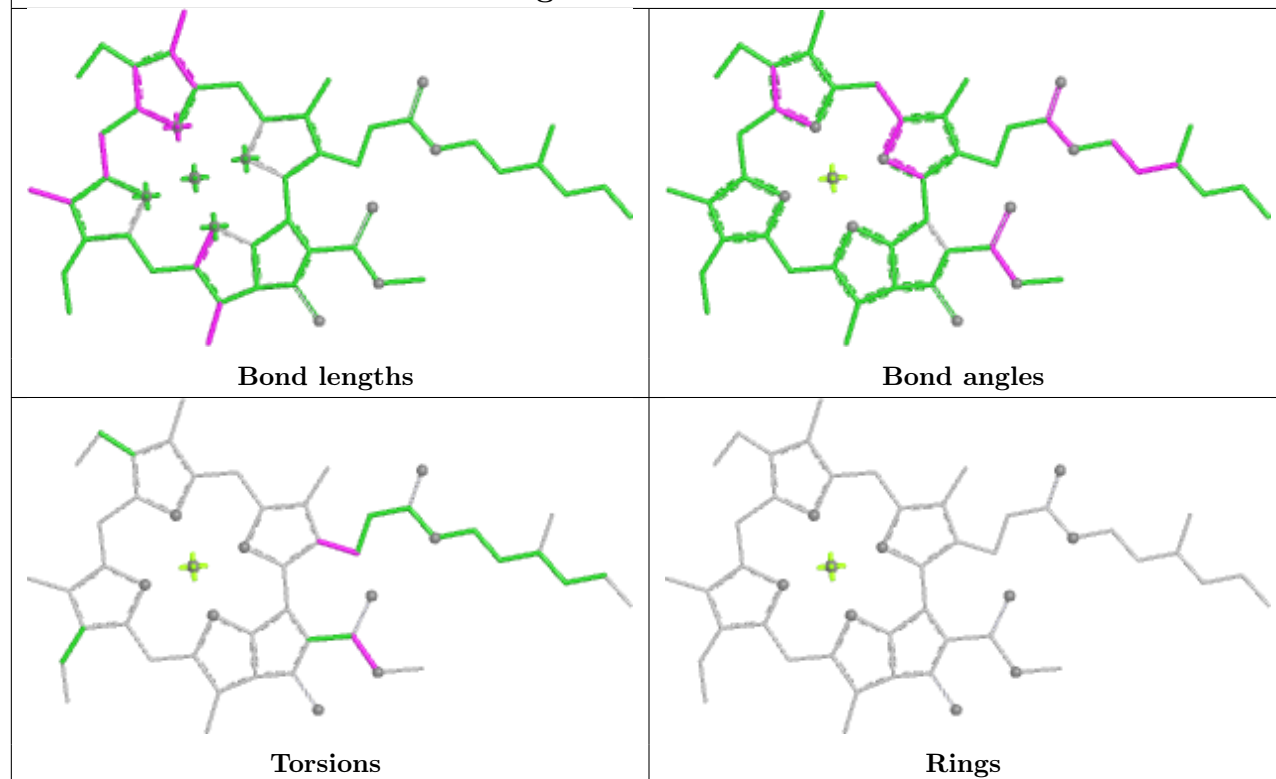




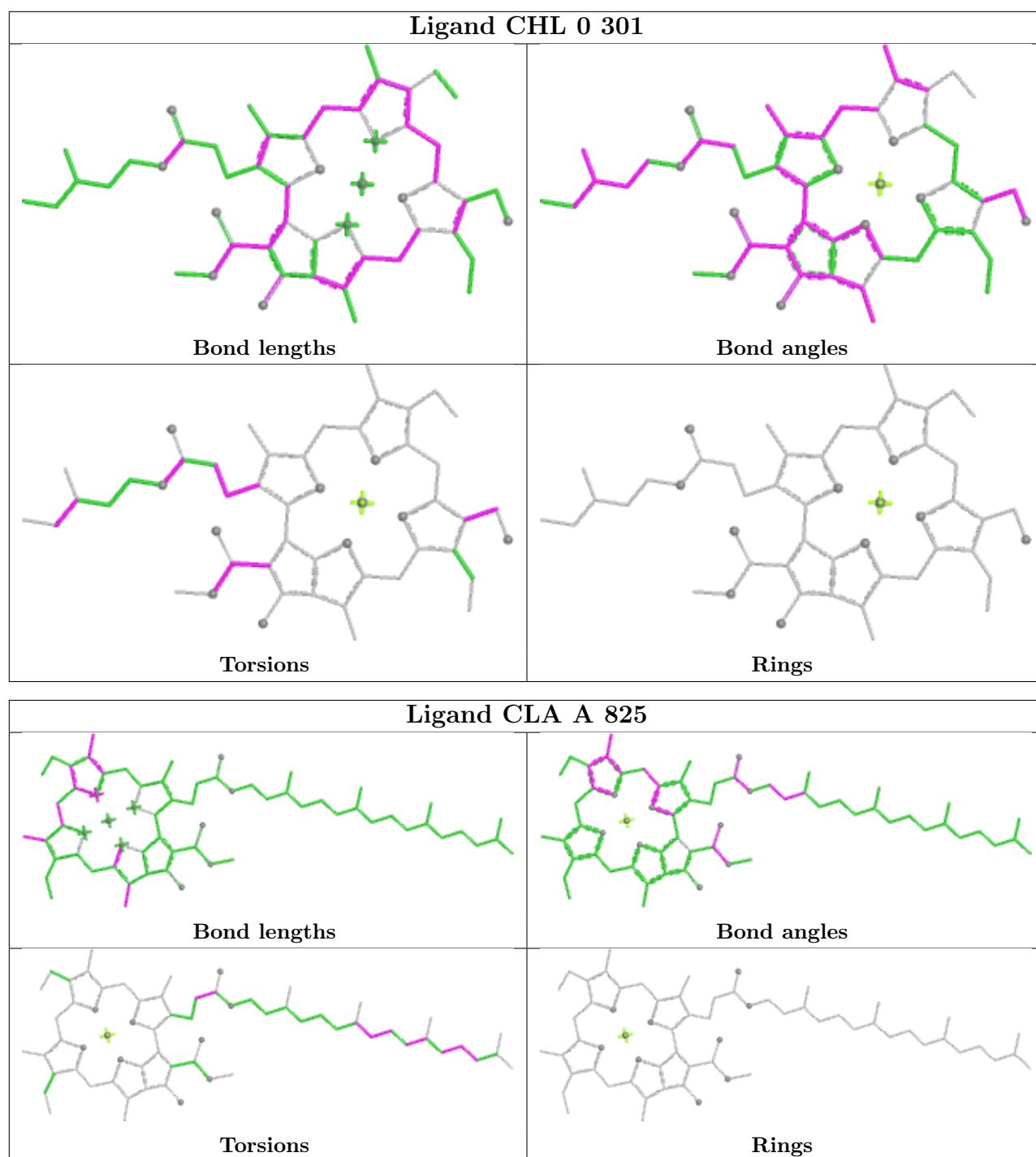
## Ligand CLA A 833



## Ligand CLA 0 304

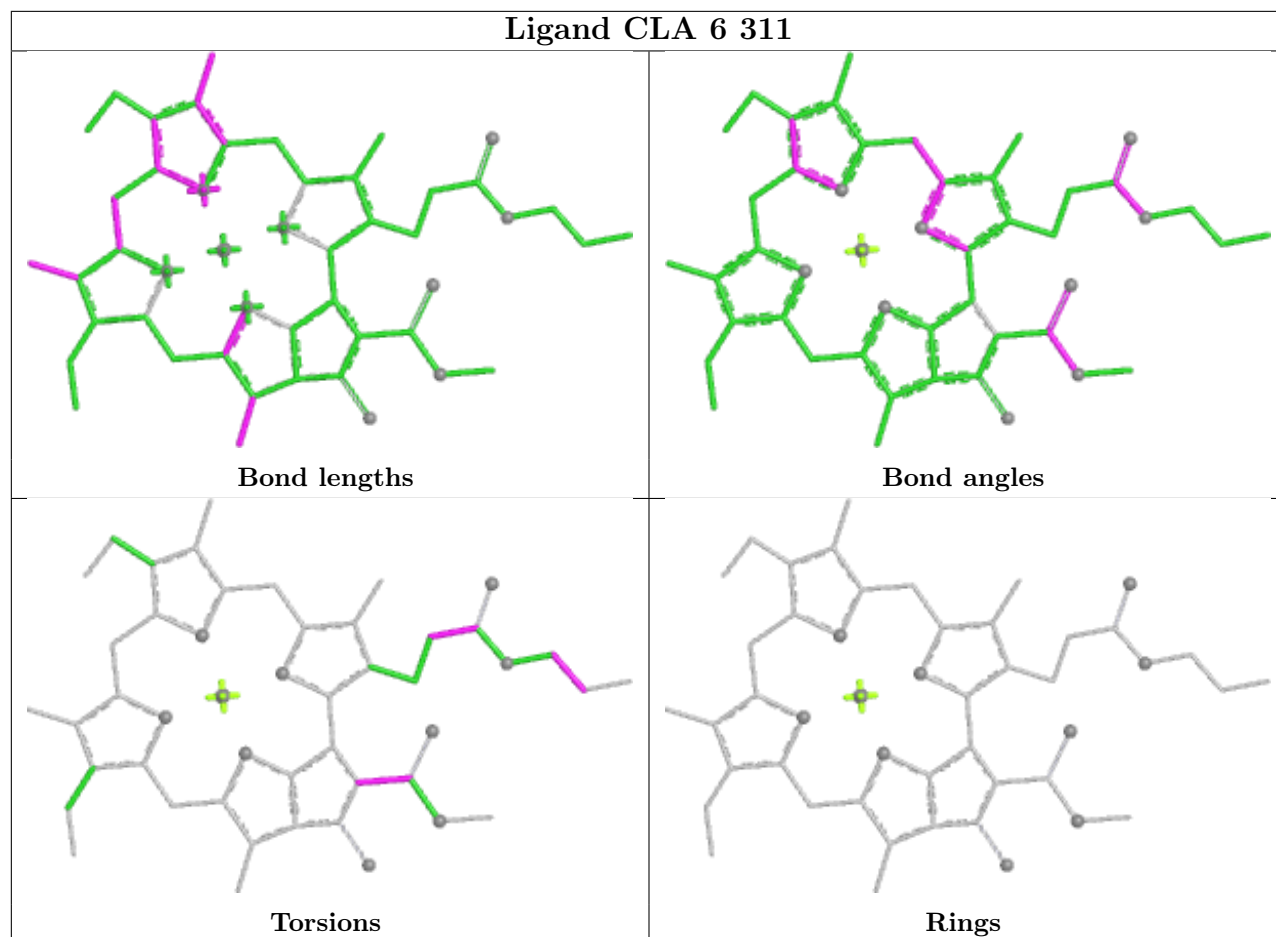






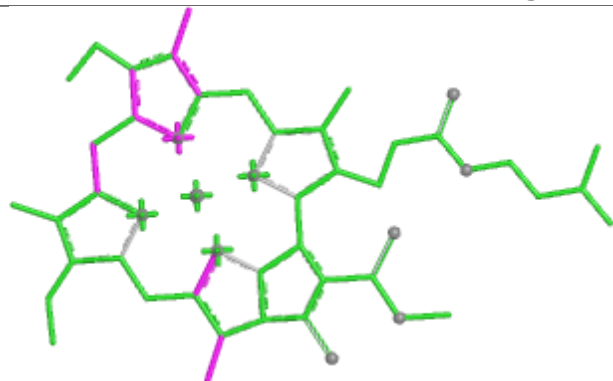


## Ligand CLA 6 311

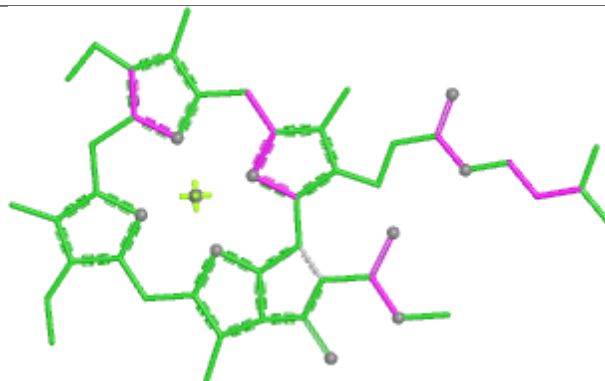




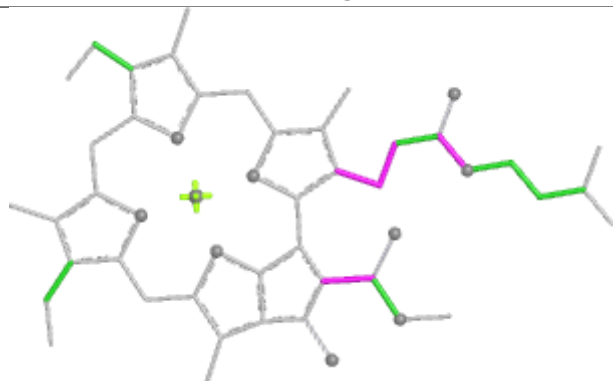
## Ligand CLA i 604



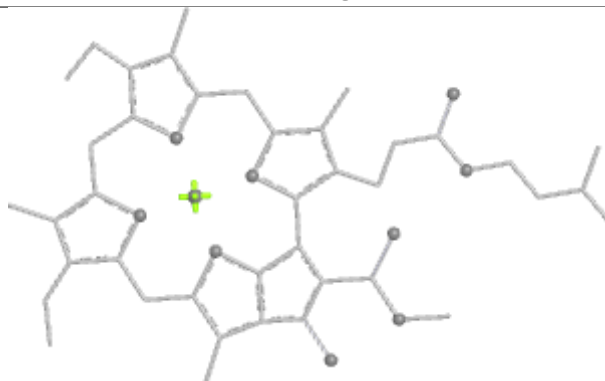
Bond lengths



Bond angles

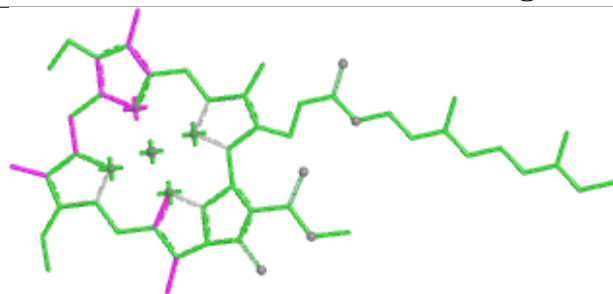


Torsions

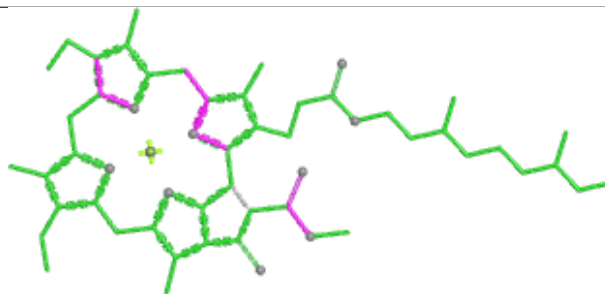


Rings

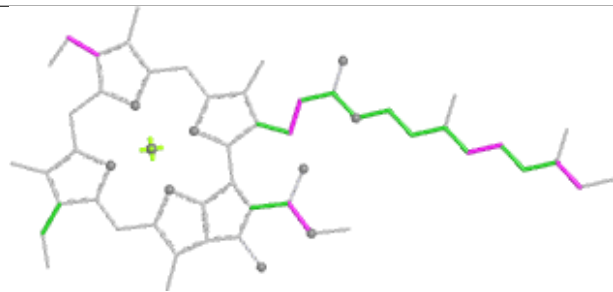
## Ligand CLA 8 312



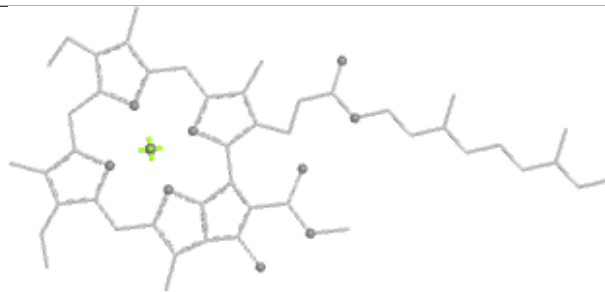
Bond lengths



Bond angles



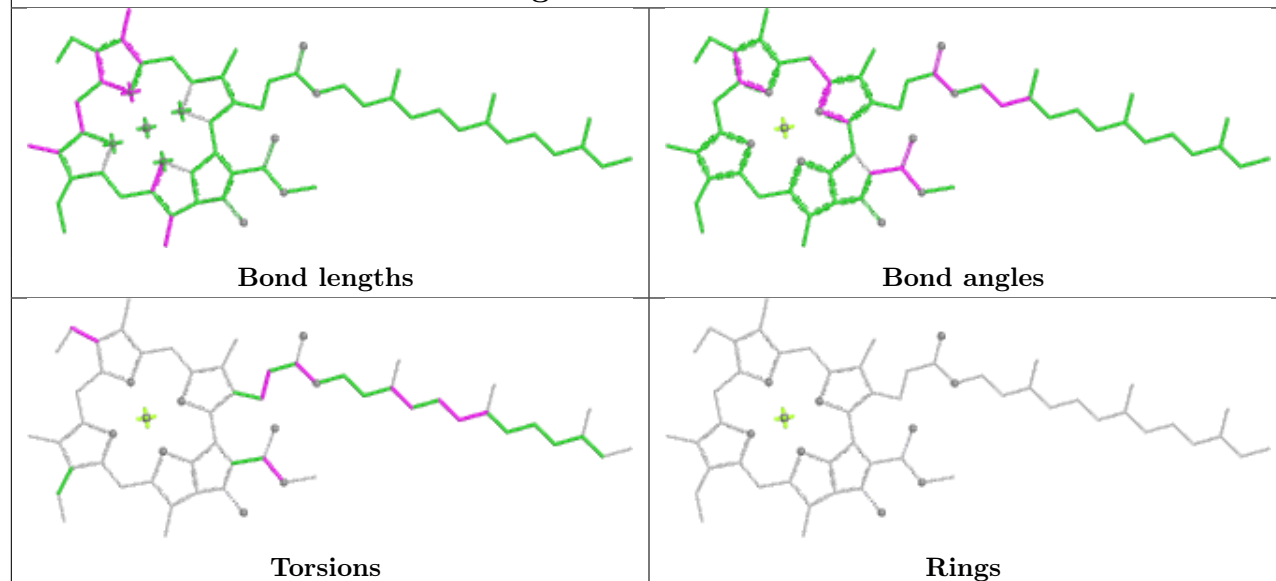
Torsions



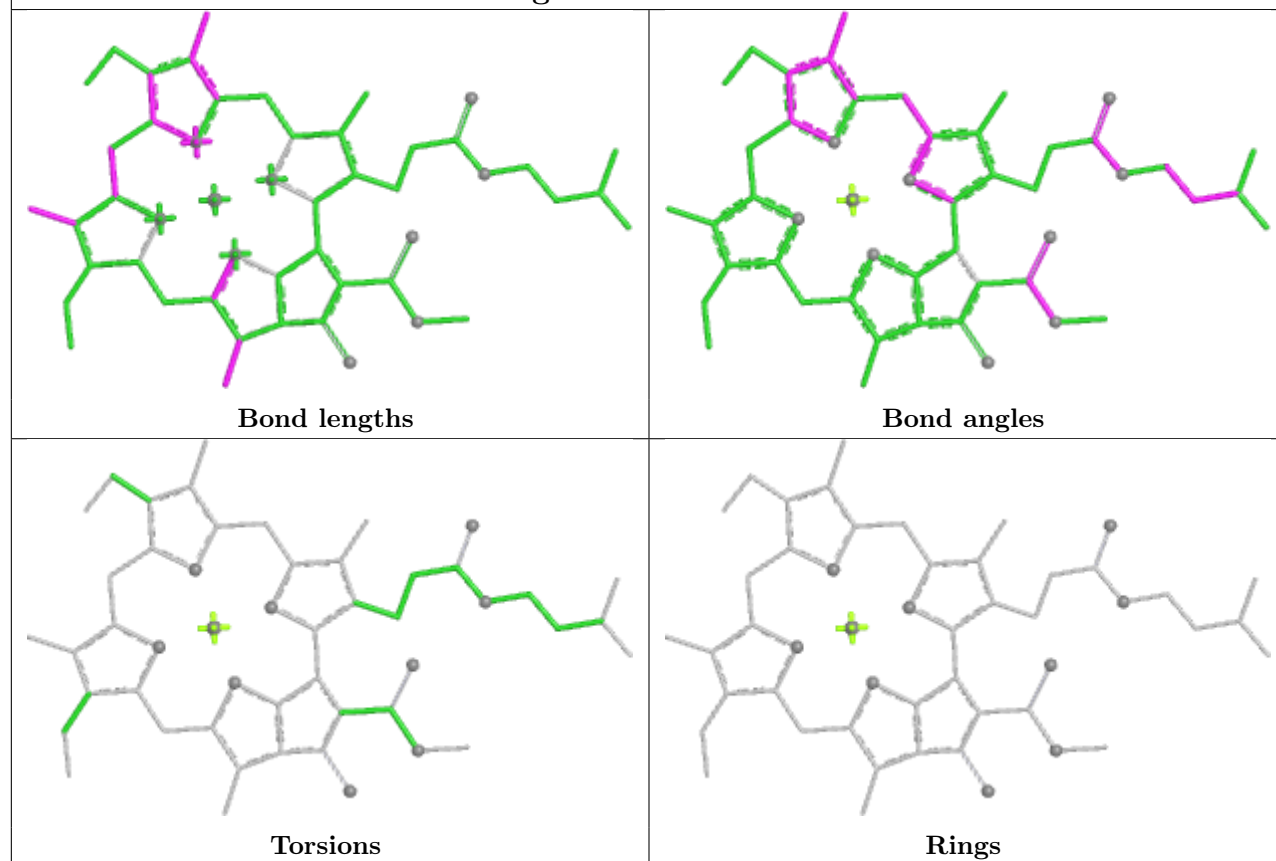
Rings



## Ligand CLA A 837

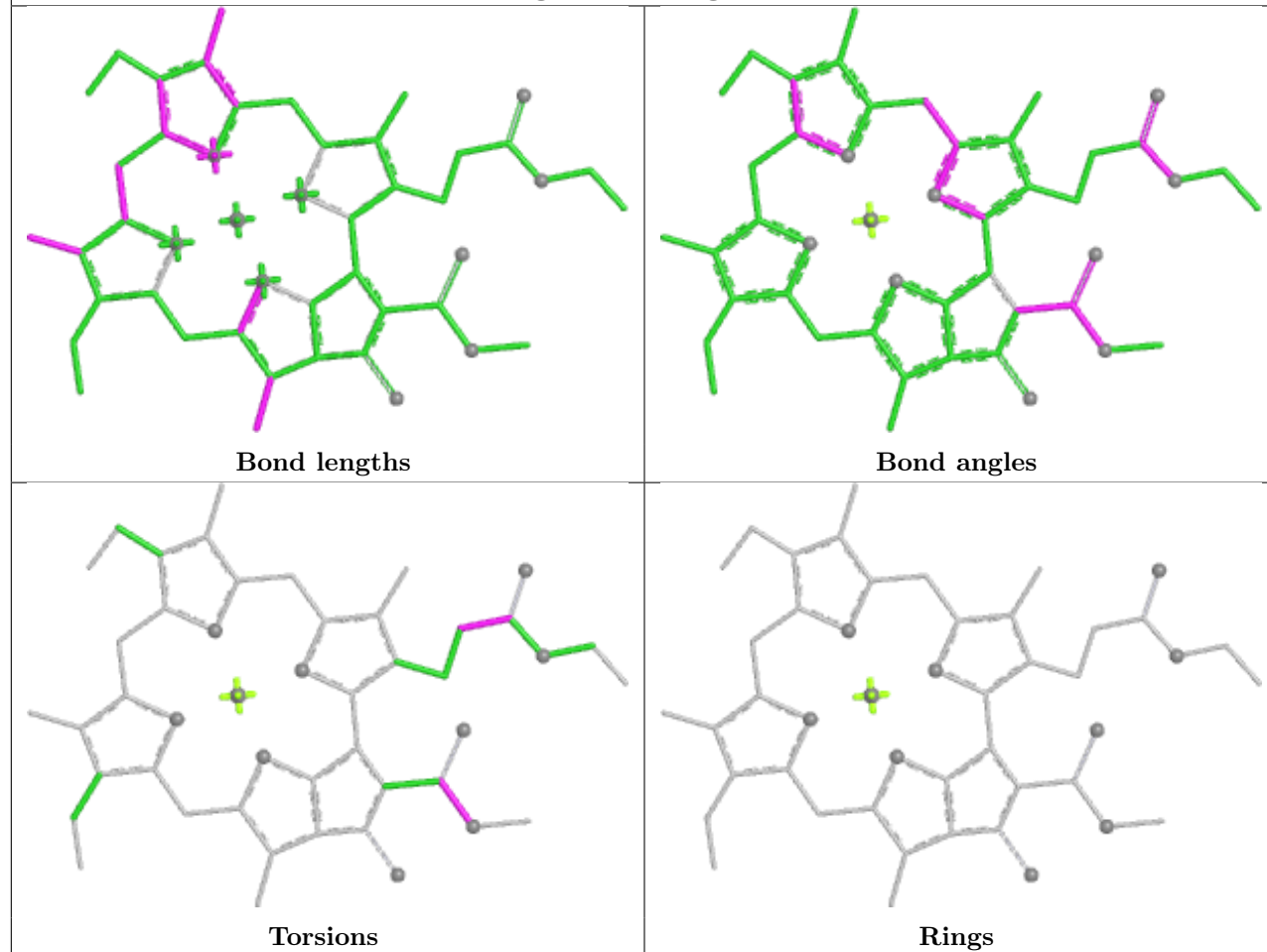


## Ligand CLA B 821

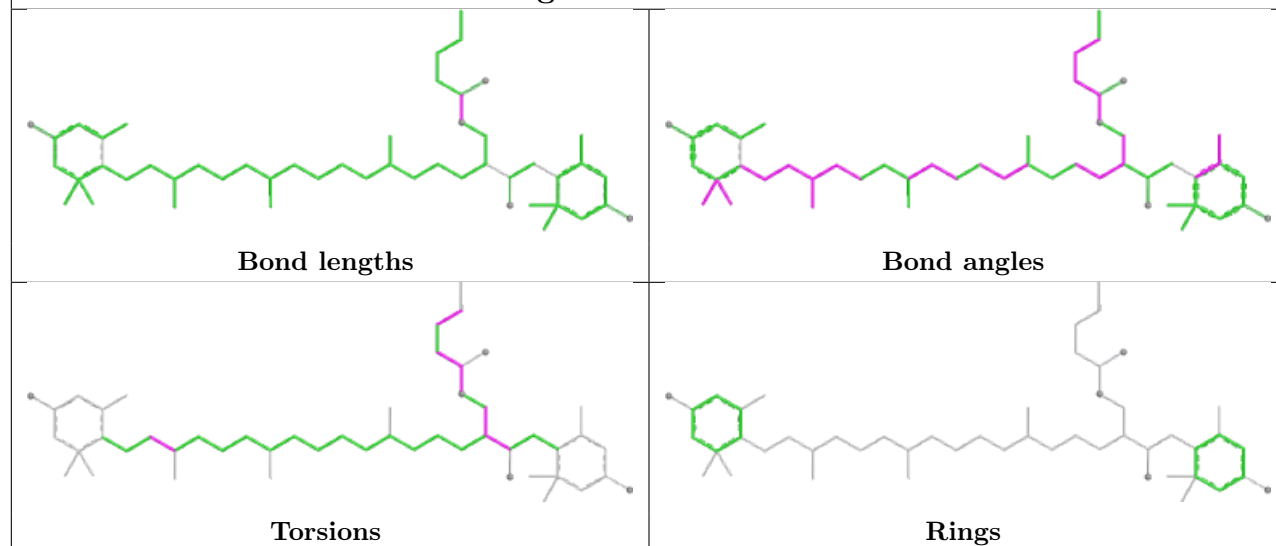




## Ligand CLA g 613

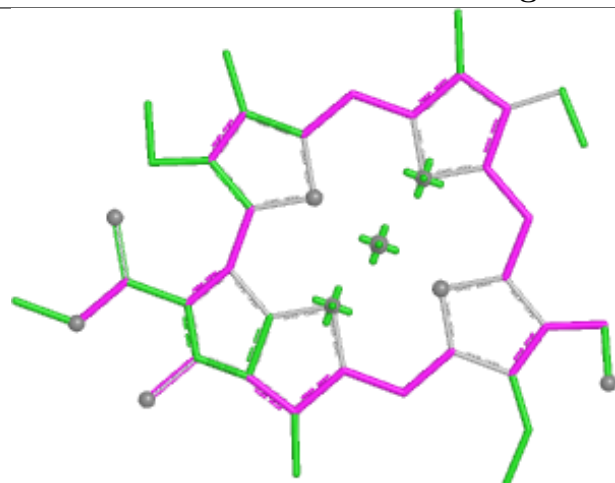


## Ligand OUR 2 502

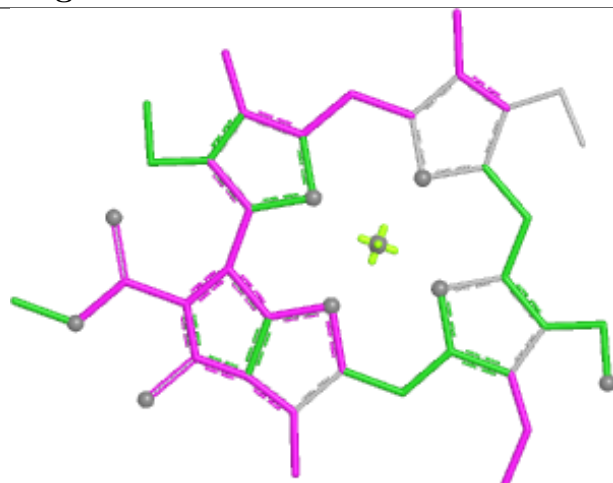




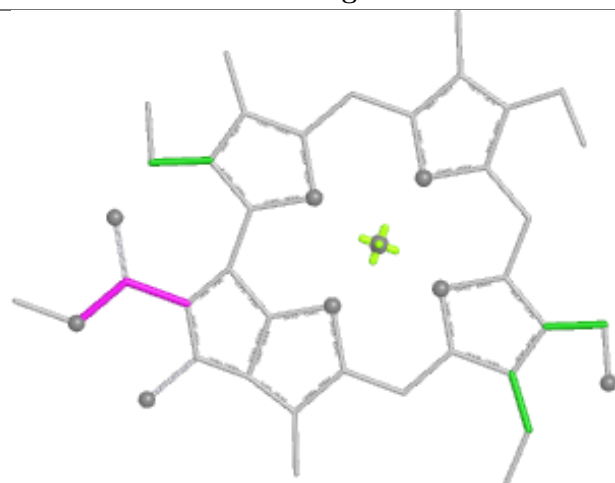
## Ligand CHL g 605



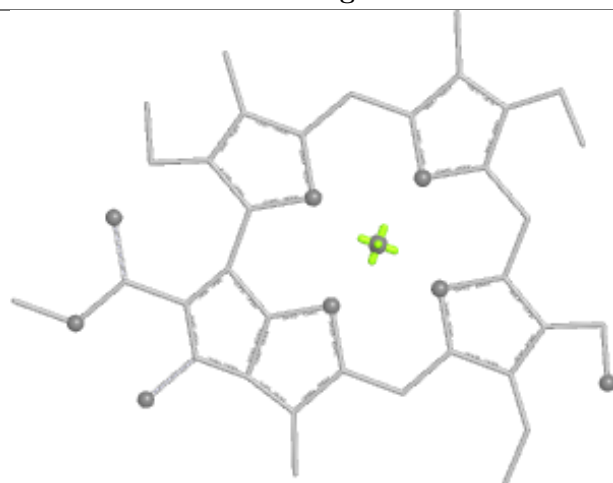
Bond lengths



Bond angles



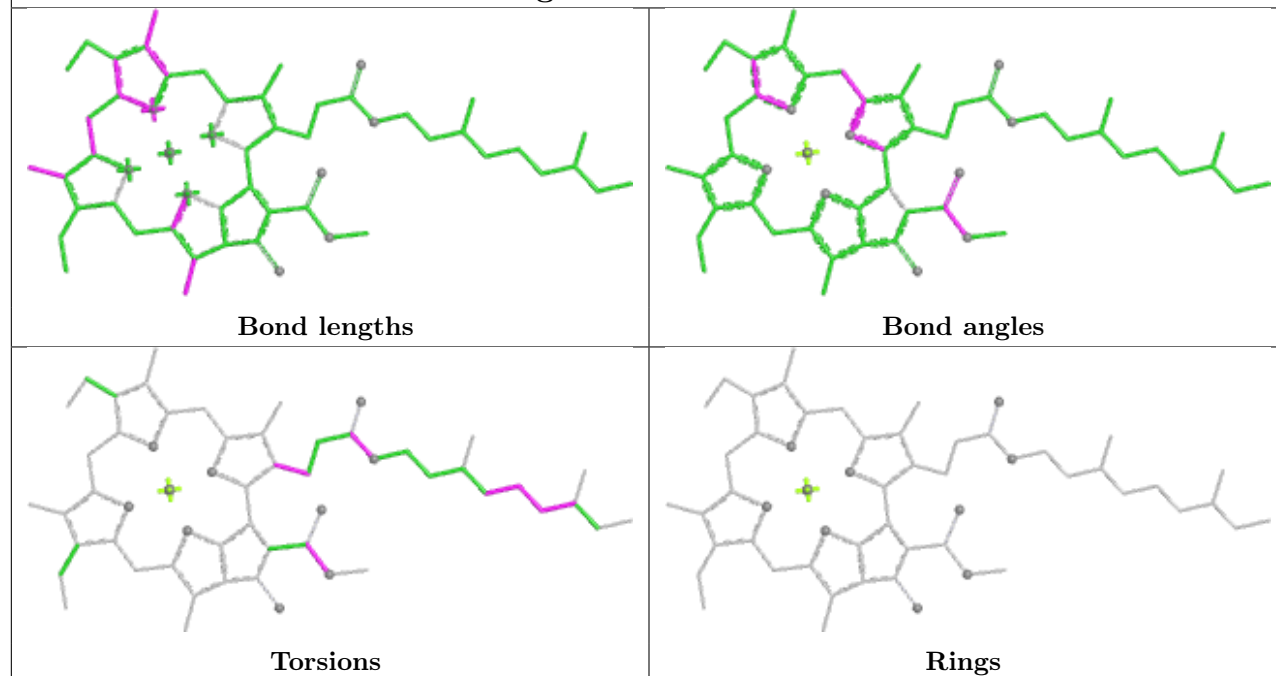
Torsions



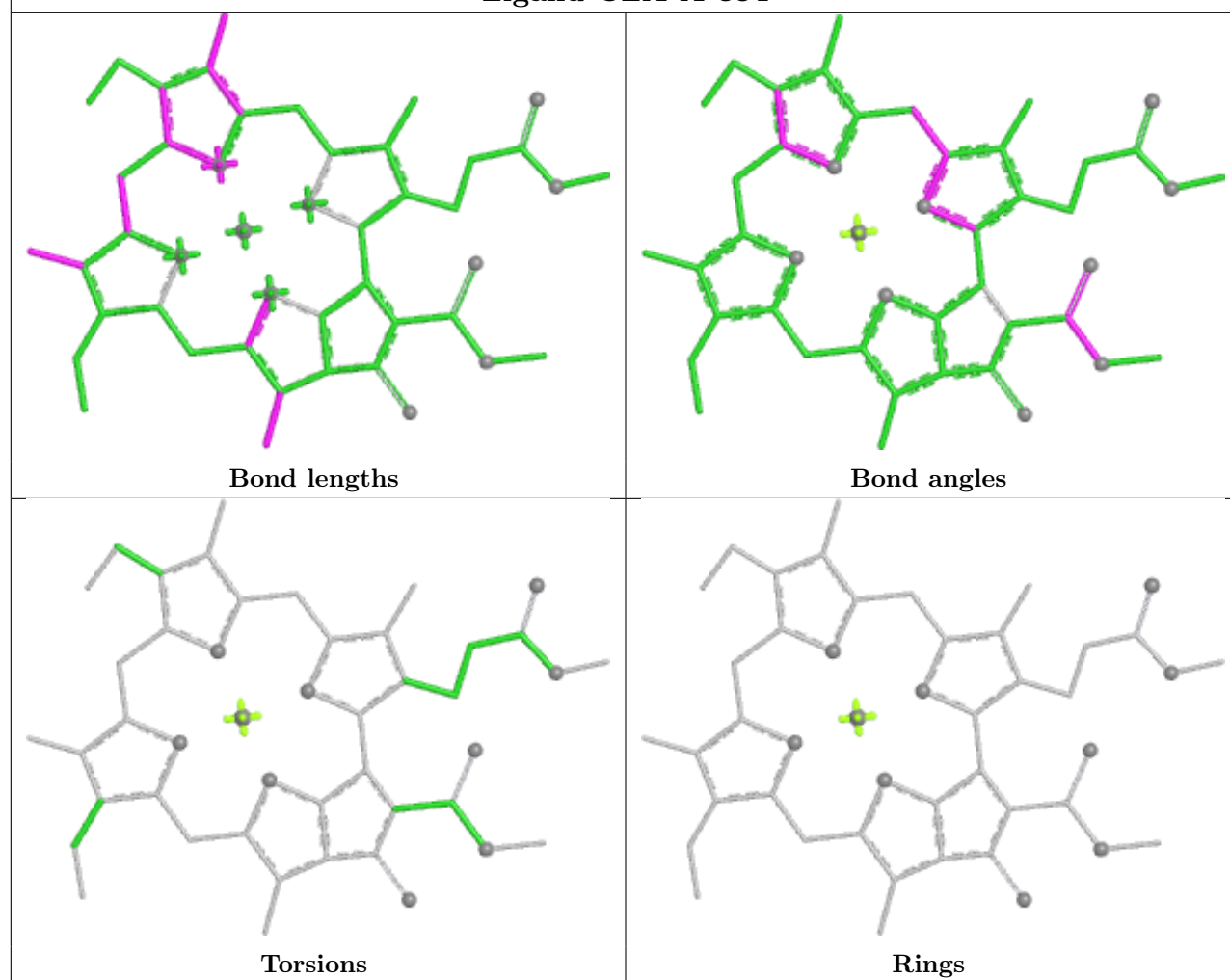
Rings



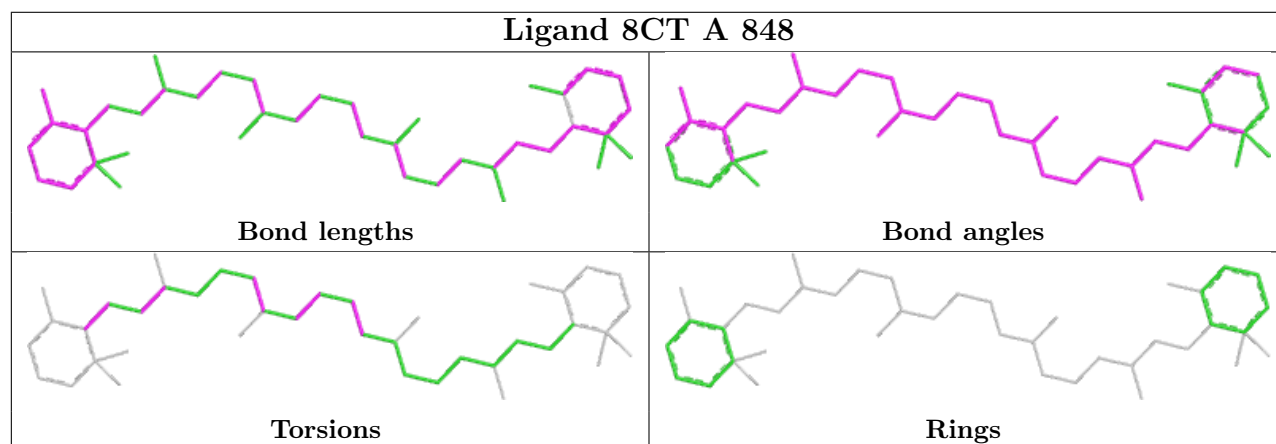
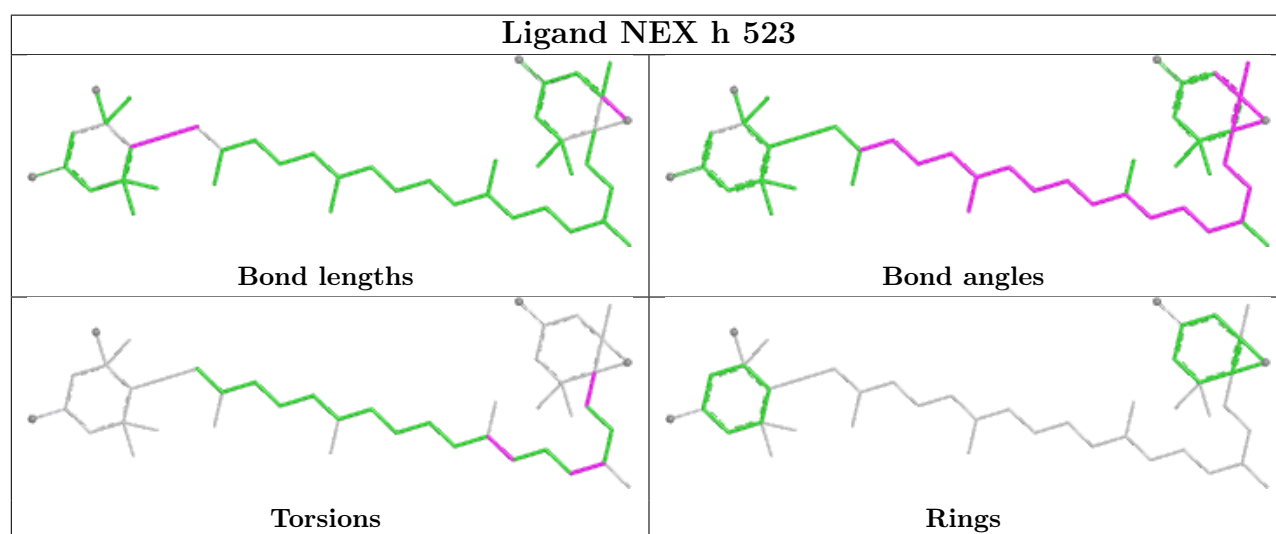
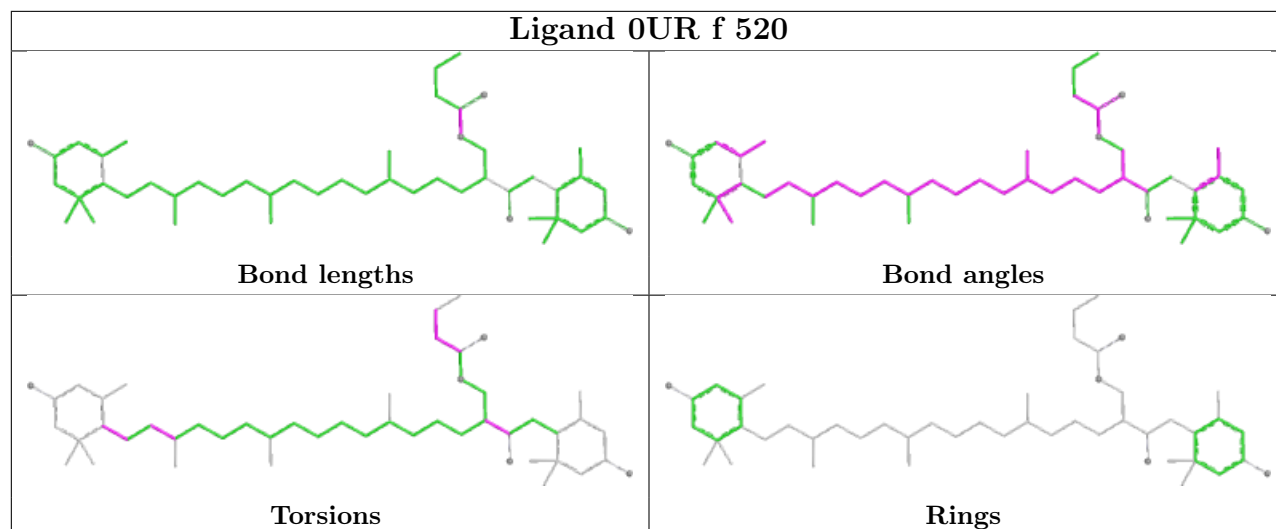
## Ligand CLA 5 312



## Ligand CLA A 834

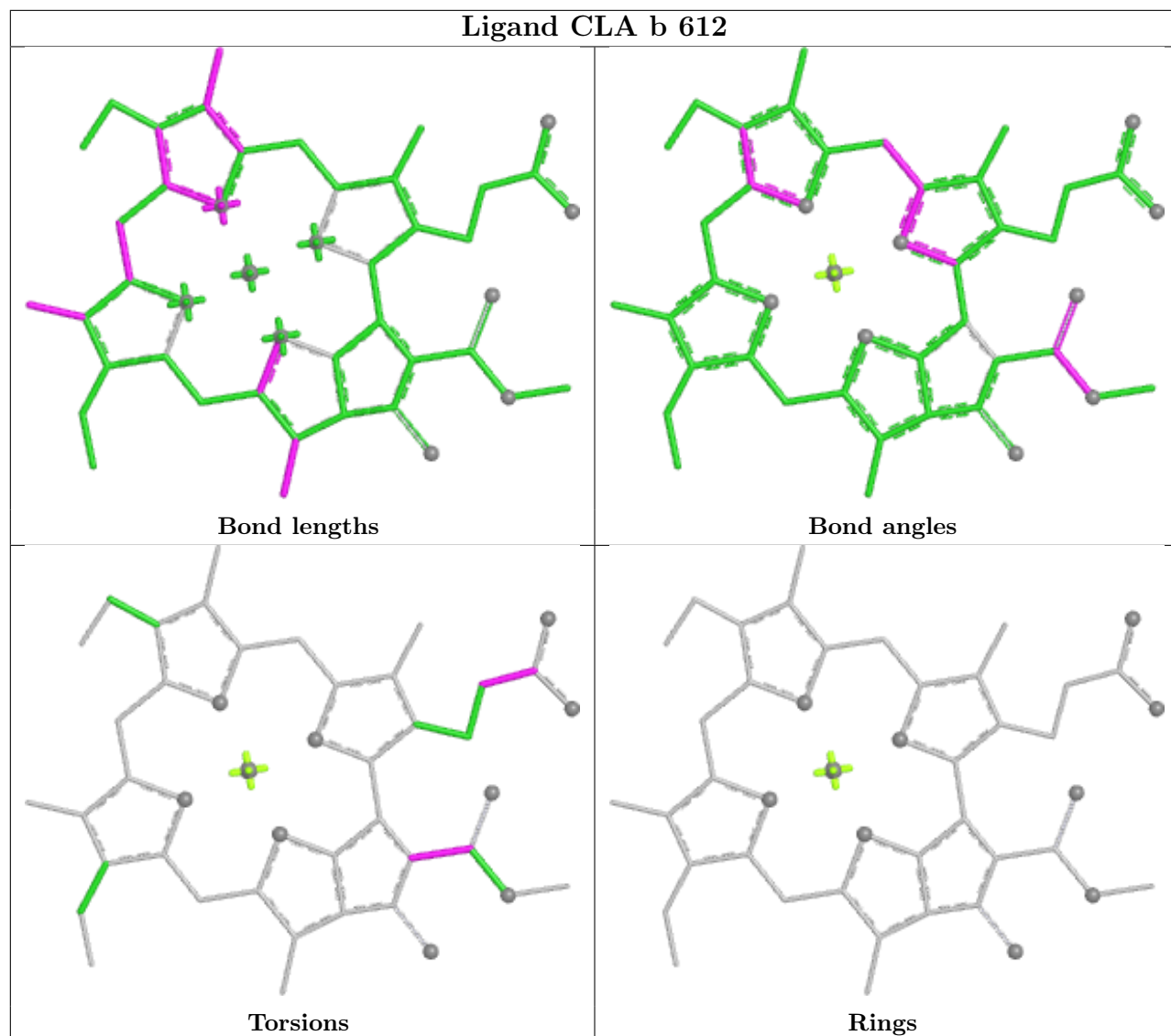




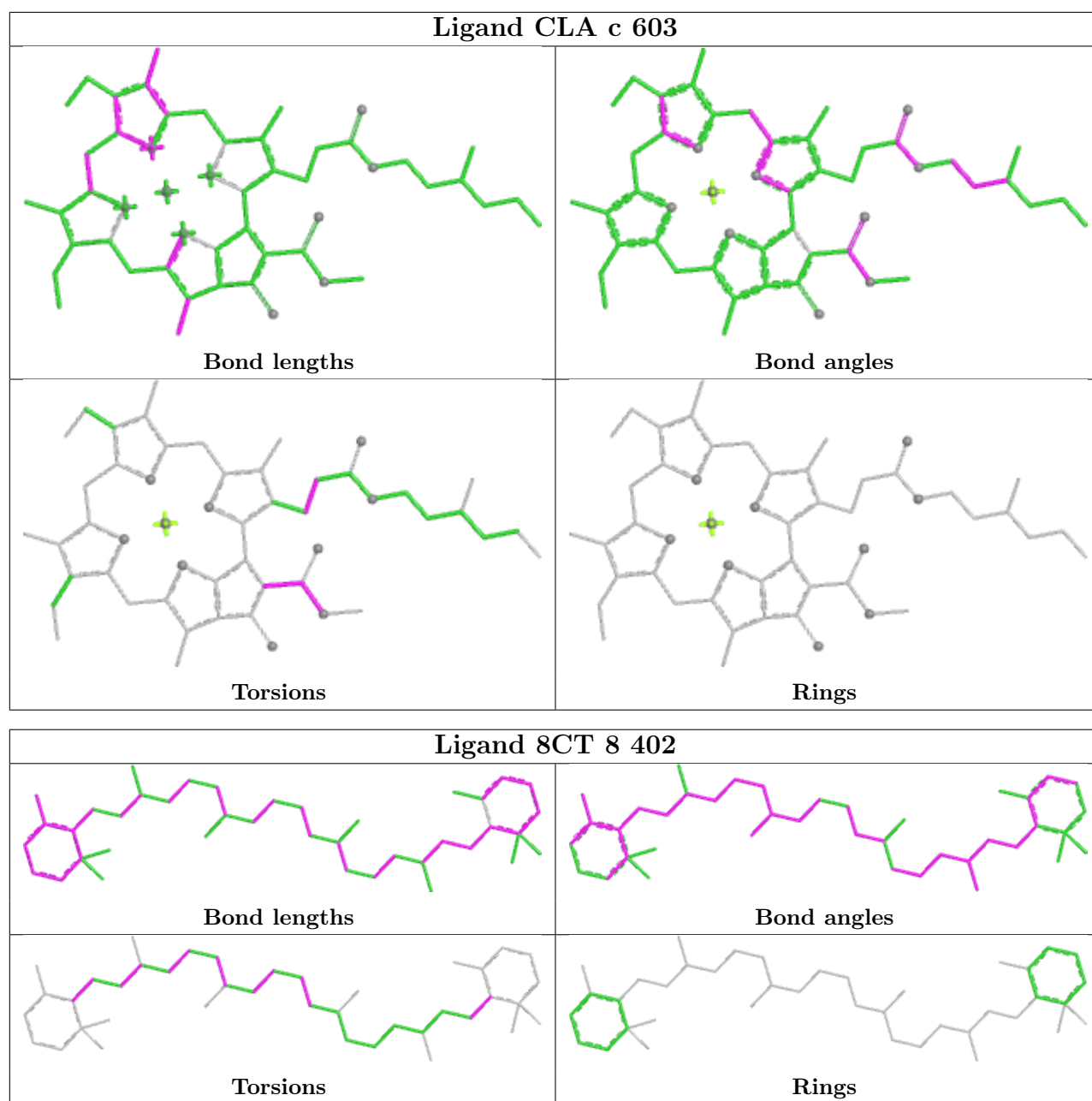




## Ligand CLA b 612

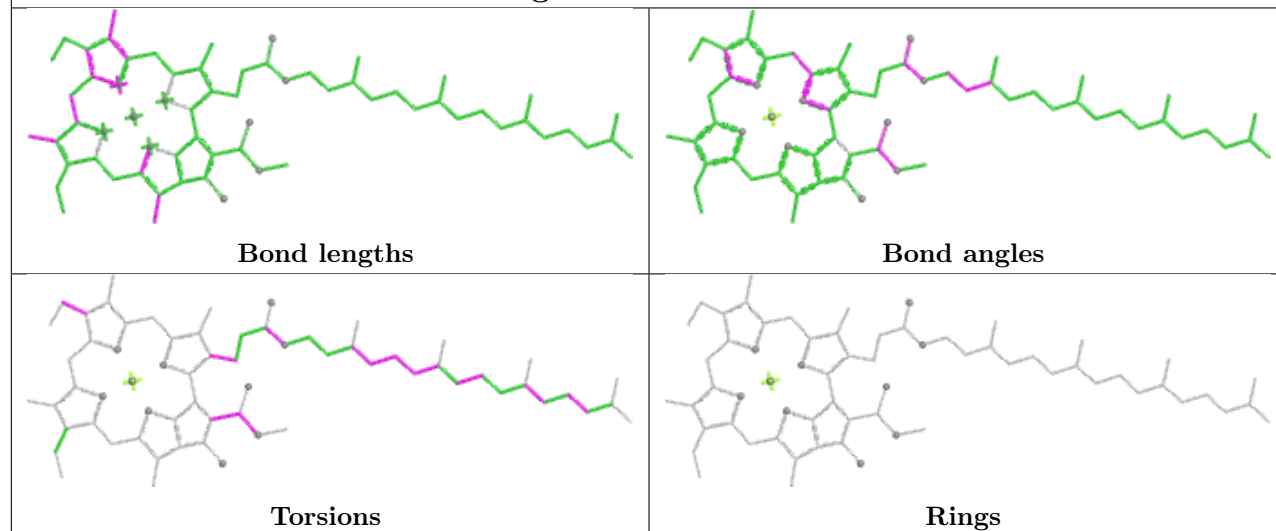




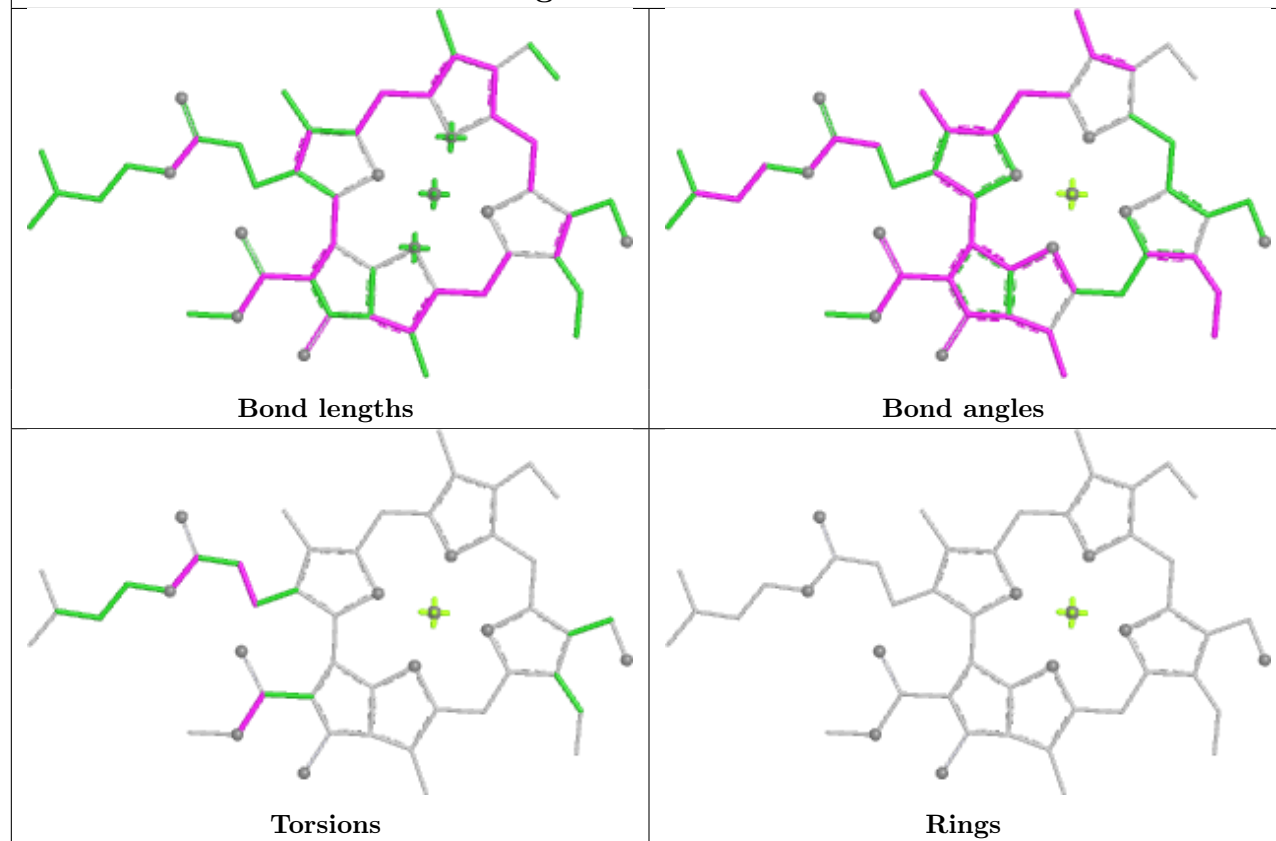




## Ligand CLA A 806

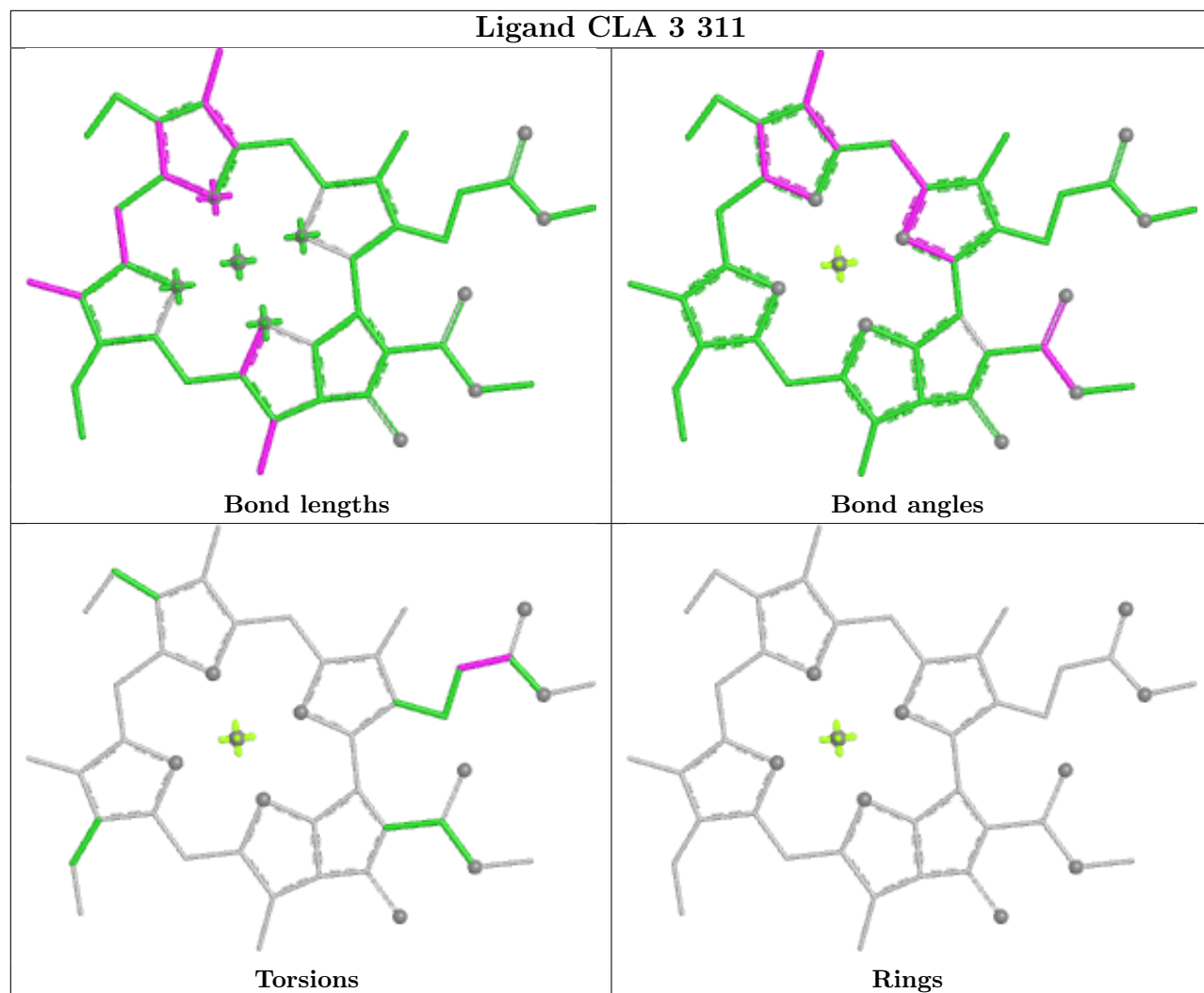


## Ligand CHL 3 305



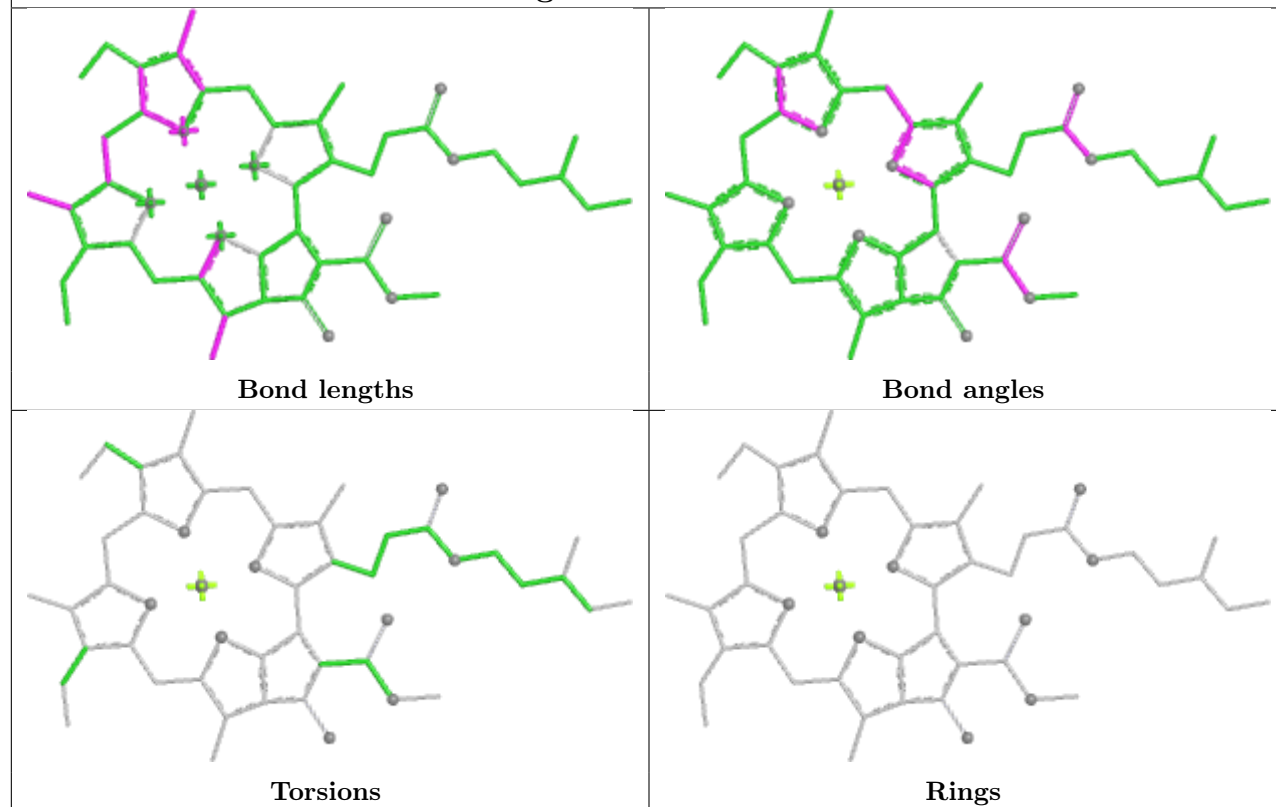


## Ligand CLA 3 311

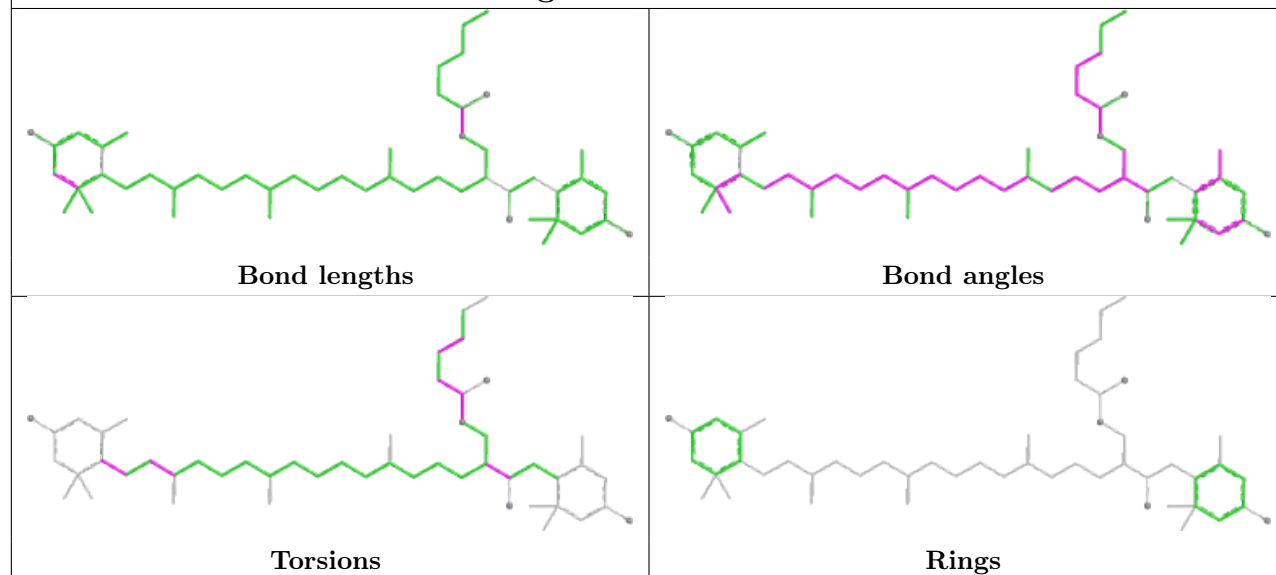




## Ligand CLA 9 304

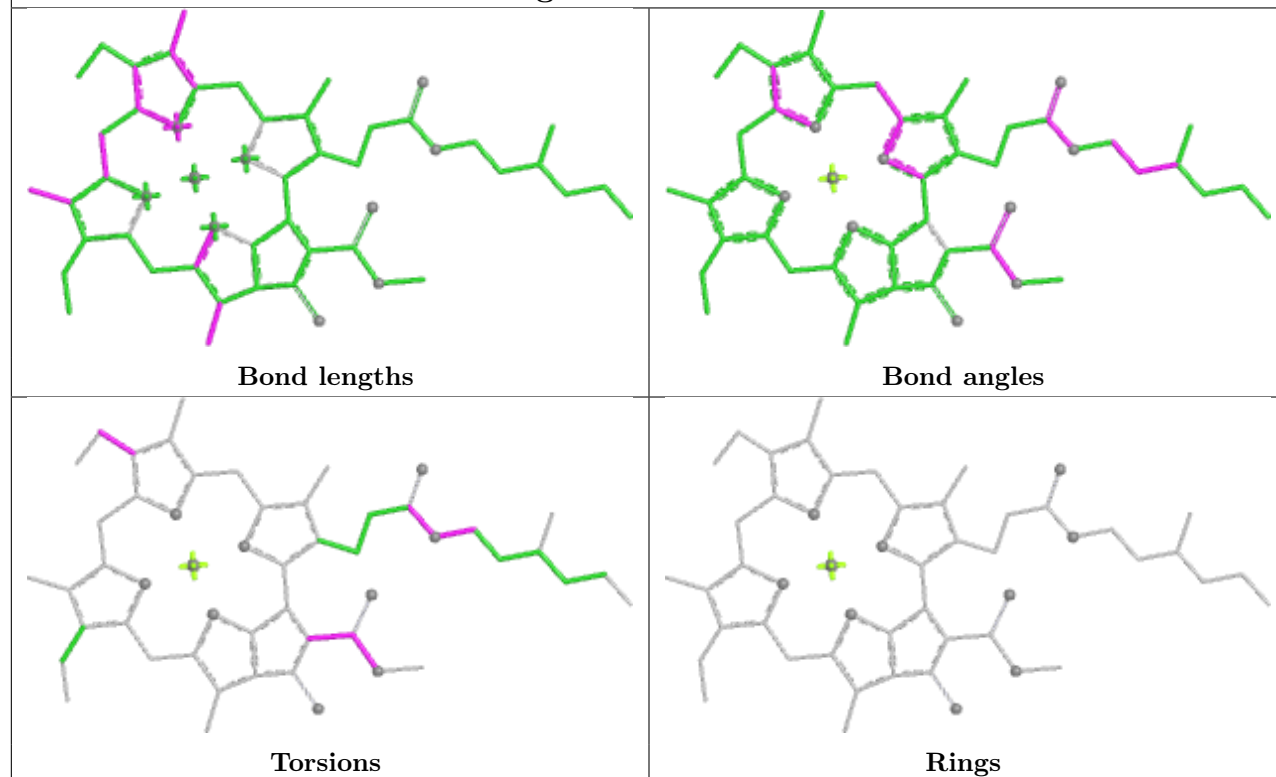


## Ligand OUR 6 501

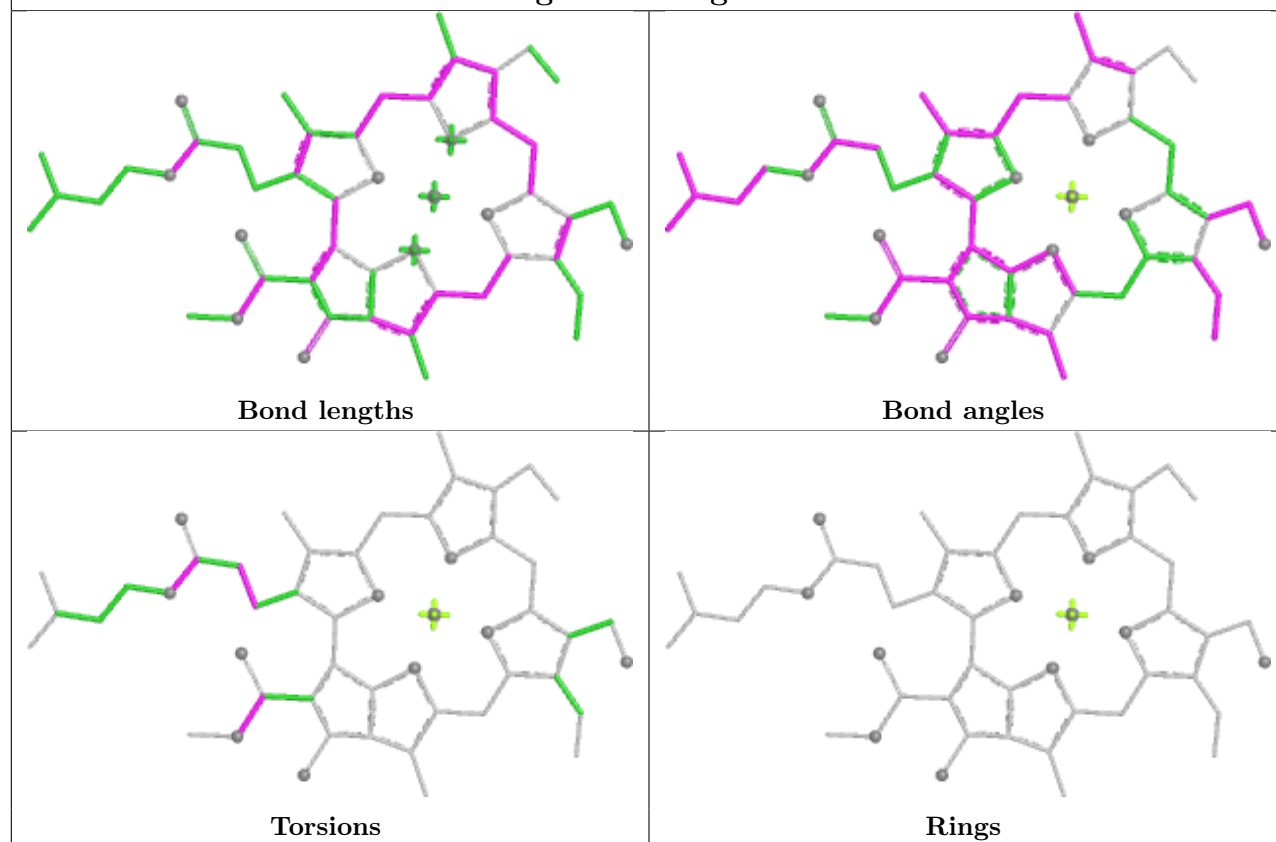




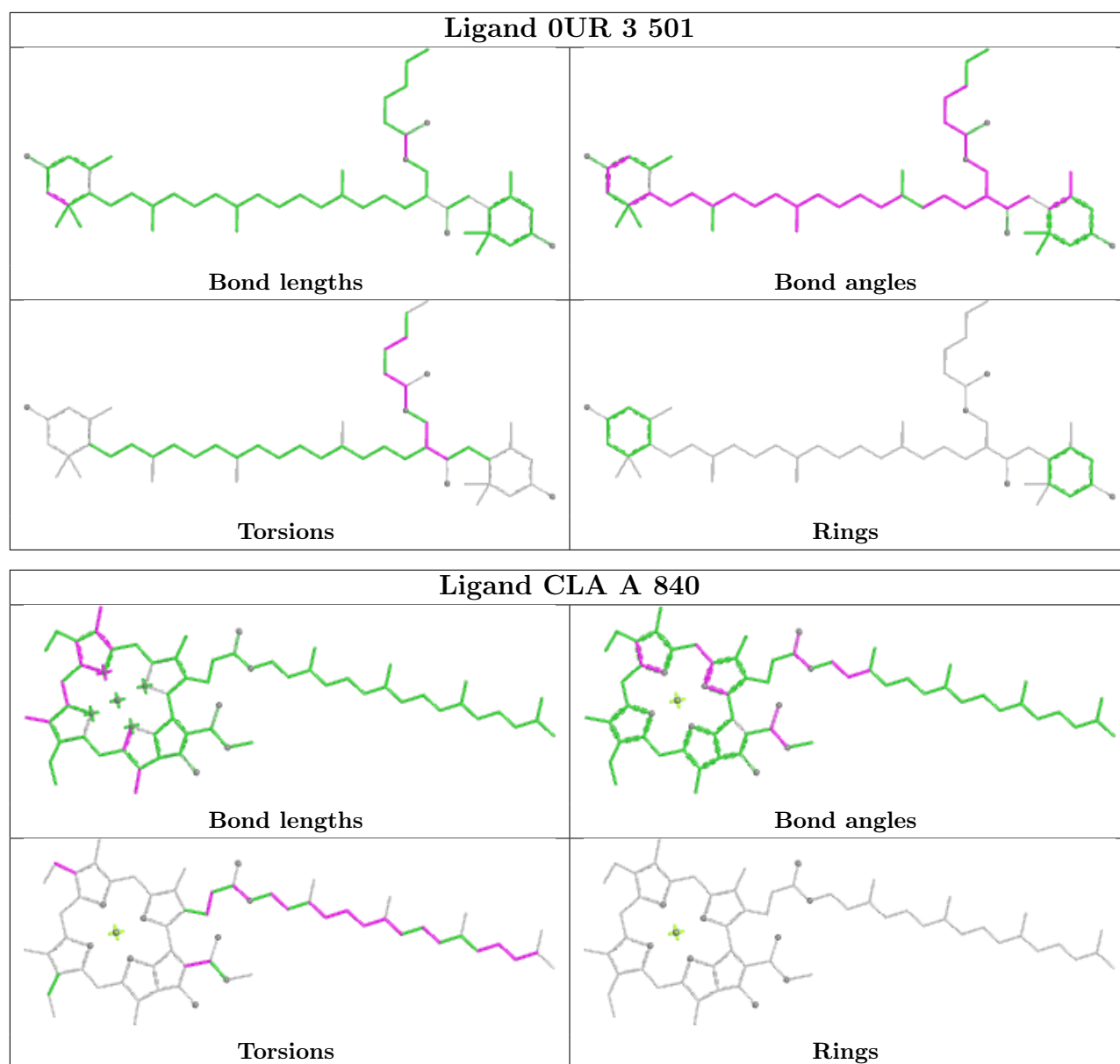
## Ligand CLA 7 311



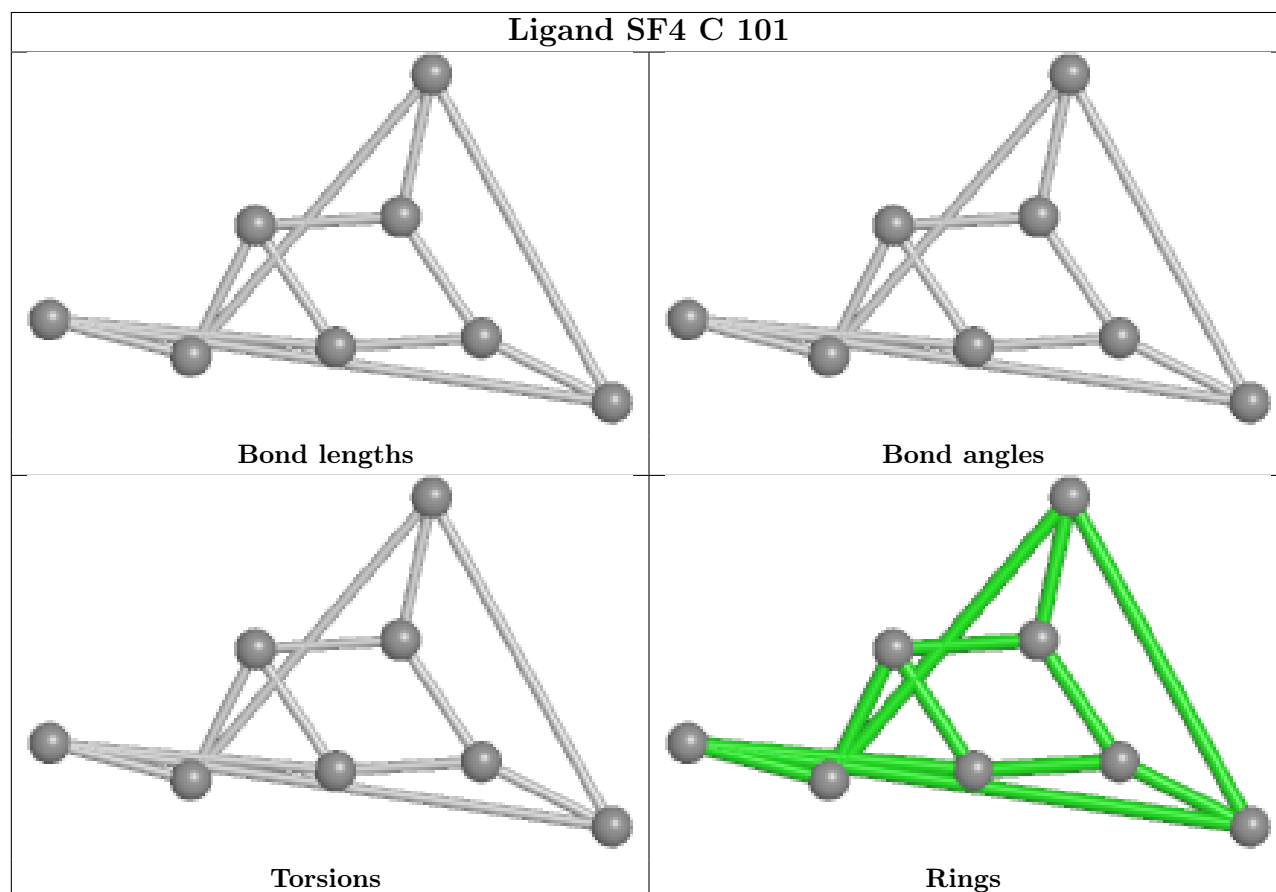
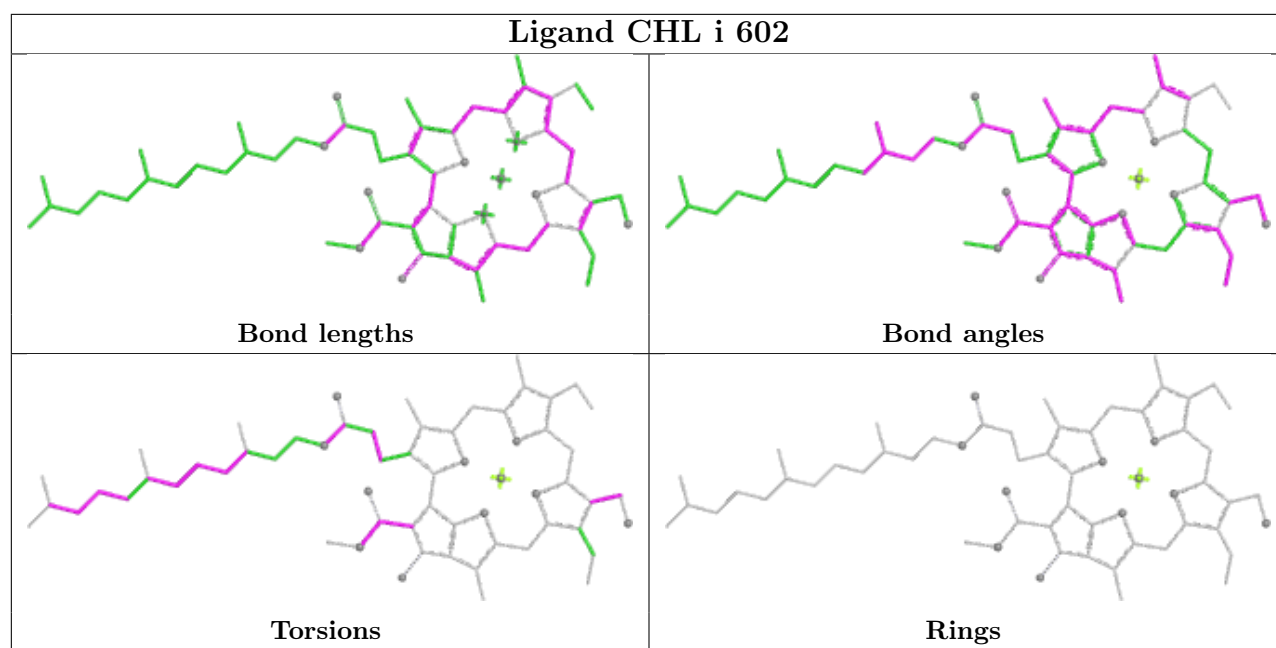
## Ligand CHL g 606



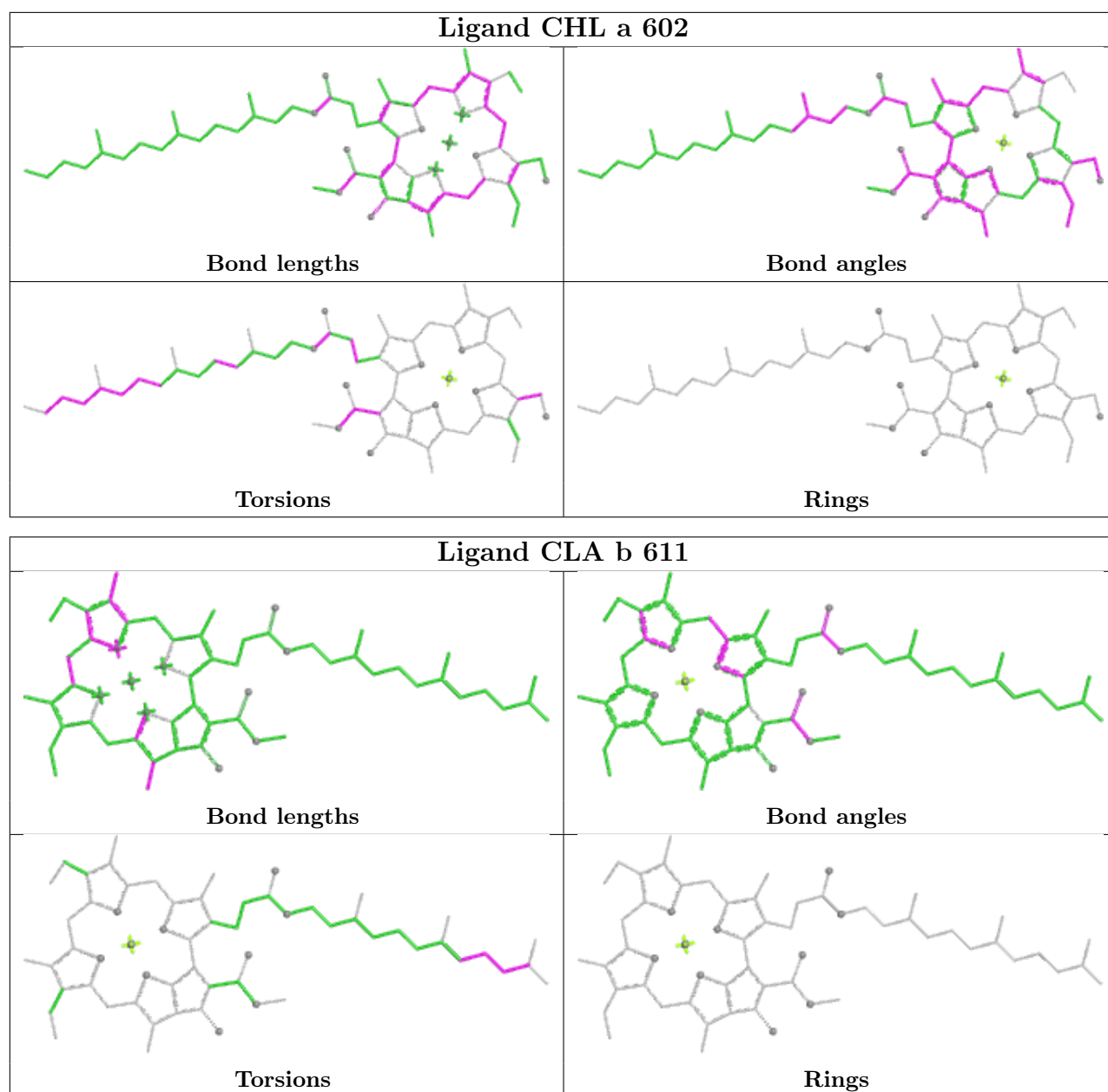




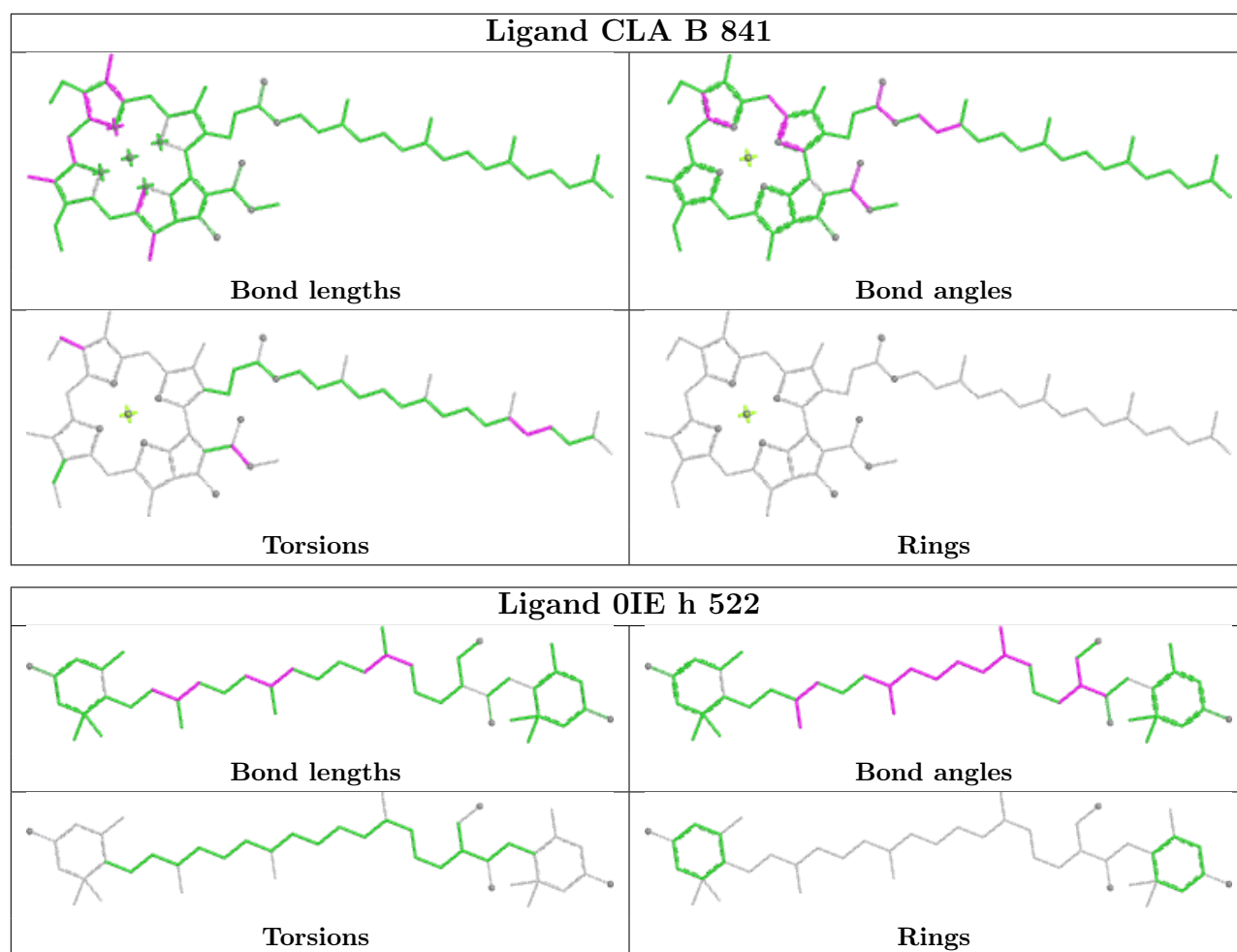




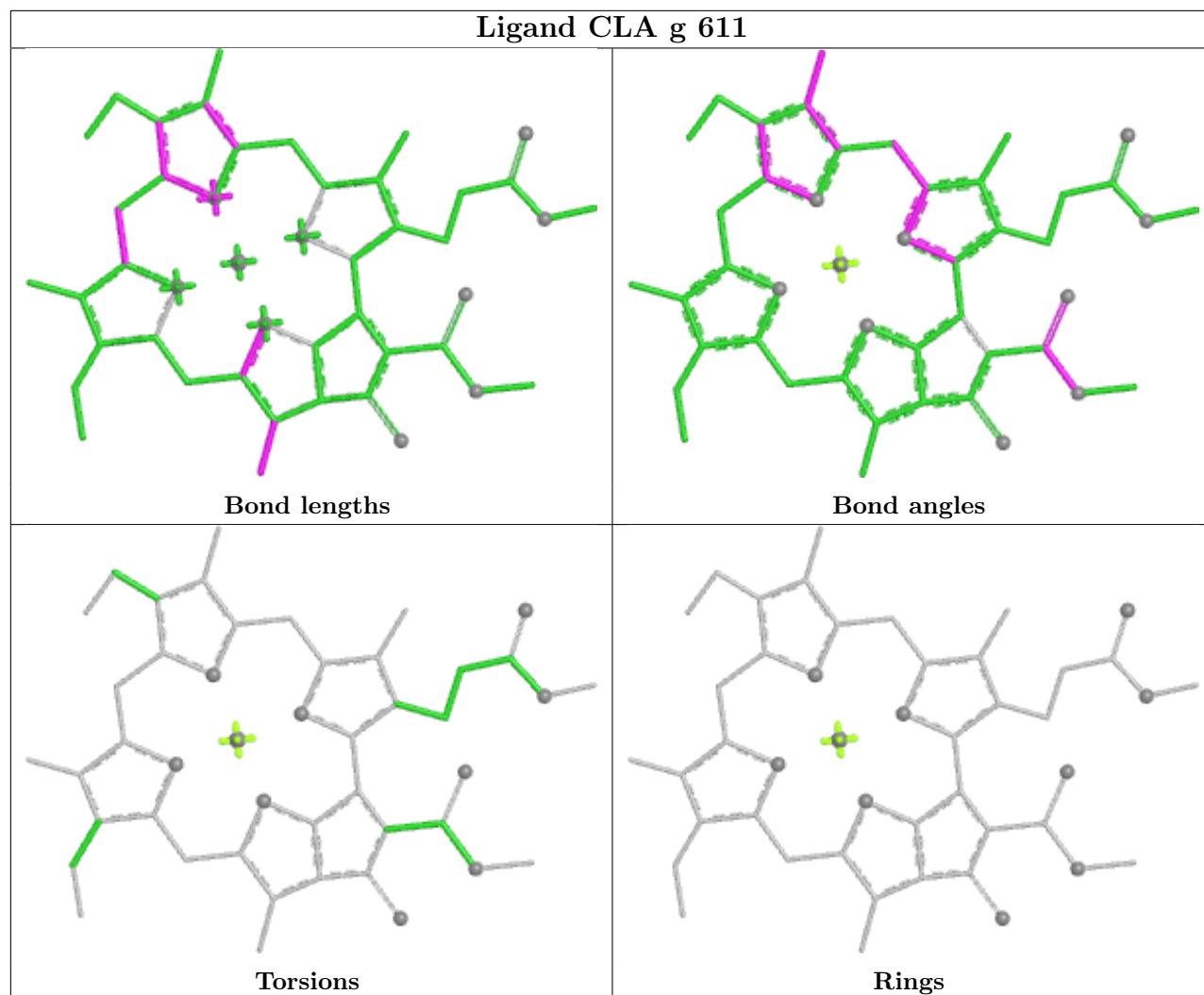






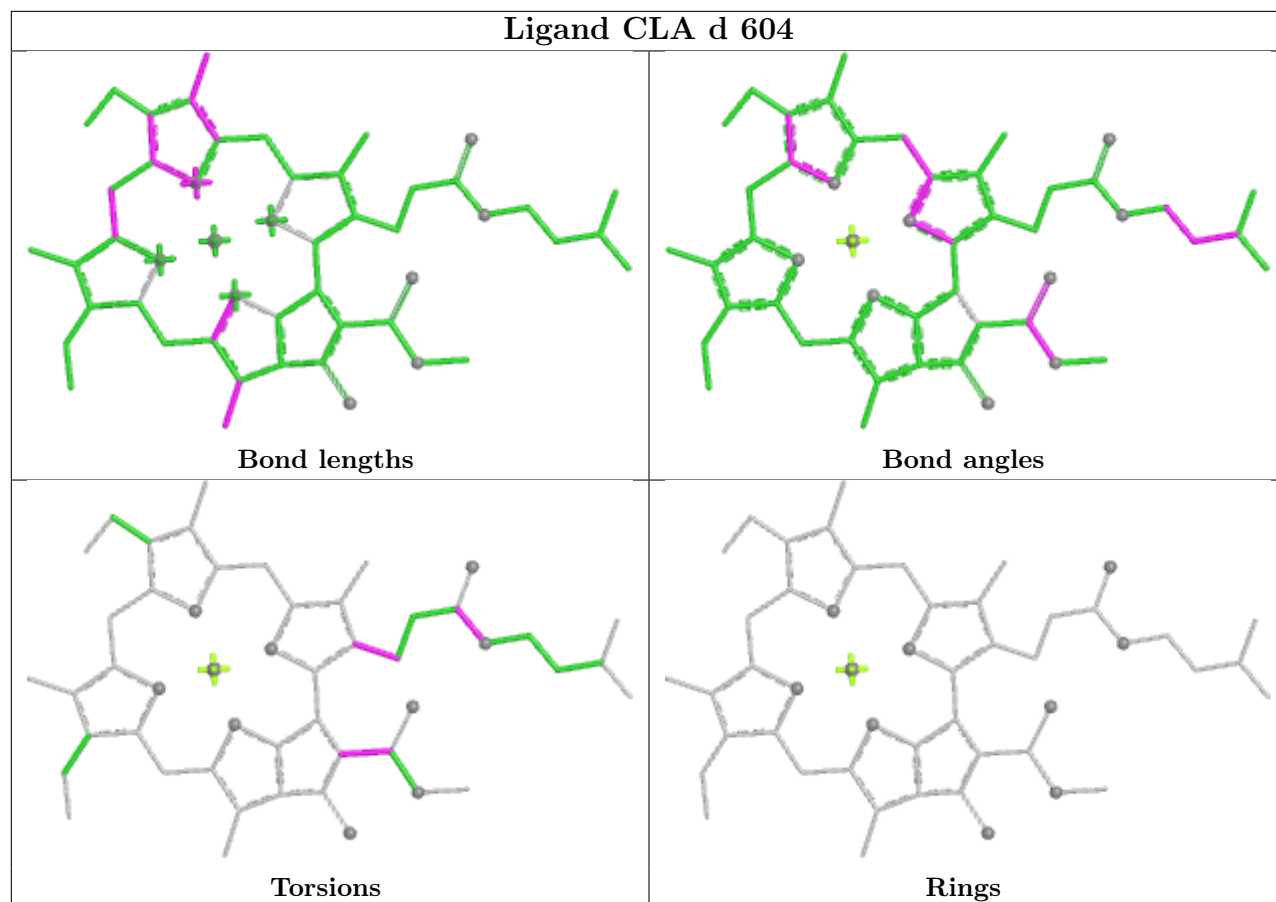




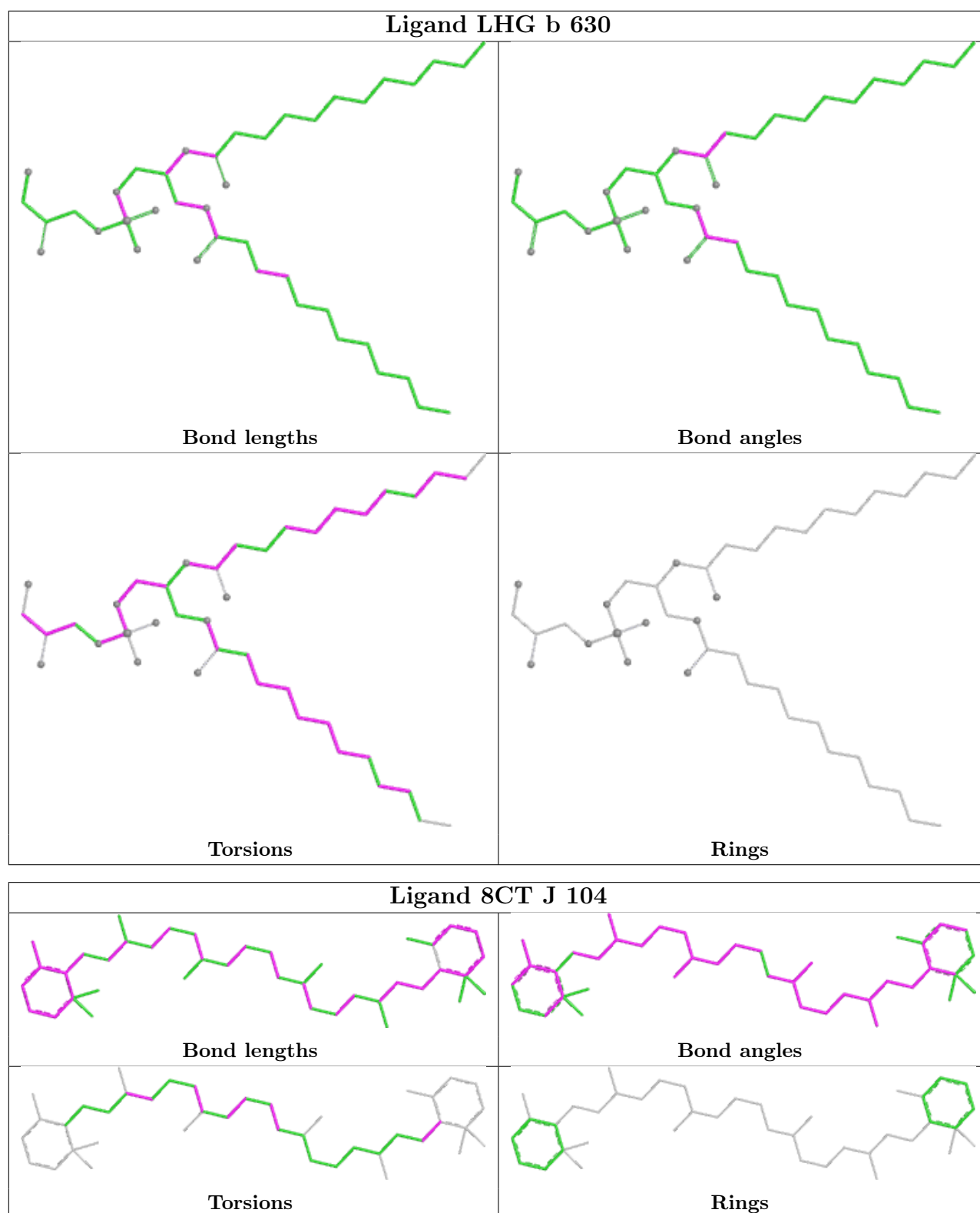




## Ligand CLA d 604







## 5.7 Other polymers ⓘ

There are no such residues in this entry.



## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.



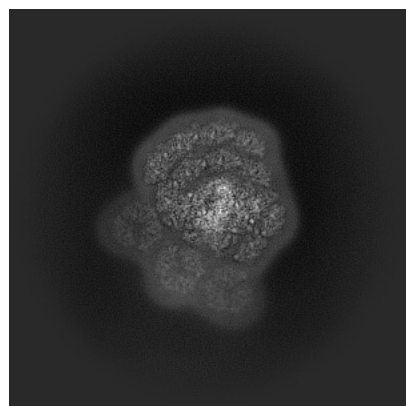
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61940. These allow visual inspection of the internal detail of the map and identification of artifacts.

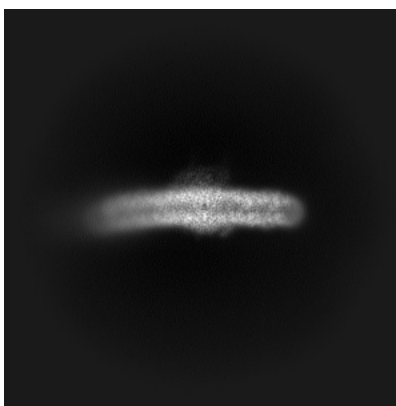
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

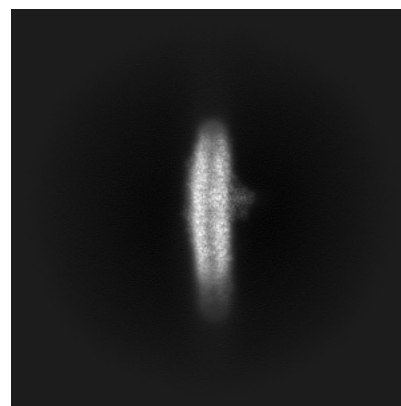
#### 6.1.1 Primary map



X

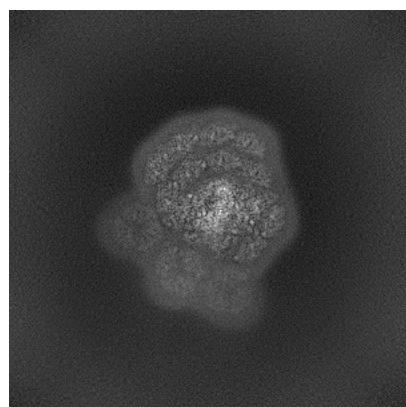


Y

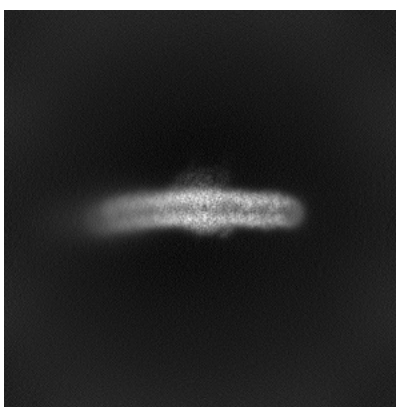


Z

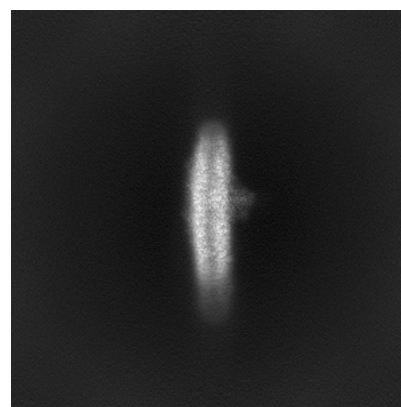
#### 6.1.2 Raw map



X



Y



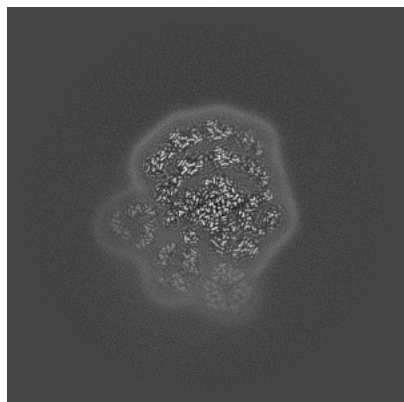
Z

The images above show the map projected in three orthogonal directions.

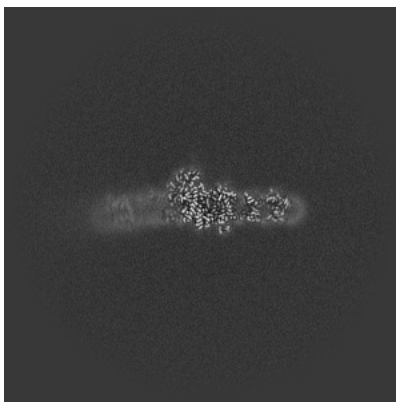


## 6.2 Central slices [i](#)

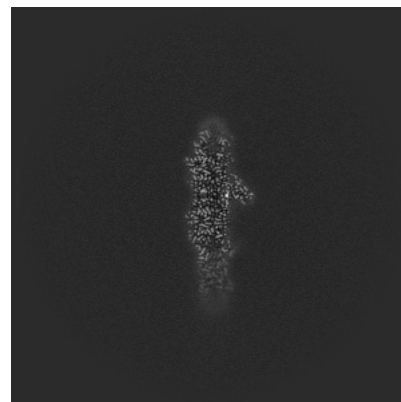
### 6.2.1 Primary map



X Index: 256

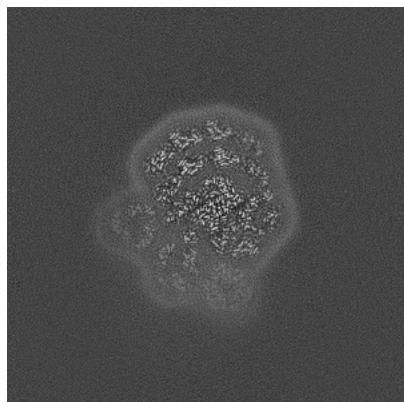


Y Index: 256

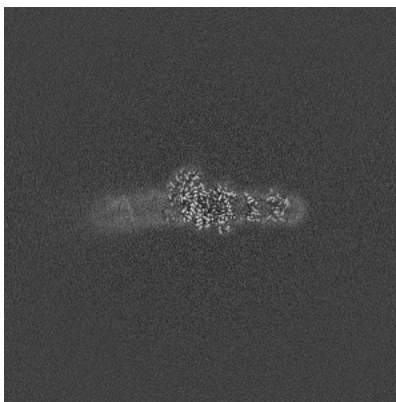


Z Index: 256

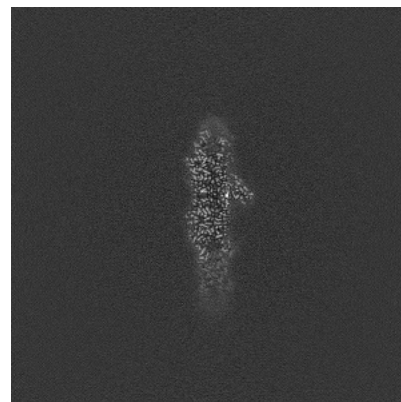
### 6.2.2 Raw map



X Index: 256



Y Index: 256



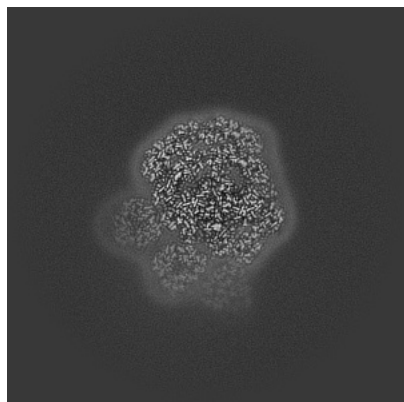
Z Index: 256

The images above show central slices of the map in three orthogonal directions.

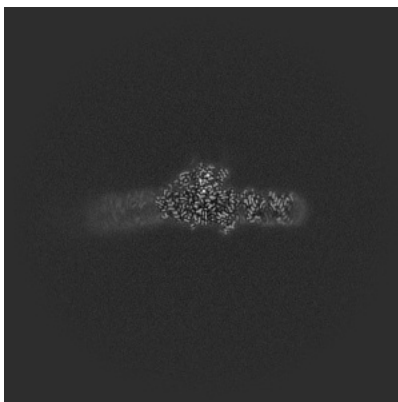


## 6.3 Largest variance slices [i](#)

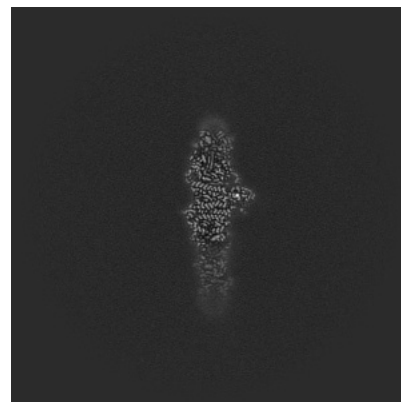
### 6.3.1 Primary map



X Index: 266

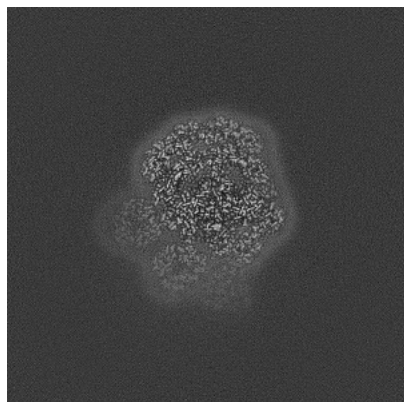


Y Index: 269

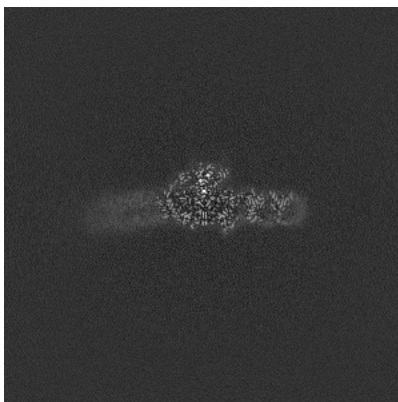


Z Index: 251

### 6.3.2 Raw map



X Index: 266



Y Index: 270



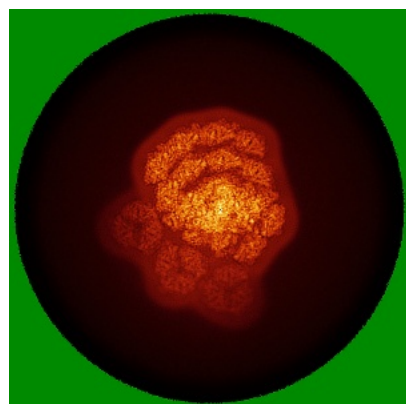
Z Index: 251

The images above show the largest variance slices of the map in three orthogonal directions.

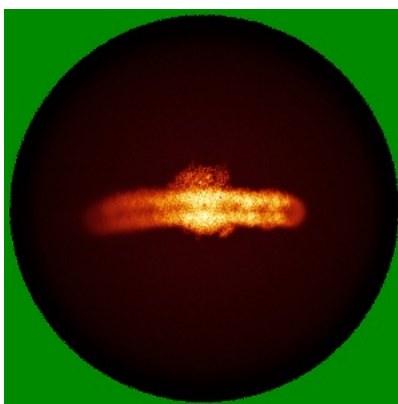


## 6.4 Orthogonal standard-deviation projections (False-color) ⓘ

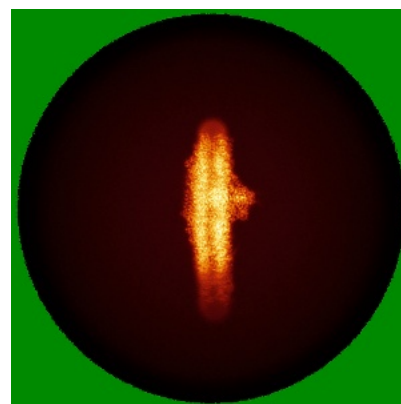
### 6.4.1 Primary map



X

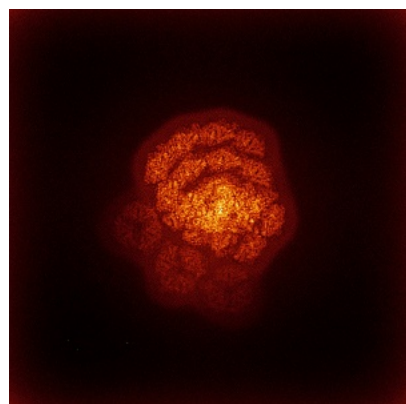


Y



Z

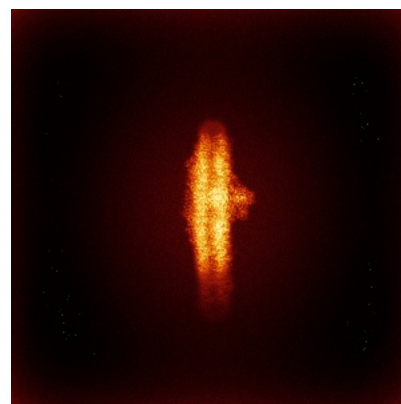
### 6.4.2 Raw map



X



Y



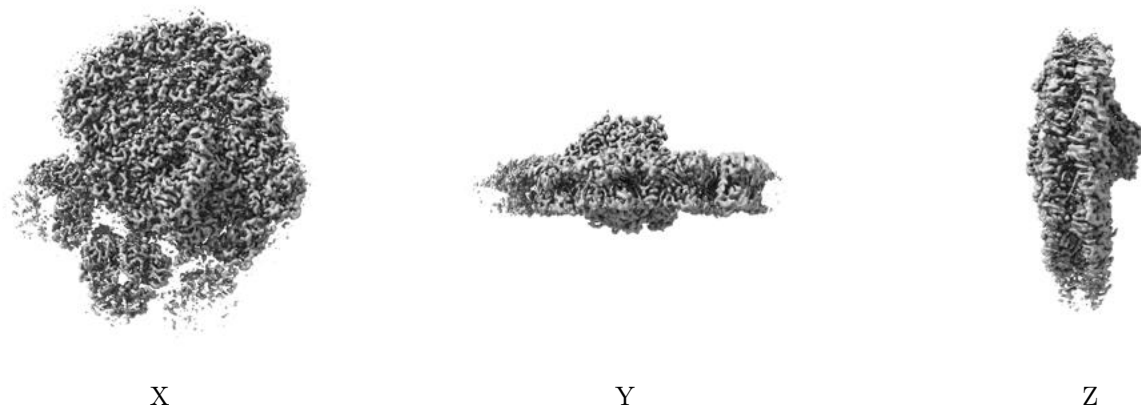
Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



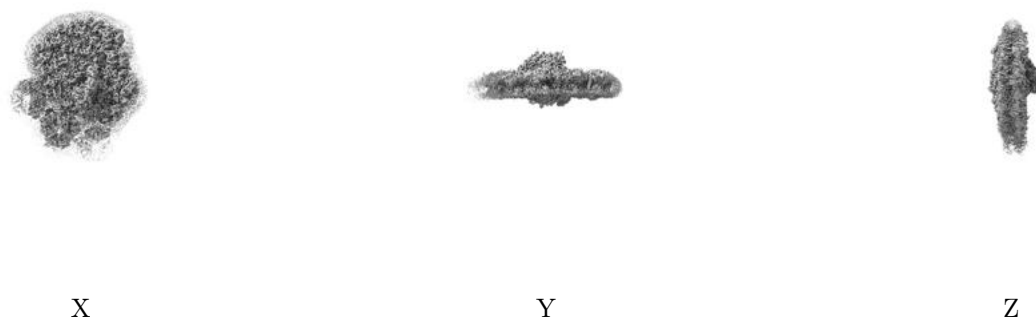
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.217. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

## 6.6 Mask visualisation [i](#)

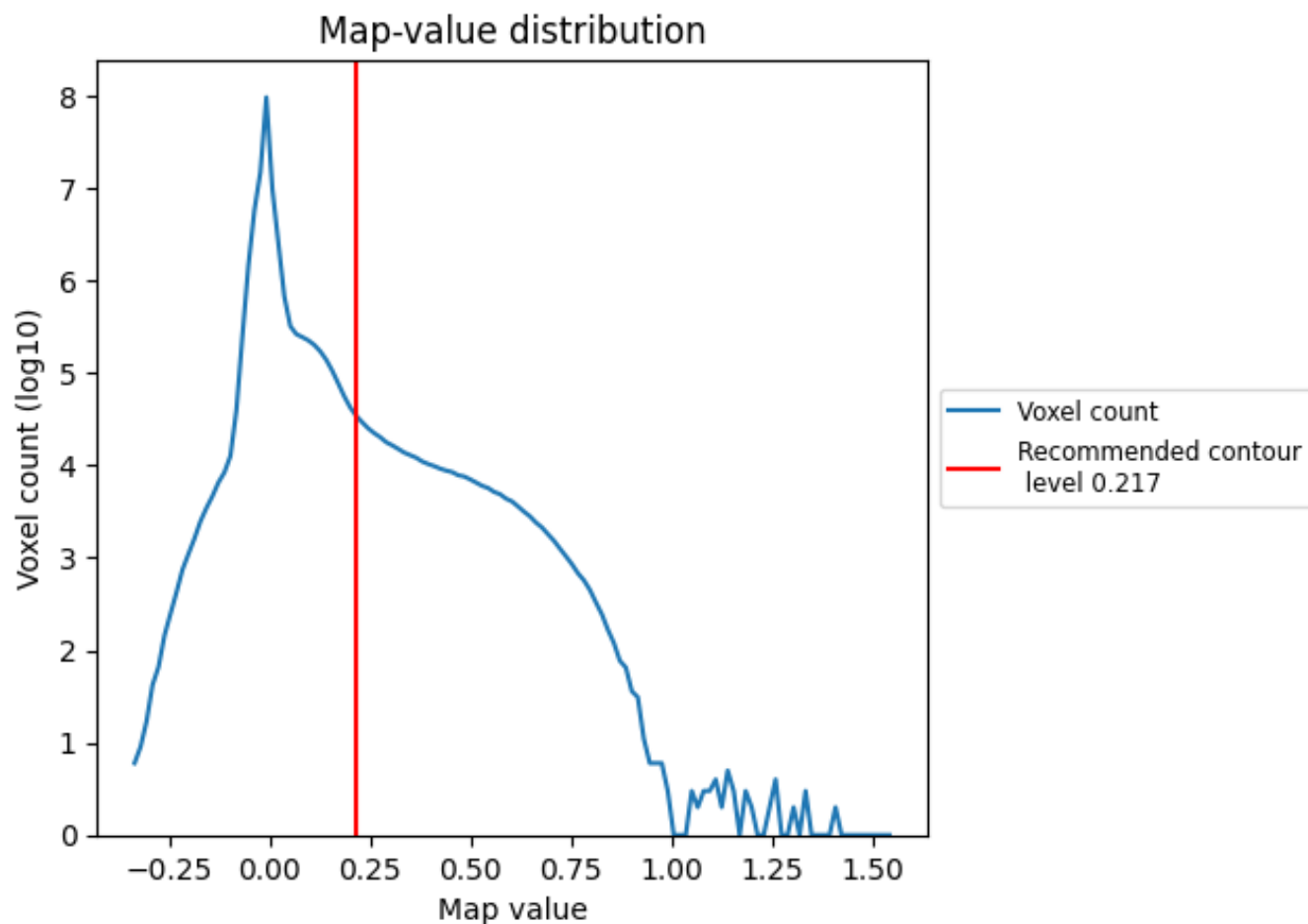
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

This section contains the results of statistical analysis of the map.

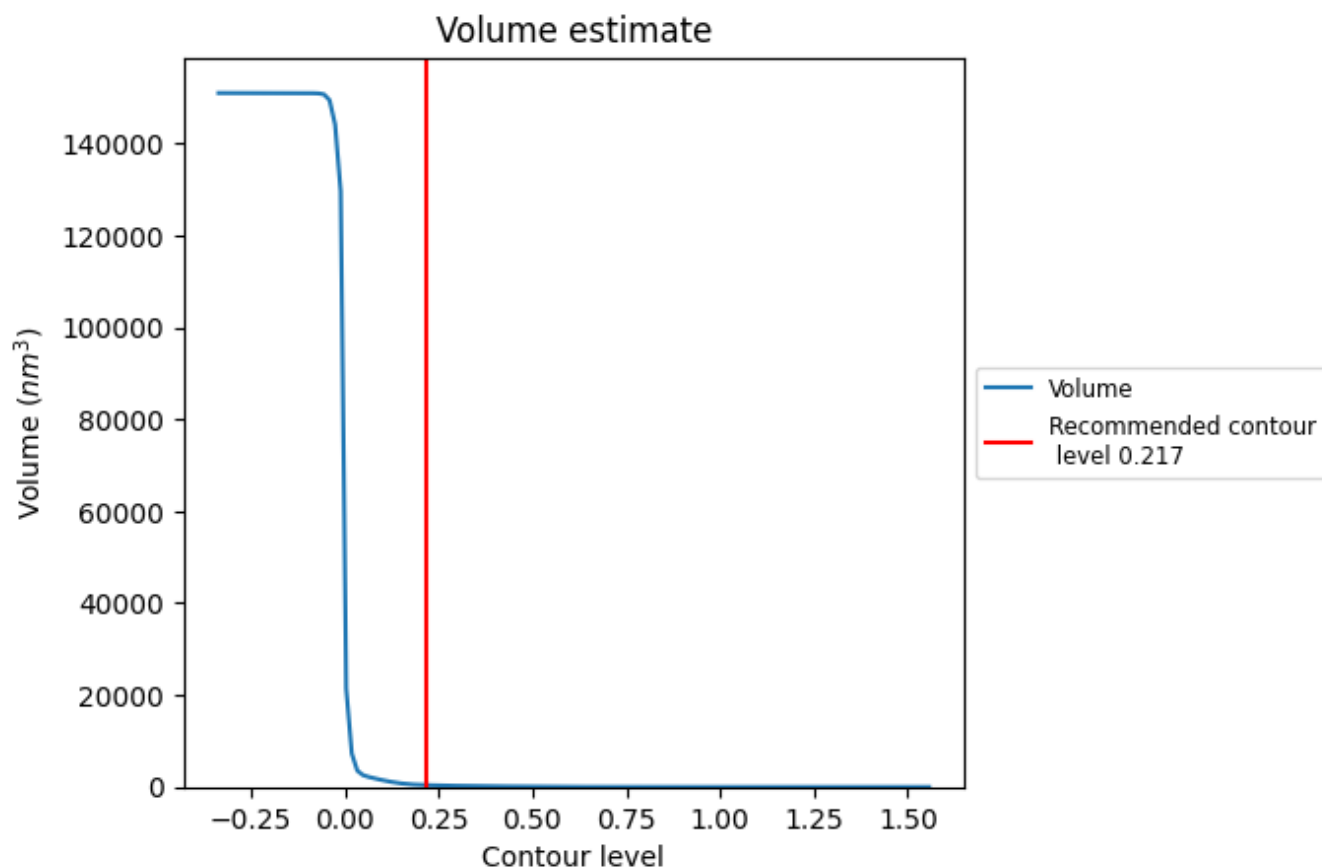
### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.



## 7.2 Volume estimate [i](#)

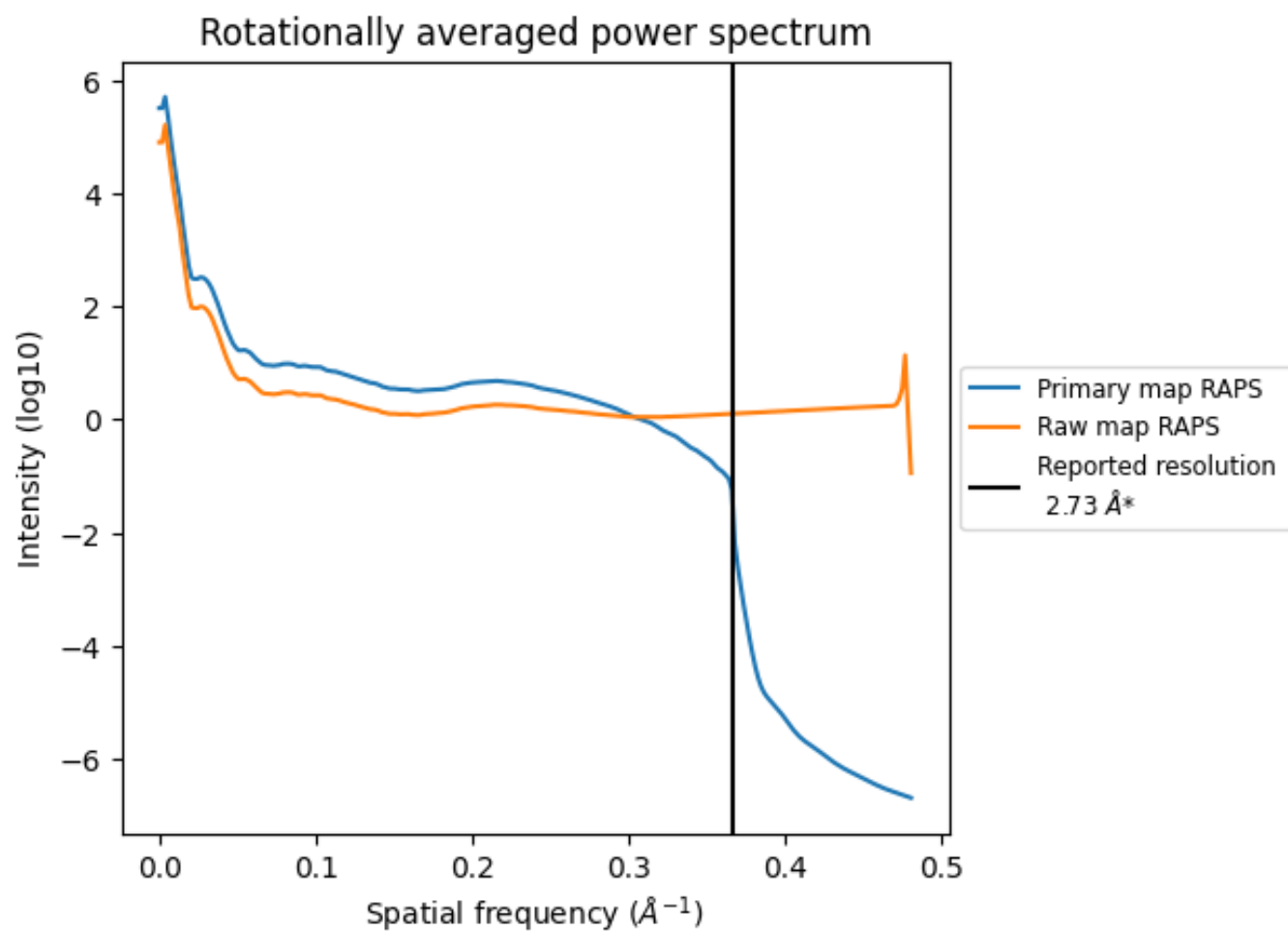


The volume at the recommended contour level is 401  $\text{nm}^3$ ; this corresponds to an approximate mass of 362 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.



### 7.3 Rotationally averaged power spectrum [i](#)



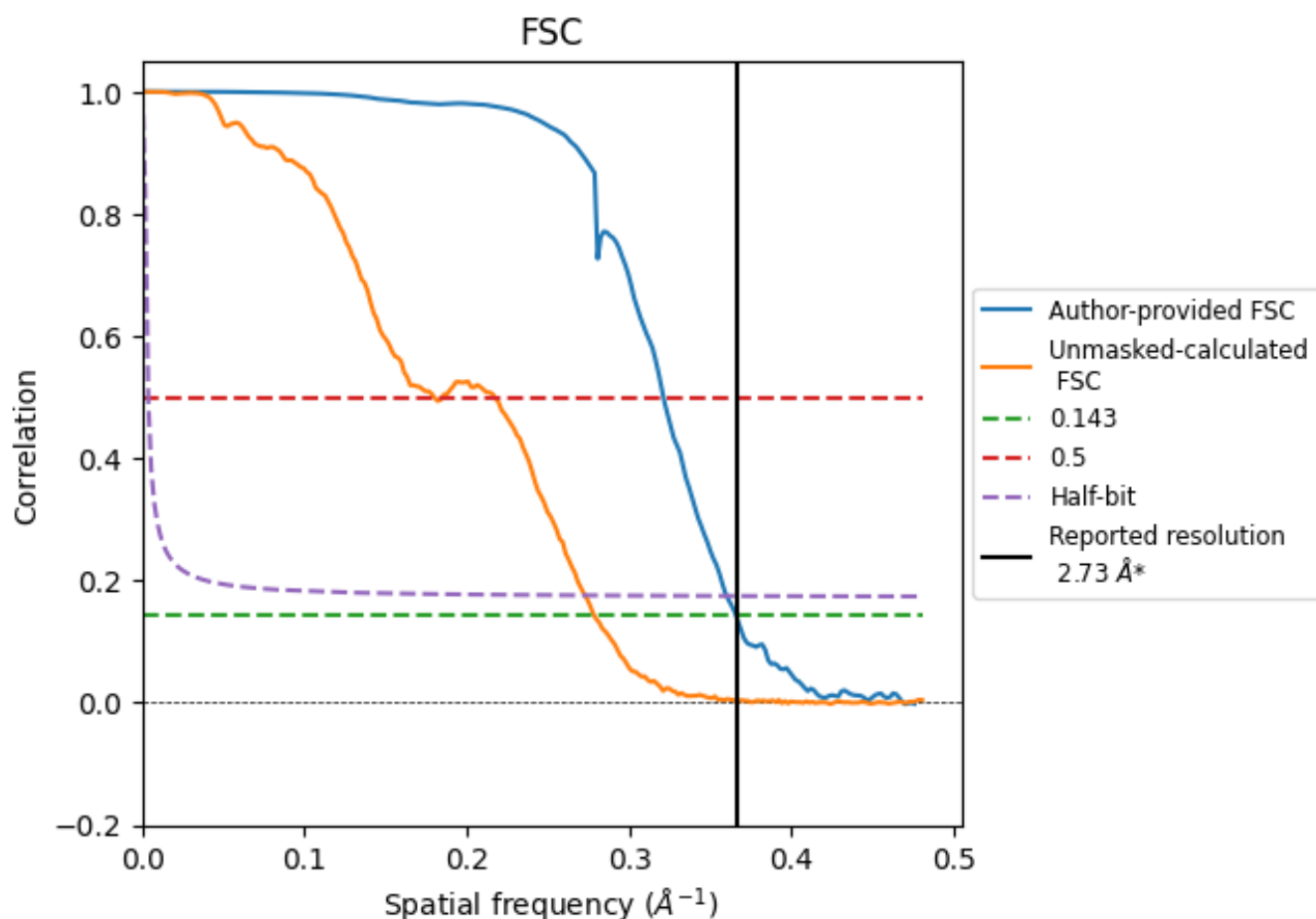
\*Reported resolution corresponds to spatial frequency of  $0.366 \text{ \AA}^{-1}$



## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.366 \text{ \AA}^{-1}$



## 8.2 Resolution estimates [i](#)

| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.73                               | -    | -        |
| Author-provided FSC curve | 2.73                               | 3.11 | 2.78     |
| Unmasked-calculated*      | 3.59                               | 5.56 | 3.66     |

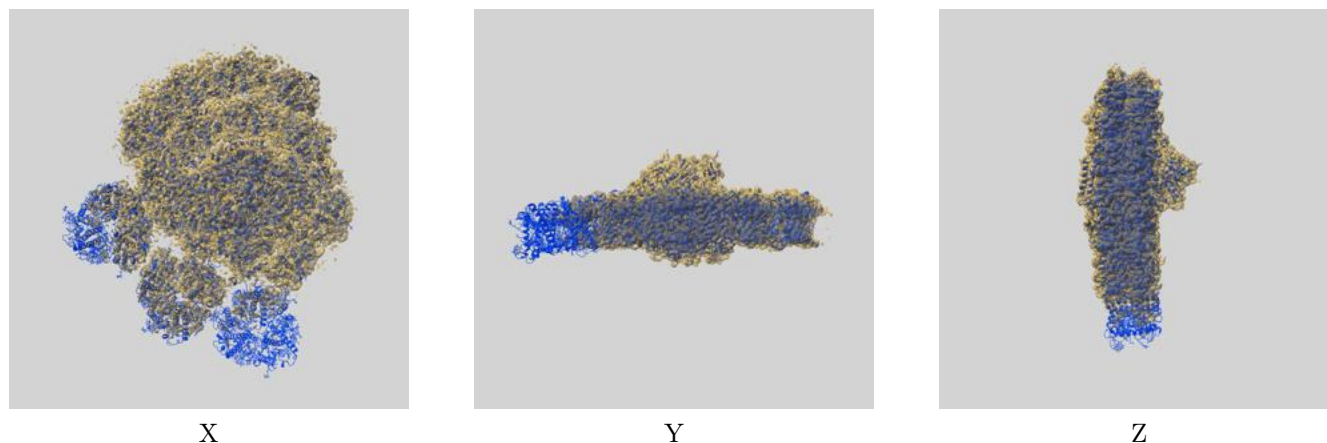
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.59 differs from the reported value 2.73 by more than 10 %



## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-61940 and PDB model 9JZR. Per-residue inclusion information can be found in section [3](#) on page [50](#).

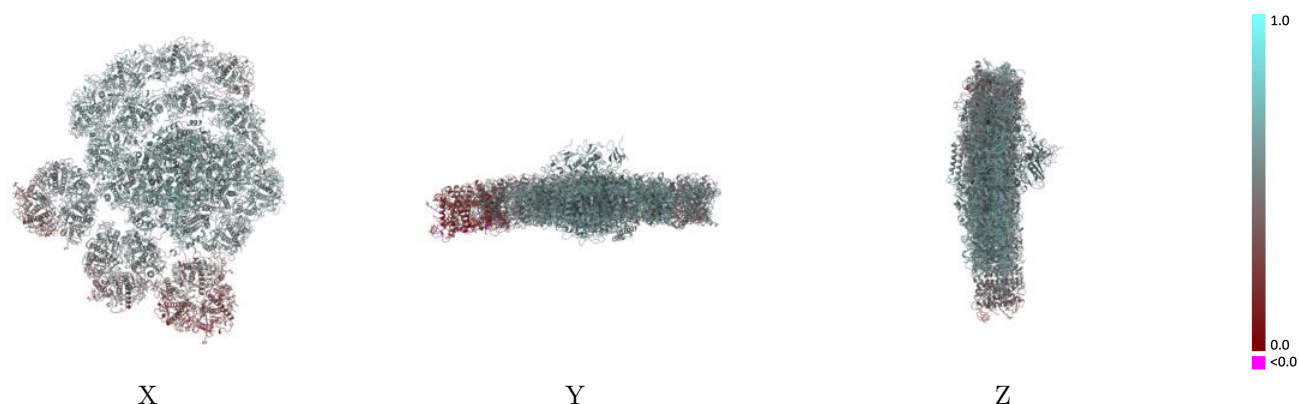
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.217 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

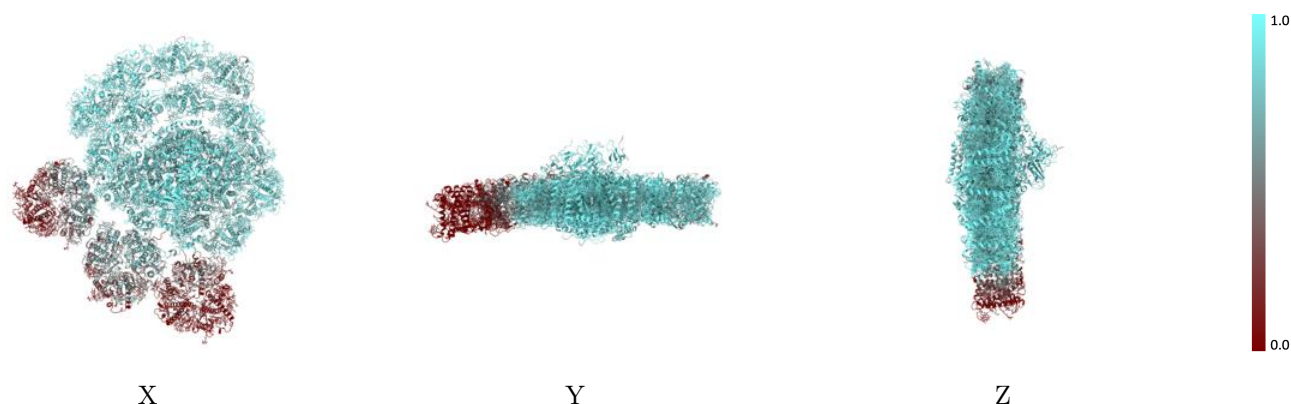


## 9.2 Q-score mapped to coordinate model [i](#)



The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

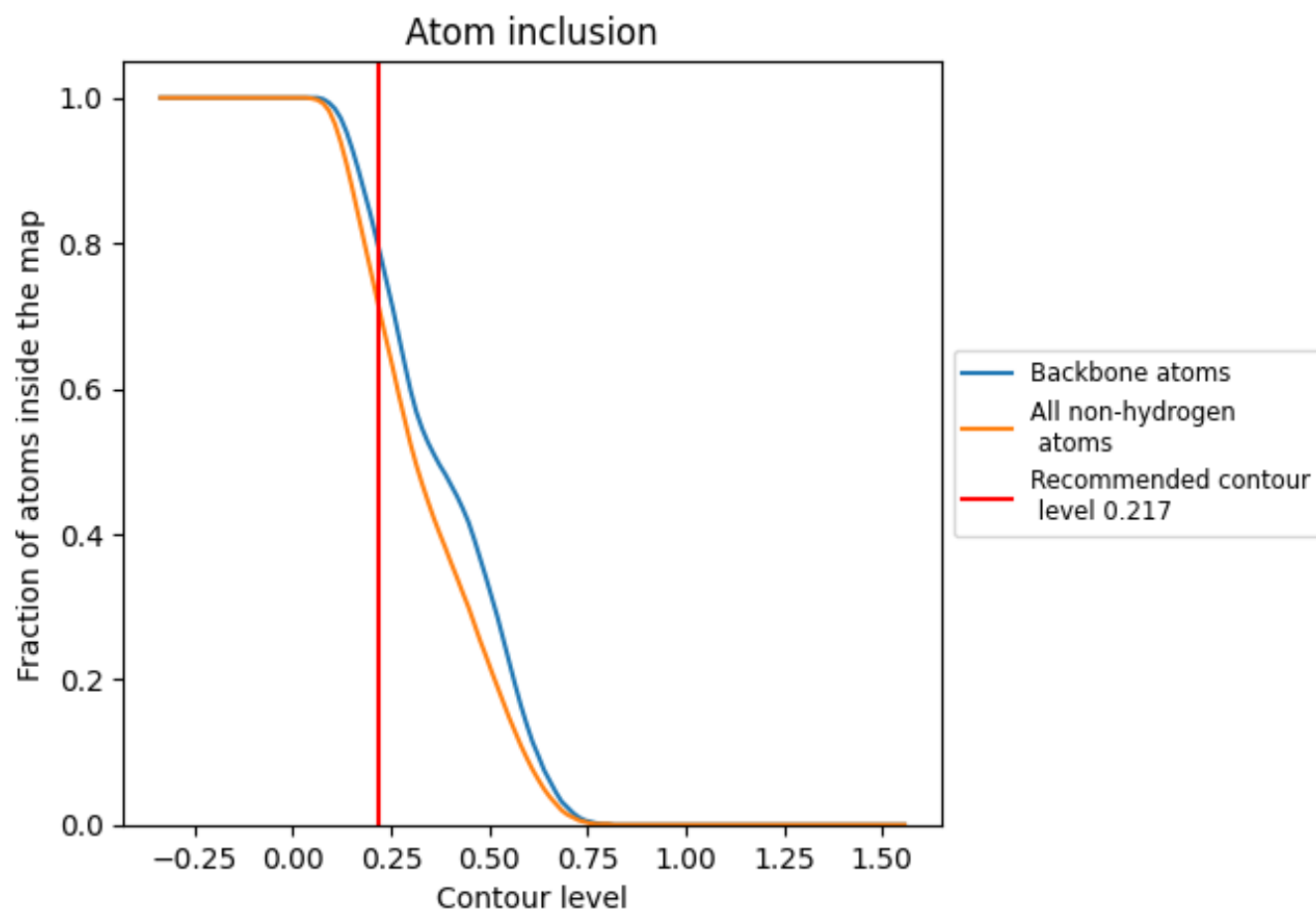
## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.217).



## 9.4 Atom inclusion [i](#)







































































At the recommended contour level, 80% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.



## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.217) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| All   |  0.7160   |  0.5260   |
| 0     |  0.8170   |  0.5440   |
| 1     |  0.8570   |  0.5600   |
| 2     |  0.9190   |  0.5900   |
| 3     |  0.9250   |  0.5940   |
| 4     |  0.8710   |  0.5490   |
| 5     |  0.7530   |  0.4730   |
| 6     |  0.9000   |  0.5700   |
| 7     |  0.8930   |  0.5770   |
| 8     |  0.8400   |  0.5370   |
| 9     |  0.8730   |  0.5690   |
| A     |  0.9360   |  0.6060   |
| B     |  0.9410   |  0.6020   |
| C     |  0.9520   |  0.5880   |
| D     |  0.9270  |  0.5990  |
| E     |  0.8480 |  0.5730 |
| F     |  0.8930 |  0.5690 |
| G     |  0.7920 |  0.5390 |
| H     |  0.8480 |  0.5790 |
| I     |  0.9130 |  0.5760 |
| J     |  0.9030 |  0.5870 |
| K     |  0.8830 |  0.5830 |
| L     |  0.8710 |  0.5780 |
| M     |  0.8950 |  0.5860 |
| O     |  0.8770 |  0.5710 |
| a     |  0.0580 |  0.3680 |
| b     |  0.4230 |  0.5140 |
| c     |  0.5090 |  0.5130 |
| d     |  0.2950 |  0.3960 |
| e     |  0.4980 |  0.4730 |
| f     |  0.6060 |  0.5100 |
| g     |  0.0030 |  0.2200 |
| h     |  0.0250 |  0.2680 |
| i     |  0.2140 |  0.3760 |

