



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 09:45 AM UTC

PDB ID : 9K7V / pdb_00009k7v
EMDB ID : EMD-62153
Title : Structural insights into photosystem II supercomplex of a a siphonous green algae *Bryopsis corticulans* from intertidal zone
Authors : Liu, X.Y.; Wang, W.D.
Deposited on : 2024-10-24
Resolution : 3.07 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

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>.

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

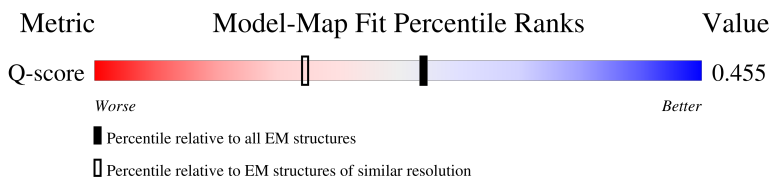
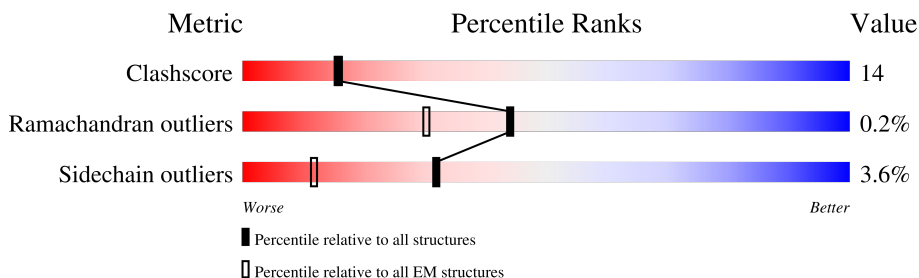
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.07 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.







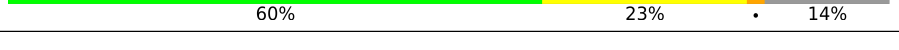


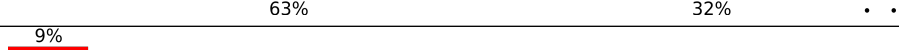
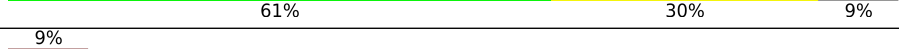

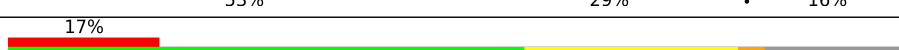
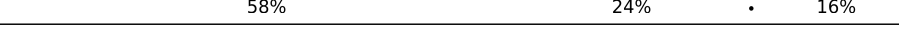



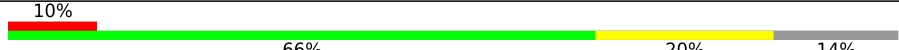



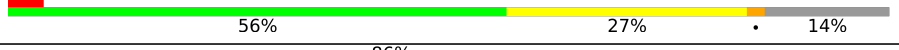





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13977 (2.57 - 3.57)

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 ≥ 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	Z	62	
1	z	62	
2	E	82	
2	e	82	





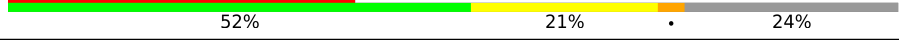

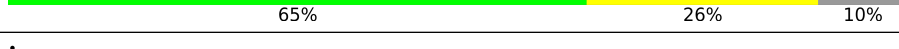

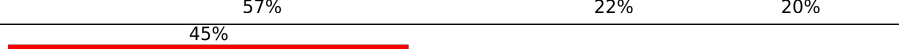
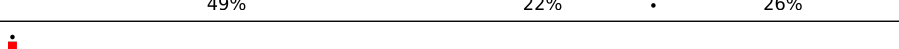




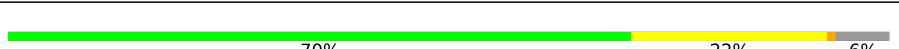





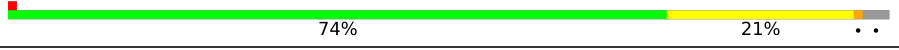
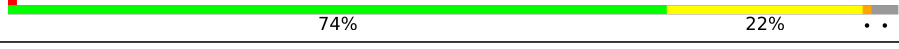



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Mol	Chain	Length	Quality of chain
3	H	75	
3	h	75	
4	I	36	
4	i	36	
5	K	43	
5	k	43	
6	L	38	
6	l	38	
7	M	33	
7	m	33	
8	R	267	
8	r	267	
9	F	42	
9	f	42	
10	1	212	
10	4	212	
11	2	256	
11	5	256	
12	3	254	
12	6	254	
12	7	254	
12	9	254	
12	p	254	
12	u	254	
13	S	308	

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Mol	Chain	Length	Quality of chain
13	s	308	
14	X	109	
14	x	109	
15	V	33	
15	v	33	
16	T	31	
16	t	31	
17	8	280	
17	G	280	
17	N	280	
17	Y	280	
17	g	280	
17	n	280	
17	q	280	
17	y	280	
18	B	508	
18	b	508	
19	A	327	
19	a	327	
20	C	461	
20	c	461	
21	D	352	
21	d	352	
22	W	118	
22	w	118	

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
24	CHL	1	304	X	-	-	-
24	CHL	1	305	X	-	-	-
24	CHL	1	308	X	-	-	-
24	CHL	1	309	X	-	-	-
24	CHL	1	310	X	-	-	-
24	CHL	1	311	X	-	-	-
24	CHL	1	312	X	-	-	-
24	CHL	1	317	X	-	-	-
24	CHL	2	305	X	-	-	-
24	CHL	2	306	X	-	-	-
24	CHL	2	309	X	-	-	-
24	CHL	2	310	X	-	-	-
24	CHL	2	311	X	-	-	-
24	CHL	2	312	X	-	-	-
24	CHL	2	313	X	-	-	-
24	CHL	2	318	X	-	-	-
24	CHL	3	304	X	-	-	-
24	CHL	3	305	X	-	-	-
24	CHL	3	308	X	-	-	-
24	CHL	3	309	X	-	-	-
24	CHL	3	310	X	-	-	-
24	CHL	3	311	X	-	-	-
24	CHL	3	312	X	-	-	-
24	CHL	3	317	X	-	-	-
24	CHL	4	304	X	-	-	-
24	CHL	4	305	X	-	-	-
24	CHL	4	308	X	-	-	-
24	CHL	4	309	X	-	-	-
24	CHL	4	310	X	-	-	-
24	CHL	4	311	X	-	-	-
24	CHL	4	312	X	-	-	-
24	CHL	4	317	X	-	-	-
24	CHL	5	305	X	-	-	-
24	CHL	5	306	X	-	-	-
24	CHL	5	309	X	-	-	-
24	CHL	5	310	X	-	-	-
24	CHL	5	311	X	-	-	-
24	CHL	5	312	X	-	-	-
24	CHL	5	313	X	-	-	-
24	CHL	5	318	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CHL	6	304	X	-	-	-
24	CHL	6	305	X	-	-	-
24	CHL	6	308	X	-	-	-
24	CHL	6	309	X	-	-	-
24	CHL	6	310	X	-	-	-
24	CHL	6	311	X	-	-	-
24	CHL	6	312	X	-	-	-
24	CHL	6	317	X	-	-	-
24	CHL	7	305	X	-	-	-
24	CHL	7	306	X	-	-	-
24	CHL	7	309	X	-	-	-
24	CHL	7	310	X	-	-	-
24	CHL	7	311	X	-	-	-
24	CHL	7	312	X	-	-	-
24	CHL	7	313	X	-	-	-
24	CHL	7	318	X	-	-	-
24	CHL	8	303	X	-	-	-
24	CHL	8	304	X	-	-	-
24	CHL	8	307	X	-	-	-
24	CHL	8	308	X	-	-	-
24	CHL	8	309	X	-	-	-
24	CHL	8	310	X	-	-	-
24	CHL	8	315	X	-	-	-
24	CHL	9	304	X	-	-	-
24	CHL	9	305	X	-	-	-
24	CHL	9	308	X	-	-	-
24	CHL	9	309	X	-	-	-
24	CHL	9	310	X	-	-	-
24	CHL	9	311	X	-	-	-
24	CHL	9	312	X	-	-	-
24	CHL	9	317	X	-	-	-
24	CHL	G	305	X	-	-	-
24	CHL	G	306	X	-	-	-
24	CHL	G	309	X	-	-	-
24	CHL	G	310	X	-	-	-
24	CHL	G	311	X	-	-	-
24	CHL	G	312	X	-	-	-
24	CHL	G	313	X	-	-	-
24	CHL	G	318	X	-	-	-
24	CHL	N	304	X	-	-	-
24	CHL	N	305	X	-	-	-
24	CHL	N	308	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CHL	N	309	X	-	-	-
24	CHL	N	310	X	-	-	-
24	CHL	N	311	X	-	-	-
24	CHL	N	312	X	-	-	-
24	CHL	N	317	X	-	-	-
24	CHL	R	601	X	-	-	-
24	CHL	R	602	X	-	-	-
24	CHL	R	605	X	-	-	-
24	CHL	R	606	X	-	-	-
24	CHL	R	607	X	-	-	-
24	CHL	R	608	X	-	-	-
24	CHL	S	601	X	-	-	-
24	CHL	S	602	X	-	-	-
24	CHL	S	605	X	-	-	-
24	CHL	S	606	X	-	-	-
24	CHL	S	607	X	-	-	-
24	CHL	S	608	X	-	-	-
24	CHL	S	613	X	-	-	-
24	CHL	Y	304	X	-	-	-
24	CHL	Y	305	X	-	-	-
24	CHL	Y	308	X	-	-	-
24	CHL	Y	309	X	-	-	-
24	CHL	Y	310	X	-	-	-
24	CHL	Y	311	X	-	-	-
24	CHL	Y	312	X	-	-	-
24	CHL	Y	317	X	-	-	-
24	CHL	Y	319	X	-	-	-
24	CHL	g	305	X	-	-	-
24	CHL	g	306	X	-	-	-
24	CHL	g	309	X	-	-	-
24	CHL	g	310	X	-	-	-
24	CHL	g	311	X	-	-	-
24	CHL	g	312	X	-	-	-
24	CHL	g	313	X	-	-	-
24	CHL	g	318	X	-	-	-
24	CHL	n	304	X	-	-	-
24	CHL	n	305	X	-	-	-
24	CHL	n	308	X	-	-	-
24	CHL	n	309	X	-	-	-
24	CHL	n	310	X	-	-	-
24	CHL	n	311	X	-	-	-
24	CHL	n	312	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CHL	n	317	X	-	-	-
24	CHL	p	305	X	-	-	-
24	CHL	p	306	X	-	-	-
24	CHL	p	309	X	-	-	-
24	CHL	p	310	X	-	-	-
24	CHL	p	311	X	-	-	-
24	CHL	p	312	X	-	-	-
24	CHL	p	313	X	-	-	-
24	CHL	p	318	X	-	-	-
24	CHL	q	303	X	-	-	-
24	CHL	q	304	X	-	-	-
24	CHL	q	307	X	-	-	-
24	CHL	q	308	X	-	-	-
24	CHL	q	309	X	-	-	-
24	CHL	q	310	X	-	-	-
24	CHL	q	311	X	-	-	-
24	CHL	q	316	X	-	-	-
24	CHL	r	302	X	-	-	-
24	CHL	r	303	X	-	-	-
24	CHL	r	306	X	-	-	-
24	CHL	r	307	X	-	-	-
24	CHL	r	308	X	-	-	-
24	CHL	r	309	X	-	-	-
24	CHL	s	402	X	-	-	-
24	CHL	s	403	X	-	-	-
24	CHL	s	406	X	-	-	-
24	CHL	s	407	X	-	-	-
24	CHL	s	408	X	-	-	-
24	CHL	s	409	X	-	-	-
24	CHL	s	414	X	-	-	-
24	CHL	u	305	X	-	-	-
24	CHL	u	306	X	-	-	-
24	CHL	u	309	X	-	-	-
24	CHL	u	310	X	-	-	-
24	CHL	u	311	X	-	-	-
24	CHL	u	312	X	-	-	-
24	CHL	u	313	X	-	-	-
24	CHL	u	318	X	-	-	-
24	CHL	y	305	X	-	-	-
24	CHL	y	306	X	-	-	-
24	CHL	y	309	X	-	-	-
24	CHL	y	310	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CHL	y	311	X	-	-	-
24	CHL	y	312	X	-	-	-
24	CHL	y	313	X	-	-	-
24	CHL	y	318	X	-	-	-
25	CLA	1	306	X	-	-	-
25	CLA	1	307	X	-	-	-
25	CLA	1	313	X	-	-	-
25	CLA	1	314	X	-	-	-
25	CLA	1	315	X	-	-	-
25	CLA	1	316	X	-	-	-
25	CLA	2	307	X	-	-	-
25	CLA	2	308	X	-	-	-
25	CLA	2	314	X	-	-	-
25	CLA	2	315	X	-	-	-
25	CLA	2	316	X	-	-	-
25	CLA	2	317	X	-	-	-
25	CLA	3	306	X	-	-	-
25	CLA	3	307	X	-	-	-
25	CLA	3	313	X	-	-	-
25	CLA	3	314	X	-	-	-
25	CLA	3	315	X	-	-	-
25	CLA	3	316	X	-	-	-
25	CLA	4	306	X	-	-	-
25	CLA	4	307	X	-	-	-
25	CLA	4	313	X	-	-	-
25	CLA	4	314	X	-	-	-
25	CLA	4	315	X	-	-	-
25	CLA	4	316	X	-	-	-
25	CLA	5	307	X	-	-	-
25	CLA	5	308	X	-	-	-
25	CLA	5	314	X	-	-	-
25	CLA	5	315	X	-	-	-
25	CLA	5	316	X	-	-	-
25	CLA	5	317	X	-	-	-
25	CLA	6	306	X	-	-	-
25	CLA	6	307	X	-	-	-
25	CLA	6	313	X	-	-	-
25	CLA	6	314	X	-	-	-
25	CLA	6	315	X	-	-	-
25	CLA	6	316	X	-	-	-
25	CLA	7	307	X	-	-	-
25	CLA	7	308	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	7	314	X	-	-	-
25	CLA	7	315	X	-	-	-
25	CLA	7	316	X	-	-	-
25	CLA	7	317	X	-	-	-
25	CLA	8	305	X	-	-	-
25	CLA	8	306	X	-	-	-
25	CLA	8	311	X	-	-	-
25	CLA	8	312	X	-	-	-
25	CLA	8	313	X	-	-	-
25	CLA	8	314	X	-	-	-
25	CLA	9	306	X	-	-	-
25	CLA	9	307	X	-	-	-
25	CLA	9	313	X	-	-	-
25	CLA	9	314	X	-	-	-
25	CLA	9	315	X	-	-	-
25	CLA	9	316	X	-	-	-
25	CLA	A	603	X	-	-	-
25	CLA	A	604	X	-	-	-
25	CLA	A	605	X	-	-	-
25	CLA	A	607	X	-	-	-
25	CLA	A	610	X	-	-	-
25	CLA	B	601	X	-	-	-
25	CLA	B	602	X	-	-	-
25	CLA	B	603	X	-	-	-
25	CLA	B	604	X	-	-	-
25	CLA	B	605	X	-	-	-
25	CLA	B	606	X	-	-	-
25	CLA	B	607	X	-	-	-
25	CLA	B	608	X	-	-	-
25	CLA	B	609	X	-	-	-
25	CLA	B	610	X	-	-	-
25	CLA	B	611	X	-	-	-
25	CLA	B	612	X	-	-	-
25	CLA	B	613	X	-	-	-
25	CLA	B	614	X	-	-	-
25	CLA	B	615	X	-	-	-
25	CLA	B	616	X	-	-	-
25	CLA	C	601	X	-	-	-
25	CLA	C	602	X	-	-	-
25	CLA	C	603	X	-	-	-
25	CLA	C	604	X	-	-	-
25	CLA	C	605	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	C	606	X	-	-	-
25	CLA	C	607	X	-	-	-
25	CLA	C	608	X	-	-	-
25	CLA	C	609	X	-	-	-
25	CLA	C	610	X	-	-	-
25	CLA	C	611	X	-	-	-
25	CLA	C	612	X	-	-	-
25	CLA	C	616	X	-	-	-
25	CLA	D	404	X	-	-	-
25	CLA	D	405	X	-	-	-
25	CLA	G	307	X	-	-	-
25	CLA	G	308	X	-	-	-
25	CLA	G	314	X	-	-	-
25	CLA	G	315	X	-	-	-
25	CLA	G	316	X	-	-	-
25	CLA	G	317	X	-	-	-
25	CLA	N	306	X	-	-	-
25	CLA	N	307	X	-	-	-
25	CLA	N	313	X	-	-	-
25	CLA	N	314	X	-	-	-
25	CLA	N	315	X	-	-	-
25	CLA	N	316	X	-	-	-
25	CLA	R	603	X	-	-	-
25	CLA	R	604	X	-	-	-
25	CLA	R	609	X	-	-	-
25	CLA	R	610	X	-	-	-
25	CLA	R	611	X	-	-	-
25	CLA	R	612	X	-	-	-
25	CLA	R	613	X	-	-	-
25	CLA	S	603	X	-	-	-
25	CLA	S	604	X	-	-	-
25	CLA	S	609	X	-	-	-
25	CLA	S	610	X	-	-	-
25	CLA	S	611	X	-	-	-
25	CLA	S	612	X	-	-	-
25	CLA	S	616	X	-	-	-
25	CLA	Y	306	X	-	-	-
25	CLA	Y	307	X	-	-	-
25	CLA	Y	313	X	-	-	-
25	CLA	Y	314	X	-	-	-
25	CLA	Y	315	X	-	-	-
25	CLA	Y	316	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	a	603	X	-	-	-
25	CLA	a	604	X	-	-	-
25	CLA	a	605	X	-	-	-
25	CLA	a	607	X	-	-	-
25	CLA	a	610	X	-	-	-
25	CLA	b	601	X	-	-	-
25	CLA	b	602	X	-	-	-
25	CLA	b	603	X	-	-	-
25	CLA	b	604	X	-	-	-
25	CLA	b	605	X	-	-	-
25	CLA	b	606	X	-	-	-
25	CLA	b	607	X	-	-	-
25	CLA	b	608	X	-	-	-
25	CLA	b	609	X	-	-	-
25	CLA	b	610	X	-	-	-
25	CLA	b	611	X	-	-	-
25	CLA	b	612	X	-	-	-
25	CLA	b	613	X	-	-	-
25	CLA	b	614	X	-	-	-
25	CLA	b	615	X	-	-	-
25	CLA	b	616	X	-	-	-
25	CLA	c	601	X	-	-	-
25	CLA	c	602	X	-	-	-
25	CLA	c	603	X	-	-	-
25	CLA	c	604	X	-	-	-
25	CLA	c	605	X	-	-	-
25	CLA	c	606	X	-	-	-
25	CLA	c	607	X	-	-	-
25	CLA	c	608	X	-	-	-
25	CLA	c	609	X	-	-	-
25	CLA	c	610	X	-	-	-
25	CLA	c	611	X	-	-	-
25	CLA	c	612	X	-	-	-
25	CLA	c	616	X	-	-	-
25	CLA	d	404	X	-	-	-
25	CLA	d	405	X	-	-	-
25	CLA	g	307	X	-	-	-
25	CLA	g	308	X	-	-	-
25	CLA	g	314	X	-	-	-
25	CLA	g	315	X	-	-	-
25	CLA	g	316	X	-	-	-
25	CLA	g	317	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	n	306	X	-	-	-
25	CLA	n	307	X	-	-	-
25	CLA	n	313	X	-	-	-
25	CLA	n	314	X	-	-	-
25	CLA	n	315	X	-	-	-
25	CLA	n	316	X	-	-	-
25	CLA	p	307	X	-	-	-
25	CLA	p	308	X	-	-	-
25	CLA	p	314	X	-	-	-
25	CLA	p	315	X	-	-	-
25	CLA	p	316	X	-	-	-
25	CLA	p	317	X	-	-	-
25	CLA	q	305	X	-	-	-
25	CLA	q	306	X	-	-	-
25	CLA	q	312	X	-	-	-
25	CLA	q	313	X	-	-	-
25	CLA	q	314	X	-	-	-
25	CLA	q	315	X	-	-	-
25	CLA	r	304	X	-	-	-
25	CLA	r	305	X	-	-	-
25	CLA	r	310	X	-	-	-
25	CLA	r	311	X	-	-	-
25	CLA	r	312	X	-	-	-
25	CLA	r	313	X	-	-	-
25	CLA	r	314	X	-	-	-
25	CLA	s	404	X	-	-	-
25	CLA	s	405	X	-	-	-
25	CLA	s	410	X	-	-	-
25	CLA	s	411	X	-	-	-
25	CLA	s	412	X	-	-	-
25	CLA	s	413	X	-	-	-
25	CLA	s	417	X	-	-	-
25	CLA	u	307	X	-	-	-
25	CLA	u	308	X	-	-	-
25	CLA	u	314	X	-	-	-
25	CLA	u	315	X	-	-	-
25	CLA	u	316	X	-	-	-
25	CLA	u	317	X	-	-	-
25	CLA	y	307	X	-	-	-
25	CLA	y	308	X	-	-	-
25	CLA	y	314	X	-	-	-
25	CLA	y	315	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	y	316	X	-	-	-
25	CLA	y	317	X	-	-	-
28	NEX	1	303	-	-	X	-
28	NEX	3	318	-	-	X	-
28	NEX	4	303	-	-	X	-
28	NEX	6	303	-	-	X	-
28	NEX	7	304	-	-	X	-
28	NEX	G	304	-	-	X	-
28	NEX	S	617	-	-	X	-
28	NEX	p	304	-	-	X	-
28	NEX	s	401	-	-	X	-

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 95298 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 Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Z	61	Total	C	N	O	S	0	0
			472	329	68	74	1		
1	z	61	Total	C	N	O	S	0	0
			472	329	68	74	1		

- Molecule 2 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	E	65	Total	C	N	O	0	0
			530	347	87	96		
2	e	65	Total	C	N	O	0	0
			530	347	87	96		

- Molecule 3 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	68	Total	C	N	O	S	0	0
			513	337	74	98	4		
3	h	68	Total	C	N	O	S	0	0
			513	337	74	98	4		

- Molecule 4 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	34	Total	C	N	O	S	0	0
			275	189	40	45	1		
4	i	34	Total	C	N	O	S	0	0
			275	189	40	45	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	26	ASP	ASN	conflict	UNP A0A2P0QH95

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Chain	Residue	Modelled	Actual	Comment	Reference
i	26	ASP	ASN	conflict	UNP A0A2P0QH95

- Molecule 5 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	K	37	Total	C	N	O	0	0
			299	208	43	48		
5	k	37	Total	C	N	O	0	0
			299	208	43	48		

- Molecule 6 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	L	37	Total	C	N	O	0	0
			304	204	48	52		
6	l	37	Total	C	N	O	0	0
			304	204	48	52		

- Molecule 7 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	M	30	Total	C	N	O	0	0
			231	159	33	39		
7	m	30	Total	C	N	O	0	0
			231	159	33	39		

- Molecule 8 is a protein called PsbR.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	R	225	Total	C	N	O	S	0	0
			1711	1092	284	326	9		
8	r	225	Total	C	N	O	S	0	0
			1707	1089	283	326	9		

- Molecule 9 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	31	Total	C	N	O	S	0	0
			246	167	40	38	1		
9	f	31	Total	C	N	O	S	0	0
			251	170	42	38	1		

- Molecule 10 is a protein called Lhcb1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	1	212	Total	C	N	O	S	0	0
			1609	1038	255	306	10		
10	4	212	Total	C	N	O	S	0	0
			1603	1035	252	306	10		

- Molecule 11 is a protein called Lhcb2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	2	221	Total	C	N	O	S	0	0
			1710	1108	278	316	8		
11	5	221	Total	C	N	O	S	0	0
			1711	1109	279	315	8		

- Molecule 12 is a protein called Lhcb3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	3	211	Total	C	N	O	S	0	0
			1606	1033	260	304	9		
12	9	219	Total	C	N	O	S	0	0
			1680	1081	271	319	9		
12	6	219	Total	C	N	O	S	0	0
			1670	1073	271	317	9		
12	u	219	Total	C	N	O	S	0	0
			1683	1084	271	319	9		
12	p	219	Total	C	N	O	S	0	0
			1680	1081	271	319	9		
12	7	219	Total	C	N	O	S	0	0
			1677	1080	271	317	9		

- Molecule 13 is a protein called LhcbS.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	S	249	Total	C	N	O	S	0	0
			1867	1203	309	349	6		
13	s	249	Total	C	N	O	S	0	0
			1867	1203	309	349	6		

- Molecule 14 is a protein called PsbX.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	X	34	Total	C	N	O	0	0
			226	146	36	44		
14	x	34	Total	C	N	O	0	0
			226	146	36	44		

- Molecule 15 is a protein called Photosystem II reaction center protein Psb30.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	V	25	Total	C	N	O	0	0
			179	118	30	31		
15	v	25	Total	C	N	O	0	0
			179	118	30	31		

- Molecule 16 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	28	Total	C	N	O	S	0	0
			236	165	34	36	1		
16	t	28	Total	C	N	O	S	0	0
			236	165	34	36	1		

- Molecule 17 is a protein called LhcbG.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	G	223	Total	C	N	O	S	0	0
			1690	1097	268	315	10		
17	N	206	Total	C	N	O	S	0	0
			1551	1002	247	292	10		
17	Y	223	Total	C	N	O	S	0	0
			1690	1097	268	315	10		
17	8	206	Total	C	N	O	S	0	0
			1554	1005	247	292	10		
17	g	223	Total	C	N	O	S	0	0
			1690	1097	268	315	10		
17	n	206	Total	C	N	O	S	0	0
			1545	998	247	290	10		
17	y	223	Total	C	N	O	S	0	0
			1690	1097	268	315	10		
17	q	206	Total	C	N	O	S	0	0
			1554	1005	247	292	10		

- Molecule 18 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	B	478	Total	C	N	O	S	0	0
			3737	2447	625	652	13		
18	b	478	Total	C	N	O	S	0	0
			3737	2447	625	652	13		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	281	ALA	SER	conflict	UNP A0A0D6E1D0
B	353	GLU	GLN	conflict	UNP A0A0D6E1D0
B	355	HIS	TYR	conflict	UNP A0A0D6E1D0
b	281	ALA	SER	conflict	UNP A0A0D6E1D0
b	353	GLU	GLN	conflict	UNP A0A0D6E1D0
b	355	HIS	TYR	conflict	UNP A0A0D6E1D0

- Molecule 19 is a protein called PsbA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	A	327	Total	C	N	O	S	0	0
			2558	1669	422	453	14		
19	a	327	Total	C	N	O	S	0	0
			2558	1669	422	453	14		

- Molecule 20 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	C	448	Total	C	N	O	S	0	0
			3472	2281	581	599	11		
20	c	448	Total	C	N	O	S	0	0
			3472	2281	581	599	11		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	VAL	MET	conflict	UNP D0EVT6
c	1	VAL	MET	conflict	UNP D0EVT6

- Molecule 21 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	D	340	Total	C	N	O	S	0	0
			2719	1803	447	458	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
21	d	340	Total	C	N	O	S	0	0
			2719	1803	447	458	11		

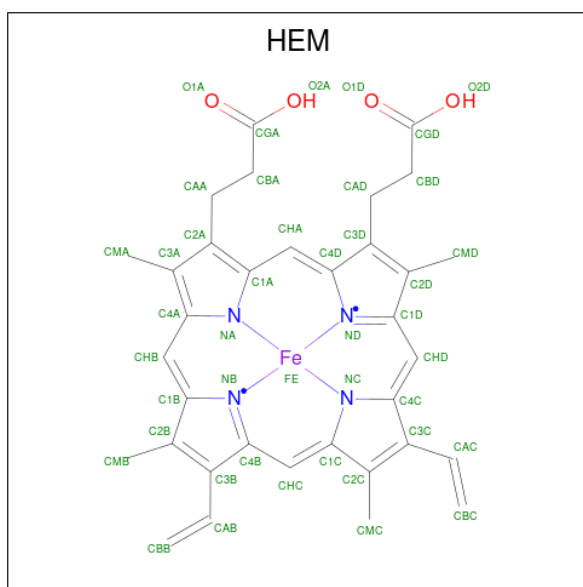
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	55	ILE	VAL	conflict	UNP A0A0B5GKA5
d	55	ILE	VAL	conflict	UNP A0A0B5GKA5

- Molecule 22 is a protein called PsbW.

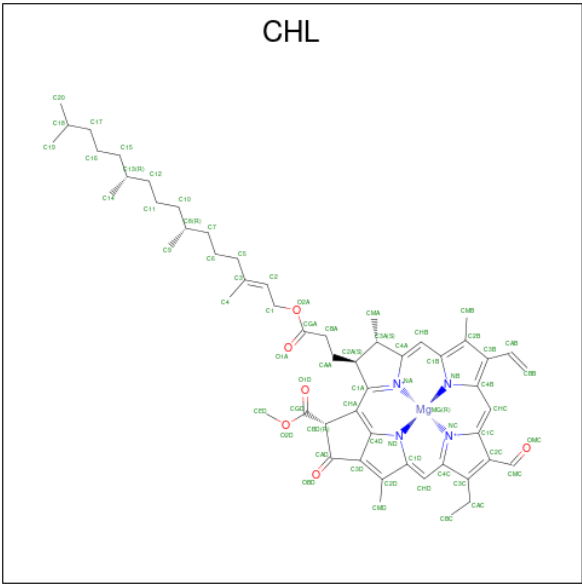
Mol	Chain	Residues	Atoms				AltConf	Trace
22	W	43	Total	C	N	O	0	0
			304	191	49	64		
22	w	43	Total	C	N	O	0	0
			304	191	49	64		

- Molecule 23 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
23	E	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
23	f	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 24 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
24	R	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	R	1	Total 47	C 36	Mg 1	N 4	O 6	0
24	R	1	Total 42	C 33	Mg 1	N 4	O 4	0
24	R	1	Total 48	C 37	Mg 1	N 4	O 6	0
24	R	1	Total 48	C 37	Mg 1	N 4	O 6	0
24	R	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	1	1	Total 42	C 33	Mg 1	N 4	O 4	0
24	1	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	1	1	Total 43	C 34	Mg 1	N 4	O 4	0
24	1	1	Total 43	C 34	Mg 1	N 4	O 4	0
24	1	1	Total 43	C 34	Mg 1	N 4	O 4	0
24	1	1	Total 44	C 35	Mg 1	N 4	O 4	0

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Mol	Chain	Residues	Atoms					AltConf
24	1	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	1	1	Total 42	C 33	Mg 1	N 4	O 4	0
24	2	1	Total 44	C 35	Mg 1	N 4	O 4	0
24	2	1	Total 47	C 36	Mg 1	N 4	O 6	0
24	2	1	Total 43	C 34	Mg 1	N 4	O 4	0
24	2	1	Total 42	C 33	Mg 1	N 4	O 4	0
24	2	1	Total 47	C 36	Mg 1	N 4	O 6	0
24	2	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	2	1	Total 42	C 33	Mg 1	N 4	O 4	0
24	2	1	Total 42	C 33	Mg 1	N 4	O 4	0
24	3	1	Total 48	C 37	Mg 1	N 4	O 6	0
24	3	1	Total 48	C 37	Mg 1	N 4	O 6	0
24	3	1	Total 43	C 34	Mg 1	N 4	O 4	0
24	3	1	Total 51	C 40	Mg 1	N 4	O 6	0
24	3	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	3	1	Total 44	C 35	Mg 1	N 4	O 4	0
24	3	1	Total 43	C 34	Mg 1	N 4	O 4	0
24	3	1	Total 42	C 33	Mg 1	N 4	O 4	0
24	S	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	S	1	Total 58	C 47	Mg 1	N 4	O 6	0
24	S	1	Total 46	C 35	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
24	S	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	S	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	S	1	Total 47	C 36	Mg 1	N 4	O 6	0
24	S	1	Total 42	C 33	Mg 1	N 4	O 4	0
24	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	G	1	Total 64	C 53	Mg 1	N 4	O 6	0
24	G	1	Total 43	C 34	Mg 1	N 4	O 4	0
24	G	1	Total 47	C 36	Mg 1	N 4	O 6	0
24	G	1	Total 54	C 43	Mg 1	N 4	O 6	0
24	G	1	Total 51	C 40	Mg 1	N 4	O 6	0
24	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	G	1	Total 42	C 33	Mg 1	N 4	O 4	0
24	9	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	9	1	Total 64	C 53	Mg 1	N 4	O 6	0
24	9	1	Total 43	C 34	Mg 1	N 4	O 4	0
24	9	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	9	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	9	1	Total 47	C 36	Mg 1	N 4	O 6	0
24	9	1	Total 43	C 34	Mg 1	N 4	O 4	0
24	9	1	Total 42	C 33	Mg 1	N 4	O 4	0
24	N	1	Total 54	C 43	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
24	N	1	Total 60	C 49	Mg 1	N 4	O 6	0
24	N	1	Total 43	C 34	Mg 1	N 4	O 4	0
24	N	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	N	1	Total 53	C 42	Mg 1	N 4	O 6	0
24	N	1	Total 50	C 39	Mg 1	N 4	O 6	0
24	N	1	Total 56	C 45	Mg 1	N 4	O 6	0
24	N	1	Total 42	C 33	Mg 1	N 4	O 4	0
24	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	Y	1	Total 64	C 53	Mg 1	N 4	O 6	0
24	Y	1	Total 43	C 34	Mg 1	N 4	O 4	0
24	Y	1	Total 47	C 36	Mg 1	N 4	O 6	0
24	Y	1	Total 54	C 43	Mg 1	N 4	O 6	0
24	Y	1	Total 51	C 40	Mg 1	N 4	O 6	0
24	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	Y	1	Total 42	C 33	Mg 1	N 4	O 4	0
24	Y	1	Total 53	C 42	Mg 1	N 4	O 6	0
24	8	1	Total 54	C 43	Mg 1	N 4	O 6	0
24	8	1	Total 60	C 49	Mg 1	N 4	O 6	0
24	8	1	Total 43	C 34	Mg 1	N 4	O 4	0
24	8	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	8	1	Total 50	C 39	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
24	8	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
24	8	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	4	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	4	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	4	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	4	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	4	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
24	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	4	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	5	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
24	5	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
24	5	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	5	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	5	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
24	5	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	5	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	5	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	6	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
24	6	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
24	6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	

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Mol	Chain	Residues	Atoms					AltConf
24	6	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
24	6	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	6	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
24	6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	6	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	g	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
24	g	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	g	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
24	g	1	Total	C	Mg	N	O	0
			54	43	1	4	6	
24	g	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
24	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	g	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	u	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	u	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
24	u	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	u	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	u	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	u	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
24	u	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	u	1	Total	C	Mg	N	O	0
			42	33	1	4	4	

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Mol	Chain	Residues	Atoms					AltConf
24	n	1	Total	C	Mg	N	O	0
			54	43	1	4	6	
24	n	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
24	n	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	n	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	n	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
24	n	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
24	n	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
24	n	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	y	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
24	y	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	y	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
24	y	1	Total	C	Mg	N	O	0
			54	43	1	4	6	
24	y	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
24	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	y	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	p	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	p	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
24	p	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	p	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	p	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

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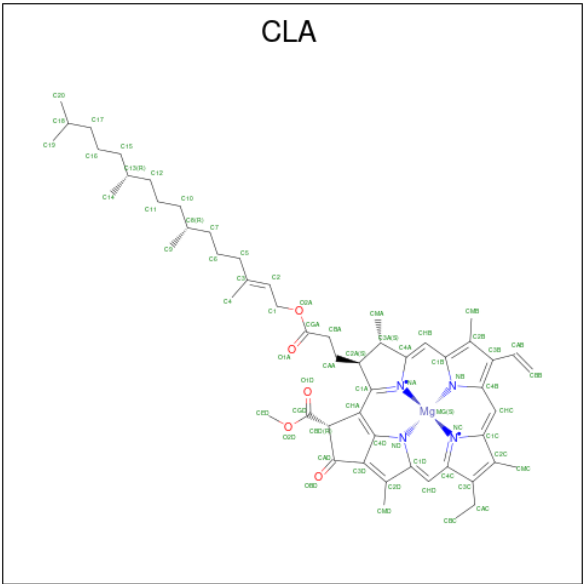
Mol	Chain	Residues	Atoms					AltConf
24	p	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
24	p	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	p	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	q	1	Total	C	Mg	N	O	0
			54	43	1	4	6	
24	q	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
24	q	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	q	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	q	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
24	q	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
24	q	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
24	q	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	s	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
24	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	s	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
24	s	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	r	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	r	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
24	r	1	Total	C	Mg	N	O	0
			42	33	1	4	4	

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Mol	Chain	Residues	Atoms					AltConf
24	r	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
24	r	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
24	r	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	7	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
24	7	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	7	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	7	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	7	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
24	7	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	7	1	Total	C	Mg	N	O	0
			42	33	1	4	4	

- Molecule 25 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
25	R	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
25	R	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	R	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	R	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
25	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	2	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	3	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
25	3	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	S	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	S	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	S	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	G	1	Total 53	C 43	Mg 1	N 4	O 5	0
25	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	G	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	G	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	9	1	Total 56	C 46	Mg 1	N 4	O 5	0
25	9	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	9	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	9	1	Total 63	C 53	Mg 1	N 4	O 5	0
25	9	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	9	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	N	1	Total 54	C 44	Mg 1	N 4	O 5	0
25	N	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	N	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	N	1	Total 63	C 53	Mg 1	N 4	O 5	0
25	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	N	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	Y	1	Total 53	C 43	Mg 1	N 4	O 5	0
25	Y	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	Y	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	Y	1	Total 63	C 53	Mg 1	N 4	O 5	0
25	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	Y	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	8	1	Total 54	C 44	Mg 1	N 4	O 5	0
25	8	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	8	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	8	1	Total 63	C 53	Mg 1	N 4	O 5	0
25	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	8	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 62	C 52	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 56	C 46	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	A	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 56	C 46	Mg 1	N 4	O 5	0
25	C	1	Total 53	C 43	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 61	C 51	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 54	C 44	Mg 1	N 4	O 5	0
25	C	1	Total 46	C 36	Mg 1	N 4	O 5	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	4	1	Total 44	C 35	Mg 1	N 4	O 4	0
25	4	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	4	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	4	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	5	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	5	1	Total 50	C 40	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	5	1	Total 63	C 53	Mg 1	N 4	O 5	0
25	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	5	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	6	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	6	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	6	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	6	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	g	1	Total 53	C 43	Mg 1	N 4	O 5	0
25	g	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	g	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	g	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	g	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	u	1	Total 56	C 46	Mg 1	N 4	O 5	0
25	u	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	u	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	u	1	Total 63	C 53	Mg 1	N 4	O 5	0
25	u	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	u	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	n	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
25	n	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	n	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	n	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
25	n	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	n	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	y	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
25	y	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	y	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	y	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
25	y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	y	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	p	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
25	p	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	p	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	p	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
25	p	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	p	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	q	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
25	q	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	q	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	q	1	Total 63	C 53	Mg 1	N 4	O 5	0
25	q	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	q	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 62	C 52	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 56	C 46	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 47	C 37	Mg 1	N 4	O 5	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0

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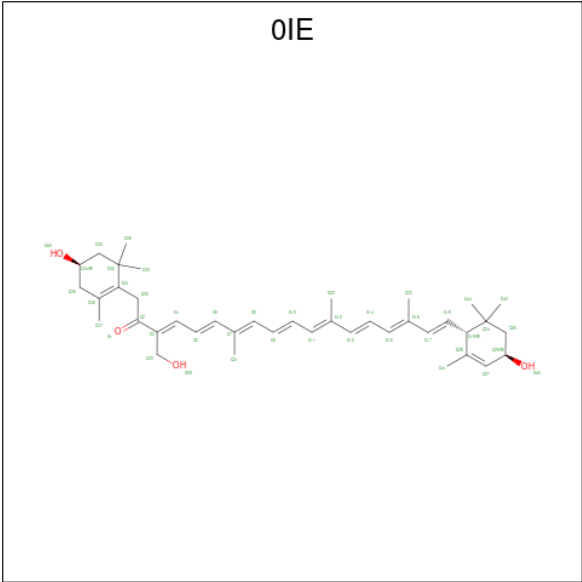
Mol	Chain	Residues	Atoms					AltConf
25	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	s	1	Total	C	Mg	N	O	0
			43	35	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
25	s	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	s	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
25	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	s	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	r	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
25	r	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	r	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	r	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	r	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	r	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	r	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
25	7	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
25	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	7	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
25	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	7	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

- Molecule 26 is Siphonaxanthin (CCD ID: 0IE) (formula: C₄₀H₅₆O₄) (labeled as "Ligand of Interest" by depositor).



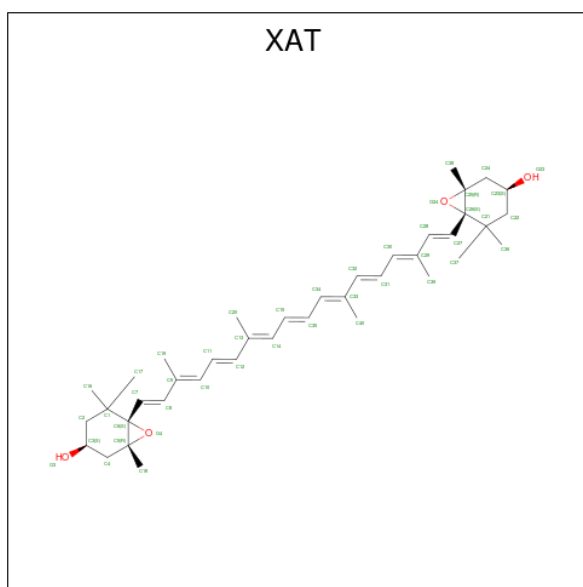
Mol	Chain	Residues	Atoms			AltConf
26	R	1	Total	C	O	0
			44	40	4	
26	1	1	Total	C	O	0
			44	40	4	
26	2	1	Total	C	O	0
			44	40	4	
26	2	1	Total	C	O	0
			44	40	4	
26	3	1	Total	C	O	0
			43	39	4	
26	3	1	Total	C	O	0
			44	40	4	
26	G	1	Total	C	O	0
			44	40	4	
26	G	1	Total	C	O	0
			44	40	4	
26	9	1	Total	C	O	0
			44	40	4	
26	9	1	Total	C	O	0
			44	40	4	
26	N	1	Total	C	O	0
			44	40	4	
26	Y	1	Total	C	O	0
			44	40	4	
26	Y	1	Total	C	O	0
			44	40	4	
26	8	1	Total	C	O	0
			44	40	4	

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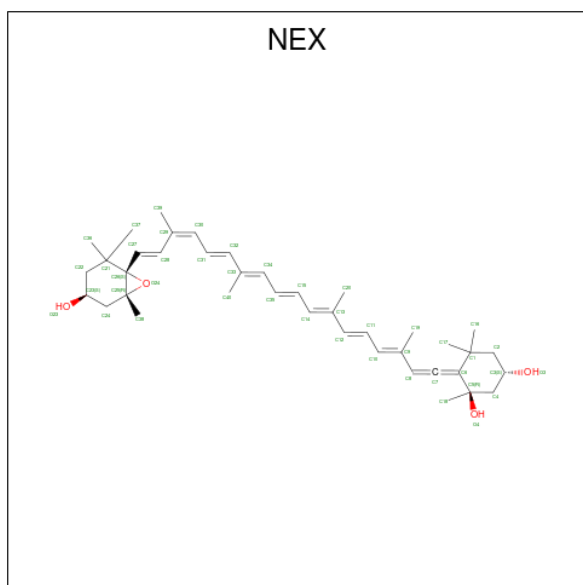
Mol	Chain	Residues	Atoms			AltConf
26	4	1	Total	C	O	0
			44	40	4	
26	5	1	Total	C	O	0
			44	40	4	
26	5	1	Total	C	O	0
			44	40	4	
26	6	1	Total	C	O	0
			43	39	4	
26	g	1	Total	C	O	0
			44	40	4	
26	g	1	Total	C	O	0
			44	40	4	
26	u	1	Total	C	O	0
			44	40	4	
26	u	1	Total	C	O	0
			44	40	4	
26	n	1	Total	C	O	0
			44	40	4	
26	y	1	Total	C	O	0
			44	40	4	
26	y	1	Total	C	O	0
			44	40	4	
26	p	1	Total	C	O	0
			44	40	4	
26	p	1	Total	C	O	0
			44	40	4	
26	q	1	Total	C	O	0
			44	40	4	
26	r	1	Total	C	O	0
			44	40	4	
26	7	1	Total	C	O	0
			44	40	4	
26	7	1	Total	C	O	0
			44	40	4	

- Molecule 27 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄) (labeled as "Ligand of Interest" by depositor).



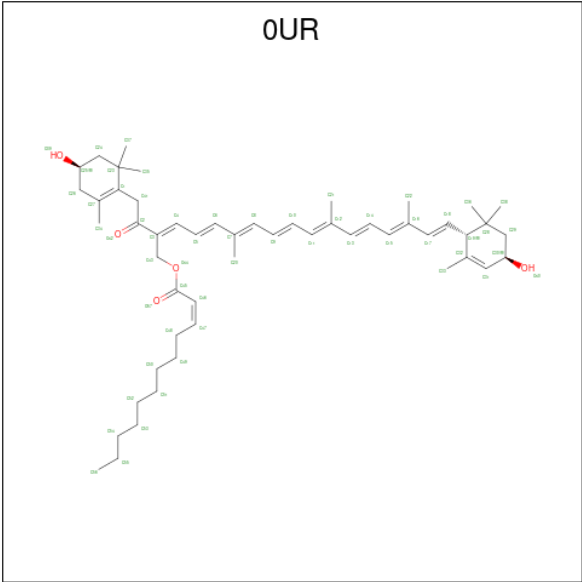
Mol	Chain	Residues	Atoms			AltConf
27	R	1	Total	C	O	0
			44	40	4	
27	r	1	Total	C	O	0
			44	40	4	

- Molecule 28 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: C₄₀H₅₆O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
28	R	1	Total	C	O	0
			44	40	4	
28	1	1	Total	C	O	0
			44	40	4	
28	2	1	Total	C	O	0
			44	40	4	
28	3	1	Total	C	O	0
			44	40	4	
28	S	1	Total	C	O	0
			44	40	4	
28	G	1	Total	C	O	0
			44	40	4	
28	9	1	Total	C	O	0
			44	40	4	
28	N	1	Total	C	O	0
			44	40	4	
28	4	1	Total	C	O	0
			44	40	4	
28	5	1	Total	C	O	0
			44	40	4	
28	6	1	Total	C	O	0
			44	40	4	
28	g	1	Total	C	O	0
			44	40	4	
28	u	1	Total	C	O	0
			44	40	4	
28	n	1	Total	C	O	0
			44	40	4	
28	y	1	Total	C	O	0
			44	40	4	
28	p	1	Total	C	O	0
			44	40	4	
28	s	1	Total	C	O	0
			44	40	4	
28	r	1	Total	C	O	0
			44	40	4	
28	r	1	Total	C	O	0
			44	40	4	
28	7	1	Total	C	O	0
			44	40	4	

- Molecule 29 is Siphonein (CCD ID: 0UR) (formula: C₅₂H₇₆O₅) (labeled as "Ligand of Interest" by depositor).



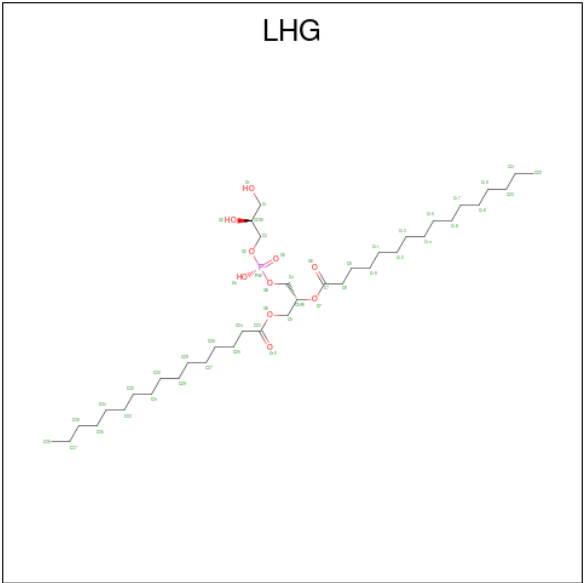
Mol	Chain	Residues	Atoms			AltConf
29	1	1	Total	C	O	0
			52	47	5	
29	2	1	Total	C	O	0
			52	47	5	
29	3	1	Total	C	O	0
			52	47	5	
29	G	1	Total	C	O	0
			52	47	5	
29	9	1	Total	C	O	0
			52	47	5	
29	N	1	Total	C	O	0
			52	47	5	
29	Y	1	Total	C	O	0
			52	47	5	
29	8	1	Total	C	O	0
			52	47	5	
29	4	1	Total	C	O	0
			52	47	5	
29	5	1	Total	C	O	0
			52	47	5	
29	6	1	Total	C	O	0
			52	47	5	
29	g	1	Total	C	O	0
			52	47	5	
29	u	1	Total	C	O	0
			52	47	5	
29	n	1	Total	C	O	0
			52	47	5	

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Mol	Chain	Residues	Atoms			AltConf
29	y	1	Total	C	O	0
			52	47	5	
29	p	1	Total	C	O	0
			52	47	5	
29	q	1	Total	C	O	0
			52	47	5	
29	7	1	Total	C	O	0
			52	47	5	

- Molecule 30 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
30	1	1	Total	C	O	P	0
			42	31	10	1	
30	2	1	Total	C	O	P	0
			40	29	10	1	
30	G	1	Total	C	O	P	0
			43	32	10	1	
30	9	1	Total	C	O	P	0
			43	32	10	1	
30	N	1	Total	C	O	P	0
			43	32	10	1	
30	Y	1	Total	C	O	P	0
			43	32	10	1	
30	A	1	Total	C	O	P	0
			45	34	10	1	

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Mol	Chain	Residues	Atoms				AltConf
30	A	1	Total	C	O	P	0
			44	33	10	1	
30	C	1	Total	C	O	P	0
			32	21	10	1	
30	D	1	Total	C	O	P	0
			49	38	10	1	
30	D	1	Total	C	O	P	0
			39	28	10	1	
30	4	1	Total	C	O	P	0
			42	31	10	1	
30	5	1	Total	C	O	P	0
			43	32	10	1	
30	g	1	Total	C	O	P	0
			43	32	10	1	
30	n	1	Total	C	O	P	0
			43	32	10	1	
30	y	1	Total	C	O	P	0
			43	32	10	1	
30	p	1	Total	C	O	P	0
			43	32	10	1	
30	a	1	Total	C	O	P	0
			45	34	10	1	
30	a	1	Total	C	O	P	0
			44	33	10	1	
30	c	1	Total	C	O	P	0
			32	21	10	1	
30	d	1	Total	C	O	P	0
			49	38	10	1	
30	d	1	Total	C	O	P	0
			39	28	10	1	
30	7	1	Total	C	O	P	0
			37	26	10	1	

- Molecule 31 is (6'R,11cis,11'cis,13cis,15cis)-4',5'-didehydro-5',6'-dihydro-beta,beta-carotene (CCD ID: 8CT) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).

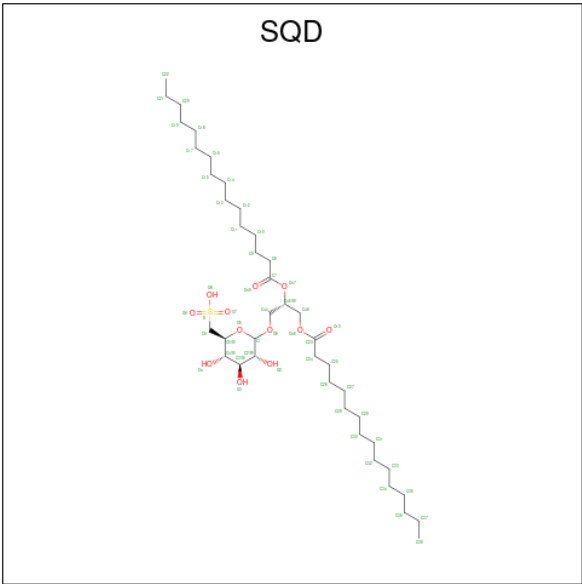


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Mol	Chain	Residues	Atoms	AltConf
31	b	1	Total C 40 40	0
31	a	1	Total C 40 40	0
31	c	1	Total C 40 40	0
31	c	1	Total C 40 40	0
31	c	1	Total C 40 40	0
31	d	1	Total C 40 40	0
31	s	1	Total C 40 40	0
31	s	1	Total C 40 40	0

- Molecule 32 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S) (labeled as "Ligand of Interest" by depositor).



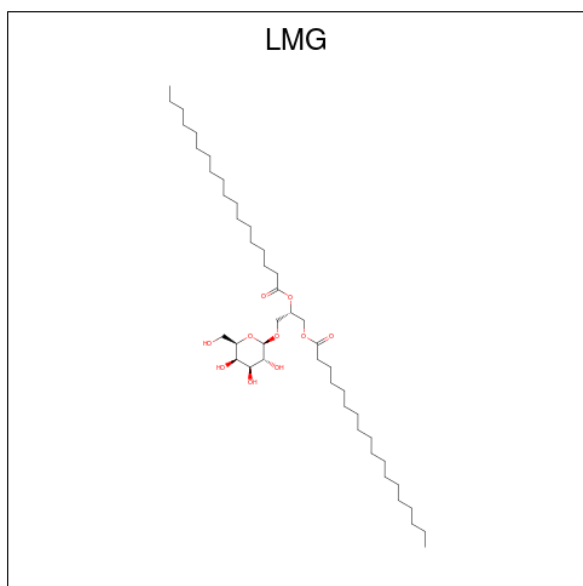
Mol	Chain	Residues	Atoms	AltConf
32	B	1	Total C O S 54 41 12 1	0
32	A	1	Total C O S 45 32 12 1	0

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Mol	Chain	Residues	Atoms				AltConf
32	D	1	Total	C	O	S	0
			44	31	12	1	
32	b	1	Total	C	O	S	0
			54	41	12	1	
32	a	1	Total	C	O	S	0
			45	32	12	1	
32	d	1	Total	C	O	S	0
			44	31	12	1	

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



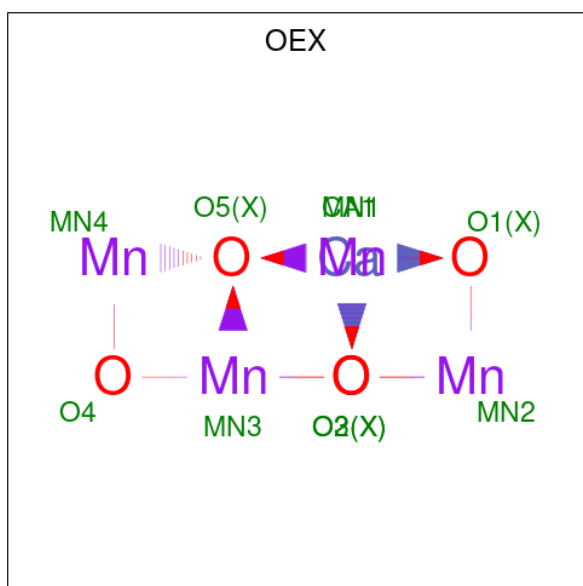
Mol	Chain	Residues	Atoms			AltConf
33	B	1	Total	C	O	0
			41	31	10	
33	C	1	Total	C	O	0
			42	32	10	
33	D	1	Total	C	O	0
			48	38	10	
33	D	1	Total	C	O	0
			46	36	10	
33	W	1	Total	C	O	0
			30	20	10	
33	i	1	Total	C	O	0
			48	38	10	
33	m	1	Total	C	O	0
			41	31	10	

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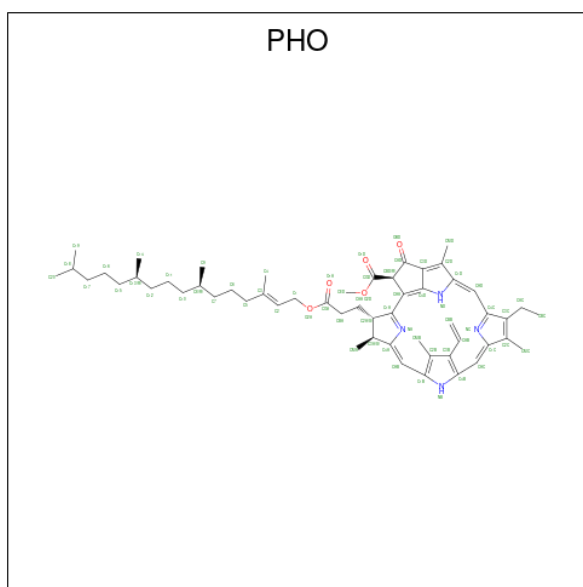
Mol	Chain	Residues	Atoms			AltConf
33	w	1	Total	C	O	0
			36	26	10	
33	d	1	Total	C	O	0
			48	38	10	
33	d	1	Total	C	O	0
			46	36	10	

- Molecule 34 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5) (labeled as "Ligand of Interest" by depositor).



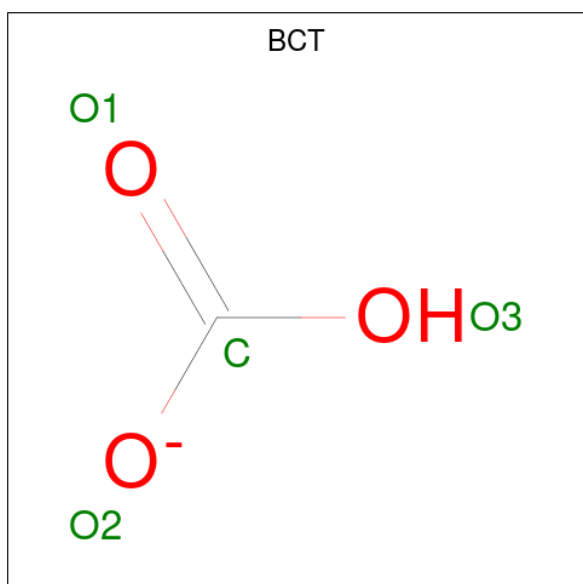
Mol	Chain	Residues	Atoms				AltConf
34	A	1	Total	Ca	Mn	O	0
			10	1	4	5	
34	a	1	Total	Ca	Mn	O	0
			10	1	4	5	

- Molecule 35 is PHEOPHYTIN A (CCD ID: PHO) (formula: $\text{C}_{55}\text{H}_{74}\text{N}_4\text{O}_5$) (labeled as "Ligand of Interest" by depositor).



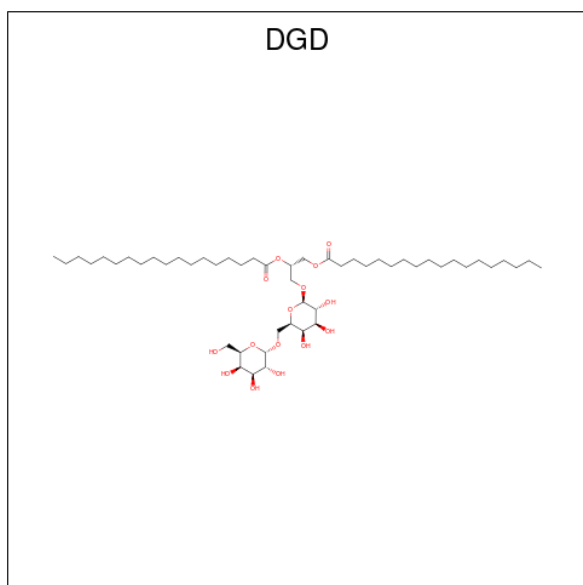
Mol	Chain	Residues	Atoms				AltConf
35	A	1	Total	C	N	O	0
			64	55	4	5	
35	D	1	Total	C	N	O	0
			64	55	4	5	
35	a	1	Total	C	N	O	0
			64	55	4	5	
35	d	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 36 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3^-) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
36	A	1	Total	C	O	0
			4	1	3	
36	a	1	Total	C	O	0
			4	1	3	

- Molecule 37 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).

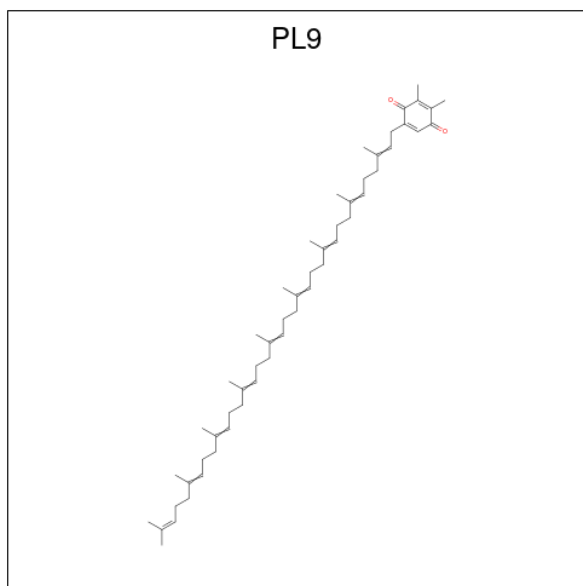


Mol	Chain	Residues	Atoms			AltConf
37	C	1	Total	C	O	0
			50	35	15	
37	C	1	Total	C	O	0
			55	40	15	
37	c	1	Total	C	O	0
			50	35	15	
37	c	1	Total	C	O	0
			55	40	15	

- Molecule 38 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
38	D	1	Total	Fe	0
			1	1	
38	d	1	Total	Fe	0
			1	1	

- Molecule 39 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$) (labeled as "Ligand of Interest" by depositor).




Mol	Chain	Residues	Atoms			AltConf
39	D	1	Total	C	O	0
			55	53	2	
39	d	1	Total	C	O	0
			55	53	2	

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.

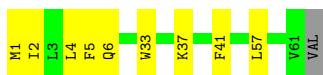
- Molecule 1: Photosystem II reaction center protein Z

Chain Z: 



- Molecule 1: Photosystem II reaction center protein Z

Chain z: 



- Molecule 2: Cytochrome b559 subunit alpha

Chain E: 



- Molecule 2: Cytochrome b559 subunit alpha

Chain e: 

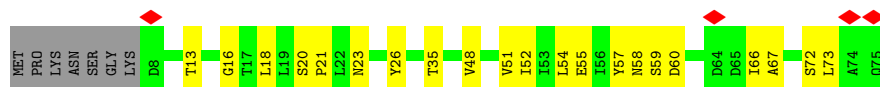


- Molecule 3: Photosystem II reaction center protein H

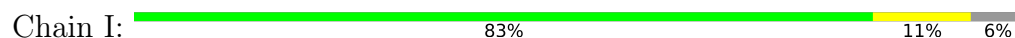
Chain H: 



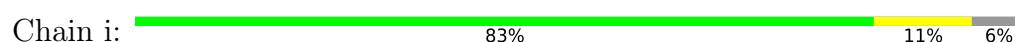
- Molecule 3: Photosystem II reaction center protein H



- Molecule 4: Photosystem II reaction center protein I



- Molecule 4: Photosystem II reaction center protein I



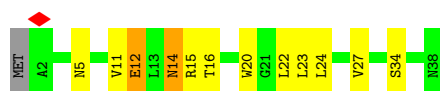
- Molecule 5: Photosystem II reaction center protein K



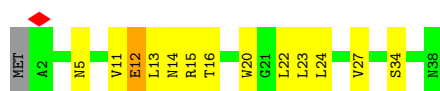
- Molecule 5: Photosystem II reaction center protein K



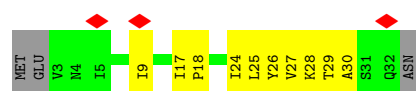
- Molecule 6: Photosystem II reaction center protein L



- Molecule 6: Photosystem II reaction center protein L



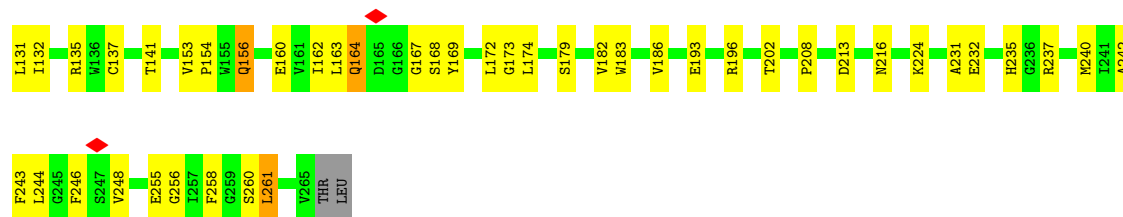
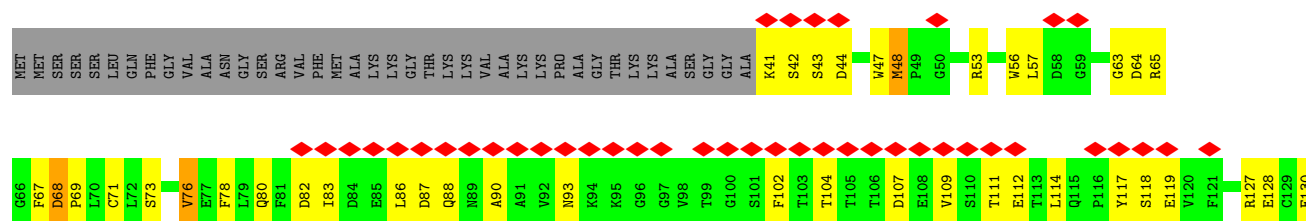
- Molecule 7: Photosystem II reaction center protein M



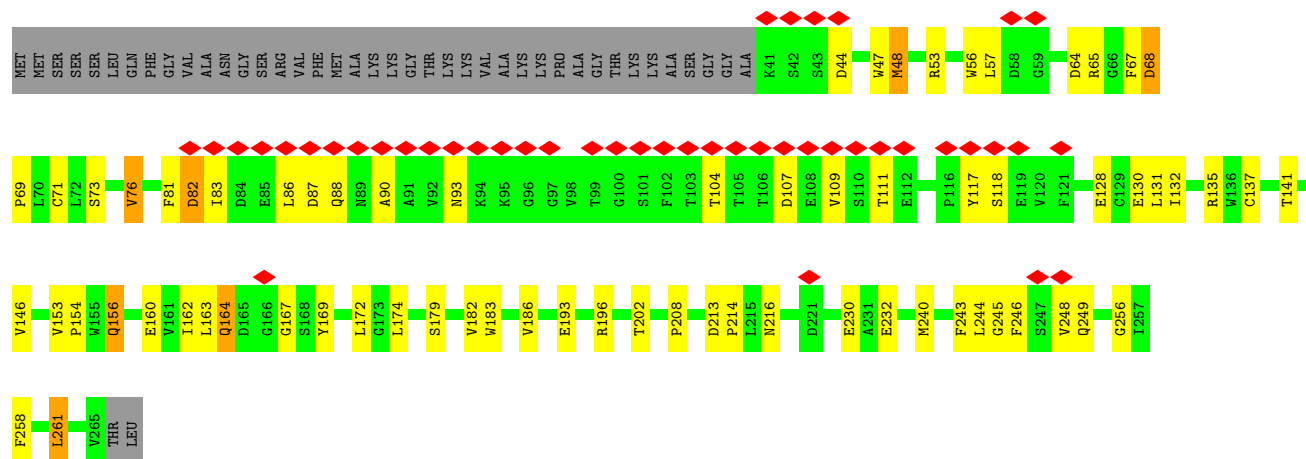
• Molecule 7: Photosystem II reaction center protein M



• Molecule 8: PsbR



• Molecule 8: PsbR



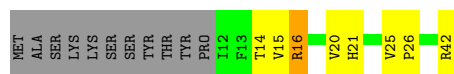
• Molecule 9: Cytochrome b559 subunit beta

Chain F:  55% 17% 26%



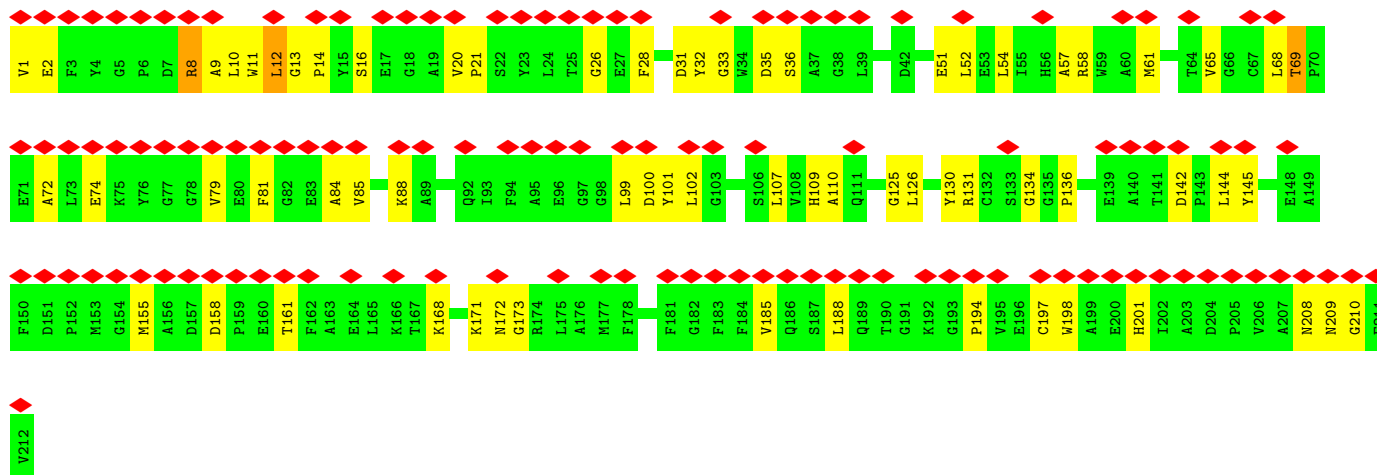
• Molecule 9: Cytochrome b559 subunit beta

Chain f:  55% 17% 26%




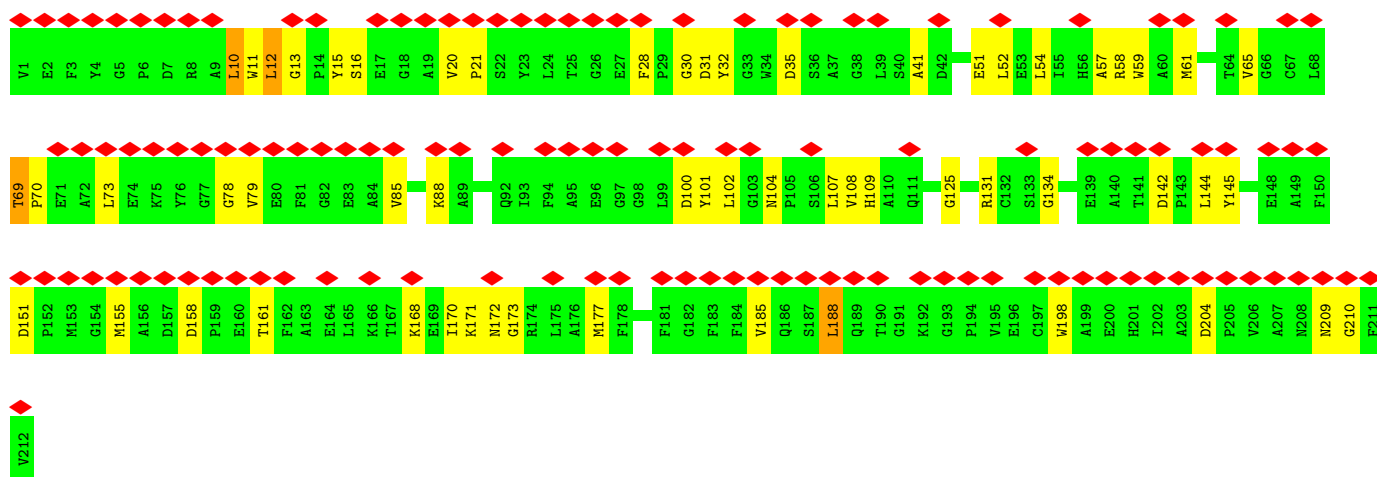
• Molecule 10: Lhcb1

Chain 1:  58% 68% 30%

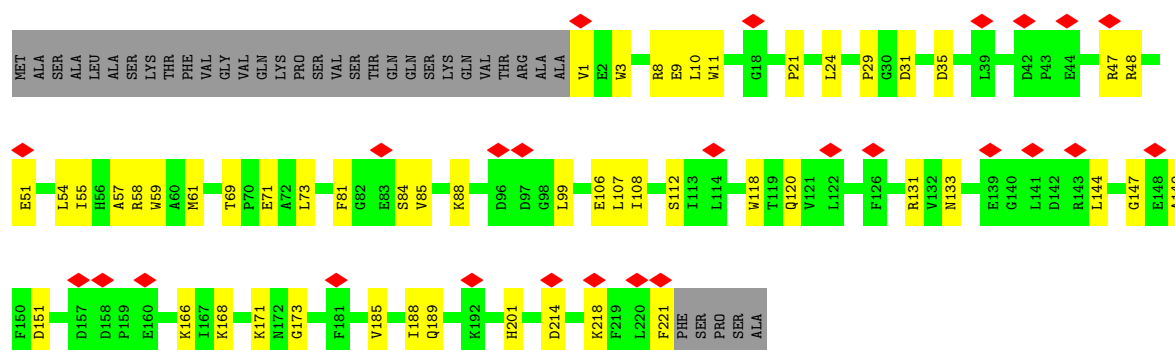


• Molecule 10: Lhcb1

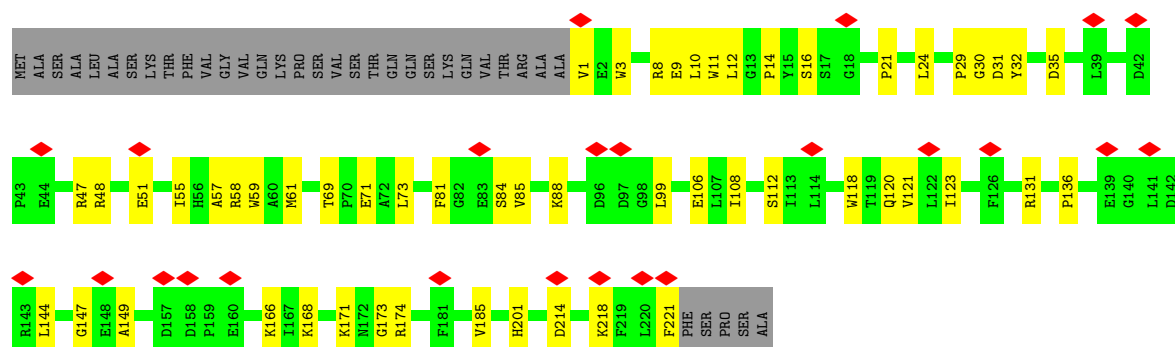
Chain 4:  58% 73% 25%



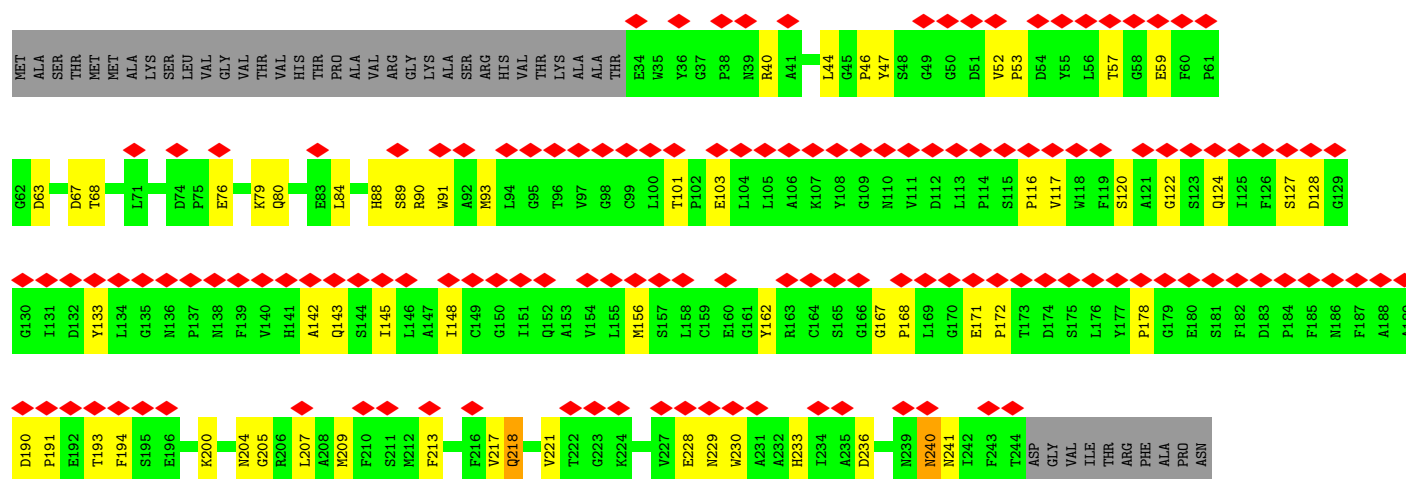
• Molecule 11: Lhcb2



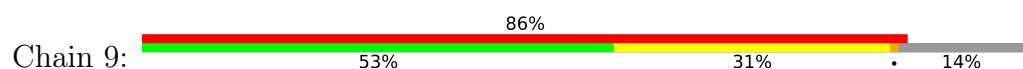
• Molecule 11: Lhcb2

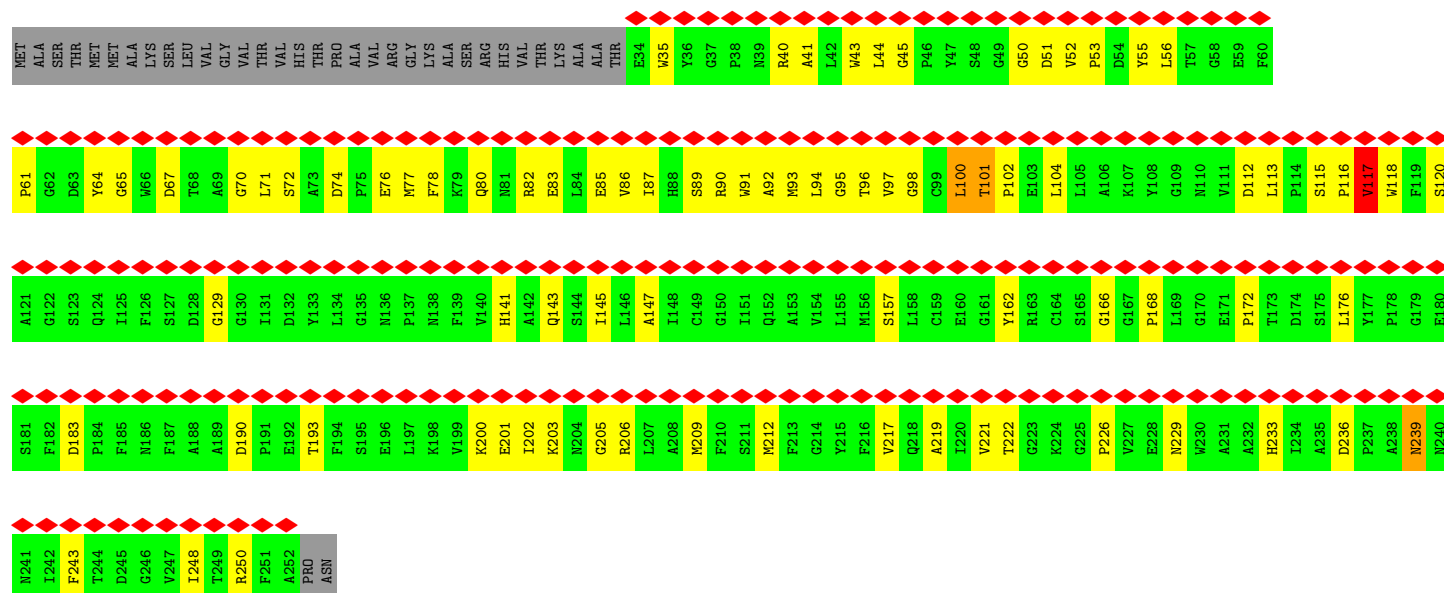


• Molecule 12: Lhcb3

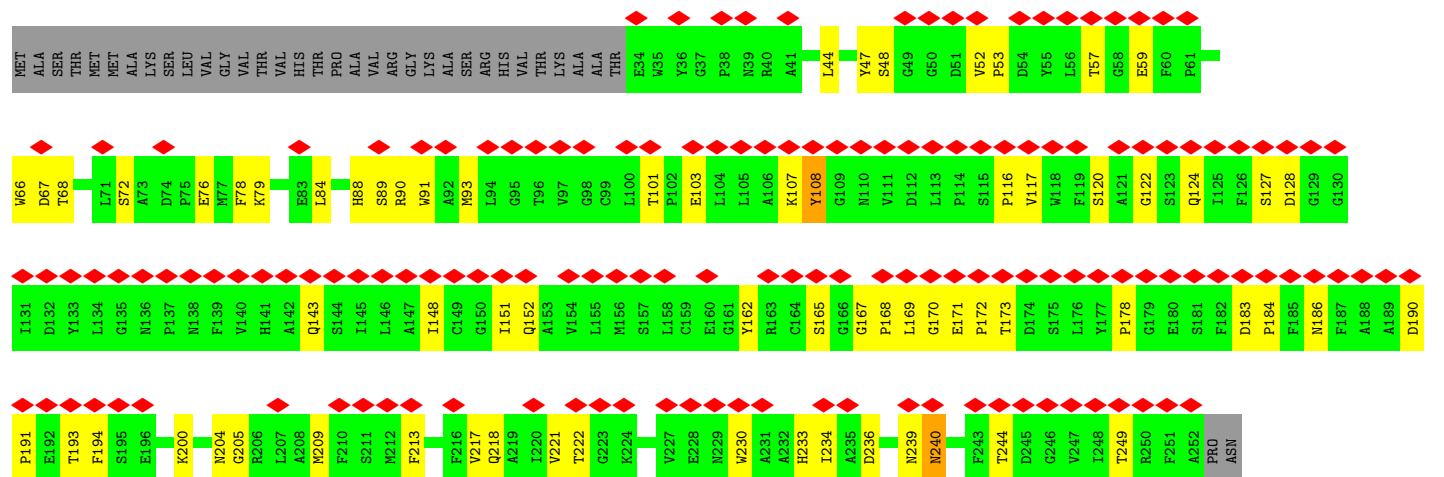


• Molecule 12: Lhcb3

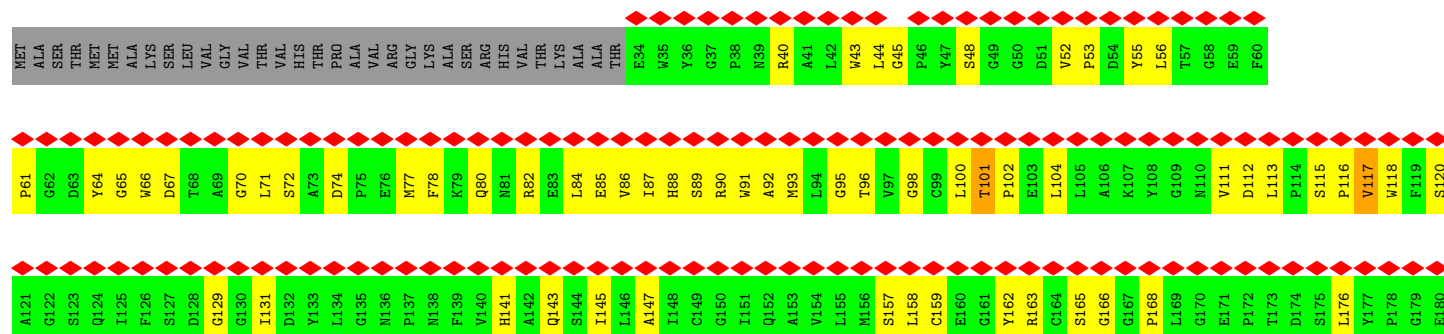
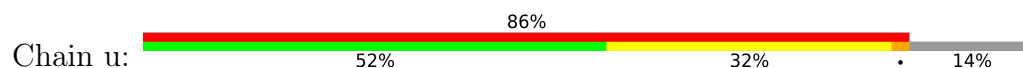


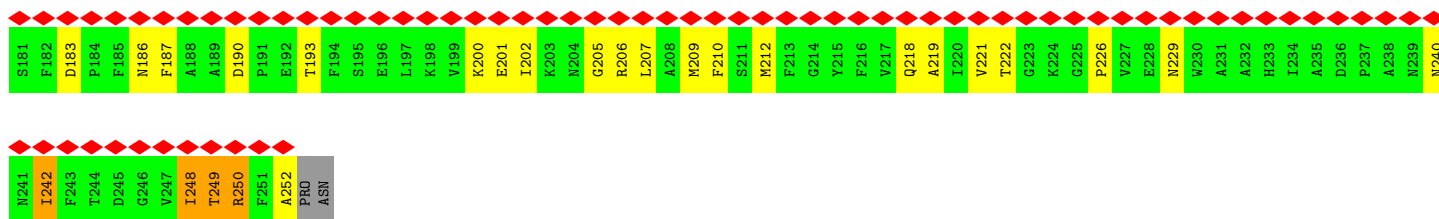


• Molecule 12: Lhcb3



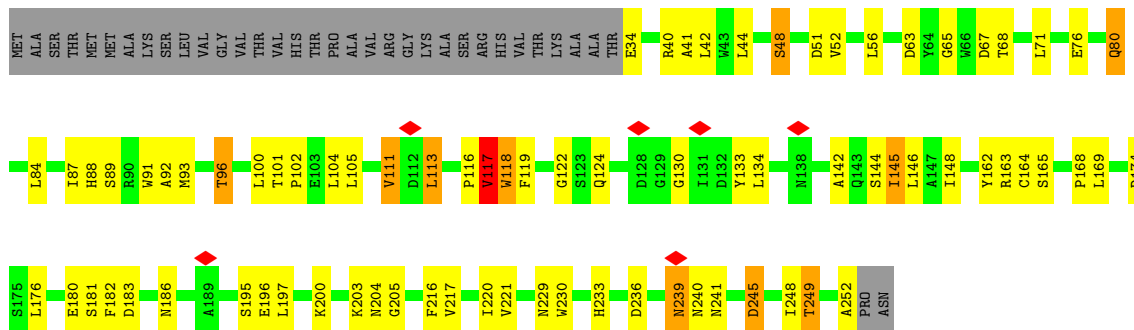
• Molecule 12: Lhcb3





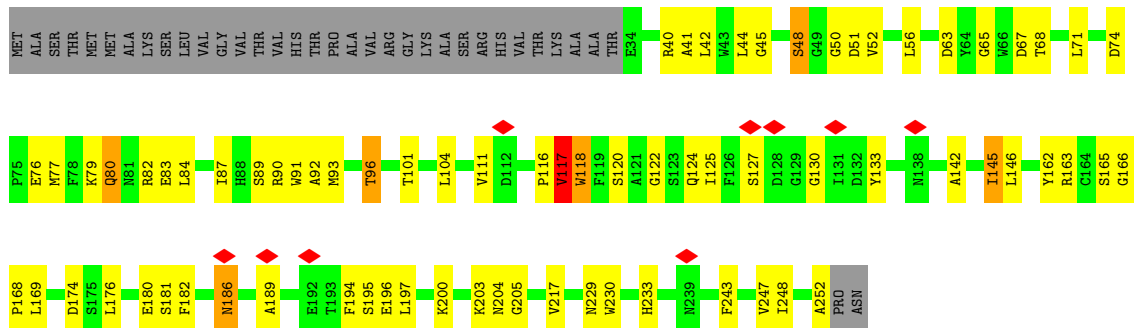
• Molecule 12: Lhcb3

Chain p: 55% 27% 14%



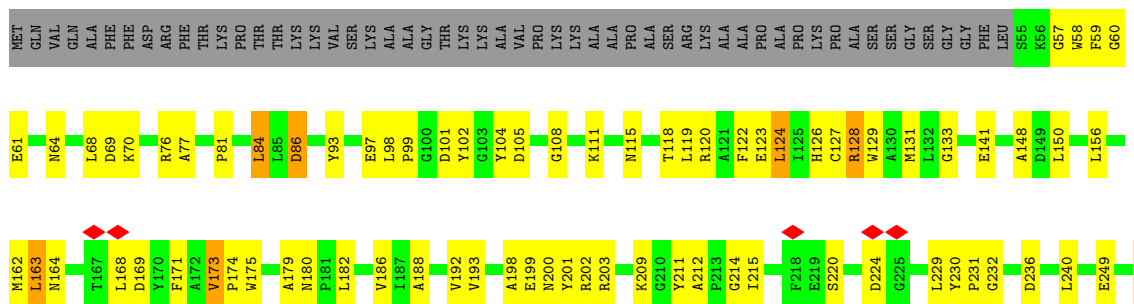
• Molecule 12: Lhcb3

Chain 7: 56% 27% 14%



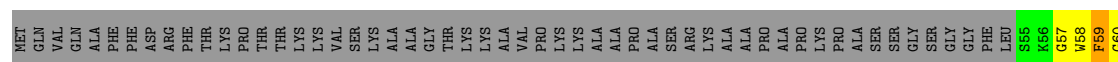
• Molecule 13: LhcbS

Chain S: 51% 27% 19%

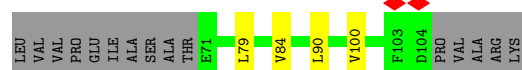
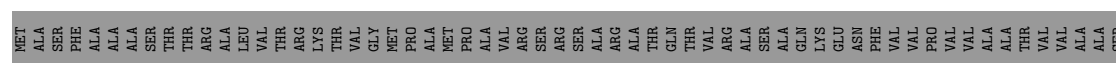




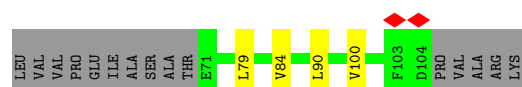
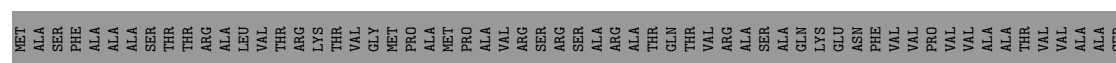
- Molecule 13: LhcbS



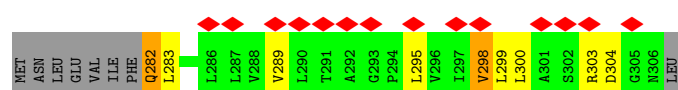
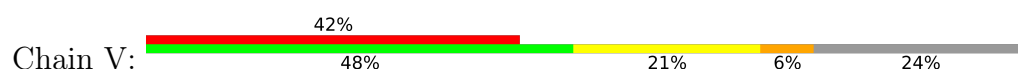
- Molecule 14: PsbX



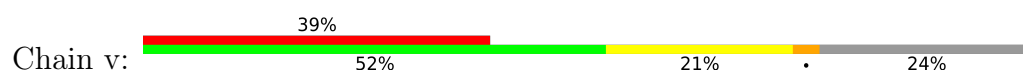
- Molecule 14: PsbX



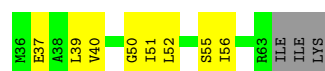
- Molecule 15: Photosystem II reaction center protein Psb30



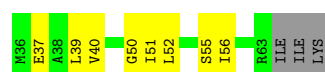
- Molecule 15: Photosystem II reaction center protein Psb30



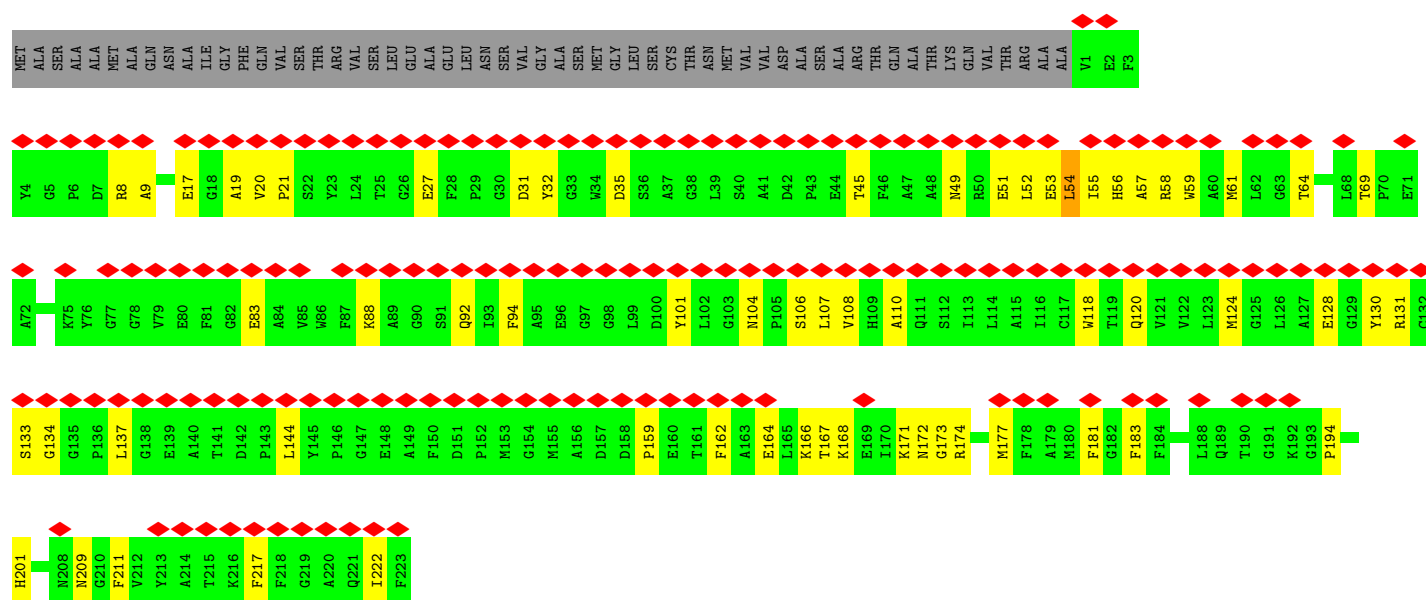
• Molecule 16: Photosystem II reaction center protein T



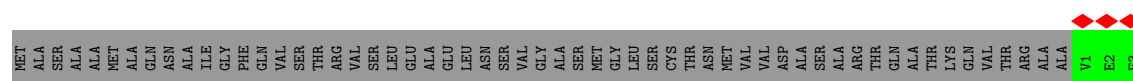
• Molecule 16: Photosystem II reaction center protein T

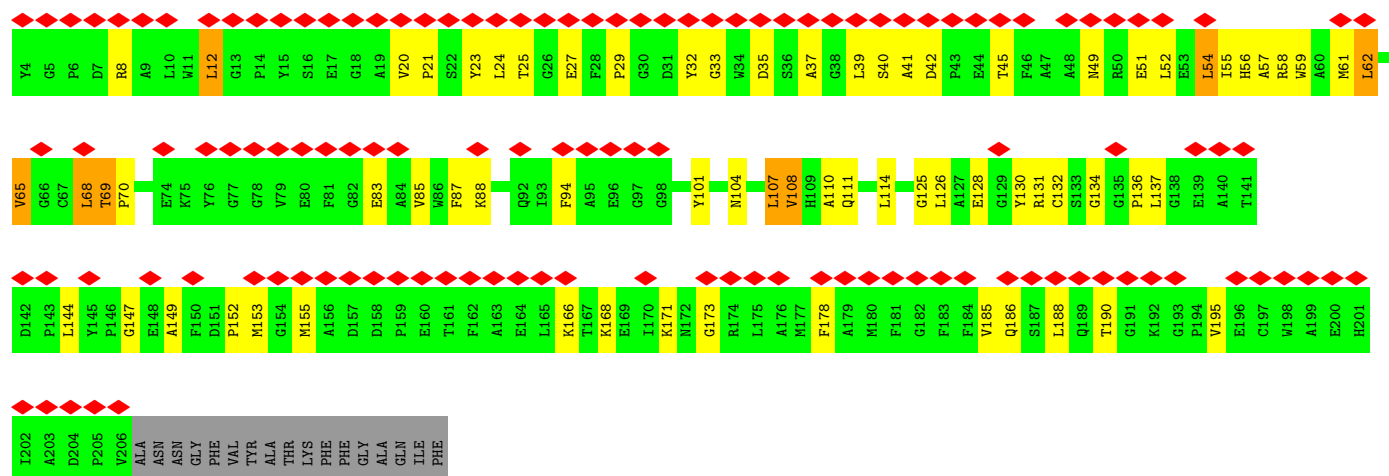


• Molecule 17: LhcbG

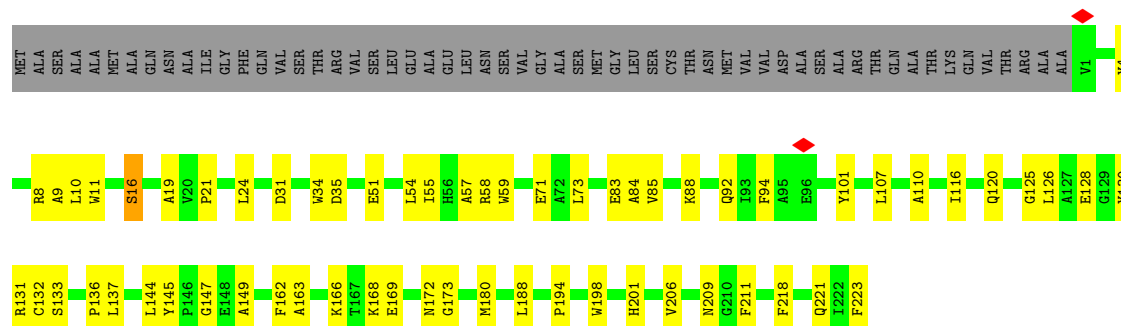


• Molecule 17: LhcbG

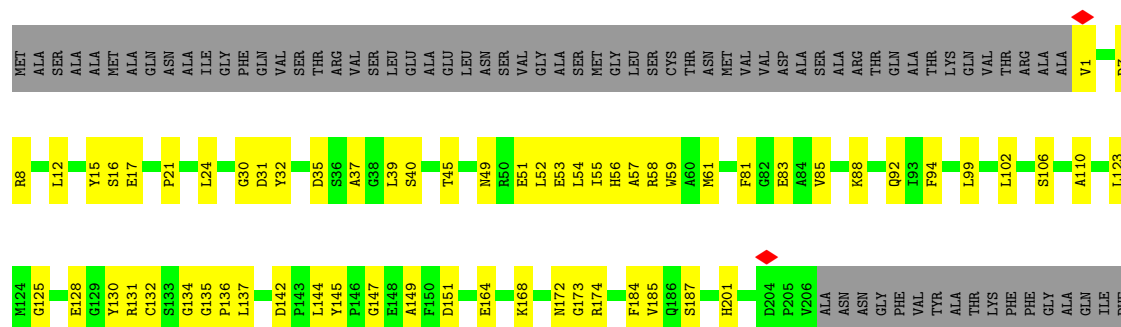




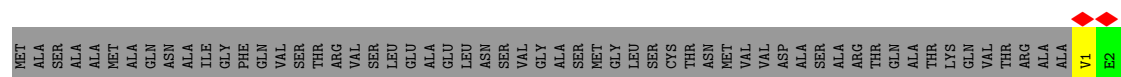
• Molecule 17: LhcbG



• Molecule 17: LhcbG

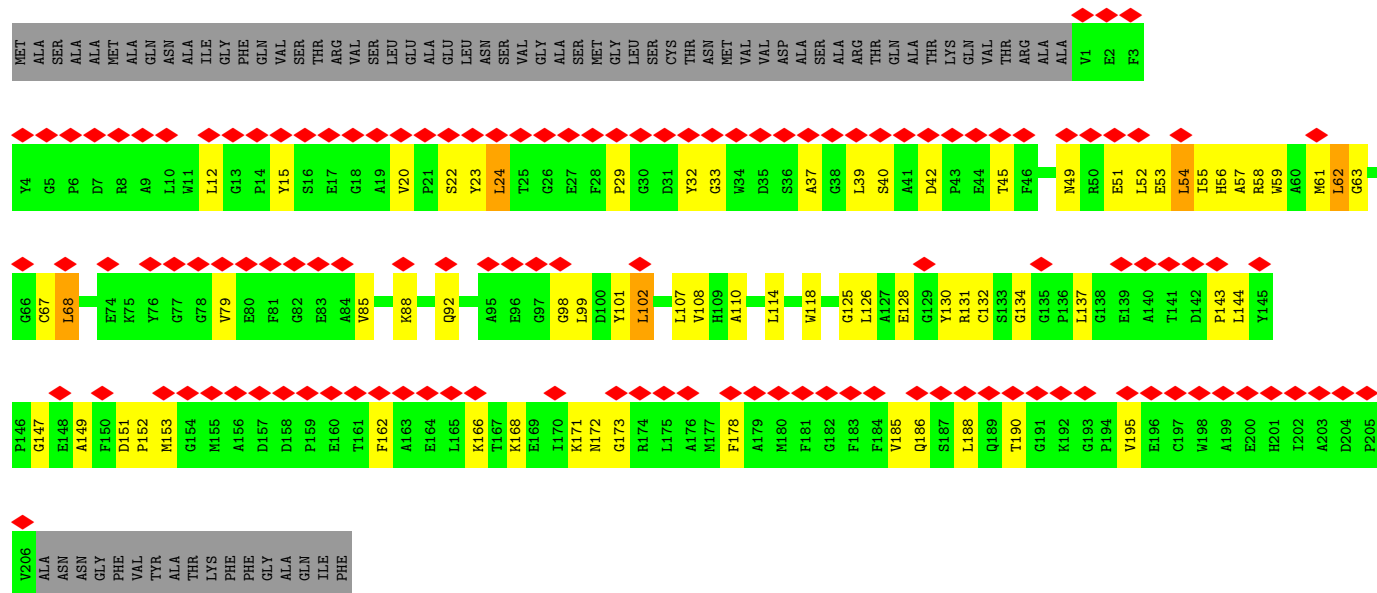


• Molecule 17: LhcbG

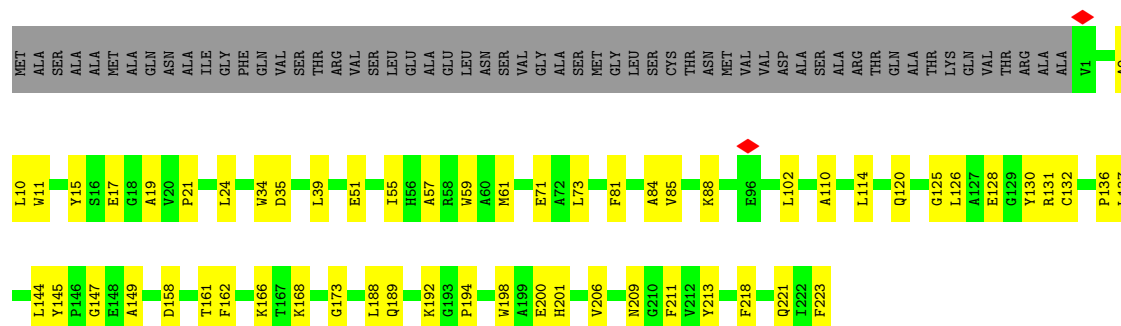




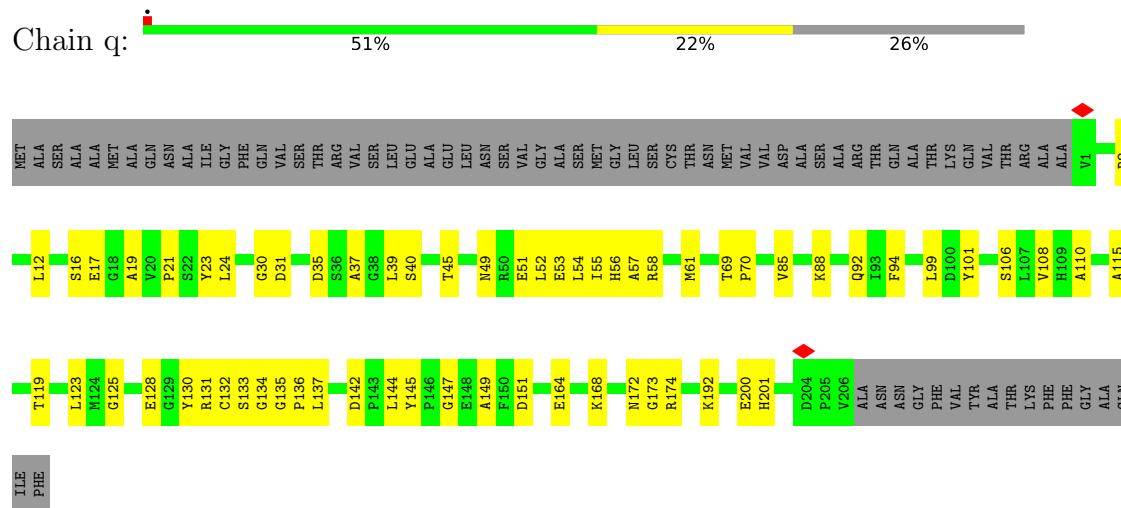
• Molecule 17: LhcbG



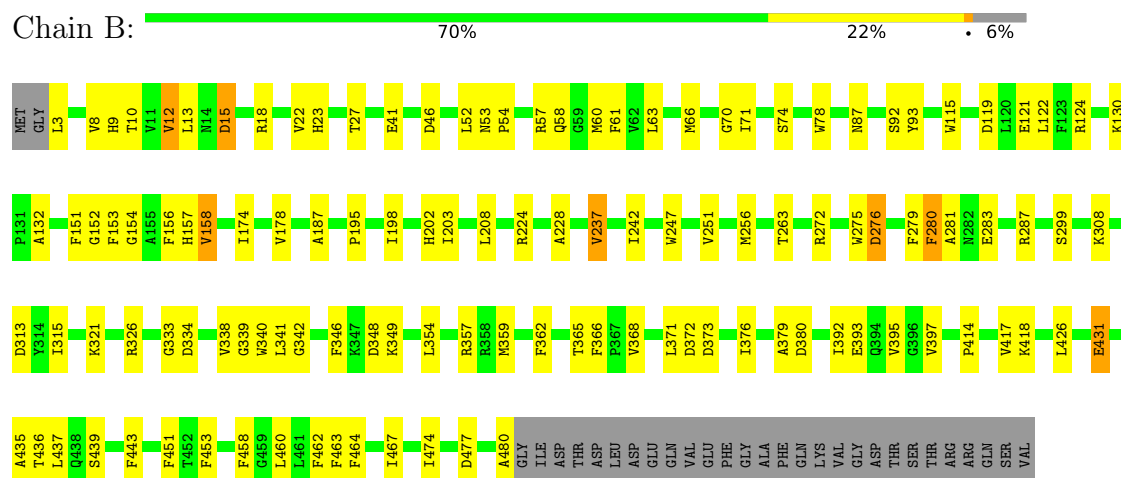
• Molecule 17: LhcbG



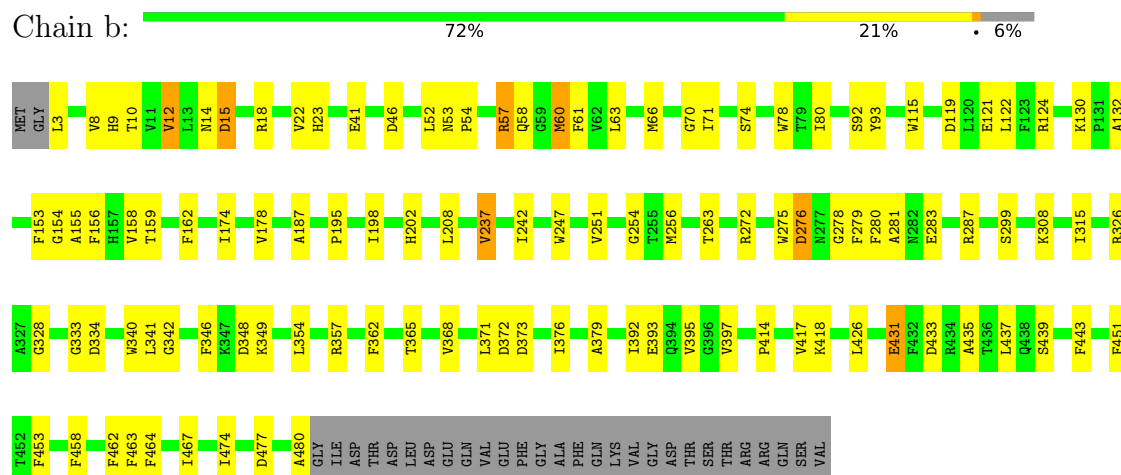
- Molecule 17: LhcbG



- Molecule 18: Photosystem II CP47 reaction center protein

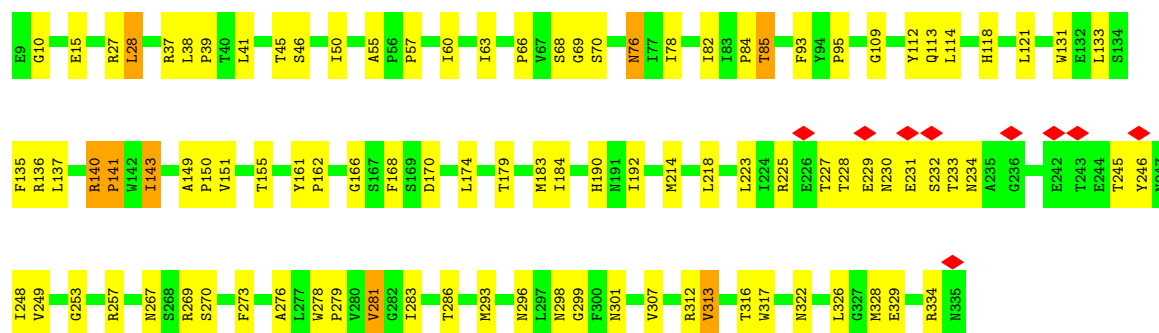


- Molecule 18: Photosystem II CP47 reaction center protein



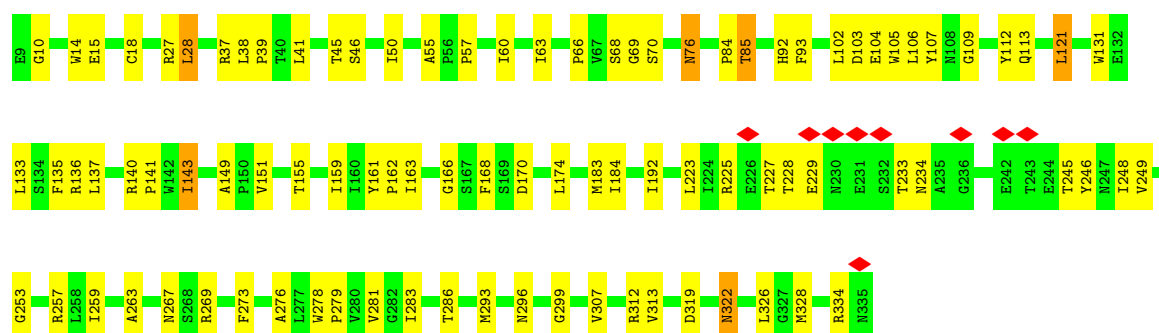
- Molecule 19: PsbA

Chain A: 




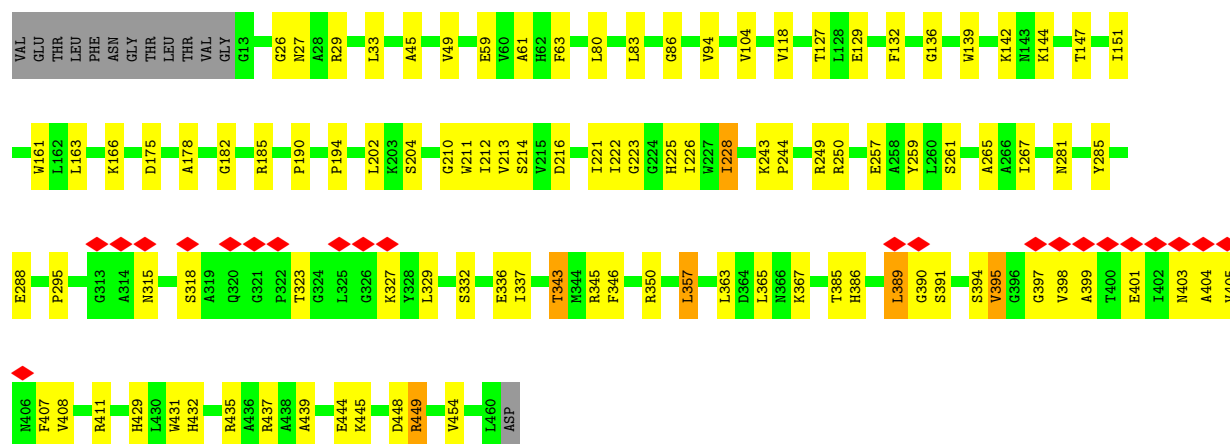
• Molecule 19: PsbA

Chain a: 




• Molecule 20: Photosystem II CP43 reaction center protein

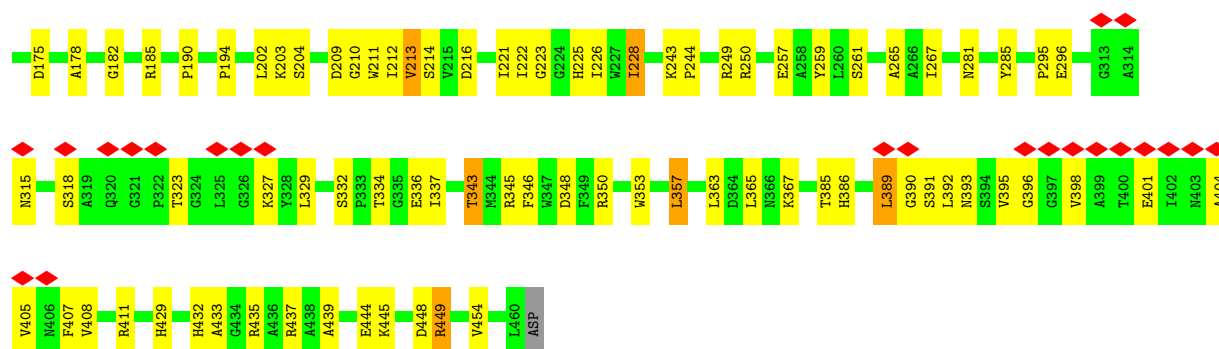
Chain C: 



• Molecule 20: Photosystem II CP43 reaction center protein

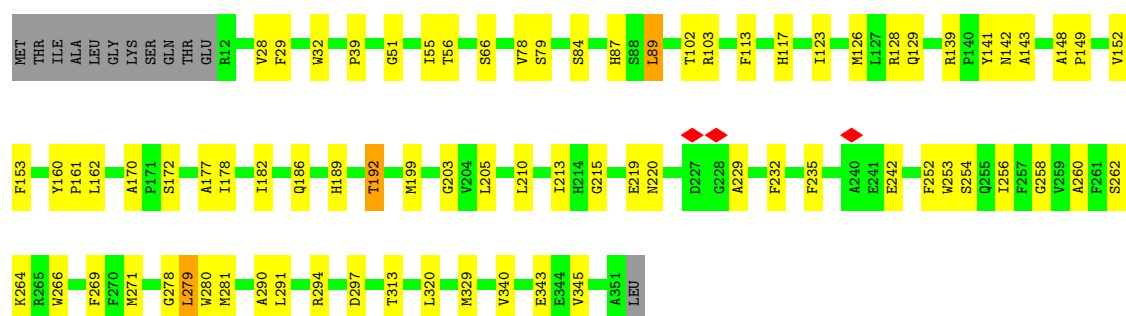
Chain c: 





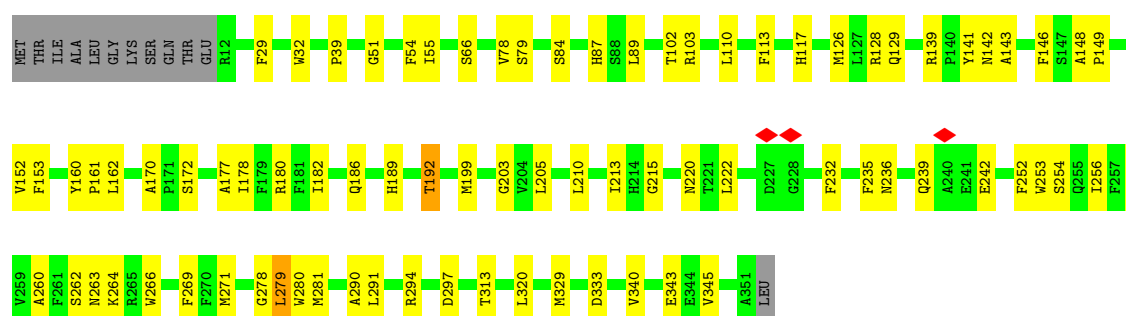
• Molecule 21: Photosystem II D2 protein

Chain D: 74% 21%



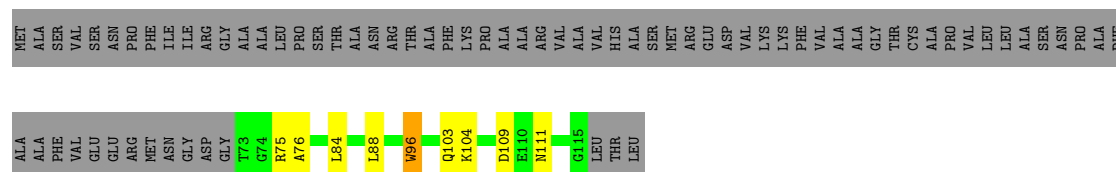
• Molecule 21: Photosystem II D2 protein

Chain d: 74% 22%



• Molecule 22: PsbW

Chain W: 29% 7% 64%



• Molecule 22: PsbW



MET	ALA	ALA	SER	VAL	SER	ASN	PRO	PHE	ILE	ILE	ARG	GLY	ALA	ALA	LEU	PRO	SER	THR	ALA	ASN	ARG	THR	ALA	PHE	LYS	PRO	ALA	ALA	ARG	VAL	ALA	VAL	HIS	ALA	SER	MET	ARG	GLU	ASP	VAL	LYS	LYS	PHE	VAL	VAL	ALA	ALA	GLY	THR	CYS	ALA	PRO	VAL	LEU	LEU	ALA	SER	ASN	PRO	ALA	PHE
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ALA	ALA	PHE	VAL	GLU	ARG	MET	ASN	GLY	ASP	GLY	T73	G74	R75	A76	L88	S93	W96	Q103	D109	E110	G115	LEU	THR	LEU
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	140758	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI 10	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	0.922	Depositor
Minimum map value	-0.284	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.204	Depositor
Map size (\AA)	624.0, 624.0, 624.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.04, 1.04, 1.04	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CLA, LMG, SQD, FE2, PL9, XAT, CHL, BCT, PHO, 8CT, LHG, OEX, 0UR, DGD, NEX, HEM, 0IE

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	Z	0.18	0/486	0.28	0/664
1	z	0.17	0/486	0.28	0/664
2	E	0.42	0/546	0.54	1/745 (0.1%)
2	e	0.23	0/546	0.35	0/745
3	H	0.22	0/523	0.29	0/713
3	h	0.23	0/523	0.32	0/713
4	I	0.33	0/283	0.28	0/383
4	i	0.34	0/283	0.38	0/383
5	K	0.26	0/310	0.52	0/426
5	k	0.25	0/310	0.35	0/426
6	L	0.27	0/312	0.30	0/424
6	l	0.27	0/312	0.29	0/424
7	M	0.16	0/234	0.31	0/320
7	m	0.15	0/234	0.30	0/320
8	R	0.18	0/1749	0.41	2/2373 (0.1%)
8	r	0.18	0/1745	0.42	2/2369 (0.1%)
9	F	0.21	0/252	0.41	0/341
9	f	0.21	0/258	0.38	0/349
10	1	0.11	0/1658	0.30	0/2257
10	4	0.11	0/1652	0.30	0/2250
11	2	0.15	0/1763	0.33	0/2394
11	5	0.14	0/1764	0.29	0/2395
12	3	0.14	0/1657	0.36	0/2261
12	6	0.14	0/1722	0.40	1/2349 (0.0%)
12	7	0.19	0/1730	0.43	0/2359
12	9	0.12	0/1733	0.37	0/2363
12	p	0.19	0/1733	0.45	0/2363
12	u	0.13	0/1736	0.38	0/2367
13	S	0.25	0/1920	0.43	1/2621 (0.0%)
13	s	0.28	0/1920	0.45	1/2621 (0.0%)
14	X	0.14	0/227	0.22	0/308

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
14	x	0.14	0/227	0.22	0/308
15	V	0.13	0/179	0.38	0/245
15	v	0.13	0/179	0.36	0/245
16	T	0.30	0/244	0.36	0/329
16	t	0.31	0/244	0.35	0/329
17	8	0.19	0/1602	0.29	0/2182
17	G	0.11	0/1743	0.27	0/2371
17	N	0.14	0/1599	0.30	0/2178
17	Y	0.24	0/1743	0.31	0/2371
17	g	0.11	0/1743	0.26	0/2371
17	n	0.13	0/1592	0.29	0/2168
17	q	0.19	0/1602	0.29	0/2182
17	y	0.23	0/1743	0.29	0/2371
18	B	0.33	0/3866	0.37	1/5266 (0.0%)
18	b	0.27	0/3866	0.34	0/5266
19	A	0.33	0/2637	0.36	0/3595
19	a	0.41	0/2637	0.39	0/3595
20	C	0.30	0/3591	0.38	0/4895
20	c	0.30	0/3591	0.39	0/4895
21	D	0.33	0/2813	0.37	0/3832
21	d	0.35	0/2813	0.37	0/3832
22	W	0.24	0/308	0.51	0/417
22	w	0.23	0/308	0.51	0/417
All	All	0.25	0/71477	0.36	9/97350 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	77	GLY	N-CA-C	7.09	123.47	114.25
8	r	68	ASP	CA-C-N	-6.62	113.97	120.52
8	r	68	ASP	C-N-CA	-6.62	113.97	120.52
8	R	68	ASP	CA-C-N	-6.58	114.00	120.52
8	R	68	ASP	C-N-CA	-6.58	114.00	120.52
12	6	249	THR	CB-CA-C	-5.87	109.79	116.54
18	B	281	ALA	N-CA-C	-5.67	108.16	114.62
13	S	299	ILE	N-CA-C	-5.50	107.02	111.91
13	s	299	ILE	N-CA-C	-5.37	107.13	111.91

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	Z	472	0	496	9	0
1	z	472	0	496	6	0
2	E	530	0	517	20	0
2	e	530	0	517	9	0
3	H	513	0	517	18	0
3	h	513	0	517	17	0
4	I	275	0	282	4	0
4	i	275	0	282	4	0
5	K	299	0	311	7	0
5	k	299	0	311	4	0
6	L	304	0	313	16	0
6	l	304	0	313	14	0
7	M	231	0	261	9	0
7	m	231	0	261	11	0
8	R	1711	0	1670	83	0
8	r	1707	0	1659	70	0
9	F	246	0	256	4	0
9	f	251	0	261	4	0
10	1	1609	0	1517	52	0
10	4	1603	0	1506	50	0
11	2	1710	0	1616	46	0
11	5	1711	0	1620	48	0
12	3	1606	0	1501	44	0
12	6	1670	0	1564	50	0
12	7	1677	0	1573	66	0
12	9	1680	0	1575	71	0
12	p	1680	0	1575	65	0
12	u	1683	0	1584	74	0
13	S	1867	0	1797	79	0
13	s	1867	0	1797	75	0
14	X	226	0	242	4	0
14	x	226	0	242	2	0
15	V	179	0	205	7	0
15	v	179	0	205	5	0
16	T	236	0	239	5	0
16	t	236	0	239	5	0
17	8	1554	0	1467	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	G	1690	0	1593	57	0
17	N	1551	0	1458	64	0
17	Y	1690	0	1593	44	0
17	g	1690	0	1593	57	0
17	n	1545	0	1455	59	0
17	q	1554	0	1467	52	0
17	y	1690	0	1593	43	0
18	B	3737	0	3605	100	0
18	b	3737	0	3605	92	0
19	A	2558	0	2469	75	0
19	a	2558	0	2469	70	0
20	C	3472	0	3381	85	0
20	c	3472	0	3381	83	0
21	D	2719	0	2631	69	0
21	d	2719	0	2631	66	0
22	W	304	0	276	8	0
22	w	304	0	276	11	0
23	E	43	0	30	2	0
23	f	43	0	30	3	0
24	1	349	0	234	24	0
24	2	353	0	234	11	0
24	3	365	0	250	31	0
24	4	349	0	234	22	0
24	5	353	0	234	15	0
24	6	365	0	250	37	0
24	7	397	0	311	35	0
24	8	351	0	270	24	0
24	9	397	0	311	25	0
24	G	433	0	370	40	0
24	N	404	0	311	20	0
24	R	277	0	186	17	0
24	S	331	0	233	14	0
24	Y	486	0	411	26	0
24	g	433	0	370	28	0
24	n	404	0	311	21	0
24	p	397	0	311	37	0
24	q	404	0	311	23	0
24	r	277	0	186	19	0
24	s	331	0	233	14	0
24	u	397	0	311	21	0
24	y	433	0	370	26	0
25	1	268	0	204	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	2	305	0	258	10	0
25	3	256	0	186	6	0
25	4	268	0	204	23	0
25	5	305	0	258	11	0
25	6	256	0	186	7	0
25	7	321	0	280	27	0
25	8	310	0	267	12	0
25	9	324	0	284	16	0
25	A	280	0	271	12	0
25	B	980	0	1023	63	0
25	C	790	0	814	30	0
25	D	130	0	144	10	0
25	G	318	0	272	27	0
25	N	310	0	267	13	0
25	R	325	0	247	17	0
25	S	333	0	261	10	0
25	Y	321	0	278	8	0
25	a	280	0	271	13	0
25	b	980	0	1023	61	0
25	c	790	0	814	33	0
25	d	130	0	144	10	0
25	g	318	0	272	15	0
25	n	310	0	267	12	0
25	p	324	0	284	24	0
25	q	310	0	267	12	0
25	r	325	0	247	18	0
25	s	332	0	261	13	0
25	u	324	0	284	16	0
25	y	321	0	278	12	0
26	1	44	0	0	0	0
26	2	88	0	0	1	0
26	3	87	0	0	2	0
26	4	44	0	0	0	0
26	5	88	0	0	0	0
26	6	43	0	0	2	0
26	7	88	0	0	2	0
26	8	44	0	0	0	0
26	9	88	0	0	3	0
26	G	88	0	0	0	0
26	N	44	0	0	0	0
26	R	44	0	0	1	0
26	Y	88	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	g	88	0	0	0	0
26	n	44	0	0	0	0
26	p	88	0	0	2	0
26	q	44	0	0	0	0
26	r	44	0	0	1	0
26	u	88	0	0	1	0
26	y	88	0	0	2	0
27	R	44	0	56	16	0
27	r	44	0	56	8	0
28	1	44	0	56	22	0
28	2	44	0	56	9	0
28	3	44	0	56	22	0
28	4	44	0	56	21	0
28	5	44	0	56	10	0
28	6	44	0	56	21	0
28	7	44	0	56	32	0
28	9	44	0	56	6	0
28	G	44	0	56	32	0
28	N	44	0	56	7	0
28	R	44	0	56	6	0
28	S	44	0	56	24	0
28	g	44	0	56	15	0
28	n	44	0	56	7	0
28	p	44	0	56	27	0
28	r	88	0	112	15	0
28	s	44	0	56	21	0
28	u	44	0	56	9	0
28	y	44	0	56	4	0
29	1	52	0	0	0	0
29	2	52	0	0	1	0
29	3	52	0	0	0	0
29	4	52	0	0	1	0
29	5	52	0	0	0	0
29	6	52	0	0	1	0
29	7	52	0	0	0	0
29	8	52	0	0	1	0
29	9	52	0	0	1	0
29	G	52	0	0	1	0
29	N	52	0	0	0	0
29	Y	52	0	0	1	0
29	g	52	0	0	0	0
29	n	52	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	p	52	0	0	1	0
29	q	52	0	0	1	0
29	u	52	0	0	1	0
29	y	52	0	0	1	0
30	1	42	0	54	3	0
30	2	40	0	50	2	0
30	4	42	0	54	3	0
30	5	43	0	56	2	0
30	7	37	0	44	3	0
30	9	43	0	56	6	0
30	A	89	0	124	8	0
30	C	32	0	34	0	0
30	D	88	0	122	13	0
30	G	43	0	56	1	0
30	N	43	0	56	4	0
30	Y	43	0	56	0	0
30	a	89	0	124	7	0
30	c	32	0	34	0	0
30	d	88	0	122	11	0
30	g	43	0	56	2	0
30	n	43	0	56	4	0
30	p	43	0	56	3	0
30	y	43	0	56	2	0
31	A	40	0	0	0	0
31	B	40	0	0	0	0
31	C	120	0	0	1	0
31	D	40	0	0	0	0
31	S	80	0	0	0	0
31	T	40	0	0	0	0
31	V	40	0	0	1	0
31	X	40	0	0	0	0
31	a	40	0	0	0	0
31	b	40	0	0	0	0
31	c	120	0	0	1	0
31	d	40	0	0	0	0
31	s	80	0	0	0	0
31	t	40	0	0	0	0
31	v	40	0	0	1	0
31	x	40	0	0	0	0
32	A	45	0	54	2	0
32	B	54	0	78	4	0
32	D	44	0	52	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	a	45	0	54	4	0
32	b	54	0	78	5	0
32	d	44	0	52	1	0
33	B	41	0	52	5	0
33	C	42	0	54	6	0
33	D	94	0	128	8	0
33	W	30	0	30	2	0
33	d	94	0	128	8	0
33	i	48	0	66	3	0
33	m	41	0	52	6	0
33	w	36	0	42	6	0
34	A	10	0	0	0	0
34	a	10	0	0	0	0
35	A	64	0	74	4	0
35	D	64	0	74	6	0
35	a	64	0	74	4	0
35	d	64	0	74	6	0
36	A	4	0	1	0	0
36	a	4	0	1	0	0
37	C	105	0	126	7	0
37	c	105	0	126	8	0
38	D	1	0	0	0	0
38	d	1	0	0	0	0
39	D	55	0	80	2	0
39	d	55	0	80	2	0
All	All	95298	0	87326	2639	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 14.

All (2639) 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)
13:S:58:TRP:HZ2	28:S:617:NEX:H183	1.14	1.10
12:u:158:LEU:HD23	28:u:304:NEX:H203	1.35	1.07
13:S:58:TRP:CZ2	28:S:617:NEX:H183	1.89	1.06
28:p:304:NEX:H31	24:p:310:CHL:HBA1	1.38	1.04
13:S:58:TRP:HE1	28:S:617:NEX:H192	1.19	1.03
28:g:304:NEX:H31	24:g:310:CHL:HBA1	1.41	1.01
28:4:303:NEX:H31	24:4:309:CHL:CBA	1.91	1.00
24:3:309:CHL:HBA2	28:3:318:NEX:H28	1.43	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:4:303:NEX:H362	25:4:307:CLA:C3B	1.91	1.00
13:s:58:TRP:HE1	28:s:401:NEX:H192	1.25	0.97
28:7:304:NEX:H362	25:7:308:CLA:C4B	1.97	0.94
28:G:304:NEX:H383	25:G:308:CLA:C1B	1.98	0.94
28:7:304:NEX:H383	25:7:308:CLA:C1B	1.98	0.94
28:7:304:NEX:H362	25:7:308:CLA:CHC	1.98	0.93
13:S:58:TRP:NE1	28:S:617:NEX:H192	1.81	0.93
28:p:304:NEX:C31	24:p:310:CHL:HBA1	1.98	0.93
28:6:303:NEX:H28	24:6:309:CHL:HBA2	1.52	0.92
28:7:304:NEX:C31	24:7:310:CHL:HBA1	1.98	0.92
13:S:59:PHE:HE2	28:S:617:NEX:O3	1.50	0.92
28:G:304:NEX:C15	24:G:312:CHL:CMB	2.50	0.89
28:p:304:NEX:H383	25:p:308:CLA:C1B	2.02	0.89
13:S:59:PHE:CE2	28:S:617:NEX:O3	2.24	0.89
8:R:67:PHE:HE2	27:R:615:XAT:H383	1.38	0.89
28:7:304:NEX:H31	24:7:310:CHL:HBA1	1.52	0.88
13:S:58:TRP:HZ2	28:S:617:NEX:C18	1.86	0.86
28:1:303:NEX:H383	25:1:307:CLA:C1B	2.05	0.86
28:g:304:NEX:C31	24:g:310:CHL:HBA1	2.05	0.86
13:S:59:PHE:CD2	28:S:617:NEX:H22	2.11	0.85
28:G:304:NEX:H362	25:G:308:CLA:CHC	2.07	0.85
19:a:296:ASN:HB3	20:c:389:LEU:HA	1.57	0.85
28:p:304:NEX:H362	25:p:308:CLA:C4B	2.06	0.85
8:r:48:MET:HE2	24:r:302:CHL:HHB	1.58	0.85
24:Y:308:CHL:HHB	8:r:172:LEU:HD13	1.59	0.85
28:7:304:NEX:H403	24:7:310:CHL:CBA	2.06	0.85
8:R:67:PHE:CE2	27:R:615:XAT:H242	2.11	0.85
25:B:615:CLA:H2	25:B:616:CLA:HBB2	1.58	0.84
25:r:305:CLA:C1B	28:r:317:NEX:H383	2.09	0.83
17:N:101:TYR:HB3	17:N:107:LEU:HD23	1.58	0.83
28:7:304:NEX:H403	24:7:310:CHL:HBA1	1.59	0.83
25:b:615:CLA:H2	25:b:616:CLA:HBB2	1.59	0.83
12:3:236:ASP:HB3	12:3:240:ASN:HB2	1.60	0.82
28:4:303:NEX:H383	25:4:307:CLA:C1B	2.09	0.82
25:R:604:CLA:C1B	28:R:616:NEX:H383	2.09	0.82
8:R:172:LEU:HD13	24:y:309:CHL:HHB	1.59	0.82
28:S:617:NEX:H31	24:8:308:CHL:HBA2	1.59	0.82
20:C:398:VAL:HG22	20:C:401:GLU:HB2	1.62	0.82
18:B:46:ASP:H	18:B:58:GLN:HE22	1.27	0.81
28:1:303:NEX:H31	24:1:309:CHL:CBA	2.10	0.81
24:3:309:CHL:HAA1	28:3:318:NEX:O24	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:28:LYS:HG2	8:R:80:GLN:HE22	1.46	0.81
28:1:303:NEX:C15	24:1:311:CHL:HMB2	2.11	0.81
11:5:185:VAL:HG21	25:5:317:CLA:HAC2	1.62	0.80
24:3:309:CHL:CAA	28:3:318:NEX:O24	2.30	0.80
11:2:185:VAL:HG21	25:2:317:CLA:HAC2	1.62	0.80
28:G:304:NEX:H222	25:G:308:CLA:C1C	2.11	0.80
13:S:211:TYR:HB3	13:S:215:ILE:HB	1.64	0.80
13:s:211:TYR:HB3	13:s:215:ILE:HB	1.63	0.79
18:b:46:ASP:H	18:b:58:GLN:HE22	1.27	0.79
20:c:398:VAL:HG22	20:c:401:GLU:HB2	1.66	0.78
24:3:309:CHL:CBA	28:3:318:NEX:H28	2.14	0.78
17:n:101:TYR:HB3	17:n:107:LEU:HD23	1.66	0.78
12:7:168:PRO:HG2	24:7:312:CHL:HBB2	1.66	0.77
28:4:303:NEX:H222	25:4:307:CLA:C4B	2.14	0.77
18:B:480:ALA:H	21:D:139:ARG:HH12	1.32	0.77
28:4:303:NEX:H362	25:4:307:CLA:C4B	2.15	0.76
25:r:305:CLA:C2B	28:r:317:NEX:H383	2.15	0.76
17:8:137:LEU:HG	24:8:309:CHL:HBB1	1.67	0.76
28:6:303:NEX:C28	24:6:309:CHL:HAA1	2.15	0.76
28:1:303:NEX:C15	24:1:311:CHL:CMB	2.64	0.76
17:g:137:LEU:HG	24:g:312:CHL:HBB1	1.67	0.76
13:s:58:TRP:NE1	28:s:401:NEX:H192	2.00	0.76
8:R:48:MET:HE2	24:R:601:CHL:HHB	1.67	0.76
8:r:87:ASP:HB2	8:r:90:ALA:HB3	1.68	0.76
28:4:303:NEX:H362	25:4:307:CLA:CAB	2.14	0.76
12:p:230:TRP:HE1	24:p:318:CHL:HMC	1.51	0.76
6:L:12:GLU:HA	7:M:29:THR:HG21	1.68	0.75
12:u:158:LEU:HD23	28:u:304:NEX:C20	2.15	0.75
3:h:57:TYR:HD2	25:b:602:CLA:H2	1.50	0.75
28:S:617:NEX:H383	25:8:306:CLA:C2B	2.17	0.75
12:p:217:VAL:HG21	25:p:317:CLA:HAC2	1.69	0.75
8:R:69:PRO:HG2	27:R:615:XAT:H221	1.69	0.74
13:S:59:PHE:CE2	28:S:617:NEX:H22	2.21	0.74
12:7:217:VAL:HG21	25:7:317:CLA:HAC2	1.68	0.74
17:8:185:VAL:HG21	25:8:314:CLA:HAC2	1.69	0.74
18:b:480:ALA:H	21:d:139:ARG:HH12	1.36	0.74
15:V:295:LEU:HA	15:V:298:VAL:HG12	1.69	0.74
24:q:310:CHL:HMA3	28:s:401:NEX:H30	1.69	0.74
12:p:168:PRO:HB2	24:p:312:CHL:HBB2	1.71	0.73
25:a:604:CLA:HHC	25:a:604:CLA:HBB1	1.71	0.73
28:1:303:NEX:H362	25:1:307:CLA:C4B	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:131:TRP:HZ2	20:C:437:ARG:HG2	1.53	0.73
12:u:242:ILE:HD13	25:u:317:CLA:HMD3	1.69	0.73
12:3:103:GLU:HA	12:3:116:PRO:HB2	1.70	0.73
13:S:59:PHE:CE2	28:S:617:NEX:C2	2.72	0.73
6:l:12:GLU:HA	7:m:29:THR:HG21	1.70	0.73
24:4:311:CHL:HHC	24:4:311:CHL:HBB1	1.71	0.73
21:d:161:PRO:HB3	21:d:170:ALA:HB2	1.69	0.73
21:D:161:PRO:HB3	21:D:170:ALA:HB2	1.70	0.73
15:v:295:LEU:HA	15:v:298:VAL:HG12	1.71	0.72
17:N:171:LYS:NZ	30:N:318:LHG:O4	2.21	0.72
28:7:304:NEX:C36	25:7:308:CLA:CHC	2.67	0.72
3:H:57:TYR:HD2	25:B:602:CLA:H2	1.53	0.72
12:9:217:VAL:HG11	25:9:316:CLA:HAC2	1.69	0.72
12:7:230:TRP:HE1	24:7:318:CHL:HMC	1.54	0.72
28:p:304:NEX:H362	25:p:308:CLA:CHC	2.19	0.72
17:q:137:LEU:HG	24:q:310:CHL:HBB1	1.71	0.72
19:A:296:ASN:HB3	20:C:389:LEU:HA	1.70	0.72
19:a:131:TRP:HZ2	20:c:437:ARG:HG2	1.53	0.72
25:p:315:CLA:H41	25:p:315:CLA:H92	1.71	0.71
18:b:392:ILE:HD11	18:b:418:LYS:HG3	1.72	0.71
12:7:40:ARG:NH2	12:7:56:LEU:O	2.23	0.71
12:7:200:LYS:O	12:7:204:ASN:ND2	2.23	0.71
17:N:52:LEU:O	17:N:56:HIS:ND1	2.23	0.71
17:g:131:ARG:NH2	24:g:313:CHL:O1D	2.23	0.71
18:b:119:ASP:OD1	18:b:124:ARG:NH2	2.24	0.71
20:c:395:VAL:HG11	20:c:404:ALA:H	1.54	0.71
17:n:171:LYS:NZ	30:n:318:LHG:O4	2.22	0.71
24:1:311:CHL:HHC	24:1:311:CHL:HBB1	1.72	0.71
25:7:315:CLA:H41	25:7:315:CLA:H92	1.71	0.71
20:C:221:ILE:O	20:C:225:HIS:ND1	2.24	0.71
12:p:40:ARG:NH2	12:p:56:LEU:O	2.24	0.71
20:c:221:ILE:O	20:c:225:HIS:ND1	2.24	0.71
17:N:126:LEU:HB2	28:N:303:NEX:H203	1.72	0.71
19:A:57:PRO:HB2	19:A:66:PRO:HB2	1.73	0.71
33:i:101:LMG:HC71	20:c:204:SER:HB2	1.71	0.71
6:l:12:GLU:OE2	18:b:3:LEU:N	2.24	0.71
17:n:126:LEU:HB2	28:n:303:NEX:H203	1.73	0.70
25:A:604:CLA:HHC	25:A:604:CLA:HBB1	1.73	0.70
17:q:168:LYS:O	17:q:172:ASN:ND2	2.23	0.70
19:a:27:ARG:NH1	21:d:254:SER:O	2.24	0.70
20:c:449:ARG:NH2	21:d:242:GLU:O	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:119:ASP:OD1	18:B:124:ARG:NH2	2.24	0.70
28:4:303:NEX:C31	24:4:309:CHL:CBA	2.70	0.70
12:p:200:LYS:O	12:p:204:ASN:ND2	2.23	0.70
12:7:117:VAL:HG21	12:7:120:SER:HB2	1.74	0.70
12:9:74:ASP:H	12:9:77:MET:HE2	1.57	0.70
10:4:10:LEU:HG	10:4:20:VAL:HG11	1.72	0.70
28:5:304:NEX:H163	17:n:153:MET:HG2	1.73	0.70
24:q:304:CHL:HHC	24:q:304:CHL:HBB1	1.74	0.70
28:2:304:NEX:C17	17:N:152:PRO:HB2	2.22	0.70
17:8:168:LYS:O	17:8:172:ASN:ND2	2.24	0.69
28:p:304:NEX:H403	24:p:310:CHL:CBA	2.22	0.69
17:y:57:ALA:HB1	17:y:173:GLY:HA3	1.73	0.69
19:a:57:PRO:HB2	19:a:66:PRO:HB2	1.74	0.69
28:G:304:NEX:H362	25:G:308:CLA:C4B	2.22	0.69
28:7:304:NEX:H383	25:7:308:CLA:CHB	2.21	0.69
28:6:303:NEX:H28	24:6:309:CHL:CBA	2.23	0.69
13:S:120:ARG:HD3	24:S:602:CHL:HED1	1.75	0.69
28:G:304:NEX:C22	25:G:308:CLA:C1C	2.70	0.69
28:6:303:NEX:O24	24:6:309:CHL:HAA1	1.93	0.69
28:G:304:NEX:C36	25:G:308:CLA:CHC	2.70	0.69
18:B:392:ILE:HD11	18:B:418:LYS:HG3	1.74	0.69
13:s:59:PHE:CD2	28:s:401:NEX:H183	2.28	0.69
28:G:304:NEX:H222	25:G:308:CLA:CHC	2.23	0.69
18:B:276:ASP:OD1	18:B:276:ASP:N	2.26	0.69
24:R:605:CHL:CBB	27:R:615:XAT:H162	2.22	0.69
21:D:192:THR:HG23	25:D:404:CLA:HBC2	1.74	0.69
13:S:58:TRP:CZ2	28:S:617:NEX:C18	2.68	0.69
9:f:20:VAL:HG23	9:f:21:HIS:HD1	1.58	0.69
19:a:143:ILE:HD12	21:d:252:PHE:CE2	2.28	0.69
8:R:261:LEU:HB3	11:2:106:GLU:HB2	1.75	0.68
19:A:143:ILE:HD12	21:D:252:PHE:CE2	2.28	0.68
24:8:304:CHL:HHC	24:8:304:CHL:HBB1	1.75	0.68
19:A:27:ARG:NH1	21:D:254:SER:O	2.25	0.68
21:d:192:THR:HG23	25:d:404:CLA:HBC2	1.74	0.68
13:S:200:ASN:OD1	13:S:203:ARG:NH2	2.26	0.68
17:G:131:ARG:NH2	24:G:313:CHL:O1D	2.26	0.68
12:6:217:VAL:HG11	25:6:316:CLA:HAC2	1.75	0.68
17:Y:57:ALA:HB1	17:Y:173:GLY:HA3	1.73	0.68
12:3:217:VAL:HG11	25:3:316:CLA:HAC2	1.74	0.68
20:C:449:ARG:NH2	21:D:242:GLU:O	2.27	0.68
11:5:8:ARG:NH2	11:5:24:LEU:O	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:s:200:ASN:OD1	13:s:203:ARG:NH2	2.26	0.68
6:l:11:VAL:HG21	7:m:25:LEU:HD22	1.76	0.68
10:4:11:TRP:HB3	10:4:32:TYR:HB3	1.74	0.68
20:c:27:ASN:ND2	25:c:610:CLA:O1A	2.27	0.68
28:g:304:NEX:H31	24:g:310:CHL:CBA	2.20	0.67
20:C:27:ASN:ND2	25:C:610:CLA:O1A	2.26	0.67
6:L:11:VAL:HG21	7:M:25:LEU:HD22	1.75	0.67
17:n:52:LEU:O	17:n:56:HIS:ND1	2.24	0.67
5:K:7:LYS:N	20:C:61:ALA:O	2.28	0.67
28:p:304:NEX:H383	25:p:308:CLA:CHB	2.23	0.67
28:1:303:NEX:H362	25:1:307:CLA:C3B	2.24	0.67
24:3:309:CHL:HAA1	28:3:318:NEX:C28	2.24	0.67
12:u:74:ASP:H	12:u:77:MET:HE2	1.58	0.67
28:6:303:NEX:O24	24:6:309:CHL:CAA	2.43	0.67
12:9:236:ASP:O	12:9:239:ASN:ND2	2.28	0.67
12:u:89:SER:HB2	12:u:205:GLY:HA3	1.77	0.67
12:6:103:GLU:HA	12:6:116:PRO:HB2	1.76	0.67
11:2:8:ARG:NH2	11:2:24:LEU:O	2.27	0.67
12:9:89:SER:HB2	12:9:205:GLY:HA3	1.77	0.67
17:N:125:GLY:HA2	24:N:312:CHL:HAB	1.77	0.67
28:G:304:NEX:H383	25:G:308:CLA:C2B	2.24	0.67
12:p:229:ASN:ND2	25:p:317:CLA:O1D	2.28	0.67
28:p:304:NEX:H403	24:p:310:CHL:HBA1	1.76	0.67
18:b:130:LYS:HB2	8:r:83:ILE:HD12	1.76	0.67
20:C:216:ASP:OD1	20:C:350:ARG:NH1	2.28	0.66
17:g:189:GLN:NE2	17:g:213:TYR:O	2.27	0.66
25:b:606:CLA:H11	25:b:610:CLA:H13	1.77	0.66
18:B:152:GLY:O	18:B:153:PHE:C	2.37	0.66
12:9:200:LYS:NZ	25:9:315:CLA:O1A	2.28	0.66
13:s:253:LYS:O	13:s:257:ASN:ND2	2.29	0.66
12:9:203:LYS:NZ	30:9:318:LHG:O4	2.28	0.66
10:1:36:SER:O	12:3:80:GLN:NE2	2.28	0.66
17:N:45:THR:O	17:N:49:ASN:ND2	2.27	0.66
10:1:11:TRP:HB3	10:1:32:TYR:HB3	1.77	0.66
3:h:58:ASN:ND2	3:h:60:ASP:OD2	2.29	0.66
17:n:51:GLU:HA	17:n:144:LEU:HD11	1.78	0.66
17:g:101:TYR:HH	28:g:304:NEX:H1	1.43	0.66
28:S:617:NEX:H30	24:8:309:CHL:HMA3	1.78	0.66
5:k:7:LYS:N	20:c:61:ALA:O	2.29	0.66
17:G:137:LEU:HG	24:G:312:CHL:HBB1	1.77	0.66
20:c:216:ASP:OD1	20:c:350:ARG:NH1	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:d:139:ARG:HE	21:d:141:TYR:HE2	1.44	0.65
13:s:120:ARG:HD3	24:s:403:CHL:HED1	1.77	0.65
12:7:229:ASN:ND2	25:7:317:CLA:O1D	2.29	0.65
28:2:304:NEX:H172	17:N:152:PRO:HB2	1.79	0.65
25:R:610:CLA:H2A	25:R:610:CLA:HED3	1.78	0.65
24:3:309:CHL:HAA1	28:3:318:NEX:C27	2.26	0.65
13:S:253:LYS:O	13:S:257:ASN:ND2	2.29	0.65
12:9:45:GLY:HA3	24:9:304:CHL:HBB1	1.79	0.65
8:R:186:VAL:HG23	24:R:608:CHL:HBB2	1.78	0.65
20:C:204:SER:HB2	33:C:618:LMG:HC71	1.78	0.65
28:6:303:NEX:C27	24:6:309:CHL:HAA1	2.27	0.65
28:g:304:NEX:H362	25:g:308:CLA:C4B	2.27	0.65
17:y:198:TRP:HE1	24:y:318:CHL:HMC	1.61	0.65
24:Y:309:CHL:HHC	24:Y:309:CHL:HBB1	1.79	0.65
28:4:303:NEX:H222	25:4:307:CLA:NB	2.12	0.65
21:D:129:GLN:NE2	35:D:403:PHO:OBD	2.30	0.65
19:a:334:ARG:HH22	21:d:320:LEU:HD12	1.62	0.65
13:S:86:ASP:N	13:S:86:ASP:OD1	2.30	0.64
25:r:304:CLA:HBC1	24:r:309:CHL:HBC2	1.79	0.64
12:7:133:TYR:HE1	28:7:304:NEX:H1	1.40	0.64
25:R:603:CLA:HBC1	24:R:608:CHL:HBC2	1.79	0.64
12:p:203:LYS:NZ	30:p:319:LHG:O4	2.31	0.64
17:8:45:THR:O	17:8:49:ASN:ND2	2.30	0.64
21:d:129:GLN:NE2	35:d:403:PHO:OBD	2.30	0.64
12:6:200:LYS:O	12:6:204:ASN:ND2	2.26	0.64
12:9:40:ARG:NH2	12:9:56:LEU:O	2.31	0.64
24:R:602:CHL:CBB	27:R:615:XAT:H32	2.27	0.64
13:S:283:TRP:HE1	24:S:613:CHL:HMC	1.62	0.64
13:s:283:TRP:HE1	24:s:414:CHL:HMC	1.62	0.64
13:s:86:ASP:OD1	13:s:86:ASP:N	2.30	0.64
28:p:304:NEX:H403	24:p:310:CHL:CGA	2.28	0.64
24:1:309:CHL:HHC	24:1:309:CHL:HBB1	1.80	0.64
17:G:94:PHE:HZ	12:9:243:PHE:HB3	1.62	0.64
12:6:128:ASP:O	12:6:143:GLN:NE2	2.30	0.64
20:c:390:GLY:HA3	20:c:408:VAL:HG22	1.79	0.64
28:7:304:NEX:H241	25:7:308:CLA:H2	1.79	0.64
25:B:606:CLA:H11	25:B:610:CLA:H13	1.80	0.63
28:4:303:NEX:C31	24:4:309:CHL:H3A	2.28	0.63
28:g:304:NEX:H383	25:g:308:CLA:C1B	2.28	0.63
8:r:82:ASP:N	8:r:82:ASP:OD1	2.30	0.63
28:p:304:NEX:C40	24:p:310:CHL:O2A	2.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:s:173:VAL:HG12	13:s:175:TRP:H	1.64	0.63
8:R:83:ILE:HD12	18:B:130:LYS:HB2	1.80	0.63
12:7:203:LYS:NZ	30:7:319:LHG:O4	2.31	0.63
12:3:128:ASP:O	12:3:143:GLN:NE2	2.31	0.63
24:3:309:CHL:HAA1	28:3:318:NEX:C26	2.27	0.63
17:q:45:THR:O	17:q:49:ASN:ND2	2.30	0.63
28:4:303:NEX:C36	25:4:307:CLA:HAB	2.28	0.63
24:n:308:CHL:HAA2	25:r:313:CLA:HBA2	1.79	0.63
6:L:12:GLU:OE2	18:B:3:LEU:N	2.32	0.63
8:R:160:GLU:OE2	8:R:164:GLN:NE2	2.31	0.63
17:g:101:TYR:HB3	17:g:107:LEU:HG	1.80	0.63
17:Y:198:TRP:HE1	24:Y:317:CHL:HMC	1.62	0.63
17:y:85:VAL:HG23	17:y:88:LYS:HB2	1.80	0.63
24:y:310:CHL:HBB1	24:y:310:CHL:HHC	1.80	0.63
11:2:57:ALA:HB1	11:2:173:GLY:HA3	1.79	0.63
13:S:98:LEU:HD22	13:S:120:ARG:HG3	1.81	0.63
17:Y:10:LEU:HD23	17:Y:16:SER:HB2	1.79	0.63
11:5:57:ALA:HB1	11:5:173:GLY:HA3	1.79	0.63
12:u:250:ARG:H	12:u:250:ARG:HE	1.47	0.63
17:n:125:GLY:HA2	24:n:312:CHL:HAB	1.79	0.63
25:B:609:CLA:H202	25:B:612:CLA:H18	1.80	0.63
3:H:58:ASN:ND2	3:H:60:ASP:OD2	2.32	0.62
20:C:395:VAL:HG11	20:C:403:ASN:HA	1.81	0.62
17:q:101:TYR:HB2	17:q:108:VAL:HG22	1.81	0.62
20:c:33:LEU:HA	20:c:127:THR:HG22	1.80	0.62
8:r:163:LEU:HB2	24:r:307:CHL:HMD1	1.79	0.62
17:G:128:GLU:OE1	17:G:131:ARG:NH1	2.32	0.62
28:G:304:NEX:C20	24:G:312:CHL:HMB1	2.28	0.62
13:S:124:LEU:HD13	13:S:229:LEU:HB3	1.81	0.62
20:C:33:LEU:HA	20:C:127:THR:HG22	1.80	0.62
10:4:125:GLY:HA2	24:4:312:CHL:HAB	1.82	0.62
28:5:304:NEX:H21	17:n:153:MET:HA	1.82	0.62
18:b:467:ILE:HD13	21:d:126:MET:HE1	1.80	0.62
32:d:409:SQD:H291	33:d:411:LMG:H192	1.80	0.62
12:3:200:LYS:O	12:3:204:ASN:ND2	2.26	0.62
19:A:45:THR:HG23	25:A:604:CLA:H201	1.81	0.62
19:A:334:ARG:HH22	21:D:320:LEU:HD12	1.63	0.62
25:q:306:CLA:NB	28:s:401:NEX:H242	2.15	0.62
19:a:45:THR:HG23	25:a:604:CLA:H201	1.81	0.62
8:r:135:ARG:NE	8:r:232:GLU:OE2	2.25	0.62
24:9:309:CHL:HBC2	24:9:310:CHL:HHD	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:q:136:PRO:HG3	13:s:58:TRP:CD2	2.35	0.62
8:R:64:ASP:O	8:R:65:ARG:NH1	2.31	0.62
28:p:304:NEX:H31	24:p:310:CHL:CBA	2.23	0.62
17:Y:21:PRO:HG2	17:Y:35:ASP:HB3	1.81	0.62
12:p:236:ASP:O	12:p:239:ASN:ND2	2.31	0.62
17:G:171:LYS:NZ	30:G:319:LHG:O4	2.32	0.62
17:G:211:PHE:HB3	17:N:94:PHE:HZ	1.65	0.62
17:N:126:LEU:HB2	28:N:303:NEX:C20	2.30	0.62
11:5:106:GLU:HB2	8:r:261:LEU:HB3	1.82	0.62
14:X:84:VAL:HG21	24:G:318:CHL:HMB2	1.81	0.62
17:Y:71:GLU:HA	17:Y:84:ALA:HB1	1.81	0.62
21:D:139:ARG:HE	21:D:141:TYR:HE2	1.45	0.62
17:Y:85:VAL:HG23	17:Y:88:LYS:HB2	1.80	0.61
2:e:98:ARG:NH2	3:h:59:SER:OG	2.33	0.61
12:7:248:ILE:O	12:7:252:ALA:N	2.33	0.61
18:B:467:ILE:HD13	21:D:126:MET:HE1	1.81	0.61
21:d:186:GLN:HB2	25:d:404:CLA:HBC1	1.81	0.61
10:1:131:ARG:NH2	24:1:312:CHL:O1D	2.30	0.61
25:A:605:CLA:HAB	25:D:404:CLA:H51	1.82	0.61
10:4:131:ARG:NH2	24:4:312:CHL:O1D	2.31	0.61
10:4:158:ASP:HB3	10:4:161:THR:HG22	1.82	0.61
28:G:304:NEX:C15	24:G:312:CHL:HMB1	2.29	0.61
17:N:128:GLU:OE1	17:N:131:ARG:NH2	2.33	0.61
13:s:180:ASN:ND2	24:s:406:CHL:OBD	2.34	0.61
25:r:305:CLA:CHC	28:r:317:NEX:H222	2.30	0.61
10:1:130:TYR:OH	28:1:303:NEX:C19	2.48	0.61
17:G:118:TRP:HZ2	24:9:317:CHL:HBD	1.65	0.61
17:Y:19:ALA:HB2	17:8:132:CYS:HB3	1.82	0.61
13:s:98:LEU:HD22	13:s:120:ARG:HG3	1.81	0.61
21:D:186:GLN:HB2	25:D:404:CLA:HBC1	1.81	0.61
18:b:372:ASP:OD1	18:b:373:ASP:N	2.32	0.61
8:R:135:ARG:NE	8:R:232:GLU:OE2	2.26	0.61
11:2:51:GLU:HA	11:2:144:LEU:HD21	1.82	0.61
12:9:118:TRP:HE1	12:9:219:ALA:HB2	1.66	0.61
20:C:390:GLY:HA3	20:C:408:VAL:HG22	1.82	0.61
30:D:408:LHG:HC41	30:D:408:LHG:HC11	1.81	0.61
10:4:100:ASP:OD2	10:4:109:HIS:ND1	2.32	0.61
13:s:59:PHE:CD2	28:s:401:NEX:C18	2.83	0.61
13:S:58:TRP:CD1	28:S:617:NEX:H192	2.35	0.61
28:p:304:NEX:H241	25:p:308:CLA:O2A	2.00	0.61
20:c:444:GLU:OE2	20:c:445:LYS:NZ	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:r:214:PRO:C	28:r:301:NEX:O3	2.43	0.61
13:S:173:VAL:HG12	13:S:175:TRP:H	1.65	0.61
11:5:9:GLU:HB3	24:5:305:CHL:HBC1	1.81	0.61
11:5:112:SER:N	24:5:309:CHL:OMC	2.34	0.61
17:g:128:GLU:OE1	17:g:131:ARG:NH1	2.33	0.61
10:1:125:GLY:HA2	24:1:312:CHL:HAB	1.81	0.61
10:1:158:ASP:HB3	10:1:161:THR:HG22	1.82	0.61
13:S:240:LEU:HD23	25:S:609:CLA:H11	1.82	0.60
17:G:201:HIS:CG	25:G:317:CLA:HAA2	2.36	0.60
19:A:63:ILE:HD12	20:C:323:THR:HB	1.82	0.60
25:9:316:CLA:HAB	30:9:318:LHG:H332	1.83	0.60
17:N:85:VAL:HG23	17:N:88:LYS:HB2	1.83	0.60
12:u:61:PRO:HB2	12:u:202:ILE:HD12	1.83	0.60
17:y:137:LEU:HG	24:y:312:CHL:HBB1	1.83	0.60
13:s:58:TRP:C	13:s:60:GLY:H	2.09	0.60
28:7:304:NEX:C40	24:7:310:CHL:HBA1	2.29	0.60
11:2:1:VAL:HG12	11:2:3:TRP:H	1.67	0.60
17:g:51:GLU:HA	17:g:144:LEU:HD21	1.84	0.60
17:n:185:VAL:HG21	25:n:316:CLA:HAC2	1.82	0.60
17:y:21:PRO:HG2	17:y:35:ASP:HB3	1.82	0.60
17:y:71:GLU:HA	17:y:84:ALA:HB1	1.82	0.60
32:a:609:SQD:H311	25:c:608:CLA:H92	1.82	0.60
21:d:79:SER:HA	21:d:172:SER:HB3	1.81	0.60
11:2:168:LYS:HD3	25:2:316:CLA:HAA2	1.82	0.60
24:4:309:CHL:HHC	24:4:309:CHL:HBB1	1.84	0.60
17:g:201:HIS:CG	25:g:317:CLA:HAA2	2.36	0.60
25:b:602:CLA:H42	33:d:401:LMG:H112	1.83	0.60
11:2:9:GLU:HB3	24:2:305:CHL:HBC1	1.82	0.60
17:q:123:LEU:HD22	28:s:401:NEX:C14	2.32	0.60
19:a:63:ILE:HD12	20:c:323:THR:HB	1.82	0.60
11:5:1:VAL:HG12	11:5:3:TRP:H	1.66	0.60
25:y:307:CLA:HBB1	24:y:313:CHL:H161	1.84	0.60
21:d:32:TRP:CD1	33:d:411:LMG:H111	2.37	0.60
28:7:304:NEX:H403	24:7:310:CHL:CGA	2.31	0.60
17:g:171:LYS:NZ	30:g:319:LHG:O4	2.33	0.60
17:y:221:GLN:NE2	17:y:223:PHE:OXT	2.35	0.60
28:G:304:NEX:H362	25:G:308:CLA:HAB	1.83	0.60
28:G:304:NEX:H222	25:G:308:CLA:NC	2.17	0.60
21:D:79:SER:HA	21:D:172:SER:HB3	1.83	0.60
28:5:304:NEX:C17	17:n:152:PRO:HB2	2.32	0.60
12:u:40:ARG:NH2	12:u:56:LEU:O	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:n:42:ASP:HB3	17:n:45:THR:HG22	1.84	0.60
10:4:58:ARG:NH1	24:4:311:CHL:OBD	2.32	0.59
17:y:19:ALA:HB2	17:q:132:CYS:HB3	1.83	0.59
12:3:44:LEU:HB3	12:3:47:TYR:HB2	1.84	0.59
11:5:168:LYS:HD3	25:5:316:CLA:HAA2	1.83	0.59
12:7:233:HIS:CG	25:7:317:CLA:HAA2	2.37	0.59
12:3:89:SER:HB3	12:3:205:GLY:HA3	1.84	0.59
25:3:307:CLA:HBA2	28:3:318:NEX:H241	1.84	0.59
17:N:42:ASP:HB3	17:N:45:THR:HG22	1.84	0.59
11:5:69:THR:HG21	25:5:308:CLA:HAC2	1.84	0.59
17:n:85:VAL:HG23	17:n:88:LYS:HB2	1.84	0.59
8:R:65:ARG:HB2	24:R:602:CHL:HMD1	1.84	0.59
8:R:87:ASP:HB2	8:R:90:ALA:HB3	1.84	0.59
17:G:101:TYR:HB3	17:G:107:LEU:HG	1.83	0.59
3:h:73:LEU:HD23	18:b:195:PRO:HD3	1.85	0.59
17:n:128:GLU:OE1	17:n:131:ARG:NH2	2.35	0.59
11:2:69:THR:HG21	25:2:308:CLA:HAC2	1.84	0.59
17:Y:221:GLN:NE2	17:Y:223:PHE:OXT	2.36	0.59
10:1:168:LYS:HD3	25:1:315:CLA:HAA2	1.85	0.59
21:D:189:HIS:HA	21:D:294:ARG:HD3	1.85	0.59
5:k:25:ILE:HD12	15:v:289:VAL:HG11	1.83	0.59
11:5:51:GLU:HA	11:5:144:LEU:HD21	1.85	0.59
12:6:236:ASP:HB3	12:6:240:ASN:HB2	1.84	0.59
12:u:157:SER:HB3	24:u:313:CHL:HAB	1.84	0.59
12:p:42:LEU:HD22	12:p:52:VAL:HG11	1.83	0.59
10:1:58:ARG:NH1	24:1:311:CHL:OBD	2.32	0.59
28:4:303:NEX:H383	25:4:307:CLA:CHB	2.32	0.59
8:r:213:ASP:OD1	26:r:315:OIE:O42	2.20	0.59
17:n:45:THR:O	17:n:49:ASN:ND2	2.27	0.59
8:r:65:ARG:HB2	24:r:303:CHL:HMD1	1.84	0.59
24:Y:312:CHL:HBB1	24:7:305:CHL:H52	1.85	0.59
12:7:41:ALA:HB1	24:7:305:CHL:HBC1	1.85	0.59
28:7:304:NEX:H31	24:7:310:CHL:CBA	2.27	0.59
19:A:267:ASN:ND2	21:D:232:PHE:O	2.36	0.59
12:p:183:ASP:OD1	29:p:301:OUR:O40	2.20	0.59
17:q:201:HIS:CG	25:q:315:CLA:HAA2	2.38	0.59
12:7:163:ARG:NH2	24:7:313:CHL:O1D	2.36	0.59
24:3:309:CHL:HBC2	24:3:310:CHL:HHD	1.85	0.58
24:3:311:CHL:HBB1	24:3:311:CHL:HHC	1.85	0.58
17:N:185:VAL:HG21	25:N:316:CLA:HAC2	1.83	0.58
17:g:88:LYS:HD3	24:g:311:CHL:HED2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:q:306:CLA:C4B	28:s:401:NEX:H242	2.33	0.58
10:1:185:VAL:HG21	25:1:316:CLA:HAC2	1.85	0.58
12:9:157:SER:HB3	24:9:312:CHL:HAB	1.85	0.58
10:4:185:VAL:HG21	25:4:316:CLA:HAC2	1.85	0.58
24:6:311:CHL:HHC	24:6:311:CHL:HBB1	1.85	0.58
14:x:84:VAL:HG21	24:g:318:CHL:HMB2	1.85	0.58
24:u:310:CHL:HHC	24:u:310:CHL:HBB1	1.86	0.58
24:y:313:CHL:HBB1	24:p:305:CHL:H52	1.85	0.58
20:c:395:VAL:HG23	20:c:407:PHE:H	1.68	0.58
21:d:262:SER:N	30:d:407:LHG:O5	2.35	0.58
8:R:224:LYS:NZ	11:2:151:ASP:O	2.35	0.58
11:2:112:SER:N	24:2:309:CHL:OMC	2.35	0.58
17:8:201:HIS:CG	25:8:314:CLA:HAA2	2.38	0.58
21:D:262:SER:N	30:D:407:LHG:O5	2.35	0.58
3:H:73:LEU:HD23	18:B:195:PRO:HD3	1.85	0.58
17:Y:137:LEU:HG	24:Y:311:CHL:HBB1	1.84	0.58
25:Y:306:CLA:HBB1	24:Y:312:CHL:H161	1.84	0.58
17:y:128:GLU:HA	17:y:131:ARG:HG2	1.86	0.58
8:r:73:SER:HB2	24:r:303:CHL:HAA2	1.86	0.58
10:1:2:GLU:O	10:1:9:ALA:N	2.36	0.58
17:n:101:TYR:HB2	17:n:108:VAL:HG12	1.85	0.58
12:p:52:VAL:HG12	12:p:65:GLY:HA3	1.85	0.58
8:r:86:LEU:HG	8:r:88:GLN:HG2	1.86	0.58
8:r:135:ARG:HD3	25:r:310:CLA:C4C	2.33	0.58
17:G:104:ASN:ND2	17:G:106:SER:OG	2.36	0.58
20:C:444:GLU:OE2	20:C:445:LYS:NZ	2.32	0.58
8:r:64:ASP:O	8:r:65:ARG:NH1	2.35	0.58
12:7:200:LYS:HD3	25:7:316:CLA:HAA2	1.86	0.58
8:R:69:PRO:HG2	27:R:615:XAT:C22	2.33	0.58
19:A:76:ASN:OD1	19:A:76:ASN:N	2.34	0.58
15:v:282:GLN:HG2	15:v:283:LEU:H	1.68	0.58
20:c:390:GLY:HA2	20:c:396:GLY:HA3	1.86	0.58
5:K:25:ILE:HD12	15:V:289:VAL:HG11	1.84	0.58
25:B:614:CLA:H42	32:B:618:SQD:H122	1.86	0.58
19:a:163:ILE:HD11	37:c:619:DGD:HA21	1.84	0.58
24:r:303:CHL:CBB	27:r:316:XAT:H32	2.34	0.58
10:1:168:LYS:O	10:1:172:ASN:ND2	2.25	0.58
12:9:90:ARG:NE	12:9:201:GLU:OE2	2.29	0.58
18:B:15:ASP:HB3	18:B:18:ARG:HB2	1.86	0.58
19:A:190:HIS:ND1	19:A:298:ASN:OD1	2.26	0.58
17:g:189:GLN:NE2	17:g:216:LYS:O	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:p:304:NEX:H241	25:p:308:CLA:H2	1.84	0.58
24:q:310:CHL:HBB1	24:q:310:CHL:HHC	1.85	0.58
13:s:128:ARG:NH2	13:s:229:LEU:O	2.36	0.58
25:r:311:CLA:H2A	25:r:311:CLA:HED3	1.85	0.58
8:R:135:ARG:HD3	25:R:609:CLA:C4C	2.33	0.58
13:S:180:ASN:ND2	24:S:605:CHL:OBD	2.35	0.58
19:A:270:SER:OG	32:A:609:SQD:O49	2.21	0.58
12:u:53:PRO:HG3	12:u:67:ASP:HB3	1.86	0.58
12:u:118:TRP:HE1	12:u:219:ALA:HB2	1.67	0.58
24:9:309:CHL:HHC	24:9:309:CHL:HBB1	1.86	0.57
20:C:295:PRO:HB3	20:C:346:PHE:HB3	1.86	0.57
28:6:303:NEX:C30	24:6:309:CHL:H3A	2.33	0.57
20:c:295:PRO:HB3	20:c:346:PHE:HB3	1.86	0.57
21:d:189:HIS:HA	21:d:294:ARG:HD3	1.84	0.57
10:1:198:TRP:HE1	24:1:317:CHL:HMC	1.69	0.57
18:B:71:ILE:HD11	25:B:607:CLA:H2A	1.87	0.57
12:6:84:LEU:O	12:6:88:HIS:ND1	2.36	0.57
28:g:304:NEX:H362	25:g:308:CLA:CHC	2.35	0.57
8:R:213:ASP:OD1	26:R:614:OIE:O42	2.21	0.57
24:1:309:CHL:HBC2	24:1:310:CHL:HHD	1.87	0.57
28:S:617:NEX:H383	25:8:306:CLA:C3B	2.34	0.57
24:Y:304:CHL:HHC	24:Y:304:CHL:HBB1	1.85	0.57
19:A:162:PRO:HB3	19:A:168:PHE:HA	1.86	0.57
10:4:168:LYS:HD3	25:4:315:CLA:HAA2	1.85	0.57
12:p:239:ASN:ND2	12:p:240:ASN:OD1	2.35	0.57
17:G:8:ARG:NH2	17:G:31:ASP:OD1	2.38	0.57
12:9:100:LEU:O	12:9:104:LEU:N	2.27	0.57
18:B:372:ASP:OD1	18:B:373:ASP:N	2.33	0.57
12:6:221:VAL:HG23	12:6:222:THR:HG23	1.87	0.57
12:6:230:TRP:HE1	24:6:317:CHL:HMC	1.69	0.57
17:g:209:ASN:HD22	17:n:114:LEU:HD21	1.69	0.57
12:u:90:ARG:NE	12:u:201:GLU:OE2	2.29	0.57
24:u:310:CHL:HBC2	24:u:311:CHL:HHD	1.86	0.57
12:p:162:TYR:HB3	24:p:312:CHL:HMC	1.86	0.57
12:p:233:HIS:CG	25:p:317:CLA:HAA2	2.40	0.57
20:c:395:VAL:HG21	20:c:404:ALA:HB3	1.85	0.57
12:3:178:PRO:HD3	24:3:311:CHL:HMD1	1.86	0.57
11:5:8:ARG:NH1	11:5:31:ASP:O	2.33	0.57
28:7:304:NEX:H222	25:7:308:CLA:NC	2.19	0.57
17:G:19:ALA:HB2	17:N:132:CYS:HB3	1.86	0.57
12:9:166:GLY:HA3	12:9:172:PRO:HD3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:57:ALA:HB1	17:N:173:GLY:HA3	1.86	0.57
17:8:85:VAL:HG23	17:8:88:LYS:HB2	1.86	0.57
18:b:53:ASN:ND2	18:b:58:GLN:OE1	2.37	0.57
8:r:160:GLU:OE2	8:r:164:GLN:NE2	2.34	0.57
4:I:27:ASP:OD1	19:A:136:ARG:NH2	2.37	0.57
15:V:300:LEU:HA	15:V:303:ARG:HB2	1.87	0.57
28:6:303:NEX:C26	24:6:309:CHL:HAA1	2.35	0.57
17:g:58:ARG:HA	17:g:61:MET:HE3	1.86	0.57
12:9:168:PRO:HG3	28:9:319:NEX:H192	1.86	0.57
25:9:306:CLA:H12	17:N:39:LEU:HD11	1.85	0.57
17:g:168:LYS:O	17:g:172:ASN:ND2	2.27	0.57
18:b:341:LEU:HD11	18:b:431:GLU:HB3	1.86	0.57
12:7:52:VAL:HG12	12:7:65:GLY:HA3	1.87	0.57
17:G:168:LYS:O	17:G:172:ASN:ND2	2.28	0.57
20:C:83:LEU:O	20:C:166:LYS:NZ	2.32	0.57
19:a:162:PRO:HB3	19:a:168:PHE:HA	1.87	0.57
19:a:299:GLY:O	20:c:391:SER:OG	2.21	0.57
8:R:73:SER:HB2	24:R:602:CHL:HAA2	1.87	0.57
17:G:21:PRO:HG2	17:G:35:ASP:HB3	1.86	0.57
17:N:24:LEU:HD22	17:N:33:GLY:HA2	1.85	0.57
23:f:201:HEM:HMC2	23:f:201:HEM:HBC2	1.86	0.57
11:5:171:LYS:NZ	30:5:319:LHG:O4	2.38	0.57
20:c:83:LEU:O	20:c:166:LYS:NZ	2.33	0.57
23:E:201:HEM:HBC2	23:E:201:HEM:HMC2	1.86	0.56
13:S:199:GLU:HG2	24:S:608:CHL:C1B	2.35	0.56
18:B:53:ASN:ND2	18:B:58:GLN:OE1	2.37	0.56
2:e:48:TYR:O	2:e:52:HIS:ND1	2.38	0.56
12:u:43:TRP:HB3	12:u:64:TYR:HB3	1.87	0.56
17:n:92:GLN:HE21	17:n:99:LEU:HG	1.70	0.56
25:b:614:CLA:H42	32:b:618:SQD:H122	1.87	0.56
25:B:604:CLA:H111	25:B:615:CLA:H42	1.86	0.56
28:4:303:NEX:O24	24:4:309:CHL:HAA1	2.05	0.56
8:r:246:PHE:CE1	25:r:313:CLA:HAC2	2.40	0.56
23:E:201:HEM:HMB2	23:E:201:HEM:HBB2	1.87	0.56
8:R:162:ILE:HG23	8:R:167:GLY:HA2	1.87	0.56
11:2:71:GLU:HA	11:2:84:SER:HB2	1.87	0.56
20:C:281:ASN:ND2	37:C:620:DGD:HE61	2.20	0.56
23:f:201:HEM:HBB2	23:f:201:HEM:HMB2	1.87	0.56
11:5:201:HIS:CG	25:5:317:CLA:HAA2	2.40	0.56
17:n:126:LEU:HB2	28:n:303:NEX:C20	2.34	0.56
17:q:54:LEU:HD23	17:q:144:LEU:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:b:15:ASP:HB3	18:b:18:ARG:HB2	1.87	0.56
18:b:71:ILE:HD11	25:b:607:CLA:H2A	1.87	0.56
17:G:58:ARG:HA	17:G:61:MET:HE3	1.87	0.56
10:4:198:TRP:HE1	24:4:317:CHL:HMC	1.70	0.56
12:6:178:PRO:HD3	24:6:311:CHL:HMD1	1.87	0.56
24:y:305:CHL:H52	24:q:311:CHL:HBB1	1.86	0.56
12:p:249:THR:H	12:p:252:ALA:HB2	1.71	0.56
6:l:14:ASN:OD1	6:l:14:ASN:N	2.39	0.56
17:q:57:ALA:HB1	17:q:173:GLY:HA3	1.86	0.56
28:7:304:NEX:H393	25:7:308:CLA:CAB	2.35	0.56
13:S:102:TYR:HB2	24:S:602:CHL:HMD3	1.88	0.56
17:g:83:GLU:N	17:g:92:GLN:OE1	2.38	0.56
17:g:118:TRP:HZ2	24:u:318:CHL:HBD	1.71	0.56
25:b:604:CLA:H111	25:b:615:CLA:H42	1.87	0.56
17:8:57:ALA:HB1	17:8:173:GLY:HA3	1.86	0.56
17:n:57:ALA:HB1	17:n:173:GLY:HA3	1.87	0.56
28:7:304:NEX:C38	25:7:308:CLA:CHB	2.84	0.56
18:B:480:ALA:HB1	19:A:229:GLU:HA	1.88	0.56
13:s:240:LEU:HD23	25:s:410:CLA:H11	1.86	0.56
8:r:162:ILE:HG23	8:r:167:GLY:HA2	1.88	0.56
12:3:190:ASP:HB3	12:3:193:THR:HG22	1.87	0.56
13:S:122:PHE:O	13:S:126:HIS:ND1	2.31	0.56
24:6:309:CHL:HBC2	24:6:310:CHL:HHD	1.88	0.56
15:v:300:LEU:HA	15:v:303:ARG:HB2	1.87	0.56
25:a:605:CLA:HAB	25:d:404:CLA:H51	1.88	0.56
11:2:201:HIS:CG	25:2:317:CLA:HAA2	2.41	0.56
15:V:282:GLN:HG2	15:V:283:LEU:H	1.71	0.56
17:Y:201:HIS:CG	25:Y:316:CLA:HAA2	2.42	0.56
17:8:54:LEU:HD23	17:8:144:LEU:HB3	1.87	0.56
18:B:153:PHE:O	18:B:158:VAL:HG23	2.06	0.56
30:A:601:LHG:H152	39:D:406:PL9:H252	1.86	0.56
22:W:96:TRP:CH2	33:W:201:LMG:H112	2.41	0.56
17:g:19:ALA:HB2	17:n:132:CYS:HB3	1.88	0.56
18:b:278:GLY:O	18:b:281:ALA:N	2.38	0.56
13:s:199:GLU:HG2	24:s:409:CHL:C1B	2.36	0.56
24:3:309:CHL:HAA2	28:3:318:NEX:O24	2.03	0.55
24:y:305:CHL:HHC	24:y:305:CHL:HBB1	1.88	0.55
18:b:276:ASP:N	18:b:276:ASP:OD1	2.24	0.55
13:s:209:LYS:NZ	13:s:220:SER:OG	2.31	0.55
10:1:61:MET:SD	25:1:313:CLA:HAB	2.46	0.55
13:S:70:LYS:HE2	13:S:77:ALA:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:9:43:TRP:HB3	12:9:64:TYR:HB3	1.87	0.55
17:Y:51:GLU:HA	17:Y:144:LEU:HD21	1.89	0.55
17:Y:128:GLU:HA	17:Y:131:ARG:HG2	1.88	0.55
12:6:89:SER:HB2	12:6:205:GLY:HA3	1.87	0.55
17:g:104:ASN:HB3	17:g:107:LEU:HD23	1.88	0.55
17:y:125:GLY:HA2	24:y:313:CHL:HAB	1.87	0.55
19:a:143:ILE:HG12	21:d:220:ASN:HD22	1.72	0.55
8:R:67:PHE:CE2	27:R:615:XAT:H383	2.29	0.55
19:A:143:ILE:HG12	21:D:220:ASN:HD22	1.71	0.55
17:g:55:ILE:HG13	17:g:131:ARG:HH21	1.70	0.55
17:g:104:ASN:ND2	17:g:106:SER:OG	2.38	0.55
28:p:304:NEX:C36	25:p:308:CLA:CHC	2.83	0.55
11:2:171:LYS:NZ	30:2:319:LHG:O4	2.39	0.55
13:S:76:ARG:NH1	13:S:101:ASP:O	2.40	0.55
17:G:209:ASN:HD22	17:N:114:LEU:HD21	1.71	0.55
18:B:340:TRP:CD1	18:B:342:GLY:H	2.25	0.55
12:6:117:VAL:HG23	12:6:120:SER:HB2	1.88	0.55
12:6:190:ASP:HB3	12:6:193:THR:HG22	1.87	0.55
25:u:307:CLA:H12	17:n:39:LEU:HD11	1.88	0.55
28:n:303:NEX:O24	25:n:307:CLA:H43	2.07	0.55
18:b:155:ALA:O	18:b:159:THR:OG1	2.23	0.55
13:s:122:PHE:O	13:s:126:HIS:ND1	2.34	0.55
6:L:34:SER:OG	19:A:76:ASN:ND2	2.39	0.55
13:S:99:PRO:HG2	13:S:120:ARG:HH22	1.70	0.55
24:Y:304:CHL:H52	24:8:310:CHL:HBB1	1.88	0.55
19:A:133:LEU:HD23	21:D:256:ILE:HG12	1.87	0.55
28:s:401:NEX:O3	25:s:411:CLA:CGA	2.54	0.55
28:1:303:NEX:H362	25:1:307:CLA:CHC	2.36	0.55
15:v:299:LEU:O	15:v:303:ARG:N	2.32	0.55
24:g:306:CHL:H93	25:g:307:CLA:HBB	1.88	0.55
12:3:84:LEU:O	12:3:88:HIS:ND1	2.39	0.55
17:N:130:TYR:HB3	24:N:311:CHL:CMC	2.37	0.55
24:N:304:CHL:HMD1	30:N:318:LHG:H251	1.88	0.55
17:n:68:LEU:HD13	17:n:195:VAL:HG22	1.87	0.55
24:n:304:CHL:HMD1	30:n:318:LHG:H251	1.89	0.55
17:G:83:GLU:N	17:G:92:GLN:OE1	2.39	0.55
17:Y:125:GLY:HA2	24:Y:312:CHL:HAB	1.88	0.55
24:4:309:CHL:HBC2	24:4:310:CHL:HHD	1.89	0.55
17:n:130:TYR:HB3	24:n:311:CHL:CMC	2.36	0.55
20:c:448:ASP:O	20:c:449:ARG:HB2	2.07	0.55
25:r:305:CLA:HMB1	24:r:306:CHL:HBB1	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:4:61:MET:SD	25:4:313:CLA:HAB	2.46	0.55
17:y:201:HIS:CG	25:y:317:CLA:HAA2	2.41	0.55
25:c:603:CLA:H203	25:c:610:CLA:HAB	1.87	0.55
8:r:186:VAL:HG23	24:r:309:CHL:HBB2	1.87	0.55
8:R:69:PRO:C	8:R:71:CYS:H	2.15	0.55
25:R:604:CLA:C2B	28:R:616:NEX:H383	2.37	0.55
11:5:71:GLU:HA	11:5:84:SER:HB2	1.87	0.55
19:a:133:LEU:HD23	21:d:256:ILE:HG12	1.88	0.55
18:B:341:LEU:HD11	18:B:431:GLU:HB3	1.87	0.54
20:C:448:ASP:O	20:C:449:ARG:HB2	2.07	0.54
3:h:51:VAL:HG21	25:d:405:CLA:H43	1.89	0.54
28:4:303:NEX:H362	25:4:307:CLA:HAB	1.85	0.54
18:b:340:TRP:CD1	18:b:342:GLY:H	2.25	0.54
25:b:604:CLA:HBA2	25:b:606:CLA:H151	1.89	0.54
20:c:395:VAL:HG23	20:c:407:PHE:N	2.22	0.54
17:G:51:GLU:HA	17:G:144:LEU:HD21	1.89	0.54
17:G:55:ILE:HG13	17:G:131:ARG:HH21	1.70	0.54
17:G:110:ALA:HA	24:G:309:CHL:HHC	1.90	0.54
28:G:304:NEX:C15	24:G:312:CHL:HMB3	2.36	0.54
12:9:86:VAL:HB	12:9:176:LEU:HD22	1.89	0.54
17:8:24:LEU:HD11	17:8:35:ASP:HB2	1.90	0.54
19:A:192:ILE:HG13	19:A:293:MET:HE1	1.89	0.54
12:6:239:ASN:HA	12:6:244:THR:HG21	1.89	0.54
28:6:303:NEX:C31	24:6:309:CHL:H3A	2.38	0.54
24:y:305:CHL:H62	30:y:319:LHG:H181	1.89	0.54
24:p:310:CHL:HBC2	24:p:311:CHL:HHD	1.88	0.54
17:q:92:GLN:HB2	17:q:99:LEU:HD12	1.89	0.54
25:b:609:CLA:H112	25:b:612:CLA:H72	1.88	0.54
3:H:23:ASN:ND2	18:B:122:LEU:O	2.39	0.54
17:G:32:TYR:HB2	24:G:306:CHL:HMD1	1.89	0.54
18:B:121:GLU:OE1	18:B:121:GLU:N	2.41	0.54
6:l:34:SER:OG	19:a:76:ASN:ND2	2.39	0.54
17:g:8:ARG:NH2	17:g:31:ASP:OD1	2.39	0.54
17:q:51:GLU:HA	17:q:144:LEU:HD11	1.90	0.54
18:b:121:GLU:OE1	18:b:121:GLU:N	2.40	0.54
20:c:281:ASN:ND2	37:c:619:DGD:HE61	2.21	0.54
12:9:200:LYS:HD2	25:9:315:CLA:HBD	1.90	0.54
17:N:51:GLU:HA	17:N:144:LEU:HD11	1.89	0.54
24:4:312:CHL:HMB3	24:5:305:CHL:HHB	1.88	0.54
12:p:41:ALA:HB1	24:p:305:CHL:HBC1	1.89	0.54
30:a:601:LHG:H152	39:d:406:PL9:H252	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:604:CLA:HBA2	25:B:606:CLA:H151	1.89	0.54
6:l:20:TRP:CE2	30:d:407:LHG:H241	2.43	0.54
17:g:21:PRO:HG2	17:g:35:ASP:HB3	1.88	0.54
12:p:163:ARG:NH2	24:p:313:CHL:O1D	2.41	0.54
8:r:214:PRO:O	28:r:301:NEX:O3	2.25	0.54
2:E:78:SER:HA	21:D:56:THR:HG21	1.90	0.54
8:R:208:PRO:HB3	24:R:607:CHL:HBC2	1.89	0.54
17:G:222:ILE:HG21	17:N:188:LEU:HD12	1.89	0.54
18:B:57:ARG:NH2	18:B:334:ASP:OD1	2.39	0.54
25:B:603:CLA:HAB	25:B:605:CLA:H152	1.90	0.54
25:C:603:CLA:H203	25:C:610:CLA:HAB	1.89	0.54
12:p:165:SER:OG	17:q:17:GLU:O	2.22	0.54
12:p:200:LYS:HD3	25:p:316:CLA:HAA2	1.88	0.54
25:q:306:CLA:C2B	28:s:401:NEX:H383	2.38	0.54
19:a:85:THR:HA	19:a:109:GLY:HA3	1.90	0.54
12:u:200:LYS:NZ	25:u:316:CLA:O1A	2.41	0.54
20:c:332:SER:OG	20:c:336:GLU:OE1	2.26	0.54
13:s:102:TYR:HB2	24:s:403:CHL:HMD3	1.88	0.54
25:r:305:CLA:C4B	28:r:317:NEX:H222	2.38	0.54
12:7:169:LEU:O	12:7:181:SER:OG	2.22	0.54
3:H:51:VAL:HG21	25:D:405:CLA:H43	1.89	0.54
11:2:189:GLN:NE2	26:2:303:OIE:O40	2.41	0.54
13:S:93:TYR:OH	13:S:105:ASP:OD2	2.26	0.54
17:Y:168:LYS:HD3	25:Y:315:CLA:HAA2	1.90	0.54
10:4:30:GLY:HA3	10:4:170:ILE:HD13	1.90	0.54
17:n:79:VAL:HG21	17:n:102:LEU:HD12	1.90	0.54
18:b:480:ALA:HB1	19:a:229:GLU:HA	1.90	0.54
13:s:57:GLY:H	13:s:64:ASN:H	1.54	0.54
13:s:115:ASN:O	13:s:118:THR:OG1	2.26	0.54
3:H:48:VAL:O	3:H:52:ILE:HG12	2.08	0.54
13:S:224:ASP:OD1	13:S:224:ASP:N	2.39	0.54
32:B:618:SQD:H321	16:t:50:GLY:HA3	1.89	0.54
28:p:304:NEX:H241	25:p:308:CLA:C2	2.37	0.54
8:R:246:PHE:CE1	25:R:612:CLA:HAC2	2.42	0.54
17:8:145:TYR:HB3	25:8:311:CLA:HED2	1.90	0.54
12:u:240:ASN:HD22	25:u:317:CLA:HED1	1.72	0.54
17:y:51:GLU:HA	17:y:144:LEU:HD21	1.89	0.54
12:p:169:LEU:O	12:p:181:SER:OG	2.21	0.54
19:a:307:VAL:HG12	19:a:313:VAL:HA	1.90	0.54
6:L:20:TRP:CE2	30:D:407:LHG:H241	2.43	0.53
7:M:26:TYR:O	7:M:30:ALA:N	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:S:209:LYS:NZ	13:S:220:SER:OG	2.29	0.53
12:9:61:PRO:HB2	12:9:202:ILE:HD12	1.90	0.53
12:9:74:ASP:HB3	12:9:77:MET:HG2	1.90	0.53
12:9:166:GLY:HA2	24:9:311:CHL:HMC	1.90	0.53
25:B:609:CLA:H112	25:B:612:CLA:H72	1.90	0.53
18:b:58:GLN:HB2	18:b:60:MET:HE3	1.90	0.53
20:c:357:LEU:HA	20:c:367:LYS:HG2	1.90	0.53
13:s:70:LYS:HE2	13:s:77:ALA:HB2	1.90	0.53
11:2:61:MET:SD	25:2:314:CLA:HAB	2.48	0.53
12:9:113:LEU:HB3	12:9:116:PRO:HB3	1.89	0.53
19:A:307:VAL:HG12	19:A:313:VAL:HA	1.91	0.53
20:C:257:GLU:OE1	20:C:435:ARG:NH1	2.38	0.53
20:C:357:LEU:HA	20:C:367:LYS:HG2	1.89	0.53
17:g:57:ALA:HB1	17:g:173:GLY:HA3	1.90	0.53
12:u:115:SER:HB2	12:u:120:SER:HB3	1.90	0.53
20:c:385:THR:HG1	20:c:386:HIS:HD1	1.55	0.53
8:r:208:PRO:HB3	24:r:308:CHL:HBC2	1.90	0.53
28:7:304:NEX:C40	24:7:310:CHL:O2A	2.56	0.53
8:R:82:ASP:N	8:R:82:ASP:OD1	2.37	0.53
17:n:168:LYS:HD3	25:n:315:CLA:HAA2	1.90	0.53
19:a:319:ASP:O	19:a:322:ASN:ND2	2.41	0.53
10:1:57:ALA:HB1	10:1:173:GLY:HA3	1.90	0.53
17:Y:168:LYS:O	17:Y:172:ASN:ND2	2.27	0.53
18:B:464:PHE:HD2	25:B:611:CLA:HAC2	1.73	0.53
17:g:222:ILE:HG21	17:n:188:LEU:HD12	1.91	0.53
25:b:603:CLA:HAB	25:b:605:CLA:H152	1.90	0.53
20:c:315:ASN:HB3	20:c:318:SER:HB2	1.90	0.53
8:r:246:PHE:HD1	25:r:313:CLA:HMD3	1.72	0.53
10:1:142:ASP:OD2	10:1:145:TYR:N	2.37	0.53
11:2:47:ARG:HH22	11:2:48:ARG:HH21	1.57	0.53
20:C:315:ASN:HB3	20:C:318:SER:HB2	1.91	0.53
12:6:44:LEU:HD23	24:6:304:CHL:HHB	1.89	0.53
17:g:101:TYR:OH	28:g:304:NEX:O23	2.22	0.53
12:u:221:VAL:HG13	12:u:222:THR:HG23	1.90	0.53
17:n:143:PRO:HG2	17:n:144:LEU:HD22	1.90	0.53
24:q:308:CHL:CBA	28:s:401:NEX:H403	2.38	0.53
18:b:463:PHE:CZ	18:b:467:ILE:HD11	2.43	0.53
19:a:192:ILE:HG13	19:a:293:MET:HE1	1.91	0.53
20:c:332:SER:OG	20:c:336:GLU:N	2.41	0.53
13:s:76:ARG:NH1	13:s:101:ASP:O	2.41	0.53
13:s:93:TYR:OH	13:s:105:ASP:OD2	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:s:169:ASP:HA	13:s:179:ALA:HA	1.91	0.53
13:S:169:ASP:HA	13:S:179:ALA:HA	1.90	0.53
28:G:304:NEX:H362	25:G:308:CLA:C3B	2.38	0.53
11:5:61:MET:SD	25:5:314:CLA:HAB	2.48	0.53
12:6:124:GLN:O	12:6:127:SER:OG	2.25	0.53
12:u:45:GLY:HA3	24:u:305:CHL:HBB1	1.90	0.53
17:n:22:SER:O	17:n:24:LEU:N	2.40	0.53
18:b:393:GLU:HG2	18:b:414:PRO:HB3	1.91	0.53
12:3:68:THR:N	26:3:302:OIE:O42	2.41	0.53
12:9:129:GLY:O	12:9:143:GLN:NE2	2.36	0.53
2:e:78:SER:OG	21:d:54:PHE:O	2.27	0.53
3:h:54:LEU:HA	25:b:602:CLA:H43	1.90	0.53
10:4:142:ASP:OD2	10:4:145:TYR:N	2.38	0.53
17:g:109:HIS:O	17:g:111:GLN:NE2	2.41	0.53
18:b:275:TRP:CE2	18:b:315:ILE:HD13	2.44	0.53
2:E:88:ASP:OD1	2:E:88:ASP:N	2.40	0.53
12:3:79:LYS:NZ	12:3:80:GLN:OE1	2.42	0.53
28:G:304:NEX:H15	24:G:312:CHL:CMB	2.37	0.53
17:8:128:GLU:OE1	17:8:131:ARG:NH1	2.37	0.53
19:A:273:PHE:CE1	30:D:408:LHG:HC61	2.44	0.53
17:q:130:TYR:O	17:q:134:GLY:N	2.35	0.53
8:r:243:PHE:CE2	27:r:316:XAT:H10	2.44	0.53
8:R:258:PHE:HA	8:R:261:LEU:HB2	1.90	0.53
13:S:267:GLY:O	13:S:271:GLN:HG2	2.09	0.53
28:G:304:NEX:H362	25:G:308:CLA:CAB	2.38	0.53
12:9:35:TRP:NE1	12:9:64:TYR:OH	2.30	0.53
20:C:163:LEU:HD23	20:C:225:HIS:CD2	2.44	0.53
21:D:253:TRP:HB2	21:D:260:ALA:HB2	1.91	0.53
3:h:23:ASN:ND2	18:b:122:LEU:O	2.38	0.53
10:4:11:TRP:O	10:4:16:SER:OG	2.25	0.53
16:T:50:GLY:HA3	32:b:618:SQD:H321	1.91	0.52
17:N:62:LEU:HD12	25:N:307:CLA:HAB	1.92	0.52
20:C:142:LYS:HB3	20:C:244:PRO:HG2	1.91	0.52
20:C:395:VAL:HG21	20:C:404:ALA:HB3	1.90	0.52
20:C:408:VAL:H	37:C:619:DGD:C3E	2.22	0.52
12:u:131:ILE:HG13	24:u:310:CHL:HMD1	1.89	0.52
32:b:618:SQD:H292	32:b:618:SQD:H162	1.89	0.52
13:s:58:TRP:HE1	28:s:401:NEX:C19	2.10	0.52
8:r:213:ASP:O	8:r:216:ASN:ND2	2.42	0.52
13:S:59:PHE:HE2	28:S:617:NEX:HO3	0.68	0.52
12:9:92:ALA:O	12:9:96:THR:N	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:286:THR:OG1	25:A:603:CLA:O1D	2.26	0.52
20:C:257:GLU:OE2	20:C:432:HIS:ND1	2.36	0.52
6:l:5:ASN:HD22	18:b:18:ARG:CZ	2.23	0.52
12:p:89:SER:HB2	12:p:205:GLY:HA3	1.91	0.52
20:c:408:VAL:H	37:c:618:DGD:C3E	2.22	0.52
24:1:312:CHL:HMB3	24:2:305:CHL:HBB	1.92	0.52
12:3:91:TRP:O	26:3:302:OIE:O29	2.28	0.52
12:9:83:GLU:HA	12:9:176:LEU:HD21	1.90	0.52
26:9:303:OIE:O42	30:9:318:LHG:O2	2.28	0.52
18:B:58:GLN:HB2	18:B:60:MET:HE3	1.91	0.52
21:D:141:TYR:O	21:D:142:ASN:C	2.52	0.52
28:6:303:NEX:C29	24:6:309:CHL:H3A	2.40	0.52
17:g:52:LEU:O	17:g:56:HIS:ND1	2.42	0.52
18:b:198:ILE:HG23	18:b:202:HIS:HE1	1.74	0.52
8:r:135:ARG:NH1	24:r:308:CHL:OBD	2.38	0.52
8:R:76:VAL:O	8:R:104:THR:OG1	2.27	0.52
20:C:337:ILE:HG22	20:C:363:LEU:HB2	1.92	0.52
18:b:464:PHE:HD2	25:b:611:CLA:HAC2	1.73	0.52
24:1:310:CHL:HHC	24:1:310:CHL:HBB1	1.90	0.52
28:G:304:NEX:C14	24:G:312:CHL:HMB1	2.40	0.52
19:A:85:THR:HA	19:A:109:GLY:HA3	1.91	0.52
21:d:253:TRP:HB2	21:d:260:ALA:HB2	1.92	0.52
12:9:115:SER:HB2	12:9:120:SER:HB3	1.91	0.52
17:N:61:MET:HG3	17:N:173:GLY:HA2	1.92	0.52
17:8:21:PRO:HG2	17:8:35:ASP:HB3	1.91	0.52
18:B:198:ILE:HG23	18:B:202:HIS:HE1	1.74	0.52
20:C:395:VAL:HG23	20:C:407:PHE:H	1.75	0.52
17:g:171:LYS:NZ	25:g:315:CLA:O1D	2.37	0.52
21:d:113:PHE:O	21:d:117:HIS:ND1	2.39	0.52
8:r:69:PRO:HG2	27:r:316:XAT:H221	1.91	0.52
8:R:107:ASP:OD1	8:R:107:ASP:N	2.40	0.52
17:8:151:ASP:OD1	29:8:301:OUR:O40	2.28	0.52
20:C:332:SER:OG	20:C:336:GLU:OE1	2.26	0.52
13:s:58:TRP:NE1	28:s:401:NEX:H181	2.25	0.52
17:g:217:PHE:CD1	24:n:310:CHL:H2	2.44	0.52
12:p:133:TYR:CE1	28:p:304:NEX:O23	2.56	0.52
12:p:148:ILE:HG12	24:p:309:CHL:HAC1	1.90	0.52
28:1:303:NEX:C31	24:1:309:CHL:CBA	2.86	0.52
11:2:99:LEU:HD21	25:2:308:CLA:HAA2	1.92	0.52
11:2:189:GLN:NE2	11:2:218:LYS:O	2.43	0.52
17:G:130:TYR:OH	28:G:304:NEX:C19	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:G:304:NEX:C13	24:G:312:CHL:HMB1	2.39	0.52
12:9:226:PRO:O	29:9:301:0UR:O39	2.28	0.52
18:B:477:ASP:OD1	18:B:477:ASP:N	2.36	0.52
20:C:202:LEU:HB3	22:W:76:ALA:H	1.74	0.52
20:C:332:SER:OG	20:C:336:GLU:N	2.41	0.52
7:m:26:TYR:O	7:m:30:ALA:N	2.42	0.52
10:4:168:LYS:NZ	25:4:315:CLA:O1A	2.41	0.52
17:g:101:TYR:HE2	28:g:304:NEX:H1	1.56	0.52
17:g:110:ALA:HA	24:g:309:CHL:HHC	1.91	0.52
12:u:229:ASN:ND2	25:u:317:CLA:O1D	2.42	0.52
17:q:8:ARG:NE	17:q:31:ASP:O	2.35	0.52
3:H:52:ILE:HD12	14:X:79:LEU:HD21	1.91	0.52
13:S:115:ASN:O	13:S:118:THR:OG1	2.25	0.52
17:G:57:ALA:HB1	17:G:173:GLY:HA3	1.92	0.52
17:8:51:GLU:HA	17:8:144:LEU:HD11	1.92	0.52
17:8:130:TYR:O	17:8:134:GLY:N	2.35	0.52
18:B:393:GLU:HG2	18:B:414:PRO:HB3	1.92	0.52
25:A:607:CLA:HAA2	33:C:618:LMG:H111	1.92	0.52
17:y:145:TYR:HB3	25:y:314:CLA:HED2	1.92	0.52
18:b:54:PRO:HD2	18:b:57:ARG:HB2	1.92	0.52
20:c:163:LEU:HD23	20:c:225:HIS:CD2	2.45	0.52
24:s:407:CHL:HHC	24:s:407:CHL:HBB1	1.92	0.52
3:H:54:LEU:HA	25:B:602:CLA:H43	1.92	0.51
21:D:152:VAL:HG21	21:D:279:LEU:HD13	1.91	0.51
17:g:120:GLN:OE1	24:g:311:CHL:HMC	2.10	0.51
12:p:40:ARG:NE	12:p:63:ASP:OD1	2.43	0.51
24:q:308:CHL:HHC	24:q:308:CHL:HBB1	1.92	0.51
19:a:225:ARG:H	19:a:225:ARG:HD2	1.75	0.51
2:E:80:ARG:H	2:E:83:GLU:HB2	1.74	0.51
8:R:68:ASP:HA	27:R:615:XAT:O23	2.10	0.51
19:A:233:THR:OG1	30:A:612:LHG:O1	2.28	0.51
11:5:8:ARG:NH1	11:5:31:ASP:OD1	2.43	0.51
11:5:99:LEU:HD21	25:5:308:CLA:HAA2	1.92	0.51
28:6:303:NEX:H241	25:6:307:CLA:HBA2	1.92	0.51
12:u:117:VAL:HG13	12:u:118:TRP:H	1.74	0.51
17:y:206:VAL:O	17:y:209:ASN:ND2	2.43	0.51
24:p:305:CHL:C1D	30:p:319:LHG:HC82	2.41	0.51
13:s:108:GLY:O	13:s:111:LYS:HG3	2.11	0.51
12:7:76:GLU:O	12:7:80:GLN:NE2	2.43	0.51
8:R:163:LEU:HB2	24:R:606:CHL:HMD1	1.93	0.51
28:1:303:NEX:H15	24:1:311:CHL:HMB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:G:45:THR:HA	12:9:70:GLY:HA3	1.93	0.51
20:C:261:SER:O	20:C:429:HIS:ND1	2.43	0.51
2:e:88:ASP:OD1	2:e:88:ASP:N	2.38	0.51
28:5:304:NEX:H172	17:n:152:PRO:HB2	1.92	0.51
17:y:59:TRP:CE2	24:y:312:CHL:HED2	2.45	0.51
18:b:480:ALA:H	21:d:139:ARG:NH1	2.08	0.51
12:7:89:SER:HB2	12:7:205:GLY:HA3	1.92	0.51
10:1:51:GLU:HA	10:1:144:LEU:HD21	1.92	0.51
28:S:617:NEX:C14	17:8:123:LEU:HD22	2.39	0.51
12:u:200:LYS:HD2	25:u:316:CLA:HBD	1.93	0.51
20:c:261:SER:O	20:c:429:HIS:ND1	2.43	0.51
20:c:337:ILE:HG22	20:c:363:LEU:HB2	1.92	0.51
13:s:224:ASP:N	13:s:224:ASP:OD1	2.38	0.51
13:s:267:GLY:O	13:s:271:GLN:HG2	2.09	0.51
8:r:67:PHE:HE2	27:r:316:XAT:H383	1.74	0.51
8:r:69:PRO:C	8:r:71:CYS:H	2.16	0.51
8:r:107:ASP:OD1	8:r:107:ASP:N	2.42	0.51
10:1:100:ASP:OD2	10:1:109:HIS:ND1	2.32	0.51
8:r:245:GLY:O	8:r:249:GLN:N	2.39	0.51
11:2:185:VAL:HA	11:2:188:ILE:HB	1.91	0.51
18:B:275:TRP:CE2	18:B:315:ILE:HD13	2.46	0.51
18:B:397:VAL:HG23	18:B:417:VAL:HG11	1.93	0.51
17:q:151:ASP:OD1	29:q:301:OUR:O40	2.28	0.51
17:G:217:PHE:CD1	24:N:310:CHL:H2	2.46	0.51
28:6:303:NEX:H31	24:6:309:CHL:CBA	2.40	0.51
12:u:226:PRO:O	29:u:301:OUR:O39	2.28	0.51
1:Z:1:MET:HB2	1:Z:4:LEU:HB3	1.92	0.51
8:R:135:ARG:NH1	24:R:607:CHL:OBD	2.38	0.51
12:9:93:MET:SD	25:9:313:CLA:HAB	2.51	0.51
17:Y:59:TRP:CE2	24:Y:311:CHL:HED2	2.45	0.51
18:B:379:ALA:HB2	18:B:395:VAL:HG21	1.93	0.51
12:u:209:MET:HB2	24:u:306:CHL:OMC	2.11	0.51
20:c:265:ALA:HB2	20:c:429:HIS:CG	2.46	0.51
12:7:145:ILE:HG23	12:7:146:LEU:HD12	1.93	0.51
8:R:67:PHE:HE2	27:R:615:XAT:C38	2.17	0.51
11:2:8:ARG:NH1	11:2:31:ASP:OD1	2.44	0.51
18:B:237:VAL:HG22	25:B:606:CLA:HMD1	1.93	0.51
17:g:54:LEU:HD23	17:g:144:LEU:HB3	1.93	0.51
17:q:85:VAL:HG23	17:q:88:LYS:HB2	1.93	0.51
18:b:57:ARG:NH2	18:b:334:ASP:OD1	2.40	0.51
12:7:166:GLY:HA2	24:7:312:CHL:HMC	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:R:117:TYR:OH	8:R:128:GLU:OE1	2.25	0.51
30:N:318:LHG:H272	30:N:318:LHG:HC62	1.92	0.51
17:Y:9:ALA:HB1	24:Y:304:CHL:HBC1	1.93	0.51
25:B:608:CLA:H2	33:B:619:LMG:H161	1.92	0.51
21:D:210:LEU:HD21	39:D:406:PL9:H13	1.92	0.51
17:q:192:LYS:NZ	17:q:200:GLU:OE2	2.38	0.51
18:b:272:ARG:NH1	18:b:276:ASP:OD2	2.44	0.51
2:E:79:PRO:CD	21:D:56:THR:HG21	2.40	0.50
25:R:604:CLA:CHC	28:R:616:NEX:H362	2.41	0.50
10:1:21:PRO:HG3	10:1:35:ASP:HB3	1.93	0.50
17:N:25:THR:OG1	17:N:27:GLU:OE1	2.24	0.50
17:Y:24:LEU:HD11	17:Y:35:ASP:HB2	1.94	0.50
25:C:604:CLA:CAA	37:C:619:DGD:HD61	2.41	0.50
21:D:252:PHE:CG	21:D:252:PHE:O	2.64	0.50
24:4:310:CHL:HHC	24:4:310:CHL:HBB1	1.92	0.50
17:g:45:THR:HA	12:u:70:GLY:HA3	1.93	0.50
17:g:93:ILE:HG21	17:g:113:ILE:HD12	1.93	0.50
17:y:189:GLN:NE2	17:y:213:TYR:O	2.44	0.50
24:q:310:CHL:CMA	28:s:401:NEX:H30	2.41	0.50
18:b:474:ILE:HD11	25:b:612:CLA:HAA2	1.91	0.50
20:c:336:GLU:OE1	20:c:336:GLU:N	2.43	0.50
12:7:133:TYR:HH	28:7:304:NEX:C23	2.23	0.50
20:C:118:VAL:HG21	25:C:611:CLA:H152	1.92	0.50
28:g:304:NEX:H362	25:g:308:CLA:C3B	2.40	0.50
18:b:397:VAL:HG23	18:b:417:VAL:HG11	1.93	0.50
21:d:39:PRO:HB2	25:d:405:CLA:HAB	1.94	0.50
21:d:141:TYR:O	21:d:142:ASN:C	2.51	0.50
13:s:99:PRO:HG2	13:s:120:ARG:HH22	1.76	0.50
6:L:5:ASN:HD22	18:B:18:ARG:CZ	2.24	0.50
18:B:154:GLY:HA2	18:B:158:VAL:CG2	2.42	0.50
19:A:283:ILE:HA	19:A:286:THR:HG22	1.92	0.50
12:6:91:TRP:O	26:6:302:OIE:O29	2.29	0.50
12:u:74:ASP:HB3	12:u:77:MET:HG2	1.94	0.50
18:b:237:VAL:HG22	25:b:606:CLA:HMD1	1.94	0.50
18:b:362:PHE:O	21:d:294:ARG:NH2	2.45	0.50
24:7:305:CHL:C1D	30:7:319:LHG:HC82	2.41	0.50
10:1:79:VAL:HG11	10:1:102:LEU:HD12	1.93	0.50
17:G:133:SER:HB3	12:9:50:GLY:H	1.76	0.50
12:9:55:TYR:OH	12:9:67:ASP:OD2	2.20	0.50
25:Y:314:CLA:H43	33:W:201:LMG:C10	2.42	0.50
18:B:54:PRO:HD2	18:B:57:ARG:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:392:ILE:HB	18:B:397:VAL:HG22	1.93	0.50
20:C:385:THR:HG1	20:C:386:HIS:HD1	1.59	0.50
28:n:303:NEX:O24	25:n:307:CLA:C4	2.59	0.50
17:q:145:TYR:HB3	25:q:312:CLA:HED2	1.94	0.50
18:b:23:HIS:ND1	25:b:615:CLA:OBD	2.44	0.50
18:b:256:MET:HA	18:b:263:THR:HG21	1.94	0.50
21:d:252:PHE:O	21:d:252:PHE:CG	2.64	0.50
11:2:214:ASP:N	11:2:214:ASP:OD1	2.43	0.50
24:3:309:CHL:H3A	28:3:318:NEX:C30	2.41	0.50
15:V:299:LEU:O	15:V:303:ARG:N	2.33	0.50
15:V:304:ASP:N	15:V:304:ASP:OD1	2.44	0.50
17:Y:206:VAL:O	17:Y:209:ASN:ND2	2.42	0.50
24:Y:309:CHL:HBA2	28:r:301:NEX:H403	1.94	0.50
17:8:45:THR:HG22	17:8:49:ASN:HD21	1.77	0.50
18:B:22:VAL:HG13	25:B:614:CLA:HMB2	1.94	0.50
20:C:265:ALA:HB2	20:C:429:HIS:CG	2.46	0.50
1:z:1:MET:SD	1:z:1:MET:N	2.80	0.50
10:4:134:GLY:HA2	24:4:311:CHL:HAC1	1.94	0.50
24:g:310:CHL:HBC2	24:g:311:CHL:HHD	1.92	0.50
12:u:248:ILE:HD12	12:u:252:ALA:HB3	1.94	0.50
8:r:243:PHE:CZ	27:r:316:XAT:H10	2.47	0.50
11:2:58:ARG:HA	11:2:61:MET:HE3	1.93	0.50
28:G:304:NEX:H222	25:G:308:CLA:C4B	2.41	0.50
18:B:480:ALA:H	21:D:139:ARG:NH1	2.06	0.50
3:h:48:VAL:O	3:h:52:ILE:HG12	2.12	0.50
33:i:101:LMG:HC71	20:c:204:SER:CB	2.41	0.50
11:5:214:ASP:N	11:5:214:ASP:OD1	2.43	0.50
12:p:245:ASP:OD1	12:p:245:ASP:N	2.33	0.50
17:q:21:PRO:HG2	17:q:35:ASP:HB3	1.93	0.50
18:b:357:ARG:HD3	18:b:371:LEU:HD11	1.93	0.50
19:a:174:LEU:HD22	35:a:606:PHO:H143	1.93	0.50
19:a:283:ILE:HA	19:a:286:THR:HG22	1.92	0.50
24:7:310:CHL:HBC2	24:7:311:CHL:HHD	1.93	0.50
8:R:57:LEU:HD11	8:R:68:ASP:HB2	1.93	0.50
13:S:57:GLY:H	13:S:64:ASN:H	1.60	0.50
13:S:58:TRP:CD2	17:8:136:PRO:HG3	2.46	0.50
13:S:120:ARG:HH21	13:S:124:LEU:HD12	1.77	0.50
12:9:83:GLU:HG2	12:9:176:LEU:HD21	1.93	0.50
17:8:92:GLN:HB2	17:8:99:LEU:HD12	1.93	0.50
25:B:604:CLA:H41	25:B:604:CLA:H92	1.93	0.50
19:A:174:LEU:HD22	35:A:606:PHO:H143	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:225:ARG:H	19:A:225:ARG:HD2	1.76	0.50
12:6:167:GLY:H	24:6:311:CHL:HMC	1.76	0.50
18:b:477:ASP:OD1	18:b:477:ASP:N	2.41	0.50
25:b:604:CLA:H41	25:b:604:CLA:H92	1.93	0.50
8:R:69:PRO:HD2	27:R:615:XAT:O23	2.12	0.50
18:B:151:PHE:HE1	18:B:203:ILE:HG23	1.76	0.50
18:B:474:ILE:HD11	25:B:612:CLA:HAA2	1.93	0.50
32:B:618:SQD:H292	32:B:618:SQD:H162	1.92	0.50
28:1:303:NEX:H383	25:1:307:CLA:CHB	2.41	0.50
12:3:117:VAL:HG23	12:3:120:SER:HB2	1.93	0.50
18:B:357:ARG:HD3	18:B:371:LEU:HD11	1.94	0.50
18:B:458:PHE:HB3	25:B:604:CLA:HBC2	1.94	0.50
10:4:13:GLY:O	10:4:16:SER:OG	2.29	0.50
28:4:303:NEX:H383	25:4:307:CLA:C2B	2.41	0.50
12:6:191:PRO:HA	12:6:194:PHE:HB3	1.94	0.50
12:u:113:LEU:HB3	12:u:116:PRO:HB3	1.94	0.50
25:c:611:CLA:HBB1	25:c:611:CLA:HMB3	1.94	0.50
21:d:210:LEU:HD21	39:d:406:PL9:H13	1.92	0.50
12:7:93:MET:SD	25:7:314:CLA:HAB	2.52	0.50
10:1:65:VAL:O	10:1:69:THR:OG1	2.22	0.49
18:B:463:PHE:CZ	18:B:467:ILE:HD11	2.47	0.49
18:b:379:ALA:HB2	18:b:395:VAL:HG21	1.94	0.49
8:r:258:PHE:HA	8:r:261:LEU:HB2	1.94	0.49
2:E:78:SER:HA	21:D:56:THR:CG2	2.42	0.49
7:M:27:VAL:HG12	7:m:28:LYS:HB2	1.94	0.49
8:R:47:TRP:CE3	24:R:601:CHL:HAA1	2.47	0.49
8:R:48:MET:SD	17:N:136:PRO:HB3	2.51	0.49
8:R:169:TYR:N	8:R:172:LEU:O	2.43	0.49
21:D:126:MET:HE3	21:D:143:ALA:O	2.12	0.49
11:5:58:ARG:HA	11:5:61:MET:HE3	1.93	0.49
12:6:44:LEU:HB3	12:6:47:TYR:HB2	1.93	0.49
22:w:109:ASP:O	20:c:249:ARG:NH1	2.44	0.49
19:a:46:SER:O	19:a:50:ILE:HG13	2.12	0.49
19:a:103:ASP:O	19:a:104:GLU:C	2.54	0.49
19:a:233:THR:OG1	30:a:612:LHG:O1	2.30	0.49
8:r:53:ARG:NH1	8:r:64:ASP:OD2	2.44	0.49
12:7:40:ARG:NE	12:7:63:ASP:OD1	2.45	0.49
28:7:304:NEX:H241	25:7:308:CLA:C2	2.42	0.49
28:7:304:NEX:H382	25:7:308:CLA:HBA2	1.94	0.49
12:3:57:THR:OG1	12:3:59:GLU:OE1	2.23	0.49
12:9:83:GLU:HA	12:9:176:LEU:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:8:55:ILE:HG22	24:8:310:CHL:HMD2	1.93	0.49
17:8:83:GLU:O	17:8:92:GLN:NE2	2.45	0.49
24:8:309:CHL:HBB1	24:8:309:CHL:HHC	1.94	0.49
6:l:22:LEU:HB3	16:t:51:ILE:HD13	1.94	0.49
10:4:210:GLY:HA2	25:4:316:CLA:CAD	2.42	0.49
8:R:47:TRP:CD2	8:R:67:PHE:HD1	2.31	0.49
10:1:171:LYS:NZ	30:1:318:LHG:O5	2.44	0.49
11:2:151:ASP:OD1	29:2:301:OUR:O40	2.29	0.49
17:G:159:PRO:HA	17:G:162:PHE:HB3	1.94	0.49
12:9:233:HIS:CG	25:9:316:CLA:HAA2	2.47	0.49
17:N:69:THR:HG23	17:N:70:PRO:HD3	1.94	0.49
18:B:23:HIS:ND1	25:B:615:CLA:OBD	2.44	0.49
12:u:212:MET:HG2	26:u:302:OIE:C6	2.42	0.49
25:y:315:CLA:H43	33:w:201:LMG:C10	2.43	0.49
12:p:93:MET:SD	25:p:314:CLA:HAB	2.52	0.49
17:q:55:ILE:HG22	24:q:311:CHL:HMD2	1.93	0.49
18:b:392:ILE:HB	18:b:397:VAL:HG22	1.94	0.49
8:r:47:TRP:CE3	24:r:302:CHL:HAA1	2.48	0.49
28:7:304:NEX:C33	24:7:310:CHL:HBA1	2.42	0.49
3:H:67:ALA:HB3	3:H:72:SER:HB3	1.93	0.49
10:4:79:VAL:HG11	10:4:102:LEU:HD12	1.95	0.49
11:5:131:ARG:NH2	24:5:313:CHL:O1D	2.44	0.49
28:p:304:NEX:H403	24:p:310:CHL:O2A	2.12	0.49
18:b:22:VAL:HG13	25:b:614:CLA:HMB2	1.93	0.49
18:b:254:GLY:HA3	33:d:401:LMG:H132	1.95	0.49
18:b:372:ASP:N	18:b:376:ILE:O	2.39	0.49
6:L:22:LEU:HB3	16:T:51:ILE:HD13	1.95	0.49
12:3:233:HIS:CG	25:3:316:CLA:HAA2	2.47	0.49
13:S:131:MET:SD	25:S:609:CLA:HAB	2.53	0.49
12:9:80:GLN:HA	12:9:83:GLU:HB3	1.94	0.49
21:D:39:PRO:HB2	25:D:405:CLA:HAB	1.94	0.49
10:4:65:VAL:O	10:4:69:THR:OG1	2.22	0.49
11:5:108:ILE:HG13	25:5:308:CLA:H11	1.95	0.49
12:p:146:LEU:H	12:p:146:LEU:HD12	1.78	0.49
17:q:12:LEU:HD23	24:q:303:CHL:HBB	1.95	0.49
20:c:142:LYS:HB3	20:c:244:PRO:HG2	1.94	0.49
28:S:617:NEX:H403	24:8:308:CHL:CBA	2.42	0.49
17:G:88:LYS:HD3	24:G:311:CHL:HED2	1.95	0.49
12:9:43:TRP:NE1	12:9:51:ASP:OD2	2.45	0.49
12:9:206:ARG:HA	12:9:209:MET:HE2	1.95	0.49
28:N:303:NEX:O24	25:N:307:CLA:C4	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:426:LEU:HD13	18:B:443:PHE:HZ	1.78	0.49
10:4:51:GLU:HA	10:4:144:LEU:HD21	1.94	0.49
22:w:96:TRP:CZ3	33:w:201:LMG:HC91	2.48	0.49
20:c:175:ASP:OD2	20:c:185:ARG:NH2	2.40	0.49
8:R:231:ALA:O	8:R:235:HIS:ND1	2.42	0.49
17:8:164:GLU:HG2	17:8:168:LYS:HE3	1.95	0.49
18:B:8:VAL:HG23	18:B:9:HIS:CD2	2.48	0.49
6:l:24:LEU:HD13	30:a:601:LHG:H151	1.93	0.49
11:5:47:ARG:HH22	11:5:48:ARG:HH21	1.61	0.49
12:u:249:THR:H	12:u:252:ALA:HB2	1.78	0.49
12:p:84:LEU:HD11	17:q:37:ALA:HA	1.93	0.49
12:p:180:GLU:O	12:p:181:SER:OG	2.31	0.49
21:d:172:SER:HB2	21:d:177:ALA:HB1	1.95	0.49
24:8:308:CHL:HHC	24:8:308:CHL:HBB1	1.95	0.49
30:n:318:LHG:HC62	30:n:318:LHG:H272	1.95	0.49
13:s:295:LEU:O	13:s:299:ILE:HG13	2.13	0.49
25:R:604:CLA:C4B	28:R:616:NEX:H362	2.43	0.49
17:G:120:GLN:OE1	24:G:311:CHL:HMC	2.12	0.49
25:N:315:CLA:HED2	25:N:315:CLA:H2A	1.95	0.49
17:Y:55:ILE:HG22	24:Y:312:CHL:HMD2	1.95	0.49
19:A:137:LEU:HD22	20:C:454:VAL:HG22	1.94	0.49
19:A:253:GLY:O	19:A:257:ARG:HG2	2.12	0.49
1:z:5:PHE:HD1	1:z:57:LEU:HB3	1.78	0.49
12:u:92:ALA:O	12:u:96:THR:N	2.41	0.49
12:u:93:MET:SD	25:u:314:CLA:HAB	2.52	0.49
12:p:230:TRP:NE1	24:p:318:CHL:HMC	2.24	0.49
18:b:458:PHE:HB3	25:b:604:CLA:HBC2	1.94	0.49
19:a:170:ASP:OD2	20:c:345:ARG:NH1	2.42	0.49
21:d:126:MET:HE3	21:d:143:ALA:O	2.13	0.49
13:s:128:ARG:HD3	25:s:410:CLA:C4C	2.43	0.49
8:r:137:CYS:O	8:r:141:THR:HG22	2.13	0.49
12:7:180:GLU:O	12:7:181:SER:OG	2.30	0.49
8:R:137:CYS:O	8:R:141:THR:HG22	2.13	0.48
10:1:88:LYS:HD3	24:1:310:CHL:HED2	1.95	0.48
17:8:8:ARG:NE	17:8:31:ASP:O	2.31	0.48
17:8:37:ALA:HA	12:7:84:LEU:HD11	1.95	0.48
18:B:362:PHE:O	21:D:294:ARG:NH2	2.46	0.48
1:z:1:MET:HB2	1:z:4:LEU:HB3	1.95	0.48
2:e:90:GLN:OE1	19:a:312:ARG:NH1	2.46	0.48
17:n:61:MET:HG3	17:n:173:GLY:HA2	1.95	0.48
17:y:168:LYS:HD3	25:y:316:CLA:HAA2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:a:137:LEU:HD22	20:c:454:VAL:HG22	1.95	0.48
13:s:59:PHE:HD2	28:s:401:NEX:C18	2.23	0.48
8:r:57:LEU:HD11	8:r:68:ASP:HB2	1.95	0.48
1:Z:5:PHE:HD1	1:Z:57:LEU:HB3	1.78	0.48
25:R:612:CLA:HBB	24:N:308:CHL:HED1	1.95	0.48
13:S:108:GLY:O	13:S:111:LYS:HG3	2.13	0.48
28:N:303:NEX:O24	25:N:307:CLA:H43	2.13	0.48
20:C:336:GLU:OE1	20:C:336:GLU:N	2.43	0.48
12:p:56:LEU:HD11	12:p:67:ASP:HB2	1.95	0.48
28:p:304:NEX:H362	25:p:308:CLA:C3B	2.43	0.48
25:b:605:CLA:H8	25:b:606:CLA:H193	1.94	0.48
20:c:395:VAL:HG11	20:c:404:ALA:N	2.26	0.48
13:s:97:GLU:OE1	13:s:97:GLU:N	2.46	0.48
13:s:124:LEU:HD13	13:s:229:LEU:HB3	1.94	0.48
28:1:303:NEX:C36	25:1:307:CLA:CHC	2.91	0.48
12:3:230:TRP:HE1	24:3:317:CHL:HMC	1.78	0.48
28:G:304:NEX:H221	25:G:308:CLA:C1C	2.44	0.48
18:B:156:PHE:O	18:B:157:HIS:C	2.56	0.48
18:B:242:ILE:HG23	18:B:462:PHE:HD2	1.79	0.48
21:D:89:LEU:H	21:D:89:LEU:HG	1.41	0.48
4:i:27:ASP:OD1	19:a:136:ARG:NH2	2.41	0.48
8:r:169:TYR:N	8:r:172:LEU:O	2.46	0.48
12:7:56:LEU:HD11	12:7:67:ASP:HB2	1.95	0.48
9:F:14:THR:HG21	14:X:100:VAL:HG11	1.95	0.48
19:A:46:SER:O	19:A:50:ILE:HG13	2.12	0.48
24:u:306:CHL:HBB1	24:u:306:CHL:H51	1.95	0.48
3:H:26:TYR:CE2	8:R:83:ILE:HG12	2.48	0.48
8:R:243:PHE:CE2	27:R:615:XAT:H10	2.49	0.48
11:2:108:ILE:HG13	25:2:308:CLA:H11	1.95	0.48
17:G:54:LEU:HD12	17:G:144:LEU:HD13	1.95	0.48
17:N:65:VAL:O	17:N:69:THR:HG22	2.14	0.48
25:B:605:CLA:H8	25:B:606:CLA:H193	1.94	0.48
25:C:611:CLA:HBB1	25:C:611:CLA:HMB3	1.94	0.48
21:D:172:SER:HB2	21:D:177:ALA:HB1	1.95	0.48
17:g:164:GLU:O	17:g:167:THR:OG1	2.29	0.48
17:q:24:LEU:HD11	17:q:35:ASP:HB2	1.94	0.48
25:b:609:CLA:H202	25:b:612:CLA:H18	1.95	0.48
19:a:85:THR:HG21	19:a:113:GLN:HB2	1.96	0.48
20:c:80:LEU:HD21	25:c:603:CLA:H2A	1.95	0.48
8:r:160:GLU:N	24:r:307:CHL:O1D	2.46	0.48
5:K:8:LEU:HD11	5:K:19:VAL:HG21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:256:MET:HA	18:B:263:THR:HG21	1.94	0.48
20:C:249:ARG:NH1	22:W:109:ASP:O	2.46	0.48
33:D:411:LMG:H182	33:D:411:LMG:H211	1.52	0.48
11:5:14:PRO:HD2	24:5:305:CHL:HBB1	1.95	0.48
18:b:12:VAL:HG21	18:b:22:VAL:HG21	1.96	0.48
25:b:604:CLA:C1C	25:b:613:CLA:HBB1	2.44	0.48
11:2:73:LEU:HD23	11:2:81:PHE:HZ	1.79	0.48
12:9:221:VAL:HG13	12:9:222:THR:HG23	1.96	0.48
17:N:186:GLN:O	17:N:190:THR:OG1	2.25	0.48
17:8:58:ARG:HA	17:8:61:MET:HE3	1.95	0.48
2:e:95:ILE:O	21:d:84:SER:OG	2.23	0.48
12:u:249:THR:HB	12:u:250:ARG:HH21	1.78	0.48
18:b:283:GLU:CD	18:b:287:ARG:HH21	2.22	0.48
25:c:610:CLA:H151	25:c:610:CLA:H112	1.54	0.48
35:d:403:PHO:H112	35:d:403:PHO:H71	1.60	0.48
6:L:23:LEU:HD22	30:D:407:LHG:H262	1.95	0.48
18:B:334:ASP:OD1	18:B:334:ASP:N	2.47	0.48
10:4:41:ALA:HB1	12:6:76:GLU:HG3	1.96	0.48
12:6:68:THR:N	26:6:302:OIE:O42	2.45	0.48
17:g:159:PRO:HA	17:g:162:PHE:HB3	1.95	0.48
12:u:112:ASP:OD1	12:u:113:LEU:N	2.47	0.48
25:p:307:CLA:H12	17:q:39:LEU:HD11	1.95	0.48
18:b:208:LEU:HD23	25:b:602:CLA:HAC2	1.96	0.48
33:d:411:LMG:H321	33:d:411:LMG:H291	1.48	0.48
8:R:193:GLU:OE1	8:R:196:ARG:NH2	2.38	0.48
16:T:52:LEU:HD11	30:D:407:LHG:H171	1.96	0.48
17:N:68:LEU:HD13	17:N:195:VAL:HG22	1.96	0.48
18:B:154:GLY:HA2	18:B:158:VAL:HG23	1.95	0.48
12:p:145:ILE:HG23	12:p:146:LEU:HD12	1.96	0.48
21:d:55:ILE:O	21:d:66:SER:HB3	2.14	0.48
25:r:305:CLA:C1C	28:r:317:NEX:H222	2.44	0.48
28:r:317:NEX:H401	28:r:317:NEX:H35	1.57	0.48
11:5:88:LYS:HA	24:5:311:CHL:HED2	1.96	0.48
12:6:76:GLU:HA	12:6:79:LYS:HE3	1.96	0.48
12:6:162:TYR:HB3	24:6:311:CHL:CMC	2.43	0.48
17:n:24:LEU:HD22	17:n:33:GLY:HA2	1.95	0.48
12:7:74:ASP:HB3	12:7:77:MET:HE2	1.95	0.48
2:E:75:VAL:HG13	2:E:76:PHE:H	1.79	0.47
6:L:15:ARG:NH1	32:b:618:SQD:O2	2.44	0.47
6:L:24:LEU:HD13	30:A:601:LHG:H151	1.96	0.47
28:1:303:NEX:H383	25:1:307:CLA:C2B	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:3:156:MET:SD	28:3:318:NEX:H32	2.54	0.47
12:9:93:MET:HG3	12:9:205:GLY:HA2	1.95	0.47
18:B:283:GLU:CD	18:B:287:ARG:HH21	2.21	0.47
20:C:80:LEU:HD21	25:C:603:CLA:H2A	1.96	0.47
3:h:26:TYR:CE2	8:r:83:ILE:HG12	2.49	0.47
9:f:14:THR:HG21	14:x:100:VAL:HG11	1.94	0.47
11:5:147:GLY:C	11:5:149:ALA:H	2.22	0.47
12:6:59:GLU:OE1	12:6:59:GLU:N	2.47	0.47
17:q:45:THR:HG22	17:q:49:ASN:HD21	1.79	0.47
18:b:242:ILE:HG23	18:b:462:PHE:HD2	1.79	0.47
19:a:253:GLY:O	19:a:257:ARG:HG2	2.14	0.47
13:s:156:LEU:HD11	13:s:272:ALA:HB1	1.95	0.47
12:7:117:VAL:O	12:7:118:TRP:HB3	2.13	0.47
2:E:98:ARG:NH2	3:H:59:SER:OG	2.47	0.47
11:2:131:ARG:NH2	24:2:313:CHL:O1D	2.48	0.47
28:2:304:NEX:H35	28:2:304:NEX:H401	1.57	0.47
13:S:97:GLU:OE1	13:S:97:GLU:N	2.46	0.47
21:D:113:PHE:O	21:D:117:HIS:ND1	2.39	0.47
11:5:61:MET:HG3	11:5:173:GLY:HA2	1.96	0.47
11:5:118:TRP:HZ2	24:6:317:CHL:HBD	1.79	0.47
21:d:152:VAL:HG21	21:d:279:LEU:HD13	1.96	0.47
33:d:411:LMG:H162	33:d:411:LMG:H191	1.52	0.47
3:H:61:VAL:HG21	14:X:79:LEU:HD22	1.97	0.47
6:L:14:ASN:OD1	6:L:14:ASN:N	2.38	0.47
8:R:107:ASP:OD1	8:R:118:SER:OG	2.26	0.47
10:1:136:PRO:HG3	28:1:303:NEX:H183	1.97	0.47
24:3:309:CHL:H3A	28:3:318:NEX:C31	2.44	0.47
17:G:168:LYS:HD3	25:G:316:CLA:HAA2	1.96	0.47
20:C:204:SER:CB	33:C:618:LMG:HC71	2.44	0.47
4:i:31:ASN:HB3	19:a:135:PHE:CZ	2.49	0.47
24:q:308:CHL:HBA1	28:s:401:NEX:H403	1.96	0.47
20:c:211:TRP:CD2	20:c:212:ILE:HG23	2.49	0.47
13:s:131:MET:SD	25:s:410:CLA:HAB	2.54	0.47
8:r:154:PRO:HB3	8:r:256:GLY:HA3	1.95	0.47
10:1:168:LYS:NZ	25:1:315:CLA:O1D	2.40	0.47
10:1:210:GLY:HA2	25:1:316:CLA:CAD	2.44	0.47
28:1:303:NEX:O24	24:1:309:CHL:HAA1	2.15	0.47
28:S:617:NEX:H15	28:S:617:NEX:H201	1.62	0.47
28:G:304:NEX:C22	25:G:308:CLA:NC	2.77	0.47
17:N:168:LYS:HD3	25:N:315:CLA:HBD	1.96	0.47
19:A:170:ASP:OD2	20:C:345:ARG:NH1	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:A:601:LHG:O3	30:A:601:LHG:O1	2.23	0.47
20:C:211:TRP:CD2	20:C:212:ILE:HG23	2.49	0.47
20:C:365:LEU:H	20:C:365:LEU:HD12	1.79	0.47
6:l:11:VAL:H	7:m:28:LYS:HZ1	1.62	0.47
28:4:303:NEX:C36	25:4:307:CLA:C4B	2.89	0.47
28:6:303:NEX:O24	24:6:309:CHL:HAA2	2.13	0.47
25:g:315:CLA:H2A	25:g:315:CLA:HED3	1.96	0.47
12:u:86:VAL:HG21	12:u:176:LEU:HD13	1.96	0.47
24:u:305:CHL:H3A	24:u:305:CHL:HBA1	1.57	0.47
18:b:348:ASP:OD1	18:b:349:LYS:N	2.47	0.47
19:a:131:TRP:CH2	25:c:605:CLA:HAA2	2.50	0.47
12:3:59:GLU:OE1	12:3:59:GLU:N	2.47	0.47
26:9:302:OIE:C14	24:9:305:CHL:HMC	2.44	0.47
30:9:318:LHG:H261	30:9:318:LHG:HC82	1.96	0.47
17:N:8:ARG:NH2	17:N:24:LEU:O	2.46	0.47
17:N:168:LYS:HD3	25:N:315:CLA:HAA2	1.95	0.47
18:B:12:VAL:HG21	18:B:22:VAL:HG21	1.96	0.47
18:B:372:ASP:N	18:B:376:ILE:O	2.39	0.47
25:B:604:CLA:C1C	25:B:613:CLA:HBB1	2.44	0.47
32:B:618:SQD:O2	6:l:15:ARG:NH1	2.43	0.47
19:A:85:THR:HG21	19:A:113:GLN:HB2	1.96	0.47
10:4:88:LYS:HD3	24:4:310:CHL:HED2	1.95	0.47
28:4:303:NEX:H222	25:4:307:CLA:CHC	2.43	0.47
28:6:303:NEX:H401	28:6:303:NEX:H35	1.75	0.47
17:n:63:GLY:O	17:n:67:CYS:N	2.40	0.47
17:q:58:ARG:HA	17:q:61:MET:HE3	1.96	0.47
17:q:128:GLU:OE1	17:q:131:ARG:NH1	2.43	0.47
30:a:601:LHG:O3	30:a:601:LHG:O1	2.23	0.47
8:r:117:TYR:OH	8:r:128:GLU:OE1	2.26	0.47
11:2:133:ASN:ND2	12:3:46:PRO:O	2.48	0.47
13:S:59:PHE:CE2	28:S:617:NEX:C3	2.96	0.47
17:G:181:PHE:HE2	24:G:306:CHL:H172	1.79	0.47
25:G:315:CLA:HED3	25:G:315:CLA:H2A	1.97	0.47
12:9:226:PRO:HA	12:9:229:ASN:HD22	1.79	0.47
28:9:319:NEX:H35	28:9:319:NEX:H401	1.57	0.47
17:N:21:PRO:HD2	17:N:24:LEU:HD13	1.96	0.47
17:Y:21:PRO:HD2	17:Y:24:LEU:HD12	1.96	0.47
18:B:339:GLY:N	18:B:431:GLU:OE1	2.44	0.47
20:C:190:PRO:HB2	20:C:223:GLY:HA2	1.97	0.47
12:6:184:PRO:O	29:6:301:OUR:O40	2.32	0.47
17:y:24:LEU:HD11	17:y:35:ASP:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:p:87:ILE:HG22	24:p:313:CHL:HMD2	1.97	0.47
35:a:606:PHO:H61	35:a:606:PHO:H2	1.54	0.47
8:r:47:TRP:CD2	8:r:67:PHE:HD1	2.32	0.47
8:R:83:ILE:HD13	18:B:132:ALA:HB2	1.96	0.47
10:1:28:PHE:O	10:1:31:ASP:HB2	2.15	0.47
30:1:318:LHG:H111	30:1:318:LHG:HC82	1.76	0.47
12:3:124:GLN:O	12:3:127:SER:OG	2.24	0.47
24:3:309:CHL:HBA1	28:3:318:NEX:H31	1.96	0.47
13:S:128:ARG:HD2	25:S:609:CLA:C4C	2.45	0.47
13:S:295:LEU:O	13:S:299:ILE:HG13	2.14	0.47
17:G:171:LYS:NZ	25:G:315:CLA:O1D	2.38	0.47
18:B:272:ARG:NH1	18:B:276:ASP:OD2	2.48	0.47
19:A:227:THR:OG1	19:A:231:GLU:OE2	2.29	0.47
19:A:269:ARG:HE	21:D:235:PHE:HB2	1.79	0.47
10:4:171:LYS:NZ	30:4:318:LHG:O5	2.48	0.47
17:n:108:VAL:HG23	24:n:308:CHL:C1D	2.45	0.47
17:y:17:GLU:O	17:q:133:SER:OG	2.32	0.47
17:y:55:ILE:HG22	24:y:313:CHL:HMD2	1.96	0.47
12:p:76:GLU:O	12:p:80:GLN:NE2	2.48	0.47
12:p:130:GLY:HA3	12:p:142:ALA:O	2.15	0.47
18:b:251:VAL:HG22	25:b:602:CLA:H61	1.97	0.47
20:c:257:GLU:OE1	20:c:435:ARG:NH1	2.41	0.47
8:r:107:ASP:OD1	8:r:118:SER:OG	2.25	0.47
24:r:306:CHL:HBC2	24:r:307:CHL:HHD	1.97	0.47
12:7:124:GLN:O	12:7:127:SER:OG	2.22	0.47
12:7:230:TRP:NE1	24:7:318:CHL:HMC	2.27	0.47
24:7:305:CHL:H51	24:7:305:CHL:H12	1.68	0.47
8:R:56:TRP:NE1	8:R:68:ASP:OD2	2.45	0.47
13:S:286:HIS:CD2	13:S:290:PRO:HA	2.50	0.47
18:B:70:GLY:HA2	18:B:178:VAL:HG21	1.97	0.47
18:B:458:PHE:CE2	25:B:604:CLA:HAB	2.50	0.47
20:C:175:ASP:OD2	20:C:185:ARG:NH2	2.40	0.47
20:C:267:ILE:HD13	25:C:609:CLA:HED2	1.97	0.47
12:u:64:TYR:CE2	24:u:305:CHL:HHD	2.50	0.47
25:u:315:CLA:H41	25:u:315:CLA:H61	1.51	0.47
12:p:117:VAL:O	12:p:118:TRP:HB3	2.14	0.47
17:q:52:LEU:O	17:q:56:HIS:ND1	2.35	0.47
19:a:105:TRP:O	19:a:106:LEU:C	2.57	0.47
21:d:148:ALA:HB1	21:d:279:LEU:HB2	1.97	0.47
8:r:243:PHE:CD2	27:r:316:XAT:H12	2.50	0.47
11:2:120:GLN:HE21	24:2:313:CHL:HMC	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:2:304:NEX:H15	28:2:304:NEX:H201	1.62	0.47
12:9:112:ASP:OD1	12:9:113:LEU:N	2.48	0.47
12:9:147:ALA:HB1	24:9:308:CHL:HBC3	1.97	0.47
17:8:15:TYR:O	12:7:165:SER:OG	2.33	0.47
25:C:609:CLA:H112	25:C:609:CLA:H142	1.63	0.47
21:D:199:MET:HE3	21:D:281:MET:HB3	1.96	0.47
11:5:55:ILE:HG22	24:5:313:CHL:HMD2	1.97	0.47
12:u:52:VAL:HG12	12:u:65:GLY:HA3	1.97	0.47
25:d:405:CLA:HBA1	25:d:405:CLA:H3A	1.74	0.47
25:r:305:CLA:CMB	24:r:306:CHL:HBB1	2.45	0.47
28:7:304:NEX:H392	25:7:308:CLA:HMB2	1.97	0.47
24:7:305:CHL:H3A	24:7:305:CHL:HBA1	1.75	0.47
10:1:155:MET:N	10:1:155:MET:SD	2.88	0.47
12:3:162:TYR:HB3	24:3:311:CHL:CMC	2.45	0.47
13:S:58:TRP:C	13:S:60:GLY:H	2.23	0.47
13:S:129:TRP:O	13:S:133:GLY:N	2.41	0.47
24:9:304:CHL:HMD1	30:9:318:LHG:H251	1.96	0.47
18:B:251:VAL:HG22	25:B:602:CLA:H61	1.96	0.47
19:A:301:ASN:HB3	20:C:394:SER:HB2	1.96	0.47
3:h:13:THR:HG23	3:h:16:GLY:H	1.80	0.47
10:4:15:TYR:HD2	12:6:165:SER:HB2	1.79	0.47
28:4:303:NEX:C36	25:4:307:CLA:CHC	2.92	0.47
18:b:154:GLY:HA3	18:b:202:HIS:HB2	1.96	0.47
18:b:334:ASP:OD1	18:b:334:ASP:N	2.47	0.47
25:s:417:CLA:H3A	25:s:417:CLA:HBA2	1.59	0.47
4:I:31:ASN:HB3	19:A:135:PHE:CZ	2.49	0.46
6:L:11:VAL:H	7:M:28:LYS:HZ3	1.63	0.46
8:R:47:TRP:HE3	24:R:601:CHL:HAA1	1.79	0.46
10:1:14:PRO:HD2	24:1:304:CHL:HBB1	1.96	0.46
17:G:51:GLU:HG2	24:G:313:CHL:HED2	1.95	0.46
24:G:306:CHL:H93	25:G:307:CLA:HBB	1.96	0.46
24:G:313:CHL:HHC	24:G:313:CHL:HBB1	1.97	0.46
12:9:52:VAL:HG12	12:9:65:GLY:HA3	1.97	0.46
12:9:97:VAL:HG22	25:9:307:CLA:HMC1	1.97	0.46
28:N:303:NEX:H11	28:N:303:NEX:H191	1.80	0.46
19:A:38:LEU:HB3	19:A:39:PRO:HD3	1.97	0.46
17:g:17:GLU:OE1	17:g:17:GLU:N	2.46	0.46
17:y:9:ALA:HB1	24:y:305:CHL:HBC1	1.96	0.46
17:y:114:LEU:HD21	12:p:241:ASN:HD22	1.80	0.46
24:p:305:CHL:H121	24:p:305:CHL:H162	1.46	0.46
18:b:458:PHE:CE2	25:b:604:CLA:HAB	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:c:83:LEU:HD13	25:c:602:CLA:H143	1.96	0.46
13:s:131:MET:HG3	13:s:258:GLY:HA2	1.97	0.46
10:1:8:ARG:NH1	10:1:26:GLY:H	2.13	0.46
10:1:12:LEU:HA	24:1:304:CHL:NB	2.30	0.46
12:9:162:TYR:HB3	24:9:311:CHL:CMC	2.45	0.46
17:N:178:PHE:CE2	25:N:316:CLA:HAB	2.51	0.46
25:B:603:CLA:H61	25:B:603:CLA:H41	1.67	0.46
20:C:408:VAL:H	37:C:619:DGD:HE3	1.79	0.46
2:e:52:HIS:NE2	23:f:201:HEM:ND	2.63	0.46
17:g:49:ASN:ND2	24:g:306:CHL:H3A	2.31	0.46
12:u:162:TYR:HB3	24:u:312:CHL:CMC	2.45	0.46
17:n:178:PHE:CE2	25:n:316:CLA:HAB	2.50	0.46
28:n:303:NEX:H403	24:n:309:CHL:HBA2	1.98	0.46
19:a:28:LEU:HD11	21:d:258:GLY:HA2	1.97	0.46
21:d:242:GLU:OE1	21:d:264:LYS:NZ	2.32	0.46
7:M:28:LYS:HB2	7:m:27:VAL:HG12	1.97	0.46
17:G:164:GLU:O	17:G:167:THR:OG1	2.29	0.46
17:8:7:ASP:OD1	17:8:7:ASP:N	2.48	0.46
18:B:348:ASP:OD1	18:B:349:LYS:N	2.47	0.46
19:A:234:ASN:ND2	30:A:601:LHG:O4	2.48	0.46
28:u:304:NEX:C32	24:u:312:CHL:HMA1	2.46	0.46
24:y:305:CHL:HMA3	30:y:319:LHG:H112	1.97	0.46
17:q:142:ASP:OD1	17:q:145:TYR:N	2.40	0.46
18:b:8:VAL:HG23	18:b:9:HIS:CD2	2.49	0.46
20:c:190:PRO:HB2	20:c:223:GLY:HA2	1.97	0.46
8:r:69:PRO:O	27:r:316:XAT:O23	2.32	0.46
12:7:133:TYR:HH	28:7:304:NEX:H1	1.61	0.46
24:7:305:CHL:H162	24:7:305:CHL:H121	1.47	0.46
8:R:168:SER:HA	8:R:173:GLY:HA2	1.98	0.46
11:2:61:MET:HG3	11:2:173:GLY:HA2	1.96	0.46
28:2:304:NEX:H11	28:2:304:NEX:H191	1.82	0.46
17:8:39:LEU:HD11	25:7:307:CLA:H12	1.96	0.46
18:B:453:PHE:HB2	21:D:291:LEU:HD12	1.98	0.46
20:C:395:VAL:HG11	20:C:404:ALA:H	1.81	0.46
10:4:57:ALA:HB1	10:4:173:GLY:HA3	1.97	0.46
10:4:131:ARG:HG3	24:4:311:CHL:C1D	2.46	0.46
28:6:303:NEX:C28	24:6:309:CHL:CAA	2.89	0.46
28:y:304:NEX:H35	28:y:304:NEX:H401	1.58	0.46
22:w:103:GLN:OE1	20:c:250:ARG:NH1	2.48	0.46
18:b:346:PHE:HB2	18:b:354:LEU:O	2.16	0.46
18:b:426:LEU:HD13	18:b:443:PHE:HZ	1.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:c:604:CLA:H141	25:c:604:CLA:H192	1.98	0.46
21:d:51:GLY:HA3	21:d:78:VAL:HG22	1.97	0.46
8:R:162:ILE:HD11	25:R:604:CLA:H2A	1.97	0.46
11:2:8:ARG:NH1	11:2:31:ASP:O	2.36	0.46
28:3:318:NEX:H11	28:3:318:NEX:H191	1.80	0.46
13:S:58:TRP:CG	17:8:136:PRO:HG3	2.50	0.46
17:N:54:LEU:HD23	17:N:55:ILE:HD13	1.98	0.46
17:8:12:LEU:HD12	17:8:16:SER:HA	1.98	0.46
17:8:17:GLU:O	12:7:165:SER:OG	2.21	0.46
18:B:151:PHE:O	18:B:152:GLY:C	2.55	0.46
25:B:611:CLA:H112	25:B:611:CLA:H72	1.73	0.46
17:g:51:GLU:HG2	24:g:313:CHL:HED2	1.98	0.46
22:w:110:GLU:OE2	20:c:243:LYS:NZ	2.47	0.46
25:b:604:CLA:H71	25:b:604:CLA:H112	1.59	0.46
19:a:37:ARG:HH11	19:a:41:LEU:HD12	1.79	0.46
20:c:257:GLU:OE2	20:c:432:HIS:ND1	2.36	0.46
2:E:79:PRO:HD2	21:D:56:THR:HG21	1.98	0.46
2:E:106:LYS:HA	21:D:103:ARG:HH21	1.80	0.46
17:Y:194:PRO:O	29:Y:301:OUR:O39	2.33	0.46
25:A:603:CLA:HBD	25:A:604:CLA:HAC2	1.98	0.46
33:C:618:LMG:H172	33:C:618:LMG:H142	1.55	0.46
35:D:403:PHO:H112	35:D:403:PHO:H71	1.60	0.46
28:g:304:NEX:H15	28:g:304:NEX:H201	1.62	0.46
12:u:147:ALA:HB1	24:u:309:CHL:HBC3	1.96	0.46
24:y:313:CHL:HAA2	12:p:68:THR:HG21	1.98	0.46
25:a:603:CLA:HBD	25:a:604:CLA:HAC2	1.98	0.46
13:s:286:HIS:CD2	13:s:290:PRO:HA	2.50	0.46
8:r:44:ASP:CG	8:r:53:ARG:HH22	2.23	0.46
12:7:76:GLU:O	12:7:79:LYS:HG3	2.16	0.46
12:7:87:ILE:HG22	24:7:313:CHL:HMD2	1.97	0.46
24:3:309:CHL:H3A	28:3:318:NEX:C29	2.45	0.46
13:S:141:GLU:CD	13:S:280:TYR:HB3	2.41	0.46
18:B:60:MET:HB3	18:B:60:MET:HE2	1.64	0.46
18:B:208:LEU:HD23	25:B:602:CLA:HAC2	1.97	0.46
25:A:603:CLA:H203	30:D:407:LHG:H162	1.97	0.46
20:C:250:ARG:NH1	22:W:103:GLN:OE1	2.48	0.46
25:D:405:CLA:H161	25:D:405:CLA:H202	1.67	0.46
6:l:23:LEU:HD22	30:d:407:LHG:H262	1.96	0.46
28:6:303:NEX:H28	24:6:309:CHL:HAA1	1.97	0.46
17:g:61:MET:SD	25:g:314:CLA:HAB	2.56	0.46
17:g:200:GLU:O	17:g:208:ASN:ND2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:u:80:GLN:NE2	17:n:37:ALA:O	2.49	0.46
25:b:611:CLA:H112	25:b:611:CLA:H72	1.74	0.46
25:c:612:CLA:H43	24:s:402:CHL:HBB2	1.98	0.46
13:s:129:TRP:CE2	24:s:408:CHL:HED2	2.51	0.46
12:7:130:GLY:HA3	12:7:142:ALA:O	2.16	0.46
12:7:146:LEU:HD12	12:7:146:LEU:H	1.80	0.46
8:R:69:PRO:CD	27:R:615:XAT:O23	2.64	0.46
10:1:131:ARG:HG3	24:1:311:CHL:C1D	2.45	0.46
17:G:61:MET:SD	25:G:314:CLA:HAB	2.55	0.46
17:Y:126:LEU:O	17:Y:130:TYR:N	2.40	0.46
17:8:30:GLY:O	17:8:174:ARG:NH2	2.41	0.46
25:B:606:CLA:H13	25:B:613:CLA:HBB2	1.98	0.46
24:g:313:CHL:H111	24:g:313:CHL:H91	1.75	0.46
12:p:133:TYR:HE1	28:p:304:NEX:H1	1.50	0.46
8:r:193:GLU:OE1	8:r:196:ARG:NH2	2.37	0.46
8:R:44:ASP:HB2	8:R:53:ARG:HH22	1.81	0.46
28:R:616:NEX:H201	28:R:616:NEX:H15	1.62	0.46
13:S:127:CYS:HB3	13:S:258:GLY:HA3	1.98	0.46
13:S:156:LEU:HD11	13:S:272:ALA:HB1	1.97	0.46
25:G:315:CLA:H112	25:G:315:CLA:H72	1.82	0.46
12:9:80:GLN:NE2	17:N:37:ALA:O	2.49	0.46
17:N:59:TRP:CE2	24:N:311:CHL:HED2	2.51	0.46
18:B:23:HIS:O	18:B:27:THR:OG1	2.30	0.46
18:B:157:HIS:HE1	25:B:607:CLA:NA	2.14	0.46
18:B:326:ARG:HH21	21:D:297:ASP:CG	2.24	0.46
19:A:143:ILE:HD12	21:D:252:PHE:HE2	1.76	0.46
25:A:604:CLA:CHA	25:A:604:CLA:HBA1	2.46	0.46
25:C:604:CLA:H192	25:C:604:CLA:H141	1.98	0.46
10:4:155:MET:N	10:4:155:MET:SD	2.89	0.46
12:u:93:MET:HG3	12:u:205:GLY:HA2	1.98	0.46
22:w:76:ALA:H	20:c:202:LEU:HB3	1.81	0.46
19:a:105:TRP:O	19:a:107:TYR:N	2.48	0.46
2:E:104:GLN:O	2:E:107:SER:OG	2.26	0.46
4:I:28:PRO:O	4:I:31:ASN:ND2	2.48	0.46
10:1:74:GLU:HB3	10:1:81:PHE:HD2	1.81	0.46
17:Y:94:PHE:HZ	12:7:243:PHE:HB3	1.81	0.46
17:8:61:MET:SD	25:8:311:CLA:HAB	2.55	0.46
24:8:310:CHL:HBB1	24:8:310:CHL:HHC	1.98	0.46
25:B:613:CLA:H41	25:B:613:CLA:H62	1.53	0.46
21:D:186:GLN:OE1	21:D:192:THR:OG1	2.22	0.46
2:e:106:LYS:HA	21:d:103:ARG:HH21	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:u:304:NEX:H11	28:u:304:NEX:H191	1.82	0.46
28:p:304:NEX:H15	28:p:304:NEX:H201	1.62	0.46
28:p:304:NEX:H35	28:p:304:NEX:H401	1.57	0.46
24:p:306:CHL:H91	24:p:306:CHL:H111	1.72	0.46
18:b:315:ILE:HG22	18:b:426:LEU:HB3	1.98	0.46
20:c:118:VAL:HG21	25:c:611:CLA:H152	1.97	0.46
21:d:186:GLN:OE1	21:d:192:THR:OG1	2.22	0.46
13:s:69:ASP:OD1	13:s:69:ASP:N	2.48	0.46
8:r:244:LEU:O	8:r:248:VAL:HG22	2.16	0.46
8:R:90:ALA:O	19:A:228:THR:OG1	2.23	0.45
11:2:21:PRO:HG2	11:2:35:ASP:HB3	1.99	0.45
13:S:68:LEU:HD21	13:S:249:GLU:HB3	1.98	0.45
24:G:305:CHL:H51	24:G:305:CHL:H12	1.76	0.45
25:Y:316:CLA:H2	25:Y:316:CLA:H61	1.59	0.45
11:5:73:LEU:HD23	11:5:81:PHE:HZ	1.80	0.45
24:6:304:CHL:H3A	24:6:304:CHL:HBA1	1.45	0.45
24:p:306:CHL:H143	24:p:306:CHL:H112	1.66	0.45
18:b:453:PHE:HB2	21:d:291:LEU:HD12	1.98	0.45
25:b:606:CLA:H13	25:b:613:CLA:HBB2	1.98	0.45
20:c:147:THR:O	20:c:151:ILE:HG13	2.16	0.45
21:d:29:PHE:O	21:d:128:ARG:NH1	2.46	0.45
28:s:401:NEX:H11	28:s:401:NEX:H191	1.80	0.45
8:r:146:VAL:HG11	25:r:305:CLA:HAC2	1.97	0.45
2:E:60:PHE:CZ	9:F:35:THR:HG21	2.52	0.45
8:R:93:ASN:OD1	8:R:93:ASN:N	2.48	0.45
8:R:154:PRO:HB3	8:R:256:GLY:HA3	1.98	0.45
24:3:304:CHL:HBA1	24:3:304:CHL:H3A	1.47	0.45
24:S:606:CHL:HHC	24:S:606:CHL:HBB1	1.97	0.45
28:S:617:NEX:C38	25:8:306:CLA:C2B	2.91	0.45
17:G:211:PHE:HB3	17:N:94:PHE:CZ	2.49	0.45
28:G:304:NEX:H15	28:G:304:NEX:H201	1.62	0.45
18:B:157:HIS:CE1	25:B:607:CLA:NA	2.84	0.45
19:A:131:TRP:CH2	25:C:605:CLA:HAA2	2.50	0.45
20:C:147:THR:O	20:C:151:ILE:HG13	2.16	0.45
1:z:2:ILE:O	1:z:6:GLN:HG2	2.17	0.45
12:6:168:PRO:HG2	24:6:311:CHL:HBB2	1.97	0.45
28:6:303:NEX:H11	28:6:303:NEX:H191	1.80	0.45
24:g:313:CHL:H43	24:u:305:CHL:H2	1.97	0.45
17:n:92:GLN:NE2	25:n:307:CLA:O1D	2.48	0.45
17:q:12:LEU:HD12	17:q:16:SER:HA	1.98	0.45
17:q:30:GLY:O	17:q:174:ARG:NH2	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:w:96:TRP:CZ2	33:w:201:LMG:H112	2.51	0.45
25:b:613:CLA:H92	25:b:613:CLA:H61	1.81	0.45
12:7:195:SER:C	12:7:197:LEU:H	2.24	0.45
6:L:27:VAL:HG21	30:A:601:LHG:H192	1.98	0.45
13:S:131:MET:HG3	13:S:258:GLY:HA2	1.98	0.45
19:A:28:LEU:HD11	21:D:258:GLY:HA2	1.99	0.45
20:C:45:ALA:O	20:C:49:VAL:HG23	2.17	0.45
30:D:408:LHG:H112	30:D:408:LHG:HC81	1.77	0.45
11:5:118:TRP:HA	11:5:121:VAL:HG12	1.99	0.45
12:6:72:SER:HB2	12:6:78:PHE:HA	1.99	0.45
12:u:210:PHE:HE2	25:u:317:CLA:HAB	1.81	0.45
22:w:96:TRP:CH2	33:w:201:LMG:H112	2.52	0.45
19:a:143:ILE:HD12	21:d:252:PHE:HE2	1.78	0.45
25:c:604:CLA:CAA	37:c:618:DGD:HD61	2.47	0.45
13:s:127:CYS:HB3	13:s:258:GLY:HA3	1.97	0.45
12:7:163:ARG:HG3	24:7:312:CHL:C1D	2.46	0.45
12:3:200:LYS:HD3	25:3:315:CLA:HAA2	1.97	0.45
24:Y:311:CHL:C4A	24:Y:311:CHL:HBA2	2.47	0.45
17:8:142:ASP:OD1	17:8:145:TYR:N	2.38	0.45
19:A:151:VAL:O	19:A:155:THR:HG23	2.16	0.45
19:A:299:GLY:O	20:C:391:SER:OG	2.27	0.45
21:D:29:PHE:O	21:D:128:ARG:NH1	2.46	0.45
28:g:304:NEX:C36	25:g:308:CLA:CHC	2.94	0.45
12:u:166:GLY:HA2	24:u:312:CHL:HMC	1.97	0.45
17:y:132:CYS:HB3	12:p:51:ASP:OD2	2.16	0.45
19:a:151:VAL:O	19:a:155:THR:HG23	2.16	0.45
20:c:365:LEU:HD12	20:c:365:LEU:H	1.81	0.45
11:2:85:VAL:HG21	11:2:88:LYS:HE3	1.99	0.45
28:G:304:NEX:C36	25:G:308:CLA:HAB	2.46	0.45
28:G:304:NEX:H401	28:G:304:NEX:H35	1.58	0.45
24:G:305:CHL:H62	24:G:305:CHL:H102	1.82	0.45
20:C:104:VAL:HG11	31:C:613:8CT:C05	2.47	0.45
33:D:411:LMG:H141	33:D:411:LMG:H171	1.77	0.45
11:5:21:PRO:HG2	11:5:35:ASP:HB3	1.98	0.45
12:u:100:LEU:O	12:u:104:LEU:N	2.28	0.45
12:u:145:ILE:H	12:u:145:ILE:HD12	1.82	0.45
17:n:168:LYS:HD3	25:n:315:CLA:HBD	1.98	0.45
24:n:305:CHL:H93	25:n:306:CLA:HHB	1.99	0.45
17:y:162:PHE:CE2	17:y:166:LYS:HD2	2.52	0.45
25:y:315:CLA:H112	25:y:315:CLA:H72	1.58	0.45
25:b:614:CLA:H41	25:b:614:CLA:H61	1.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:d:401:LMG:H141	33:d:401:LMG:H111	1.64	0.45
12:7:90:ARG:NH1	24:7:312:CHL:OBD	2.38	0.45
8:R:53:ARG:NH1	8:R:64:ASP:OD2	2.50	0.45
30:1:318:LHG:H142	30:1:318:LHG:H172	1.91	0.45
13:S:129:TRP:CE2	24:S:607:CHL:HED2	2.52	0.45
17:Y:116:ILE:HG12	24:Y:308:CHL:HAC1	1.98	0.45
17:Y:211:PHE:HB3	17:8:94:PHE:HZ	1.81	0.45
18:B:333:GLY:O	18:B:439:SER:HB3	2.17	0.45
25:B:604:CLA:H71	25:B:604:CLA:H112	1.67	0.45
21:D:51:GLY:HA3	21:D:78:VAL:HG22	1.98	0.45
7:m:17:ILE:HB	7:m:18:PRO:HD3	1.99	0.45
28:5:304:NEX:H362	25:5:308:CLA:C3B	2.46	0.45
12:u:55:TYR:OH	12:u:67:ASP:OD2	2.22	0.45
12:u:129:GLY:O	12:u:143:GLN:NE2	2.45	0.45
25:u:315:CLA:H72	25:u:316:CLA:ND	2.32	0.45
28:n:303:NEX:H35	28:n:303:NEX:H401	1.76	0.45
25:y:307:CLA:H12	12:p:71:LEU:HD11	1.99	0.45
25:p:314:CLA:H43	25:p:316:CLA:HBA1	1.98	0.45
17:q:61:MET:SD	25:q:312:CLA:HAB	2.56	0.45
20:c:267:ILE:HD13	25:c:609:CLA:HED2	1.98	0.45
12:7:92:ALA:O	12:7:96:THR:HG22	2.17	0.45
28:2:304:NEX:H173	17:N:152:PRO:HB2	1.97	0.45
25:3:307:CLA:CBA	28:3:318:NEX:H241	2.47	0.45
24:3:309:CHL:HAA1	28:3:318:NEX:H381	1.98	0.45
17:G:162:PHE:CE2	17:G:166:LYS:HD2	2.51	0.45
18:B:346:PHE:HB2	18:B:354:LEU:O	2.17	0.45
25:B:609:CLA:H142	25:B:612:CLA:H72	1.99	0.45
25:C:601:CLA:H2A	25:C:601:CLA:O1D	2.16	0.45
21:D:55:ILE:O	21:D:66:SER:HB3	2.17	0.45
21:D:87:HIS:CD2	21:D:87:HIS:H	2.35	0.45
21:D:87:HIS:CE1	21:D:162:LEU:HA	2.51	0.45
4:i:9:TYR:HD2	22:w:88:LEU:HD11	1.82	0.45
7:m:3:VAL:HG22	33:m:101:LMG:O3	2.17	0.45
28:u:304:NEX:H15	28:u:304:NEX:H201	1.62	0.45
17:n:168:LYS:O	17:n:172:ASN:ND2	2.26	0.45
17:y:110:ALA:HA	24:y:309:CHL:CHC	2.47	0.45
17:y:126:LEU:O	17:y:130:TYR:N	2.40	0.45
28:y:304:NEX:H11	28:y:304:NEX:H191	1.82	0.45
28:p:304:NEX:H11	28:p:304:NEX:H191	1.82	0.45
18:b:153:PHE:O	18:b:158:VAL:HG23	2.17	0.45
25:b:602:CLA:H11	25:b:602:CLA:H52	1.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:a:227:THR:OG1	19:a:228:THR:N	2.50	0.45
20:c:59:GLU:O	20:c:63:PHE:HB2	2.17	0.45
20:c:408:VAL:H	37:c:618:DGD:HE3	1.79	0.45
25:c:601:CLA:H2A	25:c:601:CLA:O1D	2.16	0.45
30:d:408:LHG:H112	30:d:408:LHG:HC81	1.40	0.45
24:r:303:CHL:HBB2	27:r:316:XAT:H32	1.98	0.45
12:7:133:TYR:HE1	28:7:304:NEX:H241	1.81	0.45
12:7:174:ASP:OD1	12:7:176:LEU:N	2.42	0.45
28:7:304:NEX:C32	24:7:310:CHL:HBA1	2.43	0.45
35:A:606:PHO:H141	35:A:606:PHO:H161	1.69	0.45
20:C:151:ILE:HD13	25:C:616:CLA:HAB	1.99	0.45
12:6:143:GLN:N	24:6:308:CHL:OMC	2.44	0.45
24:y:305:CHL:HBA1	24:y:305:CHL:H3A	1.64	0.45
12:p:195:SER:C	12:p:197:LEU:H	2.23	0.45
18:b:70:GLY:HA2	18:b:178:VAL:HG21	1.98	0.45
20:c:228:ILE:H	20:c:228:ILE:HG12	1.63	0.45
8:r:65:ARG:NH2	8:r:230:GLU:OE2	2.50	0.45
12:7:91:TRP:CE2	24:7:312:CHL:HED2	2.52	0.45
8:R:135:ARG:HD2	24:R:607:CHL:OBD	2.17	0.45
24:3:309:CHL:CAA	28:3:318:NEX:C28	2.92	0.45
13:S:69:ASP:OD1	13:S:69:ASP:N	2.49	0.45
12:9:98:GLY:H	12:9:101:THR:HG23	1.82	0.45
24:Y:304:CHL:HHB	24:8:310:CHL:HMB3	1.99	0.45
25:B:606:CLA:H102	25:B:606:CLA:H61	1.67	0.45
20:C:59:GLU:O	20:C:63:PHE:HB2	2.16	0.45
33:m:101:LMG:O4	18:b:328:GLY:HA3	2.17	0.45
11:5:123:ILE:HG23	28:5:304:NEX:C15	2.46	0.45
28:6:303:NEX:H31	24:6:309:CHL:HBA2	1.99	0.45
28:n:303:NEX:H15	28:n:303:NEX:H201	1.86	0.45
17:y:158:ASP:HB3	17:y:161:THR:HG22	1.99	0.45
24:y:306:CHL:H142	24:y:306:CHL:H112	1.67	0.45
12:p:174:ASP:OD1	12:p:176:LEU:N	2.43	0.45
18:b:326:ARG:HH21	21:d:297:ASP:CG	2.24	0.45
25:c:612:CLA:OBD	13:s:81:PRO:HB2	2.17	0.45
35:d:403:PHO:H41	35:d:403:PHO:H61	1.45	0.45
13:s:232:GLY:HA2	13:s:236:ASP:HB2	1.99	0.45
24:7:306:CHL:H111	24:7:306:CHL:H91	1.77	0.45
28:2:304:NEX:H362	25:2:308:CLA:C3B	2.47	0.45
28:G:304:NEX:H11	28:G:304:NEX:H191	1.82	0.45
25:G:314:CLA:H43	25:G:316:CLA:HBA1	1.98	0.45
17:N:110:ALA:O	17:N:111:GLN:NE2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:278:TRP:HB3	19:A:279:PRO:HD3	1.98	0.45
33:C:618:LMG:H331	33:C:618:LMG:H362	1.48	0.45
6:l:27:VAL:HG21	30:a:601:LHG:H192	1.98	0.45
10:4:12:LEU:HA	24:4:304:CHL:NB	2.32	0.45
11:5:85:VAL:HG21	11:5:88:LYS:HE3	1.99	0.45
12:6:91:TRP:CE2	24:6:311:CHL:HED2	2.51	0.45
17:g:110:ALA:HA	24:g:309:CHL:CHC	2.47	0.45
28:g:304:NEX:C28	24:g:310:CHL:HAA1	2.47	0.45
12:u:212:MET:HE2	12:u:212:MET:HB2	1.85	0.45
17:n:137:LEU:HG	24:n:311:CHL:HBB1	1.99	0.45
17:y:189:GLN:OE1	26:y:303:OIE:O40	2.35	0.45
28:p:304:NEX:C38	25:p:308:CLA:CHB	2.93	0.45
18:b:132:ALA:HB2	8:r:83:ILE:HD13	1.99	0.45
19:a:278:TRP:HB3	19:a:279:PRO:HD3	1.98	0.45
21:d:110:LEU:HD12	21:d:110:LEU:HA	1.77	0.45
28:7:304:NEX:C38	25:7:308:CLA:C1B	2.84	0.45
8:R:41:LYS:O	8:R:43:SER:N	2.50	0.44
10:1:13:GLY:O	10:1:16:SER:OG	2.35	0.44
17:G:17:GLU:OE1	17:G:17:GLU:N	2.47	0.44
28:G:304:NEX:H15	24:G:312:CHL:HMB3	1.98	0.44
12:9:91:TRP:CD1	24:9:312:CHL:HMD3	2.51	0.44
28:N:303:NEX:H35	28:N:303:NEX:H401	1.75	0.44
18:B:61:PHE:HE1	18:B:451:PHE:HB2	1.82	0.44
25:C:604:CLA:HAA2	37:C:619:DGD:HD61	1.99	0.44
35:D:403:PHO:H72	25:D:404:CLA:H111	1.99	0.44
17:g:168:LYS:HD3	25:g:316:CLA:HAA2	1.97	0.44
17:n:54:LEU:HD23	17:n:55:ILE:HD13	1.98	0.44
18:b:462:PHE:HA	25:b:611:CLA:HMC1	1.99	0.44
19:a:38:LEU:HB3	19:a:39:PRO:HD3	1.99	0.44
13:s:58:TRP:C	13:s:60:GLY:N	2.75	0.44
13:s:175:TRP:HE1	25:s:417:CLA:C4B	2.30	0.44
8:R:156:GLN:H	8:R:156:GLN:HG3	1.40	0.44
24:G:306:CHL:H92	24:G:306:CHL:H62	1.70	0.44
25:9:307:CLA:H42	24:9:309:CHL:HBD	1.98	0.44
5:k:23:PRO:O	5:k:26:PRO:HD2	2.17	0.44
12:6:57:THR:OG1	12:6:59:GLU:OE1	2.24	0.44
17:n:54:LEU:HD21	17:n:58:ARG:CZ	2.46	0.44
25:r:313:CLA:HBA2	25:r:313:CLA:H3A	1.61	0.44
12:7:162:TYR:HB3	24:7:312:CHL:CMC	2.47	0.44
28:R:616:NEX:H35	28:R:616:NEX:H401	1.58	0.44
28:1:303:NEX:H401	28:1:303:NEX:H35	1.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:3:191:PRO:HA	12:3:194:PHE:HB3	1.99	0.44
25:G:317:CLA:H61	25:G:317:CLA:H2	1.73	0.44
12:9:91:TRP:O	12:9:95:GLY:N	2.51	0.44
18:B:315:ILE:HG22	18:B:426:LEU:HB3	1.98	0.44
25:B:605:CLA:HBC3	25:B:606:CLA:H42	1.99	0.44
33:B:619:LMG:H161	33:B:619:LMG:H132	1.58	0.44
12:u:158:LEU:CD2	28:u:304:NEX:H203	2.26	0.44
28:u:304:NEX:H401	28:u:304:NEX:H35	1.58	0.44
25:b:613:CLA:H143	25:b:613:CLA:H111	1.75	0.44
25:b:615:CLA:H8	25:b:616:CLA:HBB1	1.99	0.44
20:c:178:ALA:HB3	20:c:182:GLY:HA2	1.99	0.44
8:r:135:ARG:HD2	24:r:308:CHL:OBD	2.17	0.44
8:R:128:GLU:O	8:R:132:ILE:HG12	2.18	0.44
25:R:604:CLA:HMB1	24:R:605:CHL:HBB1	2.00	0.44
11:2:106:GLU:CD	11:2:106:GLU:H	2.26	0.44
13:S:175:TRP:HE1	25:S:616:CLA:C4B	2.30	0.44
12:9:53:PRO:HG3	12:9:67:ASP:HB3	1.99	0.44
24:9:305:CHL:HBB1	24:9:305:CHL:H51	1.99	0.44
25:9:316:CLA:H11	25:9:316:CLA:C4D	2.48	0.44
25:N:306:CLA:HAC1	24:N:310:CHL:HBB2	2.00	0.44
25:A:603:CLA:HBB1	25:A:603:CLA:HMB3	2.00	0.44
25:C:604:CLA:H71	37:C:619:DGD:HBT1	1.99	0.44
3:h:66:ILE:HD11	18:b:187:ALA:O	2.18	0.44
17:g:93:ILE:HG12	17:g:113:ILE:HB	1.99	0.44
17:n:24:LEU:HD12	17:n:24:LEU:H	1.81	0.44
17:n:59:TRP:CE2	24:n:311:CHL:HED2	2.52	0.44
17:y:194:PRO:O	29:y:301:OUR:O39	2.35	0.44
12:p:92:ALA:O	12:p:96:THR:HG22	2.18	0.44
25:b:601:CLA:HBB1	25:b:602:CLA:CHC	2.47	0.44
21:d:236:ASN:HB3	21:d:239:GLN:HB3	2.00	0.44
13:s:174:PRO:HG3	25:s:417:CLA:NA	2.33	0.44
8:R:160:GLU:N	24:R:606:CHL:O1D	2.49	0.44
28:1:303:NEX:H362	25:1:307:CLA:CAB	2.48	0.44
12:3:133:TYR:HE1	28:3:318:NEX:H1	1.64	0.44
13:S:162:MET:O	13:S:163:LEU:C	2.60	0.44
13:S:188:ALA:O	13:S:192:VAL:HG23	2.17	0.44
25:9:307:CLA:HBA2	25:9:307:CLA:H3A	1.57	0.44
17:Y:147:GLY:C	17:Y:149:ALA:H	2.26	0.44
18:B:53:ASN:ND2	18:B:53:ASN:O	2.50	0.44
25:B:612:CLA:H141	25:B:612:CLA:H161	1.75	0.44
25:B:615:CLA:H8	25:B:616:CLA:HBB1	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:D:203:GLY:HA3	21:D:278:GLY:HA3	1.99	0.44
24:n:305:CHL:H92	24:n:305:CHL:H62	1.72	0.44
25:b:609:CLA:H193	25:b:612:CLA:H141	1.98	0.44
13:s:198:ALA:HA	13:s:201:TYR:CD2	2.53	0.44
8:r:48:MET:HE3	8:r:48:MET:HB2	1.81	0.44
7:M:17:ILE:HB	7:M:18:PRO:HD3	1.98	0.44
12:3:91:TRP:CE2	24:3:311:CHL:HED2	2.53	0.44
12:9:86:VAL:HG21	12:9:176:LEU:HD13	1.99	0.44
12:9:117:VAL:HG23	12:9:118:TRP:H	1.83	0.44
12:9:145:ILE:H	12:9:145:ILE:HD12	1.82	0.44
17:Y:120:GLN:OE1	24:Y:310:CHL:HMC	2.17	0.44
17:8:40:SER:OG	24:8:304:CHL:HAA2	2.17	0.44
17:8:147:GLY:C	17:8:149:ALA:H	2.25	0.44
19:A:281:VAL:HG13	32:A:609:SQD:H182	1.98	0.44
25:C:607:CLA:H142	25:C:607:CLA:H111	1.82	0.44
10:4:10:LEU:HB2	10:4:16:SER:HB3	2.00	0.44
24:4:304:CHL:OBD	24:4:305:CHL:HHD	2.17	0.44
12:6:122:GLY:HA2	24:6:309:CHL:HAC2	1.99	0.44
17:n:186:GLN:O	17:n:190:THR:OG1	2.24	0.44
24:n:304:CHL:H3A	24:n:304:CHL:HBA1	1.69	0.44
25:n:306:CLA:HAC1	24:n:310:CHL:HBB2	2.00	0.44
12:p:80:GLN:H	12:p:80:GLN:HG2	1.45	0.44
12:p:100:LEU:O	12:p:104:LEU:N	2.29	0.44
17:q:147:GLY:C	17:q:149:ALA:H	2.25	0.44
18:b:333:GLY:O	18:b:439:SER:HB3	2.17	0.44
19:a:55:ALA:O	19:a:70:SER:OG	2.28	0.44
13:s:141:GLU:CD	13:s:280:TYR:HB3	2.41	0.44
28:s:401:NEX:H35	28:s:401:NEX:H401	1.76	0.44
25:s:413:CLA:H2	24:s:414:CHL:HMD1	1.98	0.44
12:7:186:ASN:OD1	12:7:186:ASN:N	2.50	0.44
10:1:134:GLY:HA2	24:1:311:CHL:HAC1	2.00	0.44
28:2:304:NEX:H163	17:N:153:MET:HG2	2.00	0.44
12:3:122:GLY:HA2	24:3:309:CHL:HAC2	1.98	0.44
13:S:231:PRO:HB3	24:S:607:CHL:HBC2	1.99	0.44
13:S:232:GLY:HA2	13:S:236:ASP:HB2	2.00	0.44
24:G:306:CHL:H143	24:G:306:CHL:H112	1.73	0.44
25:9:314:CLA:H61	25:9:314:CLA:H41	1.45	0.44
25:8:305:CLA:HED1	24:8:310:CHL:H92	2.00	0.44
25:B:614:CLA:H41	25:B:614:CLA:H61	1.47	0.44
19:A:68:SER:OG	19:A:69:GLY:N	2.51	0.44
35:A:606:PHO:H61	35:A:606:PHO:H2	1.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:C:610:CLA:O2A	25:C:610:CLA:H2A	2.18	0.44
1:z:41:PHE:CZ	13:s:84:LEU:HG	2.53	0.44
3:h:67:ALA:HB3	3:h:72:SER:HB3	1.99	0.44
11:5:120:GLN:HE21	24:5:313:CHL:HMC	1.82	0.44
28:6:303:NEX:H31	24:6:309:CHL:HBA1	2.00	0.44
24:n:304:CHL:ND	30:n:318:LHG:HC82	2.33	0.44
12:p:105:LEU:O	12:p:111:VAL:HG13	2.17	0.44
17:q:135:GLY:H	24:q:310:CHL:CMC	2.31	0.44
18:b:53:ASN:ND2	18:b:53:ASN:O	2.50	0.44
13:s:268:PHE:HD2	13:s:279:PRO:HG2	1.83	0.44
8:r:76:VAL:O	8:r:104:THR:OG1	2.36	0.44
12:7:180:GLU:C	12:7:182:PHE:H	2.25	0.44
5:K:40:VAL:HG11	5:K:43:ARG:CZ	2.48	0.44
13:S:81:PRO:HB2	25:C:612:CLA:OBD	2.18	0.44
13:S:198:ALA:HA	13:S:201:TYR:CD2	2.53	0.44
24:N:304:CHL:ND	30:N:318:LHG:HC82	2.32	0.44
24:Y:312:CHL:H92	24:Y:312:CHL:H62	1.70	0.44
17:8:12:LEU:HD23	24:8:303:CHL:HHB	1.99	0.44
18:B:63:LEU:HD12	18:B:66:MET:HE3	2.00	0.44
18:B:228:ALA:HA	33:D:411:LMG:HC71	1.99	0.44
25:B:604:CLA:H93	25:B:604:CLA:H61	1.77	0.44
20:C:210:GLY:HA3	20:C:214:SER:HB3	1.98	0.44
12:6:209:MET:HB2	24:6:305:CHL:HMC	2.00	0.44
12:u:84:LEU:O	12:u:88:HIS:ND1	2.48	0.44
17:y:120:GLN:OE1	24:y:311:CHL:HMC	2.17	0.44
24:y:305:CHL:HHB	24:q:311:CHL:HMB3	2.00	0.44
17:q:40:SER:OG	24:q:304:CHL:HAA2	2.18	0.44
22:w:75:ARG:H	22:w:75:ARG:HD2	1.83	0.44
20:c:45:ALA:O	20:c:49:VAL:HG23	2.17	0.44
25:c:604:CLA:H71	37:c:618:DGD:HBT1	1.99	0.44
21:d:199:MET:HE3	21:d:281:MET:HB3	1.99	0.44
1:Z:41:PHE:CZ	13:S:84:LEU:HG	2.53	0.44
3:H:13:THR:HG23	3:H:16:GLY:H	1.83	0.44
8:R:213:ASP:O	8:R:216:ASN:ND2	2.51	0.44
24:S:601:CHL:H3A	24:S:601:CHL:HBA1	1.56	0.44
28:S:617:NEX:H401	28:S:617:NEX:H35	1.57	0.44
17:G:104:ASN:HB3	17:G:107:LEU:HD23	1.98	0.44
25:B:612:CLA:H41	25:B:612:CLA:H61	1.44	0.44
20:C:385:THR:HG1	20:C:386:HIS:CE1	2.36	0.44
25:C:601:CLA:H143	25:C:601:CLA:H162	1.84	0.44
33:C:618:LMG:H151	33:C:618:LMG:H122	1.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:4:51:GLU:HG3	10:4:144:LEU:HD21	2.00	0.44
28:6:303:NEX:H28	24:6:309:CHL:CAA	2.48	0.44
25:6:316:CLA:H3A	25:6:316:CLA:HBA2	1.71	0.44
24:g:305:CHL:H12	24:g:305:CHL:H51	1.77	0.44
24:n:308:CHL:HAA2	25:r:313:CLA:H3A	2.00	0.44
25:q:306:CLA:C3B	28:s:401:NEX:H383	2.48	0.44
25:a:604:CLA:CHA	25:a:604:CLA:HBA1	2.46	0.44
20:c:151:ILE:HD13	25:c:616:CLA:HAB	2.00	0.44
13:s:199:GLU:HG2	24:s:409:CHL:CHB	2.48	0.44
1:Z:33:TRP:O	1:Z:37:LYS:HB2	2.18	0.43
2:E:73:TYR:CD1	2:E:80:ARG:HG2	2.53	0.43
8:R:244:LEU:O	8:R:248:VAL:HG22	2.16	0.43
11:2:147:GLY:C	11:2:149:ALA:H	2.24	0.43
17:G:59:TRP:CD1	24:G:313:CHL:HMD3	2.53	0.43
28:G:304:NEX:C15	24:G:312:CHL:HMB2	2.44	0.43
24:G:313:CHL:H91	24:G:313:CHL:H111	1.76	0.43
17:Y:132:CYS:HB3	12:7:51:ASP:OD2	2.17	0.43
25:B:601:CLA:HBB1	25:B:602:CLA:CHC	2.48	0.43
20:C:132:PHE:CE1	25:C:612:CLA:HAA1	2.53	0.43
20:C:285:TYR:O	20:C:411:ARG:NH2	2.50	0.43
35:D:403:PHO:H41	35:D:403:PHO:H61	1.44	0.43
11:5:12:LEU:HB2	11:5:16:SER:HB3	2.00	0.43
12:u:102:PRO:O	12:u:116:PRO:HB2	2.18	0.43
12:u:218:GLN:O	12:u:222:THR:OG1	2.25	0.43
17:n:40:SER:HA	17:n:45:THR:HG23	2.00	0.43
17:y:211:PHE:HB3	17:q:94:PHE:HZ	1.82	0.43
25:b:606:CLA:H61	25:b:606:CLA:H102	1.62	0.43
19:a:259:ILE:HD12	19:a:263:ALA:HB3	1.99	0.43
25:d:405:CLA:H143	25:d:405:CLA:H161	1.78	0.43
28:r:317:NEX:H11	28:r:317:NEX:H191	1.82	0.43
25:7:314:CLA:H43	25:7:316:CLA:HBA1	2.00	0.43
3:H:58:ASN:C	3:H:59:SER:HG	2.25	0.43
10:1:54:LEU:HD23	10:1:144:LEU:HB3	1.99	0.43
11:2:59:TRP:CE2	24:2:312:CHL:HED2	2.53	0.43
25:2:315:CLA:H111	25:2:315:CLA:H72	1.72	0.43
12:3:213:PHE:HD1	25:3:306:CLA:HBB2	1.82	0.43
17:G:49:ASN:ND2	24:G:306:CHL:H3A	2.34	0.43
21:D:242:GLU:OE1	21:D:264:LYS:NZ	2.32	0.43
17:g:162:PHE:CE2	17:g:166:LYS:HD2	2.53	0.43
24:g:305:CHL:H62	24:g:305:CHL:H102	1.82	0.43
12:u:45:GLY:O	12:u:48:SER:OG	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:u:165:SER:OG	17:n:15:TYR:O	2.30	0.43
17:q:136:PRO:HG3	13:s:58:TRP:CG	2.53	0.43
17:q:168:LYS:HD3	25:q:314:CLA:HAA2	2.00	0.43
24:q:303:CHL:H41	24:q:303:CHL:H61	1.61	0.43
20:c:104:VAL:HG11	31:c:613:8CT:C05	2.48	0.43
25:c:610:CLA:O2A	25:c:610:CLA:H2A	2.18	0.43
13:s:188:ALA:O	13:s:192:VAL:HG23	2.18	0.43
30:7:319:LHG:H242	30:7:319:LHG:H272	1.71	0.43
30:9:318:LHG:H122	30:9:318:LHG:HC91	1.82	0.43
17:N:134:GLY:HA2	24:N:311:CHL:HAC1	1.98	0.43
17:8:53:GLU:HB2	24:8:304:CHL:CHB	2.48	0.43
20:C:83:LEU:HD13	25:C:602:CLA:H143	2.00	0.43
20:C:151:ILE:HG21	25:C:616:CLA:C3B	2.48	0.43
21:D:148:ALA:HB1	21:D:279:LEU:HB2	2.00	0.43
1:z:33:TRP:O	1:z:37:LYS:HB2	2.18	0.43
28:4:303:NEX:H221	25:4:307:CLA:C1C	2.48	0.43
24:g:318:CHL:HBD	17:n:118:TRP:HE1	1.83	0.43
12:u:147:ALA:HB3	24:u:309:CHL:HMC	2.00	0.43
25:n:316:CLA:H3A	25:n:316:CLA:HBA2	1.81	0.43
17:y:15:TYR:O	17:q:133:SER:OG	2.24	0.43
18:b:61:PHE:HE1	18:b:451:PHE:HB2	1.81	0.43
19:a:68:SER:HB3	21:d:313:THR:HG22	2.01	0.43
35:a:606:PHO:H161	35:a:606:PHO:H141	1.70	0.43
13:s:58:TRP:NE1	28:s:401:NEX:C19	2.77	0.43
8:r:128:GLU:O	8:r:132:ILE:HG12	2.17	0.43
12:7:83:GLU:HA	12:7:176:LEU:HD11	2.00	0.43
26:7:302:OIE:C13	24:7:306:CHL:HMC	2.48	0.43
5:K:23:PRO:O	5:K:26:PRO:HD2	2.17	0.43
11:2:218:LYS:HE3	11:2:221:PHE:H	1.84	0.43
24:9:304:CHL:H3A	24:9:304:CHL:HBA1	1.62	0.43
17:N:147:GLY:C	17:N:149:ALA:H	2.27	0.43
19:A:114:LEU:O	19:A:118:HIS:ND1	2.46	0.43
20:C:431:TRP:HH2	30:D:408:LHG:HC62	1.84	0.43
33:m:101:LMG:H121	25:b:608:CLA:ND	2.33	0.43
11:5:106:GLU:CD	11:5:106:GLU:H	2.26	0.43
12:6:183:ASP:OD1	12:6:186:ASN:HA	2.17	0.43
17:g:101:TYR:CE2	28:g:304:NEX:O23	2.68	0.43
24:y:312:CHL:C4A	24:y:312:CHL:HBA2	2.47	0.43
12:p:113:LEU:HD21	12:p:134:LEU:HD23	2.00	0.43
12:p:162:TYR:HB3	24:p:312:CHL:CMC	2.46	0.43
12:p:195:SER:O	12:p:196:GLU:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:b:63:LEU:HD12	18:b:66:MET:HE3	2.00	0.43
18:b:80:ILE:HD13	18:b:80:ILE:HA	1.89	0.43
19:a:225:ARG:HD2	19:a:225:ARG:N	2.33	0.43
19:a:246:TYR:CE2	19:a:248:ILE:HG12	2.54	0.43
20:c:132:PHE:CE1	25:c:612:CLA:HAA1	2.54	0.43
20:c:151:ILE:HG21	25:c:616:CLA:C3B	2.48	0.43
37:c:619:DGD:HB91	37:c:619:DGD:HB62	1.36	0.43
5:K:28:LEU:HB3	31:V:401:8CT:C18	2.49	0.43
11:2:54:LEU:HD23	11:2:144:LEU:HD22	2.00	0.43
13:S:174:PRO:HG3	25:S:616:CLA:NA	2.33	0.43
25:S:612:CLA:H2	24:S:613:CHL:HMD1	2.00	0.43
17:N:39:LEU:HD12	24:N:305:CHL:H11	1.99	0.43
24:N:304:CHL:H41	24:N:304:CHL:H61	1.74	0.43
17:Y:136:PRO:CG	28:r:301:NEX:H192	2.49	0.43
18:B:463:PHE:CE1	33:D:401:LMG:H421	2.54	0.43
25:A:604:CLA:H111	25:A:604:CLA:H151	1.89	0.43
20:C:178:ALA:HB3	20:C:182:GLY:HA2	2.01	0.43
20:C:439:ALA:HA	20:C:444:GLU:HB3	2.00	0.43
21:D:123:ILE:HD11	33:D:401:LMG:H392	2.00	0.43
25:5:315:CLA:H72	25:5:315:CLA:H111	1.73	0.43
17:n:178:PHE:HE2	25:n:316:CLA:HAB	1.83	0.43
17:y:188:LEU:HD12	17:y:218:PHE:HD2	1.84	0.43
12:p:216:PHE:O	12:p:220:ILE:HG13	2.18	0.43
18:b:433:ASP:OD1	18:b:433:ASP:N	2.48	0.43
19:a:10:GLY:HA3	19:a:15:GLU:CD	2.43	0.43
25:c:602:CLA:H92	25:c:602:CLA:H61	1.77	0.43
13:s:212:ALA:O	13:s:214:GLY:N	2.44	0.43
8:r:109:VAL:HG22	8:r:111:THR:HG22	2.01	0.43
8:r:179:SER:O	8:r:183:TRP:HD1	2.02	0.43
8:R:86:LEU:HG	8:R:88:GLN:HG2	2.00	0.43
11:2:55:ILE:HG22	24:2:313:CHL:HMD2	1.98	0.43
12:3:40:ARG:NE	12:3:63:ASP:O	2.28	0.43
13:S:124:LEU:O	13:S:128:ARG:HG2	2.18	0.43
17:G:174:ARG:HA	17:G:177:MET:HE2	2.00	0.43
12:9:77:MET:O	12:9:80:GLN:NE2	2.52	0.43
28:9:319:NEX:H11	28:9:319:NEX:H191	1.82	0.43
24:Y:304:CHL:H3A	24:Y:304:CHL:HBA1	1.65	0.43
18:B:435:ALA:O	18:B:436:THR:OG1	2.28	0.43
18:B:435:ALA:C	18:B:437:LEU:H	2.27	0.43
25:B:615:CLA:H2	25:B:616:CLA:CBB	2.39	0.43
19:A:225:ARG:HD2	19:A:225:ARG:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:D:263:ASN:HB3	21:D:266:TRP:HB3	1.99	0.43
10:4:168:LYS:O	10:4:172:ASN:ND2	2.25	0.43
12:6:170:GLY:HA3	24:6:311:CHL:HBC3	1.99	0.43
12:u:43:TRP:CG	12:u:66:TRP:HB2	2.54	0.43
25:u:307:CLA:H92	25:u:307:CLA:H61	1.79	0.43
17:n:147:GLY:C	17:n:149:ALA:H	2.27	0.43
18:b:92:SER:OG	18:b:93:TYR:N	2.51	0.43
25:b:603:CLA:H161	25:b:603:CLA:H143	1.72	0.43
25:b:605:CLA:HBC3	25:b:606:CLA:H42	2.01	0.43
13:s:162:MET:O	13:s:163:LEU:C	2.60	0.43
2:E:103:GLU:HA	2:E:106:LYS:HB2	2.00	0.43
8:R:243:PHE:CZ	27:R:615:XAT:H10	2.54	0.43
13:S:268:PHE:HD2	13:S:279:PRO:HG2	1.83	0.43
25:B:605:CLA:H61	25:B:605:CLA:H92	1.81	0.43
20:C:139:TRP:O	20:C:259:TYR:OH	2.36	0.43
25:C:610:CLA:H151	25:C:610:CLA:H112	1.54	0.43
33:m:101:LMG:H291	33:m:101:LMG:H322	1.56	0.43
9:f:25:VAL:HB	9:f:26:PRO:HD3	1.99	0.43
10:4:58:ARG:HA	10:4:61:MET:HE3	2.01	0.43
11:5:11:TRP:HZ3	24:5:305:CHL:HAA1	1.84	0.43
11:5:106:GLU:HG3	8:r:258:PHE:HD1	1.83	0.43
12:6:148:ILE:HA	12:6:151:ILE:HG22	2.00	0.43
12:6:200:LYS:HD3	25:6:315:CLA:HAA2	2.01	0.43
17:y:168:LYS:HD3	25:y:316:CLA:HBD	2.00	0.43
17:q:53:GLU:HB2	24:q:304:CHL:CHB	2.49	0.43
24:q:311:CHL:HBB1	24:q:311:CHL:HHC	2.00	0.43
25:b:602:CLA:HED3	25:b:603:CLA:H3A	2.00	0.43
19:a:273:PHE:CE1	30:d:408:LHG:HC61	2.54	0.43
25:a:604:CLA:H111	25:a:604:CLA:H151	1.90	0.43
20:c:439:ALA:HA	20:c:444:GLU:HB3	2.00	0.43
25:r:305:CLA:CHC	28:r:317:NEX:H362	2.49	0.43
12:7:101:THR:HA	12:7:104:LEU:HG	2.01	0.43
24:7:306:CHL:H143	24:7:306:CHL:H112	1.66	0.43
8:R:255:GLU:HG3	25:R:612:CLA:HED1	2.00	0.43
10:1:33:GLY:N	24:1:305:CHL:OBD	2.51	0.43
12:3:76:GLU:H	12:3:76:GLU:CD	2.26	0.43
13:S:199:GLU:CD	13:S:202:ARG:HH12	2.26	0.43
17:G:53:GLU:OE2	17:G:174:ARG:NE	2.37	0.43
17:G:124:MET:HE1	28:G:304:NEX:H32	2.00	0.43
24:G:313:CHL:H43	24:9:304:CHL:H2	2.00	0.43
17:8:52:LEU:O	17:8:56:HIS:ND1	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:8:312:CLA:H112	25:8:312:CLA:H72	1.71	0.43
25:C:601:CLA:H161	25:C:607:CLA:HMB3	2.00	0.43
17:g:27:GLU:OE1	17:g:27:GLU:N	2.50	0.43
25:q:305:CLA:HED1	24:q:311:CHL:H92	2.00	0.43
25:q:313:CLA:H143	25:q:313:CLA:H161	1.88	0.43
25:b:612:CLA:H141	25:b:612:CLA:H161	1.76	0.43
32:a:609:SQD:H292	32:a:609:SQD:H261	1.74	0.43
21:d:203:GLY:HA3	21:d:278:GLY:HA3	2.01	0.43
13:s:182:LEU:HD22	13:s:186:VAL:HG11	2.01	0.43
8:r:156:GLN:H	8:r:156:GLN:HG3	1.52	0.43
3:H:66:ILE:HD11	18:B:187:ALA:O	2.18	0.43
28:1:303:NEX:H11	28:1:303:NEX:H191	1.82	0.43
17:N:54:LEU:HD21	17:N:58:ARG:CZ	2.48	0.43
25:C:603:CLA:H193	25:C:603:CLA:H161	1.68	0.43
3:h:20:SER:N	3:h:21:PRO:HD2	2.33	0.43
4:i:28:PRO:O	4:i:31:ASN:ND2	2.49	0.43
33:m:101:LMG:H161	25:b:608:CLA:H2	2.00	0.43
10:4:168:LYS:HE3	25:4:314:CLA:HED2	2.00	0.43
11:5:59:TRP:CE2	24:5:312:CHL:HED2	2.54	0.43
11:5:123:ILE:CG2	28:5:304:NEX:C34	2.97	0.43
28:u:304:NEX:H30	24:u:312:CHL:HMA2	2.00	0.43
17:n:32:TYR:HB2	24:n:305:CHL:HMD3	2.01	0.43
17:n:151:ASP:OD1	29:n:301:OUR:O40	2.36	0.43
12:p:180:GLU:C	12:p:182:PHE:H	2.27	0.43
26:p:302:OIE:C13	24:p:306:CHL:HMC	2.49	0.43
18:b:464:PHE:HB2	21:d:280:TRP:CZ2	2.54	0.43
20:c:296:GLU:OE2	20:c:353:TRP:NE1	2.42	0.43
24:s:402:CHL:H3A	24:s:402:CHL:HBA1	1.52	0.43
12:7:44:LEU:HB2	12:7:48:SER:HB3	2.01	0.43
12:7:133:TYR:CE1	25:7:308:CLA:H2	2.54	0.43
8:R:88:GLN:HB3	19:A:230:ASN:HB3	2.01	0.43
8:R:109:VAL:HG22	8:R:111:THR:HG22	2.00	0.43
24:9:312:CHL:H2A	24:9:312:CHL:HED3	1.99	0.43
17:Y:110:ALA:HA	24:Y:308:CHL:CHC	2.49	0.43
17:8:168:LYS:HD3	25:8:313:CLA:HAA2	2.01	0.43
24:8:303:CHL:H3A	24:8:303:CHL:HBA1	1.45	0.43
18:B:462:PHE:HA	25:B:611:CLA:HMC1	2.00	0.43
19:A:140:ARG:HA	19:A:141:PRO:HD3	1.89	0.43
21:D:32:TRP:CD1	33:D:411:LMG:H152	2.54	0.43
21:D:153:PHE:CE1	35:D:403:PHO:H91	2.54	0.43
12:u:206:ARG:HA	12:u:209:MET:HE2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:n:312:CHL:H92	24:n:312:CHL:H62	1.73	0.43
17:y:147:GLY:C	17:y:149:ALA:H	2.26	0.43
12:p:44:LEU:HB2	12:p:48:SER:HB3	1.99	0.43
21:d:343:GLU:H	21:d:343:GLU:CD	2.27	0.43
8:r:44:ASP:OD1	8:r:44:ASP:N	2.52	0.43
12:7:45:GLY:O	12:7:48:SER:OG	2.37	0.43
8:R:86:LEU:HD13	18:B:13:LEU:HD23	2.00	0.42
25:R:612:CLA:H3A	25:R:612:CLA:HBA2	1.78	0.42
12:3:168:PRO:HG2	24:3:311:CHL:HBB2	2.01	0.42
17:N:104:ASN:HD22	17:N:107:LEU:HD13	1.84	0.42
17:Y:8:ARG:NE	17:Y:31:ASP:O	2.37	0.42
25:B:608:CLA:H93	25:B:608:CLA:H62	1.76	0.42
10:4:54:LEU:HD23	10:4:144:LEU:HB3	2.01	0.42
11:5:218:LYS:HE3	11:5:221:PHE:H	1.84	0.42
12:u:183:ASP:OD1	12:u:183:ASP:N	2.51	0.42
25:y:317:CLA:H61	25:y:317:CLA:H2	1.60	0.42
28:p:304:NEX:H382	25:p:308:CLA:HBA2	2.01	0.42
24:q:304:CHL:HBB1	24:q:304:CHL:CHC	2.46	0.42
18:b:174:ILE:HA	18:b:308:LYS:HD2	2.01	0.42
19:a:149:ALA:HB1	19:a:283:ILE:HB	2.01	0.42
19:a:269:ARG:HE	21:d:235:PHE:HB2	1.84	0.42
13:s:175:TRP:NE1	25:s:417:CLA:HBB1	2.34	0.42
24:r:307:CHL:HBB1	24:r:307:CHL:HHC	2.01	0.42
7:M:24:ILE:HG22	7:M:25:LEU:HD23	2.00	0.42
25:R:604:CLA:HMA2	24:R:605:CHL:C3C	2.50	0.42
18:B:338:VAL:HB	18:B:431:GLU:CD	2.44	0.42
19:A:10:GLY:HA3	19:A:15:GLU:CD	2.43	0.42
19:A:246:TYR:CE2	19:A:248:ILE:HG12	2.53	0.42
21:D:343:GLU:H	21:D:343:GLU:CD	2.28	0.42
22:W:109:ASP:O	22:W:111:ASN:N	2.52	0.42
17:g:131:ARG:HA	24:g:312:CHL:C4C	2.49	0.42
17:g:162:PHE:CZ	17:g:166:LYS:HD2	2.54	0.42
12:u:85:GLU:HB2	24:u:306:CHL:CHB	2.49	0.42
12:u:87:ILE:HG13	12:u:91:TRP:HD1	1.83	0.42
25:u:308:CLA:H43	24:u:310:CHL:HAA2	2.01	0.42
24:p:311:CHL:HHC	24:p:311:CHL:HBB1	2.01	0.42
17:q:115:ALA:O	17:q:119:THR:OG1	2.27	0.42
20:c:139:TRP:O	20:c:259:TYR:OH	2.36	0.42
20:c:334:THR:OG1	20:c:336:GLU:OE1	2.35	0.42
25:c:603:CLA:H62	25:c:603:CLA:H41	1.90	0.42
13:s:230:TYR:HB3	25:s:410:CLA:HED2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:7:195:SER:O	12:7:196:GLU:HB2	2.19	0.42
8:R:137:CYS:SG	8:R:240:MET:HA	2.60	0.42
10:1:74:GLU:HG2	10:1:84:ALA:HB1	2.02	0.42
12:3:142:ALA:HA	24:3:308:CHL:CHC	2.50	0.42
12:3:167:GLY:H	24:3:311:CHL:HMC	1.83	0.42
17:N:104:ASN:ND2	17:N:107:LEU:HD13	2.34	0.42
17:8:32:TYR:HB2	24:8:304:CHL:HMD3	2.02	0.42
24:8:304:CHL:H111	24:8:304:CHL:H91	1.82	0.42
25:C:601:CLA:H142	25:C:601:CLA:H112	1.79	0.42
30:D:408:LHG:H241	30:D:408:LHG:H272	1.81	0.42
25:g:315:CLA:H112	25:g:315:CLA:H72	1.85	0.42
17:y:21:PRO:HD2	17:y:24:LEU:HD12	2.01	0.42
17:y:125:GLY:CA	24:y:313:CHL:HAB	2.49	0.42
19:a:183:MET:HA	25:a:603:CLA:HMD1	2.00	0.42
25:a:603:CLA:H203	30:d:407:LHG:H162	2.01	0.42
35:a:606:PHO:HAB	21:d:205:LEU:HD13	2.00	0.42
20:c:210:GLY:HA3	20:c:214:SER:HB3	2.01	0.42
20:c:385:THR:HG1	20:c:386:HIS:CE1	2.37	0.42
13:s:68:LEU:HD21	13:s:249:GLU:HB3	2.00	0.42
25:s:411:CLA:C4D	25:s:412:CLA:HMD3	2.49	0.42
6:L:20:TRP:HZ2	30:D:407:LHG:HC91	1.84	0.42
10:1:58:ARG:HA	10:1:61:MET:HE3	2.01	0.42
25:S:616:CLA:H3A	25:S:616:CLA:HBA2	1.59	0.42
16:T:56:ILE:HD11	30:D:407:LHG:H301	2.01	0.42
17:G:59:TRP:CE2	24:G:312:CHL:HED2	2.54	0.42
17:N:23:TYR:OH	17:N:35:ASP:OD2	2.30	0.42
17:N:29:PRO:HG2	17:N:166:LYS:HE2	2.01	0.42
24:N:304:CHL:HBA1	24:N:304:CHL:H3A	1.67	0.42
18:B:464:PHE:HB2	21:D:280:TRP:CZ2	2.53	0.42
19:A:68:SER:HB3	21:D:313:THR:HG22	2.01	0.42
25:A:603:CLA:H142	25:A:603:CLA:H112	1.82	0.42
33:m:101:LMG:H161	33:m:101:LMG:H132	1.58	0.42
9:f:16:ARG:CZ	9:f:16:ARG:HA	2.50	0.42
12:6:53:PRO:HG2	12:6:67:ASP:HB3	2.01	0.42
12:6:218:GLN:O	12:6:222:THR:OG1	2.23	0.42
25:g:308:CLA:H42	24:g:310:CHL:HBD	2.01	0.42
25:q:306:CLA:C2B	28:s:401:NEX:C38	2.97	0.42
18:b:14:ASN:HB2	8:r:86:LEU:HD22	2.01	0.42
25:b:608:CLA:H93	25:b:608:CLA:H62	1.69	0.42
25:a:603:CLA:HBB1	25:a:603:CLA:HMB3	2.00	0.42
21:d:87:HIS:CE1	21:d:162:LEU:HA	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:d:403:PHO:H2A	35:d:403:PHO:O2D	2.19	0.42
25:r:314:CLA:H3A	25:r:314:CLA:HBA2	1.43	0.42
12:7:80:GLN:H	12:7:80:GLN:HG2	1.67	0.42
12:7:122:GLY:C	12:7:124:GLN:H	2.28	0.42
24:7:310:CHL:HMB2	24:7:313:CHL:HMC	2.01	0.42
6:L:5:ASN:ND2	18:B:15:ASP:OD2	2.43	0.42
8:R:169:TYR:HB2	8:R:174:LEU:HD21	2.01	0.42
8:R:260:SER:HA	25:R:612:CLA:HED2	2.01	0.42
28:1:303:NEX:H222	25:1:307:CLA:C4B	2.50	0.42
11:2:10:LEU:O	24:2:305:CHL:HBC2	2.19	0.42
25:2:308:CLA:H2A	25:2:308:CLA:O1D	2.19	0.42
13:S:182:LEU:HD22	13:S:186:VAL:HG11	2.01	0.42
17:Y:136:PRO:HB2	24:Y:311:CHL:HBB2	2.01	0.42
17:8:135:GLY:H	24:8:309:CHL:HMC	1.83	0.42
18:B:395:VAL:HG23	18:B:397:VAL:HG13	2.02	0.42
25:B:604:CLA:H42	25:B:605:CLA:H2	2.01	0.42
33:i:101:LMG:H111	25:a:607:CLA:HAA2	2.01	0.42
25:g:314:CLA:H43	25:g:316:CLA:HBA1	2.00	0.42
28:y:304:NEX:H241	25:y:308:CLA:O2A	2.18	0.42
18:b:463:PHE:CE1	18:b:467:ILE:HD11	2.54	0.42
8:R:78:PHE:N	8:R:102:PHE:O	2.44	0.42
10:1:101:TYR:O	10:1:107:LEU:HD12	2.20	0.42
12:3:90:ARG:HA	12:3:93:MET:HE3	2.01	0.42
24:G:313:CHL:HHC	24:9:304:CHL:H52	2.01	0.42
24:9:305:CHL:H62	24:9:305:CHL:H101	1.82	0.42
24:9:310:CHL:HHC	24:9:310:CHL:HBB1	2.02	0.42
17:Y:162:PHE:CE2	17:Y:166:LYS:HD2	2.55	0.42
17:8:110:ALA:HA	24:8:307:CHL:CHC	2.49	0.42
18:B:174:ILE:HA	18:B:308:LYS:HD2	2.02	0.42
25:B:608:CLA:ND	33:B:619:LMG:H121	2.34	0.42
35:A:606:PHO:HAB	21:D:205:LEU:HD13	2.00	0.42
5:k:28:LEU:HB3	31:v:401:8CT:C18	2.49	0.42
11:5:10:LEU:O	24:5:305:CHL:HBC2	2.20	0.42
12:6:217:VAL:O	12:6:221:VAL:HG22	2.20	0.42
24:n:304:CHL:H41	24:n:304:CHL:H61	1.74	0.42
12:p:248:ILE:HB	12:p:252:ALA:H	1.84	0.42
22:w:96:TRP:CH2	33:w:201:LMG:HC91	2.55	0.42
25:b:612:CLA:H93	25:b:612:CLA:H111	1.78	0.42
21:d:263:ASN:HB3	21:d:266:TRP:HB3	2.01	0.42
13:s:95:SER:OG	13:s:97:GLU:OE1	2.31	0.42
8:r:169:TYR:HB2	8:r:174:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:7:116:PRO:O	12:7:117:VAL:C	2.62	0.42
28:7:304:NEX:H392	25:7:308:CLA:CMB	2.49	0.42
24:7:311:CHL:HHC	24:7:311:CHL:HBB1	2.01	0.42
7:M:9:ILE:HD11	7:m:8:LEU:C	2.45	0.42
12:9:183:ASP:OD1	12:9:183:ASP:N	2.52	0.42
17:N:178:PHE:HE2	25:N:316:CLA:HAB	1.83	0.42
17:Y:145:TYR:HB3	25:Y:313:CLA:HED2	2.01	0.42
10:4:209:ASN:HB3	24:4:317:CHL:HED2	2.00	0.42
28:5:304:NEX:H201	28:5:304:NEX:H15	1.62	0.42
12:6:171:GLU:HB3	12:6:172:PRO:HD2	2.02	0.42
17:n:134:GLY:HA2	24:n:311:CHL:HAC1	2.01	0.42
24:y:305:CHL:H51	24:y:305:CHL:H12	1.69	0.42
17:q:69:THR:OG1	17:q:70:PRO:HD3	2.20	0.42
17:q:106:SER:OG	13:s:148:ALA:N	2.53	0.42
17:q:110:ALA:HA	24:q:307:CHL:CHC	2.49	0.42
19:a:166:GLY:HA3	20:c:346:PHE:HE1	1.84	0.42
32:a:609:SQD:H441	32:a:609:SQD:H2	1.70	0.42
25:c:601:CLA:H161	25:c:607:CLA:HMB3	2.01	0.42
21:d:153:PHE:CE1	35:d:403:PHO:H91	2.55	0.42
12:7:200:LYS:HD3	25:7:316:CLA:HBD	2.01	0.42
5:K:22:LEU:O	5:K:25:ILE:HG12	2.20	0.42
8:R:242:ALA:C	25:R:612:CLA:HBC1	2.45	0.42
24:2:305:CHL:O1D	30:2:319:LHG:H102	2.20	0.42
24:S:605:CHL:HBC2	24:S:606:CHL:HHD	2.02	0.42
24:G:310:CHL:HBC2	24:G:311:CHL:HHD	2.01	0.42
12:9:78:PHE:O	12:9:82:ARG:NH1	2.52	0.42
12:9:190:ASP:HB2	12:9:193:THR:HB	2.02	0.42
17:Y:133:SER:OG	12:7:50:GLY:N	2.43	0.42
17:8:59:TRP:CE2	24:8:309:CHL:HED2	2.55	0.42
18:B:92:SER:OG	18:B:93:TYR:N	2.52	0.42
25:B:615:CLA:H141	25:B:615:CLA:H161	1.87	0.42
25:D:405:CLA:H161	25:D:405:CLA:H143	1.77	0.42
10:4:104:ASN:HB3	10:4:107:LEU:HG	2.02	0.42
25:5:308:CLA:H2A	25:5:308:CLA:O1D	2.19	0.42
16:t:52:LEU:HD11	30:d:407:LHG:H171	2.02	0.42
25:u:317:CLA:H11	25:u:317:CLA:C4D	2.50	0.42
12:p:122:GLY:C	12:p:124:GLN:H	2.28	0.42
24:p:305:CHL:HBA1	24:p:305:CHL:H3A	1.72	0.42
25:p:317:CLA:H11	25:p:317:CLA:C4D	2.49	0.42
17:q:125:GLY:HA2	24:q:311:CHL:HAB	2.02	0.42
18:b:156:PHE:HB3	18:b:162:PHE:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:604:CLA:H93	25:b:604:CLA:H61	1.77	0.42
25:b:610:CLA:H151	25:b:615:CLA:HBD	2.01	0.42
19:a:14:TRP:NE1	19:a:18:CYS:SG	2.93	0.42
25:c:608:CLA:O1D	30:d:408:LHG:HC12	2.20	0.42
13:s:128:ARG:HA	13:s:131:MET:HE3	2.00	0.42
10:1:51:GLU:HG2	24:1:312:CHL:HED2	2.02	0.42
10:1:194:PRO:HA	10:1:197:CYS:HB2	2.02	0.42
12:3:171:GLU:HB3	12:3:172:PRO:HD2	2.02	0.42
13:S:230:TYR:HB3	25:S:609:CLA:HED2	2.01	0.42
12:9:102:PRO:O	12:9:116:PRO:HB2	2.20	0.42
17:N:59:TRP:CD1	24:N:312:CHL:HMD3	2.55	0.42
24:Y:305:CHL:H142	24:Y:305:CHL:H112	1.72	0.42
24:Y:317:CHL:HAB	20:C:194:PRO:HG3	2.02	0.42
18:B:247:TRP:HB2	25:B:612:CLA:HBC1	2.02	0.42
25:B:613:CLA:H143	25:B:613:CLA:H111	1.75	0.42
19:A:55:ALA:O	19:A:70:SER:OG	2.28	0.42
19:A:93:PHE:HZ	25:A:607:CLA:HAA1	1.84	0.42
20:C:136:GLY:O	20:C:144:LYS:NZ	2.49	0.42
20:C:288:GLU:OE1	20:C:288:GLU:N	2.44	0.42
28:4:303:NEX:H201	28:4:303:NEX:H15	1.62	0.42
11:5:121:VAL:HG23	24:5:313:CHL:HBB2	2.01	0.42
12:6:233:HIS:CG	25:6:316:CLA:HAA2	2.55	0.42
24:y:318:CHL:HAB	20:c:194:PRO:HG3	2.01	0.42
33:w:201:LMG:H152	33:w:201:LMG:H182	1.33	0.42
18:b:247:TRP:HB2	25:b:612:CLA:HBC1	2.02	0.42
24:s:403:CHL:HHC	24:s:403:CHL:HBB1	2.02	0.42
28:r:317:NEX:H201	28:r:317:NEX:H15	1.62	0.42
1:Z:30:PRO:HD3	15:V:304:ASP:OD2	2.20	0.42
2:E:66:PHE:CZ	2:E:75:VAL:HG11	2.54	0.42
27:R:615:XAT:H35	27:R:615:XAT:H401	1.80	0.42
10:1:155:MET:HB2	25:1:313:CLA:O1A	2.20	0.42
10:1:168:LYS:HE3	25:1:314:CLA:HED2	2.02	0.42
24:8:303:CHL:H61	24:8:303:CHL:H41	1.63	0.42
18:B:18:ARG:HD2	18:B:115:TRP:CE3	2.55	0.42
25:B:610:CLA:H151	25:B:615:CLA:HBD	2.02	0.42
19:A:140:ARG:NH1	21:D:219:GLU:O	2.50	0.42
10:4:188:LEU:HD13	10:4:188:LEU:HA	1.91	0.42
11:5:136:PRO:HB2	24:5:312:CHL:HBB2	2.02	0.42
17:g:59:TRP:CE2	24:g:312:CHL:HED2	2.54	0.42
12:p:102:PRO:O	12:p:113:LEU:HD13	2.20	0.42
12:p:116:PRO:O	12:p:117:VAL:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:p:304:NEX:C33	24:p:310:CHL:O2A	2.68	0.42
25:p:307:CLA:HMD2	24:q:303:CHL:H2	2.02	0.42
17:q:164:GLU:HG2	17:q:168:LYS:HE3	2.02	0.42
25:b:604:CLA:H12	25:b:605:CLA:C1D	2.49	0.42
8:r:47:TRP:HE3	24:r:302:CHL:HAA1	1.83	0.42
12:7:79:LYS:HA	12:7:82:ARG:CZ	2.50	0.42
27:R:615:XAT:H173	27:R:615:XAT:H3	1.85	0.41
13:S:148:ALA:N	17:8:106:SER:OG	2.53	0.41
13:S:175:TRP:NE1	25:S:616:CLA:HBB1	2.35	0.41
13:S:212:ALA:O	13:S:214:GLY:N	2.44	0.41
24:G:310:CHL:HMB1	24:G:313:CHL:HMC	2.02	0.41
24:N:312:CHL:H92	24:N:312:CHL:H62	1.73	0.41
17:Y:101:TYR:O	17:Y:107:LEU:HD12	2.20	0.41
18:B:87:ASN:OD1	18:B:87:ASN:N	2.53	0.41
20:C:26:GLY:HA3	25:C:611:CLA:HMD2	2.01	0.41
22:W:104:LYS:HD3	22:W:104:LYS:HA	1.76	0.41
28:4:303:NEX:H28	24:4:309:CHL:CBA	2.50	0.41
11:5:29:PRO:HG2	11:5:166:LYS:HE2	2.01	0.41
28:5:304:NEX:H35	28:5:304:NEX:H401	1.57	0.41
17:n:98:GLY:HA3	17:n:110:ALA:O	2.20	0.41
18:b:18:ARG:HD2	18:b:115:TRP:CE3	2.55	0.41
19:a:104:GLU:O	19:a:105:TRP:C	2.61	0.41
28:7:304:NEX:H201	28:7:304:NEX:H15	1.62	0.41
3:H:55:GLU:HB3	3:H:60:ASP:HB2	2.02	0.41
4:I:9:TYR:HD2	22:W:88:LEU:HD11	1.83	0.41
17:G:194:PRO:O	29:G:301:OUR:O39	2.38	0.41
17:N:155:MET:HB3	25:N:313:CLA:O1A	2.20	0.41
25:Y:306:CLA:H12	12:7:71:LEU:HD11	2.02	0.41
19:A:329:GLU:HG3	20:C:399:ALA:HB2	2.01	0.41
20:C:29:ARG:NH1	25:C:611:CLA:OBD	2.49	0.41
20:C:389:LEU:HD13	20:C:397:GLY:N	2.34	0.41
7:m:24:ILE:HG22	7:m:25:LEU:HD23	2.01	0.41
16:t:56:ILE:HD11	30:d:407:LHG:H331	2.01	0.41
25:g:307:CLA:H12	12:u:71:LEU:HD11	2.01	0.41
12:u:77:MET:HA	12:u:80:GLN:OE1	2.20	0.41
12:u:91:TRP:O	12:u:95:GLY:N	2.54	0.41
12:u:190:ASP:HB2	12:u:193:THR:HB	2.02	0.41
25:u:314:CLA:H43	25:u:316:CLA:HBA1	2.02	0.41
17:n:29:PRO:HG2	17:n:166:LYS:HE2	2.01	0.41
12:p:91:TRP:CE2	24:p:312:CHL:HED2	2.55	0.41
18:b:395:VAL:HG23	18:b:397:VAL:HG13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:a:269:ARG:HH11	21:d:222:LEU:HD13	1.85	0.41
25:c:609:CLA:H112	25:c:609:CLA:H142	1.63	0.41
1:Z:1:MET:SD	1:Z:1:MET:N	2.81	0.41
1:Z:32:GLY:HA2	1:Z:35:GLU:HG2	2.02	0.41
9:F:12:ILE:HB	9:F:15:VAL:HG12	2.01	0.41
12:3:218:GLN:HG2	12:3:229:ASN:ND2	2.35	0.41
24:G:305:CHL:H3A	24:G:305:CHL:HBA1	1.36	0.41
12:9:209:MET:HB2	24:9:305:CHL:OMC	2.21	0.41
25:9:313:CLA:H43	25:9:315:CLA:HBA1	2.02	0.41
17:Y:11:TRP:CG	17:Y:34:TRP:HB2	2.56	0.41
17:Y:125:GLY:CA	24:Y:312:CHL:HAB	2.49	0.41
17:8:45:THR:HG22	17:8:49:ASN:ND2	2.34	0.41
18:B:198:ILE:HG23	18:B:202:HIS:CE1	2.54	0.41
25:B:604:CLA:H12	25:B:605:CLA:C1D	2.50	0.41
19:A:84:PRO:HA	19:A:112:TYR:CG	2.56	0.41
19:A:276:ALA:HB2	21:D:215:GLY:C	2.45	0.41
32:D:409:SQD:H291	33:D:411:LMG:C22	2.50	0.41
3:h:58:ASN:O	3:h:59:SER:OG	2.37	0.41
10:4:73:LEU:O	10:4:78:GLY:N	2.53	0.41
10:4:151:ASP:OD1	29:4:301:OUR:O40	2.38	0.41
12:u:209:MET:HE3	24:u:306:CHL:OMC	2.20	0.41
17:n:162:PHE:CZ	17:n:166:LYS:HD2	2.56	0.41
26:p:302:OIE:C14	24:p:306:CHL:HMC	2.50	0.41
24:p:305:CHL:H51	24:p:305:CHL:H12	1.68	0.41
17:q:58:ARG:NH1	24:q:310:CHL:OBD	2.46	0.41
18:b:435:ALA:C	18:b:437:LEU:H	2.27	0.41
25:b:612:CLA:H41	25:b:612:CLA:H61	1.43	0.41
25:b:615:CLA:H152	25:b:615:CLA:H112	1.85	0.41
20:c:285:TYR:O	20:c:411:ARG:NH2	2.51	0.41
20:c:327:LYS:C	20:c:329:LEU:H	2.28	0.41
13:s:58:TRP:O	13:s:60:GLY:N	2.52	0.41
13:s:124:LEU:O	13:s:128:ARG:HG3	2.20	0.41
13:s:199:GLU:OE2	13:s:202:ARG:NH2	2.37	0.41
8:r:137:CYS:SG	8:r:240:MET:HA	2.60	0.41
2:E:71:LEU:O	2:E:75:VAL:HG12	2.21	0.41
24:1:304:CHL:OBD	24:1:305:CHL:HHD	2.20	0.41
12:3:103:GLU:OE2	12:3:228:GLU:HG2	2.20	0.41
24:3:309:CHL:CBA	28:3:318:NEX:H31	2.50	0.41
25:9:314:CLA:H72	25:9:315:CLA:ND	2.34	0.41
17:N:40:SER:HA	17:N:45:THR:HG23	2.02	0.41
18:B:74:SER:HG	18:B:78:TRP:CG	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:608:CLA:C4A	25:B:608:CLA:HBA2	2.51	0.41
19:A:149:ALA:HB1	19:A:283:ILE:HB	2.01	0.41
20:C:86:GLY:O	20:C:94:VAL:N	2.50	0.41
20:C:327:LYS:C	20:C:329:LEU:H	2.29	0.41
35:D:403:PHO:H2A	35:D:403:PHO:O2D	2.21	0.41
10:4:69:THR:OG1	10:4:70:PRO:HD3	2.20	0.41
10:4:155:MET:HB2	25:4:313:CLA:O1A	2.20	0.41
11:5:47:ARG:NH2	11:5:48:ARG:HE	2.18	0.41
12:6:108:TYR:HD1	12:6:108:TYR:HA	1.80	0.41
12:6:152:GLN:HE22	24:6:310:CHL:HAC1	1.85	0.41
17:y:136:PRO:HB2	24:y:312:CHL:HBB2	2.02	0.41
25:y:315:CLA:HBD	25:y:316:CLA:OBD	2.20	0.41
18:b:9:HIS:HB3	25:b:606:CLA:HAB	2.01	0.41
18:b:278:GLY:O	18:b:280:PHE:N	2.53	0.41
18:b:437:LEU:HD23	18:b:437:LEU:HA	1.92	0.41
25:b:606:CLA:H72	25:b:606:CLA:H12	2.02	0.41
20:c:203:LYS:HG2	20:c:209:ASP:HB3	2.02	0.41
25:c:607:CLA:H141	25:c:607:CLA:H162	1.87	0.41
25:c:612:CLA:HBA1	25:c:612:CLA:HBD	2.02	0.41
10:1:99:LEU:HB3	10:1:110:ALA:HB3	2.02	0.41
11:2:29:PRO:HG2	11:2:166:LYS:HE2	2.01	0.41
11:2:107:LEU:HD23	11:2:107:LEU:HA	1.88	0.41
28:2:304:NEX:H21	17:N:153:MET:HA	2.03	0.41
12:3:76:GLU:HA	12:3:79:LYS:HE3	2.02	0.41
12:3:143:GLN:N	24:3:308:CHL:OMC	2.48	0.41
24:G:313:CHL:H62	24:G:313:CHL:H92	1.76	0.41
12:9:141:HIS:CG	12:9:143:GLN:HE22	2.38	0.41
12:9:212:MET:HE2	26:9:302:OIE:C4	2.50	0.41
20:C:343:THR:O	20:C:343:THR:OG1	2.39	0.41
21:D:160:TYR:HA	21:D:290:ALA:HB2	2.02	0.41
21:D:271:MET:HE2	21:D:271:MET:HB3	1.92	0.41
11:5:30:GLY:O	11:5:174:ARG:NH2	2.48	0.41
28:5:304:NEX:H11	28:5:304:NEX:H191	1.82	0.41
12:6:171:GLU:O	12:6:173:THR:N	2.50	0.41
28:g:304:NEX:H35	28:g:304:NEX:H401	1.58	0.41
12:u:141:HIS:CG	12:u:143:GLN:HE22	2.38	0.41
12:p:34:GLU:O	12:p:40:ARG:HA	2.19	0.41
25:p:315:CLA:H2A	25:p:315:CLA:O2D	2.19	0.41
25:b:613:CLA:H62	25:b:613:CLA:H41	1.54	0.41
19:a:84:PRO:HA	19:a:112:TYR:CG	2.56	0.41
19:a:161:TYR:HB3	19:a:162:PRO:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:a:276:ALA:HB2	21:d:215:GLY:C	2.45	0.41
20:c:26:GLY:HA3	25:c:611:CLA:HMD2	2.02	0.41
20:c:142:LYS:HD3	20:c:249:ARG:HG2	2.03	0.41
2:E:97:ASP:O	2:E:101:ALA:HB2	2.21	0.41
3:H:26:TYR:HE2	8:R:83:ILE:HG12	1.85	0.41
8:R:63:GLY:O	8:R:237:ARG:NH1	2.51	0.41
8:R:104:THR:HG23	8:R:119:GLU:HG3	2.02	0.41
8:R:243:PHE:CD2	27:R:615:XAT:H12	2.56	0.41
10:1:209:ASN:HB3	24:1:317:CHL:HED2	2.02	0.41
12:3:217:VAL:O	12:3:218:GLN:C	2.64	0.41
13:S:123:GLU:HB2	24:S:602:CHL:CHB	2.50	0.41
12:9:85:GLU:HB2	24:9:305:CHL:CHB	2.50	0.41
17:N:83:GLU:OE1	17:N:88:LYS:HB3	2.21	0.41
17:8:184:PHE:O	17:8:187:SER:OG	2.30	0.41
24:8:304:CHL:HBB1	24:8:304:CHL:CHC	2.46	0.41
25:B:604:CLA:HBB1	25:B:613:CLA:HBC3	2.03	0.41
21:D:178:ILE:O	21:D:182:ILE:HG13	2.21	0.41
22:W:75:ARG:H	22:W:75:ARG:HD2	1.84	0.41
3:h:55:GLU:HB3	3:h:60:ASP:HB2	2.03	0.41
10:4:108:VAL:HG13	24:4:308:CHL:C1D	2.50	0.41
24:5:305:CHL:O1D	30:5:319:LHG:H102	2.20	0.41
12:u:131:ILE:O	12:u:141:HIS:HA	2.20	0.41
17:n:53:GLU:HB2	24:n:305:CHL:CHB	2.50	0.41
25:b:603:CLA:H112	25:b:603:CLA:H91	1.81	0.41
19:a:37:ARG:HH12	30:d:407:LHG:H383	1.84	0.41
20:c:343:THR:O	20:c:343:THR:OG1	2.39	0.41
21:d:180:ARG:NH1	21:d:333:ASP:OD1	2.54	0.41
1:Z:2:ILE:O	1:Z:6:GLN:HG2	2.20	0.41
2:E:79:PRO:HD3	21:D:56:THR:HG21	2.02	0.41
11:2:11:TRP:HZ3	24:2:305:CHL:HAA1	1.86	0.41
17:G:9:ALA:HB1	24:G:305:CHL:HBC1	2.03	0.41
12:9:85:GLU:N	24:9:305:CHL:HMB2	2.35	0.41
28:N:303:NEX:H23	25:N:307:CLA:H43	2.01	0.41
17:Y:4:TYR:OH	17:Y:163:ALA:O	2.39	0.41
17:8:125:GLY:HA2	24:8:310:CHL:HAB	2.01	0.41
25:B:611:CLA:H71	30:A:601:LHG:H312	2.02	0.41
25:B:611:CLA:H192	25:B:611:CLA:H162	1.82	0.41
19:A:161:TYR:HB3	19:A:162:PRO:HD3	2.02	0.41
20:C:395:VAL:HG23	20:C:407:PHE:N	2.35	0.41
10:4:101:TYR:O	10:4:107:LEU:HD12	2.21	0.41
28:4:303:NEX:C22	25:4:307:CLA:CHC	2.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:y:302:0IE:C13	24:y:306:CHL:HBB1	2.51	0.41
19:a:68:SER:OG	19:a:69:GLY:N	2.50	0.41
19:a:121:LEU:HD13	19:a:121:LEU:HA	1.85	0.41
19:a:184:ILE:HG23	19:a:328:MET:SD	2.61	0.41
21:d:146:PHE:C	21:d:149:PRO:HD2	2.46	0.41
25:d:405:CLA:H161	25:d:405:CLA:H202	1.67	0.41
13:s:76:ARG:HD3	13:s:96:GLY:HA3	2.03	0.41
13:s:253:LYS:HD3	25:s:412:CLA:HAA2	2.03	0.41
24:s:406:CHL:HBC2	24:s:407:CHL:HHD	2.02	0.41
8:r:69:PRO:C	8:r:71:CYS:N	2.79	0.41
25:7:317:CLA:H11	25:7:317:CLA:C4D	2.51	0.41
10:1:8:ARG:CZ	10:1:26:GLY:H	2.33	0.41
13:S:271:GLN:HG2	13:S:271:GLN:H	1.58	0.41
17:G:168:LYS:HD3	25:G:316:CLA:HBD	2.03	0.41
12:9:94:LEU:HG	25:9:307:CLA:HAB	2.02	0.41
18:B:9:HIS:HB3	25:B:606:CLA:HAB	2.02	0.41
18:B:315:ILE:HG13	18:B:321:LYS:HG3	2.02	0.41
18:B:380:ASP:N	18:B:380:ASP:OD1	2.54	0.41
25:B:612:CLA:H111	25:B:612:CLA:H93	1.77	0.41
19:A:37:ARG:HH11	19:A:41:LEU:HD12	1.84	0.41
19:A:140:ARG:HD2	20:C:444:GLU:O	2.19	0.41
37:C:620:DGD:HB22	37:C:620:DGD:HB52	1.46	0.41
10:4:28:PHE:O	10:4:31:ASP:HB2	2.21	0.41
12:6:169:LEU:HB2	24:6:311:CHL:HBB1	2.02	0.41
25:6:307:CLA:H2A	25:6:307:CLA:O1D	2.21	0.41
17:g:58:ARG:NE	17:g:169:GLU:OE2	2.42	0.41
17:g:123:LEU:HD13	17:g:123:LEU:HA	1.88	0.41
12:p:144:SER:N	24:p:309:CHL:OMC	2.54	0.41
12:p:163:ARG:HG3	24:p:312:CHL:C1D	2.51	0.41
28:p:304:NEX:C24	25:p:308:CLA:O2A	2.67	0.41
25:a:603:CLA:H122	25:a:603:CLA:H162	1.86	0.41
30:a:612:LHG:HC12	21:d:269:PHE:CG	2.55	0.41
20:c:86:GLY:O	20:c:94:VAL:N	2.50	0.41
25:c:601:CLA:H143	25:c:601:CLA:H162	1.82	0.41
28:r:301:NEX:H35	28:r:301:NEX:H401	1.75	0.41
2:E:45:SER:HB2	2:E:48:TYR:HB3	2.03	0.41
2:E:95:ILE:O	21:D:84:SER:OG	2.24	0.41
6:L:34:SER:HB3	19:A:78:ILE:HD13	2.03	0.41
8:R:112:GLU:C	8:R:114:LEU:H	2.29	0.41
8:R:131:LEU:O	8:R:135:ARG:HG3	2.21	0.41
9:F:25:VAL:HB	9:F:26:PRO:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:1:68:LEU:O	10:1:72:ALA:N	2.53	0.41
10:1:130:TYR:OH	28:1:303:NEX:H192	2.20	0.41
12:3:53:PRO:HG2	12:3:67:ASP:HB3	2.02	0.41
13:S:58:TRP:CD1	17:8:130:TYR:HH	2.39	0.41
13:S:104:TYR:HB3	24:S:602:CHL:C3D	2.51	0.41
13:S:199:GLU:OE2	13:S:202:ARG:NH2	2.37	0.41
24:G:313:CHL:H111	24:G:313:CHL:H143	1.86	0.41
12:9:87:ILE:HG13	12:9:91:TRP:HD1	1.85	0.41
12:9:100:LEU:HD12	12:9:101:THR:HG22	2.03	0.41
25:9:314:CLA:O2D	25:9:314:CLA:H2A	2.20	0.41
17:N:32:TYR:HB2	24:N:305:CHL:HMD3	2.02	0.41
17:Y:54:LEU:HD23	17:Y:144:LEU:HD22	2.03	0.41
17:Y:58:ARG:NE	17:Y:169:GLU:OE2	2.41	0.41
17:Y:83:GLU:HB2	17:Y:92:GLN:HG3	2.03	0.41
26:Y:302:OIE:C13	24:Y:305:CHL:HBB1	2.51	0.41
24:Y:312:CHL:HAA2	12:7:68:THR:HG21	2.03	0.41
25:Y:313:CLA:HBB1	25:Y:313:CLA:HMB3	2.02	0.41
25:8:305:CLA:H41	25:7:307:CLA:H51	2.03	0.41
18:B:460:LEU:O	18:B:463:PHE:HB3	2.21	0.41
19:A:93:PHE:CD2	19:A:95:PRO:HD3	2.56	0.41
19:A:135:PHE:CE1	20:C:437:ARG:HG3	2.56	0.41
19:A:149:ALA:HB3	19:A:150:PRO:HD3	2.02	0.41
19:A:316:THR:OG1	19:A:317:TRP:N	2.54	0.41
20:C:210:GLY:O	20:C:211:TRP:C	2.64	0.41
6:l:13:LEU:HD22	7:m:25:LEU:HB2	2.02	0.41
10:4:21:PRO:HG3	10:4:35:ASP:HB3	2.03	0.41
10:4:57:ALA:HB2	10:4:177:MET:HE2	2.02	0.41
10:4:70:PRO:HG3	25:4:307:CLA:C1D	2.51	0.41
11:5:11:TRP:HB3	11:5:32:TYR:HB3	2.02	0.41
24:5:312:CHL:C4A	24:5:312:CHL:HBA2	2.50	0.41
25:5:314:CLA:H43	25:5:316:CLA:HBA1	2.03	0.41
12:6:90:ARG:HA	12:6:93:MET:HE3	2.02	0.41
12:6:213:PHE:HD1	25:6:306:CLA:HBB2	1.85	0.41
17:g:10:LEU:HD13	17:g:16:SER:HB2	2.03	0.41
24:g:305:CHL:H162	24:g:305:CHL:H122	1.77	0.41
24:g:305:CHL:HAC1	30:g:319:LHG:HC31	2.03	0.41
24:g:306:CHL:H62	24:g:306:CHL:H92	1.72	0.41
12:u:93:MET:O	12:u:96:THR:OG1	2.39	0.41
17:n:51:GLU:O	17:n:55:ILE:HG12	2.21	0.41
17:y:11:TRP:CG	17:y:34:TRP:HB2	2.55	0.41
17:y:39:LEU:HD11	25:q:305:CLA:H12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:y:192:LYS:NZ	17:y:200:GLU:OE2	2.35	0.41
28:y:304:NEX:H15	28:y:304:NEX:H201	1.62	0.41
12:p:164:CYS:HB3	17:q:19:ALA:HB2	2.02	0.41
17:q:23:TYR:OH	17:q:35:ASP:OD2	2.35	0.41
22:w:93:SER:HA	22:w:96:TRP:HB3	2.03	0.41
18:b:71:ILE:HD11	25:b:607:CLA:C2A	2.51	0.41
32:a:609:SQD:H1	21:d:232:PHE:HB3	2.01	0.41
21:d:271:MET:HE2	21:d:271:MET:HB3	1.91	0.41
30:d:408:LHG:H271	30:d:408:LHG:H302	1.72	0.41
13:s:199:GLU:CD	13:s:202:ARG:HH12	2.28	0.41
8:r:56:TRP:NE1	8:r:68:ASP:OD2	2.46	0.41
28:7:304:NEX:H401	28:7:304:NEX:H35	1.58	0.41
10:1:126:LEU:HB2	28:1:303:NEX:H203	2.03	0.41
17:G:27:GLU:OE1	17:G:27:GLU:N	2.48	0.41
17:G:52:LEU:O	17:G:56:HIS:ND1	2.55	0.41
17:G:110:ALA:HA	24:G:309:CHL:CHC	2.51	0.41
17:G:120:GLN:HE22	24:G:311:CHL:CMC	2.34	0.41
25:G:307:CLA:H12	12:9:71:LEU:HD11	2.03	0.41
28:9:319:NEX:H201	28:9:319:NEX:H15	1.62	0.41
17:N:68:LEU:HD22	17:N:68:LEU:HA	1.94	0.41
25:B:608:CLA:C1D	33:B:619:LMG:H121	2.51	0.41
19:A:184:ILE:HG23	19:A:328:MET:SD	2.61	0.41
21:D:229:ALA:O	30:D:408:LHG:O1	2.34	0.41
2:e:103:GLU:HA	2:e:106:LYS:HD2	2.03	0.41
30:4:318:LHG:H142	30:4:318:LHG:H172	1.91	0.41
12:6:107:LYS:HB3	12:6:107:LYS:HE2	1.88	0.41
28:6:303:NEX:C28	24:6:309:CHL:H3A	2.51	0.41
16:t:37:GLU:C	16:t:39:LEU:H	2.29	0.41
17:g:147:GLY:C	17:g:149:ALA:H	2.29	0.41
12:u:98:GLY:H	12:u:101:THR:HG23	1.86	0.41
25:b:610:CLA:H102	25:b:615:CLA:HAA1	2.03	0.41
19:a:267:ASN:ND2	21:d:232:PHE:O	2.54	0.41
20:c:213:VAL:HG23	37:c:619:DGD:HD61	2.03	0.41
25:c:607:CLA:H142	25:c:607:CLA:H111	1.81	0.41
35:d:403:PHO:H72	25:d:404:CLA:H111	2.03	0.41
13:s:119:LEU:HD13	13:s:119:LEU:HA	1.87	0.41
25:s:411:CLA:HBD	25:s:412:CLA:OBD	2.21	0.41
8:r:93:ASN:OD1	8:r:93:ASN:N	2.54	0.41
8:r:261:LEU:HD12	8:r:261:LEU:HA	1.82	0.41
12:7:125:ILE:HG12	12:7:145:ILE:HB	2.02	0.41
1:Z:20:VAL:HG13	25:C:611:CLA:H143	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:90:GLN:OE1	19:A:312:ARG:NH1	2.54	0.40
10:1:10:LEU:HG	10:1:20:VAL:HG11	2.03	0.40
10:1:201:HIS:HA	10:1:208:ASN:HB3	2.02	0.40
12:3:209:MET:HB2	24:3:305:CHL:HMC	2.03	0.40
24:S:602:CHL:HHC	24:S:602:CHL:HBB1	2.02	0.40
17:N:137:LEU:HG	24:N:311:CHL:HBB1	2.03	0.40
17:Y:188:LEU:HD12	17:Y:218:PHE:HD2	1.86	0.40
18:B:463:PHE:CE1	18:B:467:ILE:HD11	2.55	0.40
25:D:405:CLA:H112	25:D:405:CLA:H142	1.79	0.40
30:4:318:LHG:H111	30:4:318:LHG:HC82	1.80	0.40
12:6:66:TRP:CZ3	24:6:304:CHL:HBD	2.56	0.40
24:6:311:CHL:HBB1	24:6:311:CHL:CHC	2.51	0.40
12:u:78:PHE:CZ	12:u:82:ARG:HD3	2.56	0.40
12:u:168:PRO:HG3	28:u:304:NEX:H192	2.02	0.40
17:y:81:PHE:CE1	17:y:102:LEU:HA	2.57	0.40
19:a:93:PHE:HZ	25:a:607:CLA:HAA1	1.86	0.40
20:c:433:ALA:HA	25:c:605:CLA:HED2	2.03	0.40
21:d:146:PHE:O	21:d:149:PRO:HD2	2.21	0.40
12:7:189:ALA:O	12:7:194:PHE:HB2	2.20	0.40
28:7:304:NEX:C32	24:7:310:CHL:H3A	2.51	0.40
8:R:130:GLU:HB2	24:R:602:CHL:C1B	2.51	0.40
24:2:312:CHL:C4A	24:2:312:CHL:HBA2	2.50	0.40
24:3:309:CHL:H3A	28:3:318:NEX:C28	2.51	0.40
28:S:617:NEX:H222	25:8:306:CLA:CHC	2.52	0.40
12:9:76:GLU:CD	17:N:41:ALA:HB1	2.47	0.40
24:9:311:CHL:HMA1	28:9:319:NEX:C32	2.51	0.40
17:N:12:LEU:HD12	24:N:304:CHL:HHB	2.03	0.40
17:N:87:PHE:CD1	17:N:88:LYS:HG3	2.56	0.40
17:N:125:GLY:CA	24:N:312:CHL:HAB	2.48	0.40
25:N:316:CLA:H3A	25:N:316:CLA:HBA2	1.88	0.40
17:8:81:PHE:CE1	17:8:102:LEU:HA	2.56	0.40
18:B:280:PHE:O	18:B:313:ASP:HB2	2.21	0.40
25:B:602:CLA:H18	25:B:602:CLA:H152	1.86	0.40
25:B:615:CLA:H152	25:B:615:CLA:H112	1.87	0.40
19:A:166:GLY:HA3	20:C:346:PHE:HE1	1.85	0.40
20:C:142:LYS:HD3	20:C:249:ARG:HG2	2.04	0.40
25:C:603:CLA:H72	25:C:603:CLA:H112	1.94	0.40
3:h:35:THR:O	3:h:35:THR:OG1	2.32	0.40
17:g:59:TRP:CD1	24:g:313:CHL:HMD3	2.55	0.40
12:u:72:SER:HB2	12:u:78:PHE:CD1	2.56	0.40
12:p:84:LEU:O	12:p:88:HIS:ND1	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:q:45:THR:HG22	17:q:49:ASN:ND2	2.36	0.40
18:b:198:ILE:HG23	18:b:202:HIS:CE1	2.55	0.40
25:b:608:CLA:C4A	25:b:608:CLA:HBA2	2.50	0.40
25:b:609:CLA:H41	25:b:609:CLA:H61	1.80	0.40
19:a:92:HIS:NE2	20:c:348:ASP:OD2	2.55	0.40
19:a:135:PHE:CE1	20:c:437:ARG:HG3	2.56	0.40
13:s:81:PRO:CD	24:s:402:CHL:HBB1	2.51	0.40
8:r:130:GLU:HB2	24:r:303:CHL:C1B	2.51	0.40
28:r:301:NEX:H11	28:r:301:NEX:H191	1.80	0.40
12:7:167:GLY:HA3	12:7:168:PRO:HD2	1.97	0.40
12:3:145:ILE:HA	12:3:148:ILE:HG22	2.04	0.40
24:3:309:CHL:HAA1	28:3:318:NEX:C25	2.51	0.40
13:S:253:LYS:HD3	25:S:611:CLA:HAA2	2.02	0.40
17:G:130:TYR:CE2	28:G:304:NEX:H191	2.57	0.40
24:9:311:CHL:HMA2	28:9:319:NEX:H30	2.02	0.40
19:A:179:THR:O	19:A:183:MET:HG3	2.22	0.40
20:C:161:TRP:CH2	20:C:226:ILE:HG23	2.55	0.40
20:C:228:ILE:H	20:C:228:ILE:HG12	1.64	0.40
21:D:148:ALA:HB3	21:D:149:PRO:HD3	2.04	0.40
10:4:204:ASP:OD1	10:4:204:ASP:N	2.55	0.40
17:n:62:LEU:HB3	25:n:307:CLA:HBB2	2.02	0.40
28:p:304:NEX:C31	24:p:310:CHL:H3A	2.51	0.40
24:p:305:CHL:HMA3	30:p:319:LHG:H112	2.03	0.40
18:b:53:ASN:HD21	18:b:58:GLN:CD	2.29	0.40
18:b:74:SER:HG	18:b:78:TRP:CG	2.39	0.40
25:c:608:CLA:H111	25:c:608:CLA:H93	1.78	0.40
25:c:609:CLA:H141	25:c:609:CLA:H161	1.89	0.40
21:d:160:TYR:HA	21:d:290:ALA:HB2	2.03	0.40
33:d:411:LMG:H142	33:d:411:LMG:H171	1.47	0.40
26:7:302:OIE:C14	24:7:306:CHL:HMC	2.52	0.40
8:R:179:SER:O	8:R:183:TRP:HD1	2.04	0.40
28:1:303:NEX:H31	28:1:303:NEX:H28	1.98	0.40
11:2:118:TRP:HZ2	24:3:317:CHL:HBD	1.86	0.40
16:T:37:GLU:C	16:T:39:LEU:H	2.30	0.40
17:G:64:THR:HA	17:G:183:PHE:HE2	1.87	0.40
28:G:304:NEX:H31	24:G:310:CHL:HBA1	2.04	0.40
17:N:108:VAL:HG23	24:N:308:CHL:C1D	2.51	0.40
24:N:308:CHL:HHD	24:N:309:CHL:OBD	2.21	0.40
18:B:71:ILE:HD11	25:B:607:CLA:C2A	2.51	0.40
18:B:359:MET:HE2	18:B:366:PHE:H	1.87	0.40
25:B:604:CLA:HMB1	25:B:608:CLA:HHC	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:C:243:LYS:HB3	20:C:243:LYS:HE2	1.90	0.40
25:C:602:CLA:C1D	25:C:603:CLA:H151	2.51	0.40
21:D:87:HIS:HD2	33:D:401:LMG:HC3	1.86	0.40
17:g:47:ALA:HA	17:g:50:ARG:CZ	2.52	0.40
12:u:186:ASN:ND2	12:u:187:PHE:H	2.20	0.40
25:u:315:CLA:H71	25:u:315:CLA:H111	1.89	0.40
25:u:315:CLA:O2D	25:u:315:CLA:H2A	2.21	0.40
17:y:61:MET:SD	25:y:314:CLA:HAB	2.62	0.40
25:p:317:CLA:HMB1	24:p:318:CHL:HAC2	2.03	0.40
18:b:60:MET:HB3	18:b:60:MET:HE2	1.64	0.40
18:b:115:TRP:NE1	32:b:618:SQD:O8	2.54	0.40
18:b:480:ALA:N	21:d:139:ARG:HH12	2.13	0.40
25:b:607:CLA:H141	25:b:607:CLA:H161	1.83	0.40
19:a:76:ASN:OD1	19:a:76:ASN:N	2.35	0.40
20:c:161:TRP:CH2	20:c:226:ILE:HG23	2.56	0.40
21:d:178:ILE:O	21:d:182:ILE:HG13	2.21	0.40
28:7:304:NEX:C35	24:7:310:CHL:O2A	2.68	0.40
25:7:315:CLA:H2A	25:7:315:CLA:O2D	2.21	0.40
8:R:127:ARG:HA	8:R:127:ARG:HD3	1.99	0.40
25:R:612:CLA:O1D	25:R:612:CLA:H2A	2.22	0.40
10:1:8:ARG:HD2	10:1:31:ASP:O	2.22	0.40
11:2:47:ARG:NH2	11:2:48:ARG:HE	2.20	0.40
11:2:144:LEU:HD23	11:2:144:LEU:HA	1.82	0.40
17:G:134:GLY:HA2	24:G:312:CHL:HAC1	2.02	0.40
12:9:41:ALA:HB1	24:9:304:CHL:HBC1	2.03	0.40
12:9:72:SER:HB2	12:9:78:PHE:CD1	2.56	0.40
17:8:8:ARG:NH2	17:8:24:LEU:O	2.55	0.40
25:B:602:CLA:HED3	25:B:603:CLA:H3A	2.04	0.40
33:B:619:LMG:H291	33:B:619:LMG:H322	1.61	0.40
19:A:82:ILE:HB	19:A:174:LEU:HB2	2.03	0.40
19:A:214:MET:O	19:A:218:LEU:HG	2.22	0.40
30:A:612:LHG:HC12	21:D:269:PHE:CG	2.57	0.40
21:D:152:VAL:HG22	25:D:404:CLA:HED3	2.03	0.40
3:h:13:THR:OG1	25:b:616:CLA:OBD	2.27	0.40
10:4:59:TRP:CE2	24:4:311:CHL:HED2	2.57	0.40
24:g:313:CHL:HHC	24:u:305:CHL:H52	2.03	0.40
12:u:159:CYS:O	12:u:163:ARG:N	2.51	0.40
17:n:39:LEU:HD12	24:n:305:CHL:H11	2.03	0.40
12:p:89:SER:HB2	12:p:205:GLY:CA	2.52	0.40
12:p:142:ALA:HA	24:p:309:CHL:CHC	2.51	0.40
24:p:310:CHL:HMB2	24:p:313:CHL:HMC	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:604:CLA:HMB1	25:b:608:CLA:HHC	2.04	0.40
19:a:159:ILE:C	19:a:162:PRO:HD2	2.47	0.40
19:a:234:ASN:ND2	30:a:601:LHG:O4	2.54	0.40
25:a:604:CLA:H92	25:a:604:CLA:H62	1.80	0.40
21:d:148:ALA:HB3	21:d:149:PRO:HD3	2.04	0.40
25:d:405:CLA:H142	25:d:405:CLA:H112	1.79	0.40
8:r:131:LEU:O	8:r:135:ARG:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	Z	59/62 (95%)	58 (98%)	1 (2%)	0	100	100
1	z	59/62 (95%)	58 (98%)	1 (2%)	0	100	100
2	E	63/82 (77%)	61 (97%)	2 (3%)	0	100	100
2	e	63/82 (77%)	63 (100%)	0	0	100	100
3	H	66/75 (88%)	63 (96%)	3 (4%)	0	100	100
3	h	66/75 (88%)	63 (96%)	3 (4%)	0	100	100
4	I	32/36 (89%)	32 (100%)	0	0	100	100
4	i	32/36 (89%)	30 (94%)	2 (6%)	0	100	100
5	K	35/43 (81%)	33 (94%)	2 (6%)	0	100	100
5	k	35/43 (81%)	34 (97%)	1 (3%)	0	100	100
6	L	35/38 (92%)	35 (100%)	0	0	100	100
6	l	35/38 (92%)	35 (100%)	0	0	100	100
7	M	28/33 (85%)	27 (96%)	1 (4%)	0	100	100
7	m	28/33 (85%)	27 (96%)	1 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	R	223/267 (84%)	199 (89%)	23 (10%)	1 (0%)	30	58
8	r	223/267 (84%)	203 (91%)	20 (9%)	0	100	100
9	F	29/42 (69%)	27 (93%)	2 (7%)	0	100	100
9	f	29/42 (69%)	28 (97%)	1 (3%)	0	100	100
10	1	210/212 (99%)	197 (94%)	13 (6%)	0	100	100
10	4	210/212 (99%)	197 (94%)	13 (6%)	0	100	100
11	2	219/256 (86%)	205 (94%)	14 (6%)	0	100	100
11	5	219/256 (86%)	204 (93%)	15 (7%)	0	100	100
12	3	209/254 (82%)	189 (90%)	20 (10%)	0	100	100
12	6	217/254 (85%)	196 (90%)	21 (10%)	0	100	100
12	7	217/254 (85%)	188 (87%)	27 (12%)	2 (1%)	14	41
12	9	217/254 (85%)	185 (85%)	31 (14%)	1 (0%)	24	54
12	p	217/254 (85%)	188 (87%)	26 (12%)	3 (1%)	9	31
12	u	217/254 (85%)	187 (86%)	30 (14%)	0	100	100
13	S	247/308 (80%)	211 (85%)	34 (14%)	2 (1%)	16	44
13	s	247/308 (80%)	209 (85%)	35 (14%)	3 (1%)	10	34
14	X	32/109 (29%)	32 (100%)	0	0	100	100
14	x	32/109 (29%)	32 (100%)	0	0	100	100
15	V	23/33 (70%)	18 (78%)	5 (22%)	0	100	100
15	v	23/33 (70%)	19 (83%)	4 (17%)	0	100	100
16	T	26/31 (84%)	24 (92%)	2 (8%)	0	100	100
16	t	26/31 (84%)	24 (92%)	2 (8%)	0	100	100
17	8	204/280 (73%)	195 (96%)	9 (4%)	0	100	100
17	G	221/280 (79%)	215 (97%)	6 (3%)	0	100	100
17	N	204/280 (73%)	196 (96%)	8 (4%)	0	100	100
17	Y	221/280 (79%)	212 (96%)	9 (4%)	0	100	100
17	g	221/280 (79%)	214 (97%)	7 (3%)	0	100	100
17	n	204/280 (73%)	192 (94%)	11 (5%)	1 (0%)	24	54
17	q	204/280 (73%)	196 (96%)	8 (4%)	0	100	100
17	y	221/280 (79%)	212 (96%)	9 (4%)	0	100	100
18	B	476/508 (94%)	455 (96%)	19 (4%)	2 (0%)	30	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	b	476/508 (94%)	457 (96%)	17 (4%)	2 (0%)	30	58
19	A	325/327 (99%)	307 (94%)	17 (5%)	1 (0%)	36	64
19	a	325/327 (99%)	304 (94%)	20 (6%)	1 (0%)	36	64
20	C	446/461 (97%)	409 (92%)	36 (8%)	1 (0%)	43	71
20	c	446/461 (97%)	407 (91%)	38 (8%)	1 (0%)	43	71
21	D	338/352 (96%)	313 (93%)	25 (7%)	0	100	100
21	d	338/352 (96%)	318 (94%)	20 (6%)	0	100	100
22	W	41/118 (35%)	30 (73%)	11 (27%)	0	100	100
22	w	41/118 (35%)	30 (73%)	11 (27%)	0	100	100
All	All	8900/10550 (84%)	8243 (93%)	636 (7%)	21 (0%)	44	71

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	B	279	PHE
18	B	299	SER
17	n	23	TYR
12	p	117	VAL
12	p	118	TRP
12	p	186	ASN
18	b	279	PHE
18	b	299	SER
12	7	117	VAL
12	7	118	TRP
13	S	163	LEU
20	C	449	ARG
20	c	449	ARG
13	s	163	LEU
8	R	42	SER
19	A	141	PRO
19	a	141	PRO
13	s	59	PHE
13	S	173	VAL
13	s	173	VAL
12	9	117	VAL

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	Z	51/52 (98%)	51 (100%)	0	100	100
1	z	51/52 (98%)	51 (100%)	0	100	100
2	E	58/73 (80%)	57 (98%)	1 (2%)	53	71
2	e	58/73 (80%)	57 (98%)	1 (2%)	53	71
3	H	56/62 (90%)	55 (98%)	1 (2%)	51	70
3	h	56/62 (90%)	55 (98%)	1 (2%)	51	70
4	I	31/32 (97%)	31 (100%)	0	100	100
4	i	31/32 (97%)	31 (100%)	0	100	100
5	K	33/39 (85%)	31 (94%)	2 (6%)	17	44
5	k	33/39 (85%)	32 (97%)	1 (3%)	36	62
6	L	34/35 (97%)	31 (91%)	3 (9%)	9	31
6	l	34/35 (97%)	32 (94%)	2 (6%)	18	45
7	M	27/30 (90%)	27 (100%)	0	100	100
7	m	27/30 (90%)	26 (96%)	1 (4%)	30	58
8	R	181/214 (85%)	173 (96%)	8 (4%)	25	54
8	r	180/214 (84%)	170 (94%)	10 (6%)	19	46
9	F	25/36 (69%)	22 (88%)	3 (12%)	5	19
9	f	26/36 (72%)	23 (88%)	3 (12%)	5	21
10	1	160/160 (100%)	153 (96%)	7 (4%)	25	54
10	4	159/160 (99%)	153 (96%)	6 (4%)	29	57
11	2	168/199 (84%)	168 (100%)	0	100	100
11	5	168/199 (84%)	168 (100%)	0	100	100
12	3	165/202 (82%)	158 (96%)	7 (4%)	26	55
12	6	172/202 (85%)	166 (96%)	6 (4%)	32	59
12	7	173/202 (86%)	164 (95%)	9 (5%)	21	49
12	9	174/202 (86%)	167 (96%)	7 (4%)	28	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	p	174/202 (86%)	161 (92%)	13 (8%)	12	37
12	u	175/202 (87%)	166 (95%)	9 (5%)	21	50
13	S	184/232 (79%)	172 (94%)	12 (6%)	15	42
13	s	184/232 (79%)	174 (95%)	10 (5%)	20	48
14	X	24/80 (30%)	23 (96%)	1 (4%)	26	55
14	x	24/80 (30%)	22 (92%)	2 (8%)	10	33
15	V	20/28 (71%)	18 (90%)	2 (10%)	7	26
15	v	20/28 (71%)	19 (95%)	1 (5%)	22	50
16	T	25/28 (89%)	23 (92%)	2 (8%)	11	35
16	t	25/28 (89%)	23 (92%)	2 (8%)	11	35
17	8	153/210 (73%)	152 (99%)	1 (1%)	76	80
17	G	165/210 (79%)	161 (98%)	4 (2%)	43	66
17	N	152/210 (72%)	143 (94%)	9 (6%)	18	45
17	Y	165/210 (79%)	162 (98%)	3 (2%)	51	70
17	g	165/210 (79%)	159 (96%)	6 (4%)	31	58
17	n	151/210 (72%)	144 (95%)	7 (5%)	24	53
17	q	153/210 (73%)	153 (100%)	0	100	100
17	y	165/210 (79%)	163 (99%)	2 (1%)	63	75
18	B	384/410 (94%)	371 (97%)	13 (3%)	32	60
18	b	384/410 (94%)	372 (97%)	12 (3%)	35	61
19	A	266/266 (100%)	251 (94%)	15 (6%)	19	46
19	a	266/266 (100%)	252 (95%)	14 (5%)	20	48
20	C	347/359 (97%)	338 (97%)	9 (3%)	40	65
20	c	347/359 (97%)	337 (97%)	10 (3%)	37	63
21	D	275/285 (96%)	266 (97%)	9 (3%)	33	60
21	d	275/285 (96%)	267 (97%)	8 (3%)	37	63
22	W	29/88 (33%)	27 (93%)	2 (7%)	14	40
22	w	29/88 (33%)	29 (100%)	0	100	100
All	All	7057/8308 (85%)	6800 (96%)	257 (4%)	32	58

All (257) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	75	VAL
3	H	12	VAL
5	K	24	ILE
5	K	40	VAL
6	L	12	GLU
6	L	14	ASN
6	L	16	THR
8	R	48	MET
8	R	76	VAL
8	R	153	VAL
8	R	156	GLN
8	R	164	GLN
8	R	182	VAL
8	R	202	THR
8	R	261	LEU
9	F	15	VAL
9	F	16	ARG
9	F	42	ARG
10	1	1	VAL
10	1	8	ARG
10	1	12	LEU
10	1	52	LEU
10	1	69	THR
10	1	85	VAL
10	1	188	LEU
12	3	52	VAL
12	3	101	THR
12	3	207	LEU
12	3	218	GLN
12	3	221	VAL
12	3	240	ASN
12	3	241	ASN
13	S	61	GLU
13	S	84	LEU
13	S	86	ASP
13	S	119	LEU
13	S	124	LEU
13	S	128	ARG
13	S	150	LEU
13	S	164	ASN
13	S	168	LEU
13	S	171	PHE
13	S	193	VAL

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Mol	Chain	Res	Type
13	S	271	GLN
14	X	90	LEU
15	V	282	GLN
15	V	298	VAL
16	T	40	VAL
16	T	55	SER
17	G	20	VAL
17	G	54	LEU
17	G	69	THR
17	G	108	VAL
12	9	44	LEU
12	9	100	LEU
12	9	101	THR
12	9	117	VAL
12	9	239	ASN
12	9	248	ILE
12	9	250	ARG
17	N	12	LEU
17	N	20	VAL
17	N	54	LEU
17	N	62	LEU
17	N	65	VAL
17	N	68	LEU
17	N	69	THR
17	N	107	LEU
17	N	108	VAL
17	Y	16	SER
17	Y	73	LEU
17	Y	180	MET
17	8	1	VAL
18	B	10	THR
18	B	12	VAL
18	B	15	ASP
18	B	41	GLU
18	B	52	LEU
18	B	158	VAL
18	B	224	ARG
18	B	237	VAL
18	B	276	ASP
18	B	280	PHE
18	B	365	THR
18	B	368	VAL

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Mol	Chain	Res	Type
18	B	431	GLU
19	A	28	LEU
19	A	60	ILE
19	A	76	ASN
19	A	85	THR
19	A	121	LEU
19	A	140	ARG
19	A	143	ILE
19	A	223	LEU
19	A	232	SER
19	A	245	THR
19	A	249	VAL
19	A	281	VAL
19	A	313	VAL
19	A	322	ASN
19	A	326	LEU
20	C	129	GLU
20	C	213	VAL
20	C	222	ILE
20	C	228	ILE
20	C	343	THR
20	C	357	LEU
20	C	389	LEU
20	C	395	VAL
20	C	405	VAL
21	D	28	VAL
21	D	89	LEU
21	D	102	THR
21	D	192	THR
21	D	213	ILE
21	D	279	LEU
21	D	329	MET
21	D	340	VAL
21	D	345	VAL
22	W	84	LEU
22	W	96	TRP
2	e	75	VAL
3	h	18	LEU
5	k	40	VAL
6	l	12	GLU
6	l	16	THR
7	m	3	VAL

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Mol	Chain	Res	Type
9	f	15	VAL
9	f	16	ARG
9	f	42	ARG
10	4	10	LEU
10	4	12	LEU
10	4	52	LEU
10	4	69	THR
10	4	85	VAL
10	4	188	LEU
12	6	48	SER
12	6	52	VAL
12	6	101	THR
12	6	108	TYR
12	6	234	ILE
12	6	240	ASN
14	x	79	LEU
14	x	90	LEU
15	v	298	VAL
16	t	40	VAL
16	t	55	SER
17	g	1	VAL
17	g	20	VAL
17	g	25	THR
17	g	69	THR
17	g	108	VAL
17	g	123	LEU
12	u	44	LEU
12	u	101	THR
12	u	111	VAL
12	u	117	VAL
12	u	207	LEU
12	u	242	ILE
12	u	248	ILE
12	u	249	THR
12	u	250	ARG
17	n	12	LEU
17	n	20	VAL
17	n	24	LEU
17	n	54	LEU
17	n	62	LEU
17	n	68	LEU
17	n	102	LEU

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Mol	Chain	Res	Type
17	y	10	LEU
17	y	73	LEU
12	p	48	SER
12	p	80	GLN
12	p	96	THR
12	p	101	THR
12	p	111	VAL
12	p	113	LEU
12	p	117	VAL
12	p	119	PHE
12	p	145	ILE
12	p	221	VAL
12	p	239	ASN
12	p	245	ASP
12	p	249	THR
18	b	10	THR
18	b	12	VAL
18	b	15	ASP
18	b	41	GLU
18	b	52	LEU
18	b	57	ARG
18	b	60	MET
18	b	237	VAL
18	b	276	ASP
18	b	365	THR
18	b	368	VAL
18	b	431	GLU
19	a	28	LEU
19	a	60	ILE
19	a	76	ASN
19	a	85	THR
19	a	102	LEU
19	a	121	LEU
19	a	140	ARG
19	a	143	ILE
19	a	223	LEU
19	a	245	THR
19	a	249	VAL
19	a	281	VAL
19	a	322	ASN
19	a	326	LEU
20	c	129	GLU

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Mol	Chain	Res	Type
20	c	213	VAL
20	c	222	ILE
20	c	228	ILE
20	c	343	THR
20	c	357	LEU
20	c	389	LEU
20	c	392	LEU
20	c	393	ASN
20	c	405	VAL
21	d	89	LEU
21	d	102	THR
21	d	192	THR
21	d	213	ILE
21	d	279	LEU
21	d	329	MET
21	d	340	VAL
21	d	345	VAL
13	s	61	GLU
13	s	84	LEU
13	s	86	ASP
13	s	119	LEU
13	s	124	LEU
13	s	164	ASN
13	s	168	LEU
13	s	171	PHE
13	s	193	VAL
13	s	271	GLN
8	r	48	MET
8	r	76	VAL
8	r	81	PHE
8	r	82	ASP
8	r	153	VAL
8	r	156	GLN
8	r	164	GLN
8	r	182	VAL
8	r	202	THR
8	r	261	LEU
12	7	42	LEU
12	7	48	SER
12	7	80	GLN
12	7	96	THR
12	7	111	VAL

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Mol	Chain	Res	Type
12	7	117	VAL
12	7	145	ILE
12	7	186	ASN
12	7	247	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
2	E	100	ASN
2	E	104	GLN
4	I	31	ASN
4	I	34	GLN
8	R	80	GLN
8	R	89	ASN
10	1	186	GLN
11	2	133	ASN
11	2	189	GLN
11	2	215	GLN
12	3	241	ASN
13	S	65	GLN
13	S	180	ASN
12	9	141	HIS
12	9	143	GLN
12	9	229	ASN
12	9	239	ASN
17	N	104	ASN
17	N	111	GLN
18	B	26	HIS
18	B	53	ASN
18	B	58	GLN
18	B	331	ASN
18	B	425	GLN
19	A	26	ASN
19	A	261	GLN
19	A	315	ASN
20	C	366	ASN
20	C	451	ASN
21	D	197	HIS
21	D	230	ASN
1	z	6	GLN
2	e	100	ASN
4	i	31	ASN

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Mol	Chain	Res	Type
4	i	34	GLN
11	5	215	GLN
17	g	104	ASN
12	u	141	HIS
12	u	143	GLN
17	n	189	GLN
17	q	92	GLN
18	b	26	HIS
18	b	53	ASN
18	b	58	GLN
18	b	331	ASN
18	b	425	GLN
19	a	26	ASN
19	a	75	ASN
19	a	241	GLN
19	a	315	ASN
20	c	366	ASN
20	c	451	ASN
13	s	248	GLN
8	r	216	ASN
12	7	81	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 528 ligands modelled in this entry, 2 are monoatomic - leaving 526 for Mogul analysis.

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
25	CLA	9	315	-	49,53,73	1.39	8 (16%)	58,89,113	1.43	4 (6%)
25	CLA	q	312	-	59,63,73	1.24	9 (15%)	70,101,113	1.38	6 (8%)
37	DGD	c	618	-	51,51,67	0.94	2 (3%)	65,65,81	1.21	6 (9%)
39	PL9	d	406	-	55,55,55	1.65	11 (20%)	68,69,69	1.53	12 (17%)
25	CLA	N	307	-	54,58,73	1.30	8 (14%)	64,95,113	1.39	6 (9%)
26	OIE	p	303	-	42,45,45	1.12	6 (14%)	51,63,63	1.50	10 (19%)
25	CLA	7	314	-	59,63,73	1.24	9 (15%)	70,101,113	1.34	6 (8%)
25	CLA	b	615	18	69,73,73	1.15	8 (11%)	82,113,113	1.26	5 (6%)
31	8CT	C	615	-	40,41,41	4.77	23 (57%)	51,56,56	2.80	19 (37%)
24	CHL	n	312	-	50,64,74	3.54	18 (36%)	46,102,114	2.81	19 (41%)
25	CLA	s	404	-	49,53,73	1.37	9 (18%)	58,89,113	1.43	4 (6%)
26	OIE	3	303	-	42,45,45	1.12	6 (14%)	51,63,63	1.61	10 (19%)
24	CHL	G	318	17	36,50,74	4.11	17 (47%)	29,85,114	3.09	15 (51%)
30	LHG	4	318	-	41,41,48	1.24	6 (14%)	44,47,54	0.99	3 (6%)
25	CLA	2	314	-	59,63,73	1.23	9 (15%)	70,101,113	1.33	5 (7%)
24	CHL	5	309	11	37,51,74	4.16	18 (48%)	30,86,114	3.22	16 (53%)
30	LHG	C	617	-	31,31,48	1.36	6 (19%)	34,37,54	1.15	3 (8%)
25	CLA	6	307	-	47,51,73	1.38	7 (14%)	55,86,113	1.44	4 (7%)
24	CHL	2	311	-	41,55,74	3.95	19 (46%)	35,91,114	2.99	14 (40%)
25	CLA	u	315	-	67,71,73	1.19	8 (11%)	79,110,113	1.31	6 (7%)
26	OIE	1	302	-	42,45,45	1.13	6 (14%)	51,63,63	1.53	12 (23%)
30	LHG	D	407	-	48,48,48	1.12	5 (10%)	51,54,54	0.97	2 (3%)
25	CLA	C	611	20	69,73,73	1.15	9 (13%)	82,113,113	1.32	6 (7%)
24	CHL	n	309	-	40,54,74	3.89	18 (45%)	34,90,114	3.47	16 (47%)
24	CHL	s	402	13	40,54,74	3.86	19 (47%)	34,90,114	3.17	16 (47%)
24	CHL	7	310	-	40,54,74	4.01	19 (47%)	34,90,114	3.06	14 (41%)
28	NEX	g	304	-	40,46,46	1.12	3 (7%)	50,70,70	4.72	18 (36%)
25	CLA	C	605	20	60,64,73	1.23	9 (15%)	71,102,113	1.38	6 (8%)
25	CLA	c	609	20	69,73,73	1.17	9 (13%)	82,113,113	1.35	7 (8%)
24	CHL	N	312	-	50,64,74	3.55	18 (36%)	46,102,114	2.81	19 (41%)
32	SQD	D	409	-	42,44,54	1.06	3 (7%)	52,55,65	1.51	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CHL	8	308	-	40,54,74	3.85	19 (47%)	34,90,114	3.26	16 (47%)
25	CLA	B	615	18	69,73,73	1.15	8 (11%)	82,113,113	1.27	5 (6%)
24	CHL	Y	311	-	45,59,74	3.63	19 (42%)	40,96,114	2.97	17 (42%)
25	CLA	b	612	18	69,73,73	1.15	9 (13%)	82,113,113	1.33	9 (10%)
24	CHL	g	312	-	45,59,74	3.82	18 (40%)	40,96,114	2.93	18 (45%)
25	CLA	3	306	-	45,49,73	1.41	8 (17%)	54,84,113	1.48	6 (11%)
25	CLA	6	314	-	45,49,73	1.40	7 (15%)	54,84,113	1.47	5 (9%)
26	OIE	9	302	-	42,45,45	1.12	6 (14%)	51,63,63	1.53	11 (21%)
24	CHL	N	308	17	37,51,74	4.11	18 (48%)	30,86,114	3.16	13 (43%)
23	HEM	f	201	9,2	50,50,50	1.39	7 (14%)	67,82,82	1.00	0
25	CLA	A	603	19	69,73,73	1.17	9 (13%)	82,113,113	1.37	9 (10%)
24	CHL	y	311	-	48,62,74	3.54	19 (39%)	43,99,114	3.12	20 (46%)
26	OIE	q	302	-	42,45,45	1.14	5 (11%)	51,63,63	1.48	11 (21%)
25	CLA	y	316	17	49,53,73	1.36	9 (18%)	58,89,113	1.51	4 (6%)
26	OIE	8	302	-	42,45,45	1.14	5 (11%)	51,63,63	1.48	11 (21%)
27	XAT	r	316	-	41,47,47	0.92	1 (2%)	54,74,74	2.63	20 (37%)
24	CHL	N	309	-	40,54,74	3.89	19 (47%)	34,90,114	3.40	16 (47%)
24	CHL	y	313	-	60,74,74	3.17	19 (31%)	58,114,114	2.53	19 (32%)
24	CHL	9	308	12	37,51,74	4.28	18 (48%)	30,86,114	3.30	14 (46%)
24	CHL	5	318	11	36,50,74	4.21	17 (47%)	29,85,114	3.21	17 (58%)
30	LHG	1	318	-	41,41,48	1.24	6 (14%)	44,47,54	0.98	3 (6%)
25	CLA	C	616	20	50,54,73	1.33	7 (14%)	59,90,113	1.47	5 (8%)
25	CLA	7	308	-	54,58,73	1.30	9 (16%)	64,95,113	1.37	5 (7%)
25	CLA	c	601	20	69,73,73	1.15	9 (13%)	82,113,113	1.38	9 (10%)
25	CLA	a	603	19	69,73,73	1.16	10 (14%)	82,113,113	1.37	8 (9%)
24	CHL	9	317	-	36,50,74	4.35	17 (47%)	29,85,114	3.31	15 (51%)
24	CHL	4	304	-	36,50,74	4.30	18 (50%)	29,85,114	3.24	14 (48%)
33	LMG	m	101	-	41,41,55	0.99	2 (4%)	49,49,63	1.24	4 (8%)
25	CLA	p	315	30	67,71,73	1.17	9 (13%)	79,110,113	1.38	6 (7%)
24	CHL	y	306	-	58,72,74	3.15	19 (32%)	55,111,114	2.69	20 (36%)
24	CHL	8	304	17	54,68,74	3.33	19 (35%)	50,106,114	2.83	19 (38%)
24	CHL	R	605	-	36,50,74	4.07	17 (47%)	29,85,114	3.34	16 (55%)
24	CHL	9	305	-	58,72,74	3.31	18 (31%)	55,111,114	2.57	19 (34%)
25	CLA	2	315	-	67,71,73	1.17	9 (13%)	79,110,113	1.29	4 (5%)
31	8CT	c	614	-	40,41,41	4.71	23 (57%)	51,56,56	2.81	21 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CHL	s	408	-	40,54,74	3.89	19 (47%)	34,90,114	3.20	16 (47%)
25	CLA	p	308	-	54,58,73	1.30	9 (16%)	64,95,113	1.36	5 (7%)
24	CHL	q	304	17	54,68,74	3.33	19 (35%)	50,106,114	2.84	19 (38%)
24	CHL	3	317	12	36,50,74	4.23	17 (47%)	29,85,114	3.21	14 (48%)
24	CHL	S	606	-	40,54,74	3.97	19 (47%)	34,90,114	3.03	14 (41%)
24	CHL	3	308	-	37,51,74	4.21	18 (48%)	30,86,114	3.25	15 (50%)
25	CLA	a	605	-	53,57,73	1.28	8 (15%)	61,93,113	1.41	5 (8%)
28	NEX	4	303	25	40,46,46	1.12	3 (7%)	50,70,70	4.73	18 (36%)
24	CHL	q	308	-	40,54,74	3.86	19 (47%)	34,90,114	3.30	16 (47%)
25	CLA	3	313	-	45,49,73	1.41	8 (17%)	54,84,113	1.49	6 (11%)
25	CLA	b	603	18	69,73,73	1.16	8 (11%)	82,113,113	1.29	8 (9%)
25	CLA	b	604	18	66,70,73	1.19	7 (10%)	78,109,113	1.39	7 (8%)
24	CHL	r	306	-	36,50,74	4.15	18 (50%)	29,85,114	3.02	14 (48%)
25	CLA	R	603	-	51,55,73	1.32	8 (15%)	60,91,113	1.43	4 (6%)
24	CHL	4	305	-	40,54,74	3.97	18 (45%)	34,90,114	3.14	14 (41%)
26	OIE	y	303	-	42,45,45	1.15	5 (11%)	51,63,63	1.43	9 (17%)
25	CLA	1	315	10	49,53,73	1.40	9 (18%)	58,89,113	1.44	4 (6%)
33	LMG	B	619	-	41,41,55	0.98	2 (4%)	49,49,63	1.31	4 (8%)
24	CHL	Y	319	-	47,61,74	3.61	19 (40%)	41,98,114	3.01	18 (43%)
25	CLA	5	316	-	49,53,73	1.37	9 (18%)	58,89,113	1.45	4 (6%)
29	OUR	8	301	-	50,53,58	0.96	1 (2%)	59,72,77	1.82	14 (23%)
24	CHL	g	309	-	37,51,74	4.27	18 (48%)	30,86,114	3.32	15 (50%)
25	CLA	y	307	17	57,61,73	1.27	9 (15%)	67,98,113	1.39	6 (8%)
30	LHG	y	319	25	42,42,48	1.20	5 (11%)	45,48,54	1.09	3 (6%)
26	OIE	5	302	-	42,45,45	1.13	6 (14%)	51,63,63	1.49	10 (19%)
25	CLA	g	315	-	64,68,73	1.21	9 (14%)	76,107,113	1.28	5 (6%)
24	CHL	2	312	-	40,54,74	3.92	19 (47%)	34,90,114	3.13	15 (44%)
37	DGD	c	619	-	56,56,67	0.96	3 (5%)	70,70,81	1.24	5 (7%)
25	CLA	a	604	-	69,73,73	1.17	9 (13%)	82,113,113	1.28	6 (7%)
24	CHL	4	311	-	38,52,74	4.04	18 (47%)	31,87,114	3.25	14 (45%)
25	CLA	4	314	-	45,49,73	1.41	8 (17%)	54,84,113	1.48	5 (9%)
24	CHL	7	313	-	37,51,74	4.01	18 (48%)	30,86,114	3.21	14 (46%)
25	CLA	d	405	21	69,73,73	1.15	9 (13%)	82,113,113	1.32	7 (8%)
25	CLA	B	611	18	69,73,73	1.16	8 (11%)	82,113,113	1.38	6 (7%)
24	CHL	n	305	-	54,68,74	3.39	19 (35%)	50,106,114	2.73	18 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	7	317	12	56,60,73	1.29	9 (16%)	65,97,113	1.40	5 (7%)
25	CLA	p	307	12	60,64,73	1.24	9 (15%)	71,102,113	1.38	6 (8%)
26	OIE	9	303	-	42,45,45	1.12	6 (14%)	51,63,63	1.67	13 (25%)
25	CLA	1	316	10	46,50,73	1.41	9 (19%)	53,85,113	1.44	4 (7%)
25	CLA	s	410	-	59,63,73	1.23	9 (15%)	70,101,113	1.33	6 (8%)
32	SQD	b	618	-	52,54,54	0.96	3 (5%)	62,65,65	1.50	11 (17%)
24	CHL	8	307	17	37,51,74	4.03	18 (48%)	30,86,114	3.19	14 (46%)
25	CLA	8	313	17	49,53,73	1.37	9 (18%)	58,89,113	1.45	4 (6%)
28	NEX	r	301	-	40,46,46	1.23	3 (7%)	50,70,70	2.65	16 (32%)
30	LHG	n	318	-	42,42,48	1.22	6 (14%)	45,48,54	0.98	2 (4%)
26	OIE	7	302	-	42,45,45	1.14	6 (14%)	51,63,63	1.57	13 (25%)
25	CLA	C	609	20	69,73,73	1.16	9 (13%)	82,113,113	1.35	7 (8%)
28	NEX	5	304	-	40,46,46	1.11	3 (7%)	50,70,70	4.73	18 (36%)
25	CLA	g	317	17	59,63,73	1.25	9 (15%)	69,100,113	1.35	6 (8%)
25	CLA	B	614	18	60,64,73	1.23	9 (15%)	71,102,113	1.32	5 (7%)
25	CLA	C	601	20	69,73,73	1.15	8 (11%)	82,113,113	1.35	7 (8%)
26	OIE	3	302	-	41,44,45	1.13	6 (14%)	48,60,63	1.56	11 (22%)
37	DGD	C	619	-	51,51,67	0.94	2 (3%)	65,65,81	1.23	5 (7%)
24	CHL	q	303	17	48,62,74	3.65	19 (39%)	43,99,114	2.86	16 (37%)
24	CHL	6	312	-	37,51,74	4.20	18 (48%)	30,86,114	3.16	12 (40%)
25	CLA	q	305	17	58,62,73	1.26	9 (15%)	68,99,113	1.37	6 (8%)
29	OUR	4	301	-	50,53,58	1.01	1 (2%)	59,72,77	1.95	16 (27%)
24	CHL	q	307	17	37,51,74	4.05	18 (48%)	30,86,114	3.17	14 (46%)
25	CLA	b	606	18	69,73,73	1.14	10 (14%)	82,113,113	1.35	8 (9%)
25	CLA	p	314	-	59,63,73	1.25	9 (15%)	70,101,113	1.35	6 (8%)
24	CHL	Y	304	17	60,74,74	3.10	19 (31%)	58,114,114	2.80	17 (29%)
29	OUR	p	301	-	50,53,58	0.96	1 (2%)	59,72,77	1.65	12 (20%)
24	CHL	S	602	13	52,66,74	3.37	19 (36%)	48,104,114	2.94	19 (39%)
24	CHL	y	305	17	60,74,74	3.10	19 (31%)	58,114,114	2.78	15 (25%)
28	NEX	R	616	-	40,46,46	1.12	3 (7%)	50,70,70	4.72	18 (36%)
25	CLA	C	606	20	57,61,73	1.26	9 (15%)	67,98,113	1.39	6 (8%)
25	CLA	Y	316	17	59,63,73	1.24	9 (15%)	69,100,113	1.38	5 (7%)
25	CLA	S	610	-	49,53,73	1.36	9 (18%)	58,89,113	1.40	4 (6%)
24	CHL	5	305	11	38,52,74	4.02	18 (47%)	31,87,114	3.12	15 (48%)
25	CLA	b	605	18	69,73,73	1.16	9 (13%)	82,113,113	1.27	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	OIE	u	302	-	42,45,45	1.12	6 (14%)	51,63,63	1.48	12 (23%)
29	OUR	1	301	-	50,53,58	1.01	2 (4%)	59,72,77	1.95	15 (25%)
24	CHL	9	310	-	40,54,74	4.08	18 (45%)	34,90,114	3.05	14 (41%)
29	OUR	g	301	-	50,53,58	0.96	1 (2%)	59,72,77	1.82	17 (28%)
24	CHL	9	312	-	37,51,74	4.18	18 (48%)	30,86,114	3.27	14 (46%)
31	8CT	A	608	-	40,41,41	4.77	23 (57%)	51,56,56	2.80	18 (35%)
26	OIE	n	302	-	42,45,45	1.12	6 (14%)	51,63,63	1.54	12 (23%)
24	CHL	9	304	12	60,74,74	3.30	18 (30%)	58,114,114	2.43	17 (29%)
25	CLA	G	307	-	57,61,73	1.29	8 (14%)	67,98,113	1.33	5 (7%)
25	CLA	B	613	18	69,73,73	1.17	9 (13%)	82,113,113	1.26	6 (7%)
25	CLA	4	316	-	46,50,73	1.41	8 (17%)	53,85,113	1.43	4 (7%)
25	CLA	c	610	-	69,73,73	1.15	10 (14%)	82,113,113	1.29	7 (8%)
30	LHG	9	318	25	42,42,48	1.22	6 (14%)	45,48,54	0.99	2 (4%)
25	CLA	S	604	-	47,51,73	1.36	7 (14%)	55,86,113	1.43	4 (7%)
25	CLA	1	314	-	45,49,73	1.41	8 (17%)	54,84,113	1.49	5 (9%)
25	CLA	d	404	21	69,73,73	1.15	10 (14%)	82,113,113	1.32	8 (9%)
28	NEX	u	304	-	40,46,46	1.11	3 (7%)	50,70,70	4.73	18 (36%)
25	CLA	D	405	21	69,73,73	1.15	9 (13%)	82,113,113	1.32	7 (8%)
29	OUR	7	301	-	50,53,58	0.96	1 (2%)	59,72,77	1.64	12 (20%)
24	CHL	5	312	-	40,54,74	3.91	19 (47%)	34,90,114	3.14	15 (44%)
34	OEX	a	602	19	0,15,15	-	-	-	-	-
25	CLA	c	604	-	69,73,73	1.14	9 (13%)	82,113,113	1.32	6 (7%)
25	CLA	G	315	-	64,68,73	1.21	9 (14%)	76,107,113	1.28	5 (6%)
24	CHL	g	318	17	36,50,74	4.11	17 (47%)	29,85,114	3.08	14 (48%)
24	CHL	u	312	-	41,55,74	3.98	18 (43%)	35,91,114	3.03	14 (40%)
35	PHO	a	606	-	58,69,69	2.04	11 (18%)	55,99,99	1.43	6 (10%)
28	NEX	2	304	-	40,46,46	1.11	3 (7%)	50,70,70	4.72	18 (36%)
25	CLA	b	616	18	51,55,73	1.33	7 (13%)	60,91,113	1.46	5 (8%)
25	CLA	S	609	-	59,63,73	1.23	9 (15%)	70,101,113	1.32	6 (8%)
25	CLA	c	611	20	69,73,73	1.15	9 (13%)	82,113,113	1.31	6 (7%)
25	CLA	C	607	-	69,73,73	1.14	8 (11%)	82,113,113	1.31	4 (4%)
25	CLA	s	412	13	49,53,73	1.37	9 (18%)	58,89,113	1.45	4 (6%)
24	CHL	1	317	-	36,50,74	4.34	17 (47%)	29,85,114	3.20	15 (51%)
30	LHG	A	612	-	43,43,48	1.20	5 (11%)	46,49,54	1.03	3 (6%)
25	CLA	n	315	17	49,53,73	1.38	9 (18%)	58,89,113	1.43	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	8CT	V	401	-	40,41,41	4.80	23 (57%)	51,56,56	2.64	19 (37%)
26	0IE	7	303	-	42,45,45	1.12	6 (14%)	51,63,63	1.47	10 (19%)
25	CLA	Y	314	30	67,71,73	1.16	7 (10%)	79,110,113	1.25	5 (6%)
24	CHL	G	310	-	41,55,74	4.00	18 (43%)	35,91,114	3.01	16 (45%)
23	HEM	E	201	2	50,50,50	1.36	8 (16%)	67,82,82	1.01	1 (1%)
24	CHL	3	311	-	38,52,74	4.06	17 (44%)	31,87,114	3.24	13 (41%)
24	CHL	8	310	-	50,64,74	3.45	19 (38%)	46,102,114	2.79	19 (41%)
25	CLA	r	304	-	51,55,73	1.32	8 (15%)	60,91,113	1.44	4 (6%)
30	LHG	7	319	25	36,36,48	1.30	6 (16%)	39,42,54	1.09	2 (5%)
25	CLA	5	308	-	54,58,73	1.30	9 (16%)	64,95,113	1.42	6 (9%)
30	LHG	D	408	-	38,38,48	1.26	6 (15%)	41,44,54	1.07	2 (4%)
26	0IE	2	302	-	42,45,45	1.13	6 (14%)	51,63,63	1.48	10 (19%)
25	CLA	9	316	12	59,63,73	1.27	9 (15%)	69,100,113	1.32	5 (7%)
24	CHL	q	310	-	44,58,74	3.66	19 (43%)	37,94,114	3.20	14 (37%)
24	CHL	8	309	-	44,58,74	3.65	19 (43%)	37,94,114	3.24	14 (37%)
25	CLA	5	307	11	47,51,73	1.38	9 (19%)	55,86,113	1.44	4 (7%)
26	0IE	g	303	-	42,45,45	1.12	6 (14%)	51,63,63	1.47	10 (19%)
24	CHL	g	313	-	60,74,74	3.36	19 (31%)	58,114,114	2.47	16 (27%)
33	LMG	D	401	-	48,48,55	0.92	2 (4%)	56,56,63	1.18	5 (8%)
25	CLA	n	314	-	67,71,73	1.19	8 (11%)	79,110,113	1.28	6 (7%)
29	0UR	q	301	-	50,53,58	0.96	1 (2%)	59,72,77	1.83	15 (25%)
29	0UR	G	301	-	50,53,58	0.96	1 (2%)	59,72,77	1.85	17 (28%)
24	CHL	n	311	-	44,58,74	3.75	18 (40%)	37,94,114	3.04	16 (43%)
24	CHL	4	308	10	37,51,74	4.22	17 (45%)	30,86,114	3.33	16 (53%)
25	CLA	b	610	-	69,73,73	1.15	9 (13%)	82,113,113	1.31	6 (7%)
24	CHL	y	310	-	41,55,74	3.79	19 (46%)	35,91,114	3.32	16 (45%)
31	8CT	c	615	-	40,41,41	4.77	23 (57%)	51,56,56	2.79	19 (37%)
25	CLA	Y	315	17	49,53,73	1.36	8 (16%)	58,89,113	1.51	4 (6%)
25	CLA	8	311	-	59,63,73	1.24	9 (15%)	70,101,113	1.37	6 (8%)
25	CLA	R	612	-	49,53,73	1.38	7 (14%)	58,89,113	1.45	4 (6%)
24	CHL	p	312	-	41,55,74	3.78	19 (46%)	35,91,114	3.38	16 (45%)
25	CLA	n	306	17	58,62,73	1.27	9 (15%)	68,99,113	1.36	6 (8%)
25	CLA	9	307	-	54,58,73	1.32	8 (14%)	64,95,113	1.40	5 (7%)
26	0IE	N	302	-	42,45,45	1.12	6 (14%)	51,63,63	1.55	12 (23%)
30	LHG	Y	318	25	42,42,48	1.20	5 (11%)	45,48,54	1.11	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CHL	q	316	-	36,50,74	4.29	18 (50%)	29,85,114	3.17	13 (44%)
28	NEX	r	317	-	40,46,46	1.12	3 (7%)	50,70,70	4.73	18 (36%)
24	CHL	8	303	17	48,62,74	3.66	19 (39%)	43,99,114	2.88	17 (39%)
25	CLA	5	314	-	59,63,73	1.24	9 (15%)	70,101,113	1.34	5 (7%)
25	CLA	y	314	17	59,63,73	1.24	9 (15%)	70,101,113	1.36	7 (10%)
25	CLA	p	316	-	49,53,73	1.37	9 (18%)	58,89,113	1.44	4 (6%)
25	CLA	3	307	-	47,51,73	1.37	8 (17%)	55,86,113	1.44	4 (7%)
29	OUR	5	301	-	50,53,58	1.01	3 (6%)	59,72,77	1.80	14 (23%)
24	CHL	1	312	10	40,54,74	3.98	19 (47%)	34,90,114	3.10	17 (50%)
33	LMG	C	618	-	42,42,55	1.00	2 (4%)	50,50,63	1.24	4 (8%)
24	CHL	4	317	-	36,50,74	4.33	17 (47%)	29,85,114	3.21	15 (51%)
24	CHL	s	406	-	40,54,74	3.91	19 (47%)	34,90,114	3.09	16 (47%)
24	CHL	p	309	12	37,51,74	4.26	18 (48%)	30,86,114	3.34	15 (50%)
25	CLA	9	314	30	67,71,73	1.19	8 (11%)	79,110,113	1.31	6 (7%)
36	BCT	A	611	38	3,3,3	1.12	0	2,3,3	4.21	2 (100%)
24	CHL	1	304	-	36,50,74	4.29	18 (50%)	29,85,114	3.25	14 (48%)
24	CHL	S	601	13	40,54,74	3.84	19 (47%)	34,90,114	3.19	16 (47%)
24	CHL	7	311	-	40,54,74	3.97	19 (47%)	34,90,114	3.11	14 (41%)
29	OUR	3	301	-	50,53,58	0.95	1 (2%)	59,72,77	1.74	12 (20%)
24	CHL	9	311	-	41,55,74	3.98	18 (43%)	35,91,114	3.06	14 (40%)
24	CHL	1	305	10	40,54,74	3.97	18 (45%)	34,90,114	3.15	15 (44%)
24	CHL	g	305	17	60,74,74	3.26	18 (30%)	58,114,114	2.42	16 (27%)
24	CHL	s	409	-	41,55,74	3.90	19 (46%)	35,91,114	3.16	17 (48%)
25	CLA	r	314	-	51,55,73	1.36	7 (13%)	60,91,113	1.35	5 (8%)
25	CLA	n	307	-	54,58,73	1.30	9 (16%)	64,95,113	1.40	6 (9%)
25	CLA	3	314	-	45,49,73	1.40	7 (15%)	54,84,113	1.44	6 (11%)
31	8CT	C	614	-	40,41,41	4.71	23 (57%)	51,56,56	2.79	21 (41%)
25	CLA	n	316	-	47,51,73	1.38	9 (19%)	55,86,113	1.39	4 (7%)
25	CLA	c	605	20	60,64,73	1.23	9 (15%)	71,102,113	1.37	6 (8%)
24	CHL	s	414	-	36,50,74	4.01	18 (50%)	29,85,114	3.16	15 (51%)
25	CLA	g	308	-	54,58,73	1.30	8 (14%)	64,95,113	1.38	6 (9%)
24	CHL	7	306	-	58,72,74	3.17	19 (32%)	55,111,114	2.80	18 (32%)
29	OUR	u	301	-	50,53,58	0.95	1 (2%)	59,72,77	1.86	15 (25%)
31	8CT	d	410	-	40,41,41	4.83	23 (57%)	51,56,56	2.56	19 (37%)
25	CLA	S	612	-	59,63,73	1.25	9 (15%)	69,100,113	1.35	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	B	605	18	69,73,73	1.16	9 (13%)	82,113,113	1.25	5 (6%)
26	OIE	4	302	-	42,45,45	1.13	6 (14%)	51,63,63	1.54	12 (23%)
26	OIE	G	303	-	42,45,45	1.12	6 (14%)	51,63,63	1.48	10 (19%)
24	CHL	G	313	-	60,74,74	3.35	19 (31%)	58,114,114	2.48	15 (25%)
24	CHL	Y	312	-	60,74,74	3.17	19 (31%)	58,114,114	2.56	19 (32%)
25	CLA	b	607	18	69,73,73	1.15	9 (13%)	82,113,113	1.32	6 (7%)
25	CLA	s	411	-	47,52,73	1.42	10 (21%)	55,87,113	1.42	4 (7%)
29	OUR	9	301	-	50,53,58	0.94	1 (2%)	59,72,77	1.82	13 (22%)
24	CHL	G	305	17	60,74,74	3.26	18 (30%)	58,114,114	2.43	17 (29%)
25	CLA	b	613	18	69,73,73	1.16	9 (13%)	82,113,113	1.27	6 (7%)
25	CLA	q	313	-	67,71,73	1.17	9 (13%)	79,110,113	1.27	6 (7%)
25	CLA	q	306	28	54,58,73	1.29	9 (16%)	64,95,113	1.38	7 (10%)
24	CHL	p	311	-	40,54,74	3.97	19 (47%)	34,90,114	3.03	14 (41%)
26	OIE	G	302	-	42,45,45	1.12	6 (14%)	51,63,63	1.53	10 (19%)
25	CLA	s	405	-	47,51,73	1.36	8 (17%)	55,86,113	1.43	4 (7%)
25	CLA	n	313	-	59,63,73	1.25	9 (15%)	70,101,113	1.35	6 (8%)
24	CHL	S	605	-	40,54,74	3.91	19 (47%)	34,90,114	3.11	16 (47%)
28	NEX	p	304	-	40,46,46	1.12	3 (7%)	50,70,70	4.73	19 (38%)
25	CLA	2	308	-	54,58,73	1.30	9 (16%)	64,95,113	1.43	6 (9%)
25	CLA	A	610	-	45,49,73	1.42	7 (15%)	54,84,113	1.50	6 (11%)
28	NEX	N	303	-	40,46,46	1.23	3 (7%)	50,70,70	2.66	16 (32%)
24	CHL	2	313	-	36,50,74	4.15	18 (50%)	29,85,114	3.04	13 (44%)
24	CHL	Y	309	-	41,55,74	3.78	19 (46%)	35,91,114	3.38	16 (45%)
25	CLA	2	317	-	53,57,73	1.30	9 (16%)	61,93,113	1.41	5 (8%)
28	NEX	3	318	-	40,46,46	1.23	3 (7%)	50,70,70	2.65	16 (32%)
25	CLA	S	603	-	49,53,73	1.38	9 (18%)	58,89,113	1.43	4 (6%)
25	CLA	B	612	18	69,73,73	1.14	9 (13%)	82,113,113	1.34	8 (9%)
30	LHG	d	407	-	48,48,48	1.12	5 (10%)	51,54,54	0.98	2 (3%)
25	CLA	a	607	19	64,68,73	1.19	8 (12%)	76,107,113	1.41	8 (10%)
25	CLA	S	611	13	49,53,73	1.36	9 (18%)	58,89,113	1.45	4 (6%)
24	CHL	4	310	-	37,51,74	4.08	17 (45%)	30,86,114	3.20	13 (43%)
25	CLA	1	307	-	45,49,73	1.40	8 (17%)	54,84,113	1.46	6 (11%)
24	CHL	q	309	-	47,61,74	3.60	19 (40%)	41,98,114	2.98	19 (46%)
25	CLA	5	317	11	53,57,73	1.30	9 (16%)	61,93,113	1.43	5 (8%)
25	CLA	6	313	-	45,49,73	1.41	7 (15%)	54,84,113	1.50	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CHL	G	309	-	37,51,74	4.27	18 (48%)	30,86,114	3.31	15 (50%)
24	CHL	6	308	-	37,51,74	4.22	18 (48%)	30,86,114	3.25	15 (50%)
29	OUR	2	301	-	50,53,58	1.02	3 (6%)	59,72,77	1.80	14 (23%)
25	CLA	C	608	20	65,69,73	1.19	10 (15%)	77,108,113	1.36	7 (9%)
24	CHL	n	308	17	37,51,74	4.16	17 (45%)	30,86,114	3.14	15 (50%)
24	CHL	R	608	-	40,54,74	3.93	19 (47%)	34,90,114	3.23	14 (41%)
30	LHG	a	601	-	44,44,48	1.17	5 (11%)	47,50,54	0.99	2 (4%)
30	LHG	g	319	-	42,42,48	1.21	6 (14%)	45,48,54	1.00	2 (4%)
25	CLA	y	315	30	67,71,73	1.16	7 (10%)	79,110,113	1.25	5 (6%)
26	OIE	5	303	-	42,45,45	1.12	6 (14%)	51,63,63	1.45	10 (19%)
24	CHL	5	313	-	36,50,74	4.15	18 (50%)	29,85,114	3.05	14 (48%)
25	CLA	A	607	19	64,68,73	1.18	8 (12%)	76,107,113	1.40	8 (10%)
24	CHL	u	313	-	37,51,74	4.20	17 (45%)	30,86,114	3.23	14 (46%)
25	CLA	9	313	-	59,63,73	1.26	7 (11%)	70,101,113	1.35	6 (8%)
35	PHO	A	606	-	58,69,69	2.05	11 (18%)	55,99,99	1.43	6 (10%)
28	NEX	G	304	-	40,46,46	1.12	3 (7%)	50,70,70	4.73	18 (36%)
24	CHL	6	305	-	42,56,74	3.84	19 (45%)	36,92,114	3.11	17 (47%)
25	CLA	G	308	-	54,58,73	1.31	8 (14%)	64,95,113	1.38	6 (9%)
25	CLA	B	604	18	66,70,73	1.19	7 (10%)	78,109,113	1.41	7 (8%)
25	CLA	b	602	18	69,73,73	1.15	9 (13%)	82,113,113	1.29	6 (7%)
26	OIE	6	302	-	41,44,45	1.14	6 (14%)	48,60,63	1.58	11 (22%)
24	CHL	u	306	-	58,72,74	3.32	18 (31%)	55,111,114	2.53	19 (34%)
35	PHO	d	403	-	58,69,69	2.04	9 (15%)	55,99,99	1.49	7 (12%)
24	CHL	y	312	-	45,59,74	3.64	19 (42%)	40,96,114	2.98	17 (42%)
28	NEX	n	303	-	40,46,46	1.22	3 (7%)	50,70,70	2.65	16 (32%)
25	CLA	4	307	28	45,49,73	1.41	9 (20%)	54,84,113	1.47	6 (11%)
24	CHL	r	308	-	42,56,74	3.79	19 (45%)	36,92,114	3.20	15 (41%)
25	CLA	A	604	-	69,73,73	1.16	9 (13%)	82,113,113	1.30	6 (7%)
25	CLA	C	610	-	69,73,73	1.15	9 (13%)	82,113,113	1.30	7 (8%)
31	8CT	S	615	-	40,41,41	4.85	24 (60%)	51,56,56	6.92	22 (43%)
28	NEX	s	401	25	40,46,46	1.23	3 (7%)	50,70,70	2.65	16 (32%)
25	CLA	g	314	-	59,63,73	1.26	9 (15%)	70,101,113	1.34	6 (8%)
31	8CT	v	401	-	40,41,41	4.81	23 (57%)	51,56,56	2.63	19 (37%)
25	CLA	9	306	-	60,64,73	1.26	8 (13%)	71,102,113	1.32	5 (7%)
24	CHL	G	306	17	58,72,74	3.29	19 (32%)	55,111,114	2.65	19 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CHL	r	307	-	42,56,74	3.84	18 (42%)	36,92,114	3.09	15 (41%)
24	CHL	6	310	-	40,54,74	4.08	18 (45%)	34,90,114	3.05	12 (35%)
30	LHG	d	408	-	38,38,48	0.99	3 (7%)	41,44,54	1.26	4 (9%)
26	OIE	R	614	-	42,45,45	1.14	6 (14%)	51,63,63	1.48	11 (21%)
25	CLA	R	604	-	45,49,73	1.40	9 (20%)	54,84,113	1.52	6 (11%)
24	CHL	6	317	12	36,50,74	4.22	18 (50%)	29,85,114	3.20	13 (44%)
24	CHL	r	309	-	40,54,74	3.93	19 (47%)	34,90,114	3.23	14 (41%)
25	CLA	c	607	-	69,73,73	1.15	8 (11%)	82,113,113	1.32	4 (4%)
26	OIE	u	303	-	42,45,45	1.11	6 (14%)	51,63,63	1.58	10 (19%)
30	LHG	a	612	-	43,43,48	1.20	5 (11%)	46,49,54	1.03	3 (6%)
24	CHL	l	311	-	38,52,74	4.02	18 (47%)	31,87,114	3.29	14 (45%)
24	CHL	g	310	-	41,55,74	4.01	18 (43%)	35,91,114	3.04	16 (45%)
24	CHL	n	317	-	36,50,74	4.33	18 (50%)	29,85,114	3.26	16 (55%)
24	CHL	5	310	-	36,50,74	4.07	18 (50%)	29,85,114	3.03	14 (48%)
24	CHL	l	310	-	37,51,74	4.09	17 (45%)	30,86,114	3.19	13 (43%)
24	CHL	r	302	8	40,54,74	4.07	18 (45%)	34,90,114	3.08	14 (41%)
25	CLA	r	312	8	49,53,73	1.38	9 (18%)	58,89,113	1.43	4 (6%)
32	SQD	a	609	-	43,45,54	1.05	3 (6%)	53,56,65	1.59	10 (18%)
25	CLA	C	612	20	58,62,73	1.24	9 (15%)	68,99,113	1.42	5 (7%)
32	SQD	d	409	-	42,44,54	1.06	3 (7%)	52,55,65	1.50	8 (15%)
25	CLA	7	307	12	60,64,73	1.24	9 (15%)	71,102,113	1.38	6 (8%)
25	CLA	D	404	21	69,73,73	1.15	10 (14%)	82,113,113	1.31	8 (9%)
25	CLA	c	612	20	58,62,73	1.25	9 (15%)	68,99,113	1.41	6 (8%)
25	CLA	b	601	-	49,53,73	1.36	9 (18%)	58,89,113	1.44	4 (6%)
35	PHO	D	403	-	58,69,69	2.04	10 (17%)	55,99,99	1.49	7 (12%)
25	CLA	4	313	-	59,63,73	1.27	9 (15%)	70,101,113	1.34	6 (8%)
25	CLA	G	317	-	59,63,73	1.25	8 (13%)	69,100,113	1.35	5 (7%)
24	CHL	7	305	12	60,74,74	3.13	19 (31%)	58,114,114	2.82	17 (29%)
25	CLA	B	606	18	69,73,73	1.14	9 (13%)	82,113,113	1.35	8 (9%)
25	CLA	B	603	18	69,73,73	1.16	8 (11%)	82,113,113	1.29	8 (9%)
24	CHL	2	310	-	36,50,74	4.08	18 (50%)	29,85,114	3.03	14 (48%)
24	CHL	p	313	-	37,51,74	4.02	18 (48%)	30,86,114	3.20	14 (46%)
24	CHL	G	311	-	48,62,74	3.68	18 (37%)	43,99,114	2.84	16 (37%)
25	CLA	q	314	17	49,53,73	1.38	9 (18%)	58,89,113	1.46	4 (6%)
24	CHL	g	311	-	48,62,74	3.70	18 (37%)	43,99,114	2.77	16 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	8	305	17	58,62,73	1.26	9 (15%)	68,99,113	1.36	6 (8%)
33	LMG	W	201	-	30,30,55	1.14	2 (6%)	38,38,63	1.39	6 (15%)
24	CHL	3	309	-	45,59,74	3.84	18 (40%)	40,96,114	2.91	17 (42%)
27	XAT	R	615	-	41,47,47	0.91	1 (2%)	54,74,74	2.65	21 (38%)
25	CLA	R	610	-	49,53,73	1.36	8 (16%)	58,89,113	1.43	6 (10%)
24	CHL	q	311	-	50,64,74	3.44	19 (38%)	46,102,114	2.80	19 (41%)
24	CHL	1	308	10	37,51,74	4.21	18 (48%)	30,86,114	3.32	15 (50%)
25	CLA	B	616	18	51,55,73	1.33	7 (13%)	60,91,113	1.46	4 (6%)
24	CHL	3	310	-	40,54,74	4.07	18 (45%)	34,90,114	3.06	12 (35%)
26	OIE	p	302	-	42,45,45	1.14	6 (14%)	51,63,63	1.57	13 (25%)
24	CHL	Y	308	17	37,51,74	4.04	18 (48%)	30,86,114	3.17	13 (43%)
31	8CT	B	617	-	40,41,41	4.78	23 (57%)	51,56,56	2.97	18 (35%)
24	CHL	y	318	17	36,50,74	3.96	18 (50%)	29,85,114	3.10	17 (58%)
24	CHL	u	310	-	40,54,74	4.09	18 (45%)	34,90,114	3.07	14 (41%)
25	CLA	B	608	-	59,63,73	1.25	9 (15%)	70,101,113	1.34	6 (8%)
24	CHL	p	305	12	60,74,74	3.14	19 (31%)	58,114,114	2.79	17 (29%)
24	CHL	s	403	13	52,66,74	3.37	19 (36%)	48,104,114	2.93	19 (39%)
26	OIE	r	315	-	42,45,45	1.14	6 (14%)	51,63,63	1.49	11 (21%)
25	CLA	g	316	17	49,53,73	1.38	9 (18%)	58,89,113	1.46	4 (6%)
30	LHG	c	617	-	31,31,48	1.36	6 (19%)	34,37,54	1.15	3 (8%)
39	PL9	D	406	-	55,55,55	1.64	12 (21%)	68,69,69	1.53	13 (19%)
24	CHL	n	304	17	48,62,74	3.72	19 (39%)	43,99,114	2.79	16 (37%)
24	CHL	u	305	12	60,74,74	3.35	18 (30%)	58,114,114	2.47	18 (31%)
24	CHL	Y	305	-	58,72,74	3.16	19 (32%)	55,111,114	2.69	20 (36%)
24	CHL	g	306	-	58,72,74	3.27	19 (32%)	55,111,114	2.71	19 (34%)
24	CHL	y	309	17	37,51,74	4.04	18 (48%)	30,86,114	3.18	13 (43%)
26	OIE	2	303	-	42,45,45	1.12	6 (14%)	51,63,63	1.45	10 (19%)
24	CHL	N	305	-	54,68,74	3.39	19 (35%)	50,106,114	2.71	18 (36%)
30	LHG	5	319	-	42,42,48	1.21	6 (14%)	45,48,54	1.05	3 (6%)
24	CHL	n	310	-	47,61,74	3.73	18 (38%)	41,98,114	2.90	16 (39%)
25	CLA	c	603	20	69,73,73	1.15	9 (13%)	82,113,113	1.32	8 (9%)
25	CLA	8	306	-	54,58,73	1.29	9 (16%)	64,95,113	1.38	7 (10%)
28	NEX	6	303	-	40,46,46	1.23	3 (7%)	50,70,70	2.66	16 (32%)
25	CLA	4	315	10	49,53,73	1.39	9 (18%)	58,89,113	1.44	4 (6%)
30	LHG	2	319	-	39,39,48	1.25	6 (15%)	42,45,54	1.07	3 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	8CT	T	101	-	40,41,41	4.78	23 (57%)	51,56,56	3.07	17 (33%)
24	CHL	2	305	11	38,52,74	4.03	18 (47%)	31,87,114	3.12	14 (45%)
25	CLA	u	308	-	54,58,73	1.32	8 (14%)	64,95,113	1.39	6 (9%)
31	8CT	t	101	-	40,41,41	4.78	23 (57%)	51,56,56	3.08	17 (33%)
29	OUR	n	301	-	50,53,58	0.95	1 (2%)	59,72,77	1.84	13 (22%)
25	CLA	N	313	-	59,63,73	1.25	8 (13%)	70,101,113	1.36	6 (8%)
33	LMG	D	411	-	46,46,55	0.96	2 (4%)	54,54,63	1.14	4 (7%)
24	CHL	S	607	-	40,54,74	3.90	19 (47%)	34,90,114	3.09	17 (50%)
25	CLA	N	306	17	58,62,73	1.27	9 (15%)	68,99,113	1.36	6 (8%)
25	CLA	u	317	12	59,63,73	1.28	8 (13%)	69,100,113	1.34	5 (7%)
37	DGD	C	620	-	56,56,67	0.95	2 (3%)	70,70,81	1.22	5 (7%)
24	CHL	Y	317	17	36,50,74	3.97	18 (50%)	29,85,114	3.10	17 (58%)
25	CLA	r	311	-	49,53,73	1.36	9 (18%)	58,89,113	1.44	6 (10%)
25	CLA	G	316	17	49,53,73	1.38	9 (18%)	58,89,113	1.44	4 (6%)
24	CHL	6	311	-	38,52,74	4.04	17 (44%)	31,87,114	3.24	13 (41%)
25	CLA	1	313	-	59,63,73	1.26	8 (13%)	70,101,113	1.35	6 (8%)
25	CLA	1	306	-	47,52,73	1.37	7 (14%)	55,87,113	1.43	5 (9%)
25	CLA	u	307	-	60,64,73	1.26	8 (13%)	71,102,113	1.33	5 (7%)
28	NEX	S	617	-	40,46,46	1.11	3 (7%)	50,70,70	4.73	18 (36%)
25	CLA	C	604	-	69,73,73	1.14	9 (13%)	82,113,113	1.31	6 (7%)
31	8CT	s	416	-	40,41,41	4.87	24 (60%)	51,56,56	6.92	21 (41%)
24	CHL	6	304	12	42,56,74	3.93	19 (45%)	36,92,114	2.95	15 (41%)
24	CHL	3	312	-	37,51,74	4.20	17 (45%)	30,86,114	3.15	12 (40%)
25	CLA	b	614	18	60,64,73	1.23	10 (16%)	71,102,113	1.33	5 (7%)
29	OUR	6	301	-	50,53,58	0.95	1 (2%)	59,72,77	1.82	15 (25%)
30	LHG	N	318	-	42,42,48	1.22	6 (14%)	45,48,54	0.98	2 (4%)
25	CLA	Y	306	17	57,61,73	1.27	9 (15%)	67,98,113	1.39	6 (8%)
25	CLA	r	310	8	59,63,73	1.24	9 (15%)	70,101,113	1.34	6 (8%)
26	OIE	Y	302	-	42,45,45	1.15	6 (14%)	51,63,63	1.51	11 (21%)
33	LMG	d	401	-	48,48,55	0.92	2 (4%)	56,56,63	1.20	5 (8%)
25	CLA	7	315	30	67,71,73	1.17	9 (13%)	79,110,113	1.36	6 (7%)
24	CHL	2	318	11	36,50,74	4.21	17 (47%)	29,85,114	3.20	17 (58%)
25	CLA	C	602	20	69,73,73	1.16	8 (11%)	82,113,113	1.31	6 (7%)
24	CHL	2	309	11	37,51,74	4.15	18 (48%)	30,86,114	3.20	16 (53%)
28	NEX	y	304	-	40,46,46	1.12	3 (7%)	50,70,70	4.72	18 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	c	616	20	50,54,73	1.32	8 (16%)	59,90,113	1.47	6 (10%)
25	CLA	R	609	8	59,63,73	1.24	9 (15%)	70,101,113	1.35	6 (8%)
24	CHL	8	315	-	36,50,74	4.29	18 (50%)	29,85,114	3.20	14 (48%)
25	CLA	3	315	12	49,53,73	1.39	9 (18%)	58,89,113	1.44	4 (6%)
25	CLA	N	315	17	49,53,73	1.38	9 (18%)	58,89,113	1.42	4 (6%)
30	LHG	G	319	-	42,42,48	1.21	6 (14%)	45,48,54	1.00	2 (4%)
24	CHL	N	304	17	48,62,74	3.72	19 (39%)	43,99,114	2.78	16 (37%)
25	CLA	Y	313	17	59,63,73	1.24	9 (15%)	70,101,113	1.36	7 (10%)
24	CHL	1	309	-	37,51,74	4.19	18 (48%)	30,86,114	3.25	14 (46%)
25	CLA	Y	307	-	54,58,73	1.29	9 (16%)	64,95,113	1.43	8 (12%)
24	CHL	5	311	-	41,55,74	3.96	19 (46%)	35,91,114	2.98	14 (40%)
25	CLA	c	606	20	57,61,73	1.27	9 (15%)	67,98,113	1.39	6 (8%)
25	CLA	8	312	-	67,71,73	1.18	9 (13%)	79,110,113	1.28	6 (7%)
34	OEX	A	602	19	0,15,15	-	-	-	-	-
25	CLA	R	611	8	49,53,73	1.38	9 (18%)	58,89,113	1.42	4 (6%)
25	CLA	a	610	-	45,49,73	1.42	7 (15%)	54,84,113	1.49	6 (11%)
25	CLA	N	316	-	47,51,73	1.39	8 (17%)	55,86,113	1.39	4 (7%)
24	CHL	N	317	-	36,50,74	4.33	18 (50%)	29,85,114	3.25	15 (51%)
31	8CT	C	613	-	40,41,41	4.74	23 (57%)	51,56,56	2.80	20 (39%)
25	CLA	G	314	-	59,63,73	1.25	9 (15%)	70,101,113	1.33	6 (8%)
24	CHL	R	607	-	42,56,74	3.79	19 (45%)	36,92,114	3.21	15 (41%)
24	CHL	R	602	-	41,55,74	3.81	18 (43%)	35,91,114	3.31	16 (45%)
24	CHL	s	407	-	40,54,74	3.97	19 (47%)	34,90,114	3.02	14 (41%)
24	CHL	p	310	-	40,54,74	4.02	19 (47%)	34,90,114	3.06	14 (41%)
25	CLA	6	316	-	49,53,73	1.38	9 (18%)	58,89,113	1.43	4 (6%)
30	LHG	A	601	-	44,44,48	1.18	5 (11%)	47,50,54	0.99	2 (4%)
25	CLA	b	609	18	69,73,73	1.15	8 (11%)	82,113,113	1.31	7 (8%)
25	CLA	B	602	18	69,73,73	1.15	9 (13%)	82,113,113	1.29	6 (7%)
25	CLA	p	317	12	59,63,73	1.25	9 (15%)	69,100,113	1.38	6 (8%)
24	CHL	2	306	-	41,55,74	3.82	19 (46%)	35,91,114	3.23	17 (48%)
28	NEX	1	303	-	40,46,46	1.12	3 (7%)	50,70,70	4.72	18 (36%)
31	8CT	b	617	-	40,41,41	4.80	23 (57%)	51,56,56	2.92	18 (35%)
24	CHL	R	601	8	40,54,74	4.09	19 (47%)	34,90,114	3.07	14 (41%)
24	CHL	S	613	-	36,50,74	4.03	18 (50%)	29,85,114	3.15	15 (51%)
30	LHG	p	319	25	42,42,48	1.22	6 (14%)	45,48,54	1.03	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	B	607	18	69,73,73	1.15	9 (13%)	82,113,113	1.32	6 (7%)
29	OUR	Y	301	-	50,53,58	1.01	2 (4%)	59,72,77	1.71	13 (22%)
31	8CT	a	608	-	40,41,41	4.77	23 (57%)	51,56,56	2.80	18 (35%)
24	CHL	4	309	-	37,51,74	4.18	18 (48%)	30,86,114	3.26	15 (50%)
33	LMG	i	101	-	48,48,55	0.93	2 (4%)	56,56,63	1.21	4 (7%)
24	CHL	u	311	-	40,54,74	4.06	18 (45%)	34,90,114	3.05	14 (41%)
25	CLA	B	610	-	69,73,73	1.15	9 (13%)	82,113,113	1.32	6 (7%)
25	CLA	c	608	20	65,69,73	1.18	8 (12%)	77,108,113	1.35	7 (9%)
25	CLA	u	314	-	59,63,73	1.26	6 (10%)	70,101,113	1.34	7 (10%)
31	8CT	D	410	-	40,41,41	4.84	23 (57%)	51,56,56	2.54	20 (39%)
32	SQD	B	618	-	52,54,54	0.96	3 (5%)	62,65,65	1.50	11 (17%)
25	CLA	g	307	-	57,61,73	1.29	8 (14%)	67,98,113	1.32	5 (7%)
25	CLA	q	315	17	47,51,73	1.37	9 (19%)	55,86,113	1.42	4 (7%)
25	CLA	b	611	18	69,73,73	1.16	8 (11%)	82,113,113	1.38	6 (7%)
24	CHL	7	312	-	41,55,74	3.76	19 (46%)	35,91,114	3.41	16 (45%)
24	CHL	Y	310	-	48,62,74	3.52	19 (39%)	43,99,114	3.19	20 (46%)
26	OIE	y	302	-	42,45,45	1.16	6 (14%)	51,63,63	1.49	11 (21%)
25	CLA	6	306	-	45,49,73	1.40	8 (17%)	54,84,113	1.48	6 (11%)
25	CLA	R	613	-	51,55,73	1.36	7 (13%)	60,91,113	1.35	5 (8%)
24	CHL	3	304	12	42,56,74	3.90	19 (45%)	36,92,114	2.92	15 (41%)
24	CHL	7	318	12	36,50,74	4.16	18 (50%)	29,85,114	3.03	13 (44%)
25	CLA	N	314	-	67,71,73	1.18	8 (11%)	79,110,113	1.27	6 (7%)
26	OIE	g	302	-	42,45,45	1.12	6 (14%)	51,63,63	1.53	11 (21%)
24	CHL	u	318	-	36,50,74	4.35	17 (47%)	29,85,114	3.30	15 (51%)
25	CLA	r	313	-	49,53,73	1.38	7 (14%)	58,89,113	1.48	5 (8%)
29	OUR	N	301	-	50,53,58	0.95	1 (2%)	59,72,77	1.85	13 (22%)
25	CLA	7	316	12	49,53,73	1.36	9 (18%)	58,89,113	1.43	4 (6%)
25	CLA	u	316	-	49,53,73	1.39	9 (18%)	58,89,113	1.42	4 (6%)
25	CLA	c	602	20	69,73,73	1.17	8 (11%)	82,113,113	1.31	6 (7%)
24	CHL	5	306	-	41,55,74	3.83	19 (46%)	35,91,114	3.22	17 (48%)
25	CLA	s	413	-	59,63,73	1.24	9 (15%)	69,100,113	1.36	5 (7%)
24	CHL	N	311	-	44,58,74	3.76	19 (43%)	37,94,114	3.01	16 (43%)
24	CHL	r	303	-	41,55,74	3.81	18 (43%)	35,91,114	3.33	16 (45%)
25	CLA	3	316	-	49,53,73	1.38	9 (18%)	58,89,113	1.44	4 (6%)
24	CHL	p	318	12	36,50,74	4.16	18 (50%)	29,85,114	3.03	12 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	4	306	-	47,52,73	1.38	8 (17%)	55,87,113	1.44	5 (9%)
25	CLA	B	609	18	69,73,73	1.15	8 (11%)	82,113,113	1.31	7 (8%)
31	8CT	S	614	-	40,41,41	4.85	23 (57%)	51,56,56	3.04	20 (39%)
24	CHL	7	309	12	37,51,74	4.26	18 (48%)	30,86,114	3.36	14 (46%)
25	CLA	2	316	-	49,53,73	1.37	9 (18%)	58,89,113	1.45	4 (6%)
31	8CT	c	613	-	40,41,41	4.75	23 (57%)	51,56,56	2.78	22 (43%)
36	BCT	a	611	38	3,3,3	1.12	0	2,3,3	4.19	2 (100%)
24	CHL	p	306	-	58,72,74	3.18	19 (32%)	55,111,114	2.79	18 (32%)
25	CLA	y	308	-	54,58,73	1.29	9 (16%)	64,95,113	1.42	8 (12%)
24	CHL	3	305	-	42,56,74	3.85	18 (42%)	36,92,114	3.08	17 (47%)
25	CLA	B	601	-	49,53,73	1.36	9 (18%)	58,89,113	1.44	4 (6%)
25	CLA	r	305	-	45,49,73	1.41	9 (20%)	54,84,113	1.53	7 (12%)
25	CLA	S	616	-	49,53,73	1.36	9 (18%)	58,89,113	1.41	4 (6%)
25	CLA	A	605	-	53,57,73	1.29	8 (15%)	61,93,113	1.42	5 (8%)
25	CLA	y	317	17	59,63,73	1.23	9 (15%)	69,100,113	1.38	5 (7%)
33	LMG	w	201	-	36,36,55	1.06	2 (5%)	44,44,63	1.36	5 (11%)
25	CLA	C	603	20	69,73,73	1.15	9 (13%)	82,113,113	1.32	7 (8%)
24	CHL	6	309	-	45,59,74	3.83	18 (40%)	40,96,114	2.92	18 (45%)
24	CHL	u	309	12	37,51,74	4.28	18 (48%)	30,86,114	3.26	14 (46%)
26	OIE	Y	303	-	42,45,45	1.14	5 (11%)	51,63,63	1.43	9 (17%)
24	CHL	N	310	-	47,61,74	3.72	19 (40%)	41,98,114	2.89	16 (39%)
25	CLA	8	314	-	47,51,73	1.38	9 (19%)	55,86,113	1.43	5 (9%)
31	8CT	x	601	-	40,41,41	4.77	23 (57%)	51,56,56	2.72	18 (35%)
25	CLA	6	315	12	49,53,73	1.39	9 (18%)	58,89,113	1.45	4 (6%)
28	NEX	7	304	-	40,46,46	1.11	3 (7%)	50,70,70	4.72	18 (36%)
24	CHL	R	606	-	42,56,74	3.84	18 (42%)	36,92,114	3.14	15 (41%)
24	CHL	S	608	-	41,55,74	3.90	19 (46%)	35,91,114	3.19	17 (48%)
32	SQD	A	609	-	43,45,54	1.06	3 (6%)	53,56,65	1.49	10 (18%)
25	CLA	5	315	-	67,71,73	1.18	9 (13%)	79,110,113	1.29	5 (6%)
31	8CT	s	415	-	40,41,41	4.86	23 (57%)	51,56,56	3.04	20 (39%)
24	CHL	G	312	-	45,59,74	3.82	19 (42%)	40,96,114	2.89	18 (45%)
28	NEX	9	319	-	40,46,46	1.11	3 (7%)	50,70,70	4.72	18 (36%)
24	CHL	4	312	-	40,54,74	3.99	19 (47%)	34,90,114	3.09	16 (47%)
25	CLA	2	307	11	47,51,73	1.37	8 (17%)	55,86,113	1.42	4 (7%)
25	CLA	s	417	-	49,53,73	1.37	8 (16%)	58,89,113	1.41	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	LMG	d	411	-	46,46,55	0.95	2 (4%)	54,54,63	1.13	4 (7%)
24	CHL	9	309	-	40,54,74	4.08	18 (45%)	34,90,114	3.05	15 (44%)
31	8CT	X	601	-	40,41,41	4.78	23 (57%)	51,56,56	2.71	18 (35%)
29	OUR	y	301	-	50,53,58	1.00	1 (2%)	59,72,77	1.71	13 (22%)
25	CLA	b	608	-	59,63,73	1.25	9 (15%)	70,101,113	1.35	6 (8%)

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
25	CLA	9	315	-	1/1/11/20	6/15/91/115	-
25	CLA	q	312	-	1/1/13/20	2/27/103/115	-
37	DGD	c	618	-	-	27/39/79/95	0/2/2/2
39	PL9	d	406	-	-	10/53/73/73	0/1/1/1
25	CLA	N	307	-	1/1/12/20	5/21/97/115	-
26	OIE	p	303	-	-	2/33/72/72	0/2/2/2
25	CLA	7	314	-	1/1/13/20	6/27/103/115	-
25	CLA	b	615	18	1/1/15/20	5/39/115/115	-
31	8CT	C	615	-	-	13/29/63/63	0/2/2/2
24	CHL	n	312	-	3/3/18/26	14/27/125/137	-
25	CLA	s	404	-	1/1/11/20	6/15/91/115	-
26	OIE	3	303	-	-	1/33/72/72	0/2/2/2
24	CHL	G	318	17	3/3/15/26	6/10/108/137	-
30	LHG	4	318	-	-	21/46/46/53	-
25	CLA	2	314	-	1/1/13/20	4/27/103/115	-
24	CHL	5	309	11	3/3/15/26	3/12/110/137	-
30	LHG	C	617	-	-	17/36/36/53	-
25	CLA	6	307	-	1/1/10/20	6/13/89/115	-
24	CHL	2	311	-	3/3/16/26	8/17/115/137	-
25	CLA	u	315	-	1/1/14/20	11/37/113/115	-
26	OIE	1	302	-	-	2/33/72/72	0/2/2/2
30	LHG	D	407	-	-	29/53/53/53	-
25	CLA	C	611	20	1/1/15/20	10/39/115/115	-
24	CHL	n	309	-	3/3/16/26	6/15/113/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	s	402	13	3/3/16/26	13/15/113/137	-
24	CHL	7	310	-	3/3/16/26	7/15/113/137	-
28	NEX	g	304	-	-	5/27/83/83	0/3/3/3
25	CLA	C	605	20	1/1/13/20	7/29/105/115	-
25	CLA	c	609	20	1/1/15/20	5/39/115/115	-
24	CHL	N	312	-	3/3/18/26	14/27/125/137	-
32	SQD	D	409	-	-	13/39/59/69	0/1/1/1
24	CHL	8	308	-	3/3/16/26	5/15/113/137	-
25	CLA	B	615	18	1/1/15/20	4/39/115/115	-
24	CHL	Y	311	-	3/3/17/26	5/21/119/137	-
25	CLA	b	612	18	1/1/15/20	12/39/115/115	-
24	CHL	g	312	-	3/3/17/26	4/21/119/137	-
25	CLA	3	306	-	1/1/10/20	6/10/86/115	-
25	CLA	6	314	-	1/1/10/20	2/10/86/115	-
26	OIE	9	302	-	-	4/33/72/72	0/2/2/2
24	CHL	N	308	17	3/3/15/26	2/12/110/137	-
23	HEM	f	201	9,2	-	1/14/54/54	-
25	CLA	A	603	19	1/1/15/20	12/39/115/115	-
24	CHL	y	311	-	3/3/17/26	12/25/123/137	-
26	OIE	q	302	-	-	2/33/72/72	0/2/2/2
25	CLA	y	316	17	1/1/11/20	6/15/91/115	-
26	OIE	8	302	-	-	2/33/72/72	0/2/2/2
27	XAT	r	316	-	-	0/31/93/93	0/4/4/4
24	CHL	N	309	-	3/3/16/26	7/15/113/137	-
24	CHL	y	313	-	3/3/20/26	19/39/137/137	-
24	CHL	9	308	12	3/3/15/26	2/12/110/137	-
24	CHL	5	318	11	3/3/15/26	4/10/108/137	-
30	LHG	1	318	-	-	22/46/46/53	-
25	CLA	C	616	20	1/1/11/20	2/17/93/115	-
25	CLA	7	308	-	1/1/12/20	5/21/97/115	-
25	CLA	c	601	20	1/1/15/20	14/39/115/115	-
25	CLA	a	603	19	1/1/15/20	12/39/115/115	-
24	CHL	9	317	-	3/3/15/26	4/10/108/137	-
24	CHL	4	304	-	3/3/15/26	3/10/108/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LMG	m	101	-	-	19/36/56/70	0/1/1/1
25	CLA	p	315	30	1/1/14/20	14/37/113/115	-
24	CHL	y	306	-	3/3/19/26	22/37/135/137	-
24	CHL	8	304	17	3/3/18/26	15/32/130/137	-
24	CHL	R	605	-	3/3/15/26	2/10/108/137	-
24	CHL	9	305	-	3/3/19/26	14/37/135/137	-
25	CLA	2	315	-	1/1/14/20	10/37/113/115	-
31	8CT	c	614	-	-	15/29/63/63	0/2/2/2
24	CHL	s	408	-	3/3/16/26	7/15/113/137	-
25	CLA	p	308	-	1/1/12/20	5/21/97/115	-
24	CHL	q	304	17	3/3/18/26	17/32/130/137	-
24	CHL	3	317	12	3/3/15/26	2/10/108/137	-
24	CHL	S	606	-	3/3/16/26	8/15/113/137	-
24	CHL	3	308	-	3/3/15/26	4/12/110/137	-
25	CLA	a	605	-	1/1/11/20	6/20/96/115	-
28	NEX	4	303	25	-	5/27/83/83	0/3/3/3
24	CHL	q	308	-	3/3/16/26	5/15/113/137	-
25	CLA	3	313	-	1/1/10/20	2/10/86/115	-
25	CLA	b	603	18	1/1/15/20	11/39/115/115	-
25	CLA	b	604	18	1/1/14/20	14/36/112/115	-
24	CHL	r	306	-	3/3/15/26	4/10/108/137	-
25	CLA	R	603	-	1/1/11/20	5/18/94/115	-
24	CHL	4	305	-	3/3/16/26	8/15/113/137	-
26	OIE	y	303	-	-	0/33/72/72	0/2/2/2
25	CLA	1	315	10	1/1/11/20	8/15/91/115	-
33	LMG	B	619	-	-	20/36/56/70	0/1/1/1
24	CHL	Y	319	-	3/3/17/26	7/24/122/137	-
25	CLA	5	316	-	1/1/11/20	4/15/91/115	-
29	OUR	8	301	-	-	9/42/81/86	0/2/2/2
24	CHL	g	309	-	3/3/15/26	2/12/110/137	-
25	CLA	y	307	17	1/1/12/20	4/25/101/115	-
30	LHG	y	319	25	-	23/47/47/53	-
26	OIE	5	302	-	-	2/33/72/72	0/2/2/2
25	CLA	g	315	-	1/1/14/20	7/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	2	312	-	3/3/16/26	8/15/113/137	-
37	DGD	c	619	-	-	17/44/84/95	0/2/2/2
25	CLA	a	604	-	1/1/15/20	8/39/115/115	-
24	CHL	4	311	-	3/3/15/26	3/13/111/137	-
25	CLA	4	314	-	1/1/10/20	4/10/86/115	-
24	CHL	7	313	-	3/3/15/26	6/12/110/137	-
25	CLA	d	405	21	1/1/15/20	13/39/115/115	-
25	CLA	B	611	18	1/1/15/20	4/39/115/115	-
24	CHL	n	305	-	3/3/18/26	16/32/130/137	-
25	CLA	7	317	12	1/1/12/20	5/24/100/115	-
25	CLA	p	307	12	1/1/13/20	7/29/105/115	-
26	OIE	9	303	-	-	5/33/72/72	0/2/2/2
25	CLA	1	316	10	1/1/10/20	0/12/88/115	-
25	CLA	s	410	-	1/1/13/20	5/27/103/115	-
32	SQD	b	618	-	-	14/49/69/69	0/1/1/1
24	CHL	8	307	17	3/3/15/26	2/12/110/137	-
25	CLA	8	313	17	1/1/11/20	4/15/91/115	-
28	NEX	r	301	-	-	4/27/83/83	0/3/3/3
30	LHG	n	318	-	-	18/47/47/53	-
26	OIE	7	302	-	-	4/33/72/72	0/2/2/2
25	CLA	C	609	20	1/1/15/20	5/39/115/115	-
28	NEX	5	304	-	-	5/27/83/83	0/3/3/3
25	CLA	g	317	17	1/1/12/20	6/27/103/115	-
25	CLA	B	614	18	1/1/13/20	13/29/105/115	-
25	CLA	C	601	20	1/1/15/20	14/39/115/115	-
26	OIE	3	302	-	-	4/33/69/72	0/2/2/2
37	DGD	C	619	-	-	27/39/79/95	0/2/2/2
24	CHL	q	303	17	3/3/17/26	10/25/123/137	-
24	CHL	6	312	-	3/3/15/26	5/12/110/137	-
25	CLA	q	305	17	1/1/12/20	9/26/102/115	-
29	OUR	4	301	-	-	13/42/81/86	0/2/2/2
24	CHL	q	307	17	3/3/15/26	1/12/110/137	-
25	CLA	b	606	18	1/1/15/20	16/39/115/115	-
25	CLA	p	314	-	1/1/13/20	4/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	Y	304	17	3/3/20/26	15/39/137/137	-
29	OUR	p	301	-	-	8/42/81/86	0/2/2/2
24	CHL	S	602	13	3/3/18/26	14/30/128/137	-
24	CHL	y	305	17	3/3/20/26	14/39/137/137	-
28	NEX	R	616	-	-	5/27/83/83	0/3/3/3
25	CLA	C	606	20	1/1/12/20	7/25/101/115	-
25	CLA	Y	316	17	1/1/12/20	6/27/103/115	-
25	CLA	S	610	-	1/1/11/20	2/15/91/115	-
24	CHL	5	305	11	3/3/15/26	9/13/111/137	-
25	CLA	b	605	18	1/1/15/20	13/39/115/115	-
26	OIE	u	302	-	-	4/33/72/72	0/2/2/2
29	OUR	l	301	-	-	13/42/81/86	0/2/2/2
24	CHL	9	310	-	3/3/16/26	4/15/113/137	-
29	OUR	g	301	-	-	10/42/81/86	0/2/2/2
24	CHL	9	312	-	3/3/15/26	3/12/110/137	-
31	8CT	A	608	-	-	8/29/63/63	0/2/2/2
26	OIE	n	302	-	-	2/33/72/72	0/2/2/2
24	CHL	9	304	12	3/3/20/26	15/39/137/137	-
25	CLA	G	307	-	1/1/12/20	5/25/101/115	-
25	CLA	B	613	18	1/1/15/20	9/39/115/115	-
25	CLA	4	316	-	1/1/10/20	0/12/88/115	-
25	CLA	c	610	-	1/1/15/20	8/39/115/115	-
30	LHG	9	318	25	-	24/47/47/53	-
25	CLA	S	604	-	1/1/10/20	3/13/89/115	-
25	CLA	l	314	-	1/1/10/20	4/10/86/115	-
25	CLA	d	404	21	1/1/15/20	9/39/115/115	-
28	NEX	u	304	-	-	5/27/83/83	0/3/3/3
25	CLA	D	405	21	1/1/15/20	13/39/115/115	-
29	OUR	7	301	-	-	8/42/81/86	0/2/2/2
24	CHL	5	312	-	3/3/16/26	8/15/113/137	-
25	CLA	c	604	-	1/1/15/20	16/39/115/115	-
25	CLA	G	315	-	1/1/14/20	7/33/109/115	-
24	CHL	g	318	17	3/3/15/26	6/10/108/137	-
24	CHL	u	312	-	3/3/16/26	6/17/115/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	PHO	a	606	-	-	6/37/103/103	0/5/6/6
28	NEX	2	304	-	-	5/27/83/83	0/3/3/3
25	CLA	b	616	18	1/1/11/20	6/18/94/115	-
25	CLA	S	609	-	1/1/13/20	4/27/103/115	-
25	CLA	c	611	20	1/1/15/20	10/39/115/115	-
25	CLA	C	607	-	1/1/15/20	11/39/115/115	-
25	CLA	s	412	13	1/1/11/20	6/15/91/115	-
24	CHL	1	317	-	3/3/15/26	6/10/108/137	-
30	LHG	A	612	-	-	14/48/48/53	-
25	CLA	n	315	17	1/1/11/20	8/15/91/115	-
31	8CT	V	401	-	-	10/29/63/63	0/2/2/2
26	OIE	7	303	-	-	2/33/72/72	0/2/2/2
25	CLA	Y	314	30	1/1/14/20	11/37/113/115	-
24	CHL	G	310	-	3/3/16/26	7/17/115/137	-
23	HEM	E	201	2	-	0/14/54/54	-
24	CHL	3	311	-	3/3/15/26	7/13/111/137	-
24	CHL	8	310	-	3/3/18/26	13/27/125/137	-
25	CLA	r	304	-	1/1/11/20	4/18/94/115	-
30	LHG	7	319	25	-	24/41/41/53	-
25	CLA	5	308	-	1/1/12/20	4/21/97/115	-
30	LHG	D	408	-	-	21/43/43/53	-
26	OIE	2	302	-	-	2/33/72/72	0/2/2/2
25	CLA	9	316	12	1/1/12/20	9/27/103/115	-
24	CHL	q	310	-	3/3/16/26	5/20/118/137	-
24	CHL	8	309	-	3/3/16/26	5/20/118/137	-
25	CLA	5	307	11	1/1/10/20	8/13/89/115	-
26	OIE	g	303	-	-	0/33/72/72	0/2/2/2
24	CHL	g	313	-	3/3/20/26	20/39/137/137	-
33	LMG	D	401	-	-	10/43/63/70	0/1/1/1
25	CLA	n	314	-	1/1/14/20	2/37/113/115	-
29	OUR	q	301	-	-	9/42/81/86	0/2/2/2
29	OUR	G	301	-	-	10/42/81/86	0/2/2/2
24	CHL	n	311	-	3/3/16/26	7/20/118/137	-
24	CHL	4	308	10	3/3/15/26	4/12/110/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	b	610	-	1/1/15/20	4/39/115/115	-
24	CHL	y	310	-	3/3/16/26	6/17/115/137	-
31	8CT	c	615	-	-	12/29/63/63	0/2/2/2
25	CLA	Y	315	17	1/1/11/20	6/15/91/115	-
25	CLA	8	311	-	1/1/13/20	2/27/103/115	-
25	CLA	R	612	-	1/1/11/20	6/15/91/115	-
24	CHL	p	312	-	3/3/16/26	7/17/115/137	-
25	CLA	n	306	17	1/1/12/20	8/26/102/115	-
25	CLA	9	307	-	1/1/12/20	7/21/97/115	-
26	0IE	N	302	-	-	2/33/72/72	0/2/2/2
30	LHG	Y	318	25	-	21/47/47/53	-
24	CHL	q	316	-	3/3/15/26	1/10/108/137	-
28	NEX	r	317	-	-	5/27/83/83	0/3/3/3
24	CHL	8	303	17	3/3/17/26	10/25/123/137	-
25	CLA	5	314	-	1/1/13/20	4/27/103/115	-
25	CLA	y	314	17	1/1/13/20	5/27/103/115	-
25	CLA	p	316	-	1/1/11/20	4/15/91/115	-
25	CLA	3	307	-	1/1/10/20	4/13/89/115	-
29	0UR	5	301	-	-	14/42/81/86	0/2/2/2
24	CHL	1	312	10	3/3/16/26	8/15/113/137	-
33	LMG	C	618	-	-	17/37/57/70	0/1/1/1
24	CHL	4	317	-	3/3/15/26	6/10/108/137	-
24	CHL	s	406	-	3/3/16/26	5/15/113/137	-
24	CHL	p	309	12	3/3/15/26	3/12/110/137	-
25	CLA	9	314	30	1/1/14/20	11/37/113/115	-
24	CHL	1	304	-	3/3/15/26	3/10/108/137	-
24	CHL	S	601	13	3/3/16/26	12/15/113/137	-
24	CHL	7	311	-	3/3/16/26	2/15/113/137	-
29	0UR	3	301	-	-	9/42/81/86	0/2/2/2
24	CHL	9	311	-	3/3/16/26	6/17/115/137	-
24	CHL	1	305	10	3/3/16/26	8/15/113/137	-
24	CHL	g	305	17	3/3/20/26	16/39/137/137	-
24	CHL	s	409	-	3/3/16/26	7/17/115/137	-
25	CLA	r	314	-	1/1/11/20	7/18/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	n	307	-	1/1/12/20	5/21/97/115	-
25	CLA	3	314	-	1/1/10/20	2/10/86/115	-
31	8CT	C	614	-	-	15/29/63/63	0/2/2/2
25	CLA	n	316	-	1/1/10/20	2/13/89/115	-
25	CLA	c	605	20	1/1/13/20	7/29/105/115	-
24	CHL	s	414	-	3/3/15/26	2/10/108/137	-
25	CLA	g	308	-	1/1/12/20	6/21/97/115	-
24	CHL	7	306	-	3/3/19/26	24/37/135/137	-
29	0UR	u	301	-	-	9/42/81/86	0/2/2/2
31	8CT	d	410	-	-	9/29/63/63	0/2/2/2
25	CLA	S	612	-	1/1/12/20	9/27/103/115	-
25	CLA	B	605	18	1/1/15/20	13/39/115/115	-
26	0IE	4	302	-	-	2/33/72/72	0/2/2/2
26	0IE	G	303	-	-	0/33/72/72	0/2/2/2
24	CHL	G	313	-	3/3/20/26	20/39/137/137	-
24	CHL	Y	312	-	3/3/20/26	17/39/137/137	-
25	CLA	b	607	18	1/1/15/20	12/39/115/115	-
25	CLA	s	411	-	1/1/10/20	4/14/90/115	-
29	0UR	9	301	-	-	9/42/81/86	0/2/2/2
24	CHL	G	305	17	3/3/20/26	18/39/137/137	-
25	CLA	b	613	18	1/1/15/20	9/39/115/115	-
25	CLA	q	313	-	1/1/14/20	8/37/113/115	-
25	CLA	q	306	28	1/1/12/20	6/21/97/115	-
24	CHL	p	311	-	3/3/16/26	3/15/113/137	-
26	0IE	G	302	-	-	2/33/72/72	0/2/2/2
25	CLA	s	405	-	1/1/10/20	2/13/89/115	-
25	CLA	n	313	-	1/1/13/20	5/27/103/115	-
24	CHL	S	605	-	3/3/16/26	5/15/113/137	-
28	NEX	p	304	-	-	5/27/83/83	0/3/3/3
25	CLA	2	308	-	1/1/12/20	4/21/97/115	-
25	CLA	A	610	-	1/1/10/20	2/10/86/115	-
28	NEX	N	303	-	-	4/27/83/83	0/3/3/3
24	CHL	2	313	-	3/3/15/26	3/10/108/137	-
24	CHL	Y	309	-	3/3/16/26	5/17/115/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	2	317	-	1/1/11/20	7/20/96/115	-
28	NEX	3	318	-	-	4/27/83/83	0/3/3/3
25	CLA	S	603	-	1/1/11/20	6/15/91/115	-
25	CLA	B	612	18	1/1/15/20	12/39/115/115	-
30	LHG	d	407	-	-	27/53/53/53	-
25	CLA	a	607	19	1/1/14/20	6/33/109/115	-
25	CLA	S	611	13	1/1/11/20	6/15/91/115	-
24	CHL	4	310	-	3/3/15/26	4/12/110/137	-
25	CLA	1	307	-	1/1/10/20	4/10/86/115	-
24	CHL	q	309	-	3/3/17/26	10/24/122/137	-
25	CLA	5	317	11	1/1/11/20	7/20/96/115	-
25	CLA	6	313	-	1/1/10/20	2/10/86/115	-
24	CHL	G	309	-	3/3/15/26	2/12/110/137	-
24	CHL	6	308	-	3/3/15/26	4/12/110/137	-
29	OUR	2	301	-	-	14/42/81/86	0/2/2/2
25	CLA	C	608	20	1/1/14/20	11/35/111/115	-
24	CHL	n	308	17	3/3/15/26	2/12/110/137	-
24	CHL	R	608	-	3/3/16/26	6/15/113/137	-
30	LHG	a	601	-	-	24/49/49/53	-
30	LHG	g	319	-	-	23/47/47/53	-
25	CLA	y	315	30	1/1/14/20	11/37/113/115	-
26	OIE	5	303	-	-	0/33/72/72	0/2/2/2
24	CHL	5	313	-	3/3/15/26	2/10/108/137	-
25	CLA	A	607	19	1/1/14/20	5/33/109/115	-
24	CHL	u	313	-	3/3/15/26	4/12/110/137	-
25	CLA	9	313	-	1/1/13/20	3/27/103/115	-
35	PHO	A	606	-	-	7/37/103/103	0/5/6/6
28	NEX	G	304	-	-	5/27/83/83	0/3/3/3
24	CHL	6	305	-	3/3/16/26	7/18/116/137	-
25	CLA	G	308	-	1/1/12/20	8/21/97/115	-
25	CLA	B	604	18	1/1/14/20	14/36/112/115	-
25	CLA	b	602	18	1/1/15/20	11/39/115/115	-
26	OIE	6	302	-	-	4/33/69/72	0/2/2/2
24	CHL	u	306	-	3/3/19/26	15/37/135/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	PHO	d	403	-	-	9/37/103/103	0/5/6/6
24	CHL	y	312	-	3/3/17/26	5/21/119/137	-
28	NEX	n	303	-	-	4/27/83/83	0/3/3/3
25	CLA	4	307	28	1/1/10/20	4/10/86/115	-
24	CHL	r	308	-	3/3/16/26	9/18/116/137	-
25	CLA	A	604	-	1/1/15/20	7/39/115/115	-
25	CLA	C	610	-	1/1/15/20	9/39/115/115	-
31	8CT	S	615	-	-	12/29/63/63	0/2/2/2
28	NEX	s	401	25	-	4/27/83/83	0/3/3/3
25	CLA	g	314	-	1/1/13/20	3/27/103/115	-
31	8CT	v	401	-	-	10/29/63/63	0/2/2/2
25	CLA	9	306	-	1/1/13/20	7/29/105/115	-
24	CHL	G	306	17	3/3/19/26	26/37/135/137	-
24	CHL	r	307	-	3/3/16/26	10/18/116/137	-
24	CHL	6	310	-	3/3/16/26	7/15/113/137	-
30	LHG	d	408	-	-	25/43/43/53	-
26	0IE	R	614	-	-	1/33/72/72	0/2/2/2
25	CLA	R	604	-	1/1/10/20	4/10/86/115	-
24	CHL	6	317	12	3/3/15/26	0/10/108/137	-
24	CHL	r	309	-	3/3/16/26	6/15/113/137	-
25	CLA	c	607	-	1/1/15/20	11/39/115/115	-
26	0IE	u	303	-	-	2/33/72/72	0/2/2/2
30	LHG	a	612	-	-	14/48/48/53	-
24	CHL	l	311	-	3/3/15/26	3/13/111/137	-
24	CHL	g	310	-	3/3/16/26	7/17/115/137	-
24	CHL	n	317	-	3/3/15/26	6/10/108/137	-
24	CHL	5	310	-	3/3/15/26	2/10/108/137	-
24	CHL	l	310	-	3/3/15/26	4/12/110/137	-
24	CHL	r	302	8	3/3/16/26	7/15/113/137	-
25	CLA	r	312	8	1/1/11/20	8/15/91/115	-
32	SQD	a	609	-	-	19/40/60/69	0/1/1/1
25	CLA	C	612	20	1/1/12/20	8/26/102/115	-
32	SQD	d	409	-	-	13/39/59/69	0/1/1/1
25	CLA	7	307	12	1/1/13/20	7/29/105/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	D	404	21	1/1/15/20	7/39/115/115	-
25	CLA	c	612	20	1/1/12/20	9/26/102/115	-
25	CLA	b	601	-	1/1/11/20	9/15/91/115	-
35	PHO	D	403	-	-	9/37/103/103	0/5/6/6
25	CLA	4	313	-	1/1/13/20	5/27/103/115	-
25	CLA	G	317	-	1/1/12/20	6/27/103/115	-
24	CHL	7	305	12	3/3/20/26	17/39/137/137	-
25	CLA	B	606	18	1/1/15/20	16/39/115/115	-
25	CLA	B	603	18	1/1/15/20	12/39/115/115	-
24	CHL	2	310	-	3/3/15/26	2/10/108/137	-
24	CHL	p	313	-	3/3/15/26	6/12/110/137	-
24	CHL	G	311	-	3/3/17/26	12/25/123/137	-
25	CLA	q	314	17	1/1/11/20	4/15/91/115	-
24	CHL	g	311	-	3/3/17/26	10/25/123/137	-
25	CLA	8	305	17	1/1/12/20	9/26/102/115	-
33	LMG	W	201	-	-	11/25/45/70	0/1/1/1
24	CHL	3	309	-	3/3/17/26	9/21/119/137	-
27	XAT	R	615	-	-	0/31/93/93	0/4/4/4
25	CLA	R	610	-	1/1/11/20	2/15/91/115	-
24	CHL	q	311	-	3/3/18/26	13/27/125/137	-
24	CHL	1	308	10	3/3/15/26	4/12/110/137	-
25	CLA	B	616	18	1/1/11/20	6/18/94/115	-
24	CHL	3	310	-	3/3/16/26	7/15/113/137	-
26	OIE	p	302	-	-	4/33/72/72	0/2/2/2
24	CHL	Y	308	17	3/3/15/26	4/12/110/137	-
31	8CT	B	617	-	-	13/29/63/63	0/2/2/2
24	CHL	y	318	17	3/3/15/26	4/10/108/137	-
24	CHL	u	310	-	3/3/16/26	9/15/113/137	-
25	CLA	B	608	-	1/1/13/20	10/27/103/115	-
24	CHL	p	305	12	3/3/20/26	17/39/137/137	-
24	CHL	s	403	13	3/3/18/26	14/30/128/137	-
26	OIE	r	315	-	-	1/33/72/72	0/2/2/2
25	CLA	g	316	17	1/1/11/20	5/15/91/115	-
30	LHG	c	617	-	-	17/36/36/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	PL9	D	406	-	-	10/53/73/73	0/1/1/1
24	CHL	n	304	17	3/3/17/26	8/25/123/137	-
24	CHL	u	305	12	3/3/20/26	15/39/137/137	-
24	CHL	Y	305	-	3/3/19/26	22/37/135/137	-
24	CHL	g	306	-	3/3/19/26	25/37/135/137	-
24	CHL	y	309	17	3/3/15/26	4/12/110/137	-
26	0IE	2	303	-	-	0/33/72/72	0/2/2/2
24	CHL	N	305	-	3/3/18/26	13/32/130/137	-
30	LHG	5	319	-	-	21/47/47/53	-
24	CHL	n	310	-	3/3/17/26	11/24/122/137	-
25	CLA	c	603	20	1/1/15/20	12/39/115/115	-
25	CLA	8	306	-	1/1/12/20	7/21/97/115	-
28	NEX	6	303	-	-	4/27/83/83	0/3/3/3
25	CLA	4	315	10	1/1/11/20	8/15/91/115	-
30	LHG	2	319	-	-	20/44/44/53	-
31	8CT	T	101	-	-	12/29/63/63	0/2/2/2
24	CHL	2	305	11	3/3/15/26	9/13/111/137	-
25	CLA	u	308	-	1/1/12/20	5/21/97/115	-
31	8CT	t	101	-	-	12/29/63/63	0/2/2/2
29	0UR	n	301	-	-	9/42/81/86	0/2/2/2
25	CLA	N	313	-	1/1/13/20	5/27/103/115	-
33	LMG	D	411	-	-	26/41/61/70	0/1/1/1
24	CHL	S	607	-	3/3/16/26	6/15/113/137	-
25	CLA	N	306	17	1/1/12/20	7/26/102/115	-
25	CLA	u	317	12	1/1/12/20	6/27/103/115	-
37	DGD	C	620	-	-	25/44/84/95	0/2/2/2
24	CHL	Y	317	17	3/3/15/26	4/10/108/137	-
25	CLA	r	311	-	1/1/11/20	4/15/91/115	-
25	CLA	G	316	17	1/1/11/20	5/15/91/115	-
24	CHL	6	311	-	3/3/15/26	5/13/111/137	-
25	CLA	1	313	-	1/1/13/20	4/27/103/115	-
25	CLA	1	306	-	1/1/10/20	5/14/90/115	-
25	CLA	u	307	-	1/1/13/20	6/29/105/115	-
28	NEX	S	617	-	-	5/27/83/83	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	C	604	-	1/1/15/20	16/39/115/115	-
31	8CT	s	416	-	-	12/29/63/63	0/2/2/2
24	CHL	6	304	12	3/3/16/26	10/18/116/137	-
24	CHL	3	312	-	3/3/15/26	7/12/110/137	-
25	CLA	b	614	18	1/1/13/20	12/29/105/115	-
29	0UR	6	301	-	-	9/42/81/86	0/2/2/2
30	LHG	N	318	-	-	17/47/47/53	-
25	CLA	Y	306	17	1/1/12/20	4/25/101/115	-
25	CLA	r	310	8	1/1/13/20	4/27/103/115	-
26	0IE	Y	302	-	-	2/33/72/72	0/2/2/2
33	LMG	d	401	-	-	12/43/63/70	0/1/1/1
25	CLA	7	315	30	1/1/14/20	14/37/113/115	-
24	CHL	2	318	11	3/3/15/26	4/10/108/137	-
25	CLA	C	602	20	1/1/15/20	17/39/115/115	-
24	CHL	2	309	11	3/3/15/26	3/12/110/137	-
28	NEX	y	304	-	-	5/27/83/83	0/3/3/3
25	CLA	c	616	20	1/1/11/20	2/17/93/115	-
25	CLA	R	609	8	1/1/13/20	4/27/103/115	-
24	CHL	8	315	-	3/3/15/26	0/10/108/137	-
25	CLA	3	315	12	1/1/11/20	8/15/91/115	-
25	CLA	N	315	17	1/1/11/20	8/15/91/115	-
30	LHG	G	319	-	-	23/47/47/53	-
24	CHL	N	304	17	3/3/17/26	8/25/123/137	-
25	CLA	Y	313	17	1/1/13/20	5/27/103/115	-
24	CHL	1	309	-	3/3/15/26	4/12/110/137	-
25	CLA	Y	307	-	1/1/12/20	7/21/97/115	-
24	CHL	5	311	-	3/3/16/26	8/17/115/137	-
25	CLA	c	606	20	1/1/12/20	7/25/101/115	-
25	CLA	8	312	-	1/1/14/20	10/37/113/115	-
25	CLA	R	611	8	1/1/11/20	8/15/91/115	-
25	CLA	a	610	-	1/1/10/20	2/10/86/115	-
25	CLA	N	316	-	1/1/10/20	1/13/89/115	-
24	CHL	N	317	-	3/3/15/26	5/10/108/137	-
31	8CT	C	613	-	-	8/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	G	314	-	1/1/13/20	3/27/103/115	-
24	CHL	R	607	-	3/3/16/26	9/18/116/137	-
24	CHL	R	602	-	3/3/16/26	6/17/115/137	-
24	CHL	s	407	-	3/3/16/26	7/15/113/137	-
24	CHL	p	310	-	3/3/16/26	7/15/113/137	-
25	CLA	6	316	-	1/1/11/20	8/15/91/115	-
30	LHG	A	601	-	-	24/49/49/53	-
25	CLA	b	609	18	1/1/15/20	19/39/115/115	-
25	CLA	B	602	18	1/1/15/20	11/39/115/115	-
25	CLA	p	317	12	1/1/12/20	7/27/103/115	-
24	CHL	2	306	-	3/3/16/26	10/17/115/137	-
28	NEX	l	303	-	-	5/27/83/83	0/3/3/3
31	8CT	b	617	-	-	13/29/63/63	0/2/2/2
24	CHL	R	601	8	3/3/16/26	7/15/113/137	-
24	CHL	S	613	-	3/3/15/26	2/10/108/137	-
30	LHG	p	319	25	-	26/47/47/53	-
25	CLA	B	607	18	1/1/15/20	13/39/115/115	-
29	0UR	Y	301	-	-	11/42/81/86	0/2/2/2
31	8CT	a	608	-	-	8/29/63/63	0/2/2/2
24	CHL	4	309	-	3/3/15/26	6/12/110/137	-
33	LMG	i	101	-	-	14/43/63/70	0/1/1/1
24	CHL	u	311	-	3/3/16/26	5/15/113/137	-
25	CLA	B	610	-	1/1/15/20	3/39/115/115	-
25	CLA	c	608	20	1/1/14/20	11/35/111/115	-
25	CLA	u	314	-	1/1/13/20	3/27/103/115	-
31	8CT	D	410	-	-	10/29/63/63	0/2/2/2
32	SQD	B	618	-	-	14/49/69/69	0/1/1/1
25	CLA	g	307	-	1/1/12/20	5/25/101/115	-
25	CLA	q	315	17	1/1/10/20	3/13/89/115	-
25	CLA	b	611	18	1/1/15/20	4/39/115/115	-
24	CHL	7	312	-	3/3/16/26	7/17/115/137	-
24	CHL	Y	310	-	3/3/17/26	11/25/123/137	-
26	0IE	y	302	-	-	2/33/72/72	0/2/2/2
25	CLA	6	306	-	1/1/10/20	6/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	R	613	-	1/1/11/20	7/18/94/115	-
24	CHL	3	304	12	3/3/16/26	11/18/116/137	-
24	CHL	7	318	12	3/3/15/26	4/10/108/137	-
25	CLA	N	314	-	1/1/14/20	2/37/113/115	-
26	OIE	g	302	-	-	2/33/72/72	0/2/2/2
24	CHL	u	318	-	3/3/15/26	4/10/108/137	-
25	CLA	r	313	-	1/1/11/20	6/15/91/115	-
29	OUR	N	301	-	-	10/42/81/86	0/2/2/2
25	CLA	7	316	12	1/1/11/20	4/15/91/115	-
25	CLA	u	316	-	1/1/11/20	6/15/91/115	-
25	CLA	c	602	20	1/1/15/20	16/39/115/115	-
24	CHL	5	306	-	3/3/16/26	10/17/115/137	-
25	CLA	s	413	-	1/1/12/20	9/27/103/115	-
24	CHL	N	311	-	3/3/16/26	7/20/118/137	-
24	CHL	r	303	-	3/3/16/26	6/17/115/137	-
25	CLA	3	316	-	1/1/11/20	6/15/91/115	-
24	CHL	p	318	12	3/3/15/26	4/10/108/137	-
25	CLA	4	306	-	1/1/10/20	5/14/90/115	-
25	CLA	B	609	18	1/1/15/20	16/39/115/115	-
31	8CT	S	614	-	-	7/29/63/63	0/2/2/2
24	CHL	7	309	12	3/3/15/26	3/12/110/137	-
25	CLA	2	316	-	1/1/11/20	4/15/91/115	-
31	8CT	c	613	-	-	8/29/63/63	0/2/2/2
24	CHL	p	306	-	3/3/19/26	24/37/135/137	-
25	CLA	y	308	-	1/1/12/20	7/21/97/115	-
24	CHL	3	305	-	3/3/16/26	8/18/116/137	-
25	CLA	B	601	-	1/1/11/20	9/15/91/115	-
25	CLA	r	305	-	1/1/10/20	2/10/86/115	-
25	CLA	S	616	-	1/1/11/20	8/15/91/115	-
25	CLA	A	605	-	1/1/11/20	5/20/96/115	-
25	CLA	y	317	17	1/1/12/20	6/27/103/115	-
33	LMG	w	201	-	-	17/31/51/70	0/1/1/1
25	CLA	C	603	20	1/1/15/20	13/39/115/115	-
24	CHL	6	309	-	3/3/17/26	7/21/119/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	u	309	12	3/3/15/26	2/12/110/137	-
26	OIE	Y	303	-	-	0/33/72/72	0/2/2/2
24	CHL	N	310	-	3/3/17/26	11/24/122/137	-
25	CLA	8	314	-	1/1/10/20	3/13/89/115	-
31	8CT	x	601	-	-	10/29/63/63	0/2/2/2
25	CLA	6	315	12	1/1/11/20	8/15/91/115	-
28	NEX	7	304	-	-	5/27/83/83	0/3/3/3
24	CHL	R	606	-	3/3/16/26	10/18/116/137	-
24	CHL	S	608	-	3/3/16/26	7/17/115/137	-
32	SQD	A	609	-	-	16/40/60/69	0/1/1/1
25	CLA	5	315	-	1/1/14/20	10/37/113/115	-
31	8CT	s	415	-	-	7/29/63/63	0/2/2/2
24	CHL	G	312	-	3/3/17/26	4/21/119/137	-
28	NEX	9	319	-	-	5/27/83/83	0/3/3/3
24	CHL	4	312	-	3/3/16/26	8/15/113/137	-
25	CLA	2	307	11	1/1/10/20	7/13/89/115	-
25	CLA	s	417	-	1/1/11/20	8/15/91/115	-
33	LMG	d	411	-	-	20/41/61/70	0/1/1/1
24	CHL	9	309	-	3/3/16/26	9/15/113/137	-
31	8CT	X	601	-	-	10/29/63/63	0/2/2/2
29	OUR	y	301	-	-	11/42/81/86	0/2/2/2
25	CLA	b	608	-	1/1/13/20	9/27/103/115	-

All (5928) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	D	410	8CT	C02-C03	15.16	1.59	1.34
31	d	410	8CT	C02-C03	15.02	1.59	1.34
31	S	614	8CT	C02-C03	14.75	1.59	1.34
31	s	415	8CT	C02-C03	14.74	1.59	1.34
31	A	608	8CT	C02-C03	14.72	1.59	1.34
31	a	608	8CT	C02-C03	14.67	1.59	1.34
31	B	617	8CT	C02-C03	14.64	1.59	1.34
31	b	617	8CT	C02-C03	14.62	1.59	1.34
31	x	601	8CT	C02-C03	14.57	1.58	1.34
31	V	401	8CT	C02-C03	14.56	1.58	1.34
31	v	401	8CT	C02-C03	14.56	1.58	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	X	601	8CT	C02-C03	14.55	1.58	1.34
31	c	615	8CT	C02-C03	14.55	1.58	1.34
31	C	615	8CT	C02-C03	14.54	1.58	1.34
31	c	613	8CT	C02-C03	14.48	1.58	1.34
31	C	613	8CT	C02-C03	14.43	1.58	1.34
31	s	416	8CT	C02-C03	14.42	1.58	1.34
31	d	410	8CT	C32-C31	14.40	1.60	1.32
31	D	410	8CT	C32-C31	14.40	1.60	1.32
31	T	101	8CT	C02-C03	14.39	1.58	1.34
31	v	401	8CT	C32-C31	14.38	1.60	1.32
31	V	401	8CT	C32-C31	14.38	1.60	1.32
31	t	101	8CT	C02-C03	14.36	1.58	1.34
31	b	617	8CT	C32-C31	14.36	1.60	1.32
31	S	615	8CT	C02-C03	14.30	1.58	1.34
31	B	617	8CT	C32-C31	14.28	1.59	1.32
31	X	601	8CT	C32-C31	14.20	1.59	1.32
31	A	608	8CT	C32-C31	14.20	1.59	1.32
31	x	601	8CT	C32-C31	14.19	1.59	1.32
31	a	608	8CT	C32-C31	14.19	1.59	1.32
31	C	613	8CT	C32-C31	14.13	1.59	1.32
31	S	615	8CT	C32-C31	14.12	1.59	1.32
31	c	614	8CT	C32-C31	14.12	1.59	1.32
31	s	416	8CT	C32-C31	14.10	1.59	1.32
31	c	613	8CT	C32-C31	14.10	1.59	1.32
31	C	614	8CT	C32-C31	14.09	1.59	1.32
31	S	614	8CT	C32-C31	14.06	1.59	1.32
31	s	415	8CT	C32-C31	14.06	1.59	1.32
31	t	101	8CT	C32-C31	14.03	1.59	1.32
31	C	614	8CT	C02-C03	14.00	1.58	1.34
31	c	615	8CT	C32-C31	14.00	1.59	1.32
31	T	101	8CT	C32-C31	13.99	1.59	1.32
31	C	615	8CT	C32-C31	13.99	1.59	1.32
31	c	614	8CT	C02-C03	13.95	1.57	1.34
24	u	309	CHL	C2C-C3C	11.72	1.47	1.36
24	9	308	CHL	C2C-C3C	11.71	1.47	1.36
24	9	317	CHL	C2C-C3C	11.65	1.47	1.36
24	G	309	CHL	C2C-C3C	11.65	1.47	1.36
24	p	309	CHL	C2C-C3C	11.65	1.47	1.36
24	u	318	CHL	C2C-C3C	11.65	1.47	1.36
24	1	317	CHL	C2C-C3C	11.63	1.47	1.36
24	g	309	CHL	C2C-C3C	11.60	1.47	1.36
24	3	312	CHL	C2C-C3C	11.57	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	n	317	CHL	C2C-C3C	11.57	1.47	1.36
24	7	309	CHL	C2C-C3C	11.55	1.47	1.36
24	N	317	CHL	C2C-C3C	11.55	1.47	1.36
24	4	317	CHL	C2C-C3C	11.54	1.47	1.36
24	1	304	CHL	C2C-C3C	11.54	1.47	1.36
24	3	309	CHL	C2C-C3C	11.53	1.47	1.36
24	G	313	CHL	C2C-C3C	11.53	1.47	1.36
24	4	304	CHL	C2C-C3C	11.52	1.47	1.36
24	u	313	CHL	C2C-C3C	11.52	1.47	1.36
24	g	313	CHL	C2C-C3C	11.50	1.47	1.36
24	9	312	CHL	C2C-C3C	11.48	1.47	1.36
24	6	312	CHL	C2C-C3C	11.48	1.47	1.36
24	6	309	CHL	C2C-C3C	11.46	1.47	1.36
24	R	601	CHL	C2C-C3C	11.45	1.47	1.36
24	4	308	CHL	C2C-C3C	11.45	1.47	1.36
24	3	308	CHL	C2C-C3C	11.44	1.47	1.36
24	1	308	CHL	C2C-C3C	11.43	1.47	1.36
24	u	305	CHL	C2C-C3C	11.42	1.47	1.36
24	8	315	CHL	C2C-C3C	11.41	1.47	1.36
24	q	316	CHL	C2C-C3C	11.41	1.47	1.36
24	6	308	CHL	C2C-C3C	11.40	1.47	1.36
24	9	310	CHL	C2C-C3C	11.37	1.47	1.36
24	1	309	CHL	C2C-C3C	11.33	1.47	1.36
24	u	311	CHL	C2C-C3C	11.31	1.47	1.36
24	6	310	CHL	C2C-C3C	11.30	1.47	1.36
24	u	310	CHL	C2C-C3C	11.26	1.47	1.36
24	4	309	CHL	C2C-C3C	11.26	1.47	1.36
24	3	310	CHL	C2C-C3C	11.25	1.47	1.36
24	5	309	CHL	C2C-C3C	11.24	1.47	1.36
24	r	302	CHL	C2C-C3C	11.23	1.47	1.36
24	n	304	CHL	C2C-C3C	11.23	1.47	1.36
24	n	308	CHL	C2C-C3C	11.22	1.47	1.36
24	6	317	CHL	C2C-C3C	11.20	1.47	1.36
24	2	318	CHL	C2C-C3C	11.20	1.47	1.36
24	N	304	CHL	C2C-C3C	11.20	1.47	1.36
24	3	317	CHL	C2C-C3C	11.19	1.47	1.36
24	5	318	CHL	C2C-C3C	11.19	1.47	1.36
24	2	309	CHL	C2C-C3C	11.19	1.47	1.36
24	6	304	CHL	C2C-C3C	11.18	1.47	1.36
24	N	310	CHL	C2C-C3C	11.18	1.47	1.36
24	n	310	CHL	C2C-C3C	11.18	1.47	1.36
24	N	308	CHL	C2C-C3C	11.17	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	9	309	CHL	C2C-C3C	11.16	1.47	1.36
24	g	311	CHL	C2C-C3C	11.15	1.47	1.36
24	9	304	CHL	C2C-C3C	11.15	1.47	1.36
24	g	312	CHL	C2C-C3C	11.14	1.47	1.36
24	g	310	CHL	C2C-C3C	11.14	1.47	1.36
24	G	312	CHL	C2C-C3C	11.13	1.47	1.36
24	5	311	CHL	C2C-C3C	11.11	1.47	1.36
24	G	311	CHL	C2C-C3C	11.09	1.47	1.36
24	G	310	CHL	C2C-C3C	11.07	1.47	1.36
24	4	311	CHL	C2C-C3C	11.04	1.47	1.36
24	p	310	CHL	C2C-C3C	11.04	1.47	1.36
24	4	312	CHL	C2C-C3C	11.02	1.47	1.36
24	3	304	CHL	C2C-C3C	11.02	1.47	1.36
24	7	310	CHL	C2C-C3C	11.00	1.47	1.36
24	2	311	CHL	C2C-C3C	11.00	1.47	1.36
24	9	311	CHL	C2C-C3C	10.98	1.47	1.36
24	S	608	CHL	C2C-C3C	10.97	1.47	1.36
24	s	409	CHL	C2C-C3C	10.97	1.47	1.36
24	8	303	CHL	C2C-C3C	10.97	1.47	1.36
24	9	305	CHL	C2C-C3C	10.94	1.47	1.36
24	r	309	CHL	C2C-C3C	10.93	1.47	1.36
24	7	318	CHL	C2C-C3C	10.93	1.47	1.36
24	u	312	CHL	C2C-C3C	10.93	1.47	1.36
24	2	305	CHL	C2C-C3C	10.92	1.46	1.36
24	1	311	CHL	C2C-C3C	10.91	1.46	1.36
24	1	312	CHL	C2C-C3C	10.91	1.46	1.36
24	3	311	CHL	C2C-C3C	10.91	1.46	1.36
24	6	311	CHL	C2C-C3C	10.90	1.46	1.36
24	q	303	CHL	C2C-C3C	10.90	1.46	1.36
24	R	608	CHL	C2C-C3C	10.89	1.46	1.36
24	G	305	CHL	C2C-C3C	10.89	1.46	1.36
24	r	306	CHL	C2C-C3C	10.89	1.46	1.36
24	1	310	CHL	C2C-C3C	10.89	1.46	1.36
24	p	318	CHL	C2C-C3C	10.88	1.46	1.36
24	5	305	CHL	C2C-C3C	10.86	1.46	1.36
24	2	313	CHL	C2C-C3C	10.86	1.46	1.36
24	5	313	CHL	C2C-C3C	10.85	1.46	1.36
24	g	305	CHL	C2C-C3C	10.84	1.46	1.36
24	u	306	CHL	C2C-C3C	10.83	1.46	1.36
24	N	312	CHL	C2C-C3C	10.82	1.46	1.36
24	Y	308	CHL	C2C-C3C	10.81	1.46	1.36
24	4	310	CHL	C2C-C3C	10.79	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	S	606	CHL	C2C-C3C	10.78	1.46	1.36
24	y	309	CHL	C2C-C3C	10.78	1.46	1.36
24	R	606	CHL	C2C-C3C	10.77	1.46	1.36
24	n	312	CHL	C2C-C3C	10.77	1.46	1.36
24	G	306	CHL	C2C-C3C	10.76	1.46	1.36
24	8	307	CHL	C2C-C3C	10.76	1.46	1.36
24	s	407	CHL	C2C-C3C	10.75	1.46	1.36
24	1	305	CHL	C2C-C3C	10.75	1.46	1.36
24	p	311	CHL	C2C-C3C	10.75	1.46	1.36
24	q	307	CHL	C2C-C3C	10.75	1.46	1.36
24	r	307	CHL	C2C-C3C	10.75	1.46	1.36
24	2	312	CHL	C2C-C3C	10.74	1.46	1.36
24	p	313	CHL	C2C-C3C	10.73	1.46	1.36
24	7	313	CHL	C2C-C3C	10.73	1.46	1.36
24	4	305	CHL	C2C-C3C	10.73	1.46	1.36
24	7	311	CHL	C2C-C3C	10.73	1.46	1.36
24	N	311	CHL	C2C-C3C	10.70	1.46	1.36
24	G	318	CHL	C2C-C3C	10.69	1.46	1.36
24	g	306	CHL	C2C-C3C	10.69	1.46	1.36
24	5	312	CHL	C2C-C3C	10.68	1.46	1.36
24	3	305	CHL	C2C-C3C	10.67	1.46	1.36
24	g	318	CHL	C2C-C3C	10.66	1.46	1.36
24	6	305	CHL	C2C-C3C	10.66	1.46	1.36
24	n	305	CHL	C2C-C3C	10.65	1.46	1.36
24	n	311	CHL	C2C-C3C	10.63	1.46	1.36
24	N	305	CHL	C2C-C3C	10.62	1.46	1.36
24	y	312	CHL	C2C-C3C	10.58	1.46	1.36
24	Y	311	CHL	C2C-C3C	10.57	1.46	1.36
24	S	607	CHL	C2C-C3C	10.56	1.46	1.36
24	N	309	CHL	C2C-C3C	10.53	1.46	1.36
24	s	408	CHL	C2C-C3C	10.52	1.46	1.36
24	S	605	CHL	C2C-C3C	10.49	1.46	1.36
24	R	607	CHL	C2C-C3C	10.47	1.46	1.36
24	r	308	CHL	C2C-C3C	10.47	1.46	1.36
24	Y	319	CHL	C2C-C3C	10.45	1.46	1.36
24	y	311	CHL	C2C-C3C	10.45	1.46	1.36
24	q	309	CHL	C2C-C3C	10.45	1.46	1.36
24	2	306	CHL	C2C-C3C	10.44	1.46	1.36
24	s	406	CHL	C2C-C3C	10.44	1.46	1.36
24	2	310	CHL	C2C-C3C	10.43	1.46	1.36
24	R	605	CHL	C2C-C3C	10.43	1.46	1.36
24	y	313	CHL	C2C-C3C	10.42	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	5	310	CHL	C2C-C3C	10.42	1.46	1.36
24	5	306	CHL	C2C-C3C	10.42	1.46	1.36
24	n	309	CHL	C2C-C3C	10.42	1.46	1.36
24	r	303	CHL	C2C-C3C	10.41	1.46	1.36
24	Y	312	CHL	C2C-C3C	10.39	1.46	1.36
24	S	601	CHL	C2C-C3C	10.36	1.46	1.36
24	s	402	CHL	C2C-C3C	10.35	1.46	1.36
24	Y	310	CHL	C2C-C3C	10.34	1.46	1.36
24	q	304	CHL	C2C-C3C	10.28	1.46	1.36
24	q	311	CHL	C2C-C3C	10.28	1.46	1.36
24	8	310	CHL	C2C-C3C	10.27	1.46	1.36
24	8	304	CHL	C2C-C3C	10.26	1.46	1.36
24	p	305	CHL	C2C-C3C	10.26	1.46	1.36
24	R	602	CHL	C2C-C3C	10.25	1.46	1.36
24	7	305	CHL	C2C-C3C	10.22	1.46	1.36
24	p	306	CHL	C2C-C3C	10.20	1.46	1.36
24	q	310	CHL	C2C-C3C	10.20	1.46	1.36
24	8	309	CHL	C2C-C3C	10.19	1.46	1.36
24	q	308	CHL	C2C-C3C	10.18	1.46	1.36
24	7	306	CHL	C2C-C3C	10.15	1.46	1.36
24	S	613	CHL	C2C-C3C	10.10	1.46	1.36
24	8	308	CHL	C2C-C3C	10.09	1.46	1.36
24	s	414	CHL	C2C-C3C	10.08	1.46	1.36
24	p	312	CHL	C2C-C3C	10.05	1.46	1.36
24	Y	309	CHL	C2C-C3C	10.03	1.46	1.36
24	y	318	CHL	C2C-C3C	10.00	1.46	1.36
24	Y	317	CHL	C2C-C3C	9.99	1.46	1.36
24	y	310	CHL	C2C-C3C	9.98	1.46	1.36
24	7	312	CHL	C2C-C3C	9.94	1.46	1.36
24	s	403	CHL	C2C-C3C	9.94	1.46	1.36
24	S	602	CHL	C2C-C3C	9.92	1.46	1.36
24	y	305	CHL	C2C-C3C	9.83	1.45	1.36
24	Y	304	CHL	C2C-C3C	9.76	1.45	1.36
24	Y	305	CHL	C2C-C3C	9.73	1.45	1.36
24	y	306	CHL	C2C-C3C	9.71	1.45	1.36
31	X	601	8CT	C34-C35	-9.16	1.36	1.54
31	a	608	8CT	C34-C35	-9.10	1.37	1.54
31	x	601	8CT	C34-C35	-9.10	1.37	1.54
31	A	608	8CT	C34-C35	-9.08	1.37	1.54
31	c	614	8CT	C34-C35	-9.05	1.37	1.54
31	c	613	8CT	C34-C35	-9.05	1.37	1.54
35	d	403	PHO	C1B-C2B	9.03	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	C	615	8CT	C34-C35	-9.02	1.37	1.54
31	C	613	8CT	C34-C35	-8.99	1.37	1.54
31	C	614	8CT	C34-C35	-8.98	1.37	1.54
31	c	615	8CT	C34-C35	-8.96	1.37	1.54
24	N	317	CHL	C1A-CHA	8.91	1.50	1.40
24	n	317	CHL	C1A-CHA	8.91	1.50	1.40
31	s	415	8CT	C34-C35	-8.89	1.37	1.54
35	D	403	PHO	C1B-C2B	8.89	1.49	1.39
24	8	315	CHL	C1A-CHA	8.87	1.50	1.40
24	q	316	CHL	C1A-CHA	8.87	1.50	1.40
31	S	614	8CT	C34-C35	-8.85	1.37	1.54
24	g	309	CHL	C1A-CHA	8.84	1.50	1.40
24	l	317	CHL	C1A-CHA	8.82	1.50	1.40
24	p	309	CHL	C1A-CHA	8.82	1.50	1.40
24	7	309	CHL	C1A-CHA	8.81	1.50	1.40
24	9	308	CHL	C1A-CHA	8.80	1.50	1.40
24	u	309	CHL	C1A-CHA	8.80	1.50	1.40
24	4	317	CHL	C1A-CHA	8.79	1.50	1.40
24	G	309	CHL	C1A-CHA	8.79	1.50	1.40
35	A	606	PHO	C1B-C2B	8.75	1.49	1.39
24	9	317	CHL	C1A-CHA	8.74	1.49	1.40
31	v	401	8CT	C34-C35	-8.73	1.37	1.54
35	a	606	PHO	C1B-C2B	8.72	1.49	1.39
24	6	308	CHL	C1A-CHA	8.72	1.49	1.40
24	u	318	CHL	C1A-CHA	8.70	1.49	1.40
31	V	401	8CT	C34-C35	-8.65	1.37	1.54
24	l	317	CHL	C1B-C2B	8.61	1.49	1.39
31	s	416	8CT	C34-C35	-8.59	1.38	1.54
24	4	317	CHL	C1B-C2B	8.58	1.49	1.39
24	u	309	CHL	C1B-C2B	8.58	1.49	1.39
24	3	308	CHL	C1A-CHA	8.57	1.49	1.40
24	u	312	CHL	C1A-CHA	8.57	1.49	1.40
24	9	311	CHL	C1B-C2B	8.57	1.49	1.39
24	G	312	CHL	C1B-C2B	8.56	1.49	1.39
31	d	410	8CT	C34-C35	-8.56	1.38	1.54
31	S	615	8CT	C34-C35	-8.55	1.38	1.54
24	9	304	CHL	C1B-C2B	8.55	1.49	1.39
31	B	617	8CT	C34-C35	-8.55	1.38	1.54
24	7	309	CHL	C1B-C2B	8.54	1.49	1.39
31	D	410	8CT	C34-C35	-8.54	1.38	1.54
24	9	308	CHL	C1B-C2B	8.54	1.49	1.39
24	g	309	CHL	C1B-C2B	8.53	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	b	617	8CT	C34-C35	-8.53	1.38	1.54
24	p	309	CHL	C1B-C2B	8.53	1.49	1.39
24	g	312	CHL	C1B-C2B	8.53	1.49	1.39
24	4	308	CHL	C1A-CHA	8.53	1.49	1.40
24	q	316	CHL	C1B-C2B	8.52	1.49	1.39
24	4	304	CHL	C1A-CHA	8.52	1.49	1.40
24	9	311	CHL	C1A-CHA	8.52	1.49	1.40
24	6	312	CHL	C1B-C2B	8.51	1.49	1.39
24	u	305	CHL	C1B-C2B	8.50	1.49	1.39
24	4	304	CHL	C1B-C2B	8.50	1.49	1.39
24	u	312	CHL	C1B-C2B	8.50	1.49	1.39
24	n	317	CHL	C1B-C2B	8.49	1.49	1.39
24	g	310	CHL	C1B-C2B	8.48	1.49	1.39
24	G	310	CHL	C1B-C2B	8.48	1.49	1.39
24	G	309	CHL	C1B-C2B	8.48	1.49	1.39
24	u	305	CHL	C1A-CHA	8.47	1.49	1.40
24	9	310	CHL	C1B-C2B	8.47	1.49	1.39
24	u	311	CHL	C1B-C2B	8.47	1.49	1.39
24	u	318	CHL	C1B-C2B	8.47	1.49	1.39
24	6	309	CHL	C1B-C2B	8.47	1.49	1.39
24	8	315	CHL	C1B-C2B	8.47	1.49	1.39
24	3	317	CHL	C1B-C2B	8.47	1.49	1.39
24	G	311	CHL	C1B-C2B	8.47	1.49	1.39
31	t	101	8CT	C34-C35	-8.46	1.38	1.54
24	g	311	CHL	C1B-C2B	8.46	1.49	1.39
24	6	310	CHL	C1B-C2B	8.46	1.49	1.39
31	T	101	8CT	C34-C35	-8.45	1.38	1.54
24	3	308	CHL	C1B-C2B	8.45	1.49	1.39
24	1	304	CHL	C1A-CHA	8.44	1.49	1.40
24	9	317	CHL	C1B-C2B	8.44	1.49	1.39
24	3	312	CHL	C1B-C2B	8.43	1.49	1.39
24	5	309	CHL	C1A-CHA	8.43	1.49	1.40
24	3	310	CHL	C1B-C2B	8.42	1.49	1.39
24	1	304	CHL	C1B-C2B	8.42	1.49	1.39
24	1	308	CHL	C1A-CHA	8.41	1.49	1.40
24	g	313	CHL	C1B-C2B	8.41	1.49	1.39
24	N	317	CHL	C1B-C2B	8.41	1.49	1.39
24	9	312	CHL	C1B-C2B	8.41	1.49	1.39
24	6	308	CHL	C1B-C2B	8.41	1.49	1.39
24	u	313	CHL	C1B-C2B	8.40	1.49	1.39
24	n	308	CHL	C1B-C2B	8.40	1.49	1.39
24	G	313	CHL	C1B-C2B	8.40	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	N	304	CHL	C1A-CHA	8.39	1.49	1.40
24	4	308	CHL	C1B-C2B	8.39	1.49	1.39
24	6	317	CHL	C1B-C2B	8.39	1.49	1.39
24	1	308	CHL	C1B-C2B	8.38	1.49	1.39
24	9	309	CHL	C1B-C2B	8.38	1.49	1.39
24	n	304	CHL	C1A-CHA	8.38	1.49	1.40
24	5	313	CHL	C1B-C2B	8.38	1.49	1.39
24	3	309	CHL	C1B-C2B	8.38	1.49	1.39
24	2	309	CHL	C1B-C2B	8.36	1.49	1.39
24	N	308	CHL	C1B-C2B	8.36	1.49	1.39
24	n	308	CHL	C1A-CHA	8.36	1.49	1.40
24	3	311	CHL	C1B-C2B	8.33	1.49	1.39
24	6	304	CHL	C1B-C2B	8.33	1.49	1.39
24	r	302	CHL	C1B-C2B	8.33	1.49	1.39
24	5	309	CHL	C1B-C2B	8.32	1.49	1.39
24	u	310	CHL	C1B-C2B	8.32	1.49	1.39
24	N	309	CHL	C1B-C2B	8.31	1.49	1.39
24	3	304	CHL	C1B-C2B	8.31	1.49	1.39
24	n	309	CHL	C1B-C2B	8.31	1.49	1.39
24	2	318	CHL	C1B-C2B	8.31	1.49	1.39
24	2	318	CHL	C1A-CHA	8.31	1.49	1.40
24	R	607	CHL	C1B-C2B	8.30	1.49	1.39
24	p	305	CHL	C1B-C2B	8.29	1.49	1.39
24	2	309	CHL	C1A-CHA	8.29	1.49	1.40
24	2	311	CHL	C1B-C2B	8.29	1.49	1.39
24	N	312	CHL	C1B-C2B	8.29	1.49	1.39
24	p	318	CHL	C1B-C2B	8.28	1.49	1.39
24	n	304	CHL	C1B-C2B	8.28	1.49	1.39
24	R	601	CHL	C1A-CHA	8.28	1.49	1.40
24	S	608	CHL	C1B-C2B	8.28	1.49	1.39
24	5	318	CHL	C1B-C2B	8.28	1.49	1.39
24	r	308	CHL	C1B-C2B	8.28	1.49	1.39
24	r	302	CHL	C1A-CHA	8.27	1.49	1.40
24	4	312	CHL	C1B-C2B	8.27	1.49	1.39
24	5	311	CHL	C1B-C2B	8.27	1.49	1.39
24	R	601	CHL	C1B-C2B	8.27	1.49	1.39
24	2	305	CHL	C1B-C2B	8.27	1.49	1.39
24	1	310	CHL	C1B-C2B	8.26	1.49	1.39
24	s	409	CHL	C1B-C2B	8.26	1.49	1.39
24	R	606	CHL	C1B-C2B	8.26	1.48	1.39
24	7	305	CHL	C1B-C2B	8.25	1.48	1.39
24	5	318	CHL	C1A-CHA	8.25	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	1	309	CHL	C1B-C2B	8.25	1.48	1.39
24	5	305	CHL	C1B-C2B	8.25	1.48	1.39
24	n	312	CHL	C1B-C2B	8.24	1.48	1.39
24	N	310	CHL	C1B-C2B	8.24	1.48	1.39
24	n	310	CHL	C1B-C2B	8.24	1.48	1.39
24	7	318	CHL	C1B-C2B	8.23	1.48	1.39
24	1	305	CHL	C1B-C2B	8.23	1.48	1.39
24	8	303	CHL	C1B-C2B	8.23	1.48	1.39
24	4	309	CHL	C1B-C2B	8.22	1.48	1.39
24	N	304	CHL	C1B-C2B	8.22	1.48	1.39
24	2	313	CHL	C1B-C2B	8.22	1.48	1.39
24	7	312	CHL	C1B-C2B	8.22	1.48	1.39
24	r	307	CHL	C1B-C2B	8.21	1.48	1.39
24	r	309	CHL	C1B-C2B	8.20	1.48	1.39
24	R	608	CHL	C1B-C2B	8.20	1.48	1.39
24	1	312	CHL	C1B-C2B	8.20	1.48	1.39
24	3	311	CHL	C3B-C4B	8.19	1.49	1.41
24	4	310	CHL	C1B-C2B	8.19	1.48	1.39
24	5	312	CHL	C1B-C2B	8.18	1.48	1.39
24	Y	308	CHL	C1B-C2B	8.18	1.48	1.39
24	9	309	CHL	C3B-C4B	8.18	1.49	1.41
24	g	306	CHL	C1B-C2B	8.17	1.48	1.39
24	y	309	CHL	C1B-C2B	8.17	1.48	1.39
24	R	605	CHL	C1B-C2B	8.16	1.48	1.39
24	2	312	CHL	C1B-C2B	8.16	1.48	1.39
24	S	605	CHL	C1B-C2B	8.16	1.48	1.39
24	6	311	CHL	C1B-C2B	8.16	1.48	1.39
24	p	312	CHL	C1B-C2B	8.16	1.48	1.39
24	r	306	CHL	C1B-C2B	8.16	1.48	1.39
24	q	303	CHL	C1B-C2B	8.16	1.48	1.39
24	S	607	CHL	C1B-C2B	8.15	1.48	1.39
24	r	303	CHL	C1B-C2B	8.15	1.48	1.39
24	G	305	CHL	C1B-C2B	8.15	1.48	1.39
24	s	408	CHL	C1B-C2B	8.15	1.48	1.39
24	S	606	CHL	C1B-C2B	8.15	1.48	1.39
24	p	311	CHL	C1B-C2B	8.14	1.48	1.39
24	R	602	CHL	C1B-C2B	8.14	1.48	1.39
24	G	306	CHL	C1B-C2B	8.14	1.48	1.39
24	4	309	CHL	C3B-C4B	8.14	1.49	1.41
24	7	311	CHL	C1B-C2B	8.13	1.48	1.39
24	6	305	CHL	C1B-C2B	8.12	1.48	1.39
24	9	304	CHL	C1A-CHA	8.12	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	p	313	CHL	C1B-C2B	8.12	1.48	1.39
24	q	309	CHL	C1B-C2B	8.12	1.48	1.39
24	u	310	CHL	C3B-C4B	8.12	1.49	1.41
35	A	606	PHO	C3B-C4B	8.11	1.49	1.41
24	4	305	CHL	C1B-C2B	8.11	1.48	1.39
24	g	305	CHL	C1B-C2B	8.11	1.48	1.39
24	s	403	CHL	C1B-C2B	8.11	1.48	1.39
24	6	311	CHL	C3B-C4B	8.11	1.49	1.41
24	s	406	CHL	C1B-C2B	8.11	1.48	1.39
24	s	407	CHL	C1B-C2B	8.11	1.48	1.39
24	4	311	CHL	C1B-C2B	8.10	1.48	1.39
24	1	311	CHL	C1B-C2B	8.10	1.48	1.39
24	Y	319	CHL	C1B-C2B	8.10	1.48	1.39
24	9	305	CHL	C1B-C2B	8.09	1.48	1.39
24	1	309	CHL	C3B-C4B	8.09	1.49	1.41
24	S	602	CHL	C1B-C2B	8.08	1.48	1.39
24	3	305	CHL	C1B-C2B	8.08	1.48	1.39
24	n	311	CHL	C1B-C2B	8.06	1.48	1.39
24	4	311	CHL	C3B-C4B	8.05	1.49	1.41
24	8	303	CHL	C1A-CHA	8.05	1.49	1.40
24	7	318	CHL	C1A-CHA	8.04	1.49	1.40
24	8	309	CHL	C1B-C2B	8.04	1.48	1.39
24	p	310	CHL	C1B-C2B	8.04	1.48	1.39
24	N	305	CHL	C1B-C2B	8.04	1.48	1.39
24	u	306	CHL	C1B-C2B	8.03	1.48	1.39
24	G	318	CHL	C1B-C2B	8.03	1.48	1.39
24	g	318	CHL	C1B-C2B	8.03	1.48	1.39
24	1	311	CHL	C3B-C4B	8.02	1.49	1.41
24	6	311	CHL	C1A-CHA	8.02	1.49	1.40
24	g	305	CHL	C1A-CHA	8.02	1.49	1.40
24	Y	310	CHL	C1B-C2B	8.01	1.48	1.39
24	y	309	CHL	C1A-CHA	8.01	1.49	1.40
24	y	311	CHL	C1B-C2B	8.01	1.48	1.39
24	q	307	CHL	C1B-C2B	8.01	1.48	1.39
24	n	305	CHL	C1B-C2B	8.01	1.48	1.39
24	2	310	CHL	C1A-CHA	8.00	1.49	1.40
24	7	313	CHL	C1B-C2B	8.00	1.48	1.39
24	Y	317	CHL	C1B-C2B	8.00	1.48	1.39
24	9	317	CHL	C3B-C4B	8.00	1.49	1.41
24	N	311	CHL	C1B-C2B	8.00	1.48	1.39
24	q	307	CHL	C1A-CHA	7.99	1.49	1.40
24	q	303	CHL	C1A-CHA	7.99	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	q	310	CHL	C1B-C2B	7.98	1.48	1.39
24	6	304	CHL	C1A-CHA	7.98	1.49	1.40
24	5	310	CHL	C1B-C2B	7.98	1.48	1.39
24	Y	308	CHL	C1A-CHA	7.98	1.49	1.40
24	7	310	CHL	C1B-C2B	7.97	1.48	1.39
24	y	318	CHL	C1B-C2B	7.96	1.48	1.39
24	G	305	CHL	C1A-CHA	7.96	1.49	1.40
24	u	318	CHL	C3B-C4B	7.96	1.49	1.41
24	u	309	CHL	C3B-C4B	7.96	1.49	1.41
24	N	317	CHL	C3B-C4B	7.96	1.49	1.41
24	p	318	CHL	C1A-CHA	7.95	1.49	1.40
35	a	606	PHO	C3B-C4B	7.95	1.49	1.41
24	n	317	CHL	C3B-C4B	7.95	1.49	1.41
24	2	310	CHL	C1B-C2B	7.95	1.48	1.39
24	y	305	CHL	C1B-C2B	7.95	1.48	1.39
24	u	310	CHL	C1A-CHA	7.95	1.49	1.40
24	r	308	CHL	C1A-CHA	7.95	1.49	1.40
24	5	306	CHL	C1B-C2B	7.95	1.48	1.39
24	S	601	CHL	C1B-C2B	7.94	1.48	1.39
24	Y	309	CHL	C3B-C4B	7.94	1.49	1.41
24	3	311	CHL	C1A-CHA	7.93	1.49	1.40
24	9	310	CHL	C1A-CHA	7.93	1.49	1.40
24	6	317	CHL	C1A-CHA	7.93	1.49	1.40
24	g	311	CHL	C1A-CHA	7.92	1.49	1.40
24	1	305	CHL	C1A-CHA	7.92	1.49	1.40
24	4	305	CHL	C1A-CHA	7.91	1.49	1.40
24	8	307	CHL	C1B-C2B	7.91	1.48	1.39
24	1	317	CHL	C3B-C4B	7.91	1.49	1.41
24	G	309	CHL	C3B-C4B	7.90	1.49	1.41
24	6	310	CHL	C1A-CHA	7.90	1.49	1.40
24	G	312	CHL	C1A-CHA	7.90	1.49	1.40
24	5	310	CHL	C1A-CHA	7.90	1.49	1.40
24	s	402	CHL	C1B-C2B	7.90	1.48	1.39
24	Y	304	CHL	C1B-C2B	7.89	1.48	1.39
24	9	308	CHL	C3B-C4B	7.89	1.49	1.41
24	p	310	CHL	C3B-C4B	7.88	1.49	1.41
35	D	403	PHO	C3B-C4B	7.88	1.49	1.41
24	y	310	CHL	C3B-C4B	7.88	1.49	1.41
24	g	312	CHL	C1A-CHA	7.88	1.49	1.40
24	8	307	CHL	C1A-CHA	7.87	1.49	1.40
24	2	305	CHL	C1A-CHA	7.87	1.48	1.40
24	2	306	CHL	C1B-C2B	7.87	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	3	317	CHL	C1A-CHA	7.87	1.48	1.40
24	g	312	CHL	C3B-C4B	7.87	1.49	1.41
24	G	318	CHL	C1A-CHA	7.86	1.48	1.40
24	4	310	CHL	C1A-CHA	7.86	1.48	1.40
24	g	318	CHL	C1A-CHA	7.86	1.48	1.40
24	6	309	CHL	C1A-CHA	7.85	1.48	1.40
24	3	310	CHL	C1A-CHA	7.85	1.48	1.40
24	1	310	CHL	C3B-C4B	7.85	1.49	1.41
24	4	305	CHL	C3B-C4B	7.85	1.49	1.41
35	d	403	PHO	C3B-C4B	7.85	1.49	1.41
24	G	311	CHL	C1A-CHA	7.84	1.48	1.40
24	9	309	CHL	C1A-CHA	7.84	1.48	1.40
24	4	317	CHL	C3B-C4B	7.84	1.49	1.41
24	u	306	CHL	C3B-C4B	7.83	1.49	1.41
24	R	601	CHL	C3B-C4B	7.83	1.49	1.41
24	s	414	CHL	C1B-C2B	7.83	1.48	1.39
24	Y	311	CHL	C1B-C2B	7.82	1.48	1.39
24	1	310	CHL	C1A-CHA	7.82	1.48	1.40
24	u	311	CHL	C1A-CHA	7.81	1.48	1.40
24	3	309	CHL	C1A-CHA	7.81	1.48	1.40
24	y	312	CHL	C1B-C2B	7.81	1.48	1.39
24	9	311	CHL	C3B-C4B	7.80	1.49	1.41
24	N	311	CHL	C1A-CHA	7.80	1.48	1.40
24	n	310	CHL	C1A-CHA	7.80	1.48	1.40
24	g	309	CHL	C3B-C4B	7.80	1.49	1.41
24	g	313	CHL	C1A-CHA	7.79	1.48	1.40
24	r	306	CHL	C3B-C4B	7.79	1.49	1.41
24	7	310	CHL	C3B-C4B	7.79	1.49	1.41
24	N	310	CHL	C1A-CHA	7.79	1.48	1.40
24	5	305	CHL	C1A-CHA	7.79	1.48	1.40
24	R	607	CHL	C1A-CHA	7.78	1.48	1.40
24	3	304	CHL	C1A-CHA	7.78	1.48	1.40
24	4	308	CHL	C3B-C4B	7.78	1.49	1.41
24	4	310	CHL	C3B-C4B	7.78	1.49	1.41
24	S	613	CHL	C1B-C2B	7.77	1.48	1.39
24	r	302	CHL	C3B-C4B	7.77	1.49	1.41
24	G	312	CHL	C3B-C4B	7.77	1.49	1.41
24	u	312	CHL	C3B-C4B	7.76	1.48	1.41
24	8	304	CHL	C3B-C4B	7.76	1.48	1.41
24	6	308	CHL	C3B-C4B	7.76	1.48	1.41
24	1	304	CHL	C3B-C4B	7.75	1.48	1.41
24	s	407	CHL	C3B-C4B	7.75	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	p	311	CHL	C1A-CHA	7.74	1.48	1.40
24	G	313	CHL	C1A-CHA	7.74	1.48	1.40
24	N	304	CHL	C3B-C4B	7.74	1.48	1.41
24	n	311	CHL	C3B-C4B	7.74	1.48	1.41
24	u	305	CHL	C3B-C4B	7.74	1.48	1.41
24	g	310	CHL	C1A-CHA	7.73	1.48	1.40
24	2	312	CHL	C1A-CHA	7.73	1.48	1.40
24	1	308	CHL	C3B-C4B	7.73	1.48	1.41
24	4	304	CHL	C3B-C4B	7.72	1.48	1.41
24	p	318	CHL	C3B-C4B	7.72	1.48	1.41
24	1	305	CHL	C3B-C4B	7.72	1.48	1.41
24	3	308	CHL	C3B-C4B	7.71	1.48	1.41
24	q	308	CHL	C1B-C2B	7.71	1.48	1.39
24	q	304	CHL	C3B-C4B	7.71	1.48	1.41
24	7	309	CHL	C3B-C4B	7.71	1.48	1.41
24	7	311	CHL	C1A-CHA	7.71	1.48	1.40
24	3	312	CHL	C1A-CHA	7.71	1.48	1.40
24	7	318	CHL	C3B-C4B	7.71	1.48	1.41
24	5	312	CHL	C1A-CHA	7.71	1.48	1.40
24	9	312	CHL	C1A-CHA	7.70	1.48	1.40
24	8	315	CHL	C3B-C4B	7.70	1.48	1.41
24	9	310	CHL	C3B-C4B	7.70	1.48	1.41
24	R	606	CHL	C1A-CHA	7.69	1.48	1.40
24	S	606	CHL	C3B-C4B	7.69	1.48	1.41
24	r	306	CHL	C1A-CHA	7.69	1.48	1.40
24	y	310	CHL	C1B-C2B	7.68	1.48	1.39
24	g	310	CHL	C3B-C4B	7.68	1.48	1.41
24	6	312	CHL	C1A-CHA	7.68	1.48	1.40
24	S	607	CHL	C1A-CHA	7.68	1.48	1.40
24	G	310	CHL	C3B-C4B	7.68	1.48	1.41
24	n	304	CHL	C3B-C4B	7.67	1.48	1.41
24	p	312	CHL	C1A-CHA	7.67	1.48	1.40
24	s	408	CHL	C1A-CHA	7.67	1.48	1.40
24	p	311	CHL	C3B-C4B	7.67	1.48	1.41
24	G	306	CHL	C3B-C4B	7.66	1.48	1.41
24	G	310	CHL	C1A-CHA	7.66	1.48	1.40
24	Y	305	CHL	C1B-C2B	7.65	1.48	1.39
24	r	307	CHL	C3B-C4B	7.65	1.48	1.41
24	n	310	CHL	C3B-C4B	7.65	1.48	1.41
24	y	313	CHL	C1B-C2B	7.65	1.48	1.39
24	p	309	CHL	C3B-C4B	7.64	1.48	1.41
24	G	313	CHL	C3B-C4B	7.64	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	7	312	CHL	C1A-CHA	7.64	1.48	1.40
24	N	311	CHL	C3B-C4B	7.64	1.48	1.41
24	N	308	CHL	C1A-CHA	7.64	1.48	1.40
24	g	311	CHL	C3B-C4B	7.63	1.48	1.41
24	g	306	CHL	C3B-C4B	7.63	1.48	1.41
24	Y	312	CHL	C1B-C2B	7.63	1.48	1.39
24	N	310	CHL	C3B-C4B	7.63	1.48	1.41
24	q	316	CHL	C3B-C4B	7.62	1.48	1.41
24	n	311	CHL	C1A-CHA	7.62	1.48	1.40
24	y	306	CHL	C1B-C2B	7.62	1.48	1.39
24	2	309	CHL	C3B-C4B	7.62	1.48	1.41
24	u	313	CHL	C1A-CHA	7.62	1.48	1.40
24	u	311	CHL	C3B-C4B	7.62	1.48	1.41
24	3	309	CHL	C3B-C4B	7.61	1.48	1.41
24	3	317	CHL	C3B-C4B	7.61	1.48	1.41
24	7	306	CHL	C1B-C2B	7.61	1.48	1.39
24	q	304	CHL	C1B-C2B	7.61	1.48	1.39
24	6	312	CHL	C3B-C4B	7.61	1.48	1.41
24	5	311	CHL	C1A-CHA	7.61	1.48	1.40
24	p	306	CHL	C1B-C2B	7.60	1.48	1.39
24	1	309	CHL	C1A-CHA	7.60	1.48	1.40
24	N	305	CHL	C1A-CHA	7.60	1.48	1.40
24	9	305	CHL	C3B-C4B	7.60	1.48	1.41
24	9	305	CHL	C1A-CHA	7.60	1.48	1.40
24	1	312	CHL	C1A-CHA	7.59	1.48	1.40
24	3	310	CHL	C3B-C4B	7.59	1.48	1.41
24	r	307	CHL	C1A-CHA	7.59	1.48	1.40
24	2	305	CHL	C3B-C4B	7.59	1.48	1.41
24	R	606	CHL	C3B-C4B	7.59	1.48	1.41
24	7	311	CHL	C3B-C4B	7.58	1.48	1.41
24	5	313	CHL	C3B-C4B	7.58	1.48	1.41
24	S	613	CHL	C1A-CHA	7.58	1.48	1.40
24	g	305	CHL	C3B-C4B	7.58	1.48	1.41
24	Y	309	CHL	C1B-C2B	7.58	1.48	1.39
24	2	311	CHL	C1A-CHA	7.58	1.48	1.40
24	6	317	CHL	C3B-C4B	7.58	1.48	1.41
24	u	306	CHL	C1A-CHA	7.58	1.48	1.40
24	8	308	CHL	C3B-C4B	7.57	1.48	1.41
24	5	305	CHL	C3B-C4B	7.57	1.48	1.41
24	s	407	CHL	C1A-CHA	7.57	1.48	1.40
24	S	602	CHL	C1A-CHA	7.57	1.48	1.40
24	5	309	CHL	C3B-C4B	7.57	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	9	312	CHL	C3B-C4B	7.57	1.48	1.41
24	6	309	CHL	C3B-C4B	7.57	1.48	1.41
24	4	312	CHL	C1A-CHA	7.56	1.48	1.40
24	g	313	CHL	C3B-C4B	7.56	1.48	1.41
24	4	309	CHL	C1A-CHA	7.56	1.48	1.40
24	r	303	CHL	C1A-CHA	7.56	1.48	1.40
24	u	313	CHL	C3B-C4B	7.55	1.48	1.41
24	8	310	CHL	C1B-C2B	7.55	1.48	1.39
24	8	308	CHL	C1B-C2B	7.55	1.48	1.39
24	6	310	CHL	C3B-C4B	7.55	1.48	1.41
24	5	313	CHL	C1A-CHA	7.55	1.48	1.40
24	4	311	CHL	C1A-CHA	7.54	1.48	1.40
24	2	313	CHL	C1A-CHA	7.54	1.48	1.40
24	8	304	CHL	C1B-C2B	7.54	1.48	1.39
24	n	308	CHL	C3B-C4B	7.54	1.48	1.41
24	G	311	CHL	C3B-C4B	7.54	1.48	1.41
24	s	403	CHL	C1A-CHA	7.54	1.48	1.40
24	Y	305	CHL	C1A-CHA	7.54	1.48	1.40
24	7	305	CHL	C1A-CHA	7.53	1.48	1.40
24	y	306	CHL	C1A-CHA	7.53	1.48	1.40
24	n	305	CHL	C3B-C4B	7.53	1.48	1.41
24	s	406	CHL	C1A-CHA	7.53	1.48	1.40
24	9	304	CHL	C3B-C4B	7.53	1.48	1.41
24	S	605	CHL	C1A-CHA	7.52	1.48	1.40
24	q	308	CHL	C3B-C4B	7.52	1.48	1.41
24	G	305	CHL	C3B-C4B	7.52	1.48	1.41
24	G	318	CHL	C3B-C4B	7.51	1.48	1.41
24	7	306	CHL	C3B-C4B	7.51	1.48	1.41
24	2	313	CHL	C3B-C4B	7.51	1.48	1.41
24	p	306	CHL	C3B-C4B	7.51	1.48	1.41
24	n	305	CHL	C1A-CHA	7.51	1.48	1.40
24	q	311	CHL	C1B-C2B	7.50	1.48	1.39
24	S	608	CHL	C1A-CHA	7.50	1.48	1.40
24	3	312	CHL	C3B-C4B	7.50	1.48	1.41
24	6	304	CHL	C3B-C4B	7.49	1.48	1.41
24	6	305	CHL	C1A-CHA	7.48	1.48	1.40
24	s	414	CHL	C1A-CHA	7.48	1.48	1.40
24	R	605	CHL	C3B-C4B	7.48	1.48	1.41
24	N	308	CHL	C3B-C4B	7.48	1.48	1.41
24	s	409	CHL	C1A-CHA	7.48	1.48	1.40
24	q	310	CHL	C3B-C4B	7.48	1.48	1.41
24	S	606	CHL	C1A-CHA	7.48	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	R	605	CHL	C1A-CHA	7.48	1.48	1.40
24	s	408	CHL	C3B-C4B	7.47	1.48	1.41
24	3	305	CHL	C1A-CHA	7.47	1.48	1.40
24	g	318	CHL	C3B-C4B	7.47	1.48	1.41
24	R	602	CHL	C1A-CHA	7.46	1.48	1.40
24	2	318	CHL	C3B-C4B	7.46	1.48	1.41
24	p	305	CHL	C1A-CHA	7.46	1.48	1.40
24	3	304	CHL	C3B-C4B	7.46	1.48	1.41
24	Y	310	CHL	C1A-CHA	7.46	1.48	1.40
24	2	311	CHL	C3B-C4B	7.46	1.48	1.41
24	5	318	CHL	C3B-C4B	7.46	1.48	1.41
24	8	309	CHL	C3B-C4B	7.45	1.48	1.41
24	p	312	CHL	C3B-C4B	7.45	1.48	1.41
24	Y	319	CHL	C1A-CHA	7.45	1.48	1.40
24	n	309	CHL	C1A-CHA	7.45	1.48	1.40
24	1	311	CHL	C1A-CHA	7.45	1.48	1.40
24	q	309	CHL	C1A-CHA	7.44	1.48	1.40
24	q	309	CHL	C3B-C4B	7.44	1.48	1.41
24	5	311	CHL	C3B-C4B	7.43	1.48	1.41
24	N	309	CHL	C1A-CHA	7.43	1.48	1.40
24	Y	317	CHL	C1A-CHA	7.42	1.48	1.40
24	Y	319	CHL	C3B-C4B	7.42	1.48	1.41
24	q	307	CHL	C3B-C4B	7.42	1.48	1.41
24	7	312	CHL	C3B-C4B	7.41	1.48	1.41
24	5	310	CHL	C3B-C4B	7.41	1.48	1.41
24	2	310	CHL	C3B-C4B	7.41	1.48	1.41
24	Y	308	CHL	C3B-C4B	7.41	1.48	1.41
24	p	310	CHL	C1A-CHA	7.40	1.48	1.40
24	8	303	CHL	C3B-C4B	7.40	1.48	1.41
24	Y	311	CHL	C1A-CHA	7.40	1.48	1.40
24	q	303	CHL	C3B-C4B	7.39	1.48	1.41
24	N	305	CHL	C3B-C4B	7.39	1.48	1.41
24	2	312	CHL	C3B-C4B	7.39	1.48	1.41
24	S	613	CHL	C3B-C4B	7.39	1.48	1.41
24	Y	304	CHL	C3B-C4B	7.38	1.48	1.41
24	g	306	CHL	C1A-CHA	7.38	1.48	1.40
24	8	309	CHL	C1A-CHA	7.37	1.48	1.40
24	y	305	CHL	C3B-C4B	7.37	1.48	1.41
24	y	309	CHL	C3B-C4B	7.37	1.48	1.41
24	G	306	CHL	C1A-CHA	7.36	1.48	1.40
24	s	402	CHL	C1A-CHA	7.35	1.48	1.40
24	s	402	CHL	C3B-C4B	7.35	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	S	607	CHL	C3B-C4B	7.35	1.48	1.41
24	7	310	CHL	C1A-CHA	7.34	1.48	1.40
24	R	607	CHL	C3B-C4B	7.34	1.48	1.41
24	r	309	CHL	C1A-CHA	7.34	1.48	1.40
24	Y	304	CHL	C1A-CHA	7.33	1.48	1.40
24	5	312	CHL	C3B-C4B	7.33	1.48	1.41
24	8	307	CHL	C3B-C4B	7.32	1.48	1.41
24	y	311	CHL	C1A-CHA	7.32	1.48	1.40
24	y	312	CHL	C1A-CHA	7.32	1.48	1.40
24	y	310	CHL	C1A-CHA	7.32	1.48	1.40
24	Y	305	CHL	C3B-C4B	7.32	1.48	1.41
24	y	306	CHL	C3B-C4B	7.32	1.48	1.41
24	Y	311	CHL	C3B-C4B	7.32	1.48	1.41
24	s	403	CHL	C3B-C4B	7.32	1.48	1.41
24	y	318	CHL	C1A-CHA	7.32	1.48	1.40
24	7	313	CHL	C1A-CHA	7.31	1.48	1.40
24	q	310	CHL	C1A-CHA	7.30	1.48	1.40
24	N	312	CHL	C3B-C4B	7.29	1.48	1.41
24	s	409	CHL	C3B-C4B	7.29	1.48	1.41
24	S	601	CHL	C3B-C4B	7.29	1.48	1.41
24	S	602	CHL	C3B-C4B	7.29	1.48	1.41
24	R	608	CHL	C1A-CHA	7.28	1.48	1.40
24	n	309	CHL	C3B-C4B	7.28	1.48	1.41
24	y	305	CHL	C1A-CHA	7.28	1.48	1.40
24	p	306	CHL	C1A-CHA	7.27	1.48	1.40
24	y	311	CHL	C3B-C4B	7.27	1.48	1.41
24	5	306	CHL	C3B-C4B	7.26	1.48	1.41
24	n	312	CHL	C3B-C4B	7.26	1.48	1.41
24	y	312	CHL	C3B-C4B	7.26	1.48	1.41
24	S	601	CHL	C1A-CHA	7.26	1.48	1.40
24	N	309	CHL	C3B-C4B	7.25	1.48	1.41
24	r	308	CHL	C3B-C4B	7.25	1.48	1.41
24	6	305	CHL	C3B-C4B	7.24	1.48	1.41
24	3	305	CHL	C3B-C4B	7.24	1.48	1.41
24	2	306	CHL	C3B-C4B	7.23	1.48	1.41
24	Y	309	CHL	C1A-CHA	7.23	1.48	1.40
24	S	608	CHL	C3B-C4B	7.23	1.48	1.41
24	p	313	CHL	C3B-C4B	7.22	1.48	1.41
24	s	414	CHL	C3B-C4B	7.21	1.48	1.41
24	4	312	CHL	C3B-C4B	7.21	1.48	1.41
24	N	312	CHL	C1A-CHA	7.21	1.48	1.40
24	u	313	CHL	C1D-C2D	7.20	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	2	306	CHL	C1A-CHA	7.20	1.48	1.40
24	S	605	CHL	C3B-C4B	7.19	1.48	1.41
24	1	312	CHL	C3B-C4B	7.19	1.48	1.41
24	5	306	CHL	C1A-CHA	7.19	1.48	1.40
24	q	311	CHL	C3B-C4B	7.19	1.48	1.41
24	Y	310	CHL	C3B-C4B	7.18	1.48	1.41
24	r	309	CHL	C3B-C4B	7.18	1.48	1.41
24	p	313	CHL	C1A-CHA	7.18	1.48	1.40
24	s	406	CHL	C3B-C4B	7.18	1.48	1.41
24	n	312	CHL	C1A-CHA	7.17	1.48	1.40
24	8	310	CHL	C3B-C4B	7.17	1.48	1.41
24	y	313	CHL	C1A-CHA	7.17	1.48	1.40
24	Y	312	CHL	C1A-CHA	7.15	1.48	1.40
24	q	311	CHL	C1A-CHA	7.14	1.48	1.40
24	R	602	CHL	C3B-C4B	7.13	1.48	1.41
24	r	303	CHL	C3B-C4B	7.12	1.48	1.41
24	7	313	CHL	C3B-C4B	7.12	1.48	1.41
24	u	318	CHL	C1D-C2D	7.12	1.47	1.39
24	6	312	CHL	C1D-C2D	7.11	1.47	1.39
24	Y	312	CHL	C3B-C4B	7.11	1.48	1.41
24	8	304	CHL	C1A-CHA	7.10	1.48	1.40
24	R	608	CHL	C3B-C4B	7.09	1.48	1.41
24	8	310	CHL	C1A-CHA	7.09	1.48	1.40
24	3	312	CHL	C1D-C2D	7.08	1.47	1.39
24	7	306	CHL	C1A-CHA	7.08	1.48	1.40
24	y	313	CHL	C3B-C4B	7.07	1.48	1.41
24	9	317	CHL	C1D-C2D	7.04	1.47	1.39
24	q	304	CHL	C1A-CHA	7.04	1.48	1.40
31	S	615	8CT	C15-C16	7.03	1.61	1.46
24	g	313	CHL	C1D-C2D	7.01	1.47	1.39
24	G	313	CHL	C1D-C2D	7.00	1.47	1.39
24	8	308	CHL	C1A-CHA	7.00	1.48	1.40
31	s	416	8CT	C15-C16	7.00	1.60	1.46
24	7	309	CHL	C1D-C2D	6.98	1.47	1.39
31	T	101	8CT	C05-C06	-6.98	1.36	1.52
24	p	305	CHL	C3B-C4B	6.97	1.48	1.41
31	c	614	8CT	C05-C06	-6.97	1.36	1.52
24	9	308	CHL	C1D-C2D	6.97	1.47	1.39
31	t	101	8CT	C05-C06	-6.96	1.36	1.52
31	C	614	8CT	C05-C06	-6.94	1.36	1.52
24	Y	317	CHL	C3B-C4B	6.93	1.48	1.41
24	q	308	CHL	C1A-CHA	6.93	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	1	309	CHL	C1D-C2D	6.93	1.47	1.39
24	G	309	CHL	C1D-C2D	6.93	1.47	1.39
24	3	310	CHL	C1D-C2D	6.93	1.47	1.39
24	G	310	CHL	C1D-C2D	6.93	1.47	1.39
24	1	317	CHL	C1D-C2D	6.92	1.47	1.39
24	4	317	CHL	C1D-C2D	6.92	1.47	1.39
24	6	310	CHL	C1D-C2D	6.92	1.47	1.39
24	g	309	CHL	C1D-C2D	6.91	1.47	1.39
24	u	309	CHL	C1D-C2D	6.91	1.47	1.39
24	p	309	CHL	C1D-C2D	6.91	1.47	1.39
24	u	305	CHL	C1D-C2D	6.91	1.47	1.39
31	X	601	8CT	C05-C06	-6.90	1.36	1.52
31	D	410	8CT	C05-C06	-6.89	1.36	1.52
24	9	312	CHL	C1D-C2D	6.89	1.47	1.39
24	N	317	CHL	C1D-C2D	6.88	1.47	1.39
24	4	309	CHL	C1D-C2D	6.88	1.47	1.39
31	A	608	8CT	C05-C06	-6.88	1.36	1.52
31	a	608	8CT	C05-C06	-6.88	1.36	1.52
24	g	310	CHL	C1D-C2D	6.87	1.47	1.39
31	d	410	8CT	C05-C06	-6.87	1.36	1.52
31	x	601	8CT	C05-C06	-6.86	1.36	1.52
24	3	309	CHL	C1D-C2D	6.86	1.47	1.39
24	n	310	CHL	C1D-C2D	6.85	1.47	1.39
24	7	305	CHL	C3B-C4B	6.85	1.48	1.41
24	u	311	CHL	C1D-C2D	6.84	1.47	1.39
24	9	310	CHL	C1D-C2D	6.83	1.47	1.39
24	N	310	CHL	C1D-C2D	6.83	1.47	1.39
24	N	312	CHL	C1D-C2D	6.83	1.47	1.39
24	9	304	CHL	C1D-C2D	6.83	1.47	1.39
24	G	311	CHL	C1D-C2D	6.82	1.47	1.39
24	g	311	CHL	C1D-C2D	6.82	1.47	1.39
24	n	317	CHL	C1D-C2D	6.82	1.47	1.39
24	6	308	CHL	C1D-C2D	6.82	1.47	1.39
24	1	308	CHL	C1D-C2D	6.81	1.47	1.39
24	q	316	CHL	C1D-C2D	6.81	1.47	1.39
31	c	615	8CT	C05-C06	-6.81	1.36	1.52
31	S	615	8CT	C05-C06	-6.80	1.36	1.52
31	s	416	8CT	C05-C06	-6.80	1.36	1.52
24	y	318	CHL	C3B-C4B	6.80	1.48	1.41
24	1	304	CHL	C1D-C2D	6.80	1.47	1.39
24	6	317	CHL	C1D-C2D	6.80	1.47	1.39
31	S	614	8CT	C05-C06	-6.80	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	s	415	8CT	C05-C06	-6.79	1.36	1.52
24	4	308	CHL	C1D-C2D	6.79	1.47	1.39
24	n	312	CHL	C1D-C2D	6.79	1.47	1.39
31	v	401	8CT	C05-C06	-6.79	1.36	1.52
24	6	309	CHL	C1D-C2D	6.79	1.47	1.39
31	c	613	8CT	C05-C06	-6.78	1.36	1.52
24	4	304	CHL	C1D-C2D	6.78	1.47	1.39
24	8	315	CHL	C1D-C2D	6.78	1.47	1.39
24	1	311	CHL	C1D-C2D	6.77	1.47	1.39
31	C	613	8CT	C05-C06	-6.77	1.36	1.52
24	N	304	CHL	C1D-C2D	6.77	1.47	1.39
31	V	401	8CT	C05-C06	-6.77	1.36	1.52
24	n	304	CHL	C1D-C2D	6.75	1.47	1.39
31	C	615	8CT	C05-C06	-6.75	1.36	1.52
24	3	317	CHL	C1D-C2D	6.75	1.47	1.39
31	s	415	8CT	C15-C16	6.75	1.60	1.46
24	G	312	CHL	C1D-C2D	6.74	1.47	1.39
24	4	311	CHL	C1D-C2D	6.74	1.47	1.39
24	3	308	CHL	C1D-C2D	6.73	1.47	1.39
24	3	304	CHL	C1D-C2D	6.73	1.47	1.39
24	g	312	CHL	C1D-C2D	6.72	1.47	1.39
24	2	311	CHL	C1D-C2D	6.72	1.47	1.39
24	p	313	CHL	C1D-C2D	6.72	1.47	1.39
24	N	308	CHL	C1D-C2D	6.72	1.47	1.39
24	5	305	CHL	C1D-C2D	6.72	1.47	1.39
24	q	303	CHL	C1D-C2D	6.72	1.47	1.39
24	u	310	CHL	C1D-C2D	6.71	1.47	1.39
31	S	614	8CT	C15-C16	6.71	1.60	1.46
24	6	304	CHL	C1D-C2D	6.71	1.47	1.39
24	2	309	CHL	C1D-C2D	6.69	1.47	1.39
24	9	309	CHL	C1D-C2D	6.69	1.47	1.39
24	8	303	CHL	C1D-C2D	6.67	1.47	1.39
24	n	308	CHL	C1D-C2D	6.67	1.47	1.39
24	5	311	CHL	C1D-C2D	6.66	1.47	1.39
24	r	306	CHL	C1D-C2D	6.66	1.47	1.39
24	7	313	CHL	C1D-C2D	6.66	1.47	1.39
24	2	305	CHL	C1D-C2D	6.65	1.47	1.39
24	5	309	CHL	C1D-C2D	6.65	1.47	1.39
24	s	409	CHL	C1D-C2D	6.65	1.47	1.39
24	u	312	CHL	C1D-C2D	6.64	1.47	1.39
24	5	318	CHL	C1D-C2D	6.61	1.47	1.39
24	3	305	CHL	C1D-C2D	6.61	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	1	312	CHL	C1D-C2D	6.61	1.47	1.39
24	u	306	CHL	C1D-C2D	6.61	1.47	1.39
24	g	305	CHL	C1D-C2D	6.61	1.47	1.39
24	9	305	CHL	C1D-C2D	6.60	1.47	1.39
24	G	305	CHL	C1D-C2D	6.60	1.47	1.39
24	p	310	CHL	C1D-C2D	6.60	1.47	1.39
24	S	608	CHL	C1D-C2D	6.59	1.47	1.39
31	B	617	8CT	C05-C06	-6.59	1.37	1.52
24	7	310	CHL	C1D-C2D	6.59	1.47	1.39
31	b	617	8CT	C05-C06	-6.59	1.37	1.52
24	2	313	CHL	C1D-C2D	6.59	1.47	1.39
24	9	311	CHL	C1D-C2D	6.59	1.47	1.39
24	4	305	CHL	C1D-C2D	6.58	1.47	1.39
24	G	306	CHL	C1D-C2D	6.57	1.47	1.39
24	R	601	CHL	C1D-C2D	6.57	1.47	1.39
24	6	311	CHL	C1D-C2D	6.57	1.47	1.39
31	S	614	8CT	C28-C26	6.56	1.60	1.46
24	3	311	CHL	C1D-C2D	6.56	1.47	1.39
24	r	302	CHL	C1D-C2D	6.55	1.47	1.39
24	2	318	CHL	C1D-C2D	6.55	1.47	1.39
24	6	305	CHL	C1D-C2D	6.55	1.47	1.39
24	5	313	CHL	C1D-C2D	6.54	1.47	1.39
24	R	605	CHL	C1D-C2D	6.54	1.47	1.39
31	s	415	8CT	C28-C26	6.54	1.59	1.46
24	g	306	CHL	C1D-C2D	6.53	1.47	1.39
24	y	309	CHL	C1D-C2D	6.52	1.47	1.39
24	4	312	CHL	C1D-C2D	6.51	1.46	1.39
24	n	311	CHL	C1D-C2D	6.51	1.46	1.39
24	1	310	CHL	C1D-C2D	6.50	1.46	1.39
24	p	311	CHL	C1D-C2D	6.50	1.46	1.39
24	Y	308	CHL	C1D-C2D	6.49	1.46	1.39
24	7	311	CHL	C1D-C2D	6.48	1.46	1.39
24	S	606	CHL	C1D-C2D	6.48	1.46	1.39
24	s	407	CHL	C1D-C2D	6.48	1.46	1.39
24	s	406	CHL	C1D-C2D	6.48	1.46	1.39
24	N	311	CHL	C1D-C2D	6.47	1.46	1.39
24	4	310	CHL	C1D-C2D	6.47	1.46	1.39
24	S	605	CHL	C1D-C2D	6.46	1.46	1.39
24	1	305	CHL	C1D-C2D	6.44	1.46	1.39
24	N	309	CHL	C1D-C2D	6.41	1.46	1.39
24	S	607	CHL	C1D-C2D	6.41	1.46	1.39
24	R	602	CHL	C1D-C2D	6.41	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	p	318	CHL	C1D-C2D	6.40	1.46	1.39
24	Y	312	CHL	C1D-C2D	6.39	1.46	1.39
24	G	318	CHL	C1D-C2D	6.39	1.46	1.39
24	g	318	CHL	C1D-C2D	6.39	1.46	1.39
24	y	313	CHL	C1D-C2D	6.39	1.46	1.39
24	5	312	CHL	C1D-C2D	6.37	1.46	1.39
24	7	318	CHL	C1D-C2D	6.37	1.46	1.39
24	q	311	CHL	C1D-C2D	6.36	1.46	1.39
24	8	310	CHL	C1D-C2D	6.36	1.46	1.39
24	q	307	CHL	C1D-C2D	6.36	1.46	1.39
24	8	307	CHL	C1D-C2D	6.35	1.46	1.39
24	p	305	CHL	C1D-C2D	6.35	1.46	1.39
24	r	308	CHL	C1D-C2D	6.35	1.46	1.39
24	2	312	CHL	C1D-C2D	6.34	1.46	1.39
31	b	617	8CT	C15-C16	6.33	1.59	1.46
24	n	309	CHL	C1D-C2D	6.33	1.46	1.39
24	q	304	CHL	C1D-C2D	6.33	1.46	1.39
24	R	608	CHL	C1D-C2D	6.32	1.46	1.39
24	7	305	CHL	C1D-C2D	6.32	1.46	1.39
24	R	607	CHL	C1D-C2D	6.32	1.46	1.39
24	N	305	CHL	C1D-C2D	6.31	1.46	1.39
31	v	401	8CT	C28-C26	6.30	1.59	1.46
24	r	309	CHL	C1D-C2D	6.30	1.46	1.39
31	a	608	8CT	C15-C16	6.29	1.59	1.46
31	C	613	8CT	C15-C16	6.28	1.59	1.46
31	T	101	8CT	C15-C16	6.28	1.59	1.46
24	r	303	CHL	C1D-C2D	6.28	1.46	1.39
31	S	615	8CT	C28-C26	6.27	1.59	1.46
31	s	416	8CT	C28-C26	6.27	1.59	1.46
31	B	617	8CT	C15-C16	6.27	1.59	1.46
31	v	401	8CT	C15-C16	6.27	1.59	1.46
31	c	613	8CT	C15-C16	6.26	1.59	1.46
24	Y	319	CHL	C1D-C2D	6.26	1.46	1.39
24	q	308	CHL	C1D-C2D	6.26	1.46	1.39
24	n	305	CHL	C1D-C2D	6.26	1.46	1.39
31	C	615	8CT	C15-C16	6.26	1.59	1.46
31	V	401	8CT	C28-C26	6.26	1.59	1.46
31	V	401	8CT	C15-C16	6.25	1.59	1.46
31	c	615	8CT	C15-C16	6.25	1.59	1.46
31	d	410	8CT	C28-C26	6.25	1.59	1.46
31	c	615	8CT	C04-C03	-6.25	1.45	1.53
24	8	304	CHL	C1D-C2D	6.24	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	5	306	CHL	C1D-C2D	6.24	1.46	1.39
24	s	408	CHL	C1D-C2D	6.24	1.46	1.39
31	t	101	8CT	C15-C16	6.23	1.59	1.46
31	D	410	8CT	C28-C26	6.23	1.59	1.46
31	C	614	8CT	C04-C03	-6.22	1.45	1.53
31	d	410	8CT	C15-C16	6.22	1.59	1.46
24	2	306	CHL	C1D-C2D	6.22	1.46	1.39
24	2	310	CHL	C1D-C2D	6.22	1.46	1.39
24	r	307	CHL	C1D-C2D	6.22	1.46	1.39
31	X	601	8CT	C15-C16	6.22	1.59	1.46
24	5	310	CHL	C1D-C2D	6.22	1.46	1.39
31	D	410	8CT	C15-C16	6.22	1.59	1.46
31	c	614	8CT	C04-C03	-6.22	1.45	1.53
31	A	608	8CT	C15-C16	6.21	1.59	1.46
31	C	615	8CT	C04-C03	-6.21	1.45	1.53
24	y	311	CHL	C1D-C2D	6.18	1.46	1.39
31	C	614	8CT	C15-C16	6.17	1.59	1.46
24	8	308	CHL	C1D-C2D	6.17	1.46	1.39
31	x	601	8CT	C15-C16	6.17	1.59	1.46
31	t	101	8CT	C28-C26	6.17	1.59	1.46
24	q	309	CHL	C1D-C2D	6.17	1.46	1.39
24	q	310	CHL	C1D-C2D	6.16	1.46	1.39
31	c	614	8CT	C15-C16	6.16	1.59	1.46
24	Y	310	CHL	C1D-C2D	6.15	1.46	1.39
24	R	606	CHL	C1D-C2D	6.15	1.46	1.39
31	b	617	8CT	C28-C26	6.15	1.59	1.46
31	T	101	8CT	C28-C26	6.13	1.59	1.46
24	y	312	CHL	C1D-C2D	6.13	1.46	1.39
24	p	312	CHL	C1D-C2D	6.12	1.46	1.39
31	A	608	8CT	C04-C03	-6.11	1.46	1.53
31	B	617	8CT	C28-C26	6.10	1.59	1.46
24	7	312	CHL	C1D-C2D	6.10	1.46	1.39
24	s	402	CHL	C1D-C2D	6.09	1.46	1.39
24	8	309	CHL	C1D-C2D	6.09	1.46	1.39
31	C	613	8CT	C28-C26	6.09	1.59	1.46
24	p	306	CHL	C1D-C2D	6.07	1.46	1.39
31	a	608	8CT	C04-C03	-6.06	1.46	1.53
24	S	613	CHL	C1D-C2D	6.05	1.46	1.39
24	s	414	CHL	C1D-C2D	6.05	1.46	1.39
31	X	601	8CT	C28-C26	6.04	1.58	1.46
31	s	416	8CT	C04-C03	-6.04	1.46	1.53
31	c	613	8CT	C28-C26	6.03	1.58	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	x	601	8CT	C28-C26	6.02	1.58	1.46
24	Y	317	CHL	C1D-C2D	6.02	1.46	1.39
24	S	601	CHL	C1D-C2D	6.01	1.46	1.39
24	Y	311	CHL	C1D-C2D	6.01	1.46	1.39
31	v	401	8CT	C04-C03	-6.01	1.46	1.53
31	s	416	8CT	C23-C21	6.00	1.58	1.46
24	Y	309	CHL	C1D-C2D	6.00	1.46	1.39
24	Y	304	CHL	C1D-C2D	5.99	1.46	1.39
24	7	306	CHL	C1D-C2D	5.99	1.46	1.39
31	S	615	8CT	C04-C03	-5.98	1.46	1.53
31	V	401	8CT	C04-C03	-5.98	1.46	1.53
31	T	101	8CT	C04-C03	-5.98	1.46	1.53
31	S	615	8CT	C23-C21	5.97	1.58	1.46
24	y	318	CHL	C1D-C2D	5.97	1.46	1.39
31	C	614	8CT	C28-C26	5.97	1.58	1.46
24	y	310	CHL	C1D-C2D	5.95	1.46	1.39
31	t	101	8CT	C04-C03	-5.93	1.46	1.53
31	X	601	8CT	C04-C03	-5.93	1.46	1.53
31	c	614	8CT	C28-C26	5.93	1.58	1.46
24	y	305	CHL	C1D-C2D	5.92	1.46	1.39
24	y	306	CHL	C1D-C2D	5.91	1.46	1.39
24	Y	305	CHL	C1D-C2D	5.90	1.46	1.39
31	x	601	8CT	C04-C03	-5.89	1.46	1.53
31	b	617	8CT	C34-C33	5.89	1.65	1.52
31	B	617	8CT	C34-C33	5.88	1.65	1.52
31	d	410	8CT	C04-C03	-5.88	1.46	1.53
31	A	608	8CT	C28-C26	5.88	1.58	1.46
31	T	101	8CT	C34-C33	5.87	1.65	1.52
24	s	414	CHL	C2A-C3A	-5.87	1.49	1.54
31	t	101	8CT	C34-C33	5.87	1.65	1.52
31	a	608	8CT	C28-C26	5.87	1.58	1.46
31	c	613	8CT	C04-C03	-5.87	1.46	1.53
31	C	615	8CT	C28-C26	5.85	1.58	1.46
31	c	615	8CT	C28-C26	5.83	1.58	1.46
24	S	613	CHL	C2A-C3A	-5.83	1.50	1.54
31	C	613	8CT	C04-C03	-5.81	1.46	1.53
31	D	410	8CT	C34-C33	5.79	1.65	1.52
31	d	410	8CT	C34-C33	5.78	1.65	1.52
31	t	101	8CT	C23-C21	5.75	1.58	1.46
31	T	101	8CT	C23-C21	5.75	1.58	1.46
31	b	617	8CT	C04-C03	-5.74	1.46	1.53
24	y	318	CHL	C2A-C3A	-5.74	1.50	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	D	410	8CT	C04-C03	-5.73	1.46	1.53
31	S	614	8CT	C23-C21	5.72	1.58	1.46
31	V	401	8CT	C23-C21	5.71	1.58	1.46
31	b	617	8CT	C23-C21	5.71	1.58	1.46
31	v	401	8CT	C23-C21	5.71	1.58	1.46
24	S	602	CHL	C1D-C2D	5.69	1.46	1.39
31	s	415	8CT	C04-C03	-5.68	1.46	1.53
31	D	410	8CT	C23-C21	5.68	1.58	1.46
31	s	416	8CT	C34-C33	5.67	1.65	1.52
31	s	415	8CT	C23-C21	5.67	1.58	1.46
31	s	415	8CT	C34-C33	5.67	1.65	1.52
31	v	401	8CT	C34-C33	5.67	1.65	1.52
24	Y	317	CHL	C2A-C3A	-5.67	1.50	1.54
31	S	614	8CT	C04-C03	-5.65	1.46	1.53
24	s	403	CHL	C1D-C2D	5.65	1.46	1.39
31	V	401	8CT	C34-C33	5.65	1.65	1.52
31	B	617	8CT	C23-C21	5.65	1.58	1.46
31	S	615	8CT	C34-C33	5.64	1.65	1.52
31	S	614	8CT	C34-C33	5.63	1.65	1.52
31	B	617	8CT	C04-C03	-5.62	1.46	1.53
31	d	410	8CT	C23-C21	5.62	1.58	1.46
24	p	306	CHL	C3A-C2A	-5.58	1.49	1.54
31	c	615	8CT	C23-C21	5.56	1.57	1.46
31	C	613	8CT	C23-C21	5.56	1.57	1.46
31	c	614	8CT	C34-C33	5.55	1.65	1.52
24	Y	305	CHL	C3A-C2A	-5.54	1.49	1.54
31	C	614	8CT	C34-C33	5.54	1.65	1.52
31	C	615	8CT	C23-C21	5.54	1.57	1.46
31	c	613	8CT	C23-C21	5.54	1.57	1.46
24	7	306	CHL	C3A-C2A	-5.53	1.49	1.54
31	x	601	8CT	C23-C21	5.52	1.57	1.46
31	X	601	8CT	C23-C21	5.52	1.57	1.46
24	y	306	CHL	C3A-C2A	-5.52	1.49	1.54
24	Y	304	CHL	C3A-C2A	-5.48	1.50	1.54
24	9	317	CHL	C3B-C2B	5.46	1.47	1.40
31	a	608	8CT	C34-C33	5.46	1.64	1.52
24	u	318	CHL	C3B-C2B	5.46	1.47	1.40
24	y	305	CHL	C3A-C2A	-5.45	1.50	1.54
24	n	317	CHL	C3B-C2B	5.45	1.47	1.40
24	u	309	CHL	C3B-C2B	5.45	1.47	1.40
31	C	615	8CT	C34-C33	5.45	1.64	1.52
31	x	601	8CT	C34-C33	5.45	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	608	8CT	C34-C33	5.45	1.64	1.52
31	c	613	8CT	C34-C33	5.45	1.64	1.52
24	9	309	CHL	CHC-C4B	5.44	1.48	1.39
24	Y	309	CHL	C3A-C2A	-5.44	1.50	1.54
31	X	601	8CT	C34-C33	5.43	1.64	1.52
31	c	615	8CT	C34-C33	5.43	1.64	1.52
24	n	317	CHL	CHC-C4B	5.42	1.48	1.39
24	p	310	CHL	CHC-C4B	5.42	1.48	1.39
31	c	614	8CT	C23-C21	5.42	1.57	1.46
24	N	317	CHL	CHC-C4B	5.42	1.48	1.39
31	C	614	8CT	C23-C21	5.42	1.57	1.46
31	C	613	8CT	C34-C33	5.41	1.64	1.52
24	u	310	CHL	CHC-C4B	5.41	1.48	1.39
24	y	310	CHL	C3A-C2A	-5.40	1.50	1.54
24	g	309	CHL	CHC-C4B	5.40	1.48	1.39
24	4	317	CHL	C3B-C2B	5.40	1.47	1.40
24	N	317	CHL	C3B-C2B	5.39	1.47	1.40
24	9	308	CHL	C3B-C2B	5.38	1.47	1.40
24	1	317	CHL	C3B-C2B	5.38	1.47	1.40
24	7	310	CHL	CHC-C4B	5.38	1.48	1.39
24	9	317	CHL	CHD-C1D	5.37	1.48	1.39
24	9	308	CHL	CHC-C4B	5.36	1.48	1.39
24	1	308	CHL	CHC-C4B	5.36	1.48	1.39
24	4	317	CHL	CHC-C4B	5.36	1.48	1.39
24	u	318	CHL	CHD-C1D	5.36	1.48	1.39
24	7	309	CHL	C3B-C2B	5.36	1.47	1.40
24	1	317	CHL	CHC-C4B	5.36	1.48	1.39
24	4	304	CHL	C3B-C2B	5.35	1.47	1.40
24	g	309	CHL	C3B-C2B	5.35	1.47	1.40
24	9	317	CHL	CHC-C4B	5.35	1.48	1.39
24	u	309	CHL	CHC-C4B	5.35	1.48	1.39
24	6	308	CHL	C3B-C2B	5.35	1.47	1.40
24	G	309	CHL	C3B-C2B	5.34	1.47	1.40
24	u	318	CHL	CHC-C4B	5.34	1.48	1.39
24	G	309	CHL	CHC-C4B	5.34	1.48	1.39
24	p	309	CHL	C3B-C2B	5.33	1.47	1.40
24	4	309	CHL	CHC-C4B	5.33	1.48	1.39
24	u	313	CHL	C3B-C2B	5.33	1.47	1.40
24	4	308	CHL	CHC-C4B	5.32	1.48	1.39
24	p	309	CHL	CHD-C1D	5.32	1.48	1.39
24	9	312	CHL	C3B-C2B	5.32	1.47	1.40
24	4	304	CHL	CHC-C4B	5.32	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	8	309	CHL	C3A-C2A	-5.32	1.50	1.54
24	7	306	CHL	CHB-C4A	-5.32	1.32	1.38
24	1	309	CHL	CHC-C4B	5.31	1.48	1.39
24	Y	305	CHL	CHB-C4A	-5.31	1.32	1.38
24	8	315	CHL	C3B-C2B	5.30	1.47	1.40
24	4	308	CHL	C3B-C2B	5.30	1.47	1.40
24	3	308	CHL	C3B-C2B	5.30	1.47	1.40
24	u	306	CHL	CHC-C4B	5.30	1.48	1.39
24	y	306	CHL	CHB-C4A	-5.30	1.32	1.38
24	g	309	CHL	CHD-C1D	5.30	1.48	1.39
24	1	304	CHL	C3B-C2B	5.30	1.47	1.40
24	7	309	CHL	CHD-C1D	5.30	1.48	1.39
24	n	317	CHL	CHD-C1D	5.29	1.48	1.39
31	a	608	8CT	C23-C21	5.29	1.57	1.46
24	3	310	CHL	C3B-C2B	5.28	1.47	1.40
31	B	617	8CT	C05-C04	5.27	1.66	1.54
31	A	608	8CT	C23-C21	5.27	1.57	1.46
24	2	318	CHL	C3B-C2B	5.27	1.47	1.40
24	8	315	CHL	CHC-C4B	5.27	1.48	1.39
24	7	309	CHL	C3D-C2D	5.27	1.48	1.39
24	p	309	CHL	C3D-C2D	5.27	1.48	1.39
31	b	617	8CT	C05-C04	5.26	1.66	1.54
24	9	310	CHL	CHC-C4B	5.26	1.48	1.39
24	G	309	CHL	CHD-C1D	5.26	1.48	1.39
24	1	308	CHL	C3B-C2B	5.26	1.47	1.40
24	q	316	CHL	C3B-C2B	5.26	1.47	1.40
24	9	310	CHL	C3B-C2B	5.26	1.47	1.40
24	1	317	CHL	CHD-C1D	5.26	1.48	1.39
24	3	308	CHL	CHC-C4B	5.26	1.48	1.39
24	N	317	CHL	CHD-C1D	5.25	1.48	1.39
24	3	312	CHL	CHD-C1D	5.25	1.48	1.39
24	p	306	CHL	CHB-C4A	-5.25	1.32	1.38
24	S	601	CHL	CHB-C4A	-5.25	1.32	1.38
24	y	311	CHL	C3A-C2A	-5.25	1.50	1.54
24	6	312	CHL	C3B-C2B	5.24	1.47	1.40
24	4	317	CHL	CHD-C1D	5.24	1.48	1.39
24	y	310	CHL	CHB-C4A	-5.24	1.32	1.38
24	u	311	CHL	CHC-C4B	5.24	1.48	1.39
24	q	316	CHL	CHC-C4B	5.24	1.48	1.39
24	Y	309	CHL	CHB-C4A	-5.24	1.32	1.38
24	g	313	CHL	CHD-C1D	5.24	1.48	1.39
24	N	305	CHL	CHC-C4B	5.24	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	5	309	CHL	CHC-C4B	5.24	1.48	1.39
24	q	311	CHL	CHB-C4A	-5.23	1.32	1.38
24	R	605	CHL	C2A-C3A	-5.23	1.50	1.54
24	S	602	CHL	C3A-C2A	-5.23	1.50	1.54
24	s	402	CHL	CHB-C4A	-5.23	1.32	1.38
24	9	308	CHL	CHD-C1D	5.23	1.48	1.39
24	g	313	CHL	C3B-C2B	5.23	1.47	1.40
24	3	312	CHL	C3B-C2B	5.23	1.47	1.40
24	n	304	CHL	C3B-C2B	5.23	1.47	1.40
24	p	309	CHL	CHC-C4B	5.22	1.48	1.39
24	G	313	CHL	CHD-C1D	5.22	1.48	1.39
24	u	313	CHL	CHD-C1D	5.22	1.48	1.39
24	6	310	CHL	C3D-C2D	5.22	1.48	1.39
24	1	304	CHL	CHD-C1D	5.22	1.48	1.39
24	3	305	CHL	CHC-C4B	5.22	1.48	1.39
24	6	308	CHL	CHC-C4B	5.22	1.48	1.39
24	6	305	CHL	CHC-C4B	5.22	1.48	1.39
24	u	313	CHL	CHC-C4B	5.21	1.48	1.39
24	1	304	CHL	CHC-C4B	5.21	1.48	1.39
24	8	310	CHL	C3A-C2A	-5.21	1.50	1.54
24	5	318	CHL	C3B-C2B	5.21	1.47	1.40
24	q	310	CHL	C3A-C2A	-5.21	1.50	1.54
24	q	304	CHL	CHB-C4A	-5.21	1.32	1.38
24	9	312	CHL	CHD-C1D	5.21	1.48	1.39
24	N	304	CHL	C3B-C2B	5.20	1.47	1.40
24	4	304	CHL	C3D-C2D	5.20	1.48	1.39
24	7	309	CHL	CHC-C4B	5.20	1.48	1.39
24	1	304	CHL	C3D-C2D	5.20	1.48	1.39
24	u	310	CHL	C3B-C2B	5.20	1.47	1.40
24	u	311	CHL	C3B-C2B	5.20	1.47	1.40
24	3	308	CHL	CHD-C1D	5.20	1.48	1.39
24	q	308	CHL	C3A-C2A	-5.20	1.50	1.54
24	R	601	CHL	O2D-CGD	5.20	1.46	1.33
24	3	312	CHL	C3D-C2D	5.20	1.48	1.39
24	u	313	CHL	C3D-C2D	5.20	1.48	1.39
24	6	312	CHL	CHD-C1D	5.20	1.48	1.39
24	n	304	CHL	CHC-C4B	5.19	1.48	1.39
24	9	310	CHL	C3D-C2D	5.19	1.48	1.39
24	y	312	CHL	C3A-C2A	-5.19	1.50	1.54
24	5	318	CHL	CHC-C4B	5.19	1.48	1.39
24	g	313	CHL	CHC-C4B	5.19	1.48	1.39
24	2	309	CHL	CHC-C4B	5.19	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	n	305	CHL	CHC-C4B	5.19	1.48	1.39
24	G	313	CHL	C3B-C2B	5.19	1.47	1.40
24	6	310	CHL	CHC-C4B	5.19	1.48	1.39
24	r	302	CHL	CHC-C4B	5.19	1.48	1.39
24	u	311	CHL	C3D-C2D	5.19	1.48	1.39
24	g	310	CHL	CHC-C4B	5.18	1.48	1.39
24	G	310	CHL	CHC-C4B	5.18	1.48	1.39
24	8	304	CHL	CHB-C4A	-5.18	1.32	1.38
24	8	310	CHL	CHB-C4A	-5.18	1.32	1.38
24	R	601	CHL	CHC-C4B	5.18	1.48	1.39
24	6	312	CHL	CHC-C4B	5.18	1.48	1.39
24	6	317	CHL	CHC-C4B	5.18	1.48	1.39
24	g	309	CHL	C3D-C2D	5.18	1.48	1.39
24	3	317	CHL	CHC-C4B	5.18	1.48	1.39
24	9	317	CHL	C3D-C2D	5.18	1.48	1.39
24	9	309	CHL	C3B-C2B	5.18	1.47	1.40
24	u	305	CHL	CHD-C1D	5.18	1.48	1.39
24	q	316	CHL	CHD-C1D	5.18	1.48	1.39
24	6	310	CHL	C3B-C2B	5.18	1.47	1.40
24	9	308	CHL	C3D-C2D	5.17	1.48	1.39
24	7	305	CHL	C3A-C2A	-5.17	1.50	1.54
24	1	317	CHL	C3D-C2D	5.17	1.48	1.39
24	6	312	CHL	C3D-C2D	5.17	1.48	1.39
24	3	310	CHL	C3D-C2D	5.17	1.48	1.39
24	G	309	CHL	C3D-C2D	5.17	1.48	1.39
24	r	302	CHL	O2D-CGD	5.17	1.45	1.33
24	u	309	CHL	C3D-C2D	5.17	1.48	1.39
24	u	318	CHL	C3D-C2D	5.17	1.48	1.39
24	9	312	CHL	CHC-C4B	5.17	1.48	1.39
24	4	304	CHL	CHD-C1D	5.16	1.48	1.39
24	8	315	CHL	CHD-C1D	5.16	1.48	1.39
24	N	304	CHL	CHC-C4B	5.16	1.48	1.39
24	3	308	CHL	C3D-C2D	5.16	1.48	1.39
24	9	312	CHL	C3D-C2D	5.16	1.48	1.39
24	u	312	CHL	CHC-C4B	5.16	1.48	1.39
24	G	309	CHL	O2D-CGD	5.16	1.45	1.33
24	4	308	CHL	CHD-C1D	5.16	1.48	1.39
24	n	308	CHL	CHC-C4B	5.16	1.48	1.39
24	n	310	CHL	CHC-C4B	5.16	1.48	1.39
24	4	317	CHL	O2D-CGD	5.16	1.45	1.33
24	n	309	CHL	C3A-C2A	-5.16	1.50	1.54
24	1	317	CHL	O2D-CGD	5.15	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	8	308	CHL	C3A-C2A	-5.15	1.50	1.54
24	3	312	CHL	CHC-C4B	5.15	1.48	1.39
24	Y	310	CHL	C3A-C2A	-5.15	1.50	1.54
24	6	308	CHL	CHD-C1D	5.15	1.48	1.39
24	u	312	CHL	C3B-C2B	5.15	1.47	1.40
24	2	311	CHL	CHC-C4B	5.15	1.48	1.39
24	4	308	CHL	C3D-C2D	5.15	1.48	1.39
24	g	309	CHL	O2D-CGD	5.15	1.45	1.33
24	8	315	CHL	O2D-CGD	5.14	1.45	1.33
24	u	309	CHL	CHD-C1D	5.14	1.47	1.39
24	n	308	CHL	C3B-C2B	5.14	1.47	1.40
24	8	308	CHL	CHB-C4A	-5.14	1.32	1.38
24	5	310	CHL	C2A-C3A	-5.14	1.50	1.54
24	9	317	CHL	O2D-CGD	5.14	1.45	1.33
24	2	318	CHL	CHC-C4B	5.14	1.47	1.39
24	6	308	CHL	C3D-C2D	5.14	1.48	1.39
24	q	316	CHL	O2D-CGD	5.14	1.45	1.33
24	g	313	CHL	C3D-C2D	5.14	1.48	1.39
24	4	310	CHL	CHC-C4B	5.14	1.47	1.39
24	3	310	CHL	CHC-C4B	5.14	1.47	1.39
31	c	613	8CT	C05-C04	5.14	1.65	1.54
24	1	317	CHL	OBD-CAD	5.14	1.29	1.22
24	7	311	CHL	CHC-C4B	5.14	1.47	1.39
24	r	302	CHL	C3D-C2D	5.14	1.48	1.39
24	9	311	CHL	CHC-C4B	5.14	1.47	1.39
24	8	303	CHL	C3D-C2D	5.14	1.48	1.39
24	u	310	CHL	O2D-CGD	5.14	1.45	1.33
24	p	305	CHL	C3A-C2A	-5.14	1.50	1.54
24	6	309	CHL	CHC-C4B	5.13	1.47	1.39
24	g	310	CHL	C3D-C2D	5.13	1.48	1.39
24	N	310	CHL	CHC-C4B	5.13	1.47	1.39
24	Y	312	CHL	C3A-C2A	-5.13	1.50	1.54
24	3	309	CHL	CHC-C4B	5.13	1.47	1.39
24	8	303	CHL	CHD-C1D	5.13	1.47	1.39
24	r	306	CHL	CHC-C4B	5.13	1.47	1.39
24	q	311	CHL	C3A-C2A	-5.13	1.50	1.54
24	G	313	CHL	CHC-C4B	5.13	1.47	1.39
24	9	311	CHL	C3B-C2B	5.13	1.47	1.40
24	Y	312	CHL	CHB-C4A	-5.13	1.32	1.38
24	3	308	CHL	O2D-CGD	5.13	1.45	1.33
24	3	317	CHL	C3B-C2B	5.13	1.47	1.40
24	G	313	CHL	C3D-C2D	5.13	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	g	311	CHL	C3D-C2D	5.13	1.48	1.39
24	4	304	CHL	O2D-CGD	5.13	1.45	1.33
24	n	317	CHL	O2D-CGD	5.13	1.45	1.33
24	u	305	CHL	C3B-C2B	5.13	1.47	1.40
24	9	305	CHL	CHC-C4B	5.13	1.47	1.39
24	4	317	CHL	C3D-C2D	5.13	1.48	1.39
24	s	403	CHL	C3A-C2A	-5.12	1.50	1.54
24	9	311	CHL	O2D-CGD	5.12	1.45	1.33
24	n	317	CHL	C3D-C2D	5.12	1.48	1.39
24	N	304	CHL	C3D-C2D	5.12	1.48	1.39
24	5	311	CHL	CHC-C4B	5.12	1.47	1.39
24	u	318	CHL	O2D-CGD	5.12	1.45	1.33
31	S	614	8CT	C05-C04	5.12	1.65	1.54
24	4	317	CHL	OBD-CAD	5.12	1.29	1.22
24	6	308	CHL	O2D-CGD	5.12	1.45	1.33
24	6	309	CHL	C3D-C2D	5.12	1.48	1.39
24	u	306	CHL	O2D-CGD	5.12	1.45	1.33
31	s	415	8CT	C05-C04	5.12	1.65	1.54
24	6	308	CHL	OBD-CAD	5.11	1.29	1.22
24	1	310	CHL	CHC-C4B	5.11	1.47	1.39
31	C	613	8CT	C05-C04	5.11	1.65	1.54
24	Y	311	CHL	C3A-C2A	-5.11	1.50	1.54
24	u	309	CHL	O2D-CGD	5.11	1.45	1.33
24	9	310	CHL	O2D-CGD	5.11	1.45	1.33
24	N	317	CHL	C3D-C2D	5.11	1.48	1.39
24	8	307	CHL	CHC-C4B	5.11	1.47	1.39
24	u	311	CHL	O2D-CGD	5.11	1.45	1.33
24	6	317	CHL	C3B-C2B	5.11	1.47	1.40
24	6	310	CHL	CHD-C1D	5.11	1.47	1.39
24	1	308	CHL	C3D-C2D	5.11	1.48	1.39
24	1	304	CHL	O2D-CGD	5.11	1.45	1.33
24	u	305	CHL	CHC-C4B	5.11	1.47	1.39
24	n	309	CHL	O2D-CGD	5.11	1.45	1.33
24	9	308	CHL	O2D-CGD	5.10	1.45	1.33
24	8	315	CHL	C3D-C2D	5.10	1.48	1.39
24	g	310	CHL	CHD-C1D	5.10	1.47	1.39
24	6	310	CHL	O2D-CGD	5.10	1.45	1.33
24	6	311	CHL	O2D-CGD	5.10	1.45	1.33
24	1	308	CHL	CHD-C1D	5.10	1.47	1.39
24	1	309	CHL	C3B-C2B	5.10	1.47	1.40
24	9	309	CHL	O2D-CGD	5.10	1.45	1.33
24	G	310	CHL	C3B-C2B	5.10	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	G	310	CHL	O2D-CGD	5.10	1.45	1.33
24	G	312	CHL	CHC-C4B	5.10	1.47	1.39
24	u	312	CHL	O2D-CGD	5.10	1.45	1.33
24	G	310	CHL	CHD-C1D	5.10	1.47	1.39
24	3	309	CHL	C3D-C2D	5.10	1.48	1.39
24	g	311	CHL	CHC-C4B	5.09	1.47	1.39
24	6	305	CHL	O2D-CGD	5.09	1.45	1.33
24	g	310	CHL	C3B-C2B	5.09	1.47	1.40
24	N	305	CHL	O2D-CGD	5.09	1.45	1.33
24	1	308	CHL	O2D-CGD	5.09	1.45	1.33
24	1	305	CHL	O2D-CGD	5.09	1.45	1.33
24	N	317	CHL	O2D-CGD	5.09	1.45	1.33
24	G	310	CHL	C3D-C2D	5.09	1.48	1.39
24	9	305	CHL	O2D-CGD	5.09	1.45	1.33
24	4	312	CHL	C3D-C2D	5.09	1.48	1.39
24	3	305	CHL	O2D-CGD	5.09	1.45	1.33
24	N	304	CHL	O2D-CGD	5.09	1.45	1.33
24	p	318	CHL	C3B-C2B	5.09	1.47	1.40
24	4	305	CHL	O2D-CGD	5.09	1.45	1.33
24	n	304	CHL	CHD-C1D	5.09	1.47	1.39
24	p	318	CHL	CHC-C4B	5.09	1.47	1.39
24	g	310	CHL	O2D-CGD	5.09	1.45	1.33
24	R	601	CHL	C3D-C2D	5.09	1.48	1.39
24	N	311	CHL	O2D-CGD	5.09	1.45	1.33
24	q	308	CHL	CHB-C4A	-5.09	1.32	1.38
24	7	309	CHL	O2D-CGD	5.09	1.45	1.33
24	3	310	CHL	O2D-CGD	5.09	1.45	1.33
24	1	308	CHL	OBD-CAD	5.09	1.29	1.22
24	n	304	CHL	O2D-CGD	5.09	1.45	1.33
24	n	304	CHL	C3D-C2D	5.09	1.48	1.39
24	4	308	CHL	O2D-CGD	5.09	1.45	1.33
24	p	311	CHL	CHC-C4B	5.08	1.47	1.39
24	7	318	CHL	CHC-C4B	5.08	1.47	1.39
24	y	312	CHL	CHB-C4A	-5.08	1.32	1.38
24	g	312	CHL	O2D-CGD	5.08	1.45	1.33
24	y	311	CHL	CHB-C4A	-5.08	1.32	1.38
24	q	307	CHL	CHC-C4B	5.08	1.47	1.39
24	g	311	CHL	O2D-CGD	5.08	1.45	1.33
24	u	309	CHL	OBD-CAD	5.08	1.29	1.22
24	1	311	CHL	O2D-CGD	5.08	1.45	1.33
24	3	310	CHL	CHD-C1D	5.08	1.47	1.39
24	q	308	CHL	CHC-C4B	5.08	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	3	310	CHL	OBD-CAD	5.08	1.29	1.22
24	G	318	CHL	C2A-C3A	-5.08	1.50	1.54
24	2	311	CHL	C3D-C2D	5.08	1.48	1.39
24	3	309	CHL	O2D-CGD	5.07	1.45	1.33
24	N	309	CHL	O2D-CGD	5.07	1.45	1.33
24	n	311	CHL	O2D-CGD	5.07	1.45	1.33
24	6	309	CHL	O2D-CGD	5.07	1.45	1.33
24	7	318	CHL	C3B-C2B	5.07	1.47	1.40
24	u	305	CHL	O2D-CGD	5.07	1.45	1.33
24	g	309	CHL	OBD-CAD	5.07	1.29	1.22
24	q	316	CHL	C3D-C2D	5.07	1.48	1.39
24	n	305	CHL	O2D-CGD	5.07	1.45	1.33
24	5	309	CHL	C3B-C2B	5.07	1.47	1.40
24	n	304	CHL	OBD-CAD	5.07	1.28	1.22
24	4	311	CHL	O2D-CGD	5.07	1.45	1.33
24	5	311	CHL	C3D-C2D	5.07	1.48	1.39
24	q	303	CHL	C3D-C2D	5.07	1.48	1.39
24	5	309	CHL	CHD-C1D	5.07	1.47	1.39
24	Y	304	CHL	CHB-C4A	-5.07	1.32	1.38
24	5	311	CHL	O2D-CGD	5.07	1.45	1.33
24	G	311	CHL	C3D-C2D	5.07	1.48	1.39
24	1	312	CHL	C3D-C2D	5.07	1.48	1.39
24	9	312	CHL	O2D-CGD	5.07	1.45	1.33
24	N	312	CHL	O2D-CGD	5.06	1.45	1.33
24	4	308	CHL	OBD-CAD	5.06	1.28	1.22
24	N	304	CHL	CHD-C1D	5.06	1.47	1.39
24	3	311	CHL	O2D-CGD	5.06	1.45	1.33
24	G	312	CHL	O2D-CGD	5.06	1.45	1.33
24	u	306	CHL	C3D-C2D	5.06	1.48	1.39
24	3	317	CHL	O2D-CGD	5.06	1.45	1.33
24	y	313	CHL	CHB-C4A	-5.06	1.32	1.38
24	G	312	CHL	C3B-C2B	5.06	1.47	1.40
24	s	407	CHL	O2D-CGD	5.06	1.45	1.33
24	g	318	CHL	C2A-C3A	-5.06	1.50	1.54
24	G	306	CHL	O2D-CGD	5.06	1.45	1.33
24	9	308	CHL	OBD-CAD	5.06	1.28	1.22
24	6	310	CHL	OBD-CAD	5.06	1.28	1.22
24	8	303	CHL	CHC-C4B	5.06	1.47	1.39
24	N	310	CHL	C3D-C2D	5.06	1.48	1.39
24	S	602	CHL	OBD-CAD	5.06	1.28	1.22
24	5	318	CHL	C3D-C2D	5.06	1.48	1.39
24	9	310	CHL	CHD-C1D	5.06	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	g	305	CHL	O2D-CGD	5.06	1.45	1.33
24	p	309	CHL	O2D-CGD	5.06	1.45	1.33
24	R	601	CHL	C3B-C2B	5.06	1.47	1.40
24	r	306	CHL	O2D-CGD	5.06	1.45	1.33
24	4	309	CHL	CHD-C1D	5.06	1.47	1.39
24	n	308	CHL	O2D-CGD	5.06	1.45	1.33
31	x	601	8CT	C05-C04	5.06	1.65	1.54
24	9	304	CHL	C3D-C2D	5.06	1.48	1.39
24	n	308	CHL	C3D-C2D	5.06	1.48	1.39
24	Y	309	CHL	O2D-CGD	5.05	1.45	1.33
24	5	310	CHL	O2D-CGD	5.05	1.45	1.33
24	y	310	CHL	O2D-CGD	5.05	1.45	1.33
24	g	312	CHL	CHC-C4B	5.05	1.47	1.39
24	q	303	CHL	CHD-C1D	5.05	1.47	1.39
24	3	311	CHL	CHC-C4B	5.05	1.47	1.39
24	6	311	CHL	CHC-C4B	5.05	1.47	1.39
24	2	311	CHL	O2D-CGD	5.05	1.45	1.33
24	6	317	CHL	O2D-CGD	5.05	1.45	1.33
24	u	305	CHL	OBD-CAD	5.05	1.28	1.22
24	q	303	CHL	CHC-C4B	5.05	1.47	1.39
24	u	313	CHL	O2D-CGD	5.05	1.45	1.33
24	g	310	CHL	OBD-CAD	5.05	1.28	1.22
24	N	305	CHL	C3D-C2D	5.05	1.48	1.39
24	r	302	CHL	C3B-C2B	5.05	1.47	1.40
24	2	313	CHL	C3B-C2B	5.05	1.47	1.40
24	2	310	CHL	O2D-CGD	5.05	1.45	1.33
24	4	309	CHL	O2D-CGD	5.05	1.45	1.33
24	n	312	CHL	O2D-CGD	5.05	1.45	1.33
24	Y	310	CHL	CHB-C4A	-5.05	1.32	1.38
24	9	304	CHL	CHD-C1D	5.05	1.47	1.39
24	2	311	CHL	C3B-C2B	5.05	1.47	1.40
31	X	601	8CT	C05-C04	5.04	1.65	1.54
24	G	309	CHL	OBD-CAD	5.04	1.28	1.22
24	2	305	CHL	O2D-CGD	5.04	1.45	1.33
24	N	310	CHL	O2D-CGD	5.04	1.45	1.33
24	p	318	CHL	O2D-CGD	5.04	1.45	1.33
24	S	606	CHL	O2D-CGD	5.04	1.45	1.33
24	9	304	CHL	O2D-CGD	5.04	1.45	1.33
24	N	308	CHL	CHC-C4B	5.04	1.47	1.39
24	n	310	CHL	O2D-CGD	5.04	1.45	1.33
24	s	406	CHL	O2D-CGD	5.04	1.45	1.33
24	3	308	CHL	OBD-CAD	5.04	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	u	305	CHL	C3D-C2D	5.04	1.48	1.39
24	g	313	CHL	O2D-CGD	5.04	1.45	1.33
24	G	312	CHL	C3D-C2D	5.04	1.48	1.39
24	g	311	CHL	C3B-C2B	5.04	1.47	1.40
24	9	317	CHL	OBD-CAD	5.04	1.28	1.22
24	y	313	CHL	C3A-C2A	-5.04	1.50	1.54
24	4	310	CHL	O2D-CGD	5.04	1.45	1.33
24	6	312	CHL	O2D-CGD	5.04	1.45	1.33
24	g	306	CHL	O2D-CGD	5.04	1.45	1.33
24	2	313	CHL	O2D-CGD	5.04	1.45	1.33
24	p	310	CHL	O2D-CGD	5.04	1.45	1.33
24	1	309	CHL	CHD-C1D	5.03	1.47	1.39
24	N	308	CHL	C3D-C2D	5.03	1.48	1.39
24	3	311	CHL	C3B-C2B	5.03	1.47	1.40
24	7	310	CHL	O2D-CGD	5.03	1.45	1.33
24	2	318	CHL	C3D-C2D	5.03	1.48	1.39
24	n	312	CHL	C3D-C2D	5.03	1.48	1.39
24	g	312	CHL	C3D-C2D	5.03	1.48	1.39
24	6	304	CHL	CHC-C4B	5.03	1.47	1.39
24	3	304	CHL	O2D-CGD	5.03	1.45	1.33
24	n	310	CHL	C3D-C2D	5.03	1.48	1.39
29	3	301	OUR	O44-C45	5.03	1.45	1.34
24	2	310	CHL	CHC-C4B	5.03	1.47	1.39
24	S	606	CHL	CHC-C4B	5.03	1.47	1.39
24	3	309	CHL	OBD-CAD	5.03	1.28	1.22
24	g	305	CHL	CHC-C4B	5.03	1.47	1.39
24	G	313	CHL	O2D-CGD	5.03	1.45	1.33
24	G	306	CHL	CHC-C4B	5.03	1.47	1.39
24	y	305	CHL	CHB-C4A	-5.03	1.32	1.38
24	N	310	CHL	CHD-C1D	5.03	1.47	1.39
24	1	310	CHL	O2D-CGD	5.03	1.45	1.33
24	2	310	CHL	C2A-C3A	-5.03	1.50	1.54
24	5	313	CHL	O2D-CGD	5.02	1.45	1.33
24	R	605	CHL	O2D-CGD	5.02	1.45	1.33
24	y	309	CHL	O2D-CGD	5.02	1.45	1.33
24	3	317	CHL	CHD-C1D	5.02	1.47	1.39
24	G	311	CHL	CHC-C4B	5.02	1.47	1.39
24	Y	308	CHL	O2D-CGD	5.02	1.45	1.33
24	p	312	CHL	C3A-C2A	-5.02	1.50	1.54
24	1	310	CHL	C3D-C2D	5.02	1.48	1.39
24	4	317	CHL	CHB-C1B	5.02	1.47	1.39
24	N	317	CHL	OBD-CAD	5.02	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	p	310	CHL	C3B-C2B	5.02	1.47	1.40
24	5	309	CHL	C3D-C2D	5.02	1.48	1.39
24	p	311	CHL	O2D-CGD	5.02	1.45	1.33
24	u	310	CHL	C3D-C2D	5.02	1.48	1.39
24	4	309	CHL	C3D-C2D	5.02	1.48	1.39
24	N	304	CHL	OBD-CAD	5.02	1.28	1.22
24	u	318	CHL	OBD-CAD	5.02	1.28	1.22
24	2	305	CHL	CHC-C4B	5.02	1.47	1.39
24	n	310	CHL	CHD-C1D	5.02	1.47	1.39
24	2	318	CHL	CHD-C1D	5.02	1.47	1.39
24	y	311	CHL	O2D-CGD	5.02	1.45	1.33
24	4	310	CHL	C3D-C2D	5.02	1.48	1.39
24	R	606	CHL	O2D-CGD	5.02	1.45	1.33
24	N	308	CHL	C3B-C2B	5.02	1.47	1.40
24	3	312	CHL	O2D-CGD	5.02	1.45	1.33
24	1	309	CHL	C3D-C2D	5.02	1.48	1.39
24	5	312	CHL	O2D-CGD	5.01	1.45	1.33
24	s	403	CHL	OBD-CAD	5.01	1.28	1.22
24	G	305	CHL	O2D-CGD	5.01	1.45	1.33
24	G	311	CHL	O2D-CGD	5.01	1.45	1.33
24	1	312	CHL	CHC-C4B	5.01	1.47	1.39
24	g	318	CHL	CHC-C4B	5.01	1.47	1.39
24	5	306	CHL	C3A-C2A	-5.01	1.50	1.54
24	1	312	CHL	OBD-CAD	5.01	1.28	1.22
24	n	305	CHL	C3D-C2D	5.01	1.48	1.39
24	1	309	CHL	O2D-CGD	5.01	1.45	1.33
29	G	301	OUR	O44-C45	5.01	1.45	1.34
24	7	318	CHL	O2D-CGD	5.01	1.45	1.33
24	2	309	CHL	CHD-C1D	5.01	1.47	1.39
24	n	317	CHL	OBD-CAD	5.01	1.28	1.22
24	9	309	CHL	OBD-CAD	5.01	1.28	1.22
24	Y	311	CHL	CHB-C4A	-5.01	1.32	1.38
24	y	310	CHL	CHC-C4B	5.01	1.47	1.39
24	G	318	CHL	CHC-C4B	5.01	1.47	1.39
24	4	312	CHL	CHC-C4B	5.01	1.47	1.39
24	5	305	CHL	O2D-CGD	5.01	1.45	1.33
24	5	318	CHL	CHD-C1D	5.01	1.47	1.39
24	N	308	CHL	OBD-CAD	5.01	1.28	1.22
24	7	309	CHL	OBD-CAD	5.01	1.28	1.22
24	4	309	CHL	C3B-C2B	5.00	1.47	1.40
24	2	309	CHL	C3B-C2B	5.00	1.47	1.40
29	4	301	OUR	O44-C45	5.00	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	p	312	CHL	O2D-CGD	5.00	1.45	1.33
24	N	311	CHL	CHC-C4B	5.00	1.47	1.39
31	d	410	8CT	C05-C04	5.00	1.65	1.54
24	9	312	CHL	OBD-CAD	5.00	1.28	1.22
24	Y	310	CHL	O2D-CGD	5.00	1.45	1.33
31	s	416	8CT	C05-C04	5.00	1.65	1.54
24	4	312	CHL	C3B-C2B	5.00	1.47	1.40
31	S	615	8CT	C05-C04	5.00	1.65	1.54
24	G	305	CHL	CHC-C4B	5.00	1.47	1.39
24	q	304	CHL	CHC-C4B	5.00	1.47	1.39
24	G	306	CHL	OBD-CAD	5.00	1.28	1.22
24	4	312	CHL	OBD-CAD	5.00	1.28	1.22
24	6	304	CHL	O2D-CGD	5.00	1.45	1.33
24	3	305	CHL	C3D-C2D	5.00	1.48	1.39
24	6	309	CHL	OBD-CAD	5.00	1.28	1.22
24	9	305	CHL	C3D-C2D	5.00	1.48	1.39
24	5	309	CHL	O2D-CGD	5.00	1.45	1.33
24	9	309	CHL	C3D-C2D	5.00	1.48	1.39
24	6	317	CHL	CHD-C1D	5.00	1.47	1.39
24	p	318	CHL	C3D-C2D	4.99	1.48	1.39
24	r	306	CHL	C3D-C2D	4.99	1.48	1.39
24	u	311	CHL	CHD-C1D	4.99	1.47	1.39
24	n	308	CHL	OBD-CAD	4.99	1.28	1.22
24	N	308	CHL	O2D-CGD	4.99	1.45	1.33
24	5	318	CHL	O2D-CGD	4.99	1.45	1.33
24	8	308	CHL	CHC-C4B	4.99	1.47	1.39
24	g	311	CHL	CHD-C1D	4.99	1.47	1.39
24	5	306	CHL	OBD-CAD	4.99	1.28	1.22
29	Y	301	0UR	O44-C45	4.99	1.45	1.34
24	7	318	CHL	C3D-C2D	4.99	1.48	1.39
24	r	307	CHL	O2D-CGD	4.99	1.45	1.33
29	1	301	0UR	O44-C45	4.99	1.45	1.34
29	N	301	0UR	O44-C45	4.99	1.45	1.34
24	N	312	CHL	C3D-C2D	4.99	1.48	1.39
24	6	304	CHL	CHD-C1D	4.99	1.47	1.39
24	n	310	CHL	C3B-C2B	4.99	1.47	1.40
24	7	310	CHL	C3B-C2B	4.99	1.47	1.40
24	8	315	CHL	OBD-CAD	4.99	1.28	1.22
24	r	307	CHL	OBD-CAD	4.99	1.28	1.22
24	u	310	CHL	OBD-CAD	4.99	1.28	1.22
29	6	301	0UR	O44-C45	4.99	1.45	1.34
29	u	301	0UR	O44-C45	4.99	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	2	318	CHL	O2D-CGD	4.99	1.45	1.33
24	G	310	CHL	OBD-CAD	4.99	1.28	1.22
24	5	313	CHL	C3B-C2B	4.99	1.47	1.40
24	2	312	CHL	O2D-CGD	4.99	1.45	1.33
24	S	605	CHL	O2D-CGD	4.99	1.45	1.33
29	n	301	OUR	O44-C45	4.99	1.45	1.34
24	g	318	CHL	O2D-CGD	4.99	1.45	1.33
24	R	606	CHL	OBD-CAD	4.98	1.28	1.22
24	g	311	CHL	OBD-CAD	4.98	1.28	1.22
24	p	305	CHL	OBD-CAD	4.98	1.28	1.22
24	n	308	CHL	CHD-C1D	4.98	1.47	1.39
24	Y	319	CHL	O2D-CGD	4.98	1.45	1.33
24	7	311	CHL	O2D-CGD	4.98	1.45	1.33
24	R	607	CHL	O2D-CGD	4.98	1.45	1.33
24	q	309	CHL	O2D-CGD	4.98	1.45	1.33
24	s	408	CHL	O2D-CGD	4.98	1.45	1.33
24	4	312	CHL	CHD-C1D	4.98	1.47	1.39
24	3	317	CHL	OBD-CAD	4.98	1.28	1.22
24	y	318	CHL	CHB-C4A	-4.98	1.32	1.38
24	9	304	CHL	OBD-CAD	4.98	1.28	1.22
24	g	306	CHL	CHC-C4B	4.98	1.47	1.39
24	2	309	CHL	C3D-C2D	4.98	1.48	1.39
24	r	309	CHL	OBD-CAD	4.98	1.28	1.22
24	r	308	CHL	CHB-C4A	-4.98	1.32	1.38
24	2	309	CHL	O2D-CGD	4.98	1.45	1.33
24	n	311	CHL	CHC-C4B	4.98	1.47	1.39
24	G	311	CHL	CHD-C1D	4.98	1.47	1.39
24	R	602	CHL	CHB-C4A	-4.98	1.32	1.38
29	g	301	OUR	O44-C45	4.98	1.45	1.34
24	9	304	CHL	CHC-C4B	4.98	1.47	1.39
24	Y	319	CHL	CHC-C4B	4.98	1.47	1.39
29	9	301	OUR	O44-C45	4.98	1.45	1.34
24	1	304	CHL	OBD-CAD	4.98	1.28	1.22
24	g	306	CHL	OBD-CAD	4.98	1.28	1.22
24	s	407	CHL	CHC-C4B	4.98	1.47	1.39
24	5	305	CHL	OBD-CAD	4.98	1.28	1.22
24	5	313	CHL	CHC-C4B	4.98	1.47	1.39
29	y	301	OUR	O44-C45	4.98	1.45	1.34
24	1	310	CHL	OBD-CAD	4.98	1.28	1.22
24	4	304	CHL	OBD-CAD	4.98	1.28	1.22
24	2	313	CHL	CHC-C4B	4.97	1.47	1.39
24	7	311	CHL	C3B-C2B	4.97	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	8	304	CHL	CHC-C4B	4.97	1.47	1.39
24	s	403	CHL	CHC-C4B	4.97	1.47	1.39
24	s	409	CHL	O2D-CGD	4.97	1.45	1.33
24	r	308	CHL	O2D-CGD	4.97	1.45	1.33
24	3	304	CHL	OBD-CAD	4.97	1.28	1.22
24	5	311	CHL	C3B-C2B	4.97	1.47	1.40
24	q	316	CHL	OBD-CAD	4.97	1.28	1.22
24	1	312	CHL	O2D-CGD	4.97	1.45	1.33
24	S	607	CHL	O2D-CGD	4.97	1.45	1.33
31	D	410	8CT	C05-C04	4.97	1.65	1.54
24	G	318	CHL	O2D-CGD	4.97	1.45	1.33
24	N	317	CHL	CHB-C1B	4.97	1.47	1.39
24	4	309	CHL	OBD-CAD	4.97	1.28	1.22
24	4	310	CHL	OBD-CAD	4.97	1.28	1.22
24	R	602	CHL	C3A-C2A	-4.97	1.50	1.54
24	S	602	CHL	CHC-C4B	4.97	1.47	1.39
24	G	312	CHL	CHD-C1D	4.96	1.47	1.39
24	u	310	CHL	CHD-C1D	4.96	1.47	1.39
24	q	304	CHL	O2D-CGD	4.96	1.45	1.33
24	p	309	CHL	OBD-CAD	4.96	1.28	1.22
24	R	608	CHL	O2D-CGD	4.96	1.45	1.33
24	S	608	CHL	O2D-CGD	4.96	1.45	1.33
24	G	311	CHL	C3B-C2B	4.96	1.47	1.40
24	R	605	CHL	CHB-C4A	-4.96	1.32	1.38
24	7	312	CHL	O2D-CGD	4.96	1.45	1.33
24	Y	319	CHL	CHB-C4A	-4.96	1.32	1.38
24	5	306	CHL	O2D-CGD	4.96	1.45	1.33
24	Y	317	CHL	CHB-C4A	-4.96	1.32	1.38
24	1	312	CHL	C3B-C2B	4.96	1.47	1.40
24	R	608	CHL	OBD-CAD	4.96	1.28	1.22
24	g	318	CHL	C3B-C2B	4.96	1.47	1.40
24	6	304	CHL	C3D-C2D	4.95	1.48	1.39
24	p	310	CHL	C3D-C2D	4.95	1.48	1.39
24	7	310	CHL	C3D-C2D	4.95	1.48	1.39
24	N	310	CHL	C3B-C2B	4.95	1.47	1.40
24	Y	308	CHL	CHC-C4B	4.95	1.47	1.39
24	G	318	CHL	OBD-CAD	4.95	1.28	1.22
24	1	305	CHL	CHC-C4B	4.95	1.47	1.39
24	2	306	CHL	C3A-C2A	-4.95	1.50	1.54
24	g	305	CHL	C3D-C2D	4.95	1.48	1.39
24	R	607	CHL	CHB-C4A	-4.95	1.32	1.38
24	2	311	CHL	CHD-C1D	4.95	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	6	311	CHL	C3B-C2B	4.95	1.47	1.40
24	r	303	CHL	OBD-CAD	4.95	1.28	1.22
24	G	318	CHL	C3B-C2B	4.95	1.47	1.40
31	v	401	8CT	C05-C04	4.95	1.65	1.54
24	N	309	CHL	C3A-C2A	-4.95	1.50	1.54
24	4	312	CHL	O2D-CGD	4.95	1.45	1.33
24	2	306	CHL	OBD-CAD	4.95	1.28	1.22
24	G	313	CHL	OBD-CAD	4.95	1.28	1.22
24	6	317	CHL	OBD-CAD	4.95	1.28	1.22
24	g	305	CHL	OBD-CAD	4.95	1.28	1.22
24	6	304	CHL	OBD-CAD	4.95	1.28	1.22
24	3	309	CHL	CHD-C1D	4.95	1.47	1.39
24	1	317	CHL	CHB-C1B	4.95	1.47	1.39
24	S	602	CHL	O2D-CGD	4.95	1.45	1.33
24	s	403	CHL	O2D-CGD	4.95	1.45	1.33
24	q	310	CHL	CHB-C4A	-4.95	1.32	1.38
24	R	607	CHL	C3A-C2A	-4.95	1.50	1.54
24	p	311	CHL	C3B-C2B	4.95	1.47	1.40
24	q	303	CHL	O2D-CGD	4.95	1.45	1.33
24	s	414	CHL	CHC-C4B	4.95	1.47	1.39
24	r	303	CHL	CHB-C4A	-4.94	1.32	1.38
24	r	302	CHL	OBD-CAD	4.94	1.28	1.22
24	q	308	CHL	O2D-CGD	4.94	1.45	1.33
24	6	317	CHL	C3D-C2D	4.94	1.48	1.39
24	s	402	CHL	CHC-C4B	4.94	1.47	1.39
24	N	308	CHL	CHD-C1D	4.94	1.47	1.39
29	7	301	0UR	O44-C45	4.94	1.45	1.34
24	4	305	CHL	CHC-C4B	4.94	1.47	1.39
24	5	305	CHL	CHC-C4B	4.94	1.47	1.39
24	R	602	CHL	OBD-CAD	4.94	1.28	1.22
24	R	605	CHL	CHC-C4B	4.94	1.47	1.39
24	1	312	CHL	CHD-C1D	4.94	1.47	1.39
24	n	312	CHL	CHC-C4B	4.94	1.47	1.39
24	G	305	CHL	C3D-C2D	4.94	1.48	1.39
31	T	101	8CT	C05-C04	4.94	1.65	1.54
24	q	309	CHL	CHB-C4A	-4.94	1.32	1.38
24	N	312	CHL	CHC-C4B	4.94	1.47	1.39
24	5	310	CHL	CHC-C4B	4.94	1.47	1.39
24	n	309	CHL	OBD-CAD	4.94	1.28	1.22
24	R	605	CHL	OBD-CAD	4.94	1.28	1.22
24	2	313	CHL	CHD-C1D	4.94	1.47	1.39
24	p	305	CHL	CHB-C4A	-4.93	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	S	613	CHL	CHC-C4B	4.93	1.47	1.39
24	Y	309	CHL	CHC-C4B	4.93	1.47	1.39
24	5	313	CHL	CHD-C1D	4.93	1.47	1.39
31	V	401	8CT	C05-C04	4.93	1.65	1.54
24	2	313	CHL	C3D-C2D	4.93	1.48	1.39
24	7	312	CHL	C3A-C2A	-4.93	1.50	1.54
24	Y	312	CHL	O2D-CGD	4.93	1.45	1.33
24	S	605	CHL	CHC-C4B	4.93	1.47	1.39
24	8	303	CHL	C3B-C2B	4.93	1.47	1.40
24	8	304	CHL	O2D-CGD	4.93	1.45	1.33
24	2	305	CHL	C3D-C2D	4.93	1.48	1.39
24	5	305	CHL	C3D-C2D	4.93	1.48	1.39
24	q	309	CHL	CHC-C4B	4.93	1.47	1.39
24	G	309	CHL	CHB-C1B	4.93	1.47	1.39
24	8	308	CHL	O2D-CGD	4.93	1.45	1.33
24	N	310	CHL	OBD-CAD	4.93	1.28	1.22
24	9	308	CHL	CHB-C1B	4.93	1.47	1.39
24	6	309	CHL	CHD-C1D	4.93	1.47	1.39
24	p	313	CHL	O2D-CGD	4.93	1.45	1.33
24	2	306	CHL	O2D-CGD	4.92	1.45	1.33
24	3	309	CHL	C3B-C2B	4.92	1.47	1.40
24	1	304	CHL	CHB-C1B	4.92	1.47	1.39
24	G	305	CHL	OBD-CAD	4.92	1.28	1.22
24	1	311	CHL	CHC-C4B	4.92	1.47	1.39
24	7	311	CHL	C3D-C2D	4.92	1.48	1.39
24	3	317	CHL	C3D-C2D	4.92	1.48	1.39
24	5	313	CHL	C3D-C2D	4.92	1.48	1.39
24	g	313	CHL	OBD-CAD	4.92	1.28	1.22
24	5	306	CHL	CHC-C4B	4.92	1.47	1.39
24	2	310	CHL	OBD-CAD	4.92	1.28	1.22
24	s	407	CHL	CHB-C4A	-4.92	1.32	1.38
24	7	305	CHL	OBD-CAD	4.92	1.28	1.22
24	R	602	CHL	O2D-CGD	4.92	1.45	1.33
31	t	101	8CT	C05-C04	4.92	1.65	1.54
24	2	306	CHL	CHB-C4A	-4.92	1.32	1.38
24	n	317	CHL	CHB-C1B	4.92	1.47	1.39
24	5	311	CHL	CHD-C1D	4.92	1.47	1.39
24	9	311	CHL	C3D-C2D	4.92	1.48	1.39
24	n	310	CHL	OBD-CAD	4.91	1.28	1.22
24	9	305	CHL	OBD-CAD	4.91	1.28	1.22
24	7	313	CHL	O2D-CGD	4.91	1.45	1.33
24	6	309	CHL	C3B-C2B	4.91	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	r	309	CHL	O2D-CGD	4.91	1.45	1.33
24	u	312	CHL	C3D-C2D	4.91	1.48	1.39
24	p	305	CHL	O2D-CGD	4.91	1.45	1.33
24	2	305	CHL	OBD-CAD	4.91	1.28	1.22
24	7	306	CHL	O2D-CGD	4.91	1.45	1.33
24	R	601	CHL	OBD-CAD	4.91	1.28	1.22
24	r	306	CHL	OBD-CAD	4.91	1.28	1.22
24	p	311	CHL	C3D-C2D	4.91	1.48	1.39
24	Y	308	CHL	CHD-C1D	4.91	1.47	1.39
24	u	312	CHL	CHD-C1D	4.91	1.47	1.39
24	8	303	CHL	O2D-CGD	4.91	1.45	1.33
24	8	307	CHL	O2D-CGD	4.91	1.45	1.33
24	1	309	CHL	OBD-CAD	4.91	1.28	1.22
24	N	311	CHL	CHB-C4A	-4.91	1.32	1.38
24	3	304	CHL	CHC-C4B	4.90	1.47	1.39
24	4	311	CHL	CHC-C4B	4.90	1.47	1.39
24	7	305	CHL	O2D-CGD	4.90	1.45	1.33
24	Y	317	CHL	O2D-CGD	4.90	1.45	1.33
24	5	318	CHL	OBD-CAD	4.90	1.28	1.22
24	6	305	CHL	C3D-C2D	4.90	1.48	1.39
24	3	312	CHL	CHB-C1B	4.90	1.47	1.39
24	5	311	CHL	OBD-CAD	4.90	1.28	1.22
24	q	310	CHL	O2D-CGD	4.90	1.45	1.33
24	S	601	CHL	CHC-C4B	4.90	1.47	1.39
39	D	406	PL9	C3-C4	-4.90	1.41	1.49
24	g	318	CHL	OBD-CAD	4.90	1.28	1.22
24	7	310	CHL	OBD-CAD	4.90	1.28	1.22
24	g	312	CHL	CHD-C1D	4.90	1.47	1.39
24	S	607	CHL	OBD-CAD	4.90	1.28	1.22
24	g	313	CHL	CHB-C1B	4.90	1.47	1.39
24	y	313	CHL	O2D-CGD	4.90	1.45	1.33
24	5	310	CHL	OBD-CAD	4.90	1.28	1.22
29	p	301	0UR	O44-C45	4.90	1.45	1.34
24	g	312	CHL	OBD-CAD	4.90	1.28	1.22
24	u	306	CHL	CHB-C4A	-4.90	1.32	1.38
24	G	311	CHL	OBD-CAD	4.90	1.28	1.22
24	7	305	CHL	CHB-C4A	-4.89	1.32	1.38
31	C	615	8CT	C05-C04	4.89	1.65	1.54
24	y	306	CHL	O2D-CGD	4.89	1.45	1.33
24	2	306	CHL	CHC-C4B	4.89	1.47	1.39
24	r	303	CHL	O2D-CGD	4.89	1.45	1.33
24	q	303	CHL	OBD-CAD	4.89	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	8	310	CHL	O2D-CGD	4.89	1.45	1.33
24	G	318	CHL	C3D-C2D	4.89	1.48	1.39
24	g	312	CHL	C3B-C2B	4.89	1.47	1.40
24	g	309	CHL	CHB-C1B	4.89	1.47	1.39
24	s	406	CHL	CHC-C4B	4.89	1.47	1.39
24	7	310	CHL	CHD-C1D	4.89	1.47	1.39
24	p	310	CHL	OBD-CAD	4.89	1.28	1.22
24	G	305	CHL	C3B-C2B	4.89	1.47	1.40
24	4	304	CHL	CHB-C1B	4.89	1.47	1.39
24	p	306	CHL	O2D-CGD	4.89	1.45	1.33
24	7	313	CHL	CHD-C1D	4.89	1.47	1.39
24	q	307	CHL	C3D-C2D	4.89	1.48	1.39
24	r	307	CHL	C3B-C2B	4.89	1.47	1.40
24	1	311	CHL	CHB-C4A	-4.89	1.32	1.38
24	2	305	CHL	CHD-C1D	4.88	1.47	1.39
31	a	608	8CT	C05-C04	4.88	1.65	1.54
24	n	312	CHL	CHD-C1D	4.88	1.47	1.39
24	p	318	CHL	OBD-CAD	4.88	1.28	1.22
24	s	407	CHL	OBD-CAD	4.88	1.28	1.22
24	R	601	CHL	CHD-C1D	4.88	1.47	1.39
24	u	309	CHL	CHB-C1B	4.88	1.47	1.39
24	3	312	CHL	OBD-CAD	4.88	1.28	1.22
24	s	402	CHL	O2D-CGD	4.88	1.45	1.33
24	1	311	CHL	OBD-CAD	4.88	1.28	1.22
24	G	305	CHL	CHD-C1D	4.88	1.47	1.39
24	N	312	CHL	CHD-C1D	4.88	1.47	1.39
24	N	312	CHL	OBD-CAD	4.88	1.28	1.22
24	3	304	CHL	C3D-C2D	4.88	1.48	1.39
24	2	313	CHL	OBD-CAD	4.88	1.28	1.22
24	q	307	CHL	O2D-CGD	4.88	1.45	1.33
24	p	312	CHL	CHC-C4B	4.88	1.47	1.39
24	u	310	CHL	CHB-C1B	4.88	1.47	1.39
24	3	304	CHL	CHD-C1D	4.88	1.47	1.39
24	9	310	CHL	OBD-CAD	4.88	1.28	1.22
31	A	608	8CT	C05-C04	4.88	1.65	1.54
24	n	311	CHL	CHB-C4A	-4.88	1.32	1.38
24	n	312	CHL	OBD-CAD	4.88	1.28	1.22
29	8	301	OUR	O44-C45	4.88	1.45	1.34
31	c	615	8CT	C05-C04	4.88	1.65	1.54
24	S	606	CHL	CHB-C4A	-4.88	1.32	1.38
24	q	311	CHL	O2D-CGD	4.88	1.45	1.33
24	s	406	CHL	C3D-C2D	4.87	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	r	307	CHL	CHC-C4B	4.87	1.47	1.39
24	1	310	CHL	C3B-C2B	4.87	1.47	1.40
24	7	306	CHL	CHC-C4B	4.87	1.47	1.39
24	8	307	CHL	C3D-C2D	4.87	1.48	1.39
24	G	306	CHL	CHB-C4A	-4.87	1.32	1.38
24	s	414	CHL	CHB-C4A	-4.87	1.32	1.38
24	6	312	CHL	OBD-CAD	4.87	1.28	1.22
24	3	304	CHL	CHB-C4A	-4.87	1.32	1.38
24	r	309	CHL	C3D-C2D	4.87	1.48	1.39
24	1	308	CHL	CHB-C1B	4.87	1.47	1.39
24	8	303	CHL	OBD-CAD	4.87	1.28	1.22
24	R	606	CHL	C3B-C2B	4.87	1.47	1.40
24	s	406	CHL	CHD-C1D	4.87	1.47	1.39
24	9	309	CHL	CHD-C1D	4.87	1.47	1.39
24	y	309	CHL	CHC-C4B	4.87	1.47	1.39
29	2	301	OUR	O44-C45	4.87	1.45	1.34
24	S	613	CHL	CHB-C4A	-4.87	1.32	1.38
24	8	315	CHL	CHB-C1B	4.87	1.47	1.39
24	N	311	CHL	OBD-CAD	4.87	1.28	1.22
24	y	318	CHL	O2D-CGD	4.87	1.45	1.33
24	p	306	CHL	CHC-C4B	4.87	1.47	1.39
24	r	303	CHL	C3A-C2A	-4.87	1.50	1.54
24	1	305	CHL	OBD-CAD	4.86	1.28	1.22
24	p	309	CHL	CHB-C1B	4.86	1.47	1.39
24	u	306	CHL	OBD-CAD	4.86	1.28	1.22
24	g	318	CHL	C3D-C2D	4.86	1.47	1.39
24	s	409	CHL	C3D-C2D	4.86	1.47	1.39
24	y	318	CHL	CHC-C4B	4.86	1.47	1.39
24	5	306	CHL	C3D-C2D	4.86	1.47	1.39
24	q	308	CHL	OBD-CAD	4.86	1.28	1.22
24	4	310	CHL	C3B-C2B	4.86	1.47	1.40
24	Y	305	CHL	O2D-CGD	4.86	1.45	1.33
24	p	313	CHL	CHD-C1D	4.86	1.47	1.39
24	y	312	CHL	O2D-CGD	4.86	1.45	1.33
24	y	311	CHL	OBD-CAD	4.86	1.28	1.22
24	5	306	CHL	CHB-C4A	-4.86	1.32	1.38
24	q	303	CHL	C3B-C2B	4.86	1.47	1.40
24	R	608	CHL	C3D-C2D	4.86	1.47	1.39
24	g	305	CHL	CHD-C1D	4.86	1.47	1.39
24	s	409	CHL	OBD-CAD	4.86	1.28	1.22
24	S	606	CHL	OBD-CAD	4.86	1.28	1.22
24	n	311	CHL	OBD-CAD	4.86	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	S	606	CHL	C3D-C2D	4.86	1.47	1.39
24	5	310	CHL	C3D-C2D	4.86	1.47	1.39
24	q	316	CHL	CHB-C1B	4.86	1.47	1.39
24	p	313	CHL	C3D-C2D	4.85	1.47	1.39
24	7	313	CHL	C3D-C2D	4.85	1.47	1.39
24	Y	311	CHL	O2D-CGD	4.85	1.45	1.33
24	s	406	CHL	OBD-CAD	4.85	1.28	1.22
24	s	407	CHL	C3D-C2D	4.85	1.47	1.39
24	u	312	CHL	OBD-CAD	4.85	1.28	1.22
24	3	305	CHL	CHD-C1D	4.85	1.47	1.39
24	4	311	CHL	CHD-C1D	4.85	1.47	1.39
24	7	318	CHL	OBD-CAD	4.85	1.28	1.22
24	r	309	CHL	CHC-C4B	4.85	1.47	1.39
24	8	309	CHL	O2D-CGD	4.85	1.45	1.33
24	2	312	CHL	CHB-C4A	-4.85	1.32	1.38
24	S	602	CHL	CHB-C4A	-4.85	1.32	1.38
24	G	306	CHL	C3D-C2D	4.85	1.47	1.39
24	q	307	CHL	OBD-CAD	4.85	1.28	1.22
24	4	308	CHL	CHB-C1B	4.85	1.47	1.39
24	u	313	CHL	OBD-CAD	4.85	1.28	1.22
24	9	317	CHL	CHB-C1B	4.85	1.47	1.39
24	Y	319	CHL	C3A-C2A	-4.85	1.50	1.54
24	p	311	CHL	OBD-CAD	4.85	1.28	1.22
24	S	607	CHL	CHB-C4A	-4.85	1.32	1.38
24	2	309	CHL	OBD-CAD	4.85	1.28	1.22
24	y	309	CHL	OBD-CAD	4.85	1.28	1.22
24	5	312	CHL	CHC-C4B	4.85	1.47	1.39
24	4	311	CHL	CHB-C4A	-4.85	1.32	1.38
24	5	310	CHL	CHB-C4A	-4.85	1.32	1.38
24	s	408	CHL	CHB-C4A	-4.85	1.32	1.38
24	S	601	CHL	O2D-CGD	4.85	1.45	1.33
24	N	305	CHL	OBD-CAD	4.85	1.28	1.22
24	2	312	CHL	CHC-C4B	4.84	1.47	1.39
24	2	305	CHL	C3B-C2B	4.84	1.46	1.40
24	4	305	CHL	OBD-CAD	4.84	1.28	1.22
24	4	311	CHL	OBD-CAD	4.84	1.28	1.22
24	S	606	CHL	CHD-C1D	4.84	1.47	1.39
24	9	304	CHL	C3B-C2B	4.84	1.46	1.40
24	G	310	CHL	CHB-C1B	4.84	1.47	1.39
24	2	310	CHL	C3D-C2D	4.84	1.47	1.39
24	8	307	CHL	OBD-CAD	4.84	1.28	1.22
24	3	311	CHL	OBD-CAD	4.84	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	R	606	CHL	CHC-C4B	4.84	1.47	1.39
24	5	305	CHL	CHD-C1D	4.84	1.47	1.39
24	2	311	CHL	OBD-CAD	4.84	1.28	1.22
24	r	302	CHL	CHD-C1D	4.84	1.47	1.39
24	p	310	CHL	CHD-C1D	4.84	1.47	1.39
24	n	305	CHL	OBD-CAD	4.84	1.28	1.22
24	g	305	CHL	C3B-C2B	4.84	1.46	1.40
24	7	312	CHL	CHB-C4A	-4.84	1.32	1.38
39	d	406	PL9	C3-C4	-4.84	1.42	1.49
29	5	301	0UR	O44-C45	4.84	1.45	1.34
24	6	312	CHL	CHB-C1B	4.84	1.47	1.39
24	9	311	CHL	CHD-C1D	4.84	1.47	1.39
24	g	310	CHL	CHB-C1B	4.84	1.47	1.39
24	7	318	CHL	CHD-C1D	4.84	1.47	1.39
24	u	313	CHL	CHB-C1B	4.84	1.47	1.39
24	r	306	CHL	CHD-C1D	4.84	1.47	1.39
24	7	309	CHL	CHB-C1B	4.84	1.47	1.39
29	q	301	0UR	O44-C45	4.84	1.45	1.34
24	s	414	CHL	OBD-CAD	4.84	1.28	1.22
24	5	313	CHL	OBD-CAD	4.83	1.28	1.22
24	9	305	CHL	CHB-C4A	-4.83	1.32	1.38
24	u	311	CHL	OBD-CAD	4.83	1.28	1.22
24	S	608	CHL	OBD-CAD	4.83	1.28	1.22
24	r	307	CHL	C3D-C2D	4.83	1.47	1.39
24	8	310	CHL	C3D-C2D	4.83	1.47	1.39
24	1	305	CHL	CHB-C4A	-4.83	1.32	1.38
24	Y	310	CHL	CHC-C4B	4.83	1.47	1.39
24	s	414	CHL	O2D-CGD	4.83	1.45	1.33
24	S	605	CHL	C3D-C2D	4.83	1.47	1.39
24	p	313	CHL	CHB-C4A	-4.83	1.32	1.38
24	7	313	CHL	CHB-C4A	-4.83	1.32	1.38
24	S	613	CHL	O2D-CGD	4.83	1.45	1.33
24	6	308	CHL	CHB-C1B	4.82	1.47	1.39
24	u	318	CHL	CHB-C1B	4.82	1.47	1.39
24	g	306	CHL	C3D-C2D	4.82	1.47	1.39
31	c	614	8CT	C05-C04	4.82	1.65	1.54
24	G	312	CHL	OBD-CAD	4.82	1.28	1.22
24	r	309	CHL	C3A-C2A	-4.82	1.50	1.54
24	y	311	CHL	CHC-C4B	4.82	1.47	1.39
31	C	614	8CT	C05-C04	4.82	1.65	1.54
24	1	309	CHL	CHB-C1B	4.82	1.47	1.39
24	Y	317	CHL	CHC-C4B	4.82	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	3	308	CHL	CHB-C1B	4.82	1.47	1.39
24	7	312	CHL	CHC-C4B	4.82	1.47	1.39
24	r	303	CHL	CHC-C4B	4.82	1.47	1.39
24	r	308	CHL	C3A-C2A	-4.82	1.50	1.54
24	R	608	CHL	CHC-C4B	4.82	1.47	1.39
24	6	311	CHL	OBD-CAD	4.82	1.28	1.22
24	9	312	CHL	CHB-C1B	4.82	1.47	1.39
24	p	312	CHL	CHB-C4A	-4.81	1.32	1.38
24	r	306	CHL	C3B-C2B	4.81	1.46	1.40
24	6	310	CHL	CHB-C1B	4.81	1.47	1.39
24	5	312	CHL	CHB-C4A	-4.81	1.32	1.38
24	S	608	CHL	C3D-C2D	4.81	1.47	1.39
24	y	305	CHL	OBD-CAD	4.81	1.28	1.22
24	Y	311	CHL	CHC-C4B	4.81	1.47	1.39
24	y	305	CHL	O2D-CGD	4.81	1.45	1.33
24	q	309	CHL	C3A-C2A	-4.81	1.50	1.54
24	3	305	CHL	CHB-C4A	-4.81	1.32	1.38
24	N	312	CHL	C3B-C2B	4.81	1.46	1.40
24	6	305	CHL	CHB-C4A	-4.81	1.32	1.38
24	n	308	CHL	CHB-C1B	4.81	1.47	1.39
24	y	313	CHL	CHC-C4B	4.81	1.47	1.39
24	R	608	CHL	C3A-C2A	-4.81	1.50	1.54
24	9	305	CHL	CHD-C1D	4.81	1.47	1.39
24	5	309	CHL	OBD-CAD	4.80	1.28	1.22
24	Y	308	CHL	C3D-C2D	4.80	1.47	1.39
24	p	318	CHL	CHD-C1D	4.80	1.47	1.39
24	2	306	CHL	C3D-C2D	4.80	1.47	1.39
24	6	305	CHL	OBD-CAD	4.80	1.28	1.22
24	5	305	CHL	C3B-C2B	4.80	1.46	1.40
24	y	309	CHL	C3D-C2D	4.80	1.47	1.39
24	4	309	CHL	CHB-C1B	4.80	1.47	1.39
24	q	309	CHL	OBD-CAD	4.80	1.28	1.22
24	y	309	CHL	CHD-C1D	4.80	1.47	1.39
24	8	308	CHL	OBD-CAD	4.80	1.28	1.22
24	s	403	CHL	CHB-C4A	-4.80	1.32	1.38
24	3	310	CHL	CHB-C1B	4.80	1.47	1.39
24	g	306	CHL	CHB-C4A	-4.80	1.32	1.38
24	3	317	CHL	C2A-C3A	-4.80	1.50	1.54
24	Y	308	CHL	OBD-CAD	4.80	1.28	1.22
24	1	311	CHL	CHD-C1D	4.79	1.47	1.39
24	g	318	CHL	CHD-C1D	4.79	1.47	1.39
24	9	309	CHL	CHB-C1B	4.79	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	q	307	CHL	CHB-C4A	-4.79	1.32	1.38
24	2	310	CHL	CHB-C4A	-4.79	1.32	1.38
24	2	318	CHL	OBD-CAD	4.79	1.28	1.22
24	S	601	CHL	C3A-C2A	-4.79	1.50	1.54
24	3	309	CHL	CHB-C1B	4.79	1.47	1.39
24	S	608	CHL	CHD-C1D	4.79	1.47	1.39
24	y	312	CHL	CHC-C4B	4.79	1.47	1.39
24	1	305	CHL	C3D-C2D	4.79	1.47	1.39
24	n	312	CHL	C3B-C2B	4.79	1.46	1.40
24	4	310	CHL	CHD-C1D	4.79	1.47	1.39
24	8	309	CHL	CHB-C4A	-4.79	1.32	1.38
24	1	312	CHL	CHB-C1B	4.79	1.47	1.39
24	G	313	CHL	CHB-C1B	4.79	1.47	1.39
24	S	613	CHL	OBD-CAD	4.79	1.28	1.22
24	s	409	CHL	CHC-C4B	4.79	1.47	1.39
24	8	304	CHL	C3A-C2A	-4.78	1.50	1.54
24	Y	312	CHL	CHC-C4B	4.78	1.47	1.39
24	S	602	CHL	C3D-C2D	4.78	1.47	1.39
24	4	305	CHL	C3D-C2D	4.78	1.47	1.39
24	Y	304	CHL	OBD-CAD	4.78	1.28	1.22
24	n	309	CHL	CHB-C4A	-4.78	1.32	1.38
24	u	305	CHL	CHB-C1B	4.78	1.47	1.39
24	4	311	CHL	C3D-C2D	4.78	1.47	1.39
24	q	311	CHL	C3D-C2D	4.78	1.47	1.39
24	9	311	CHL	OBD-CAD	4.78	1.28	1.22
24	5	312	CHL	OBD-CAD	4.78	1.28	1.22
24	q	304	CHL	C3A-C2A	-4.78	1.50	1.54
24	s	409	CHL	CHD-C1D	4.78	1.47	1.39
24	Y	310	CHL	OBD-CAD	4.78	1.28	1.22
24	Y	319	CHL	OBD-CAD	4.78	1.28	1.22
24	N	305	CHL	C3B-C2B	4.78	1.46	1.40
24	8	307	CHL	CHB-C4A	-4.78	1.32	1.38
24	s	407	CHL	CHD-C1D	4.78	1.47	1.39
24	S	605	CHL	OBD-CAD	4.78	1.28	1.22
24	q	304	CHL	OBD-CAD	4.78	1.28	1.22
24	1	305	CHL	C3B-C2B	4.77	1.46	1.40
24	5	309	CHL	CHB-C1B	4.77	1.47	1.39
24	N	309	CHL	CHC-C4B	4.77	1.47	1.39
24	6	305	CHL	CHD-C1D	4.77	1.47	1.39
24	R	606	CHL	C3D-C2D	4.77	1.47	1.39
24	s	408	CHL	CHC-C4B	4.77	1.47	1.39
24	7	313	CHL	C3A-C2A	-4.77	1.50	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	7	313	CHL	CHC-C4B	4.77	1.47	1.39
24	8	304	CHL	C3D-C2D	4.77	1.47	1.39
24	6	304	CHL	C3B-C2B	4.77	1.46	1.40
24	S	608	CHL	CHC-C4B	4.77	1.47	1.39
24	S	608	CHL	CHB-C4A	-4.77	1.32	1.38
24	4	305	CHL	CHB-C4A	-4.77	1.32	1.38
24	4	311	CHL	C3B-C2B	4.76	1.46	1.40
24	y	306	CHL	OBD-CAD	4.76	1.28	1.22
24	Y	304	CHL	O2D-CGD	4.76	1.44	1.33
24	1	311	CHL	C3D-C2D	4.76	1.47	1.39
24	p	311	CHL	CHD-C1D	4.76	1.47	1.39
24	q	307	CHL	C3B-C2B	4.76	1.46	1.40
24	8	304	CHL	OBD-CAD	4.76	1.28	1.22
24	Y	312	CHL	C3D-C2D	4.76	1.47	1.39
24	3	311	CHL	CHD-C1D	4.76	1.47	1.39
24	y	313	CHL	CHD-C1D	4.76	1.47	1.39
24	R	606	CHL	CHB-C4A	-4.76	1.32	1.38
24	s	402	CHL	OBD-CAD	4.76	1.28	1.22
24	R	602	CHL	CHC-C4B	4.76	1.47	1.39
24	s	407	CHL	C3B-C2B	4.76	1.46	1.40
24	u	311	CHL	CHB-C1B	4.76	1.47	1.39
24	7	311	CHL	OBD-CAD	4.75	1.28	1.22
24	9	310	CHL	CHB-C1B	4.75	1.47	1.39
24	R	605	CHL	C3D-C2D	4.75	1.47	1.39
24	S	605	CHL	CHD-C1D	4.75	1.47	1.39
24	p	313	CHL	C3A-C2A	-4.75	1.50	1.54
24	q	304	CHL	C3D-C2D	4.75	1.47	1.39
24	G	318	CHL	CHD-C1D	4.75	1.47	1.39
24	u	312	CHL	CHB-C1B	4.75	1.47	1.39
24	Y	309	CHL	OBD-CAD	4.75	1.28	1.22
24	1	310	CHL	CHD-C1D	4.75	1.47	1.39
24	G	305	CHL	CHB-C4A	-4.75	1.32	1.38
24	4	305	CHL	C3B-C2B	4.75	1.46	1.40
24	8	309	CHL	OBD-CAD	4.75	1.28	1.22
24	2	312	CHL	OBD-CAD	4.75	1.28	1.22
24	2	318	CHL	CHB-C1B	4.75	1.47	1.39
24	5	318	CHL	CHB-C1B	4.75	1.47	1.39
24	S	606	CHL	C3B-C2B	4.75	1.46	1.40
24	s	406	CHL	C3B-C2B	4.75	1.46	1.40
24	s	403	CHL	C3D-C2D	4.75	1.47	1.39
24	5	311	CHL	CHB-C1B	4.74	1.47	1.39
24	S	607	CHL	CHC-C4B	4.74	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	q	310	CHL	CHC-C4B	4.74	1.47	1.39
24	Y	312	CHL	CHD-C1D	4.74	1.47	1.39
24	8	310	CHL	CHD-C1D	4.74	1.47	1.39
24	p	312	CHL	OBD-CAD	4.74	1.28	1.22
24	l	305	CHL	C3A-C2A	-4.74	1.50	1.54
24	y	313	CHL	OBD-CAD	4.74	1.28	1.22
24	y	313	CHL	C3D-C2D	4.74	1.47	1.39
24	Y	305	CHL	OBD-CAD	4.74	1.28	1.22
24	8	310	CHL	CHC-C4B	4.74	1.47	1.39
24	p	313	CHL	CHC-C4B	4.73	1.47	1.39
24	q	307	CHL	CHD-C1D	4.73	1.47	1.39
24	2	311	CHL	CHB-C1B	4.73	1.47	1.39
24	p	313	CHL	OBD-CAD	4.73	1.28	1.22
24	7	311	CHL	CHD-C1D	4.73	1.47	1.39
24	5	305	CHL	CHB-C4A	-4.73	1.32	1.38
24	s	409	CHL	CHB-C4A	-4.73	1.32	1.38
24	3	305	CHL	OBD-CAD	4.73	1.28	1.22
24	N	309	CHL	OBD-CAD	4.73	1.28	1.22
24	8	307	CHL	C3B-C2B	4.73	1.46	1.40
24	G	318	CHL	CHB-C4A	-4.73	1.32	1.38
24	g	311	CHL	CHB-C1B	4.73	1.47	1.39
24	y	306	CHL	C3D-C2D	4.73	1.47	1.39
24	S	605	CHL	C3B-C2B	4.73	1.46	1.40
24	r	307	CHL	CHB-C4A	-4.73	1.32	1.38
24	q	311	CHL	CHD-C1D	4.73	1.47	1.39
24	6	317	CHL	C2A-C3A	-4.73	1.50	1.54
24	6	304	CHL	CHB-C4A	-4.73	1.32	1.38
24	7	318	CHL	C2A-C3A	-4.73	1.50	1.54
24	R	608	CHL	C3B-C2B	4.72	1.46	1.40
24	2	313	CHL	CHB-C1B	4.72	1.47	1.39
24	6	309	CHL	CHB-C1B	4.72	1.47	1.39
24	6	311	CHL	CHD-C1D	4.72	1.47	1.39
24	y	310	CHL	OBD-CAD	4.72	1.28	1.22
24	4	305	CHL	C3A-C2A	-4.72	1.50	1.54
24	y	318	CHL	C3D-C2D	4.72	1.47	1.39
24	2	309	CHL	CHB-C1B	4.72	1.47	1.39
24	5	312	CHL	C3A-C2A	-4.72	1.50	1.54
24	2	312	CHL	C3A-C2A	-4.72	1.50	1.54
24	G	312	CHL	CHB-C1B	4.72	1.47	1.39
24	8	307	CHL	CHD-C1D	4.72	1.47	1.39
24	s	406	CHL	CHB-C4A	-4.72	1.32	1.38
24	N	311	CHL	C3D-C2D	4.72	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	r	306	CHL	CHB-C4A	-4.71	1.32	1.38
24	3	311	CHL	C3D-C2D	4.71	1.47	1.39
24	3	305	CHL	C3B-C2B	4.71	1.46	1.40
24	u	306	CHL	CHD-C1D	4.71	1.47	1.39
24	s	402	CHL	C3A-C2A	-4.71	1.50	1.54
24	n	311	CHL	C3D-C2D	4.71	1.47	1.39
24	n	312	CHL	CHB-C4A	-4.71	1.32	1.38
24	Y	308	CHL	CHB-C4A	-4.71	1.32	1.38
24	g	305	CHL	CHB-C4A	-4.71	1.32	1.38
24	7	313	CHL	OBD-CAD	4.71	1.28	1.22
24	Y	305	CHL	C3D-C2D	4.71	1.47	1.39
24	q	311	CHL	CHC-C4B	4.71	1.47	1.39
24	S	601	CHL	OBD-CAD	4.71	1.28	1.22
24	n	309	CHL	CHC-C4B	4.70	1.47	1.39
24	S	607	CHL	C3D-C2D	4.70	1.47	1.39
24	r	309	CHL	C3B-C2B	4.70	1.46	1.40
24	N	309	CHL	CHB-C4A	-4.70	1.33	1.38
24	Y	308	CHL	C3B-C2B	4.70	1.46	1.40
24	p	318	CHL	C2A-C3A	-4.70	1.50	1.54
24	G	306	CHL	CHD-C1D	4.70	1.47	1.39
24	p	306	CHL	C3D-C2D	4.70	1.47	1.39
24	1	311	CHL	C3B-C2B	4.70	1.46	1.40
24	R	607	CHL	OBD-CAD	4.70	1.28	1.22
24	2	305	CHL	CHB-C4A	-4.70	1.33	1.38
24	3	317	CHL	CHB-C1B	4.70	1.47	1.39
24	7	306	CHL	C3D-C2D	4.69	1.47	1.39
24	S	605	CHL	CHB-C4A	-4.69	1.33	1.38
24	u	306	CHL	C3B-C2B	4.69	1.46	1.40
24	g	312	CHL	CHB-C1B	4.69	1.47	1.39
24	R	608	CHL	CHB-C4A	-4.69	1.33	1.38
24	2	312	CHL	C3B-C2B	4.69	1.46	1.40
24	N	304	CHL	CHB-C1B	4.69	1.47	1.39
24	8	309	CHL	CHC-C4B	4.69	1.47	1.39
24	7	310	CHL	CHB-C1B	4.69	1.47	1.39
24	g	318	CHL	CHB-C4A	-4.69	1.33	1.38
24	G	306	CHL	C3B-C2B	4.68	1.46	1.40
24	5	312	CHL	C3B-C2B	4.68	1.46	1.40
24	N	312	CHL	CHB-C4A	-4.68	1.33	1.38
24	2	312	CHL	C3D-C2D	4.68	1.47	1.39
24	y	312	CHL	OBD-CAD	4.68	1.28	1.22
24	n	305	CHL	CHB-C4A	-4.68	1.33	1.38
24	5	313	CHL	CHB-C1B	4.68	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	7	311	CHL	CHB-C4A	-4.68	1.33	1.38
24	8	310	CHL	OBD-CAD	4.68	1.28	1.22
24	n	305	CHL	C3B-C2B	4.68	1.46	1.40
24	6	317	CHL	CHB-C1B	4.68	1.47	1.39
24	3	304	CHL	C3B-C2B	4.68	1.46	1.40
24	p	313	CHL	C3B-C2B	4.68	1.46	1.40
24	9	311	CHL	CHB-C1B	4.67	1.47	1.39
24	N	311	CHL	C3B-C2B	4.67	1.46	1.40
24	q	310	CHL	OBD-CAD	4.67	1.28	1.22
24	r	302	CHL	CHB-C4A	-4.67	1.33	1.38
24	S	608	CHL	C3B-C2B	4.67	1.46	1.40
24	r	308	CHL	OBD-CAD	4.67	1.28	1.22
24	R	608	CHL	CHD-C1D	4.67	1.47	1.39
24	Y	317	CHL	OBD-CAD	4.67	1.28	1.22
24	y	311	CHL	C3D-C2D	4.67	1.47	1.39
24	R	602	CHL	C3D-C2D	4.67	1.47	1.39
24	r	303	CHL	C3D-C2D	4.67	1.47	1.39
24	N	311	CHL	CHD-C1D	4.67	1.47	1.39
24	g	306	CHL	CHD-C1D	4.67	1.47	1.39
24	q	311	CHL	OBD-CAD	4.67	1.28	1.22
24	6	311	CHL	C3D-C2D	4.67	1.47	1.39
24	R	607	CHL	CHC-C4B	4.66	1.47	1.39
24	R	601	CHL	CHB-C4A	-4.66	1.33	1.38
24	4	312	CHL	CHB-C1B	4.66	1.47	1.39
24	7	312	CHL	OBD-CAD	4.66	1.28	1.22
24	s	408	CHL	C3D-C2D	4.66	1.47	1.39
24	r	308	CHL	CHC-C4B	4.66	1.47	1.39
24	s	409	CHL	C3B-C2B	4.66	1.46	1.40
24	3	311	CHL	CHB-C4A	-4.66	1.33	1.38
24	7	313	CHL	C3B-C2B	4.66	1.46	1.40
24	s	408	CHL	OBD-CAD	4.66	1.28	1.22
24	1	311	CHL	C3A-C2A	-4.66	1.50	1.54
24	N	308	CHL	CHB-C1B	4.66	1.47	1.39
24	N	310	CHL	CHB-C1B	4.66	1.47	1.39
24	n	304	CHL	CHB-C1B	4.66	1.47	1.39
24	y	309	CHL	C3B-C2B	4.66	1.46	1.40
24	y	305	CHL	CHC-C4B	4.66	1.47	1.39
24	q	309	CHL	C3D-C2D	4.65	1.47	1.39
24	S	607	CHL	CHD-C1D	4.65	1.47	1.39
24	y	306	CHL	CHC-C4B	4.65	1.47	1.39
24	S	606	CHL	C3A-C2A	-4.65	1.50	1.54
24	s	403	CHL	C3B-C2B	4.65	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Y	304	CHL	CHC-C4B	4.65	1.47	1.39
24	y	309	CHL	CHB-C4A	-4.65	1.33	1.38
31	s	416	8CT	C19-C20	4.65	1.57	1.43
24	Y	311	CHL	OBD-CAD	4.65	1.28	1.22
24	Y	319	CHL	CHD-C1D	4.65	1.47	1.39
24	N	305	CHL	CHB-C4A	-4.65	1.33	1.38
24	6	311	CHL	CHB-C4A	-4.65	1.33	1.38
24	s	408	CHL	C3B-C2B	4.65	1.46	1.40
24	2	310	CHL	CHD-C1D	4.65	1.47	1.39
24	n	311	CHL	C3A-C2A	-4.65	1.50	1.54
24	g	306	CHL	C3A-C2A	-4.65	1.50	1.54
24	1	310	CHL	CHB-C4A	-4.65	1.33	1.38
24	y	318	CHL	OBD-CAD	4.65	1.28	1.22
24	7	310	CHL	CHB-C4A	-4.65	1.33	1.38
24	p	310	CHL	CHB-C4A	-4.64	1.33	1.38
24	Y	317	CHL	C3D-C2D	4.64	1.47	1.39
24	r	309	CHL	CHB-C4A	-4.64	1.33	1.38
24	7	309	CHL	CHD-C4C	4.64	1.48	1.39
24	G	311	CHL	CHB-C1B	4.64	1.47	1.39
24	p	310	CHL	CHB-C1B	4.64	1.47	1.39
24	9	304	CHL	CHB-C1B	4.64	1.47	1.39
24	s	408	CHL	CHD-C1D	4.64	1.47	1.39
24	n	305	CHL	CHD-C1D	4.63	1.47	1.39
24	q	303	CHL	CHB-C1B	4.63	1.47	1.39
24	p	309	CHL	CHD-C4C	4.63	1.48	1.39
24	6	305	CHL	C3B-C2B	4.63	1.46	1.40
24	Y	310	CHL	C3D-C2D	4.63	1.47	1.39
24	5	310	CHL	CHD-C1D	4.63	1.47	1.39
24	8	303	CHL	CHB-C1B	4.63	1.47	1.39
24	N	317	CHL	CHD-C4C	4.63	1.48	1.39
24	r	302	CHL	CHB-C1B	4.63	1.47	1.39
24	4	310	CHL	CHB-C4A	-4.63	1.33	1.38
24	2	312	CHL	CHD-C1D	4.63	1.47	1.39
24	4	305	CHL	CHD-C1D	4.63	1.47	1.39
24	N	309	CHL	C3B-C2B	4.63	1.46	1.40
24	5	310	CHL	C3B-C2B	4.63	1.46	1.40
24	S	613	CHL	C3D-C2D	4.63	1.47	1.39
24	s	414	CHL	C3D-C2D	4.63	1.47	1.39
24	Y	305	CHL	CHC-C4B	4.62	1.47	1.39
24	s	409	CHL	C3A-C2A	-4.62	1.50	1.54
24	5	312	CHL	CHD-C1D	4.62	1.47	1.39
24	n	311	CHL	C3B-C2B	4.62	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	7	305	CHL	CHC-C4B	4.62	1.47	1.39
24	1	305	CHL	CHD-C1D	4.62	1.47	1.39
31	V	401	8CT	C06-C07	4.62	1.67	1.52
24	8	308	CHL	CHD-C1D	4.62	1.47	1.39
31	S	614	8CT	C19-C20	4.61	1.57	1.43
24	p	311	CHL	CHB-C4A	-4.61	1.33	1.38
31	C	615	8CT	C06-C07	4.61	1.66	1.52
24	3	305	CHL	CHB-C1B	4.61	1.47	1.39
24	u	318	CHL	CHD-C4C	4.61	1.48	1.39
31	c	615	8CT	C06-C07	4.61	1.66	1.52
31	v	401	8CT	C06-C07	4.61	1.66	1.52
24	6	311	CHL	C3A-C2A	-4.61	1.50	1.54
31	S	615	8CT	C06-C07	4.61	1.66	1.52
31	B	617	8CT	C06-C07	4.61	1.66	1.52
24	Y	311	CHL	C3D-C2D	4.61	1.47	1.39
31	S	615	8CT	C19-C20	4.61	1.57	1.43
24	2	310	CHL	C3B-C2B	4.61	1.46	1.40
24	G	309	CHL	CHD-C4C	4.61	1.48	1.39
24	9	317	CHL	CHD-C4C	4.61	1.48	1.39
24	9	308	CHL	CHD-C4C	4.60	1.48	1.39
24	N	305	CHL	CHB-C1B	4.60	1.47	1.39
24	S	607	CHL	C3B-C2B	4.60	1.46	1.40
24	g	312	CHL	CHB-C4A	-4.60	1.33	1.38
24	y	313	CHL	C3B-C2B	4.60	1.46	1.40
24	r	309	CHL	CHD-C1D	4.60	1.47	1.39
24	r	306	CHL	CHB-C1B	4.60	1.47	1.39
31	s	416	8CT	C06-C07	4.60	1.66	1.52
24	5	313	CHL	CHB-C4A	-4.60	1.33	1.38
24	u	306	CHL	CHB-C1B	4.59	1.47	1.39
24	5	312	CHL	C3D-C2D	4.59	1.47	1.39
24	n	310	CHL	CHB-C1B	4.59	1.47	1.39
24	y	312	CHL	C3D-C2D	4.59	1.47	1.39
24	q	308	CHL	CHD-C1D	4.59	1.47	1.39
31	b	617	8CT	C06-C07	4.59	1.66	1.52
31	s	415	8CT	C19-C20	4.59	1.57	1.43
24	N	305	CHL	CHD-C1D	4.59	1.47	1.39
24	2	313	CHL	CHB-C4A	-4.58	1.33	1.38
24	p	311	CHL	CHB-C1B	4.58	1.47	1.39
24	1	304	CHL	CHD-C4C	4.58	1.48	1.39
24	n	317	CHL	CHD-C4C	4.58	1.48	1.39
24	Y	319	CHL	C3D-C2D	4.58	1.47	1.39
24	1	312	CHL	CHB-C4A	-4.58	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	7	318	CHL	CHB-C4A	-4.58	1.33	1.38
24	4	310	CHL	CHB-C1B	4.58	1.47	1.39
24	8	308	CHL	C3D-C2D	4.58	1.47	1.39
24	R	601	CHL	CHB-C1B	4.58	1.47	1.39
24	2	310	CHL	CHB-C1B	4.58	1.47	1.39
24	6	310	CHL	O2A-CGA	4.58	1.45	1.30
24	1	317	CHL	CHD-C4C	4.58	1.48	1.39
24	n	311	CHL	CHD-C1D	4.58	1.47	1.39
31	S	614	8CT	C06-C07	4.58	1.66	1.52
24	S	602	CHL	C3B-C2B	4.57	1.46	1.40
24	q	309	CHL	CHD-C1D	4.57	1.47	1.39
24	S	605	CHL	C3A-C2A	-4.57	1.50	1.54
24	4	311	CHL	C3A-C2A	-4.57	1.50	1.54
24	s	406	CHL	C3A-C2A	-4.57	1.50	1.54
24	R	607	CHL	C3B-C2B	4.57	1.46	1.40
24	n	310	CHL	CHB-C4A	-4.57	1.33	1.38
24	s	402	CHL	C3D-C2D	4.57	1.47	1.39
24	Y	312	CHL	C3B-C2B	4.57	1.46	1.40
39	d	406	PL9	C7-C3	-4.57	1.45	1.51
24	3	310	CHL	O2A-CGA	4.56	1.45	1.30
24	g	313	CHL	CHD-C4C	4.56	1.48	1.39
24	7	318	CHL	CHB-C1B	4.56	1.47	1.39
24	p	306	CHL	OBD-CAD	4.56	1.28	1.22
24	6	308	CHL	CHD-C4C	4.56	1.48	1.39
24	g	309	CHL	CHD-C4C	4.56	1.48	1.39
24	9	305	CHL	C3A-C2A	-4.56	1.50	1.54
24	8	304	CHL	CHD-C1D	4.56	1.47	1.39
24	q	308	CHL	C3D-C2D	4.56	1.47	1.39
24	n	309	CHL	C3D-C2D	4.56	1.47	1.39
24	u	309	CHL	CHD-C4C	4.56	1.48	1.39
24	n	312	CHL	CHB-C1B	4.55	1.47	1.39
24	S	601	CHL	C3D-C2D	4.55	1.47	1.39
24	1	310	CHL	CHB-C1B	4.55	1.47	1.39
24	Y	311	CHL	CHD-C1D	4.55	1.47	1.39
24	r	302	CHL	O2A-CGA	4.55	1.45	1.30
31	D	410	8CT	C06-C07	4.55	1.66	1.52
31	s	415	8CT	C06-C07	4.55	1.66	1.52
24	S	607	CHL	O2A-CGA	4.55	1.45	1.30
24	5	311	CHL	CHB-C4A	-4.55	1.33	1.38
24	N	309	CHL	C3D-C2D	4.55	1.47	1.39
24	n	305	CHL	CHB-C1B	4.55	1.47	1.39
24	9	305	CHL	CHB-C1B	4.55	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	y	311	CHL	CHD-C1D	4.55	1.47	1.39
24	y	312	CHL	CHD-C1D	4.55	1.47	1.39
24	s	408	CHL	O2A-CGA	4.55	1.45	1.30
24	p	305	CHL	CHC-C4B	4.55	1.47	1.39
24	4	317	CHL	CHD-C4C	4.55	1.48	1.39
24	S	605	CHL	O2A-CGA	4.54	1.45	1.30
24	Y	319	CHL	C3B-C2B	4.54	1.46	1.40
24	r	308	CHL	CHD-C1D	4.54	1.47	1.39
24	4	305	CHL	O2A-CGA	4.54	1.45	1.30
24	3	312	CHL	CHD-C4C	4.54	1.48	1.39
24	7	306	CHL	OBD-CAD	4.54	1.28	1.22
24	u	311	CHL	O2A-CGA	4.54	1.45	1.30
24	S	608	CHL	C3A-C2A	-4.54	1.50	1.54
24	7	311	CHL	O2A-CGA	4.54	1.45	1.30
24	r	308	CHL	C3B-C2B	4.54	1.46	1.40
24	6	305	CHL	CHB-C1B	4.54	1.47	1.39
24	r	309	CHL	O2A-CGA	4.54	1.45	1.30
24	R	608	CHL	CHB-C1B	4.54	1.47	1.39
24	3	311	CHL	CHB-C1B	4.54	1.47	1.39
24	9	305	CHL	C3B-C2B	4.54	1.46	1.40
24	1	305	CHL	O2A-CGA	4.54	1.45	1.30
24	q	308	CHL	O2A-CGA	4.54	1.45	1.30
24	s	406	CHL	O2A-CGA	4.54	1.45	1.30
24	R	608	CHL	O2A-CGA	4.54	1.45	1.30
24	7	312	CHL	C3D-C2D	4.54	1.47	1.39
24	9	310	CHL	O2A-CGA	4.54	1.45	1.30
24	2	312	CHL	O2A-CGA	4.54	1.45	1.30
24	R	605	CHL	CHD-C1D	4.53	1.47	1.39
24	9	309	CHL	O2A-CGA	4.53	1.45	1.30
24	2	306	CHL	CHD-C1D	4.53	1.47	1.39
24	u	310	CHL	O2A-CGA	4.53	1.45	1.30
24	3	311	CHL	C3A-C2A	-4.53	1.50	1.54
24	s	407	CHL	O2A-CGA	4.53	1.45	1.30
24	8	308	CHL	O2A-CGA	4.53	1.45	1.30
24	p	310	CHL	O2A-CGA	4.53	1.45	1.30
24	2	313	CHL	C2A-C3A	-4.53	1.51	1.54
24	n	312	CHL	C3A-C2A	-4.53	1.50	1.54
24	N	312	CHL	CHB-C1B	4.53	1.47	1.39
24	n	309	CHL	O2A-CGA	4.53	1.45	1.30
24	6	312	CHL	CHD-C4C	4.53	1.48	1.39
24	r	307	CHL	CHD-C1D	4.53	1.47	1.39
24	5	312	CHL	O2A-CGA	4.53	1.45	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	p	318	CHL	CHB-C1B	4.53	1.47	1.39
24	q	304	CHL	CHD-C1D	4.53	1.47	1.39
24	G	306	CHL	C3A-C2A	-4.53	1.50	1.54
24	Y	312	CHL	OBD-CAD	4.53	1.28	1.22
24	u	313	CHL	CHD-C4C	4.53	1.48	1.39
24	1	308	CHL	CHD-C4C	4.52	1.48	1.39
24	3	308	CHL	CHD-C4C	4.52	1.48	1.39
24	G	313	CHL	CHD-C4C	4.52	1.48	1.39
24	1	312	CHL	O2A-CGA	4.52	1.45	1.30
24	S	607	CHL	C3A-C2A	-4.52	1.50	1.54
24	7	305	CHL	C3D-C2D	4.52	1.47	1.39
24	S	608	CHL	CHB-C1B	4.52	1.46	1.39
24	q	307	CHL	CHB-C1B	4.52	1.46	1.39
24	4	308	CHL	CHD-C4C	4.52	1.48	1.39
24	s	402	CHL	O2A-CGA	4.52	1.45	1.30
31	d	410	8CT	C06-C07	4.52	1.66	1.52
24	4	312	CHL	O2A-CGA	4.51	1.45	1.30
24	5	306	CHL	C3B-C2B	4.51	1.46	1.40
24	8	309	CHL	C3D-C2D	4.51	1.47	1.39
24	N	309	CHL	O2A-CGA	4.51	1.45	1.30
24	7	310	CHL	O2A-CGA	4.51	1.45	1.30
24	7	311	CHL	CHB-C1B	4.51	1.46	1.39
24	G	310	CHL	CHD-C4C	4.51	1.48	1.39
24	R	601	CHL	O2A-CGA	4.51	1.45	1.30
24	p	311	CHL	O2A-CGA	4.51	1.45	1.30
24	q	310	CHL	C3D-C2D	4.51	1.47	1.39
24	S	606	CHL	O2A-CGA	4.51	1.45	1.30
24	5	306	CHL	CHD-C1D	4.51	1.46	1.39
24	p	305	CHL	CHD-C1D	4.51	1.46	1.39
24	G	306	CHL	CHB-C1B	4.51	1.46	1.39
24	g	312	CHL	C3A-C2A	-4.51	1.50	1.54
24	s	409	CHL	CHB-C1B	4.51	1.46	1.39
24	4	304	CHL	CHD-C4C	4.51	1.48	1.39
24	5	310	CHL	CHB-C1B	4.51	1.46	1.39
31	a	608	8CT	C06-C07	4.51	1.66	1.52
24	n	309	CHL	CHD-C1D	4.51	1.46	1.39
24	N	309	CHL	CHD-C1D	4.51	1.46	1.39
24	g	306	CHL	C3B-C2B	4.51	1.46	1.40
24	2	311	CHL	CHB-C4A	-4.50	1.33	1.38
24	s	406	CHL	CHB-C1B	4.50	1.46	1.39
24	1	309	CHL	CHD-C4C	4.50	1.48	1.39
31	A	608	8CT	C06-C07	4.50	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	R	606	CHL	C3A-C2A	-4.50	1.50	1.54
24	s	408	CHL	C3A-C2A	-4.50	1.50	1.54
24	n	309	CHL	C3B-C2B	4.50	1.46	1.40
24	n	304	CHL	CHD-C4C	4.50	1.48	1.39
24	N	310	CHL	CHB-C4A	-4.49	1.33	1.38
24	R	607	CHL	CHD-C1D	4.49	1.46	1.39
24	S	601	CHL	O2A-CGA	4.49	1.45	1.30
24	u	306	CHL	C3A-C2A	-4.49	1.50	1.54
24	2	309	CHL	CHB-C4A	-4.49	1.33	1.38
24	Y	310	CHL	CHD-C1D	4.49	1.46	1.39
24	s	407	CHL	C3A-C2A	-4.49	1.50	1.54
31	c	615	8CT	C19-C20	4.49	1.57	1.43
24	8	315	CHL	CHD-C4C	4.48	1.48	1.39
39	D	406	PL9	C7-C3	-4.48	1.45	1.51
24	N	305	CHL	C3A-C2A	-4.48	1.50	1.54
24	5	305	CHL	C3A-C2A	-4.48	1.50	1.54
24	G	311	CHL	CHB-C4A	-4.48	1.33	1.38
24	9	312	CHL	CHD-C4C	4.48	1.48	1.39
24	N	304	CHL	CHD-C4C	4.48	1.48	1.39
24	N	308	CHL	CHB-C4A	-4.48	1.33	1.38
24	p	312	CHL	C3D-C2D	4.48	1.47	1.39
24	8	309	CHL	CHD-C1D	4.48	1.46	1.39
24	p	318	CHL	CHB-C4A	-4.48	1.33	1.38
24	G	305	CHL	CHB-C1B	4.48	1.46	1.39
24	S	605	CHL	CHB-C1B	4.48	1.46	1.39
24	g	318	CHL	CHB-C1B	4.48	1.46	1.39
24	g	310	CHL	CHD-C4C	4.48	1.48	1.39
24	u	305	CHL	CHD-C4C	4.48	1.48	1.39
31	b	617	8CT	C19-C20	4.48	1.57	1.43
24	4	311	CHL	CHB-C1B	4.48	1.46	1.39
24	4	309	CHL	CHD-C4C	4.47	1.48	1.39
24	R	606	CHL	CHD-C1D	4.47	1.46	1.39
24	p	305	CHL	C3D-C2D	4.47	1.47	1.39
31	c	613	8CT	C06-C07	4.47	1.66	1.52
24	6	310	CHL	CHD-C4C	4.47	1.48	1.39
24	7	313	CHL	CHB-C1B	4.47	1.46	1.39
24	q	309	CHL	C3B-C2B	4.47	1.46	1.40
24	q	311	CHL	C3B-C2B	4.47	1.46	1.40
31	X	601	8CT	C06-C07	4.47	1.66	1.52
24	S	613	CHL	C3B-C2B	4.47	1.46	1.40
31	t	101	8CT	C06-C07	4.47	1.66	1.52
24	r	309	CHL	CHB-C1B	4.47	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	S	601	CHL	CHD-C1D	4.47	1.46	1.39
24	q	310	CHL	CHD-C1D	4.47	1.46	1.39
24	g	311	CHL	CHB-C4A	-4.47	1.33	1.38
24	8	308	CHL	C3B-C2B	4.46	1.46	1.40
31	x	601	8CT	C06-C07	4.46	1.66	1.52
24	2	306	CHL	C3B-C2B	4.46	1.46	1.40
24	S	613	CHL	CHD-C1D	4.46	1.46	1.39
31	C	613	8CT	C06-C07	4.46	1.66	1.52
31	v	401	8CT	C19-C20	4.46	1.57	1.43
31	T	101	8CT	C06-C07	4.46	1.66	1.52
24	5	305	CHL	CHB-C1B	4.46	1.46	1.39
24	5	313	CHL	C2A-C3A	-4.46	1.51	1.54
24	y	305	CHL	C3D-C2D	4.45	1.47	1.39
24	4	312	CHL	CHB-C4A	-4.45	1.33	1.38
24	S	606	CHL	CHB-C1B	4.45	1.46	1.39
24	u	310	CHL	CHD-C4C	4.45	1.47	1.39
24	N	311	CHL	C3A-C2A	-4.45	1.50	1.54
24	p	313	CHL	CHB-C1B	4.45	1.46	1.39
24	G	312	CHL	CHB-C4A	-4.45	1.33	1.38
24	g	305	CHL	CHB-C1B	4.45	1.46	1.39
24	u	310	CHL	CHB-C4A	-4.45	1.33	1.38
31	C	615	8CT	C19-C20	4.45	1.57	1.43
24	q	303	CHL	CHB-C4A	-4.45	1.33	1.38
31	T	101	8CT	C19-C20	4.45	1.57	1.43
24	R	602	CHL	CHD-C1D	4.45	1.46	1.39
24	r	303	CHL	CHD-C1D	4.45	1.46	1.39
24	9	317	CHL	CHC-C1C	4.45	1.47	1.39
24	6	311	CHL	CHB-C1B	4.45	1.46	1.39
24	6	304	CHL	CHB-C1B	4.44	1.46	1.39
24	s	414	CHL	C3B-C2B	4.44	1.46	1.40
24	R	601	CHL	CHD-C4C	4.44	1.47	1.39
31	B	617	8CT	C19-C20	4.44	1.56	1.43
24	N	312	CHL	C3A-C2A	-4.44	1.50	1.54
24	9	304	CHL	CHB-C4A	-4.43	1.33	1.38
24	y	309	CHL	C3A-C2A	-4.43	1.50	1.54
24	R	605	CHL	C3B-C2B	4.43	1.46	1.40
24	Y	308	CHL	CHB-C1B	4.43	1.46	1.39
24	q	316	CHL	CHD-C4C	4.43	1.47	1.39
24	y	318	CHL	CHD-C1D	4.43	1.46	1.39
24	s	403	CHL	CHB-C1B	4.43	1.46	1.39
24	N	317	CHL	CHC-C1C	4.43	1.47	1.39
24	s	414	CHL	CHD-C1D	4.43	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	5	309	CHL	CHD-C4C	4.43	1.47	1.39
24	7	310	CHL	CHC-C1C	4.43	1.47	1.39
31	t	101	8CT	C19-C20	4.43	1.56	1.43
24	8	307	CHL	CHB-C1B	4.43	1.46	1.39
24	g	310	CHL	CHB-C4A	-4.43	1.33	1.38
24	3	310	CHL	CHD-C4C	4.43	1.47	1.39
24	4	309	CHL	CHB-C4A	-4.42	1.33	1.38
24	p	312	CHL	C3B-C2B	4.42	1.46	1.40
24	G	318	CHL	CHB-C1B	4.42	1.46	1.39
24	7	305	CHL	CHD-C1D	4.42	1.46	1.39
24	2	305	CHL	CHB-C1B	4.42	1.46	1.39
24	G	313	CHL	CHB-C4A	-4.42	1.33	1.38
24	u	313	CHL	CHB-C4A	-4.42	1.33	1.38
24	n	304	CHL	CHB-C4A	-4.42	1.33	1.38
24	y	310	CHL	C3D-C2D	4.42	1.47	1.39
24	g	305	CHL	C3A-C2A	-4.42	1.50	1.54
24	S	602	CHL	CHB-C1B	4.42	1.46	1.39
24	1	309	CHL	CHB-C4A	-4.42	1.33	1.38
24	3	312	CHL	CHB-C4A	-4.42	1.33	1.38
24	8	303	CHL	CHB-C4A	-4.42	1.33	1.38
31	V	401	8CT	C19-C20	4.42	1.56	1.43
24	G	309	CHL	CHC-C1C	4.42	1.47	1.39
24	8	303	CHL	CHD-C4C	4.42	1.47	1.39
24	n	305	CHL	C3A-C2A	-4.42	1.50	1.54
24	r	307	CHL	C3A-C2A	-4.42	1.50	1.54
24	q	303	CHL	CHD-C4C	4.41	1.47	1.39
24	u	311	CHL	CHB-C4A	-4.41	1.33	1.38
24	s	402	CHL	CHD-C1D	4.41	1.46	1.39
24	g	313	CHL	CHB-C4A	-4.41	1.33	1.38
24	n	308	CHL	CHD-C4C	4.41	1.47	1.39
24	2	305	CHL	C3A-C2A	-4.41	1.50	1.54
24	n	317	CHL	CHC-C1C	4.41	1.47	1.39
24	y	309	CHL	CHB-C1B	4.41	1.46	1.39
24	3	317	CHL	CHB-C4A	-4.41	1.33	1.38
24	q	308	CHL	C3B-C2B	4.41	1.46	1.40
24	3	304	CHL	CHB-C1B	4.41	1.46	1.39
24	Y	309	CHL	C3D-C2D	4.40	1.47	1.39
31	A	608	8CT	C19-C20	4.40	1.56	1.43
24	2	318	CHL	CHD-C4C	4.40	1.47	1.39
24	6	305	CHL	C3A-C2A	-4.40	1.50	1.54
24	8	310	CHL	C3B-C2B	4.40	1.46	1.40
31	c	613	8CT	C19-C20	4.40	1.56	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	1	305	CHL	CHB-C1B	4.40	1.46	1.39
24	N	304	CHL	CHB-C4A	-4.40	1.33	1.38
24	n	308	CHL	CHB-C4A	-4.40	1.33	1.38
24	9	309	CHL	CHD-C4C	4.40	1.47	1.39
24	5	318	CHL	CHB-C4A	-4.40	1.33	1.38
24	6	317	CHL	CHD-C4C	4.40	1.47	1.39
24	9	309	CHL	CHB-C4A	-4.39	1.33	1.38
24	7	309	CHL	CHC-C1C	4.39	1.47	1.39
24	2	309	CHL	CHD-C4C	4.39	1.47	1.39
31	X	601	8CT	C19-C20	4.39	1.56	1.43
31	a	608	8CT	C19-C20	4.39	1.56	1.43
31	d	410	8CT	C19-C20	4.39	1.56	1.43
24	r	302	CHL	CHD-C4C	4.39	1.47	1.39
24	u	309	CHL	CHC-C1C	4.39	1.47	1.39
31	D	410	8CT	C19-C20	4.39	1.56	1.43
24	9	308	CHL	CHC-C1C	4.39	1.47	1.39
24	6	312	CHL	CHB-C4A	-4.39	1.33	1.38
24	G	310	CHL	CHB-C4A	-4.39	1.33	1.38
24	u	318	CHL	CHC-C1C	4.39	1.47	1.39
24	Y	304	CHL	C3D-C2D	4.39	1.47	1.39
24	R	602	CHL	CHB-C1B	4.39	1.46	1.39
24	g	306	CHL	CHB-C1B	4.39	1.46	1.39
24	Y	317	CHL	CHD-C1D	4.39	1.46	1.39
24	4	317	CHL	CHC-C1C	4.38	1.47	1.39
24	N	310	CHL	CHD-C4C	4.38	1.47	1.39
24	r	307	CHL	CHB-C1B	4.38	1.46	1.39
24	p	309	CHL	CHC-C1C	4.38	1.47	1.39
24	3	304	CHL	C3A-C2A	-4.38	1.50	1.54
24	2	318	CHL	CHB-C4A	-4.38	1.33	1.38
31	c	614	8CT	C06-C07	4.38	1.66	1.52
24	y	313	CHL	CHB-C1B	4.38	1.46	1.39
24	s	407	CHL	CHB-C1B	4.38	1.46	1.39
24	3	309	CHL	CHD-C4C	4.38	1.47	1.39
24	g	311	CHL	CHD-C4C	4.38	1.47	1.39
24	1	317	CHL	CHC-C1C	4.38	1.47	1.39
24	g	309	CHL	CHC-C1C	4.38	1.47	1.39
24	9	310	CHL	CHD-C4C	4.38	1.47	1.39
24	5	309	CHL	CHB-C4A	-4.38	1.33	1.38
24	7	311	CHL	C3A-C2A	-4.38	1.50	1.54
24	3	317	CHL	CHD-C4C	4.37	1.47	1.39
31	C	614	8CT	C06-C07	4.37	1.66	1.52
24	3	309	CHL	O2A-CGA	4.37	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	9	304	CHL	CHD-C4C	4.37	1.47	1.39
24	g	312	CHL	CHD-C4C	4.37	1.47	1.39
24	p	310	CHL	CHC-C1C	4.37	1.47	1.39
24	7	312	CHL	C3B-C2B	4.37	1.46	1.40
24	q	309	CHL	CHB-C1B	4.37	1.46	1.39
24	5	311	CHL	CHD-C4C	4.37	1.47	1.39
31	c	614	8CT	C19-C20	4.37	1.56	1.43
24	5	318	CHL	CHD-C4C	4.37	1.47	1.39
24	G	305	CHL	C3A-C2A	-4.37	1.50	1.54
24	R	606	CHL	CHB-C1B	4.37	1.46	1.39
24	8	304	CHL	C3B-C2B	4.37	1.46	1.40
24	u	311	CHL	CHD-C4C	4.37	1.47	1.39
24	6	317	CHL	CHB-C4A	-4.37	1.33	1.38
24	4	305	CHL	CHB-C1B	4.36	1.46	1.39
31	C	613	8CT	C19-C20	4.36	1.56	1.43
24	1	311	CHL	CHB-C1B	4.36	1.46	1.39
24	6	309	CHL	CHD-C4C	4.36	1.47	1.39
24	G	312	CHL	CHD-C4C	4.36	1.47	1.39
24	N	311	CHL	O2A-CGA	4.36	1.46	1.33
24	9	311	CHL	CHB-C4A	-4.35	1.33	1.38
24	Y	308	CHL	C3A-C2A	-4.35	1.51	1.54
24	s	402	CHL	C3B-C2B	4.35	1.46	1.40
24	G	311	CHL	CHD-C4C	4.35	1.47	1.39
24	7	310	CHL	CHD-C4C	4.35	1.47	1.39
24	n	311	CHL	O2A-CGA	4.35	1.46	1.33
24	6	309	CHL	CHB-C4A	-4.35	1.33	1.38
24	N	311	CHL	CHB-C1B	4.35	1.46	1.39
24	N	312	CHL	O2A-CGA	4.35	1.46	1.33
24	Y	311	CHL	C3B-C2B	4.35	1.46	1.40
24	q	304	CHL	C3B-C2B	4.35	1.46	1.40
31	x	601	8CT	C19-C20	4.35	1.56	1.43
24	5	312	CHL	CHB-C1B	4.35	1.46	1.39
24	3	305	CHL	C3A-C2A	-4.34	1.51	1.54
24	9	312	CHL	CHB-C4A	-4.34	1.33	1.38
24	Y	317	CHL	C3B-C2B	4.34	1.46	1.40
24	6	304	CHL	O2A-CGA	4.34	1.46	1.33
24	6	309	CHL	O2A-CGA	4.34	1.46	1.33
24	y	312	CHL	C3B-C2B	4.34	1.46	1.40
24	5	318	CHL	C2A-C3A	-4.34	1.51	1.54
24	r	303	CHL	CHB-C1B	4.34	1.46	1.39
24	3	309	CHL	CHB-C4A	-4.34	1.33	1.38
24	G	313	CHL	O2A-CGA	4.34	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	r	308	CHL	C3D-C2D	4.34	1.47	1.39
24	n	311	CHL	CHB-C1B	4.34	1.46	1.39
24	6	304	CHL	CHD-C4C	4.34	1.47	1.39
24	2	312	CHL	CHB-C1B	4.34	1.46	1.39
24	9	305	CHL	O2A-CGA	4.34	1.46	1.33
24	p	312	CHL	CHB-C1B	4.33	1.46	1.39
24	n	310	CHL	O2A-CGA	4.33	1.46	1.33
24	r	303	CHL	C3B-C2B	4.33	1.46	1.40
24	R	607	CHL	C3D-C2D	4.33	1.47	1.39
24	Y	304	CHL	CHD-C1D	4.33	1.46	1.39
24	Y	312	CHL	CHB-C1B	4.33	1.46	1.39
24	y	318	CHL	C3B-C2B	4.33	1.46	1.40
24	y	310	CHL	CHD-C1D	4.33	1.46	1.39
24	R	602	CHL	C3B-C2B	4.33	1.46	1.40
24	2	311	CHL	CHD-C4C	4.33	1.47	1.39
24	u	310	CHL	CHC-C1C	4.33	1.47	1.39
24	3	304	CHL	O2A-CGA	4.33	1.46	1.33
24	6	308	CHL	CHC-C1C	4.33	1.47	1.39
24	G	312	CHL	C3A-C2A	-4.33	1.51	1.54
24	y	305	CHL	CHD-C1D	4.33	1.46	1.39
24	2	313	CHL	CHD-C4C	4.32	1.47	1.39
24	5	313	CHL	CHD-C4C	4.32	1.47	1.39
24	u	306	CHL	O2A-CGA	4.32	1.45	1.33
24	3	310	CHL	CHB-C4A	-4.32	1.33	1.38
24	y	311	CHL	C3B-C2B	4.32	1.46	1.40
24	N	312	CHL	CHD-C4C	4.32	1.47	1.39
24	p	310	CHL	CHD-C4C	4.32	1.47	1.39
37	C	619	DGD	O1G-C1A	4.32	1.45	1.33
24	4	304	CHL	CHC-C1C	4.32	1.47	1.39
31	C	614	8CT	C19-C20	4.32	1.56	1.43
24	N	309	CHL	CHB-C1B	4.32	1.46	1.39
24	N	310	CHL	O2A-CGA	4.32	1.45	1.33
24	n	312	CHL	O2A-CGA	4.32	1.45	1.33
24	n	310	CHL	CHD-C4C	4.32	1.47	1.39
24	g	313	CHL	O2A-CGA	4.32	1.45	1.33
24	1	309	CHL	CHC-C1C	4.31	1.47	1.39
24	8	304	CHL	CHB-C1B	4.31	1.46	1.39
24	u	305	CHL	CHB-C4A	-4.31	1.33	1.38
24	6	305	CHL	O2A-CGA	4.31	1.45	1.33
24	6	310	CHL	CHB-C4A	-4.31	1.33	1.38
24	n	312	CHL	CHD-C4C	4.31	1.47	1.39
24	3	305	CHL	O2A-CGA	4.31	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Y	310	CHL	C3B-C2B	4.31	1.46	1.40
24	s	408	CHL	CHB-C1B	4.31	1.46	1.39
24	G	306	CHL	O2A-CGA	4.31	1.45	1.33
24	1	304	CHL	CHC-C1C	4.31	1.47	1.39
37	c	618	DGD	O1G-C1A	4.31	1.45	1.33
24	7	312	CHL	CHB-C1B	4.31	1.46	1.39
24	Y	309	CHL	CHD-C1D	4.31	1.46	1.39
24	8	315	CHL	CHC-C1C	4.30	1.47	1.39
24	R	607	CHL	O2A-CGA	4.30	1.45	1.33
24	r	306	CHL	CHC-C1C	4.30	1.47	1.39
24	g	306	CHL	O2A-CGA	4.30	1.45	1.33
24	y	306	CHL	CHD-C1D	4.30	1.46	1.39
24	S	601	CHL	C3B-C2B	4.30	1.46	1.40
24	Y	319	CHL	O2A-CGA	4.30	1.45	1.33
24	8	308	CHL	CHB-C1B	4.30	1.46	1.39
24	q	309	CHL	O2A-CGA	4.30	1.45	1.33
24	G	311	CHL	O2A-CGA	4.30	1.45	1.33
24	S	613	CHL	CHB-C1B	4.30	1.46	1.39
24	5	305	CHL	CHD-C4C	4.30	1.47	1.39
24	q	303	CHL	O2A-CGA	4.30	1.45	1.33
24	9	309	CHL	CHC-C1C	4.29	1.47	1.39
24	q	316	CHL	CHC-C1C	4.29	1.47	1.39
24	9	310	CHL	CHB-C4A	-4.29	1.33	1.38
24	9	311	CHL	CHD-C4C	4.29	1.47	1.39
24	3	304	CHL	CHD-C4C	4.29	1.47	1.39
24	8	304	CHL	O2A-CGA	4.29	1.45	1.33
24	2	306	CHL	CHB-C1B	4.29	1.46	1.39
24	4	308	CHL	CHC-C1C	4.29	1.47	1.39
24	4	309	CHL	CHC-C1C	4.29	1.47	1.39
24	N	305	CHL	O2A-CGA	4.29	1.45	1.33
24	q	304	CHL	O2A-CGA	4.29	1.45	1.33
24	r	308	CHL	O2A-CGA	4.29	1.45	1.33
24	g	311	CHL	O2A-CGA	4.29	1.45	1.33
24	p	305	CHL	O2A-CGA	4.29	1.45	1.33
24	u	312	CHL	CHB-C4A	-4.29	1.33	1.38
24	2	318	CHL	C2A-C3A	-4.29	1.51	1.54
24	y	313	CHL	O2A-CGA	4.29	1.45	1.33
24	q	310	CHL	CHB-C1B	4.29	1.46	1.39
24	R	605	CHL	CHB-C1B	4.28	1.46	1.39
24	8	303	CHL	O2A-CGA	4.28	1.45	1.33
31	S	615	8CT	C24-C25	4.28	1.56	1.43
24	8	309	CHL	O2A-CGA	4.28	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Y	319	CHL	CHB-C1B	4.28	1.46	1.39
24	y	311	CHL	O2A-CGA	4.28	1.45	1.33
24	Y	305	CHL	CHD-C1D	4.28	1.46	1.39
24	R	606	CHL	O2A-CGA	4.28	1.45	1.33
24	n	305	CHL	O2A-CGA	4.28	1.45	1.33
24	4	312	CHL	CHD-C4C	4.28	1.47	1.39
24	q	304	CHL	CHB-C1B	4.28	1.46	1.39
24	s	414	CHL	CHB-C1B	4.28	1.46	1.39
24	2	305	CHL	CHD-C4C	4.28	1.47	1.39
33	d	411	LMG	O8-C28	4.28	1.45	1.33
24	y	310	CHL	C3B-C2B	4.28	1.46	1.40
24	g	313	CHL	CHC-C1C	4.28	1.47	1.39
33	D	411	LMG	O8-C28	4.28	1.45	1.33
24	u	313	CHL	CHC-C1C	4.28	1.47	1.39
24	4	311	CHL	CHD-C4C	4.28	1.47	1.39
24	g	305	CHL	CHD-C4C	4.28	1.47	1.39
24	G	312	CHL	O2A-CGA	4.27	1.45	1.33
24	p	312	CHL	CHD-C1D	4.27	1.46	1.39
24	1	312	CHL	CHD-C4C	4.27	1.47	1.39
24	1	308	CHL	CHB-C4A	-4.27	1.33	1.38
24	u	305	CHL	O2A-CGA	4.27	1.45	1.33
24	7	305	CHL	O2A-CGA	4.27	1.45	1.33
24	y	318	CHL	CHB-C1B	4.27	1.46	1.39
24	Y	311	CHL	O2A-CGA	4.27	1.45	1.33
24	3	308	CHL	CHC-C1C	4.27	1.47	1.39
24	Y	312	CHL	O2A-CGA	4.27	1.45	1.33
24	N	308	CHL	CHD-C4C	4.27	1.47	1.39
24	q	310	CHL	O2A-CGA	4.27	1.45	1.33
31	s	416	8CT	C24-C25	4.26	1.56	1.43
24	u	312	CHL	CHD-C4C	4.26	1.47	1.39
24	G	318	CHL	CHD-C4C	4.26	1.47	1.39
24	S	602	CHL	O2A-CGA	4.26	1.45	1.33
24	9	312	CHL	CHC-C1C	4.26	1.47	1.39
24	r	307	CHL	O2A-CGA	4.26	1.45	1.33
24	8	310	CHL	O2A-CGA	4.26	1.45	1.33
24	G	310	CHL	CHC-C1C	4.26	1.47	1.39
24	g	318	CHL	CHD-C4C	4.26	1.47	1.39
24	1	308	CHL	CHC-C1C	4.26	1.47	1.39
24	q	311	CHL	O2A-CGA	4.26	1.45	1.33
24	p	311	CHL	C3A-C2A	-4.26	1.51	1.54
24	5	306	CHL	CHB-C1B	4.26	1.46	1.39
24	s	403	CHL	O2A-CGA	4.26	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	y	312	CHL	O2A-CGA	4.26	1.45	1.33
24	4	308	CHL	CHB-C4A	-4.26	1.33	1.38
24	G	305	CHL	CHD-C4C	4.25	1.47	1.39
24	5	309	CHL	CHC-C1C	4.25	1.47	1.39
24	7	312	CHL	CHD-C1D	4.25	1.46	1.39
24	4	309	CHL	C3A-C2A	-4.25	1.51	1.54
24	9	304	CHL	O2A-CGA	4.25	1.45	1.33
24	g	312	CHL	O2A-CGA	4.25	1.45	1.33
24	S	607	CHL	CHB-C1B	4.25	1.46	1.39
24	9	310	CHL	CHC-C1C	4.25	1.47	1.39
24	Y	310	CHL	O2A-CGA	4.25	1.45	1.33
24	u	311	CHL	CHC-C1C	4.25	1.47	1.39
24	r	308	CHL	CHB-C1B	4.25	1.46	1.39
24	g	305	CHL	O2A-CGA	4.25	1.45	1.33
24	R	607	CHL	CHB-C1B	4.24	1.46	1.39
24	n	304	CHL	O2A-CGA	4.24	1.45	1.33
24	n	309	CHL	CHB-C1B	4.24	1.46	1.39
24	p	306	CHL	O2A-CGA	4.24	1.45	1.33
24	N	304	CHL	O2A-CGA	4.24	1.45	1.33
24	7	306	CHL	O2A-CGA	4.24	1.45	1.33
24	p	318	CHL	CHD-C4C	4.24	1.47	1.39
24	G	306	CHL	CHD-C4C	4.24	1.47	1.39
24	g	310	CHL	CHC-C1C	4.24	1.47	1.39
24	6	308	CHL	CHB-C4A	-4.23	1.33	1.38
24	9	305	CHL	CHD-C4C	4.23	1.47	1.39
24	p	305	CHL	CHB-C1B	4.23	1.46	1.39
24	n	308	CHL	CHC-C1C	4.23	1.47	1.39
24	s	409	CHL	CHD-C4C	4.23	1.47	1.39
24	1	311	CHL	CHD-C4C	4.23	1.47	1.39
24	S	608	CHL	CHD-C4C	4.23	1.47	1.39
24	n	310	CHL	CHC-C1C	4.23	1.47	1.39
24	Y	317	CHL	CHB-C1B	4.23	1.46	1.39
24	y	313	CHL	CHD-C4C	4.22	1.47	1.39
24	8	309	CHL	CHB-C1B	4.22	1.46	1.39
24	1	304	CHL	CHB-C4A	-4.22	1.33	1.38
24	6	310	CHL	CHC-C1C	4.22	1.47	1.39
31	S	615	8CT	C14-C13	4.22	1.56	1.43
24	u	306	CHL	CHD-C4C	4.22	1.47	1.39
24	p	309	CHL	CHB-C4A	-4.22	1.33	1.38
24	8	307	CHL	CHD-C4C	4.21	1.47	1.39
24	G	305	CHL	O2A-CGA	4.21	1.45	1.33
24	3	317	CHL	CHC-C1C	4.21	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	3	305	CHL	CHD-C4C	4.21	1.47	1.39
24	u	306	CHL	CHC-C1C	4.21	1.47	1.39
24	q	307	CHL	CHD-C4C	4.21	1.47	1.39
24	7	318	CHL	CHD-C4C	4.21	1.47	1.39
24	4	310	CHL	CHD-C4C	4.21	1.47	1.39
31	s	416	8CT	C14-C13	4.21	1.56	1.43
33	B	619	LMG	O8-C28	4.21	1.45	1.33
24	Y	308	CHL	CHD-C4C	4.21	1.47	1.39
24	5	311	CHL	CHC-C1C	4.21	1.47	1.39
24	3	310	CHL	CHC-C1C	4.21	1.47	1.39
24	q	303	CHL	C3A-C2A	-4.21	1.51	1.54
24	9	308	CHL	CHB-C4A	-4.21	1.33	1.38
24	n	304	CHL	CHC-C1C	4.21	1.47	1.39
24	N	310	CHL	CHC-C1C	4.21	1.47	1.39
24	q	308	CHL	CHB-C1B	4.21	1.46	1.39
24	R	601	CHL	CHC-C1C	4.21	1.47	1.39
24	r	306	CHL	CHD-C4C	4.20	1.47	1.39
24	7	305	CHL	CHB-C1B	4.20	1.46	1.39
24	3	308	CHL	CHB-C4A	-4.20	1.33	1.38
24	7	313	CHL	CHD-C4C	4.20	1.47	1.39
24	9	317	CHL	CHB-C4A	-4.20	1.33	1.38
24	9	304	CHL	C3A-C2A	-4.20	1.51	1.54
24	u	305	CHL	CHC-C1C	4.20	1.47	1.39
24	7	306	CHL	CHD-C1D	4.20	1.46	1.39
24	8	307	CHL	C3A-C2A	-4.20	1.51	1.54
24	2	318	CHL	CHC-C1C	4.20	1.47	1.39
24	r	302	CHL	CHC-C1C	4.20	1.47	1.39
24	y	309	CHL	CHD-C4C	4.20	1.47	1.39
24	5	318	CHL	CHC-C1C	4.19	1.47	1.39
24	6	311	CHL	CHD-C4C	4.19	1.47	1.39
24	n	305	CHL	CHC-C1C	4.19	1.47	1.39
33	m	101	LMG	O8-C28	4.19	1.45	1.33
24	g	309	CHL	CHB-C4A	-4.19	1.33	1.38
24	u	318	CHL	CHB-C4A	-4.19	1.33	1.38
24	2	309	CHL	CHC-C1C	4.19	1.47	1.39
24	G	313	CHL	CHC-C1C	4.19	1.47	1.39
24	u	312	CHL	CHC-C1C	4.19	1.47	1.39
24	1	310	CHL	CHD-C4C	4.19	1.47	1.39
24	6	312	CHL	CHC-C1C	4.19	1.47	1.39
24	p	310	CHL	C3A-C2A	-4.19	1.51	1.54
31	S	614	8CT	C24-C25	4.19	1.56	1.43
31	s	415	8CT	C11-C12	4.18	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	G	309	CHL	CHB-C4A	-4.18	1.33	1.38
24	s	407	CHL	CHD-C4C	4.18	1.47	1.39
31	v	401	8CT	C24-C25	4.18	1.56	1.43
24	p	306	CHL	CHD-C1D	4.18	1.46	1.39
24	g	311	CHL	CHC-C1C	4.18	1.47	1.39
24	p	306	CHL	C3B-C2B	4.18	1.46	1.40
31	V	401	8CT	C24-C25	4.18	1.56	1.43
24	3	311	CHL	CHD-C4C	4.18	1.47	1.39
24	Y	312	CHL	CHD-C4C	4.18	1.47	1.39
24	G	311	CHL	CHC-C1C	4.17	1.47	1.39
24	6	317	CHL	CHC-C1C	4.17	1.47	1.39
24	3	312	CHL	CHC-C1C	4.17	1.47	1.39
24	N	305	CHL	CHC-C1C	4.17	1.47	1.39
31	s	415	8CT	C24-C25	4.17	1.56	1.43
24	y	312	CHL	CHB-C1B	4.17	1.46	1.39
24	p	313	CHL	CHD-C4C	4.17	1.47	1.39
24	6	305	CHL	CHD-C4C	4.17	1.47	1.39
24	S	601	CHL	CHB-C1B	4.17	1.46	1.39
24	8	310	CHL	CHB-C1B	4.17	1.46	1.39
24	N	304	CHL	CHC-C1C	4.17	1.47	1.39
24	6	305	CHL	CHC-C1C	4.17	1.47	1.39
24	s	402	CHL	CHB-C1B	4.16	1.46	1.39
24	u	309	CHL	CHB-C4A	-4.16	1.33	1.38
24	s	403	CHL	CHD-C1D	4.16	1.46	1.39
24	1	305	CHL	CHD-C4C	4.16	1.47	1.39
24	q	311	CHL	CHB-C1B	4.16	1.46	1.39
24	q	307	CHL	CHC-C1C	4.16	1.47	1.39
24	Y	309	CHL	O2A-CGA	4.16	1.45	1.33
24	G	312	CHL	CHC-C1C	4.16	1.47	1.39
24	u	312	CHL	O2A-CGA	4.16	1.45	1.33
24	p	312	CHL	O2A-CGA	4.15	1.45	1.33
31	S	614	8CT	C11-C12	4.15	1.54	1.46
24	4	305	CHL	CHD-C4C	4.15	1.47	1.39
24	N	308	CHL	CHC-C1C	4.15	1.47	1.39
24	G	311	CHL	C3A-C2A	-4.15	1.51	1.54
24	7	309	CHL	CHB-C4A	-4.15	1.33	1.38
24	R	602	CHL	O2A-CGA	4.15	1.45	1.33
24	6	309	CHL	C3A-C2A	-4.15	1.51	1.54
24	7	310	CHL	C3A-C2A	-4.15	1.51	1.54
24	S	605	CHL	CHD-C4C	4.15	1.47	1.39
24	4	304	CHL	CHB-C4A	-4.15	1.33	1.38
24	q	316	CHL	CHB-C4A	-4.15	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	y	310	CHL	O2A-CGA	4.15	1.45	1.33
24	r	303	CHL	O2A-CGA	4.15	1.45	1.33
24	G	310	CHL	O2A-CGA	4.15	1.45	1.33
24	s	406	CHL	CHD-C4C	4.15	1.47	1.39
24	r	302	CHL	C3A-C2A	-4.14	1.51	1.54
24	g	306	CHL	CHD-C4C	4.14	1.47	1.39
24	9	311	CHL	O2A-CGA	4.14	1.45	1.33
24	S	602	CHL	CHD-C1D	4.14	1.46	1.39
24	3	309	CHL	CHC-C1C	4.14	1.47	1.39
24	2	311	CHL	O2A-CGA	4.14	1.45	1.33
24	5	311	CHL	O2A-CGA	4.14	1.45	1.33
24	g	310	CHL	O2A-CGA	4.14	1.45	1.33
33	D	401	LMG	O8-C28	4.13	1.45	1.33
24	9	311	CHL	CHC-C1C	4.13	1.47	1.39
24	4	312	CHL	CHC-C1C	4.13	1.47	1.39
24	Y	311	CHL	CHB-C1B	4.13	1.46	1.39
24	s	409	CHL	O2A-CGA	4.13	1.45	1.33
24	1	309	CHL	C3A-C2A	-4.13	1.51	1.54
33	C	618	LMG	O8-C28	4.13	1.45	1.33
24	1	312	CHL	CHC-C1C	4.13	1.47	1.39
28	3	318	NEX	C7-C6	-4.13	1.25	1.30
24	8	310	CHL	CHD-C4C	4.13	1.47	1.39
24	p	311	CHL	CHD-C4C	4.13	1.47	1.39
24	3	305	CHL	CHC-C1C	4.13	1.47	1.39
28	N	303	NEX	C7-C6	-4.13	1.25	1.30
24	7	306	CHL	C3B-C2B	4.13	1.46	1.40
24	S	608	CHL	O2A-CGA	4.13	1.45	1.33
24	y	305	CHL	CHB-C1B	4.13	1.46	1.39
39	D	406	PL9	C6-C1	-4.13	1.41	1.48
24	S	606	CHL	CHD-C4C	4.13	1.47	1.39
24	8	315	CHL	CHB-C4A	-4.13	1.33	1.38
24	2	311	CHL	CHC-C1C	4.13	1.47	1.39
24	4	312	CHL	C3A-C2A	-4.12	1.51	1.54
24	7	312	CHL	O2A-CGA	4.12	1.45	1.33
24	8	303	CHL	CHC-C1C	4.12	1.47	1.39
24	r	306	CHL	C2A-C3A	-4.12	1.51	1.54
31	D	410	8CT	C24-C25	4.12	1.56	1.43
24	q	307	CHL	C3A-C2A	-4.12	1.51	1.54
39	d	406	PL9	C6-C1	-4.11	1.41	1.48
24	q	311	CHL	CHD-C4C	4.11	1.47	1.39
24	2	306	CHL	O2A-CGA	4.11	1.45	1.33
24	5	311	CHL	C3A-C2A	-4.11	1.51	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Y	309	CHL	C3B-C2B	4.11	1.45	1.40
24	y	306	CHL	O2A-CGA	4.11	1.45	1.33
31	t	101	8CT	C24-C25	4.11	1.55	1.43
31	d	410	8CT	C24-C25	4.11	1.55	1.43
24	7	311	CHL	CHD-C4C	4.11	1.47	1.39
24	1	310	CHL	C3A-C2A	-4.11	1.51	1.54
24	Y	304	CHL	CHB-C1B	4.11	1.46	1.39
33	d	401	LMG	O8-C28	4.11	1.45	1.33
31	T	101	8CT	C24-C25	4.11	1.55	1.43
24	q	316	CHL	C2A-C3A	-4.10	1.51	1.54
24	y	311	CHL	CHB-C1B	4.10	1.46	1.39
24	8	307	CHL	CHC-C1C	4.10	1.47	1.39
24	2	312	CHL	CHD-C4C	4.10	1.47	1.39
24	5	312	CHL	CHD-C4C	4.10	1.47	1.39
24	Y	304	CHL	O2A-CGA	4.10	1.45	1.33
24	p	311	CHL	CHC-C1C	4.10	1.47	1.39
24	5	306	CHL	O2A-CGA	4.09	1.45	1.33
24	3	309	CHL	C3A-C2A	-4.09	1.51	1.54
24	y	305	CHL	O2A-CGA	4.09	1.45	1.33
24	S	607	CHL	CHD-C4C	4.09	1.47	1.39
24	9	305	CHL	CHC-C1C	4.08	1.47	1.39
28	r	301	NEX	C7-C6	-4.08	1.25	1.30
24	N	317	CHL	CHB-C4A	-4.08	1.33	1.38
24	q	303	CHL	CHC-C1C	4.08	1.47	1.39
31	b	617	8CT	C24-C25	4.08	1.55	1.43
24	9	304	CHL	CHC-C1C	4.08	1.47	1.39
24	2	311	CHL	C3A-C2A	-4.08	1.51	1.54
24	Y	310	CHL	CHB-C1B	4.08	1.46	1.39
24	Y	305	CHL	O2A-CGA	4.08	1.45	1.33
24	p	318	CHL	CHC-C1C	4.07	1.47	1.39
24	Y	319	CHL	CHD-C4C	4.07	1.47	1.39
24	n	305	CHL	CHD-C4C	4.07	1.47	1.39
31	c	615	8CT	C24-C25	4.07	1.55	1.43
24	y	310	CHL	CHB-C1B	4.07	1.46	1.39
24	3	311	CHL	CHC-C1C	4.07	1.47	1.39
33	i	101	LMG	O8-C28	4.07	1.45	1.33
24	7	311	CHL	CHC-C1C	4.07	1.47	1.39
31	C	613	8CT	C24-C25	4.07	1.55	1.43
24	R	601	CHL	C3A-C2A	-4.07	1.51	1.54
24	4	310	CHL	CHC-C1C	4.07	1.47	1.39
24	6	309	CHL	CHC-C1C	4.07	1.47	1.39
24	s	402	CHL	CHC-C1C	4.06	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	6	304	CHL	C3A-C2A	-4.06	1.51	1.54
24	2	310	CHL	CHD-C4C	4.06	1.47	1.39
24	6	304	CHL	CHC-C1C	4.06	1.47	1.39
24	s	402	CHL	CHD-C4C	4.06	1.47	1.39
24	N	311	CHL	CHD-C4C	4.06	1.47	1.39
31	X	601	8CT	C24-C25	4.06	1.55	1.43
24	1	310	CHL	CHC-C1C	4.06	1.47	1.39
31	B	617	8CT	C24-C25	4.05	1.55	1.43
28	s	401	NEX	C7-C6	-4.05	1.25	1.30
24	9	317	CHL	C2A-C3A	-4.05	1.51	1.54
24	y	312	CHL	CHD-C4C	4.05	1.47	1.39
24	5	313	CHL	CHC-C1C	4.05	1.47	1.39
24	r	309	CHL	CHD-C4C	4.05	1.47	1.39
31	c	613	8CT	C24-C25	4.05	1.55	1.43
24	s	408	CHL	CHD-C4C	4.05	1.47	1.39
24	4	310	CHL	C3A-C2A	-4.05	1.51	1.54
24	g	305	CHL	CHC-C1C	4.05	1.47	1.39
24	N	309	CHL	CHD-C4C	4.05	1.47	1.39
24	n	317	CHL	CHB-C4A	-4.05	1.33	1.38
24	8	303	CHL	C3A-C2A	-4.05	1.51	1.54
31	C	615	8CT	C24-C25	4.04	1.55	1.43
28	6	303	NEX	C7-C6	-4.04	1.25	1.30
31	x	601	8CT	C24-C25	4.04	1.55	1.43
24	2	306	CHL	CHC-C1C	4.04	1.47	1.39
24	n	309	CHL	CHD-C4C	4.04	1.47	1.39
24	7	318	CHL	CHC-C1C	4.04	1.47	1.39
24	y	305	CHL	C3B-C2B	4.04	1.45	1.40
24	1	312	CHL	C3A-C2A	-4.04	1.51	1.54
24	2	310	CHL	CHC-C1C	4.04	1.47	1.39
24	R	606	CHL	CHD-C4C	4.04	1.47	1.39
24	r	303	CHL	CHD-C4C	4.04	1.47	1.39
24	Y	311	CHL	CHD-C4C	4.04	1.47	1.39
24	q	310	CHL	C3B-C2B	4.04	1.45	1.40
24	N	305	CHL	CHD-C4C	4.04	1.47	1.39
24	q	309	CHL	CHD-C4C	4.03	1.47	1.39
28	n	303	NEX	C7-C6	-4.03	1.25	1.30
24	5	306	CHL	CHD-C4C	4.03	1.47	1.39
24	r	308	CHL	CHD-C4C	4.03	1.47	1.39
24	8	315	CHL	C2A-C3A	-4.03	1.51	1.54
24	n	310	CHL	C3A-C2A	-4.03	1.51	1.54
24	y	311	CHL	CHD-C4C	4.02	1.47	1.39
24	g	318	CHL	CHC-C1C	4.02	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	g	312	CHL	CHC-C1C	4.02	1.47	1.39
24	g	311	CHL	C3A-C2A	-4.02	1.51	1.54
24	2	313	CHL	CHC-C1C	4.02	1.47	1.39
24	p	305	CHL	C3B-C2B	4.02	1.45	1.40
24	R	602	CHL	CHD-C4C	4.02	1.47	1.39
24	R	608	CHL	CHD-C4C	4.02	1.47	1.39
24	G	305	CHL	CHC-C1C	4.01	1.47	1.39
24	Y	309	CHL	CHB-C1B	4.01	1.46	1.39
24	G	318	CHL	CHC-C1C	4.01	1.47	1.39
24	R	607	CHL	CHD-C4C	4.01	1.47	1.39
24	6	311	CHL	CHC-C1C	4.01	1.47	1.39
24	3	304	CHL	CHC-C1C	4.01	1.47	1.39
31	S	615	8CT	C28-C29	4.01	1.41	1.32
24	2	306	CHL	CHD-C4C	4.01	1.47	1.39
24	n	311	CHL	CHD-C4C	4.01	1.47	1.39
24	Y	304	CHL	C3B-C2B	4.01	1.45	1.40
24	5	306	CHL	CHC-C1C	4.01	1.47	1.39
24	5	310	CHL	CHD-C4C	4.00	1.47	1.39
24	8	309	CHL	C3B-C2B	4.00	1.45	1.40
24	1	317	CHL	CHB-C4A	-4.00	1.33	1.38
24	r	307	CHL	CHD-C4C	4.00	1.47	1.39
24	N	312	CHL	CHC-C1C	3.99	1.47	1.39
24	Y	305	CHL	C3B-C2B	3.99	1.45	1.40
37	C	620	DGD	O1G-C1A	3.99	1.45	1.33
24	S	613	CHL	CHD-C4C	3.99	1.47	1.39
24	N	311	CHL	CHC-C1C	3.99	1.47	1.39
24	8	308	CHL	CHC-C1C	3.99	1.47	1.39
24	5	310	CHL	CHC-C1C	3.99	1.47	1.39
31	s	416	8CT	C11-C12	3.99	1.54	1.46
24	g	313	CHL	C3A-C2A	-3.98	1.51	1.54
31	s	416	8CT	C28-C29	3.98	1.41	1.32
24	Y	305	CHL	CHB-C1B	3.98	1.46	1.39
24	7	305	CHL	CHD-C4C	3.98	1.47	1.39
24	u	318	CHL	C2A-C3A	-3.98	1.51	1.54
24	s	414	CHL	CHD-C4C	3.98	1.47	1.39
24	S	601	CHL	CHD-C4C	3.98	1.47	1.39
24	p	305	CHL	CHD-C4C	3.98	1.47	1.39
31	a	608	8CT	C24-C25	3.98	1.55	1.43
24	p	306	CHL	CHB-C1B	3.97	1.46	1.39
31	c	614	8CT	C24-C25	3.97	1.55	1.43
24	S	601	CHL	CHC-C1C	3.97	1.47	1.39
24	s	406	CHL	CHC-C1C	3.97	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	S	605	CHL	CHC-C1C	3.97	1.47	1.39
24	R	605	CHL	CHC-C1C	3.97	1.47	1.39
24	8	304	CHL	CHD-C4C	3.97	1.47	1.39
24	n	312	CHL	CHC-C1C	3.97	1.47	1.39
24	9	309	CHL	C3A-C2A	-3.97	1.51	1.54
24	q	304	CHL	CHD-C4C	3.97	1.47	1.39
24	y	306	CHL	CHB-C1B	3.97	1.46	1.39
24	4	317	CHL	CHB-C4A	-3.97	1.33	1.38
24	G	306	CHL	CHC-C1C	3.97	1.47	1.39
31	C	614	8CT	C24-C25	3.97	1.55	1.43
24	q	308	CHL	CHD-C4C	3.96	1.47	1.39
24	R	605	CHL	CHD-C4C	3.96	1.47	1.39
24	4	305	CHL	CHC-C1C	3.96	1.47	1.39
24	8	308	CHL	CHD-C4C	3.96	1.47	1.39
31	s	415	8CT	C28-C29	3.96	1.41	1.32
24	7	305	CHL	C3B-C2B	3.96	1.45	1.40
24	Y	317	CHL	CHD-C4C	3.96	1.47	1.39
24	p	313	CHL	CHC-C1C	3.95	1.47	1.39
31	A	608	8CT	C24-C25	3.95	1.55	1.43
24	y	306	CHL	C3B-C2B	3.95	1.45	1.40
24	q	308	CHL	CHC-C1C	3.95	1.46	1.39
24	7	306	CHL	CHB-C1B	3.95	1.46	1.39
24	y	309	CHL	CHC-C1C	3.95	1.46	1.39
24	5	305	CHL	CHC-C1C	3.95	1.46	1.39
31	S	615	8CT	C11-C12	3.95	1.54	1.46
24	s	408	CHL	CHC-C1C	3.94	1.46	1.39
31	S	614	8CT	C28-C29	3.94	1.41	1.32
31	s	415	8CT	C14-C13	3.94	1.55	1.43
24	y	306	CHL	CHC-C1C	3.94	1.46	1.39
24	1	305	CHL	CHC-C1C	3.94	1.46	1.39
31	S	614	8CT	C14-C13	3.94	1.55	1.43
24	q	309	CHL	CHC-C1C	3.94	1.46	1.39
24	Y	319	CHL	CHC-C1C	3.93	1.46	1.39
24	8	309	CHL	CHD-C4C	3.93	1.46	1.39
24	s	403	CHL	CHC-C1C	3.93	1.46	1.39
24	n	311	CHL	CHC-C1C	3.93	1.46	1.39
24	y	318	CHL	CHD-C4C	3.93	1.46	1.39
24	r	307	CHL	CHC-C1C	3.93	1.46	1.39
24	q	310	CHL	CHD-C4C	3.93	1.46	1.39
24	R	606	CHL	CHC-C1C	3.93	1.46	1.39
24	2	305	CHL	CHC-C1C	3.93	1.46	1.39
24	Y	305	CHL	CHC-C1C	3.93	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	S	606	CHL	CHC-C1C	3.93	1.46	1.39
24	2	309	CHL	C3A-C2A	-3.92	1.51	1.54
24	s	407	CHL	CHC-C1C	3.92	1.46	1.39
37	c	619	DGD	O1G-C1A	3.92	1.44	1.33
24	Y	308	CHL	CHC-C1C	3.92	1.46	1.39
24	Y	310	CHL	CHD-C4C	3.92	1.46	1.39
24	g	310	CHL	C3A-C2A	-3.92	1.51	1.54
24	7	313	CHL	CHC-C1C	3.91	1.46	1.39
24	G	313	CHL	C3A-C2A	-3.91	1.51	1.54
24	R	608	CHL	CHC-C1C	3.91	1.46	1.39
24	g	306	CHL	CHC-C1C	3.91	1.46	1.39
24	8	304	CHL	CHC-C1C	3.91	1.46	1.39
24	N	304	CHL	C3A-C2A	-3.91	1.51	1.54
24	N	310	CHL	C3A-C2A	-3.91	1.51	1.54
24	Y	304	CHL	CHD-C4C	3.91	1.46	1.39
24	N	308	CHL	C3A-C2A	-3.91	1.51	1.54
24	q	304	CHL	CHC-C1C	3.90	1.46	1.39
24	r	303	CHL	CHC-C1C	3.90	1.46	1.39
24	R	602	CHL	CHC-C1C	3.90	1.46	1.39
24	y	313	CHL	CHC-C1C	3.90	1.46	1.39
31	c	615	8CT	C14-C13	3.90	1.55	1.43
24	Y	312	CHL	CHC-C1C	3.89	1.46	1.39
33	w	201	LMG	O8-C28	3.89	1.44	1.33
24	S	613	CHL	CHC-C1C	3.89	1.46	1.39
24	r	309	CHL	CHC-C1C	3.89	1.46	1.39
24	S	602	CHL	CHC-C1C	3.88	1.46	1.39
24	n	304	CHL	C3A-C2A	-3.88	1.51	1.54
31	C	615	8CT	C14-C13	3.88	1.55	1.43
24	2	312	CHL	CHC-C1C	3.88	1.46	1.39
24	3	310	CHL	C3A-C2A	-3.88	1.51	1.54
24	s	414	CHL	CHC-C1C	3.88	1.46	1.39
24	7	306	CHL	CHC-C1C	3.87	1.46	1.39
24	p	312	CHL	CHD-C4C	3.87	1.46	1.39
33	w	201	LMG	O7-C10	3.86	1.45	1.34
24	G	310	CHL	C3A-C2A	-3.86	1.51	1.54
24	5	309	CHL	C3A-C2A	-3.85	1.51	1.54
24	6	312	CHL	C3A-C2A	-3.85	1.51	1.54
31	c	613	8CT	C14-C13	3.85	1.55	1.43
24	Y	309	CHL	CHC-C1C	3.84	1.46	1.39
24	3	312	CHL	C3A-C2A	-3.84	1.51	1.54
24	y	310	CHL	CHD-C4C	3.84	1.46	1.39
31	C	613	8CT	C14-C13	3.83	1.55	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	l	311	CHL	CHC-C1C	3.83	1.46	1.39
24	Y	309	CHL	CHD-C4C	3.83	1.46	1.39
24	p	306	CHL	CHC-C1C	3.83	1.46	1.39
24	y	310	CHL	CHC-C1C	3.83	1.46	1.39
24	q	304	CHL	CHA-CBD	-3.83	1.47	1.51
24	y	311	CHL	CHC-C1C	3.83	1.46	1.39
24	y	305	CHL	CHD-C4C	3.82	1.46	1.39
30	d	408	LHG	O8-C23	3.82	1.44	1.33
24	5	312	CHL	CHC-C1C	3.82	1.46	1.39
24	4	311	CHL	CHC-C1C	3.82	1.46	1.39
24	S	607	CHL	CHC-C1C	3.82	1.46	1.39
24	u	312	CHL	C3A-C2A	-3.82	1.51	1.54
24	u	310	CHL	C3A-C2A	-3.82	1.51	1.54
31	t	101	8CT	C14-C13	3.81	1.55	1.43
31	v	401	8CT	C14-C13	3.81	1.55	1.43
31	t	101	8CT	C28-C29	3.81	1.40	1.32
24	p	306	CHL	CHD-C4C	3.81	1.46	1.39
24	u	311	CHL	C3A-C2A	-3.81	1.51	1.54
24	s	409	CHL	CHC-C1C	3.81	1.46	1.39
24	7	306	CHL	CHD-C4C	3.81	1.46	1.39
24	9	311	CHL	C3A-C2A	-3.81	1.51	1.54
24	4	304	CHL	C2A-C3A	-3.80	1.51	1.54
31	V	401	8CT	C14-C13	3.80	1.55	1.43
31	T	101	8CT	C14-C13	3.80	1.55	1.43
33	d	411	LMG	O7-C10	3.80	1.45	1.34
31	T	101	8CT	C28-C29	3.80	1.40	1.32
24	7	312	CHL	CHD-C4C	3.79	1.46	1.39
24	Y	317	CHL	CHC-C1C	3.78	1.46	1.39
24	8	304	CHL	CHA-CBD	-3.78	1.47	1.51
33	W	201	LMG	O8-C28	3.78	1.44	1.33
31	a	608	8CT	C14-C13	3.78	1.54	1.43
24	Y	310	CHL	CHC-C1C	3.78	1.46	1.39
33	C	618	LMG	O7-C10	3.78	1.45	1.34
33	W	201	LMG	O7-C10	3.78	1.45	1.34
31	C	614	8CT	C14-C13	3.77	1.54	1.43
24	Y	312	CHL	CHA-CBD	-3.77	1.47	1.51
37	C	619	DGD	O2G-C1B	3.77	1.44	1.34
31	B	617	8CT	C14-C13	3.77	1.54	1.43
37	c	618	DGD	O2G-C1B	3.77	1.44	1.34
24	l	308	CHL	C3A-C2A	-3.77	1.51	1.54
31	b	617	8CT	C14-C13	3.77	1.54	1.43
24	n	308	CHL	C3A-C2A	-3.77	1.51	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	2	306	CHL	CHA-CBD	-3.77	1.47	1.51
28	6	303	NEX	C7-C8	-3.76	1.25	1.31
31	c	614	8CT	C14-C13	3.76	1.54	1.43
24	Y	305	CHL	CHD-C4C	3.76	1.46	1.39
24	y	318	CHL	CHC-C1C	3.76	1.46	1.39
31	A	608	8CT	C14-C13	3.76	1.54	1.43
24	6	310	CHL	C3A-C2A	-3.75	1.51	1.54
24	8	310	CHL	CHC-C1C	3.75	1.46	1.39
28	s	401	NEX	C7-C8	-3.75	1.25	1.31
31	D	410	8CT	C14-C13	3.75	1.54	1.43
24	n	312	CHL	CHA-CBD	-3.74	1.47	1.51
28	p	304	NEX	C7-C6	-3.74	1.26	1.30
24	S	608	CHL	CHC-C1C	3.74	1.46	1.39
24	q	311	CHL	CHC-C1C	3.74	1.46	1.39
24	l	304	CHL	C2A-C3A	-3.74	1.51	1.54
33	D	401	LMG	O7-C10	3.74	1.44	1.34
24	Y	311	CHL	CHC-C1C	3.74	1.46	1.39
24	y	306	CHL	CHD-C4C	3.74	1.46	1.39
24	9	310	CHL	C3A-C2A	-3.74	1.51	1.54
24	N	309	CHL	CHC-C1C	3.74	1.46	1.39
31	d	410	8CT	C14-C13	3.74	1.54	1.43
24	y	313	CHL	CHA-CBD	-3.73	1.47	1.51
24	8	308	CHL	CHA-CBD	-3.73	1.47	1.51
33	D	411	LMG	O7-C10	3.73	1.44	1.34
31	B	617	8CT	C28-C29	3.73	1.40	1.32
24	n	317	CHL	C2A-C3A	-3.73	1.51	1.54
28	S	617	NEX	C7-C6	-3.73	1.26	1.30
28	4	303	NEX	C7-C6	-3.73	1.26	1.30
37	C	620	DGD	O2G-C1B	3.73	1.44	1.34
28	9	319	NEX	C7-C6	-3.72	1.26	1.30
24	Y	305	CHL	CHA-CBD	-3.72	1.47	1.51
28	y	304	NEX	C7-C6	-3.72	1.26	1.30
24	5	306	CHL	CHA-CBD	-3.72	1.47	1.51
31	v	401	8CT	C28-C29	3.72	1.40	1.32
24	s	403	CHL	CHD-C4C	3.72	1.46	1.39
31	x	601	8CT	C14-C13	3.72	1.54	1.43
24	S	602	CHL	CHD-C4C	3.72	1.46	1.39
28	g	304	NEX	C7-C6	-3.72	1.26	1.30
24	S	613	CHL	CHA-CBD	-3.72	1.47	1.51
28	5	304	NEX	C7-C6	-3.72	1.26	1.30
24	r	308	CHL	CHC-C1C	3.72	1.46	1.39
33	d	401	LMG	O7-C10	3.71	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	u	313	CHL	C3A-C2A	-3.71	1.51	1.54
31	X	601	8CT	C14-C13	3.71	1.54	1.43
24	4	317	CHL	C2A-C3A	-3.71	1.51	1.54
28	n	303	NEX	C7-C8	-3.71	1.25	1.31
24	u	305	CHL	C3A-C2A	-3.71	1.51	1.54
28	G	304	NEX	C7-C6	-3.71	1.26	1.30
24	n	309	CHL	CHC-C1C	3.70	1.46	1.39
24	R	607	CHL	CHC-C1C	3.70	1.46	1.39
24	y	312	CHL	CHC-C1C	3.70	1.46	1.39
28	r	301	NEX	C7-C8	-3.70	1.25	1.31
28	R	616	NEX	C7-C6	-3.70	1.26	1.30
28	3	318	NEX	C7-C8	-3.70	1.25	1.31
31	C	615	8CT	C11-C12	3.70	1.53	1.46
28	r	317	NEX	C7-C6	-3.70	1.26	1.30
24	q	308	CHL	CHA-CBD	-3.70	1.47	1.51
24	1	317	CHL	C2A-C3A	-3.69	1.51	1.54
24	p	312	CHL	CHC-C1C	3.69	1.46	1.39
24	7	313	CHL	CHA-CBD	-3.69	1.47	1.51
33	m	101	LMG	O7-C10	3.69	1.44	1.34
28	2	304	NEX	C7-C6	-3.69	1.26	1.30
31	b	617	8CT	C28-C29	3.69	1.40	1.32
24	N	317	CHL	C2A-C3A	-3.68	1.51	1.54
24	8	310	CHL	CHA-CBD	-3.68	1.47	1.51
33	i	101	LMG	O7-C10	3.68	1.44	1.34
31	B	617	8CT	C11-C12	3.68	1.53	1.46
31	V	401	8CT	C28-C29	3.68	1.40	1.32
28	1	303	NEX	C7-C6	-3.68	1.26	1.30
24	q	311	CHL	CHA-CBD	-3.67	1.47	1.51
28	u	304	NEX	C7-C6	-3.67	1.26	1.30
31	c	615	8CT	C11-C12	3.66	1.53	1.46
28	N	303	NEX	C7-C8	-3.66	1.25	1.31
24	N	312	CHL	CHA-CBD	-3.66	1.47	1.51
24	s	414	CHL	CHA-CBD	-3.66	1.47	1.51
24	7	312	CHL	CHC-C1C	3.65	1.46	1.39
31	c	615	8CT	C28-C29	3.65	1.40	1.32
24	p	310	CHL	CHA-CBD	-3.65	1.47	1.51
24	y	306	CHL	CHA-CBD	-3.65	1.47	1.51
31	d	410	8CT	C28-C29	3.65	1.40	1.32
31	D	410	8CT	C28-C29	3.65	1.40	1.32
24	p	305	CHL	CHC-C1C	3.65	1.46	1.39
24	p	313	CHL	CHA-CBD	-3.64	1.47	1.51
24	q	310	CHL	CHC-C1C	3.64	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	d	408	LHG	O7-C7	3.64	1.44	1.34
33	B	619	LMG	O7-C10	3.64	1.44	1.34
31	C	615	8CT	C28-C29	3.63	1.40	1.32
31	C	613	8CT	C11-C12	3.63	1.53	1.46
31	t	101	8CT	C30-C29	3.63	1.55	1.50
24	8	309	CHL	CHC-C1C	3.63	1.46	1.39
24	4	308	CHL	C3A-C2A	-3.63	1.51	1.54
24	7	311	CHL	CHA-CBD	-3.63	1.47	1.51
31	T	101	8CT	C30-C29	3.62	1.55	1.50
37	c	619	DGD	O2G-C1B	3.62	1.44	1.34
28	7	304	NEX	C7-C6	-3.62	1.26	1.30
31	b	617	8CT	C11-C12	3.62	1.53	1.46
24	7	310	CHL	CHA-CBD	-3.61	1.47	1.51
24	7	305	CHL	CHC-C1C	3.59	1.46	1.39
24	2	313	CHL	CHA-CBD	-3.59	1.47	1.51
25	4	316	CLA	C1D-ND	3.59	1.42	1.37
31	D	410	8CT	C01-C02	3.58	1.56	1.50
31	c	613	8CT	C11-C12	3.58	1.53	1.46
24	7	306	CHL	CHA-CBD	-3.58	1.47	1.51
24	9	312	CHL	C3A-C2A	-3.58	1.51	1.54
24	s	402	CHL	CHA-CBD	-3.58	1.47	1.51
24	p	306	CHL	CHA-CBD	-3.58	1.47	1.51
31	s	416	8CT	C30-C29	3.57	1.55	1.50
24	n	305	CHL	CHA-CBD	-3.57	1.47	1.51
24	1	312	CHL	CHA-CBD	-3.57	1.47	1.51
24	Y	304	CHL	CHC-C1C	3.57	1.46	1.39
24	3	312	CHL	CHA-CBD	-3.57	1.47	1.51
24	S	601	CHL	CHA-CBD	-3.56	1.47	1.51
24	4	312	CHL	CHA-CBD	-3.56	1.47	1.51
24	5	313	CHL	CHA-CBD	-3.56	1.47	1.51
25	N	316	CLA	C1D-ND	3.56	1.42	1.37
31	c	614	8CT	C11-C12	3.55	1.53	1.46
31	S	615	8CT	C30-C29	3.55	1.55	1.50
24	r	309	CHL	CHA-CBD	-3.55	1.47	1.51
24	6	308	CHL	C3A-C2A	-3.55	1.51	1.54
24	4	309	CHL	CHA-CBD	-3.55	1.47	1.51
24	N	308	CHL	CHA-CBD	-3.54	1.47	1.51
24	G	313	CHL	CHA-CBD	-3.54	1.47	1.51
25	4	315	CLA	C1D-ND	3.53	1.42	1.37
31	d	410	8CT	C01-C02	3.53	1.56	1.50
24	1	309	CHL	CHA-CBD	-3.53	1.47	1.51
31	C	614	8CT	C11-C12	3.53	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	u	314	CLA	C1D-ND	3.52	1.42	1.37
31	x	601	8CT	C11-C12	3.52	1.53	1.46
31	X	601	8CT	C11-C12	3.52	1.53	1.46
24	S	606	CHL	CHA-CBD	-3.52	1.47	1.51
24	5	311	CHL	CHA-CBD	-3.52	1.47	1.51
24	Y	304	CHL	CHA-CBD	-3.52	1.47	1.51
24	s	407	CHL	CHA-CBD	-3.51	1.47	1.51
24	y	305	CHL	CHC-C1C	3.51	1.46	1.39
25	R	613	CLA	C1D-ND	3.51	1.42	1.37
25	a	610	CLA	C1D-ND	3.51	1.42	1.37
31	c	614	8CT	C07-C02	-3.50	1.44	1.51
24	2	311	CHL	CHA-CBD	-3.50	1.47	1.51
25	r	314	CLA	C1D-ND	3.50	1.42	1.37
24	p	311	CHL	CHA-CBD	-3.50	1.47	1.51
24	u	309	CHL	C3A-C2A	-3.50	1.51	1.54
31	t	101	8CT	C35-C30	3.50	1.66	1.56
24	3	308	CHL	C3A-C2A	-3.50	1.51	1.54
25	9	314	CLA	C1D-ND	3.50	1.42	1.37
24	Y	317	CHL	CHA-CBD	-3.50	1.47	1.51
24	q	309	CHL	CHA-CBD	-3.49	1.47	1.51
24	S	608	CHL	CHA-CBD	-3.49	1.47	1.51
24	u	313	CHL	CHA-CBD	-3.49	1.47	1.51
25	1	316	CLA	C1D-ND	3.49	1.42	1.37
24	u	306	CHL	CHA-CBD	-3.49	1.47	1.51
25	n	316	CLA	C1D-ND	3.49	1.42	1.37
25	A	610	CLA	C1D-ND	3.49	1.42	1.37
31	d	410	8CT	C11-C12	3.49	1.53	1.46
24	p	309	CHL	C3A-C2A	-3.48	1.51	1.54
31	D	410	8CT	C11-C12	3.48	1.53	1.46
24	7	309	CHL	C3A-C2A	-3.48	1.51	1.54
25	3	314	CLA	C1D-ND	3.48	1.42	1.37
25	u	316	CLA	C1D-ND	3.48	1.42	1.37
31	T	101	8CT	C35-C30	3.48	1.66	1.56
25	u	315	CLA	C1D-ND	3.48	1.42	1.37
24	y	305	CHL	CHA-CBD	-3.48	1.47	1.51
25	6	314	CLA	C1D-ND	3.47	1.42	1.37
24	3	305	CHL	CHA-CBD	-3.47	1.47	1.51
24	S	602	CHL	CHA-CBD	-3.47	1.47	1.51
24	s	409	CHL	CHA-CBD	-3.47	1.47	1.51
25	1	315	CLA	C1D-ND	3.47	1.42	1.37
24	Y	319	CHL	CHA-CBD	-3.47	1.47	1.51
25	u	307	CLA	C1D-ND	3.47	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	315	CLA	C1D-ND	3.46	1.42	1.37
25	9	315	CLA	C1D-ND	3.46	1.42	1.37
24	q	310	CHL	CHA-CBD	-3.46	1.47	1.51
28	7	304	NEX	C7-C8	-3.46	1.26	1.31
25	4	314	CLA	C1D-ND	3.46	1.42	1.37
25	G	307	CLA	C1D-ND	3.46	1.42	1.37
24	g	313	CHL	CHA-CBD	-3.46	1.47	1.51
31	t	101	8CT	C11-C12	3.46	1.53	1.46
25	1	314	CLA	C1D-ND	3.46	1.42	1.37
24	6	312	CHL	CHA-CBD	-3.46	1.47	1.51
31	v	401	8CT	C11-C12	3.46	1.53	1.46
28	r	317	NEX	C7-C8	-3.45	1.26	1.31
25	g	307	CLA	C1D-ND	3.45	1.42	1.37
25	4	307	CLA	C1D-ND	3.45	1.42	1.37
25	9	313	CLA	C1D-ND	3.45	1.42	1.37
25	9	307	CLA	C1D-ND	3.45	1.42	1.37
25	G	315	CLA	C1D-ND	3.45	1.42	1.37
25	6	306	CLA	C1D-ND	3.44	1.42	1.37
31	V	401	8CT	C11-C12	3.44	1.53	1.46
31	a	608	8CT	C11-C12	3.44	1.53	1.46
31	A	608	8CT	C28-C29	3.44	1.40	1.32
31	T	101	8CT	C11-C12	3.44	1.53	1.46
25	6	313	CLA	C1D-ND	3.43	1.42	1.37
25	3	307	CLA	C1D-ND	3.43	1.42	1.37
24	y	311	CHL	CHA-CBD	-3.43	1.47	1.51
31	C	613	8CT	C28-C29	3.43	1.40	1.32
24	R	608	CHL	CHA-CBD	-3.43	1.47	1.51
25	n	314	CLA	C1D-ND	3.43	1.42	1.37
24	9	308	CHL	C3A-C2A	-3.43	1.51	1.54
28	y	304	NEX	C7-C8	-3.42	1.26	1.31
25	g	314	CLA	C1D-ND	3.42	1.42	1.37
24	s	403	CHL	CHA-CBD	-3.42	1.47	1.51
25	6	307	CLA	C1D-ND	3.42	1.42	1.37
28	G	304	NEX	C7-C8	-3.42	1.26	1.31
28	1	303	NEX	C7-C8	-3.42	1.26	1.31
25	6	315	CLA	C1D-ND	3.42	1.42	1.37
24	y	318	CHL	CHA-CBD	-3.42	1.47	1.51
25	6	316	CLA	C1D-ND	3.41	1.42	1.37
28	g	304	NEX	C7-C8	-3.41	1.26	1.31
35	D	403	PHO	C1D-C2D	3.41	1.43	1.39
31	C	614	8CT	C28-C29	3.41	1.40	1.32
25	3	306	CLA	C1D-ND	3.41	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	R	616	NEX	C7-C8	-3.41	1.26	1.31
24	Y	310	CHL	CHA-CBD	-3.41	1.47	1.51
25	r	312	CLA	C1D-ND	3.41	1.42	1.37
28	4	303	NEX	C7-C8	-3.41	1.26	1.31
31	c	614	8CT	C28-C29	3.41	1.40	1.32
25	G	314	CLA	C1D-ND	3.41	1.42	1.37
25	4	306	CLA	C1D-ND	3.41	1.42	1.37
24	N	305	CHL	CHA-CBD	-3.41	1.47	1.51
31	X	601	8CT	C28-C29	3.41	1.40	1.32
24	8	309	CHL	CHA-CBD	-3.41	1.47	1.51
31	C	614	8CT	C07-C02	-3.41	1.44	1.51
25	9	306	CLA	C1D-ND	3.41	1.42	1.37
31	c	613	8CT	C28-C29	3.41	1.40	1.32
24	9	312	CHL	CHA-CBD	-3.40	1.47	1.51
25	4	313	CLA	C1D-ND	3.40	1.42	1.37
25	2	308	CLA	C1D-ND	3.40	1.42	1.37
25	5	307	CLA	C1D-ND	3.40	1.42	1.37
31	x	601	8CT	C28-C29	3.40	1.40	1.32
24	6	305	CHL	CHA-CBD	-3.40	1.47	1.51
25	N	314	CLA	C1D-ND	3.40	1.42	1.37
25	g	315	CLA	C1D-ND	3.40	1.42	1.37
35	d	403	PHO	C1D-C2D	3.39	1.43	1.39
31	A	608	8CT	C11-C12	3.39	1.53	1.46
25	u	317	CLA	C1D-ND	3.39	1.42	1.37
24	Y	311	CHL	CHA-CBD	-3.39	1.47	1.51
24	y	312	CHL	CHA-CBD	-3.39	1.47	1.51
24	g	309	CHL	C3A-C2A	-3.39	1.51	1.54
31	a	608	8CT	C28-C29	3.39	1.40	1.32
25	n	306	CLA	C1D-ND	3.38	1.42	1.37
25	R	611	CLA	C1D-ND	3.38	1.42	1.37
25	q	315	CLA	C1D-ND	3.38	1.42	1.37
25	r	313	CLA	C1D-ND	3.38	1.42	1.37
25	3	313	CLA	C1D-ND	3.38	1.42	1.37
25	r	314	CLA	C4B-NB	3.38	1.42	1.37
24	3	309	CHL	CHA-CBD	-3.38	1.47	1.51
25	G	308	CLA	C1D-ND	3.38	1.42	1.37
25	N	306	CLA	C1D-ND	3.38	1.42	1.37
25	8	314	CLA	C1D-ND	3.38	1.42	1.37
25	9	316	CLA	C1D-ND	3.37	1.42	1.37
25	u	308	CLA	C1D-ND	3.37	1.42	1.37
31	A	608	8CT	C01-C02	3.37	1.56	1.50
25	1	306	CLA	C1D-ND	3.37	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	g	306	CHL	CHA-CBD	-3.37	1.47	1.51
25	p	308	CLA	C1D-ND	3.37	1.42	1.37
25	l	307	CLA	C1D-ND	3.37	1.42	1.37
24	G	309	CHL	C3A-C2A	-3.37	1.51	1.54
24	R	606	CHL	CHA-CBD	-3.37	1.47	1.51
25	R	612	CLA	C1D-ND	3.36	1.42	1.37
25	2	317	CLA	C1D-ND	3.36	1.42	1.37
25	r	311	CLA	C1D-ND	3.36	1.42	1.37
24	r	306	CHL	CHA-CBD	-3.36	1.47	1.51
25	3	316	CLA	C1D-ND	3.36	1.42	1.37
28	u	304	NEX	C7-C8	-3.36	1.26	1.31
28	p	304	NEX	C7-C8	-3.35	1.26	1.31
28	2	304	NEX	C7-C8	-3.35	1.26	1.31
25	r	310	CLA	C1D-ND	3.35	1.42	1.37
25	1	313	CLA	C1D-ND	3.35	1.42	1.37
25	8	312	CLA	C1D-ND	3.35	1.42	1.37
25	g	317	CLA	C1D-ND	3.35	1.42	1.37
25	5	308	CLA	C1D-ND	3.35	1.42	1.37
25	R	613	CLA	C4B-NB	3.35	1.42	1.37
25	g	316	CLA	C1D-ND	3.34	1.42	1.37
25	g	308	CLA	C1D-ND	3.34	1.42	1.37
31	a	608	8CT	C01-C02	3.34	1.56	1.50
23	f	201	HEM	FE-ND	3.34	2.05	1.94
31	s	415	8CT	C01-C02	3.33	1.56	1.50
24	S	605	CHL	CHA-CBD	-3.33	1.47	1.51
35	a	606	PHO	C1D-C2D	3.33	1.43	1.39
24	R	605	CHL	CHA-CBD	-3.33	1.47	1.51
25	S	603	CLA	C1D-ND	3.33	1.42	1.37
24	9	305	CHL	CHA-CBD	-3.33	1.47	1.51
31	v	401	8CT	C01-C02	3.33	1.56	1.50
28	S	617	NEX	C7-C8	-3.33	1.26	1.31
25	G	317	CLA	C1D-ND	3.33	1.42	1.37
25	n	315	CLA	C1D-ND	3.33	1.42	1.37
25	q	313	CLA	C1D-ND	3.32	1.42	1.37
25	N	315	CLA	C1D-ND	3.32	1.42	1.37
28	5	304	NEX	C7-C8	-3.32	1.26	1.31
24	p	305	CHL	CHA-CBD	-3.32	1.47	1.51
24	G	306	CHL	CHA-CBD	-3.32	1.47	1.51
35	A	606	PHO	C1D-C2D	3.32	1.43	1.39
30	D	408	LHG	C26-C25	-3.31	1.35	1.51
24	y	310	CHL	CHA-CBD	-3.31	1.47	1.51
25	r	304	CLA	C1D-ND	3.31	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	D	407	LHG	C26-C25	-3.31	1.35	1.51
28	9	319	NEX	C7-C8	-3.31	1.26	1.31
24	6	310	CHL	CHA-CBD	-3.31	1.47	1.51
30	d	407	LHG	C26-C25	-3.31	1.35	1.51
25	2	307	CLA	C1D-ND	3.31	1.42	1.37
24	s	406	CHL	CHA-CBD	-3.31	1.47	1.51
30	Y	318	LHG	C26-C25	-3.31	1.35	1.51
31	X	601	8CT	C01-C02	3.30	1.56	1.50
25	R	610	CLA	C1D-ND	3.30	1.42	1.37
25	r	305	CLA	C1D-ND	3.30	1.42	1.37
25	5	316	CLA	C1D-ND	3.30	1.42	1.37
25	N	307	CLA	C1D-ND	3.30	1.42	1.37
25	5	315	CLA	C1D-ND	3.30	1.42	1.37
25	7	308	CLA	C1D-ND	3.30	1.42	1.37
25	R	604	CLA	C1D-ND	3.30	1.42	1.37
35	d	403	PHO	C4D-CHA	3.30	1.44	1.39
24	r	307	CHL	CHA-CBD	-3.30	1.47	1.51
24	7	305	CHL	CHA-CBD	-3.30	1.47	1.51
25	R	609	CLA	C1D-ND	3.30	1.42	1.37
25	R	603	CLA	C1D-ND	3.30	1.42	1.37
24	3	317	CHL	CHA-CBD	-3.30	1.47	1.51
25	G	316	CLA	C1D-ND	3.29	1.42	1.37
30	A	601	LHG	C26-C25	-3.29	1.35	1.51
30	y	319	LHG	C26-C25	-3.29	1.35	1.51
30	a	601	LHG	C26-C25	-3.29	1.35	1.51
24	n	310	CHL	CHA-CBD	-3.29	1.47	1.51
25	q	314	CLA	C1D-ND	3.29	1.42	1.37
31	x	601	8CT	C01-C02	3.29	1.56	1.50
24	3	310	CHL	CHA-CBD	-3.29	1.47	1.51
30	a	612	LHG	C26-C25	-3.28	1.35	1.51
25	2	316	CLA	C1D-ND	3.28	1.42	1.37
25	5	317	CLA	C1D-ND	3.28	1.42	1.37
24	6	304	CHL	CHA-CBD	-3.28	1.47	1.51
25	B	604	CLA	C1D-ND	3.28	1.42	1.37
25	n	313	CLA	C1D-ND	3.28	1.42	1.37
25	2	314	CLA	C1D-ND	3.28	1.42	1.37
24	G	311	CHL	CHA-CBD	-3.28	1.47	1.51
31	V	401	8CT	C01-C02	3.27	1.56	1.50
30	A	612	LHG	C26-C25	-3.27	1.35	1.51
25	5	314	CLA	C1D-ND	3.27	1.42	1.37
25	8	313	CLA	C1D-ND	3.27	1.42	1.37
31	C	615	8CT	C01-C02	3.27	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	S	615	8CT	C10-C03	3.27	1.56	1.45
31	C	613	8CT	C07-C02	-3.27	1.44	1.51
31	s	416	8CT	C10-C03	3.27	1.56	1.45
31	s	415	8CT	C18-C17	3.27	1.53	1.43
25	p	314	CLA	C1D-ND	3.27	1.42	1.37
24	3	304	CHL	CHA-CBD	-3.27	1.47	1.51
24	N	309	CHL	CHA-CBD	-3.26	1.47	1.51
35	D	403	PHO	C4D-CHA	3.26	1.44	1.39
24	4	311	CHL	CHA-CBD	-3.26	1.47	1.51
25	N	313	CLA	C1D-ND	3.26	1.42	1.37
31	c	613	8CT	C07-C02	-3.26	1.44	1.51
24	6	309	CHL	CHA-CBD	-3.26	1.47	1.51
25	p	317	CLA	C1D-ND	3.26	1.42	1.37
25	S	609	CLA	C1D-ND	3.25	1.42	1.37
25	7	314	CLA	C1D-ND	3.25	1.42	1.37
31	S	614	8CT	C18-C17	3.25	1.53	1.43
23	E	201	HEM	FE-ND	3.25	2.04	1.94
30	7	319	LHG	C26-C25	-3.25	1.35	1.51
24	8	307	CHL	CHA-CBD	-3.25	1.47	1.51
25	2	315	CLA	C1D-ND	3.25	1.42	1.37
30	C	617	LHG	C26-C25	-3.25	1.35	1.51
24	4	310	CHL	CHA-CBD	-3.25	1.47	1.51
25	B	601	CLA	C1D-ND	3.25	1.42	1.37
24	6	317	CHL	CHA-CBD	-3.25	1.47	1.51
24	1	311	CHL	CHA-CBD	-3.25	1.47	1.51
31	S	614	8CT	C01-C02	3.25	1.56	1.50
25	s	404	CLA	C1D-ND	3.24	1.42	1.37
30	p	319	LHG	C26-C25	-3.24	1.35	1.51
30	c	617	LHG	C26-C25	-3.24	1.35	1.51
30	5	319	LHG	C26-C25	-3.24	1.35	1.51
25	p	315	CLA	C1D-ND	3.24	1.42	1.37
30	g	319	LHG	C26-C25	-3.23	1.35	1.51
25	7	315	CLA	C1D-ND	3.23	1.42	1.37
25	7	317	CLA	C1D-ND	3.23	1.42	1.37
30	2	319	LHG	C26-C25	-3.23	1.35	1.51
25	b	601	CLA	C1D-ND	3.23	1.42	1.37
31	c	615	8CT	C01-C02	3.23	1.56	1.50
30	n	318	LHG	C26-C25	-3.23	1.35	1.51
24	S	607	CHL	CHA-CBD	-3.22	1.47	1.51
30	G	319	LHG	C26-C25	-3.22	1.35	1.51
24	g	310	CHL	CHA-CBD	-3.22	1.47	1.51
25	s	410	CLA	C1D-ND	3.22	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	u	311	CHL	CHA-CBD	-3.22	1.47	1.51
25	n	307	CLA	C1D-ND	3.21	1.42	1.37
25	b	604	CLA	C1D-ND	3.21	1.42	1.37
30	N	318	LHG	C26-C25	-3.21	1.35	1.51
31	B	617	8CT	C01-C02	3.21	1.56	1.50
31	s	415	8CT	C10-C03	3.21	1.56	1.45
31	T	101	8CT	C01-C02	3.21	1.56	1.50
30	9	318	LHG	C26-C25	-3.21	1.35	1.51
24	G	310	CHL	CHA-CBD	-3.20	1.47	1.51
31	b	617	8CT	C01-C02	3.20	1.56	1.50
24	n	309	CHL	CHA-CBD	-3.20	1.47	1.51
30	1	318	LHG	C26-C25	-3.20	1.35	1.51
24	g	311	CHL	CHA-CBD	-3.20	1.47	1.51
25	7	316	CLA	C1D-ND	3.20	1.42	1.37
31	b	617	8CT	C18-C17	3.20	1.53	1.43
31	S	614	8CT	C10-C03	3.19	1.56	1.45
31	c	615	8CT	C18-C17	3.19	1.53	1.43
30	4	318	LHG	C26-C25	-3.19	1.35	1.51
24	9	310	CHL	CHA-CBD	-3.19	1.47	1.51
31	c	615	8CT	C35-C30	3.19	1.65	1.56
24	N	310	CHL	CHA-CBD	-3.19	1.47	1.51
25	B	607	CLA	C1D-ND	3.19	1.42	1.37
24	q	307	CHL	CHA-CBD	-3.19	1.47	1.51
25	7	307	CLA	C1D-ND	3.19	1.42	1.37
25	p	316	CLA	C1D-ND	3.19	1.42	1.37
25	S	604	CLA	C1D-ND	3.18	1.42	1.37
25	s	417	CLA	C1D-ND	3.18	1.42	1.37
24	Y	309	CHL	CHA-CBD	-3.18	1.47	1.51
25	q	306	CLA	C1D-ND	3.18	1.42	1.37
25	C	611	CLA	C1D-ND	3.18	1.42	1.37
24	q	303	CHL	CHA-CBD	-3.18	1.47	1.51
31	t	101	8CT	C01-C02	3.17	1.56	1.50
25	B	609	CLA	C1D-ND	3.17	1.42	1.37
25	c	611	CLA	C1D-ND	3.17	1.42	1.37
25	Y	307	CLA	C1D-ND	3.17	1.42	1.37
31	S	615	8CT	C18-C17	3.17	1.53	1.43
25	y	307	CLA	C1D-ND	3.17	1.42	1.37
25	q	312	CLA	C1D-ND	3.17	1.42	1.37
25	Y	306	CLA	C1D-ND	3.17	1.42	1.37
24	8	303	CHL	CHA-CBD	-3.17	1.48	1.51
25	s	405	CLA	C1D-ND	3.17	1.42	1.37
31	C	615	8CT	C35-C30	3.17	1.65	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	S	616	CLA	C1D-ND	3.17	1.42	1.37
25	B	608	CLA	C1D-ND	3.17	1.42	1.37
25	8	306	CLA	C1D-ND	3.16	1.42	1.37
31	C	615	8CT	C18-C17	3.16	1.53	1.43
31	T	101	8CT	C07-C02	-3.16	1.45	1.51
23	f	201	HEM	FE-NB	3.16	2.04	1.94
25	b	607	CLA	C1D-ND	3.16	1.42	1.37
24	u	310	CHL	CHA-CBD	-3.15	1.48	1.51
31	B	617	8CT	C18-C17	3.15	1.52	1.43
25	8	305	CLA	C1D-ND	3.15	1.42	1.37
31	S	615	8CT	C35-C30	3.14	1.65	1.56
25	q	305	CLA	C1D-ND	3.14	1.42	1.37
31	s	416	8CT	C18-C17	3.14	1.52	1.43
25	B	616	CLA	C1D-ND	3.14	1.42	1.37
24	2	310	CHL	CHA-CBD	-3.14	1.48	1.51
25	p	307	CLA	C1D-ND	3.14	1.42	1.37
24	2	312	CHL	CHA-CBD	-3.14	1.48	1.51
31	v	401	8CT	C35-C30	3.14	1.65	1.56
25	y	308	CLA	C1D-ND	3.14	1.42	1.37
31	s	416	8CT	C35-C30	3.14	1.65	1.56
24	1	304	CHL	CHA-CBD	-3.13	1.48	1.51
25	b	616	CLA	C1D-ND	3.13	1.42	1.37
25	s	412	CLA	C1D-ND	3.13	1.42	1.37
31	T	101	8CT	C18-C17	3.13	1.52	1.43
25	a	607	CLA	C1D-ND	3.13	1.42	1.37
25	9	316	CLA	C4B-NB	3.13	1.42	1.37
25	b	608	CLA	C1D-ND	3.13	1.42	1.37
24	R	601	CHL	CHA-CBD	-3.12	1.48	1.51
31	t	101	8CT	C07-C02	-3.12	1.45	1.51
25	S	610	CLA	C1D-ND	3.12	1.42	1.37
35	a	606	PHO	C4D-CHA	3.12	1.44	1.39
25	8	311	CLA	C1D-ND	3.12	1.42	1.37
31	t	101	8CT	C18-C17	3.12	1.52	1.43
25	u	317	CLA	C4B-NB	3.12	1.42	1.37
25	S	612	CLA	C1D-ND	3.12	1.42	1.37
31	V	401	8CT	C35-C30	3.12	1.65	1.56
24	4	304	CHL	CHA-CBD	-3.12	1.48	1.51
31	V	401	8CT	C18-C17	3.12	1.52	1.43
35	A	606	PHO	C4D-CHA	3.11	1.44	1.39
25	d	405	CLA	C1D-ND	3.11	1.41	1.37
31	d	410	8CT	C35-C30	3.11	1.65	1.56
31	v	401	8CT	C18-C17	3.11	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	s	408	CHL	CHA-CBD	-3.11	1.48	1.51
25	b	609	CLA	C1D-ND	3.11	1.41	1.37
25	R	612	CLA	C4B-NB	3.11	1.41	1.37
24	R	602	CHL	CHA-CBD	-3.11	1.48	1.51
24	l	310	CHL	CHA-CBD	-3.11	1.48	1.51
25	9	314	CLA	C4B-NB	3.10	1.41	1.37
25	Y	313	CLA	C1D-ND	3.10	1.41	1.37
24	5	310	CHL	CHA-CBD	-3.10	1.48	1.51
31	C	615	8CT	C10-C03	3.10	1.55	1.45
25	B	613	CLA	C1D-ND	3.10	1.41	1.37
31	C	613	8CT	C18-C17	3.10	1.52	1.43
31	A	608	8CT	C35-C30	3.10	1.65	1.56
31	D	410	8CT	C35-C30	3.10	1.65	1.56
24	r	302	CHL	CHA-CBD	-3.10	1.48	1.51
31	C	613	8CT	C01-C02	3.10	1.55	1.50
25	C	601	CLA	C1D-ND	3.10	1.41	1.37
25	s	411	CLA	C1D-ND	3.10	1.41	1.37
24	9	309	CHL	CHA-CBD	-3.10	1.48	1.51
31	a	608	8CT	C35-C30	3.09	1.65	1.56
25	l	315	CLA	C4B-NB	3.09	1.41	1.37
25	y	317	CLA	C1D-ND	3.09	1.41	1.37
25	A	603	CLA	C1D-ND	3.09	1.41	1.37
23	f	201	HEM	CAB-C3B	3.09	1.55	1.47
25	a	610	CLA	C4B-NB	3.09	1.41	1.37
25	B	615	CLA	C1D-ND	3.09	1.41	1.37
25	A	607	CLA	C1D-ND	3.08	1.41	1.37
31	c	615	8CT	C10-C03	3.08	1.55	1.45
25	b	605	CLA	C1D-ND	3.08	1.41	1.37
31	c	613	8CT	C18-C17	3.07	1.52	1.43
39	d	406	PL9	C53-C6	-3.07	1.44	1.50
31	c	614	8CT	C01-C02	3.07	1.55	1.50
25	l	316	CLA	C4B-NB	3.07	1.41	1.37
24	r	303	CHL	CHA-CBD	-3.07	1.48	1.51
25	4	314	CLA	C4B-NB	3.07	1.41	1.37
25	S	611	CLA	C1D-ND	3.07	1.41	1.37
31	S	614	8CT	C35-C30	3.07	1.64	1.56
25	l	314	CLA	C4B-NB	3.07	1.41	1.37
24	5	312	CHL	CHA-CBD	-3.06	1.48	1.51
25	b	602	CLA	C1D-ND	3.06	1.41	1.37
31	A	608	8CT	C18-C17	3.06	1.52	1.43
31	X	601	8CT	C07-C02	-3.06	1.45	1.51
31	d	410	8CT	C18-C17	3.06	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Y	316	CLA	C1D-ND	3.06	1.41	1.37
31	c	613	8CT	C01-C02	3.06	1.55	1.50
25	D	405	CLA	C1D-ND	3.06	1.41	1.37
32	a	609	SQD	O48-C23	3.06	1.42	1.33
31	S	615	8CT	C01-C02	3.05	1.55	1.50
24	n	308	CHL	CHA-CBD	-3.05	1.48	1.51
32	b	618	SQD	O48-C23	3.05	1.42	1.33
25	u	315	CLA	C4B-NB	3.05	1.41	1.37
32	A	609	SQD	O48-C23	3.05	1.42	1.33
31	s	415	8CT	C35-C30	3.05	1.64	1.56
31	B	617	8CT	C10-C03	3.05	1.55	1.45
31	x	601	8CT	C07-C02	-3.05	1.45	1.51
25	y	314	CLA	C1D-ND	3.05	1.41	1.37
31	a	608	8CT	C18-C17	3.04	1.52	1.43
32	B	618	SQD	O48-C23	3.04	1.42	1.33
25	4	316	CLA	C4B-NB	3.04	1.41	1.37
25	b	613	CLA	C1D-ND	3.04	1.41	1.37
24	l	305	CHL	CHA-CBD	-3.04	1.48	1.51
31	b	617	8CT	C10-C03	3.04	1.55	1.45
31	D	410	8CT	C18-C17	3.04	1.52	1.43
25	G	307	CLA	C4B-NB	3.04	1.41	1.37
31	c	614	8CT	C18-C17	3.04	1.52	1.43
31	X	601	8CT	C18-C17	3.04	1.52	1.43
25	u	307	CLA	C4B-NB	3.04	1.41	1.37
31	d	410	8CT	C10-C03	3.04	1.55	1.45
25	c	608	CLA	C1D-ND	3.04	1.41	1.37
25	A	610	CLA	C4B-NB	3.03	1.41	1.37
23	E	201	HEM	CAB-C3B	3.03	1.55	1.47
25	a	603	CLA	C1D-ND	3.03	1.41	1.37
25	s	413	CLA	C1D-ND	3.03	1.41	1.37
25	b	615	CLA	C1D-ND	3.03	1.41	1.37
25	c	601	CLA	C1D-ND	3.03	1.41	1.37
23	E	201	HEM	CAC-C3C	3.03	1.55	1.47
25	y	316	CLA	C1D-ND	3.03	1.41	1.37
25	c	609	CLA	C1D-ND	3.03	1.41	1.37
25	Y	314	CLA	C1D-ND	3.03	1.41	1.37
25	c	602	CLA	C1D-ND	3.03	1.41	1.37
31	s	416	8CT	C01-C02	3.03	1.55	1.50
24	g	305	CHL	CHA-CBD	-3.02	1.48	1.51
31	v	401	8CT	C07-C02	-3.02	1.45	1.51
31	C	614	8CT	C01-C02	3.02	1.55	1.50
25	C	608	CLA	C1D-ND	3.02	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	612	CLA	C1D-ND	3.02	1.41	1.37
24	2	305	CHL	CHA-CBD	-3.02	1.48	1.51
25	B	605	CLA	C1D-ND	3.02	1.41	1.37
25	C	603	CLA	C1D-ND	3.02	1.41	1.37
25	a	605	CLA	C1D-ND	3.02	1.41	1.37
25	c	606	CLA	C1D-ND	3.02	1.41	1.37
31	x	601	8CT	C18-C17	3.01	1.52	1.43
31	x	601	8CT	C35-C30	3.01	1.64	1.56
24	r	308	CHL	CHA-CBD	-3.01	1.48	1.51
25	3	316	CLA	C4B-NB	3.01	1.41	1.37
25	u	314	CLA	C4B-NB	3.01	1.41	1.37
25	9	315	CLA	C4B-NB	3.01	1.41	1.37
25	Y	315	CLA	C1D-ND	3.01	1.41	1.37
23	f	201	HEM	CAC-C3C	3.01	1.55	1.47
25	6	307	CLA	C4B-NB	3.01	1.41	1.37
31	C	614	8CT	C18-C17	3.01	1.52	1.43
25	B	602	CLA	C1D-ND	3.01	1.41	1.37
31	D	410	8CT	C10-C03	3.00	1.55	1.45
39	D	406	PL9	C53-C6	-3.00	1.44	1.50
25	n	306	CLA	C4B-NB	3.00	1.41	1.37
32	D	409	SQD	O48-C23	3.00	1.42	1.33
31	C	613	8CT	C10-C03	3.00	1.55	1.45
31	c	613	8CT	C10-C03	3.00	1.55	1.45
25	s	411	CLA	O1A-CGA	3.00	1.37	1.20
25	n	314	CLA	C4B-NB	3.00	1.41	1.37
32	d	409	SQD	O48-C23	3.00	1.42	1.33
25	3	313	CLA	C4B-NB	3.00	1.41	1.37
25	7	317	CLA	C4B-NB	3.00	1.41	1.37
25	b	614	CLA	C1D-ND	2.99	1.41	1.37
24	G	305	CHL	CHA-CBD	-2.99	1.48	1.51
25	6	316	CLA	C4B-NB	2.99	1.41	1.37
24	7	318	CHL	CHA-CBD	-2.99	1.48	1.51
25	c	612	CLA	C1D-ND	2.99	1.41	1.37
25	6	315	CLA	C4B-NB	2.99	1.41	1.37
25	g	307	CLA	C4B-NB	2.99	1.41	1.37
31	X	601	8CT	C35-C30	2.99	1.64	1.56
25	C	606	CLA	C1D-ND	2.98	1.41	1.37
25	n	307	CLA	C4B-NB	2.98	1.41	1.37
31	B	617	8CT	C35-C30	2.98	1.64	1.56
25	9	313	CLA	C4B-NB	2.98	1.41	1.37
31	A	608	8CT	C07-C02	-2.98	1.45	1.51
25	9	307	CLA	C4B-NB	2.98	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	N	307	CLA	C4B-NB	2.98	1.41	1.37
25	C	604	CLA	C1D-ND	2.98	1.41	1.37
25	4	315	CLA	C4B-NB	2.98	1.41	1.37
24	g	318	CHL	CHA-CBD	-2.98	1.48	1.51
24	G	312	CHL	CHA-CBD	-2.97	1.48	1.51
25	y	315	CLA	C1D-ND	2.97	1.41	1.37
24	n	311	CHL	CHA-CBD	-2.97	1.48	1.51
31	a	608	8CT	C07-C02	-2.97	1.45	1.51
24	2	318	CHL	CHA-CBD	-2.97	1.48	1.51
24	5	305	CHL	CHA-CBD	-2.97	1.48	1.51
25	c	603	CLA	C1D-ND	2.97	1.41	1.37
25	u	308	CLA	C4B-NB	2.97	1.41	1.37
24	G	318	CHL	CHA-CBD	-2.97	1.48	1.51
25	C	609	CLA	C1D-ND	2.96	1.41	1.37
25	C	612	CLA	C1D-ND	2.96	1.41	1.37
25	4	313	CLA	C4B-NB	2.96	1.41	1.37
31	T	101	8CT	C10-C03	2.96	1.55	1.45
25	c	604	CLA	C1D-ND	2.96	1.41	1.37
25	g	308	CLA	C4B-NB	2.96	1.41	1.37
24	4	305	CHL	CHA-CBD	-2.96	1.48	1.51
25	N	316	CLA	C4B-NB	2.96	1.41	1.37
24	N	311	CHL	CHA-CBD	-2.96	1.48	1.51
25	3	314	CLA	C4B-NB	2.96	1.41	1.37
25	n	316	CLA	C4B-NB	2.96	1.41	1.37
25	b	610	CLA	C1D-ND	2.96	1.41	1.37
25	G	316	CLA	C4B-NB	2.96	1.41	1.37
25	C	602	CLA	C1D-ND	2.96	1.41	1.37
25	u	316	CLA	C4B-NB	2.96	1.41	1.37
31	t	101	8CT	C10-C03	2.96	1.55	1.45
25	A	605	CLA	C1D-ND	2.96	1.41	1.37
25	r	313	CLA	C4B-NB	2.96	1.41	1.37
25	9	306	CLA	C4B-NB	2.95	1.41	1.37
31	V	401	8CT	C07-C02	-2.95	1.45	1.51
31	A	608	8CT	C10-C03	2.95	1.55	1.45
24	5	318	CHL	CHA-CBD	-2.95	1.48	1.51
31	V	401	8CT	C10-C03	2.94	1.55	1.45
25	3	315	CLA	C4B-NB	2.94	1.41	1.37
25	p	317	CLA	C4B-NB	2.94	1.41	1.37
31	X	601	8CT	C10-C03	2.94	1.55	1.45
25	A	604	CLA	C1D-ND	2.94	1.41	1.37
25	b	603	CLA	C1D-ND	2.94	1.41	1.37
25	n	313	CLA	C4B-NB	2.94	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	R	607	CHL	CHA-CBD	-2.94	1.48	1.51
24	g	312	CHL	CHA-CBD	-2.94	1.48	1.51
25	B	612	CLA	C1D-ND	2.94	1.41	1.37
25	6	313	CLA	C4B-NB	2.94	1.41	1.37
31	a	608	8CT	C10-C03	2.94	1.55	1.45
25	B	610	CLA	C1D-ND	2.94	1.41	1.37
25	N	314	CLA	C4B-NB	2.94	1.41	1.37
24	2	309	CHL	CHA-CBD	-2.93	1.48	1.51
25	c	607	CLA	C1D-ND	2.93	1.41	1.37
25	G	308	CLA	C4B-NB	2.93	1.41	1.37
25	B	614	CLA	C1D-ND	2.93	1.41	1.37
25	4	306	CLA	C4B-NB	2.93	1.41	1.37
31	s	415	8CT	C07-C02	-2.93	1.45	1.51
25	a	604	CLA	C1D-ND	2.93	1.41	1.37
31	b	617	8CT	C35-C30	2.93	1.64	1.56
25	1	313	CLA	C4B-NB	2.93	1.41	1.37
25	N	315	CLA	C4B-NB	2.93	1.41	1.37
25	B	611	CLA	C1D-ND	2.93	1.41	1.37
25	n	315	CLA	C4B-NB	2.93	1.41	1.37
35	a	606	PHO	CMC-C2C	-2.92	1.46	1.50
24	Y	308	CHL	CHA-CBD	-2.92	1.48	1.51
25	N	306	CLA	C4B-NB	2.92	1.41	1.37
25	c	610	CLA	C1D-ND	2.92	1.41	1.37
31	S	614	8CT	C07-C02	-2.92	1.45	1.51
31	v	401	8CT	C10-C03	2.92	1.55	1.45
25	1	307	CLA	C4B-NB	2.92	1.41	1.37
25	4	307	CLA	C4B-NB	2.92	1.41	1.37
24	p	318	CHL	CHA-CBD	-2.91	1.48	1.51
31	c	614	8CT	C10-C03	2.91	1.55	1.45
25	6	314	CLA	C4B-NB	2.91	1.41	1.37
31	x	601	8CT	C10-C03	2.91	1.55	1.45
24	5	309	CHL	CHA-CBD	-2.91	1.48	1.51
24	y	309	CHL	CHA-CBD	-2.91	1.48	1.51
25	N	313	CLA	C4B-NB	2.91	1.41	1.37
25	G	315	CLA	C4B-NB	2.90	1.41	1.37
25	C	616	CLA	C1D-ND	2.90	1.41	1.37
25	b	611	CLA	C1D-ND	2.90	1.41	1.37
31	C	615	8CT	C07-C02	-2.90	1.45	1.51
31	C	614	8CT	C10-C03	2.90	1.55	1.45
25	B	603	CLA	C1D-ND	2.90	1.41	1.37
25	g	315	CLA	C4B-NB	2.90	1.41	1.37
25	3	306	CLA	C4B-NB	2.89	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	610	CLA	C1D-ND	2.89	1.41	1.37
32	a	609	SQD	O47-C7	2.89	1.42	1.34
32	A	609	SQD	O47-C7	2.89	1.42	1.34
24	1	308	CHL	CHA-CBD	-2.89	1.48	1.51
35	D	403	PHO	CMC-C2C	-2.89	1.46	1.50
25	s	417	CLA	C4B-NB	2.88	1.41	1.37
25	G	317	CLA	C4B-NB	2.88	1.41	1.37
25	8	314	CLA	C4B-NB	2.88	1.41	1.37
32	b	618	SQD	O47-C7	2.88	1.42	1.34
25	G	314	CLA	C4B-NB	2.87	1.41	1.37
31	D	410	8CT	C07-C02	-2.87	1.45	1.51
31	S	615	8CT	C07-C02	-2.87	1.45	1.51
24	9	304	CHL	CHA-CBD	-2.87	1.48	1.51
25	G	307	CLA	C1B-C2B	2.87	1.49	1.43
32	d	409	SQD	O47-C7	2.87	1.42	1.34
25	2	307	CLA	C4B-NB	2.87	1.41	1.37
31	c	615	8CT	C07-C02	-2.87	1.45	1.51
25	C	607	CLA	C1D-ND	2.86	1.41	1.37
25	3	307	CLA	C4B-NB	2.86	1.41	1.37
25	c	605	CLA	C1D-ND	2.86	1.41	1.37
25	S	616	CLA	C4B-NB	2.86	1.41	1.37
32	B	618	SQD	O47-C7	2.86	1.42	1.34
25	g	317	CLA	C4B-NB	2.86	1.41	1.37
25	c	616	CLA	C1D-ND	2.86	1.41	1.37
25	g	314	CLA	C4B-NB	2.86	1.41	1.37
24	4	308	CHL	CHA-CBD	-2.86	1.48	1.51
25	g	316	CLA	C4B-NB	2.85	1.41	1.37
25	g	307	CLA	C1B-C2B	2.85	1.49	1.43
35	d	403	PHO	CMC-C2C	-2.85	1.46	1.50
31	d	410	8CT	C07-C02	-2.85	1.45	1.51
25	p	308	CLA	C4B-NB	2.85	1.41	1.37
24	7	312	CHL	CHA-CBD	-2.85	1.48	1.51
25	q	315	CLA	C4B-NB	2.84	1.41	1.37
24	u	305	CHL	CHA-CBD	-2.84	1.48	1.51
25	5	307	CLA	C4B-NB	2.84	1.41	1.37
31	B	617	8CT	C07-C02	-2.84	1.45	1.51
32	D	409	SQD	O47-C7	2.84	1.42	1.34
24	6	311	CHL	CHA-CBD	-2.84	1.48	1.51
31	b	617	8CT	C07-C02	-2.84	1.45	1.51
25	8	306	CLA	C4B-NB	2.84	1.41	1.37
31	X	601	8CT	C30-C29	2.84	1.54	1.50
31	x	601	8CT	C30-C29	2.84	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	1	306	CLA	C4B-NB	2.84	1.41	1.37
31	v	401	8CT	C30-C29	2.83	1.54	1.50
25	8	312	CLA	C4B-NB	2.83	1.41	1.37
24	p	312	CHL	CHA-CBD	-2.83	1.48	1.51
31	V	401	8CT	C30-C29	2.82	1.54	1.50
35	A	606	PHO	CMC-C2C	-2.82	1.46	1.50
25	7	308	CLA	C4B-NB	2.82	1.41	1.37
31	s	416	8CT	C07-C02	-2.82	1.45	1.51
25	R	604	CLA	C4B-NB	2.82	1.41	1.37
25	q	313	CLA	C4B-NB	2.82	1.41	1.37
25	r	305	CLA	C4B-NB	2.82	1.41	1.37
25	C	605	CLA	C1D-ND	2.81	1.41	1.37
24	3	311	CHL	CHA-CBD	-2.81	1.48	1.51
25	6	306	CLA	C4B-NB	2.80	1.41	1.37
25	7	307	CLA	C4B-NB	2.80	1.41	1.37
23	E	201	HEM	FE-NB	2.80	2.03	1.94
35	a	606	PHO	CMB-C2B	-2.80	1.46	1.51
25	5	315	CLA	C4B-NB	2.80	1.41	1.37
25	5	316	CLA	C4B-NB	2.80	1.41	1.37
25	B	606	CLA	C1D-ND	2.79	1.41	1.37
35	A	606	PHO	CMD-C2D	-2.79	1.46	1.51
35	a	606	PHO	CMD-C2D	-2.79	1.46	1.51
24	N	304	CHL	CHA-CBD	-2.79	1.48	1.51
25	2	315	CLA	C4B-NB	2.79	1.41	1.37
25	2	316	CLA	C4B-NB	2.79	1.41	1.37
25	9	307	CLA	C1B-C2B	2.79	1.49	1.43
25	u	316	CLA	C1B-C2B	2.79	1.49	1.43
25	a	604	CLA	C4B-NB	2.79	1.41	1.37
25	S	604	CLA	C4B-NB	2.79	1.41	1.37
25	q	306	CLA	C4B-NB	2.79	1.41	1.37
31	d	410	8CT	C30-C29	2.79	1.54	1.50
24	n	304	CHL	CHA-CBD	-2.78	1.48	1.51
25	s	405	CLA	C4B-NB	2.78	1.41	1.37
31	D	410	8CT	C30-C29	2.78	1.54	1.50
24	7	309	CHL	CHA-CBD	-2.78	1.48	1.51
25	b	606	CLA	C1D-ND	2.77	1.41	1.37
25	7	315	CLA	C4B-NB	2.77	1.41	1.37
35	a	606	PHO	CAC-C3C	-2.77	1.46	1.51
25	b	609	CLA	C4B-NB	2.77	1.41	1.37
25	1	316	CLA	C1B-C2B	2.77	1.49	1.43
35	A	606	PHO	CAC-C3C	-2.76	1.46	1.51
25	q	314	CLA	C4B-NB	2.76	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	p	315	CLA	C4B-NB	2.76	1.41	1.37
25	B	605	CLA	C4B-NB	2.76	1.41	1.37
25	9	315	CLA	C1B-C2B	2.76	1.49	1.43
25	S	603	CLA	C4B-NB	2.76	1.41	1.37
25	p	307	CLA	C4B-NB	2.76	1.41	1.37
25	r	304	CLA	C4B-NB	2.76	1.41	1.37
25	B	611	CLA	CMB-C2B	-2.76	1.45	1.50
25	b	611	CLA	CMB-C2B	-2.75	1.45	1.50
25	b	605	CLA	C4B-NB	2.75	1.41	1.37
25	r	313	CLA	C1B-C2B	2.75	1.49	1.43
25	r	312	CLA	C4B-NB	2.75	1.41	1.37
25	u	317	CLA	C1B-C2B	2.75	1.49	1.43
25	2	308	CLA	C4B-NB	2.74	1.41	1.37
25	8	313	CLA	C4B-NB	2.74	1.41	1.37
25	C	604	CLA	C4B-NB	2.74	1.41	1.37
25	d	404	CLA	C1D-ND	2.74	1.41	1.37
25	9	306	CLA	C1B-C2B	2.74	1.49	1.43
25	B	609	CLA	C4B-NB	2.74	1.41	1.37
25	s	404	CLA	C4B-NB	2.74	1.41	1.37
25	9	316	CLA	C1B-C2B	2.73	1.49	1.43
31	c	614	8CT	C35-C30	2.73	1.64	1.56
31	C	614	8CT	C35-C30	2.73	1.64	1.56
25	u	308	CLA	C1B-C2B	2.73	1.49	1.43
25	6	313	CLA	C1B-C2B	2.73	1.49	1.43
35	A	606	PHO	CMB-C2B	-2.73	1.46	1.51
25	n	315	CLA	C1B-C2B	2.73	1.49	1.43
25	4	316	CLA	C1B-C2B	2.73	1.49	1.43
24	9	308	CHL	CHA-CBD	-2.73	1.48	1.51
25	n	316	CLA	C1B-C2B	2.73	1.49	1.43
25	R	611	CLA	C4B-NB	2.73	1.41	1.37
25	5	314	CLA	C4B-NB	2.73	1.41	1.37
25	u	315	CLA	C1B-C2B	2.73	1.49	1.43
25	N	315	CLA	C1B-C2B	2.72	1.49	1.43
25	4	315	CLA	C1B-C2B	2.72	1.49	1.43
25	5	308	CLA	C4B-NB	2.72	1.41	1.37
24	g	309	CHL	CHA-CBD	-2.72	1.48	1.51
35	d	403	PHO	CMD-C2D	-2.72	1.46	1.51
25	9	314	CLA	C1B-C2B	2.72	1.49	1.43
25	R	603	CLA	C4B-NB	2.72	1.41	1.37
24	p	309	CHL	CHA-CBD	-2.72	1.48	1.51
25	4	314	CLA	C1B-C2B	2.72	1.49	1.43
25	u	307	CLA	C1B-C2B	2.72	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	N	314	CLA	C1B-C2B	2.71	1.49	1.43
25	n	306	CLA	C1B-C2B	2.71	1.49	1.43
25	D	404	CLA	C1D-ND	2.71	1.41	1.37
25	q	312	CLA	C4B-NB	2.71	1.41	1.37
24	u	309	CHL	CHA-CBD	-2.71	1.48	1.51
35	D	403	PHO	CMD-C2D	-2.71	1.46	1.51
25	l	315	CLA	C1B-C2B	2.71	1.49	1.43
25	q	314	CLA	C1B-C2B	2.71	1.49	1.43
25	2	314	CLA	C4B-NB	2.71	1.41	1.37
25	A	604	CLA	C4B-NB	2.71	1.41	1.37
25	S	612	CLA	C4B-NB	2.71	1.41	1.37
25	B	615	CLA	C4B-NB	2.71	1.41	1.37
25	8	313	CLA	C1B-C2B	2.71	1.49	1.43
25	n	314	CLA	C1B-C2B	2.71	1.49	1.43
25	3	313	CLA	C1B-C2B	2.71	1.49	1.43
25	R	612	CLA	C1B-C2B	2.71	1.49	1.43
25	B	607	CLA	C4B-NB	2.71	1.41	1.37
25	b	607	CLA	C4B-NB	2.71	1.41	1.37
25	R	613	CLA	C1B-C2B	2.70	1.49	1.43
25	p	316	CLA	C4B-NB	2.70	1.41	1.37
30	D	407	LHG	O7-C5	-2.70	1.40	1.46
25	s	413	CLA	C4B-NB	2.70	1.41	1.37
25	6	306	CLA	C1B-C2B	2.70	1.49	1.43
24	G	309	CHL	CHA-CBD	-2.70	1.48	1.51
25	5	317	CLA	C4B-NB	2.70	1.41	1.37
25	q	305	CLA	C4B-NB	2.70	1.41	1.37
25	u	314	CLA	C1B-C2B	2.70	1.49	1.43
25	a	610	CLA	C1B-C2B	2.70	1.49	1.43
25	3	315	CLA	C1B-C2B	2.70	1.49	1.43
31	c	615	8CT	C30-C29	2.70	1.54	1.50
25	G	316	CLA	C1B-C2B	2.70	1.49	1.43
25	b	615	CLA	C4B-NB	2.70	1.41	1.37
25	r	314	CLA	C1B-C2B	2.69	1.49	1.43
30	d	407	LHG	O7-C5	-2.69	1.40	1.46
25	4	307	CLA	C1B-C2B	2.69	1.49	1.43
25	s	404	CLA	C1B-C2B	2.69	1.49	1.43
25	l	314	CLA	C1B-C2B	2.69	1.49	1.43
25	b	608	CLA	C4B-NB	2.69	1.41	1.37
39	D	406	PL9	C52-C5	-2.69	1.45	1.50
25	p	314	CLA	C4B-NB	2.69	1.41	1.37
25	R	610	CLA	C4B-NB	2.69	1.41	1.37
25	A	610	CLA	C1B-C2B	2.69	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	306	CLA	C1B-C2B	2.68	1.49	1.43
25	p	308	CLA	C1B-C2B	2.68	1.49	1.43
31	C	615	8CT	C30-C29	2.68	1.54	1.50
25	6	307	CLA	C1B-C2B	2.68	1.49	1.43
25	g	316	CLA	C1B-C2B	2.68	1.49	1.43
25	N	316	CLA	C1B-C2B	2.68	1.49	1.43
25	9	313	CLA	C1B-C2B	2.68	1.49	1.43
25	3	307	CLA	C1B-C2B	2.68	1.49	1.43
25	8	305	CLA	C4B-NB	2.68	1.41	1.37
25	8	311	CLA	C4B-NB	2.68	1.41	1.37
25	1	307	CLA	C1B-C2B	2.68	1.49	1.43
24	3	308	CHL	CHA-CBD	-2.68	1.48	1.51
24	6	308	CHL	CHA-CBD	-2.68	1.48	1.51
25	7	316	CLA	C4B-NB	2.67	1.41	1.37
25	6	314	CLA	C1B-C2B	2.67	1.49	1.43
25	1	306	CLA	C1B-C2B	2.67	1.49	1.43
25	r	310	CLA	C4B-NB	2.67	1.41	1.37
39	d	406	PL9	C52-C5	-2.67	1.45	1.50
25	2	317	CLA	C4B-NB	2.67	1.41	1.37
35	d	403	PHO	CAC-C3C	-2.67	1.47	1.51
25	7	308	CLA	C1B-C2B	2.67	1.49	1.43
24	9	317	CHL	CHA-CBD	-2.67	1.48	1.51
25	N	306	CLA	C1B-C2B	2.67	1.49	1.43
25	6	315	CLA	C1B-C2B	2.67	1.49	1.43
25	s	412	CLA	C4B-NB	2.67	1.41	1.37
25	5	317	CLA	C1B-C2B	2.66	1.49	1.43
25	p	317	CLA	C1B-C2B	2.66	1.49	1.43
25	C	608	CLA	CMB-C2B	-2.66	1.45	1.50
35	D	403	PHO	CMB-C2B	-2.66	1.46	1.51
35	d	403	PHO	CMB-C2B	-2.66	1.46	1.51
25	Y	314	CLA	C4B-NB	2.66	1.41	1.37
25	g	315	CLA	C1B-C2B	2.66	1.49	1.43
25	G	315	CLA	C1B-C2B	2.65	1.49	1.43
25	q	315	CLA	C1B-C2B	2.65	1.49	1.43
25	r	311	CLA	C4B-NB	2.65	1.41	1.37
25	b	601	CLA	C4B-NB	2.65	1.41	1.37
25	2	316	CLA	C1B-C2B	2.65	1.49	1.43
25	G	314	CLA	C1B-C2B	2.65	1.49	1.43
24	Y	304	CHL	CBD-CGD	-2.65	1.49	1.52
30	a	601	LHG	O7-C5	-2.65	1.40	1.46
25	b	616	CLA	C4B-NB	2.65	1.41	1.37
25	6	316	CLA	C1B-C2B	2.65	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	601	LHG	O7-C5	-2.65	1.40	1.46
25	8	314	CLA	C1B-C2B	2.65	1.49	1.43
25	n	313	CLA	C1B-C2B	2.65	1.49	1.43
25	B	612	CLA	MG-NB	-2.65	2.00	2.05
25	b	612	CLA	MG-NB	-2.65	2.00	2.05
25	S	610	CLA	C4B-NB	2.65	1.41	1.37
25	4	306	CLA	C1B-C2B	2.65	1.49	1.43
25	s	405	CLA	C1B-C2B	2.65	1.49	1.43
25	S	604	CLA	C1B-C2B	2.65	1.49	1.43
31	a	608	8CT	C30-C29	2.64	1.54	1.50
25	4	313	CLA	C1B-C2B	2.64	1.49	1.43
25	g	308	CLA	C1B-C2B	2.64	1.49	1.43
25	7	317	CLA	C1B-C2B	2.64	1.49	1.43
24	y	305	CHL	CBD-CGD	-2.64	1.49	1.52
25	g	314	CLA	C1B-C2B	2.64	1.49	1.43
25	5	316	CLA	C1B-C2B	2.64	1.49	1.43
25	Y	307	CLA	C4B-NB	2.64	1.41	1.37
25	B	608	CLA	C4B-NB	2.64	1.41	1.37
24	4	317	CHL	CHA-CBD	-2.63	1.48	1.51
25	7	307	CLA	C1B-C2B	2.63	1.49	1.43
25	B	610	CLA	C4B-NB	2.63	1.41	1.37
25	b	610	CLA	C4B-NB	2.63	1.41	1.37
25	r	312	CLA	C1B-C2B	2.63	1.49	1.43
25	B	611	CLA	C4B-NB	2.63	1.41	1.37
30	Y	318	LHG	O8-C6	-2.63	1.39	1.45
25	c	604	CLA	C4B-NB	2.63	1.41	1.37
25	S	603	CLA	C1B-C2B	2.63	1.49	1.43
24	N	317	CHL	CHA-CBD	-2.63	1.48	1.51
25	C	605	CLA	CMD-C2D	-2.63	1.45	1.50
25	8	305	CLA	C1B-C2B	2.63	1.49	1.43
25	R	603	CLA	C1B-C2B	2.63	1.49	1.43
26	q	302	0IE	C13-C12	-2.63	1.40	1.46
24	u	318	CHL	CHA-CBD	-2.62	1.48	1.51
35	D	403	PHO	CAC-C3C	-2.62	1.47	1.51
25	c	608	CLA	CMB-C2B	-2.62	1.45	1.50
25	c	616	CLA	MG-NB	-2.62	2.00	2.05
23	f	201	HEM	FE-NC	2.62	2.03	1.95
25	S	611	CLA	C4B-NB	2.62	1.41	1.37
25	8	312	CLA	C1B-C2B	2.62	1.49	1.43
25	G	308	CLA	C1B-C2B	2.62	1.49	1.43
25	R	611	CLA	C1B-C2B	2.62	1.49	1.43
25	R	609	CLA	C4B-NB	2.62	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	D	408	LHG	O8-C6	-2.62	1.39	1.45
25	2	317	CLA	C1B-C2B	2.62	1.49	1.43
24	n	317	CHL	CHA-CBD	-2.62	1.48	1.51
24	u	312	CHL	CHA-CBD	-2.62	1.48	1.51
25	N	313	CLA	C1B-C2B	2.62	1.49	1.43
25	B	601	CLA	C4B-NB	2.62	1.41	1.37
25	S	616	CLA	C1B-C2B	2.62	1.49	1.43
25	b	603	CLA	MG-NB	-2.62	2.00	2.05
25	3	316	CLA	C1B-C2B	2.62	1.49	1.43
25	1	313	CLA	C1B-C2B	2.62	1.49	1.43
25	p	316	CLA	C1B-C2B	2.62	1.49	1.43
25	7	316	CLA	C1B-C2B	2.62	1.49	1.43
25	s	410	CLA	C1B-C2B	2.61	1.49	1.43
25	3	314	CLA	C1B-C2B	2.61	1.49	1.43
25	s	417	CLA	C1B-C2B	2.61	1.49	1.43
25	r	304	CLA	C1B-C2B	2.61	1.49	1.43
25	B	603	CLA	MG-NB	-2.61	2.00	2.05
25	n	307	CLA	C1B-C2B	2.61	1.49	1.43
25	q	305	CLA	C1B-C2B	2.61	1.49	1.43
25	B	602	CLA	C4B-NB	2.61	1.41	1.37
25	s	413	CLA	C1B-C2B	2.61	1.49	1.43
30	D	407	LHG	O8-C6	-2.61	1.39	1.45
25	y	308	CLA	C4B-NB	2.61	1.41	1.37
25	c	605	CLA	CMD-C2D	-2.61	1.45	1.50
25	S	609	CLA	C1B-C2B	2.61	1.49	1.43
25	7	314	CLA	C4B-NB	2.61	1.41	1.37
25	b	611	CLA	C4B-NB	2.61	1.41	1.37
25	c	606	CLA	CMB-C2B	-2.60	1.45	1.50
25	R	609	CLA	C1B-C2B	2.60	1.49	1.43
25	q	313	CLA	C1B-C2B	2.60	1.49	1.43
31	b	617	8CT	C30-C29	2.60	1.54	1.50
25	y	315	CLA	C4B-NB	2.60	1.41	1.37
30	y	319	LHG	O7-C5	-2.60	1.40	1.46
25	B	616	CLA	C1B-C2B	2.60	1.49	1.43
26	y	302	0IE	C6-C7	-2.60	1.40	1.46
30	d	407	LHG	O8-C6	-2.60	1.39	1.45
24	8	315	CHL	CHA-CBD	-2.60	1.48	1.51
31	A	608	8CT	C30-C29	2.60	1.54	1.50
25	b	616	CLA	C1B-C2B	2.59	1.49	1.43
25	D	405	CLA	C4B-NB	2.59	1.41	1.37
25	B	616	CLA	C4B-NB	2.59	1.41	1.37
25	C	616	CLA	MG-NB	-2.59	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	5	307	CLA	C1B-C2B	2.59	1.49	1.43
25	Y	316	CLA	C4B-NB	2.59	1.41	1.37
25	p	307	CLA	C1B-C2B	2.59	1.49	1.43
26	8	302	0IE	C13-C12	-2.59	1.40	1.46
25	R	610	CLA	C1B-C2B	2.59	1.49	1.43
25	S	610	CLA	C1B-C2B	2.58	1.49	1.43
25	g	317	CLA	C1B-C2B	2.58	1.49	1.43
25	y	317	CLA	C4B-NB	2.58	1.41	1.37
25	c	601	CLA	CMD-C2D	-2.58	1.45	1.50
26	Y	303	0IE	C13-C12	-2.58	1.40	1.46
25	N	307	CLA	C1B-C2B	2.58	1.49	1.43
25	d	405	CLA	C4B-NB	2.58	1.41	1.37
25	5	308	CLA	C1B-C2B	2.58	1.49	1.43
25	B	604	CLA	C4B-NB	2.58	1.41	1.37
25	B	614	CLA	C4B-NB	2.58	1.41	1.37
25	s	410	CLA	C4B-NB	2.58	1.41	1.37
25	S	612	CLA	C1B-C2B	2.58	1.49	1.43
25	C	601	CLA	CMD-C2D	-2.58	1.45	1.50
25	G	317	CLA	C1B-C2B	2.58	1.49	1.43
25	2	308	CLA	C1B-C2B	2.58	1.49	1.43
26	y	302	0IE	C13-C12	-2.57	1.40	1.46
26	y	302	0IE	C17-C16	-2.57	1.40	1.46
25	s	411	CLA	C1B-C2B	2.57	1.49	1.43
26	8	302	0IE	C17-C16	-2.57	1.40	1.46
26	y	303	0IE	C13-C12	-2.57	1.40	1.46
25	2	307	CLA	C1B-C2B	2.57	1.49	1.43
25	S	609	CLA	C4B-NB	2.57	1.41	1.37
30	Y	318	LHG	O7-C5	-2.57	1.40	1.46
30	y	319	LHG	O8-C6	-2.57	1.39	1.45
24	9	311	CHL	CHA-CBD	-2.57	1.48	1.51
25	r	305	CLA	C1B-C2B	2.57	1.49	1.43
25	r	310	CLA	C1B-C2B	2.56	1.49	1.43
25	b	613	CLA	C4B-NB	2.56	1.41	1.37
25	C	606	CLA	CMB-C2B	-2.56	1.45	1.50
25	b	602	CLA	C4B-NB	2.56	1.41	1.37
24	1	317	CHL	CHA-CBD	-2.56	1.48	1.51
30	A	601	LHG	O8-C6	-2.56	1.39	1.45
25	y	307	CLA	C4B-NB	2.56	1.41	1.37
30	c	617	LHG	O8-C6	-2.56	1.39	1.45
25	Y	314	CLA	C1B-C2B	2.56	1.49	1.43
25	R	604	CLA	C1B-C2B	2.56	1.49	1.43
31	c	613	8CT	C35-C30	2.56	1.63	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	2	315	CLA	C1B-C2B	2.56	1.49	1.43
25	r	311	CLA	C1B-C2B	2.56	1.49	1.43
25	y	307	CLA	C1B-C2B	2.56	1.49	1.43
30	a	612	LHG	O7-C5	-2.55	1.40	1.46
25	7	315	CLA	C1B-C2B	2.55	1.49	1.43
24	q	316	CHL	CHA-CBD	-2.55	1.48	1.51
25	b	615	CLA	C1B-C2B	2.55	1.49	1.43
26	Y	302	0IE	C6-C7	-2.55	1.40	1.46
25	2	314	CLA	C1B-C2B	2.55	1.49	1.43
26	5	302	0IE	C6-C7	-2.55	1.40	1.46
30	A	612	LHG	O7-C5	-2.55	1.40	1.46
31	C	613	8CT	C35-C30	2.55	1.63	1.56
26	Y	302	0IE	C13-C12	-2.55	1.40	1.46
25	C	606	CLA	MG-NB	-2.55	2.00	2.05
25	c	601	CLA	MG-NB	-2.55	2.00	2.05
25	b	614	CLA	C4B-NB	2.55	1.41	1.37
25	s	411	CLA	C4B-NB	2.55	1.41	1.37
25	D	404	CLA	CMD-C2D	-2.55	1.45	1.50
25	y	314	CLA	C4B-NB	2.54	1.41	1.37
25	b	604	CLA	C1B-C2B	2.54	1.49	1.43
26	q	302	0IE	C17-C16	-2.54	1.40	1.46
25	Y	313	CLA	C4B-NB	2.54	1.41	1.37
25	5	314	CLA	C1B-C2B	2.54	1.49	1.43
25	b	604	CLA	C4B-NB	2.54	1.41	1.37
26	y	303	0IE	C6-C7	-2.54	1.40	1.46
25	s	412	CLA	C1B-C2B	2.54	1.49	1.43
25	B	613	CLA	C4B-NB	2.54	1.41	1.37
25	c	603	CLA	C4B-NB	2.54	1.41	1.37
25	5	315	CLA	C1B-C2B	2.54	1.49	1.43
25	A	605	CLA	MG-NB	-2.54	2.00	2.05
25	S	611	CLA	C1B-C2B	2.53	1.49	1.43
30	C	617	LHG	O8-C6	-2.53	1.39	1.45
25	Y	306	CLA	C1B-C2B	2.53	1.49	1.43
26	2	302	0IE	C6-C7	-2.53	1.40	1.46
25	7	314	CLA	C1B-C2B	2.53	1.49	1.43
25	p	314	CLA	C1B-C2B	2.53	1.49	1.43
25	C	603	CLA	C4B-NB	2.53	1.41	1.37
25	C	612	CLA	C1B-C2B	2.53	1.49	1.43
25	d	404	CLA	C4B-NB	2.53	1.41	1.37
25	Y	306	CLA	C4B-NB	2.53	1.41	1.37
25	d	404	CLA	CMD-C2D	-2.53	1.45	1.50
26	Y	302	0IE	C17-C16	-2.53	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	601	CLA	C1B-C2B	2.53	1.49	1.43
30	D	408	LHG	O7-C5	-2.53	1.40	1.46
25	B	601	CLA	C1B-C2B	2.52	1.49	1.43
25	B	604	CLA	C1B-C2B	2.52	1.49	1.43
25	c	606	CLA	MG-NB	-2.52	2.00	2.05
25	B	602	CLA	C1B-C2B	2.52	1.49	1.43
25	p	315	CLA	C1B-C2B	2.52	1.49	1.43
25	C	601	CLA	MG-NB	-2.51	2.00	2.05
26	Y	303	0IE	C6-C7	-2.51	1.40	1.46
25	c	611	CLA	C1B-C2B	2.51	1.49	1.43
25	y	316	CLA	C1B-C2B	2.51	1.49	1.43
26	5	302	0IE	C13-C12	-2.51	1.40	1.46
30	a	601	LHG	O8-C6	-2.51	1.39	1.45
30	7	319	LHG	O8-C6	-2.51	1.39	1.45
25	C	611	CLA	C4B-NB	2.51	1.41	1.37
26	Y	303	0IE	C17-C16	-2.51	1.40	1.46
25	a	604	CLA	CMB-C2B	-2.51	1.45	1.50
25	C	605	CLA	C4B-NB	2.51	1.41	1.37
30	G	319	LHG	O8-C6	-2.51	1.39	1.45
25	B	606	CLA	C1B-C2B	2.51	1.49	1.43
25	Y	315	CLA	MG-NB	-2.50	2.00	2.05
25	y	316	CLA	MG-NB	-2.50	2.00	2.05
25	c	604	CLA	C1B-C2B	2.50	1.49	1.43
25	c	609	CLA	C4B-NB	2.50	1.41	1.37
26	2	302	0IE	C13-C12	-2.50	1.40	1.46
30	A	612	LHG	O8-C6	-2.50	1.39	1.45
25	c	608	CLA	MG-NB	-2.50	2.00	2.05
25	B	615	CLA	C1B-C2B	2.50	1.49	1.43
25	y	315	CLA	C1B-C2B	2.50	1.49	1.43
26	y	303	0IE	C17-C16	-2.50	1.40	1.46
25	c	612	CLA	C4B-NB	2.50	1.41	1.37
30	p	319	LHG	O8-C6	-2.49	1.39	1.45
25	y	316	CLA	CMC-C2C	-2.49	1.45	1.50
25	a	605	CLA	MG-NB	-2.49	2.00	2.05
26	8	302	0IE	C6-C7	-2.49	1.40	1.46
25	B	605	CLA	C1B-C2B	2.49	1.49	1.43
25	c	605	CLA	MG-NB	-2.49	2.00	2.05
25	c	607	CLA	MG-NB	-2.49	2.00	2.05
25	b	606	CLA	C1B-C2B	2.49	1.49	1.43
25	b	616	CLA	CMC-C2C	-2.49	1.45	1.50
25	B	606	CLA	MG-NB	-2.48	2.00	2.05
25	c	612	CLA	C1B-C2B	2.48	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	7	302	0IE	C13-C12	-2.48	1.40	1.46
31	c	613	8CT	C30-C29	2.48	1.54	1.50
25	D	405	CLA	C1B-C2B	2.48	1.49	1.43
25	q	306	CLA	C1B-C2B	2.48	1.49	1.43
25	C	603	CLA	MG-NB	-2.48	2.00	2.05
31	B	617	8CT	C30-C29	2.48	1.54	1.50
25	c	616	CLA	C4B-NB	2.48	1.41	1.37
30	g	319	LHG	O8-C6	-2.48	1.39	1.45
25	A	607	CLA	MG-NB	-2.48	2.00	2.05
25	8	306	CLA	C1B-C2B	2.48	1.48	1.43
25	b	609	CLA	C1B-C2B	2.48	1.48	1.43
25	Y	315	CLA	CMC-C2C	-2.48	1.45	1.50
25	a	607	CLA	MG-NB	-2.48	2.00	2.05
30	p	319	LHG	O7-C5	-2.48	1.40	1.46
25	B	610	CLA	MG-NB	-2.48	2.00	2.05
25	A	603	CLA	MG-NB	-2.48	2.00	2.05
25	d	405	CLA	C1B-C2B	2.48	1.48	1.43
25	b	606	CLA	MG-NB	-2.48	2.00	2.05
25	Y	315	CLA	C1B-C2B	2.47	1.48	1.43
25	b	602	CLA	C1B-C2B	2.47	1.48	1.43
26	r	315	0IE	C13-C12	-2.47	1.40	1.46
35	a	606	PHO	C4D-ND	-2.47	1.34	1.38
25	C	605	CLA	MG-NB	-2.47	2.00	2.05
25	B	609	CLA	C1B-C2B	2.47	1.48	1.43
30	a	612	LHG	O8-C6	-2.47	1.39	1.45
25	b	607	CLA	C1B-C2B	2.47	1.48	1.43
25	b	605	CLA	C1B-C2B	2.47	1.48	1.43
25	C	601	CLA	C1B-C2B	2.47	1.48	1.43
23	f	201	HEM	FE-NA	2.47	2.03	1.95
25	C	609	CLA	C4B-NB	2.47	1.41	1.37
28	g	304	NEX	O24-C25	-2.47	1.43	1.46
24	s	414	CHL	CBD-CGD	-2.47	1.49	1.52
25	C	616	CLA	C4B-NB	2.47	1.41	1.37
25	A	604	CLA	CMB-C2B	-2.47	1.45	1.50
24	q	307	CHL	CBD-CGD	-2.47	1.49	1.52
25	b	606	CLA	C4B-NB	2.47	1.41	1.37
25	b	610	CLA	MG-NB	-2.46	2.00	2.05
25	c	611	CLA	C4B-NB	2.46	1.41	1.37
26	R	614	0IE	C13-C12	-2.46	1.40	1.46
25	c	603	CLA	MG-NB	-2.46	2.00	2.05
25	B	607	CLA	C1B-C2B	2.46	1.48	1.43
30	4	318	LHG	O8-C6	-2.46	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	610	CLA	MG-NB	-2.46	2.00	2.05
25	C	607	CLA	C1B-C2B	2.46	1.48	1.43
25	D	404	CLA	C4B-NB	2.46	1.41	1.37
24	8	307	CHL	CBD-CGD	-2.46	1.49	1.52
25	d	405	CLA	MG-NB	-2.46	2.00	2.05
26	5	302	0IE	C17-C16	-2.46	1.40	1.46
25	C	604	CLA	C1B-C2B	2.46	1.48	1.43
25	B	616	CLA	CMC-C2C	-2.46	1.45	1.50
25	C	602	CLA	MG-NB	-2.46	2.00	2.05
25	C	611	CLA	C1B-C2B	2.46	1.48	1.43
26	p	303	0IE	C6-C7	-2.46	1.40	1.46
25	C	616	CLA	C1B-C2B	2.45	1.48	1.43
31	C	613	8CT	C30-C29	2.45	1.54	1.50
25	b	603	CLA	CMD-C2D	-2.45	1.45	1.50
25	c	607	CLA	C1B-C2B	2.45	1.48	1.43
25	C	607	CLA	MG-NB	-2.45	2.00	2.05
26	2	302	0IE	C17-C16	-2.45	1.40	1.46
25	d	404	CLA	C1B-C2B	2.45	1.48	1.43
26	q	302	0IE	C6-C7	-2.45	1.40	1.46
25	B	606	CLA	C4B-NB	2.45	1.41	1.37
28	1	303	NEX	O24-C25	-2.45	1.43	1.46
24	Y	312	CHL	CBD-CGD	-2.45	1.49	1.52
25	c	601	CLA	C1B-C2B	2.45	1.48	1.43
25	Y	307	CLA	C1B-C2B	2.45	1.48	1.43
25	y	308	CLA	C1B-C2B	2.45	1.48	1.43
25	c	602	CLA	CMC-C2C	-2.44	1.45	1.50
25	c	605	CLA	C4B-NB	2.44	1.41	1.37
25	B	603	CLA	C1B-C2B	2.44	1.48	1.43
25	c	609	CLA	MG-NB	-2.44	2.00	2.05
25	C	612	CLA	C4B-NB	2.44	1.41	1.37
26	9	303	0IE	C15-C16	2.44	1.41	1.35
28	p	304	NEX	O24-C25	-2.44	1.43	1.46
26	p	302	0IE	C13-C12	-2.44	1.40	1.46
25	A	605	CLA	C4B-NB	2.44	1.41	1.37
26	7	303	0IE	C6-C7	-2.44	1.40	1.46
25	D	404	CLA	C1B-C2B	2.44	1.48	1.43
35	A	606	PHO	C4D-ND	-2.44	1.34	1.38
24	S	613	CHL	CBD-CGD	-2.44	1.49	1.52
26	p	302	0IE	C17-C16	-2.44	1.40	1.46
25	8	311	CLA	C1B-C2B	2.43	1.48	1.43
25	C	608	CLA	MG-NB	-2.43	2.01	2.05
25	c	602	CLA	MG-NB	-2.43	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	l	318	LHG	O8-C6	-2.43	1.39	1.45
30	n	318	LHG	O8-C6	-2.43	1.39	1.45
25	a	603	CLA	CMD-C2D	-2.43	1.45	1.50
25	B	603	CLA	CMD-C2D	-2.43	1.45	1.50
25	R	613	CLA	C3B-C4B	2.43	1.49	1.42
25	A	604	CLA	MG-NB	-2.43	2.01	2.05
25	B	603	CLA	C4B-NB	2.43	1.41	1.37
25	c	616	CLA	C1B-C2B	2.43	1.48	1.43
25	D	405	CLA	MG-NB	-2.43	2.01	2.05
24	s	402	CHL	CBD-CGD	-2.43	1.49	1.52
31	c	615	8CT	C33-C32	-2.43	1.43	1.50
25	q	305	CLA	MG-NB	-2.42	2.01	2.05
26	u	303	0IE	C15-C16	2.42	1.41	1.35
25	S	603	CLA	MG-NB	-2.42	2.01	2.05
25	C	602	CLA	CMB-C2B	-2.42	1.45	1.50
24	Y	319	CHL	CBD-CGD	-2.42	1.49	1.52
26	g	303	0IE	C6-C7	-2.42	1.40	1.46
24	y	313	CHL	CBD-CGD	-2.42	1.49	1.52
25	b	603	CLA	C4B-NB	2.42	1.41	1.37
25	a	604	CLA	C3B-C4B	2.42	1.49	1.42
25	S	611	CLA	MG-NB	-2.42	2.01	2.05
35	A	606	PHO	C3B-C2B	-2.42	1.37	1.40
25	C	609	CLA	MG-NB	-2.42	2.01	2.05
25	s	413	CLA	MG-NB	-2.42	2.01	2.05
25	b	613	CLA	MG-NB	-2.42	2.01	2.05
25	C	610	CLA	MG-NB	-2.42	2.01	2.05
25	B	612	CLA	CMB-C2B	-2.42	1.45	1.50
26	6	302	0IE	C13-C12	-2.42	1.40	1.46
25	c	603	CLA	C1B-C2B	2.42	1.48	1.43
25	a	603	CLA	MG-NB	-2.42	2.01	2.05
26	7	302	0IE	C17-C16	-2.41	1.40	1.46
25	B	614	CLA	C1B-C2B	2.41	1.48	1.43
25	C	616	CLA	CMD-C2D	-2.41	1.45	1.50
24	y	318	CHL	CBD-CGD	-2.41	1.49	1.52
23	E	201	HEM	FE-NC	2.41	2.03	1.95
25	b	603	CLA	C1B-C2B	2.41	1.48	1.43
25	b	614	CLA	C1B-C2B	2.41	1.48	1.43
24	Y	317	CHL	CBD-CGD	-2.41	1.49	1.52
25	y	317	CLA	MG-NB	-2.41	2.01	2.05
25	B	611	CLA	MG-NB	-2.41	2.01	2.05
25	b	608	CLA	MG-NB	-2.41	2.01	2.05
30	7	319	LHG	O7-C5	-2.41	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	3	302	0IE	C6-C7	-2.41	1.40	1.46
25	B	602	CLA	MG-NB	-2.41	2.01	2.05
28	4	303	NEX	O24-C25	-2.41	1.43	1.46
28	7	304	NEX	O24-C25	-2.41	1.43	1.46
25	C	602	CLA	C1B-C2B	2.41	1.48	1.43
25	B	604	CLA	MG-NB	-2.41	2.01	2.05
26	3	302	0IE	C13-C12	-2.41	1.40	1.46
25	C	602	CLA	CMC-C2C	-2.41	1.45	1.50
25	a	604	CLA	MG-NB	-2.41	2.01	2.05
25	b	602	CLA	MG-NB	-2.41	2.01	2.05
25	A	604	CLA	C3B-C4B	2.40	1.49	1.42
28	5	304	NEX	O24-C25	-2.40	1.43	1.46
31	C	615	8CT	C33-C32	-2.40	1.43	1.50
30	N	318	LHG	O8-C6	-2.40	1.39	1.45
28	r	301	NEX	O24-C25	-2.40	1.43	1.46
25	b	615	CLA	MG-NB	-2.40	2.01	2.05
25	c	602	CLA	CMB-C2B	-2.40	1.45	1.50
25	y	314	CLA	CMB-C2B	-2.40	1.45	1.50
25	y	316	CLA	C4B-NB	2.40	1.41	1.37
25	s	412	CLA	MG-NB	-2.40	2.01	2.05
25	A	603	CLA	CMD-C2D	-2.40	1.45	1.50
25	c	610	CLA	CMD-C2D	-2.40	1.45	1.50
26	6	302	0IE	C6-C7	-2.40	1.40	1.46
25	B	613	CLA	MG-NB	-2.40	2.01	2.05
24	S	601	CHL	CBD-CGD	-2.40	1.49	1.52
31	C	614	8CT	C30-C29	2.40	1.54	1.50
25	q	312	CLA	C1B-C2B	2.40	1.48	1.43
30	N	318	LHG	O7-C5	-2.40	1.41	1.46
26	G	303	0IE	C6-C7	-2.40	1.40	1.46
25	c	608	CLA	C4B-NB	2.40	1.41	1.37
25	C	603	CLA	C1B-C2B	2.40	1.48	1.43
30	5	319	LHG	O7-C5	-2.40	1.41	1.46
24	q	309	CHL	CBD-CGD	-2.40	1.49	1.52
25	b	612	CLA	CMB-C2B	-2.40	1.45	1.50
24	8	310	CHL	CBD-CGD	-2.39	1.49	1.52
28	G	304	NEX	O24-C25	-2.39	1.43	1.46
25	C	610	CLA	CMD-C2D	-2.39	1.45	1.50
25	C	604	CLA	MG-NB	-2.39	2.01	2.05
25	S	612	CLA	MG-NB	-2.39	2.01	2.05
25	Y	313	CLA	MG-NB	-2.39	2.01	2.05
31	c	614	8CT	C30-C29	2.39	1.54	1.50
25	4	313	CLA	CHC-C1C	2.39	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	y	314	CLA	MG-NB	-2.39	2.01	2.05
25	b	611	CLA	MG-NB	-2.39	2.01	2.05
25	d	404	CLA	MG-NB	-2.39	2.01	2.05
25	C	610	CLA	C4B-NB	2.39	1.41	1.37
30	n	318	LHG	O7-C5	-2.39	1.41	1.46
25	3	316	CLA	C3B-C4B	2.39	1.49	1.42
25	c	606	CLA	C4B-NB	2.39	1.41	1.37
23	E	201	HEM	FE-NA	2.39	2.03	1.95
25	B	612	CLA	C4B-NB	2.39	1.41	1.37
28	r	317	NEX	O24-C25	-2.39	1.43	1.46
25	b	604	CLA	CMB-C2B	-2.39	1.45	1.50
25	1	313	CLA	C3B-C4B	2.39	1.49	1.42
25	r	314	CLA	C3B-C4B	2.39	1.49	1.42
25	Y	306	CLA	MG-NB	-2.39	2.01	2.05
26	G	303	0IE	C17-C16	-2.39	1.40	1.46
25	c	616	CLA	CMD-C2D	-2.39	1.45	1.50
30	2	319	LHG	O7-C5	-2.39	1.41	1.46
25	B	616	CLA	MG-NB	-2.39	2.01	2.05
25	b	616	CLA	MG-NB	-2.38	2.01	2.05
25	8	305	CLA	MG-NB	-2.38	2.01	2.05
25	y	307	CLA	MG-NB	-2.38	2.01	2.05
28	9	319	NEX	O24-C25	-2.38	1.43	1.46
25	r	305	CLA	CMB-C2B	-2.38	1.45	1.50
25	b	603	CLA	CMB-C2B	-2.38	1.45	1.50
26	2	303	0IE	C17-C16	-2.38	1.40	1.46
25	B	614	CLA	MG-NB	-2.38	2.01	2.05
25	C	609	CLA	CMB-C2B	-2.38	1.45	1.50
25	3	313	CLA	C3B-C4B	2.38	1.49	1.42
25	C	608	CLA	C4B-NB	2.38	1.41	1.37
25	b	604	CLA	MG-NB	-2.38	2.01	2.05
26	N	302	0IE	C13-C12	-2.38	1.40	1.46
25	C	606	CLA	C4B-NB	2.38	1.41	1.37
28	u	304	NEX	O24-C25	-2.38	1.43	1.46
25	N	313	CLA	C3B-C4B	2.38	1.49	1.42
25	A	603	CLA	CMC-C2C	-2.38	1.45	1.50
26	g	303	0IE	C17-C16	-2.38	1.40	1.46
26	5	303	0IE	C17-C16	-2.38	1.40	1.46
25	y	314	CLA	C1B-C2B	2.38	1.48	1.43
25	Y	315	CLA	CMD-C2D	-2.38	1.45	1.50
25	4	313	CLA	C3B-C4B	2.37	1.49	1.42
26	p	303	0IE	C13-C12	-2.37	1.40	1.46
28	R	616	NEX	O24-C25	-2.37	1.43	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	608	CLA	C1B-C2B	2.37	1.48	1.43
25	B	603	CLA	CMB-C2B	-2.37	1.45	1.50
25	y	317	CLA	C1B-C2B	2.37	1.48	1.43
25	9	313	CLA	C3B-C4B	2.37	1.49	1.42
25	Y	316	CLA	MG-NB	-2.37	2.01	2.05
25	c	607	CLA	C4B-NB	2.37	1.41	1.37
26	4	302	0IE	C13-C12	-2.37	1.40	1.46
25	B	605	CLA	MG-NB	-2.37	2.01	2.05
25	b	614	CLA	MG-NB	-2.37	2.01	2.05
25	9	314	CLA	C3B-C4B	2.37	1.49	1.42
25	B	611	CLA	CMC-C2C	-2.37	1.45	1.50
25	Y	314	CLA	MG-NB	-2.37	2.01	2.05
25	B	615	CLA	MG-NB	-2.37	2.01	2.05
30	C	617	LHG	O7-C5	-2.37	1.41	1.46
25	b	609	CLA	MG-NB	-2.37	2.01	2.05
30	9	318	LHG	O8-C6	-2.37	1.39	1.45
25	n	313	CLA	C3B-C4B	2.37	1.49	1.42
26	u	303	0IE	C11-C12	2.37	1.41	1.35
25	a	605	CLA	C4B-NB	2.37	1.41	1.37
25	u	314	CLA	C3B-C4B	2.37	1.49	1.42
25	8	311	CLA	MG-NB	-2.36	2.01	2.05
25	y	316	CLA	CMD-C2D	-2.36	1.45	1.50
30	1	318	LHG	O7-C5	-2.36	1.41	1.46
25	8	313	CLA	MG-NB	-2.36	2.01	2.05
25	y	315	CLA	MG-NB	-2.36	2.01	2.05
25	c	612	CLA	MG-NB	-2.36	2.01	2.05
25	u	315	CLA	C3B-C4B	2.36	1.49	1.42
26	9	303	0IE	C11-C12	2.36	1.41	1.35
25	7	307	CLA	MG-NB	-2.36	2.01	2.05
25	c	607	CLA	CMD-C2D	-2.36	1.45	1.50
28	S	617	NEX	O24-C25	-2.36	1.43	1.46
25	c	610	CLA	C4B-NB	2.36	1.41	1.37
25	4	314	CLA	C3B-C4B	2.36	1.49	1.42
25	s	404	CLA	MG-NB	-2.36	2.01	2.05
24	7	313	CHL	CBD-CGD	-2.36	1.49	1.52
25	S	610	CLA	MG-NB	-2.36	2.01	2.05
25	p	316	CLA	MG-NB	-2.36	2.01	2.05
25	1	313	CLA	CHC-C1C	2.36	1.43	1.38
28	y	304	NEX	O24-C25	-2.36	1.43	1.46
25	C	607	CLA	CMD-C2D	-2.36	1.45	1.50
26	g	302	0IE	C17-C16	-2.36	1.40	1.46
26	u	302	0IE	C8-C7	2.36	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Y	313	CLA	CMB-C2B	-2.36	1.45	1.50
25	q	314	CLA	MG-NB	-2.36	2.01	2.05
25	c	609	CLA	CMB-C2B	-2.36	1.45	1.50
26	u	303	0IE	C8-C7	2.36	1.41	1.35
25	s	411	CLA	MG-NB	-2.36	2.01	2.05
26	R	614	0IE	C17-C16	-2.36	1.40	1.46
25	a	603	CLA	CMC-C2C	-2.36	1.45	1.50
25	Y	313	CLA	C1B-C2B	2.36	1.48	1.43
25	c	602	CLA	C1B-C2B	2.36	1.48	1.43
28	n	303	NEX	O24-C25	-2.35	1.43	1.46
25	b	611	CLA	CMC-C2C	-2.35	1.45	1.50
25	6	313	CLA	C3B-C4B	2.35	1.49	1.42
28	2	304	NEX	O24-C25	-2.35	1.43	1.46
25	9	316	CLA	C3B-C4B	2.35	1.49	1.42
25	Y	315	CLA	C4B-NB	2.35	1.41	1.37
25	u	317	CLA	CHC-C1C	2.35	1.43	1.38
25	b	608	CLA	C1B-C2B	2.35	1.48	1.43
25	8	306	CLA	MG-NB	-2.35	2.01	2.05
25	Y	316	CLA	C1B-C2B	2.35	1.48	1.43
28	3	318	NEX	O24-C25	-2.35	1.43	1.46
25	9	316	CLA	CHC-C1C	2.35	1.43	1.38
25	B	608	CLA	MG-NB	-2.35	2.01	2.05
26	5	303	0IE	C13-C12	-2.35	1.40	1.46
25	b	609	CLA	CMB-C2B	-2.35	1.46	1.50
28	6	303	NEX	O24-C25	-2.35	1.43	1.46
25	b	603	CLA	CMC-C2C	-2.35	1.46	1.50
25	p	307	CLA	MG-NB	-2.35	2.01	2.05
30	g	319	LHG	O7-C5	-2.35	1.41	1.46
25	C	602	CLA	C4B-NB	2.35	1.40	1.37
25	c	602	CLA	C4B-NB	2.35	1.40	1.37
25	a	607	CLA	C1B-C2B	2.35	1.48	1.43
26	7	303	0IE	C13-C12	-2.35	1.40	1.46
25	a	604	CLA	CMD-C2D	-2.35	1.46	1.50
26	g	302	0IE	C13-C12	-2.34	1.40	1.46
26	g	303	0IE	C13-C12	-2.34	1.40	1.46
28	N	303	NEX	O24-C25	-2.34	1.43	1.46
25	6	316	CLA	C3B-C4B	2.34	1.49	1.42
25	B	609	CLA	MG-NB	-2.34	2.01	2.05
25	A	607	CLA	C4B-NB	2.34	1.40	1.37
35	D	403	PHO	C4D-ND	-2.34	1.35	1.38
25	b	606	CLA	CMD-C2D	-2.34	1.46	1.50
24	y	312	CHL	CBD-CGD	-2.34	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	u	317	CLA	C3B-C4B	2.34	1.49	1.42
25	Y	314	CLA	CMD-C2D	-2.34	1.46	1.50
30	4	318	LHG	O8-C23	2.34	1.40	1.33
26	9	302	0IE	C13-C12	-2.34	1.40	1.46
26	G	303	0IE	C13-C12	-2.34	1.40	1.46
39	d	406	PL9	C31-C29	-2.34	1.46	1.51
26	5	303	0IE	C6-C7	-2.34	1.41	1.46
25	B	603	CLA	CMC-C2C	-2.34	1.46	1.50
25	c	608	CLA	CMC-C2C	-2.34	1.46	1.50
25	C	612	CLA	MG-NB	-2.34	2.01	2.05
26	4	302	0IE	C11-C12	2.34	1.41	1.35
26	2	303	0IE	C13-C12	-2.34	1.41	1.46
26	u	302	0IE	C13-C12	-2.34	1.41	1.46
25	C	608	CLA	CMC-C2C	-2.33	1.46	1.50
25	4	315	CLA	C3B-C4B	2.33	1.49	1.42
25	c	609	CLA	CMC-C2C	-2.33	1.46	1.50
25	s	412	CLA	CMD-C2D	-2.33	1.46	1.50
25	b	612	CLA	C4B-NB	2.33	1.40	1.37
26	G	302	0IE	C6-C7	-2.33	1.41	1.46
25	y	308	CLA	MG-NB	-2.33	2.01	2.05
25	b	601	CLA	MG-NB	-2.33	2.01	2.05
35	d	403	PHO	C4D-ND	-2.33	1.35	1.38
24	R	608	CHL	CBD-CGD	-2.33	1.49	1.52
25	A	605	CLA	C1B-C2B	2.33	1.48	1.43
25	c	604	CLA	MG-NB	-2.33	2.01	2.05
25	r	305	CLA	MG-NB	-2.33	2.01	2.05
25	7	316	CLA	MG-NB	-2.33	2.01	2.05
25	A	607	CLA	C1B-C2B	2.33	1.48	1.43
25	C	611	CLA	MG-NB	-2.33	2.01	2.05
30	G	319	LHG	O7-C5	-2.33	1.41	1.46
28	s	401	NEX	O24-C25	-2.33	1.43	1.46
26	1	302	0IE	C13-C12	-2.33	1.41	1.46
25	c	611	CLA	MG-NB	-2.33	2.01	2.05
26	3	303	0IE	C15-C16	2.33	1.41	1.35
30	4	318	LHG	O7-C5	-2.33	1.41	1.46
26	9	302	0IE	C8-C7	2.33	1.41	1.35
30	1	318	LHG	O8-C23	2.33	1.40	1.33
25	R	604	CLA	CMB-C2B	-2.33	1.46	1.50
31	s	416	8CT	C33-C32	-2.33	1.44	1.50
25	c	610	CLA	C1B-C2B	2.33	1.48	1.43
25	D	404	CLA	MG-NB	-2.33	2.01	2.05
31	C	613	8CT	C33-C32	-2.33	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	604	CLA	CMD-C2D	-2.33	1.46	1.50
25	C	607	CLA	C4B-NB	2.33	1.40	1.37
30	7	319	LHG	O7-C7	2.33	1.40	1.34
26	r	315	0IE	C17-C16	-2.33	1.41	1.46
25	1	315	CLA	C3B-C4B	2.32	1.49	1.42
25	B	605	CLA	CMD-C2D	-2.32	1.46	1.50
25	C	608	CLA	CMD-C2D	-2.32	1.46	1.50
26	2	303	0IE	C6-C7	-2.32	1.41	1.46
30	c	617	LHG	O7-C5	-2.32	1.41	1.46
25	A	610	CLA	C3B-C4B	2.32	1.49	1.42
24	p	305	CHL	CBD-CGD	-2.32	1.49	1.52
25	6	315	CLA	C3B-C4B	2.32	1.49	1.42
25	q	312	CLA	MG-NB	-2.32	2.01	2.05
25	Y	307	CLA	MG-NB	-2.32	2.01	2.05
26	u	302	0IE	C11-C12	2.32	1.41	1.35
25	B	608	CLA	CMB-C2B	-2.32	1.46	1.50
25	B	604	CLA	CMB-C2B	-2.32	1.46	1.50
26	9	302	0IE	C11-C12	2.32	1.41	1.35
25	u	314	CLA	CHC-C1C	2.32	1.43	1.38
25	A	605	CLA	CMB-C2B	-2.32	1.46	1.50
26	G	302	0IE	C17-C16	-2.32	1.41	1.46
26	3	303	0IE	C11-C12	2.32	1.41	1.35
26	4	302	0IE	C17-C16	-2.32	1.41	1.46
25	2	307	CLA	MG-NB	-2.32	2.01	2.05
25	5	315	CLA	MG-NB	-2.32	2.01	2.05
25	c	601	CLA	C4B-NB	2.32	1.40	1.37
25	B	613	CLA	CMB-C2B	-2.32	1.46	1.50
26	p	303	0IE	C17-C16	-2.32	1.41	1.46
25	y	315	CLA	CMD-C2D	-2.31	1.46	1.50
25	a	605	CLA	C1B-C2B	2.31	1.48	1.43
24	r	308	CHL	CBD-CGD	-2.31	1.49	1.52
25	b	608	CLA	CMB-C2B	-2.31	1.46	1.50
25	B	613	CLA	C1B-C2B	2.31	1.48	1.43
25	B	609	CLA	CMB-C2B	-2.31	1.46	1.50
26	3	303	0IE	C8-C7	2.31	1.41	1.35
25	C	610	CLA	C1B-C2B	2.31	1.48	1.43
25	3	314	CLA	C3B-C4B	2.31	1.49	1.42
26	n	302	0IE	C11-C12	2.31	1.41	1.35
24	p	313	CHL	CBD-CGD	-2.31	1.49	1.52
25	8	311	CLA	CMB-C2B	-2.31	1.46	1.50
26	n	302	0IE	C13-C12	-2.31	1.41	1.46
26	g	302	0IE	C6-C7	-2.31	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	n	302	0IE	C6-C7	-2.31	1.41	1.46
30	9	318	LHG	O8-C23	2.31	1.40	1.33
25	b	614	CLA	CMD-C2D	-2.31	1.46	1.50
26	N	302	0IE	C6-C7	-2.31	1.41	1.46
25	3	313	CLA	CHC-C1C	2.31	1.43	1.38
26	1	302	0IE	C6-C7	-2.31	1.41	1.46
25	B	601	CLA	MG-NB	-2.31	2.01	2.05
26	1	302	0IE	C11-C12	2.31	1.41	1.35
25	B	614	CLA	CMD-C2D	-2.31	1.46	1.50
25	1	314	CLA	C3B-C4B	2.31	1.49	1.42
25	q	306	CLA	MG-NB	-2.31	2.01	2.05
25	C	609	CLA	CMC-C2C	-2.31	1.46	1.50
25	b	607	CLA	CMB-C2B	-2.31	1.46	1.50
26	p	302	0IE	C11-C12	2.31	1.41	1.35
25	3	315	CLA	C3B-C4B	2.31	1.49	1.42
25	4	316	CLA	C3B-C4B	2.31	1.49	1.42
25	D	404	CLA	CMB-C2B	-2.31	1.46	1.50
25	c	605	CLA	C1B-C2B	2.31	1.48	1.43
24	R	607	CHL	CBD-CGD	-2.31	1.49	1.52
30	5	319	LHG	O8-C6	-2.31	1.40	1.45
26	7	303	0IE	C17-C16	-2.31	1.41	1.46
25	b	607	CLA	MG-NB	-2.31	2.01	2.05
25	b	604	CLA	CMD-C2D	-2.30	1.46	1.50
25	d	405	CLA	CMD-C2D	-2.30	1.46	1.50
30	N	318	LHG	O7-C7	2.30	1.40	1.34
25	s	405	CLA	MG-NB	-2.30	2.01	2.05
24	8	309	CHL	CBD-CGD	-2.30	1.49	1.52
24	q	311	CHL	CBD-CGD	-2.30	1.49	1.52
26	6	302	0IE	C8-C7	2.30	1.41	1.35
25	b	613	CLA	CMD-C2D	-2.30	1.46	1.50
25	q	312	CLA	CMB-C2B	-2.30	1.46	1.50
31	S	615	8CT	C33-C32	-2.30	1.44	1.50
26	1	302	0IE	C17-C16	-2.30	1.41	1.46
25	a	605	CLA	CMB-C2B	-2.30	1.46	1.50
25	S	604	CLA	MG-NB	-2.30	2.01	2.05
25	r	312	CLA	MG-NB	-2.30	2.01	2.05
25	g	314	CLA	C3B-C4B	2.30	1.49	1.42
25	b	605	CLA	MG-NB	-2.30	2.01	2.05
30	n	318	LHG	O8-C23	2.30	1.40	1.33
35	a	606	PHO	C3B-C2B	-2.30	1.37	1.40
26	7	302	0IE	C11-C12	2.30	1.41	1.35
26	3	302	0IE	C17-C16	-2.30	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	r	311	CLA	MG-NB	-2.30	2.01	2.05
31	x	601	8CT	C33-C32	-2.30	1.44	1.50
26	3	302	0IE	C8-C7	2.30	1.41	1.35
25	d	404	CLA	CMB-C2B	-2.30	1.46	1.50
26	3	303	0IE	C6-C7	-2.30	1.41	1.46
25	A	603	CLA	C1B-C2B	2.30	1.48	1.43
25	Y	313	CLA	CMD-C2D	-2.29	1.46	1.50
25	c	610	CLA	CMC-C2C	-2.29	1.46	1.50
39	D	406	PL9	C36-C34	-2.29	1.46	1.51
30	p	319	LHG	O7-C7	2.29	1.40	1.34
30	N	318	LHG	O8-C23	2.29	1.40	1.33
25	9	313	CLA	CHC-C1C	2.29	1.43	1.38
25	Y	315	CLA	CMB-C2B	-2.29	1.46	1.50
25	5	307	CLA	MG-NB	-2.29	2.01	2.05
30	9	318	LHG	O7-C5	-2.29	1.41	1.46
25	R	612	CLA	C3B-C4B	2.29	1.49	1.42
25	S	611	CLA	CMD-C2D	-2.29	1.46	1.50
25	Y	316	CLA	CMD-C2D	-2.29	1.46	1.50
31	a	608	8CT	C33-C32	-2.29	1.44	1.50
26	9	303	0IE	C8-C7	2.29	1.41	1.35
26	r	315	0IE	C8-C7	2.29	1.41	1.35
25	A	610	CLA	CHC-C1C	2.29	1.43	1.38
26	N	302	0IE	C11-C12	2.29	1.41	1.35
25	7	314	CLA	MG-NB	-2.29	2.01	2.05
25	b	614	CLA	CMB-C2B	-2.29	1.46	1.50
26	1	302	0IE	C8-C7	2.29	1.41	1.35
25	B	607	CLA	MG-NB	-2.29	2.01	2.05
25	9	315	CLA	C3B-C4B	2.29	1.49	1.42
25	C	606	CLA	C1B-C2B	2.29	1.48	1.43
25	6	313	CLA	CHC-C1C	2.29	1.43	1.38
25	6	314	CLA	C3B-C4B	2.29	1.49	1.42
26	7	302	0IE	C6-C7	-2.29	1.41	1.46
25	u	315	CLA	CHC-C1C	2.29	1.43	1.38
26	3	303	0IE	C17-C16	-2.29	1.41	1.46
26	2	303	0IE	C11-C12	2.29	1.41	1.35
25	8	306	CLA	CMB-C2B	-2.29	1.46	1.50
25	5	316	CLA	CMC-C2C	-2.29	1.46	1.50
30	2	319	LHG	O8-C6	-2.29	1.40	1.45
25	b	610	CLA	CMD-C2D	-2.29	1.46	1.50
25	R	604	CLA	MG-NB	-2.29	2.01	2.05
25	N	307	CLA	CHC-C1C	2.29	1.43	1.38
25	D	404	CLA	CMC-C2C	-2.28	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	y	306	CHL	CBD-CGD	-2.28	1.49	1.52
31	A	608	8CT	C33-C32	-2.28	1.44	1.50
25	B	606	CLA	CMD-C2D	-2.28	1.46	1.50
25	B	610	CLA	C1B-C2B	2.28	1.48	1.43
25	g	317	CLA	C3B-C4B	2.28	1.49	1.42
31	X	601	8CT	C33-C32	-2.28	1.44	1.50
26	G	302	0IE	C13-C12	-2.28	1.41	1.46
26	9	303	0IE	C17-C16	-2.28	1.41	1.46
25	D	405	CLA	CMD-C2D	-2.28	1.46	1.50
26	4	302	0IE	C15-C16	2.28	1.41	1.35
25	C	604	CLA	CMD-C2D	-2.28	1.46	1.50
25	G	308	CLA	C3B-C4B	2.28	1.49	1.42
26	4	302	0IE	C6-C7	-2.28	1.41	1.46
25	1	316	CLA	C3B-C4B	2.28	1.49	1.42
25	s	417	CLA	MG-NB	-2.28	2.01	2.05
25	b	610	CLA	C1B-C2B	2.28	1.48	1.43
26	6	302	0IE	C17-C16	-2.28	1.41	1.46
25	y	317	CLA	CMD-C2D	-2.28	1.46	1.50
25	c	609	CLA	CMD-C2D	-2.28	1.46	1.50
25	u	316	CLA	C3B-C4B	2.28	1.49	1.42
25	n	314	CLA	C3B-C4B	2.28	1.49	1.42
30	n	318	LHG	O7-C7	2.28	1.40	1.34
26	n	302	0IE	C15-C16	2.28	1.41	1.35
25	B	612	CLA	CMD-C2D	-2.28	1.46	1.50
25	A	604	CLA	CMD-C2D	-2.28	1.46	1.50
25	b	605	CLA	CMD-C2D	-2.28	1.46	1.50
25	d	404	CLA	CMC-C2C	-2.28	1.46	1.50
30	5	319	LHG	O8-C23	2.28	1.40	1.33
26	u	302	0IE	C6-C7	-2.28	1.41	1.46
25	A	605	CLA	CMD-C2D	-2.28	1.46	1.50
25	2	315	CLA	C3B-C4B	2.28	1.49	1.42
25	2	315	CLA	MG-NB	-2.28	2.01	2.05
25	b	611	CLA	C1B-C2B	2.28	1.48	1.43
25	B	610	CLA	CMB-C2B	-2.28	1.46	1.50
25	N	316	CLA	C3B-C4B	2.28	1.49	1.42
25	b	612	CLA	CMD-C2D	-2.28	1.46	1.50
25	1	306	CLA	C3B-C4B	2.28	1.49	1.42
25	n	316	CLA	C3B-C4B	2.28	1.49	1.42
25	C	616	CLA	CMB-C2B	-2.28	1.46	1.50
25	a	603	CLA	C4B-NB	2.28	1.40	1.37
25	G	314	CLA	C3B-C4B	2.28	1.49	1.42
25	c	606	CLA	C1B-C2B	2.28	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Y	311	CHL	CBD-CGD	-2.28	1.49	1.52
25	2	317	CLA	MG-NB	-2.28	2.01	2.05
25	a	610	CLA	C3B-C4B	2.28	1.49	1.42
24	Y	305	CHL	CBD-CGD	-2.28	1.49	1.52
25	q	305	CLA	CMB-C2B	-2.28	1.46	1.50
26	R	614	0IE	C8-C7	2.28	1.41	1.35
26	5	303	0IE	C11-C12	2.28	1.41	1.35
31	c	613	8CT	C33-C32	-2.28	1.44	1.50
26	9	302	0IE	C15-C16	2.28	1.41	1.35
25	y	314	CLA	CMD-C2D	-2.28	1.46	1.50
25	c	605	CLA	CMB-C2B	-2.28	1.46	1.50
25	a	607	CLA	C4B-NB	2.27	1.40	1.37
26	p	302	0IE	C6-C7	-2.27	1.41	1.46
26	p	302	0IE	C8-C7	2.27	1.41	1.35
26	R	614	0IE	C11-C12	2.27	1.41	1.35
30	9	318	LHG	O7-C7	2.27	1.40	1.34
25	4	316	CLA	CHC-C1C	2.27	1.43	1.38
24	2	306	CHL	CBD-CGD	-2.27	1.49	1.52
25	p	307	CLA	CMD-C2D	-2.27	1.46	1.50
26	R	614	0IE	C6-C7	-2.27	1.41	1.46
25	B	602	CLA	CMD-C2D	-2.27	1.46	1.50
25	C	610	CLA	CMB-C2B	-2.27	1.46	1.50
25	a	607	CLA	CMB-C2B	-2.27	1.46	1.50
25	c	608	CLA	CMD-C2D	-2.27	1.46	1.50
25	G	317	CLA	C3B-C4B	2.27	1.49	1.42
25	B	606	CLA	CMC-C2C	-2.27	1.46	1.50
26	G	302	0IE	C11-C12	2.27	1.41	1.35
25	g	315	CLA	C3B-C4B	2.27	1.49	1.42
25	a	603	CLA	C1B-C2B	2.27	1.48	1.43
25	c	606	CLA	CMD-C2D	-2.27	1.46	1.50
25	R	609	CLA	C3B-C4B	2.27	1.49	1.42
25	G	307	CLA	C3B-C4B	2.27	1.49	1.42
25	C	605	CLA	CMB-C2B	-2.27	1.46	1.50
25	c	607	CLA	CMB-C2B	-2.27	1.46	1.50
26	4	302	0IE	C8-C7	2.27	1.41	1.35
25	b	616	CLA	CMB-C2B	-2.27	1.46	1.50
25	n	307	CLA	C3B-C4B	2.27	1.49	1.42
25	1	316	CLA	CHC-C1C	2.27	1.43	1.38
25	B	605	CLA	CMB-C2B	-2.27	1.46	1.50
25	B	610	CLA	CMD-C2D	-2.27	1.46	1.50
30	G	319	LHG	O8-C23	2.27	1.40	1.33
26	7	302	0IE	C8-C7	2.27	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	605	CLA	C1B-C2B	2.27	1.48	1.43
25	G	317	CLA	CHC-C1C	2.27	1.43	1.38
26	r	315	0IE	C6-C7	-2.27	1.41	1.46
25	n	313	CLA	CHC-C1C	2.26	1.43	1.38
25	C	602	CLA	CMD-C2D	-2.26	1.46	1.50
25	b	613	CLA	CMB-C2B	-2.26	1.46	1.50
25	5	315	CLA	C3B-C4B	2.26	1.49	1.42
25	R	611	CLA	MG-NB	-2.26	2.01	2.05
25	G	314	CLA	CHC-C1C	2.26	1.43	1.38
25	r	310	CLA	CMC-C2C	-2.26	1.46	1.50
30	c	617	LHG	O7-C7	2.26	1.40	1.34
25	p	314	CLA	MG-NB	-2.26	2.01	2.05
25	8	305	CLA	CMB-C2B	-2.26	1.46	1.50
26	n	302	0IE	C8-C7	2.26	1.41	1.35
25	2	316	CLA	CMC-C2C	-2.26	1.46	1.50
25	y	315	CLA	CMB-C2B	-2.26	1.46	1.50
25	3	307	CLA	C3B-C4B	2.26	1.49	1.42
30	G	319	LHG	O7-C7	2.26	1.40	1.34
26	g	302	0IE	C11-C12	2.26	1.41	1.35
25	B	615	CLA	CMC-C2C	-2.26	1.46	1.50
25	5	308	CLA	C3B-C4B	2.26	1.49	1.42
25	C	609	CLA	C3B-C4B	2.26	1.49	1.42
25	b	602	CLA	CMD-C2D	-2.26	1.46	1.50
25	8	312	CLA	MG-NB	-2.26	2.01	2.05
25	B	611	CLA	C1B-C2B	2.26	1.48	1.43
25	D	405	CLA	CMB-C2B	-2.26	1.46	1.50
25	c	603	CLA	CMD-C2D	-2.26	1.46	1.50
25	C	607	CLA	CMB-C2B	-2.26	1.46	1.50
25	y	316	CLA	CMB-C2B	-2.26	1.46	1.50
25	b	610	CLA	CMB-C2B	-2.26	1.46	1.50
25	5	314	CLA	MG-NB	-2.26	2.01	2.05
25	b	613	CLA	C1B-C2B	2.26	1.48	1.43
25	g	317	CLA	CHC-C1C	2.26	1.43	1.38
25	G	315	CLA	C3B-C4B	2.26	1.49	1.42
25	g	308	CLA	C3B-C4B	2.26	1.49	1.42
25	2	308	CLA	MG-NB	-2.26	2.01	2.05
26	3	303	0IE	C13-C12	-2.26	1.41	1.46
25	c	612	CLA	CMD-C2D	-2.26	1.46	1.50
25	6	307	CLA	C3B-C4B	2.25	1.49	1.42
25	s	410	CLA	C3B-C4B	2.25	1.49	1.42
25	B	613	CLA	CMD-C2D	-2.25	1.46	1.50
26	1	302	0IE	C15-C16	2.25	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	603	CLA	C4B-NB	2.25	1.40	1.37
25	N	313	CLA	CHC-C1C	2.25	1.43	1.38
30	2	319	LHG	O8-C23	2.25	1.39	1.33
25	s	405	CLA	CMB-C2B	-2.25	1.46	1.50
26	N	302	0IE	C15-C16	2.25	1.41	1.35
25	C	601	CLA	C4B-NB	2.25	1.40	1.37
25	C	606	CLA	CMD-C2D	-2.25	1.46	1.50
25	b	605	CLA	CMB-C2B	-2.25	1.46	1.50
25	7	315	CLA	MG-NB	-2.25	2.01	2.05
25	s	417	CLA	C3B-C4B	2.25	1.49	1.42
24	p	306	CHL	CBD-CGD	-2.25	1.49	1.52
24	q	310	CHL	CBD-CGD	-2.25	1.49	1.52
25	B	607	CLA	CMB-C2B	-2.25	1.46	1.50
25	p	308	CLA	C3B-C4B	2.25	1.49	1.42
39	D	406	PL9	C31-C29	-2.25	1.46	1.51
31	C	614	8CT	C33-C32	-2.25	1.44	1.50
25	c	609	CLA	C3B-C4B	2.25	1.49	1.42
25	S	616	CLA	MG-NB	-2.25	2.01	2.05
25	B	614	CLA	CMB-C2B	-2.25	1.46	1.50
25	C	609	CLA	CMD-C2D	-2.25	1.46	1.50
25	S	609	CLA	MG-NB	-2.25	2.01	2.05
25	R	610	CLA	C3B-C4B	2.25	1.49	1.42
25	S	604	CLA	CMB-C2B	-2.25	1.46	1.50
25	C	612	CLA	CMD-C2D	-2.25	1.46	1.50
26	6	302	0IE	C11-C12	2.25	1.41	1.35
25	q	305	CLA	CMD-C2D	-2.25	1.46	1.50
30	C	617	LHG	O7-C7	2.25	1.40	1.34
25	c	611	CLA	CMC-C2C	-2.25	1.46	1.50
24	s	408	CHL	CBD-CGD	-2.25	1.49	1.52
25	N	307	CLA	C3B-C4B	2.25	1.49	1.42
25	u	308	CLA	C3B-C4B	2.25	1.49	1.42
31	s	415	8CT	C33-C32	-2.25	1.44	1.50
25	r	310	CLA	C3B-C4B	2.25	1.49	1.42
26	G	302	0IE	C8-C7	2.25	1.41	1.35
25	u	307	CLA	C3B-C4B	2.25	1.49	1.42
25	C	612	CLA	CMB-C2B	-2.25	1.46	1.50
25	1	314	CLA	CHC-C1C	2.25	1.43	1.38
25	y	307	CLA	CMB-C2B	-2.25	1.46	1.50
25	c	602	CLA	CMD-C2D	-2.25	1.46	1.50
25	7	317	CLA	C3B-C4B	2.25	1.49	1.42
25	c	616	CLA	CMB-C2B	-2.24	1.46	1.50
30	a	612	LHG	O8-C23	2.24	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	N	308	CHL	CBD-CGD	-2.24	1.49	1.52
25	N	314	CLA	C3B-C4B	2.24	1.49	1.42
25	Y	314	CLA	CMB-C2B	-2.24	1.46	1.50
25	R	610	CLA	MG-NB	-2.24	2.01	2.05
25	S	609	CLA	C3B-C4B	2.24	1.49	1.42
25	p	317	CLA	C3B-C4B	2.24	1.49	1.42
25	c	611	CLA	CMB-C2B	-2.24	1.46	1.50
25	g	315	CLA	CHC-C1C	2.24	1.43	1.38
25	b	609	CLA	CMD-C2D	-2.24	1.46	1.50
25	a	605	CLA	CMD-C2D	-2.24	1.46	1.50
25	r	310	CLA	CMD-C2D	-2.24	1.46	1.50
30	4	318	LHG	O7-C7	2.24	1.40	1.34
25	n	307	CLA	CHC-C1C	2.24	1.43	1.38
25	B	611	CLA	CMD-C2D	-2.24	1.46	1.50
25	9	306	CLA	C3B-C4B	2.24	1.49	1.42
25	c	610	CLA	CMB-C2B	-2.24	1.46	1.50
26	5	303	OIE	C15-C16	2.24	1.41	1.35
26	g	302	OIE	C8-C7	2.24	1.41	1.35
25	g	307	CLA	CHC-C1C	2.24	1.43	1.38
25	a	610	CLA	CHC-C1C	2.24	1.43	1.38
25	b	606	CLA	CMC-C2C	-2.24	1.46	1.50
25	c	604	CLA	CMD-C2D	-2.24	1.46	1.50
25	g	307	CLA	C3B-C4B	2.24	1.49	1.42
25	R	603	CLA	MG-NB	-2.24	2.01	2.05
30	p	319	LHG	O8-C23	2.24	1.39	1.33
25	S	612	CLA	CMD-C2D	-2.24	1.46	1.50
25	c	612	CLA	CMB-C2B	-2.24	1.46	1.50
25	5	314	CLA	C3B-C4B	2.24	1.49	1.42
25	q	313	CLA	MG-NB	-2.24	2.01	2.05
25	2	308	CLA	C3B-C4B	2.24	1.49	1.42
26	N	302	OIE	C17-C16	-2.24	1.41	1.46
26	u	302	OIE	C15-C16	2.24	1.41	1.35
30	g	319	LHG	O8-C23	2.24	1.39	1.33
25	4	306	CLA	C3B-C4B	2.24	1.49	1.42
30	A	612	LHG	O8-C23	2.24	1.39	1.33
26	9	302	OIE	C17-C16	-2.24	1.41	1.46
26	9	303	OIE	C13-C12	-2.24	1.41	1.46
24	7	310	CHL	CBD-CGD	-2.24	1.49	1.52
25	c	607	CLA	CMC-C2C	-2.24	1.46	1.50
25	n	314	CLA	CHC-C1C	2.24	1.43	1.38
25	r	304	CLA	MG-NB	-2.24	2.01	2.05
25	Y	306	CLA	CMD-C2D	-2.24	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	607	CLA	CMB-C2B	-2.24	1.46	1.50
25	8	305	CLA	CMD-C2D	-2.24	1.46	1.50
25	b	615	CLA	CMD-C2D	-2.24	1.46	1.50
26	3	302	0IE	C11-C12	2.24	1.41	1.35
25	C	605	CLA	CMC-C2C	-2.24	1.46	1.50
25	C	612	CLA	CMC-C2C	-2.24	1.46	1.50
25	u	317	CLA	CMD-C2D	-2.24	1.46	1.50
25	q	315	CLA	C3B-C4B	2.24	1.49	1.42
25	2	314	CLA	C3B-C4B	2.24	1.49	1.42
25	C	610	CLA	CMC-C2C	-2.23	1.46	1.50
25	a	607	CLA	CMD-C2D	-2.23	1.46	1.50
30	7	319	LHG	O8-C23	2.23	1.39	1.33
31	S	614	8CT	C30-C29	2.23	1.53	1.50
25	B	615	CLA	CMD-C2D	-2.23	1.46	1.50
25	C	611	CLA	CMC-C2C	-2.23	1.46	1.50
25	r	311	CLA	C3B-C4B	2.23	1.49	1.42
25	1	307	CLA	CMB-C2B	-2.23	1.46	1.50
25	p	315	CLA	MG-NB	-2.23	2.01	2.05
26	r	315	0IE	C11-C12	2.23	1.41	1.35
25	B	615	CLA	C3B-C4B	2.23	1.49	1.42
25	q	306	CLA	CMB-C2B	-2.23	1.46	1.50
26	5	303	0IE	C8-C7	2.23	1.41	1.35
25	s	410	CLA	MG-NB	-2.23	2.01	2.05
25	d	405	CLA	CMB-C2B	-2.23	1.46	1.50
25	G	315	CLA	CHC-C1C	2.23	1.43	1.38
25	2	314	CLA	MG-NB	-2.23	2.01	2.05
30	g	319	LHG	O7-C7	2.23	1.40	1.34
25	g	317	CLA	MG-NB	-2.23	2.01	2.05
25	S	610	CLA	CMD-C2D	-2.23	1.46	1.50
25	n	315	CLA	C3B-C4B	2.23	1.49	1.42
26	u	302	0IE	C17-C16	-2.23	1.41	1.46
25	B	616	CLA	CMD-C2D	-2.23	1.46	1.50
25	s	413	CLA	CMD-C2D	-2.23	1.46	1.50
25	S	616	CLA	C3B-C4B	2.23	1.49	1.42
25	p	316	CLA	CMD-C2D	-2.23	1.46	1.50
25	4	306	CLA	MG-NB	-2.23	2.01	2.05
24	8	304	CHL	CBD-CGD	-2.23	1.49	1.52
25	2	314	CLA	CHC-C1C	2.23	1.42	1.38
25	g	314	CLA	CHC-C1C	2.23	1.42	1.38
31	S	614	8CT	C33-C32	-2.23	1.44	1.50
25	B	605	CLA	C3B-C4B	2.23	1.49	1.42
25	B	609	CLA	CMD-C2D	-2.23	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	609	CLA	CMC-C2C	-2.22	1.46	1.50
25	C	603	CLA	CMD-C2D	-2.22	1.46	1.50
25	7	307	CLA	CMD-C2D	-2.22	1.46	1.50
26	u	303	0IE	C17-C16	-2.22	1.41	1.46
25	Y	306	CLA	CMB-C2B	-2.22	1.46	1.50
25	6	307	CLA	CHC-C1C	2.22	1.42	1.38
25	3	306	CLA	MG-NB	-2.22	2.01	2.05
25	5	308	CLA	MG-NB	-2.22	2.01	2.05
25	G	316	CLA	C3B-C4B	2.22	1.49	1.42
25	B	610	CLA	CMC-C2C	-2.22	1.46	1.50
25	B	616	CLA	CMB-C2B	-2.22	1.46	1.50
25	b	610	CLA	CMC-C2C	-2.22	1.46	1.50
25	b	608	CLA	CMD-C2D	-2.22	1.46	1.50
25	R	609	CLA	MG-NB	-2.22	2.01	2.05
24	r	309	CHL	CBD-CGD	-2.22	1.49	1.52
26	n	302	0IE	C17-C16	-2.22	1.41	1.46
25	c	605	CLA	CMC-C2C	-2.22	1.46	1.50
25	8	314	CLA	MG-NB	-2.22	2.01	2.05
25	u	316	CLA	CHC-C1C	2.22	1.42	1.38
25	9	307	CLA	C3B-C4B	2.22	1.49	1.42
25	R	603	CLA	CMD-C2D	-2.22	1.46	1.50
25	p	314	CLA	CMB-C2B	-2.22	1.46	1.50
25	7	316	CLA	CMD-C2D	-2.22	1.46	1.50
25	7	308	CLA	C3B-C4B	2.22	1.49	1.42
25	S	610	CLA	CMB-C2B	-2.22	1.46	1.50
25	C	606	CLA	CMC-C2C	-2.22	1.46	1.50
25	b	615	CLA	CMC-C2C	-2.22	1.46	1.50
25	c	606	CLA	CMC-C2C	-2.22	1.46	1.50
25	3	314	CLA	CHC-C1C	2.22	1.42	1.38
25	7	314	CLA	CMB-C2B	-2.22	1.46	1.50
37	c	619	DGD	O2G-C2G	-2.22	1.41	1.46
25	8	314	CLA	C3B-C4B	2.22	1.49	1.42
25	A	607	CLA	CMD-C2D	-2.22	1.46	1.50
25	8	314	CLA	CHC-C1C	2.22	1.42	1.38
25	b	611	CLA	CMD-C2D	-2.22	1.46	1.50
25	N	306	CLA	CHC-C1C	2.22	1.42	1.38
25	R	613	CLA	CMB-C2B	-2.22	1.46	1.50
24	5	306	CHL	CBD-CGD	-2.22	1.49	1.52
25	5	317	CLA	MG-NB	-2.22	2.01	2.05
30	1	318	LHG	O7-C7	2.22	1.40	1.34
26	9	302	0IE	C6-C7	-2.22	1.41	1.46
25	C	603	CLA	CMB-C2B	-2.22	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	7	315	CLA	CMB-C2B	-2.22	1.46	1.50
25	9	315	CLA	CHC-C1C	2.22	1.42	1.38
25	b	610	CLA	C3B-C4B	2.22	1.49	1.42
25	s	412	CLA	CMB-C2B	-2.21	1.46	1.50
26	9	303	0IE	C6-C7	-2.21	1.41	1.46
31	c	614	8CT	C33-C32	-2.21	1.44	1.50
25	N	316	CLA	CHC-C1C	2.21	1.42	1.38
24	q	308	CHL	CBD-CGD	-2.21	1.49	1.52
25	p	308	CLA	MG-NB	-2.21	2.01	2.05
25	b	613	CLA	C3B-C4B	2.21	1.49	1.42
25	g	316	CLA	C3B-C4B	2.21	1.49	1.42
27	r	316	XAT	O4-C5	-2.21	1.43	1.46
24	q	304	CHL	CBD-CGD	-2.21	1.49	1.52
25	s	411	CLA	CMD-C2D	-2.21	1.46	1.50
25	4	314	CLA	CHC-C1C	2.21	1.42	1.38
25	3	307	CLA	CHC-C1C	2.21	1.42	1.38
26	p	302	0IE	C15-C16	2.21	1.40	1.35
25	b	615	CLA	CMB-C2B	-2.21	1.46	1.50
25	C	609	CLA	C1B-C2B	2.21	1.48	1.43
25	B	608	CLA	CMD-C2D	-2.21	1.46	1.50
25	Y	316	CLA	CMB-C2B	-2.21	1.46	1.50
25	2	316	CLA	C3B-C4B	2.21	1.49	1.42
25	q	315	CLA	MG-NB	-2.21	2.01	2.05
25	q	313	CLA	C3B-C4B	2.21	1.49	1.42
24	S	607	CHL	CBD-CGD	-2.21	1.49	1.52
25	8	312	CLA	CMD-C2D	-2.21	1.46	1.50
25	b	607	CLA	CMD-C2D	-2.21	1.46	1.50
25	9	314	CLA	CHC-C1C	2.21	1.42	1.38
24	p	310	CHL	CBD-CGD	-2.21	1.49	1.52
25	4	307	CLA	CMB-C2B	-2.21	1.46	1.50
26	g	302	0IE	C15-C16	2.21	1.40	1.35
24	7	305	CHL	CBD-CGD	-2.21	1.49	1.52
25	5	314	CLA	CHC-C1C	2.21	1.42	1.38
25	4	307	CLA	MG-NB	-2.21	2.01	2.05
25	b	616	CLA	CMD-C2D	-2.21	1.46	1.50
25	c	601	CLA	CMC-C2C	-2.21	1.46	1.50
26	2	303	0IE	C15-C16	2.20	1.40	1.35
25	6	315	CLA	CHC-C1C	2.20	1.42	1.38
25	y	317	CLA	CMB-C2B	-2.20	1.46	1.50
26	7	302	0IE	C15-C16	2.20	1.40	1.35
25	1	307	CLA	C3B-C4B	2.20	1.49	1.42
25	Y	316	CLA	CMC-C2C	-2.20	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	611	CLA	C3B-C4B	2.20	1.49	1.42
25	C	611	CLA	CMB-C2B	-2.20	1.46	1.50
25	B	610	CLA	C3B-C4B	2.20	1.49	1.42
25	b	615	CLA	C3B-C4B	2.20	1.49	1.42
25	G	316	CLA	CHC-C1C	2.20	1.42	1.38
25	8	312	CLA	C3B-C4B	2.20	1.49	1.42
25	3	306	CLA	C3B-C4B	2.20	1.49	1.42
25	q	315	CLA	CHC-C1C	2.20	1.42	1.38
25	c	608	CLA	C1B-C2B	2.20	1.48	1.43
25	N	315	CLA	C3B-C4B	2.20	1.49	1.42
26	G	302	0IE	C15-C16	2.20	1.40	1.35
25	7	316	CLA	CMC-C2C	-2.20	1.46	1.50
25	n	316	CLA	CHC-C1C	2.20	1.42	1.38
25	1	306	CLA	MG-NB	-2.20	2.01	2.05
25	p	314	CLA	C3B-C4B	2.20	1.49	1.42
25	Y	313	CLA	CMC-C2C	-2.20	1.46	1.50
25	s	411	CLA	CMB-C2B	-2.20	1.46	1.50
25	7	317	CLA	CMB-C2B	-2.20	1.46	1.50
25	6	314	CLA	CHC-C1C	2.20	1.42	1.38
25	C	601	CLA	CMC-C2C	-2.20	1.46	1.50
25	y	307	CLA	CMD-C2D	-2.20	1.46	1.50
25	c	612	CLA	CMC-C2C	-2.20	1.46	1.50
25	3	316	CLA	CHC-C1C	2.20	1.42	1.38
25	B	613	CLA	C3B-C4B	2.20	1.49	1.42
25	5	316	CLA	MG-NB	-2.20	2.01	2.05
25	R	609	CLA	CMD-C2D	-2.20	1.46	1.50
25	5	315	CLA	CMB-C2B	-2.20	1.46	1.50
25	S	611	CLA	CMB-C2B	-2.20	1.46	1.50
25	s	413	CLA	CMB-C2B	-2.20	1.46	1.50
26	6	302	0IE	C15-C16	2.20	1.40	1.35
25	C	611	CLA	C3B-C4B	2.20	1.49	1.42
25	c	604	CLA	CMB-C2B	-2.20	1.46	1.50
25	u	308	CLA	CHC-C1C	2.20	1.42	1.38
25	c	611	CLA	C3B-C4B	2.20	1.49	1.42
26	N	302	0IE	C8-C7	2.20	1.40	1.35
25	p	315	CLA	CMD-C2D	-2.19	1.46	1.50
25	7	315	CLA	CMD-C2D	-2.19	1.46	1.50
25	G	316	CLA	MG-NB	-2.19	2.01	2.05
24	7	306	CHL	CBD-CGD	-2.19	1.49	1.52
25	5	316	CLA	C3B-C4B	2.19	1.49	1.42
25	Y	314	CLA	CMC-C2C	-2.19	1.46	1.50
25	C	608	CLA	C1B-C2B	2.19	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	u	303	0IE	C6-C7	-2.19	1.41	1.46
25	G	317	CLA	MG-NB	-2.19	2.01	2.05
25	r	310	CLA	MG-NB	-2.19	2.01	2.05
25	q	312	CLA	C3B-C4B	2.19	1.49	1.42
25	q	314	CLA	C3B-C4B	2.19	1.49	1.42
25	l	315	CLA	CHC-C1C	2.19	1.42	1.38
25	9	306	CLA	CHC-C1C	2.19	1.42	1.38
25	b	605	CLA	C3B-C4B	2.19	1.49	1.42
25	N	306	CLA	MG-NB	-2.19	2.01	2.05
26	2	303	0IE	C8-C7	2.19	1.40	1.35
24	S	608	CHL	CBD-CGD	-2.19	1.49	1.52
25	r	313	CLA	C3B-C4B	2.19	1.49	1.42
25	C	616	CLA	CMC-C2C	-2.19	1.46	1.50
25	R	612	CLA	CMD-C2D	-2.19	1.46	1.50
25	c	609	CLA	C1B-C2B	2.19	1.48	1.43
25	B	602	CLA	CMB-C2B	-2.19	1.46	1.50
25	r	312	CLA	CHC-C1C	2.19	1.42	1.38
25	B	615	CLA	CMB-C2B	-2.19	1.46	1.50
25	N	306	CLA	C3B-C4B	2.19	1.49	1.42
25	y	317	CLA	CMC-C2C	-2.19	1.46	1.50
27	R	615	XAT	O4-C5	-2.19	1.43	1.46
25	l	307	CLA	MG-NB	-2.19	2.01	2.05
25	A	610	CLA	CMD-C2D	-2.19	1.46	1.50
26	g	303	0IE	C11-C12	2.19	1.40	1.35
25	b	612	CLA	CMC-C2C	-2.19	1.46	1.50
25	a	610	CLA	CMD-C2D	-2.19	1.46	1.50
30	Y	318	LHG	O8-C23	2.19	1.39	1.33
24	s	409	CHL	CBD-CGD	-2.19	1.49	1.52
25	S	609	CLA	CMD-C2D	-2.19	1.46	1.50
25	2	315	CLA	CMB-C2B	-2.18	1.46	1.50
25	b	601	CLA	CMD-C2D	-2.18	1.46	1.50
25	8	313	CLA	CMD-C2D	-2.18	1.46	1.50
25	C	604	CLA	CMC-C2C	-2.18	1.46	1.50
25	C	607	CLA	CMC-C2C	-2.18	1.46	1.50
25	c	604	CLA	CMC-C2C	-2.18	1.46	1.50
26	r	315	0IE	C15-C16	2.18	1.40	1.35
39	D	406	PL9	C46-C44	-2.18	1.46	1.51
25	g	316	CLA	MG-NB	-2.18	2.01	2.05
25	2	315	CLA	CMD-C2D	-2.18	1.46	1.50
24	s	407	CHL	CBD-CGD	-2.18	1.49	1.52
25	p	316	CLA	CMC-C2C	-2.18	1.46	1.50
25	u	307	CLA	CHC-C1C	2.18	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Y	307	CLA	CMB-C2B	-2.18	1.46	1.50
26	p	303	0IE	C15-C16	2.18	1.40	1.35
25	y	314	CLA	CMC-C2C	-2.18	1.46	1.50
25	G	308	CLA	CHC-C1C	2.18	1.42	1.38
25	8	306	CLA	CMD-C2D	-2.18	1.46	1.50
25	q	306	CLA	CMD-C2D	-2.18	1.46	1.50
25	6	306	CLA	MG-NB	-2.18	2.01	2.05
25	p	317	CLA	MG-NB	-2.18	2.01	2.05
25	s	404	CLA	CMD-C2D	-2.18	1.46	1.50
35	A	606	PHO	CBD-CGD	-2.18	1.49	1.52
25	2	316	CLA	CMD-C2D	-2.18	1.46	1.50
25	N	314	CLA	CHC-C1C	2.18	1.42	1.38
25	6	314	CLA	MG-NB	-2.18	2.01	2.05
25	n	306	CLA	MG-NB	-2.18	2.01	2.05
25	y	314	CLA	C3B-C4B	2.18	1.49	1.42
30	y	319	LHG	O8-C23	2.18	1.39	1.33
24	1	312	CHL	CBD-CGD	-2.18	1.49	1.52
39	d	406	PL9	C36-C34	-2.18	1.46	1.51
25	n	306	CLA	CHC-C1C	2.18	1.42	1.38
25	3	307	CLA	MG-NB	-2.18	2.01	2.05
25	5	315	CLA	CMD-C2D	-2.18	1.46	1.50
25	p	315	CLA	CMB-C2B	-2.18	1.46	1.50
24	2	313	CHL	CBD-CGD	-2.18	1.49	1.52
25	G	308	CLA	MG-NB	-2.18	2.01	2.05
25	9	307	CLA	CHC-C1C	2.17	1.42	1.38
25	4	307	CLA	C3B-C4B	2.17	1.49	1.42
25	G	315	CLA	MG-NB	-2.17	2.01	2.05
25	Y	307	CLA	CMD-C2D	-2.17	1.46	1.50
24	S	606	CHL	CBD-CGD	-2.17	1.49	1.52
25	S	612	CLA	CMB-C2B	-2.17	1.46	1.50
25	C	604	CLA	CMB-C2B	-2.17	1.46	1.50
25	g	316	CLA	CHC-C1C	2.17	1.42	1.38
25	6	306	CLA	C3B-C4B	2.17	1.49	1.42
25	c	603	CLA	CMB-C2B	-2.17	1.46	1.50
25	c	611	CLA	CMD-C2D	-2.17	1.46	1.50
25	c	616	CLA	CMC-C2C	-2.17	1.46	1.50
25	Y	313	CLA	C3B-C4B	2.17	1.49	1.42
25	R	604	CLA	CMD-C2D	-2.17	1.46	1.50
25	C	603	CLA	CMC-C2C	-2.17	1.46	1.50
25	r	313	CLA	CMD-C2D	-2.17	1.46	1.50
25	2	316	CLA	MG-NB	-2.17	2.01	2.05
25	3	314	CLA	MG-NB	-2.17	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	y	311	CHL	CBD-CGD	-2.17	1.49	1.52
25	R	613	CLA	CHC-C1C	2.17	1.42	1.38
30	A	601	LHG	O8-C23	2.17	1.39	1.33
25	A	605	CLA	CMC-C2C	-2.17	1.46	1.50
25	a	607	CLA	CMC-C2C	-2.17	1.46	1.50
25	7	308	CLA	MG-NB	-2.17	2.01	2.05
24	y	310	CHL	CBD-CGD	-2.17	1.49	1.52
25	n	306	CLA	C3B-C4B	2.17	1.49	1.42
25	b	607	CLA	C3B-C4B	2.17	1.49	1.42
25	r	312	CLA	C3B-C4B	2.17	1.49	1.42
39	d	406	PL9	C16-C14	-2.17	1.46	1.51
25	5	317	CLA	C3B-C4B	2.17	1.49	1.42
25	3	315	CLA	MG-NB	-2.17	2.01	2.05
25	u	307	CLA	MG-NB	-2.17	2.01	2.05
25	R	611	CLA	CHC-C1C	2.17	1.42	1.38
24	S	602	CHL	CBD-CGD	-2.17	1.49	1.52
24	Y	310	CHL	CBD-CGD	-2.17	1.49	1.52
25	5	307	CLA	CMD-C2D	-2.17	1.46	1.50
25	y	308	CLA	CMB-C2B	-2.17	1.46	1.50
25	b	612	CLA	C1B-C2B	2.17	1.48	1.43
25	g	308	CLA	CHC-C1C	2.17	1.42	1.38
24	4	312	CHL	CBD-CGD	-2.17	1.49	1.52
25	N	315	CLA	CHC-C1C	2.17	1.42	1.38
25	C	611	CLA	CMD-C2D	-2.17	1.46	1.50
30	2	319	LHG	O7-C7	2.17	1.40	1.34
25	G	307	CLA	CHC-C1C	2.17	1.42	1.38
26	G	303	0IE	C11-C12	2.17	1.40	1.35
25	p	317	CLA	CMD-C2D	-2.17	1.46	1.50
25	B	601	CLA	CMB-C2B	-2.16	1.46	1.50
25	5	307	CLA	CMB-C2B	-2.16	1.46	1.50
25	B	601	CLA	CMD-C2D	-2.16	1.46	1.50
25	a	604	CLA	CMC-C2C	-2.16	1.46	1.50
26	G	303	0IE	C15-C16	2.16	1.40	1.35
26	7	303	0IE	C11-C12	2.16	1.40	1.35
31	s	415	8CT	C30-C29	2.16	1.53	1.50
26	R	614	0IE	C15-C16	2.16	1.40	1.35
25	6	315	CLA	MG-NB	-2.16	2.01	2.05
25	5	308	CLA	CHC-C1C	2.16	1.42	1.38
25	q	313	CLA	CMD-C2D	-2.16	1.46	1.50
26	g	303	0IE	C15-C16	2.16	1.40	1.35
25	5	316	CLA	CMD-C2D	-2.16	1.46	1.50
25	S	610	CLA	CMC-C2C	-2.16	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	7	314	CLA	C3B-C4B	2.16	1.49	1.42
25	n	307	CLA	MG-NB	-2.16	2.01	2.05
25	r	312	CLA	CMB-C2B	-2.16	1.46	1.50
25	8	306	CLA	C3B-C4B	2.16	1.49	1.42
25	R	604	CLA	C3B-C4B	2.16	1.49	1.42
25	S	603	CLA	CMD-C2D	-2.16	1.46	1.50
24	5	313	CHL	CBD-CGD	-2.16	1.49	1.52
25	S	612	CLA	CMC-C2C	-2.16	1.46	1.50
25	b	607	CLA	CMC-C2C	-2.16	1.46	1.50
26	7	303	0IE	C15-C16	2.16	1.40	1.35
25	2	317	CLA	C3B-C4B	2.16	1.49	1.42
25	8	311	CLA	C3B-C4B	2.16	1.49	1.42
26	g	303	0IE	C8-C7	2.16	1.40	1.35
25	y	308	CLA	CMD-C2D	-2.16	1.46	1.50
24	5	310	CHL	CBD-CGD	-2.16	1.49	1.52
25	r	314	CLA	CMB-C2B	-2.16	1.46	1.50
25	7	317	CLA	MG-NB	-2.16	2.01	2.05
25	S	616	CLA	CHC-C1C	2.16	1.42	1.38
25	N	315	CLA	CMD-C2D	-2.15	1.46	1.50
25	r	304	CLA	CMD-C2D	-2.15	1.46	1.50
25	y	315	CLA	CMC-C2C	-2.15	1.46	1.50
25	3	315	CLA	CHC-C1C	2.15	1.42	1.38
25	A	604	CLA	CMC-C2C	-2.15	1.46	1.50
25	7	317	CLA	CHC-C1C	2.15	1.42	1.38
26	G	303	0IE	C8-C7	2.15	1.40	1.35
25	A	603	CLA	CMB-C2B	-2.15	1.46	1.50
25	a	603	CLA	CMB-C2B	-2.15	1.46	1.50
30	5	319	LHG	O7-C7	2.15	1.40	1.34
25	B	607	CLA	CMD-C2D	-2.15	1.46	1.50
25	8	313	CLA	C3B-C4B	2.15	1.49	1.42
25	B	607	CLA	CMC-C2C	-2.15	1.46	1.50
25	u	316	CLA	MG-NB	-2.15	2.01	2.05
31	V	401	8CT	C33-C32	-2.15	1.44	1.50
25	6	307	CLA	MG-NB	-2.15	2.01	2.05
25	2	308	CLA	CHC-C1C	2.15	1.42	1.38
25	2	307	CLA	CMD-C2D	-2.15	1.46	1.50
25	S	603	CLA	CMB-C2B	-2.15	1.46	1.50
25	q	314	CLA	CMD-C2D	-2.15	1.46	1.50
25	b	601	CLA	CMB-C2B	-2.15	1.46	1.50
30	c	617	LHG	O8-C23	2.15	1.39	1.33
24	8	308	CHL	CBD-CGD	-2.15	1.49	1.52
25	8	314	CLA	CMD-C2D	-2.15	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	g	315	CLA	MG-NB	-2.15	2.01	2.05
25	n	315	CLA	CMC-C2C	-2.15	1.46	1.50
25	3	306	CLA	CHC-C1C	2.15	1.42	1.38
25	6	316	CLA	CHC-C1C	2.15	1.42	1.38
25	N	315	CLA	MG-NB	-2.15	2.01	2.05
25	9	306	CLA	MG-NB	-2.15	2.01	2.05
26	3	302	0IE	C15-C16	2.15	1.40	1.35
25	G	316	CLA	CMD-C2D	-2.15	1.46	1.50
25	B	608	CLA	C3B-C4B	2.15	1.49	1.42
25	b	608	CLA	C3B-C4B	2.15	1.49	1.42
25	7	315	CLA	C3B-C4B	2.15	1.49	1.42
24	6	304	CHL	CBD-CGD	-2.15	1.49	1.52
25	N	313	CLA	MG-NB	-2.15	2.01	2.05
25	s	410	CLA	CMB-C2B	-2.15	1.46	1.50
25	s	413	CLA	CMC-C2C	-2.15	1.46	1.50
25	7	317	CLA	CMD-C2D	-2.14	1.46	1.50
25	7	308	CLA	CMB-C2B	-2.14	1.46	1.50
25	c	612	CLA	C3B-C4B	2.14	1.49	1.42
25	b	602	CLA	C3B-C4B	2.14	1.49	1.42
30	y	319	LHG	O7-C7	2.14	1.40	1.34
25	n	315	CLA	CHC-C1C	2.14	1.42	1.38
25	3	315	CLA	CMC-C2C	-2.14	1.46	1.50
25	Y	307	CLA	CMC-C2C	-2.14	1.46	1.50
25	8	311	CLA	CMD-C2D	-2.14	1.46	1.50
25	n	315	CLA	CMD-C2D	-2.14	1.46	1.50
25	b	604	CLA	CMC-C2C	-2.14	1.46	1.50
25	q	306	CLA	C3B-C4B	2.14	1.49	1.42
32	B	618	SQD	O2-C2	-2.14	1.37	1.43
25	R	610	CLA	CHC-C1C	2.14	1.42	1.38
30	a	601	LHG	O8-C23	2.14	1.39	1.33
25	Y	316	CLA	C3B-C4B	2.14	1.49	1.42
25	G	317	CLA	CMD-C2D	-2.14	1.46	1.50
35	a	606	PHO	CBD-CGD	-2.14	1.49	1.52
25	Y	307	CLA	CHC-C1C	2.14	1.42	1.38
30	C	617	LHG	O8-C23	2.14	1.39	1.33
31	T	101	8CT	C33-C32	-2.14	1.44	1.50
26	q	302	0IE	C11-C12	2.14	1.40	1.35
25	s	404	CLA	CMB-C2B	-2.14	1.46	1.50
25	Y	306	CLA	CMC-C2C	-2.14	1.46	1.50
25	q	312	CLA	CMD-C2D	-2.14	1.46	1.50
25	N	314	CLA	MG-NB	-2.14	2.01	2.05
30	4	318	LHG	P-O6	2.14	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	S	604	CLA	CMD-C2D	-2.14	1.46	1.50
25	B	608	CLA	CMC-C2C	-2.14	1.46	1.50
25	B	607	CLA	C3B-C4B	2.14	1.49	1.42
25	r	312	CLA	CMD-C2D	-2.14	1.46	1.50
25	b	607	CLA	CHC-C1C	2.14	1.42	1.38
25	6	316	CLA	MG-NB	-2.14	2.01	2.05
25	B	611	CLA	C3B-C4B	2.14	1.49	1.42
25	4	306	CLA	CHC-C1C	2.14	1.42	1.38
25	s	410	CLA	CMD-C2D	-2.14	1.46	1.50
25	p	308	CLA	CMD-C2D	-2.14	1.46	1.50
25	s	412	CLA	CMC-C2C	-2.14	1.46	1.50
25	y	317	CLA	C3B-C4B	2.14	1.49	1.42
25	4	306	CLA	CMD-C2D	-2.14	1.46	1.50
24	2	310	CHL	CBD-CGD	-2.14	1.49	1.52
26	p	303	0IE	C11-C12	2.14	1.40	1.35
25	2	307	CLA	C3B-C4B	2.14	1.49	1.42
25	7	308	CLA	CHC-C1C	2.14	1.42	1.38
25	B	612	CLA	C1B-C2B	2.14	1.48	1.43
25	N	316	CLA	MG-NB	-2.14	2.01	2.05
25	S	609	CLA	CMB-C2B	-2.14	1.46	1.50
25	b	602	CLA	CMB-C2B	-2.14	1.46	1.50
25	b	614	CLA	CMC-C2C	-2.13	1.46	1.50
26	u	303	0IE	C13-C12	-2.13	1.41	1.46
25	D	405	CLA	CMC-C2C	-2.13	1.46	1.50
25	5	307	CLA	C3B-C4B	2.13	1.49	1.42
24	s	406	CHL	CBD-CGD	-2.13	1.49	1.52
25	5	317	CLA	CMD-C2D	-2.13	1.46	1.50
25	S	611	CLA	CMC-C2C	-2.13	1.46	1.50
25	b	608	CLA	CMC-C2C	-2.13	1.46	1.50
39	D	406	PL9	C16-C14	-2.13	1.46	1.51
30	D	408	LHG	O7-C7	2.13	1.40	1.34
25	5	314	CLA	CMD-C2D	-2.13	1.46	1.50
25	7	315	CLA	CHC-C1C	2.13	1.42	1.38
25	n	315	CLA	MG-NB	-2.13	2.01	2.05
25	2	307	CLA	CHC-C1C	2.13	1.42	1.38
25	u	308	CLA	MG-NB	-2.13	2.01	2.05
25	4	315	CLA	CHC-C1C	2.13	1.42	1.38
31	v	401	8CT	C33-C32	-2.13	1.44	1.50
25	S	616	CLA	CMD-C2D	-2.13	1.46	1.50
24	S	605	CHL	CBD-CGD	-2.13	1.49	1.52
25	p	317	CLA	CMB-C2B	-2.13	1.46	1.50
25	s	412	CLA	C3B-C4B	2.13	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	s	403	CHL	CBD-CGD	-2.13	1.49	1.52
29	5	301	0UR	C19-C18	2.13	1.53	1.50
25	R	611	CLA	CMB-C2B	-2.13	1.46	1.50
26	Y	302	0IE	C11-C12	2.13	1.40	1.35
25	l	315	CLA	MG-NB	-2.13	2.01	2.05
25	u	317	CLA	MG-NB	-2.13	2.01	2.05
25	r	313	CLA	MG-NB	-2.13	2.01	2.05
25	7	314	CLA	CMD-C2D	-2.13	1.46	1.50
25	N	315	CLA	CMC-C2C	-2.13	1.46	1.50
25	7	308	CLA	CMD-C2D	-2.13	1.46	1.50
24	Y	309	CHL	CBD-CGD	-2.13	1.49	1.52
25	n	313	CLA	MG-NB	-2.13	2.01	2.05
26	2	302	0IE	C11-C12	2.13	1.40	1.35
25	R	611	CLA	CMD-C2D	-2.13	1.46	1.50
25	B	614	CLA	CMC-C2C	-2.13	1.46	1.50
25	q	315	CLA	CMD-C2D	-2.13	1.46	1.50
25	r	311	CLA	CHC-C1C	2.13	1.42	1.38
25	3	315	CLA	CMD-C2D	-2.13	1.46	1.50
25	B	606	CLA	CMB-C2B	-2.13	1.46	1.50
25	n	307	CLA	CMD-C2D	-2.13	1.46	1.50
25	r	305	CLA	CMD-C2D	-2.13	1.46	1.50
25	p	316	CLA	C3B-C4B	2.13	1.48	1.42
25	q	312	CLA	CHC-C1C	2.13	1.42	1.38
25	G	315	CLA	CMD-C2D	-2.13	1.46	1.50
25	g	316	CLA	CMD-C2D	-2.13	1.46	1.50
25	r	313	CLA	CMB-C2B	-2.13	1.46	1.50
25	c	601	CLA	CMB-C2B	-2.12	1.46	1.50
25	S	611	CLA	CHC-C1C	2.12	1.42	1.38
29	2	301	0UR	C19-C18	2.12	1.53	1.50
25	B	604	CLA	CMC-C2C	-2.12	1.46	1.50
25	y	308	CLA	C3B-C4B	2.12	1.48	1.42
25	S	609	CLA	CMC-C2C	-2.12	1.46	1.50
25	4	313	CLA	CMD-C2D	-2.12	1.46	1.50
25	y	314	CLA	CHC-C1C	2.12	1.42	1.38
25	7	316	CLA	CMB-C2B	-2.12	1.46	1.50
39	d	406	PL9	C46-C44	-2.12	1.46	1.51
25	p	308	CLA	CMB-C2B	-2.12	1.46	1.50
25	R	603	CLA	C3B-C4B	2.12	1.48	1.42
25	6	306	CLA	CHC-C1C	2.12	1.42	1.38
25	p	316	CLA	CHC-C1C	2.12	1.42	1.38
25	c	605	CLA	CHC-C1C	2.12	1.42	1.38
25	s	410	CLA	CHC-C1C	2.12	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d	405	CLA	CMC-C2C	-2.12	1.46	1.50
25	p	315	CLA	C3B-C4B	2.12	1.48	1.42
25	9	307	CLA	MG-NB	-2.12	2.01	2.05
25	c	603	CLA	C3B-C4B	2.12	1.48	1.42
25	Y	313	CLA	CHC-C1C	2.12	1.42	1.38
25	b	613	CLA	CMC-C2C	-2.12	1.46	1.50
25	7	317	CLA	CMC-C2C	-2.12	1.46	1.50
25	B	602	CLA	C3B-C4B	2.12	1.48	1.42
25	p	308	CLA	CHC-C1C	2.12	1.42	1.38
25	r	314	CLA	CHC-C1C	2.12	1.42	1.38
24	2	305	CHL	CBD-CGD	-2.12	1.49	1.52
25	y	308	CLA	CHC-C1C	2.12	1.42	1.38
25	p	314	CLA	CHC-C1C	2.12	1.42	1.38
25	2	307	CLA	CMB-C2B	-2.12	1.46	1.50
25	b	601	CLA	C3B-C4B	2.12	1.48	1.42
25	Y	316	CLA	CHC-C1C	2.12	1.42	1.38
25	C	601	CLA	CMB-C2B	-2.12	1.46	1.50
25	S	611	CLA	C3B-C4B	2.12	1.48	1.42
25	g	308	CLA	MG-NB	-2.12	2.01	2.05
30	1	318	LHG	P-O6	2.12	1.67	1.59
31	D	410	8CT	C33-C32	-2.12	1.44	1.50
25	4	315	CLA	MG-NB	-2.12	2.01	2.05
25	s	417	CLA	CMB-C2B	-2.12	1.46	1.50
25	c	610	CLA	CHC-C1C	2.12	1.42	1.38
25	G	307	CLA	MG-NB	-2.12	2.01	2.05
25	g	307	CLA	MG-NB	-2.12	2.01	2.05
25	7	316	CLA	C3B-C4B	2.12	1.48	1.42
25	a	605	CLA	CMC-C2C	-2.12	1.46	1.50
25	2	314	CLA	CMC-C2C	-2.11	1.46	1.50
25	S	603	CLA	C3B-C4B	2.11	1.48	1.42
25	B	601	CLA	C3B-C4B	2.11	1.48	1.42
25	4	316	CLA	MG-NB	-2.11	2.01	2.05
25	S	616	CLA	CMB-C2B	-2.11	1.46	1.50
31	t	101	8CT	C33-C32	-2.11	1.44	1.50
25	a	610	CLA	MG-NB	-2.11	2.01	2.05
26	7	303	0IE	C8-C7	2.11	1.40	1.35
24	Y	308	CHL	CBD-CGD	-2.11	1.49	1.52
25	9	307	CLA	CMB-C2B	-2.11	1.46	1.50
25	b	613	CLA	CHC-C1C	2.11	1.42	1.38
25	1	313	CLA	MG-NB	-2.11	2.01	2.05
25	N	307	CLA	MG-NB	-2.11	2.01	2.05
25	N	306	CLA	CMD-C2D	-2.11	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	5	314	CLA	CMB-C2B	-2.11	1.46	1.50
25	2	317	CLA	CMD-C2D	-2.11	1.46	1.50
25	p	314	CLA	CMD-C2D	-2.11	1.46	1.50
25	g	315	CLA	CMD-C2D	-2.11	1.46	1.50
25	y	307	CLA	CMC-C2C	-2.11	1.46	1.50
25	p	317	CLA	CHC-C1C	2.11	1.42	1.38
25	b	601	CLA	CHC-C1C	2.11	1.42	1.38
25	s	412	CLA	CHC-C1C	2.11	1.42	1.38
25	A	603	CLA	C3B-C4B	2.11	1.48	1.42
25	a	603	CLA	C3B-C4B	2.11	1.48	1.42
25	6	315	CLA	CMD-C2D	-2.11	1.46	1.50
25	p	316	CLA	CMB-C2B	-2.11	1.46	1.50
26	y	302	OIE	C11-C12	2.11	1.40	1.35
25	7	307	CLA	C3B-C4B	2.11	1.48	1.42
25	5	307	CLA	CHC-C1C	2.11	1.42	1.38
25	5	314	CLA	CMC-C2C	-2.11	1.46	1.50
25	p	307	CLA	CMB-C2B	-2.11	1.46	1.50
25	R	611	CLA	CMC-C2C	-2.11	1.46	1.50
25	A	607	CLA	CMC-C2C	-2.11	1.46	1.50
24	2	309	CHL	CBD-CGD	-2.11	1.49	1.52
25	c	603	CLA	CMC-C2C	-2.11	1.46	1.50
32	b	618	SQD	O2-C2	-2.11	1.37	1.43
25	1	306	CLA	CHC-C1C	2.11	1.42	1.38
25	p	315	CLA	CHC-C1C	2.11	1.42	1.38
25	q	314	CLA	CMC-C2C	-2.11	1.46	1.50
25	s	405	CLA	CMD-C2D	-2.11	1.46	1.50
25	B	607	CLA	CHC-C1C	2.11	1.42	1.38
25	3	306	CLA	CMD-C2D	-2.11	1.46	1.50
25	4	307	CLA	CHC-C1C	2.11	1.42	1.38
25	b	605	CLA	CMC-C2C	-2.11	1.46	1.50
25	6	313	CLA	MG-NB	-2.11	2.01	2.05
25	b	611	CLA	C3B-C4B	2.11	1.48	1.42
24	8	303	CHL	CBD-CGD	-2.11	1.49	1.52
25	1	307	CLA	CHC-C1C	2.10	1.42	1.38
25	b	614	CLA	C3B-C4B	2.10	1.48	1.42
25	u	316	CLA	CMD-C2D	-2.10	1.46	1.50
30	9	318	LHG	P-O6	2.10	1.67	1.59
26	2	302	OIE	C15-C16	2.10	1.40	1.35
24	9	308	CHL	CMC-C2C	2.10	1.49	1.44
25	N	307	CLA	CMD-C2D	-2.10	1.46	1.50
25	Y	307	CLA	C3B-C4B	2.10	1.48	1.42
25	C	612	CLA	C3B-C4B	2.10	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	y	316	CLA	MG-ND	-2.10	2.01	2.05
25	B	602	CLA	CHC-C1C	2.10	1.42	1.38
30	D	408	LHG	O8-C23	2.10	1.39	1.33
25	r	304	CLA	C3B-C4B	2.10	1.48	1.42
25	g	317	CLA	CMD-C2D	-2.10	1.46	1.50
25	s	417	CLA	CMD-C2D	-2.10	1.46	1.50
25	n	314	CLA	CMD-C2D	-2.10	1.46	1.50
25	b	603	CLA	MG-ND	-2.10	2.01	2.05
25	N	307	CLA	CMB-C2B	-2.10	1.46	1.50
25	b	606	CLA	CMB-C2B	-2.10	1.46	1.50
25	y	307	CLA	C3B-C4B	2.10	1.48	1.42
25	9	315	CLA	MG-NB	-2.10	2.01	2.05
25	3	316	CLA	CMC-C2C	-2.10	1.46	1.50
25	G	316	CLA	CMC-C2C	-2.10	1.46	1.50
25	7	307	CLA	CMB-C2B	-2.10	1.46	1.50
26	5	302	0IE	C11-C12	2.10	1.40	1.35
25	R	612	CLA	MG-NB	-2.10	2.01	2.05
32	D	409	SQD	O2-C2	-2.10	1.37	1.43
24	1	309	CHL	CBD-CGD	-2.10	1.49	1.52
25	n	314	CLA	MG-NB	-2.10	2.01	2.05
25	8	311	CLA	CHC-C1C	2.10	1.42	1.38
25	9	316	CLA	CMD-C2D	-2.10	1.46	1.50
25	n	316	CLA	MG-NB	-2.10	2.01	2.05
25	8	311	CLA	CMC-C2C	-2.10	1.46	1.50
25	B	612	CLA	CMC-C2C	-2.10	1.46	1.50
25	B	614	CLA	C3B-C4B	2.10	1.48	1.42
25	d	405	CLA	C3B-C4B	2.10	1.48	1.42
25	4	314	CLA	MG-NB	-2.10	2.01	2.05
25	r	312	CLA	CMC-C2C	-2.10	1.46	1.50
26	8	302	0IE	C11-C12	2.10	1.40	1.35
25	G	316	CLA	CMB-C2B	-2.10	1.46	1.50
25	y	308	CLA	CMC-C2C	-2.10	1.46	1.50
25	q	315	CLA	CMB-C2B	-2.10	1.46	1.50
25	5	317	CLA	CHC-C1C	2.10	1.42	1.38
25	G	314	CLA	CMD-C2D	-2.10	1.46	1.50
25	s	404	CLA	C3B-C4B	2.10	1.48	1.42
25	3	316	CLA	MG-NB	-2.10	2.01	2.05
25	u	308	CLA	CMB-C2B	-2.10	1.46	1.50
25	s	413	CLA	CHC-C1C	2.10	1.42	1.38
25	B	603	CLA	MG-ND	-2.10	2.01	2.05
23	f	201	HEM	CMB-C2B	2.10	1.55	1.50
25	r	311	CLA	CMD-C2D	-2.10	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	2	316	CLA	CMB-C2B	-2.10	1.46	1.50
30	D	407	LHG	O8-C23	2.10	1.39	1.33
25	6	306	CLA	CMB-C2B	-2.10	1.46	1.50
26	5	302	0IE	C8-C7	2.10	1.40	1.35
25	u	314	CLA	MG-NB	-2.10	2.01	2.05
25	p	307	CLA	C3B-C4B	2.10	1.48	1.42
25	B	609	CLA	CMC-C2C	-2.09	1.46	1.50
25	s	410	CLA	CMC-C2C	-2.09	1.46	1.50
25	B	605	CLA	CMC-C2C	-2.09	1.46	1.50
25	6	315	CLA	CMC-C2C	-2.09	1.46	1.50
25	r	305	CLA	C3B-C4B	2.09	1.48	1.42
24	7	311	CHL	CBD-CGD	-2.09	1.49	1.52
25	u	308	CLA	CMD-C2D	-2.09	1.46	1.50
25	4	314	CLA	CMD-C2D	-2.09	1.46	1.50
25	c	604	CLA	C3B-C4B	2.09	1.48	1.42
24	u	309	CHL	CMC-C2C	2.09	1.49	1.44
25	6	316	CLA	CMB-C2B	-2.09	1.46	1.50
25	p	315	CLA	CMC-C2C	-2.09	1.46	1.50
25	1	316	CLA	MG-NB	-2.09	2.01	2.05
25	2	314	CLA	CMD-C2D	-2.09	1.46	1.50
25	p	317	CLA	CMC-C2C	-2.09	1.46	1.50
24	5	311	CHL	CBD-CGD	-2.09	1.49	1.52
25	Y	306	CLA	C3B-C4B	2.09	1.48	1.42
25	R	604	CLA	CMC-C2C	-2.09	1.46	1.50
25	9	316	CLA	CMC-C2C	-2.09	1.46	1.50
25	N	314	CLA	CMD-C2D	-2.09	1.46	1.50
24	y	309	CHL	CBD-CGD	-2.09	1.49	1.52
25	8	313	CLA	CMC-C2C	-2.09	1.46	1.50
25	B	605	CLA	CHC-C1C	2.09	1.42	1.38
25	C	603	CLA	C3B-C4B	2.09	1.48	1.42
25	u	317	CLA	CMC-C2C	-2.09	1.46	1.50
25	q	305	CLA	CMC-C2C	-2.09	1.46	1.50
32	d	409	SQD	O2-C2	-2.09	1.37	1.43
30	Y	318	LHG	O7-C7	2.09	1.40	1.34
25	R	604	CLA	CHC-C1C	2.09	1.42	1.38
25	7	314	CLA	CHC-C1C	2.09	1.42	1.38
25	R	610	CLA	CMD-C2D	-2.09	1.46	1.50
25	9	315	CLA	CMD-C2D	-2.09	1.46	1.50
25	N	316	CLA	CMB-C2B	-2.09	1.46	1.50
25	B	608	CLA	CHC-C1C	2.09	1.42	1.38
25	g	316	CLA	CMC-C2C	-2.09	1.46	1.50
25	n	306	CLA	CMD-C2D	-2.09	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	604	CLA	C3B-C4B	2.09	1.48	1.42
25	8	313	CLA	CMB-C2B	-2.09	1.46	1.50
25	6	316	CLA	CMD-C2D	-2.09	1.46	1.50
25	q	312	CLA	CMC-C2C	-2.09	1.46	1.50
25	7	316	CLA	CHC-C1C	2.09	1.42	1.38
25	C	607	CLA	MG-ND	-2.09	2.01	2.05
25	8	306	CLA	CHC-C1C	2.09	1.42	1.38
25	3	313	CLA	MG-NB	-2.09	2.01	2.05
25	1	315	CLA	CMD-C2D	-2.09	1.46	1.50
25	g	314	CLA	MG-NB	-2.09	2.01	2.05
25	3	315	CLA	CMB-C2B	-2.09	1.46	1.50
25	p	307	CLA	CHC-C1C	2.08	1.42	1.38
25	8	312	CLA	CHC-C1C	2.08	1.42	1.38
25	B	613	CLA	CMC-C2C	-2.08	1.46	1.50
25	g	314	CLA	CMD-C2D	-2.08	1.46	1.50
25	C	608	CLA	C3B-C4B	2.08	1.48	1.42
25	1	306	CLA	CMD-C2D	-2.08	1.46	1.50
25	8	314	CLA	CMC-C2C	-2.08	1.46	1.50
24	1	311	CHL	CMC-C2C	2.08	1.49	1.44
25	a	604	CLA	C1B-C2B	2.08	1.48	1.43
25	C	605	CLA	C3B-C4B	2.08	1.48	1.42
25	D	405	CLA	C3B-C4B	2.08	1.48	1.42
25	9	314	CLA	MG-NB	-2.08	2.01	2.05
25	R	610	CLA	CMC-C2C	-2.08	1.46	1.50
25	C	611	CLA	CHC-C1C	2.08	1.42	1.38
25	g	316	CLA	CMB-C2B	-2.08	1.46	1.50
31	s	416	8CT	C14-C15	2.08	1.40	1.34
25	c	605	CLA	C3B-C4B	2.08	1.48	1.42
25	c	607	CLA	MG-ND	-2.08	2.01	2.05
25	G	307	CLA	CMD-C2D	-2.08	1.46	1.50
25	8	314	CLA	CMB-C2B	-2.08	1.46	1.50
25	B	601	CLA	CMC-C2C	-2.08	1.46	1.50
24	5	305	CHL	CBD-CGD	-2.08	1.49	1.52
25	S	603	CLA	CMC-C2C	-2.08	1.46	1.50
31	d	410	8CT	C33-C32	-2.08	1.44	1.50
25	2	316	CLA	CHC-C1C	2.08	1.42	1.38
25	b	601	CLA	CMC-C2C	-2.08	1.46	1.50
25	s	417	CLA	CHC-C1C	2.08	1.42	1.38
25	g	317	CLA	CMC-C2C	-2.08	1.46	1.50
32	a	609	SQD	O2-C2	-2.08	1.37	1.43
25	r	305	CLA	CHC-C1C	2.08	1.42	1.38
30	a	612	LHG	O7-C7	2.08	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	602	CLA	CMC-C2C	-2.08	1.46	1.50
25	4	307	CLA	CMD-C2D	-2.08	1.46	1.50
25	q	315	CLA	CMC-C2C	-2.08	1.46	1.50
25	s	411	CLA	CMC-C2C	-2.08	1.46	1.50
25	3	316	CLA	CMB-C2B	-2.08	1.46	1.50
25	7	315	CLA	CMC-C2C	-2.08	1.46	1.50
25	2	308	CLA	CMD-C2D	-2.08	1.46	1.50
25	r	305	CLA	CMC-C2C	-2.08	1.46	1.50
26	2	302	0IE	C8-C7	2.08	1.40	1.35
25	9	316	CLA	MG-NB	-2.08	2.01	2.05
25	C	605	CLA	CHC-C1C	2.08	1.42	1.38
25	A	603	CLA	CHC-C1C	2.08	1.42	1.38
25	a	603	CLA	CHC-C1C	2.08	1.42	1.38
25	R	613	CLA	CMD-C2D	-2.08	1.46	1.50
25	2	314	CLA	CMB-C2B	-2.08	1.46	1.50
25	6	306	CLA	CMD-C2D	-2.08	1.46	1.50
25	b	602	CLA	CMC-C2C	-2.08	1.46	1.50
25	s	411	CLA	C3B-C4B	2.08	1.48	1.42
25	8	312	CLA	CMB-C2B	-2.08	1.46	1.50
25	A	604	CLA	C1B-NB	-2.08	1.35	1.37
25	g	314	CLA	CMC-C2C	-2.07	1.46	1.50
25	G	314	CLA	MG-NB	-2.07	2.01	2.05
25	5	308	CLA	CMD-C2D	-2.07	1.46	1.50
25	p	314	CLA	CMC-C2C	-2.07	1.46	1.50
25	4	313	CLA	MG-NB	-2.07	2.01	2.05
25	y	317	CLA	CHC-C1C	2.07	1.42	1.38
25	b	612	CLA	C3B-C4B	2.07	1.48	1.42
25	1	313	CLA	CMD-C2D	-2.07	1.46	1.50
25	3	306	CLA	CMB-C2B	-2.07	1.46	1.50
25	3	316	CLA	CMD-C2D	-2.07	1.46	1.50
25	g	307	CLA	CMD-C2D	-2.07	1.46	1.50
25	b	610	CLA	CHC-C1C	2.07	1.42	1.38
25	C	606	CLA	MG-ND	-2.07	2.01	2.05
25	c	606	CLA	MG-ND	-2.07	2.01	2.05
25	6	315	CLA	CMB-C2B	-2.07	1.46	1.50
30	A	612	LHG	O7-C7	2.07	1.40	1.34
26	y	303	0IE	C11-C12	2.07	1.40	1.35
25	s	413	CLA	C3B-C4B	2.07	1.48	1.42
25	C	608	CLA	MG-ND	-2.07	2.01	2.05
30	d	407	LHG	O8-C23	2.07	1.39	1.33
25	C	610	CLA	C3B-C4B	2.07	1.48	1.42
25	4	315	CLA	CMD-C2D	-2.07	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	5	316	CLA	CHC-C1C	2.07	1.42	1.38
24	G	313	CHL	CBD-CGD	-2.07	1.49	1.52
26	Y	303	0IE	C11-C12	2.07	1.40	1.35
25	9	306	CLA	CMB-C2B	-2.07	1.46	1.50
25	S	612	CLA	CHC-C1C	2.07	1.42	1.38
25	N	313	CLA	CMD-C2D	-2.07	1.46	1.50
25	C	612	CLA	CHC-C1C	2.07	1.42	1.38
26	5	302	0IE	C15-C16	2.07	1.40	1.35
25	A	610	CLA	MG-NB	-2.07	2.01	2.05
25	n	315	CLA	CMB-C2B	-2.07	1.46	1.50
25	D	404	CLA	C3B-C4B	2.07	1.48	1.42
25	d	404	CLA	C3B-C4B	2.07	1.48	1.42
25	7	314	CLA	CMC-C2C	-2.07	1.46	1.50
26	Y	303	0IE	C8-C7	2.07	1.40	1.35
24	5	309	CHL	CBD-CGD	-2.07	1.49	1.52
25	9	307	CLA	CMD-C2D	-2.07	1.46	1.50
25	c	612	CLA	CHC-C1C	2.07	1.42	1.38
25	8	305	CLA	CMC-C2C	-2.07	1.46	1.50
26	p	303	0IE	C8-C7	2.07	1.40	1.35
24	5	312	CHL	CBD-CGD	-2.07	1.49	1.52
25	B	610	CLA	CHC-C1C	2.07	1.42	1.38
25	C	610	CLA	CHC-C1C	2.07	1.42	1.38
25	D	404	CLA	CHC-C1C	2.07	1.42	1.38
25	A	604	CLA	C1B-C2B	2.07	1.48	1.43
24	N	305	CHL	CBD-CGD	-2.06	1.49	1.52
25	5	316	CLA	CMB-C2B	-2.06	1.46	1.50
25	n	313	CLA	CMD-C2D	-2.06	1.46	1.50
25	b	609	CLA	CMC-C2C	-2.06	1.46	1.50
25	1	307	CLA	CMD-C2D	-2.06	1.46	1.50
25	r	304	CLA	CMC-C2C	-2.06	1.46	1.50
24	3	304	CHL	CBD-CGD	-2.06	1.49	1.52
25	c	606	CLA	C3B-C4B	2.06	1.48	1.42
30	n	318	LHG	P-O6	2.06	1.67	1.59
25	q	306	CLA	CMC-C2C	-2.06	1.46	1.50
25	3	313	CLA	CMD-C2D	-2.06	1.46	1.50
25	5	317	CLA	CMB-C2B	-2.06	1.46	1.50
25	g	308	CLA	CMD-C2D	-2.06	1.46	1.50
25	R	609	CLA	CHC-C1C	2.06	1.42	1.38
25	B	613	CLA	CHC-C1C	2.06	1.42	1.38
25	r	310	CLA	CHC-C1C	2.06	1.42	1.38
25	u	315	CLA	MG-NB	-2.06	2.01	2.05
25	c	608	CLA	C3B-C4B	2.06	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	307	CLA	CMD-C2D	-2.06	1.46	1.50
32	A	609	SQD	O2-C2	-2.06	1.37	1.43
25	B	601	CLA	CHC-C1C	2.06	1.42	1.38
25	N	316	CLA	CMD-C2D	-2.06	1.46	1.50
25	C	606	CLA	C3B-C4B	2.06	1.48	1.42
25	2	317	CLA	CHC-C1C	2.06	1.42	1.38
25	2	317	CLA	CMB-C2B	-2.06	1.46	1.50
25	q	313	CLA	CHC-C1C	2.06	1.42	1.38
25	r	310	CLA	CMB-C2B	-2.06	1.46	1.50
29	5	301	0UR	C29-C28	-2.06	1.52	1.54
24	2	311	CHL	CBD-CGD	-2.06	1.49	1.52
24	N	309	CHL	CBD-CGD	-2.06	1.49	1.52
25	S	612	CLA	C3B-C4B	2.06	1.48	1.42
25	8	305	CLA	C3B-C4B	2.06	1.48	1.42
25	S	610	CLA	CHC-C1C	2.06	1.42	1.38
25	S	610	CLA	C3B-C4B	2.06	1.48	1.42
25	1	314	CLA	MG-NB	-2.06	2.01	2.05
30	N	318	LHG	P-O6	2.06	1.67	1.59
25	N	315	CLA	CMB-C2B	-2.06	1.46	1.50
25	B	612	CLA	C3B-C4B	2.06	1.48	1.42
25	R	612	CLA	CMB-C2B	-2.06	1.46	1.50
25	6	307	CLA	CMD-C2D	-2.06	1.46	1.50
25	1	314	CLA	CMD-C2D	-2.06	1.46	1.50
25	G	317	CLA	CMC-C2C	-2.06	1.46	1.50
25	5	315	CLA	CMC-C2C	-2.06	1.46	1.50
25	S	604	CLA	C3B-C4B	2.06	1.48	1.42
25	4	314	CLA	CMB-C2B	-2.05	1.46	1.50
25	c	610	CLA	C3B-C4B	2.05	1.48	1.42
25	a	604	CLA	C1B-NB	-2.05	1.35	1.37
25	2	315	CLA	CMC-C2C	-2.05	1.46	1.50
25	u	316	CLA	CMC-C2C	-2.05	1.46	1.50
25	9	313	CLA	MG-NB	-2.05	2.01	2.05
25	5	308	CLA	CMB-C2B	-2.05	1.46	1.50
25	4	315	CLA	CMB-C2B	-2.05	1.46	1.50
25	2	317	CLA	CMC-C2C	-2.05	1.46	1.50
25	n	316	CLA	CMD-C2D	-2.05	1.46	1.50
24	4	311	CHL	CMC-C2C	2.05	1.49	1.44
25	6	316	CLA	CMC-C2C	-2.05	1.46	1.50
25	r	314	CLA	CMD-C2D	-2.05	1.46	1.50
30	A	601	LHG	O7-C7	2.05	1.40	1.34
25	q	313	CLA	CMB-C2B	-2.05	1.46	1.50
25	S	609	CLA	CHC-C1C	2.05	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	611	CLA	CHC-C1C	2.05	1.42	1.38
26	y	302	0IE	C8-C7	2.05	1.40	1.35
25	R	609	CLA	CMB-C2B	-2.05	1.46	1.50
25	u	315	CLA	CMD-C2D	-2.05	1.46	1.50
30	G	319	LHG	P-O6	2.05	1.67	1.59
31	B	617	8CT	C33-C32	-2.05	1.44	1.50
25	l	315	CLA	CMB-C2B	-2.05	1.46	1.50
25	n	307	CLA	CMB-C2B	-2.05	1.46	1.50
25	7	308	CLA	CMC-C2C	-2.05	1.46	1.50
25	q	306	CLA	CHC-C1C	2.05	1.42	1.38
26	8	302	0IE	C8-C7	2.05	1.40	1.35
25	C	603	CLA	CHC-C1C	2.05	1.42	1.38
23	E	201	HEM	CMB-C2B	2.05	1.55	1.50
25	s	411	CLA	CHC-C1C	2.05	1.42	1.38
39	D	406	PL9	C41-C39	-2.05	1.47	1.51
25	b	606	CLA	C3B-C4B	2.05	1.48	1.42
26	Y	302	0IE	C15-C16	2.05	1.40	1.35
25	4	315	CLA	CMC-C2C	-2.05	1.46	1.50
25	a	607	CLA	C3B-C4B	2.05	1.48	1.42
25	C	604	CLA	CHC-C1C	2.05	1.42	1.38
24	p	309	CHL	CMC-C2C	2.05	1.49	1.44
25	r	311	CLA	CMC-C2C	-2.05	1.46	1.50
30	d	407	LHG	O7-C7	2.05	1.40	1.34
31	S	615	8CT	C14-C15	2.05	1.40	1.34
25	8	313	CLA	CHC-C1C	2.05	1.42	1.38
24	N	317	CHL	CMC-C2C	2.04	1.49	1.44
25	9	313	CLA	CMD-C2D	-2.04	1.46	1.50
25	4	313	CLA	CMC-C2C	-2.04	1.46	1.50
25	u	315	CLA	CMB-C2B	-2.04	1.46	1.50
25	b	608	CLA	CHC-C1C	2.04	1.42	1.38
25	c	603	CLA	CHC-C1C	2.04	1.42	1.38
24	N	310	CHL	CBD-CGD	-2.04	1.49	1.52
25	d	404	CLA	CHC-C1C	2.04	1.42	1.38
26	q	302	0IE	C8-C7	2.04	1.40	1.35
24	7	309	CHL	CMC-C2C	2.04	1.49	1.44
25	8	312	CLA	CMC-C2C	-2.04	1.46	1.50
26	Y	302	0IE	C8-C7	2.04	1.40	1.35
25	B	606	CLA	C3B-C4B	2.04	1.48	1.42
25	2	308	CLA	CMB-C2B	-2.04	1.46	1.50
25	4	316	CLA	CMD-C2D	-2.04	1.46	1.50
25	g	315	CLA	CMB-C2B	-2.04	1.46	1.50
25	p	307	CLA	CMC-C2C	-2.04	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	q	314	CLA	CMB-C2B	-2.04	1.46	1.50
30	a	601	LHG	O7-C7	2.04	1.40	1.34
29	2	301	OUR	C29-C28	-2.04	1.52	1.54
25	r	311	CLA	CMB-C2B	-2.04	1.46	1.50
25	l	315	CLA	CMC-C2C	-2.04	1.46	1.50
25	9	306	CLA	CMD-C2D	-2.04	1.46	1.50
25	n	316	CLA	CMB-C2B	-2.04	1.46	1.50
25	B	609	CLA	C3B-C4B	2.04	1.48	1.42
25	G	307	CLA	CMB-C2B	-2.04	1.46	1.50
24	n	305	CHL	CBD-CGD	-2.04	1.49	1.52
25	6	314	CLA	CMD-C2D	-2.04	1.46	1.50
25	g	308	CLA	CMB-C2B	-2.04	1.46	1.50
30	2	319	LHG	P-O6	2.04	1.67	1.59
25	c	604	CLA	CHC-C1C	2.04	1.42	1.38
25	R	603	CLA	CMB-C2B	-2.04	1.46	1.50
25	7	307	CLA	CMC-C2C	-2.04	1.46	1.50
30	D	407	LHG	O7-C7	2.04	1.40	1.34
30	5	319	LHG	P-O6	2.04	1.67	1.59
25	C	609	CLA	CHC-C1C	2.04	1.42	1.38
25	c	609	CLA	CHC-C1C	2.04	1.42	1.38
39	d	406	PL9	C41-C39	-2.04	1.47	1.51
24	g	313	CHL	CBD-CGD	-2.04	1.49	1.52
26	y	303	OIE	C8-C7	2.04	1.40	1.35
25	s	404	CLA	CMC-C2C	-2.04	1.46	1.50
31	b	617	8CT	C33-C32	-2.04	1.44	1.50
26	y	302	OIE	C15-C16	2.04	1.40	1.35
25	q	314	CLA	CHC-C1C	2.04	1.42	1.38
25	l	316	CLA	CMD-C2D	-2.03	1.46	1.50
24	7	312	CHL	CBD-CGD	-2.03	1.49	1.52
25	s	404	CLA	CHC-C1C	2.03	1.42	1.38
25	b	609	CLA	C3B-C4B	2.03	1.48	1.42
30	g	319	LHG	P-O6	2.03	1.67	1.59
25	n	307	CLA	CMC-C2C	-2.03	1.46	1.50
25	a	603	CLA	MG-ND	-2.03	2.01	2.05
39	D	406	PL9	C26-C24	-2.03	1.47	1.51
25	3	314	CLA	CMD-C2D	-2.03	1.46	1.50
25	S	603	CLA	CHC-C1C	2.03	1.42	1.38
25	c	601	CLA	C1B-NB	-2.03	1.35	1.37
24	r	306	CHL	CBD-CGD	-2.03	1.49	1.52
24	G	309	CHL	CMC-C2C	2.03	1.49	1.44
25	l	313	CLA	CMC-C2C	-2.03	1.46	1.50
25	u	307	CLA	CMD-C2D	-2.03	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	n	313	CLA	CMB-C2B	-2.03	1.46	1.50
25	1	314	CLA	CMB-C2B	-2.03	1.46	1.50
24	6	308	CHL	CMC-C2C	2.03	1.49	1.44
25	G	314	CLA	CMC-C2C	-2.03	1.46	1.50
25	b	605	CLA	CHC-C1C	2.03	1.42	1.38
25	b	614	CLA	CHC-C1C	2.03	1.42	1.38
24	9	312	CHL	CMC-C2C	2.03	1.49	1.44
25	6	313	CLA	CMD-C2D	-2.03	1.46	1.50
25	2	315	CLA	CHC-C1C	2.03	1.42	1.38
25	B	614	CLA	CHC-C1C	2.03	1.42	1.38
25	5	315	CLA	CHC-C1C	2.03	1.42	1.38
25	b	612	CLA	CHC-C1C	2.03	1.42	1.38
24	q	303	CHL	CBD-CGD	-2.03	1.49	1.52
25	S	616	CLA	CMC-C2C	-2.03	1.46	1.50
25	G	308	CLA	CMD-C2D	-2.03	1.46	1.50
25	g	314	CLA	CMB-C2B	-2.03	1.46	1.50
25	Y	315	CLA	MG-ND	-2.03	2.01	2.05
25	c	610	CLA	MG-ND	-2.03	2.01	2.05
29	1	301	0UR	C19-C18	2.03	1.53	1.50
25	g	317	CLA	CMB-C2B	-2.03	1.46	1.50
30	C	617	LHG	P-O6	2.03	1.67	1.59
24	4	309	CHL	CBD-CGD	-2.03	1.50	1.52
24	p	311	CHL	CBD-CGD	-2.03	1.50	1.52
25	y	316	CLA	C3B-C4B	2.03	1.48	1.42
30	7	319	LHG	P-O6	2.03	1.67	1.59
25	g	307	CLA	CMB-C2B	-2.03	1.46	1.50
25	r	304	CLA	CMB-C2B	-2.03	1.46	1.50
24	2	312	CHL	CBD-CGD	-2.03	1.50	1.52
25	G	314	CLA	CMB-C2B	-2.03	1.46	1.50
25	a	605	CLA	C3B-C4B	2.02	1.48	1.42
25	c	601	CLA	C3B-C4B	2.02	1.48	1.42
25	9	314	CLA	CMD-C2D	-2.02	1.46	1.50
25	q	313	CLA	CMC-C2C	-2.02	1.46	1.50
24	p	312	CHL	CBD-CGD	-2.02	1.50	1.52
25	A	605	CLA	C3B-C4B	2.02	1.48	1.42
25	D	405	CLA	CHC-C1C	2.02	1.42	1.38
24	4	304	CHL	CMC-C2C	2.02	1.49	1.44
25	s	405	CLA	C3B-C4B	2.02	1.48	1.42
39	d	406	PL9	C11-C9	-2.02	1.47	1.51
25	5	308	CLA	CMC-C2C	-2.02	1.46	1.50
25	G	308	CLA	CMB-C2B	-2.02	1.46	1.50
25	8	306	CLA	CMC-C2C	-2.02	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	q	305	CLA	C3B-C4B	2.02	1.48	1.42
25	9	316	CLA	CMB-C2B	-2.02	1.46	1.50
25	q	305	CLA	CHC-C1C	2.02	1.42	1.38
25	4	313	CLA	CMB-C2B	-2.02	1.46	1.50
25	s	405	CLA	CMC-C2C	-2.02	1.46	1.50
24	6	317	CHL	CMC-C2C	2.02	1.49	1.44
25	B	612	CLA	CHC-C1C	2.02	1.42	1.38
24	8	315	CHL	CMC-C2C	2.02	1.49	1.44
24	n	304	CHL	CMC-C2C	2.02	1.49	1.44
25	A	607	CLA	C3B-C4B	2.02	1.48	1.42
24	G	312	CHL	CMC-C2C	2.02	1.49	1.44
30	D	408	LHG	P-O6	2.02	1.67	1.59
25	b	602	CLA	CHC-C1C	2.02	1.42	1.38
25	R	603	CLA	CMC-C2C	-2.02	1.46	1.50
25	8	305	CLA	CHC-C1C	2.02	1.42	1.38
25	u	307	CLA	CMB-C2B	-2.02	1.46	1.50
25	G	315	CLA	CMB-C2B	-2.02	1.46	1.50
25	n	313	CLA	CMC-C2C	-2.02	1.46	1.50
35	D	403	PHO	C3D-C4D	2.02	1.44	1.41
30	p	319	LHG	P-O6	2.02	1.67	1.59
24	6	305	CHL	CBD-CGD	-2.02	1.50	1.52
24	n	317	CHL	CMC-C2C	2.02	1.49	1.44
25	N	313	CLA	CMC-C2C	-2.02	1.46	1.50
24	6	312	CHL	CMC-C2C	2.02	1.49	1.44
24	g	309	CHL	CMC-C2C	2.02	1.49	1.44
25	9	315	CLA	CMB-C2B	-2.01	1.46	1.50
30	d	408	LHG	O7-C5	-2.01	1.41	1.46
25	7	307	CLA	CHC-C1C	2.01	1.42	1.38
24	7	318	CHL	CBD-CGD	-2.01	1.50	1.52
25	b	606	CLA	CHC-C1C	2.01	1.42	1.38
25	2	308	CLA	CMC-C2C	-2.01	1.46	1.50
25	u	316	CLA	CMB-C2B	-2.01	1.46	1.50
25	n	306	CLA	CMC-C2C	-2.01	1.46	1.50
25	d	404	CLA	MG-ND	-2.01	2.01	2.05
24	N	311	CHL	CBD-CGD	-2.01	1.50	1.52
25	C	602	CLA	C3B-C4B	2.01	1.48	1.42
24	G	306	CHL	CBD-CGD	-2.01	1.50	1.52
39	D	406	PL9	C11-C9	-2.01	1.47	1.51
25	N	306	CLA	CMB-C2B	-2.01	1.46	1.50
25	4	316	CLA	CMC-C2C	-2.01	1.46	1.50
25	n	306	CLA	CMB-C2B	-2.01	1.46	1.50
25	B	606	CLA	CHC-C1C	2.01	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	1	308	CHL	CMC-C2C	2.01	1.49	1.44
25	D	404	CLA	MG-ND	-2.01	2.01	2.05
25	c	602	CLA	MG-ND	-2.01	2.01	2.05
25	d	405	CLA	CHC-C1C	2.01	1.42	1.38
24	q	316	CHL	CMC-C2C	2.01	1.49	1.44
25	c	616	CLA	MG-ND	-2.01	2.01	2.05
25	4	307	CLA	CMC-C2C	-2.01	1.46	1.50
25	C	601	CLA	C3B-C4B	2.01	1.48	1.42
30	c	617	LHG	P-O6	2.01	1.67	1.59
25	b	614	CLA	MG-ND	-2.01	2.01	2.05
29	Y	301	0UR	C29-C28	-2.01	1.52	1.54
25	N	314	CLA	CMC-C2C	-2.01	1.46	1.50
25	n	316	CLA	CMC-C2C	-2.01	1.46	1.50
24	R	601	CHL	CMC-C2C	2.01	1.49	1.44
25	b	606	CLA	MG-ND	-2.01	2.01	2.05
24	1	304	CHL	CMC-C2C	2.01	1.49	1.44
24	3	308	CHL	CMC-C2C	2.01	1.49	1.44
25	9	314	CLA	CMB-C2B	-2.01	1.46	1.50
25	n	314	CLA	CMC-C2C	-2.01	1.46	1.50
25	N	306	CLA	CMC-C2C	-2.01	1.46	1.50
25	4	306	CLA	CMC-C2C	-2.01	1.46	1.50
25	p	308	CLA	CMC-C2C	-2.01	1.46	1.50
25	1	316	CLA	CMB-C2B	-2.00	1.46	1.50
23	E	201	HEM	C2A-C3A	-2.00	1.33	1.38
25	5	317	CLA	CMC-C2C	-2.00	1.46	1.50
25	Y	306	CLA	CHC-C1C	2.00	1.42	1.38
25	1	316	CLA	CMC-C2C	-2.00	1.46	1.50
25	g	315	CLA	CMC-C2C	-2.00	1.46	1.50
24	g	306	CHL	CBD-CGD	-2.00	1.50	1.52
24	p	318	CHL	CBD-CGD	-2.00	1.50	1.52
25	y	307	CLA	CHC-C1C	2.00	1.42	1.38
25	5	307	CLA	CMC-C2C	-2.00	1.46	1.50
25	3	307	CLA	CMB-C2B	-2.00	1.46	1.50
25	3	313	CLA	CMB-C2B	-2.00	1.46	1.50
25	G	315	CLA	CMC-C2C	-2.00	1.46	1.50
24	N	304	CHL	CMC-C2C	2.00	1.49	1.44
25	C	608	CLA	CHC-C1C	2.00	1.42	1.38

All (5455) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	s	416	8CT	C22-C21-C20	-27.08	78.94	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	S	615	8CT	C22-C21-C20	-27.07	78.96	122.82
31	S	615	8CT	C22-C21-C23	-26.12	78.18	118.09
31	s	416	8CT	C22-C21-C23	-26.11	78.20	118.09
31	S	615	8CT	C23-C21-C20	24.21	157.09	119.01
31	s	416	8CT	C23-C21-C20	24.21	157.08	119.01
28	G	304	NEX	O24-C25-C24	15.73	128.24	113.49
28	4	303	NEX	O24-C25-C24	15.69	128.20	113.49
28	u	304	NEX	O24-C25-C24	15.68	128.19	113.49
28	r	317	NEX	O24-C25-C24	15.68	128.19	113.49
28	p	304	NEX	O24-C25-C24	15.68	128.19	113.49
28	1	303	NEX	O24-C25-C24	15.68	128.18	113.49
28	5	304	NEX	O24-C25-C24	15.68	128.18	113.49
28	2	304	NEX	O24-C25-C24	15.67	128.17	113.49
28	g	304	NEX	O24-C25-C24	15.66	128.17	113.49
28	7	304	NEX	O24-C25-C24	15.66	128.17	113.49
28	S	617	NEX	O24-C25-C24	15.66	128.17	113.49
28	9	319	NEX	O24-C25-C24	15.66	128.17	113.49
28	R	616	NEX	O24-C25-C24	15.65	128.15	113.49
28	y	304	NEX	O24-C25-C24	15.65	128.15	113.49
28	S	617	NEX	C20-C13-C12	13.92	139.36	118.09
28	p	304	NEX	C20-C13-C12	13.92	139.35	118.09
28	r	317	NEX	C20-C13-C12	13.91	139.34	118.09
28	G	304	NEX	C20-C13-C12	13.91	139.34	118.09
28	4	303	NEX	C20-C13-C12	13.91	139.34	118.09
28	5	304	NEX	C20-C13-C12	13.91	139.34	118.09
28	g	304	NEX	C20-C13-C12	13.91	139.34	118.09
28	7	304	NEX	C20-C13-C12	13.91	139.33	118.09
28	2	304	NEX	C20-C13-C12	13.90	139.33	118.09
28	u	304	NEX	C20-C13-C12	13.90	139.33	118.09
28	y	304	NEX	C20-C13-C12	13.90	139.32	118.09
28	R	616	NEX	C20-C13-C12	13.89	139.31	118.09
28	1	303	NEX	C20-C13-C12	13.89	139.30	118.09
28	9	319	NEX	C20-C13-C12	13.87	139.28	118.09
28	y	304	NEX	C12-C13-C14	-11.92	100.26	119.01
28	G	304	NEX	C12-C13-C14	-11.91	100.27	119.01
28	2	304	NEX	C12-C13-C14	-11.91	100.27	119.01
28	4	303	NEX	C12-C13-C14	-11.91	100.28	119.01
28	S	617	NEX	C12-C13-C14	-11.91	100.28	119.01
28	p	304	NEX	C12-C13-C14	-11.90	100.29	119.01
28	5	304	NEX	C12-C13-C14	-11.90	100.29	119.01
28	r	317	NEX	C12-C13-C14	-11.90	100.29	119.01
28	9	319	NEX	C12-C13-C14	-11.90	100.30	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	7	304	NEX	C12-C13-C14	-11.89	100.31	119.01
28	g	304	NEX	C12-C13-C14	-11.88	100.33	119.01
28	u	304	NEX	C12-C13-C14	-11.88	100.33	119.01
28	R	616	NEX	C12-C13-C14	-11.87	100.34	119.01
28	l	303	NEX	C12-C13-C14	-11.86	100.35	119.01
31	S	615	8CT	C33-C32-C31	-11.26	114.08	124.83
31	s	416	8CT	C33-C32-C31	-11.20	114.14	124.83
31	T	101	8CT	C33-C32-C31	-10.95	114.37	124.83
31	t	101	8CT	C33-C32-C31	-10.94	114.39	124.83
28	5	304	NEX	C30-C31-C32	-9.96	94.35	123.20
28	R	616	NEX	C30-C31-C32	-9.95	94.37	123.20
28	r	317	NEX	C30-C31-C32	-9.95	94.37	123.20
28	S	617	NEX	C30-C31-C32	-9.95	94.37	123.20
28	u	304	NEX	C30-C31-C32	-9.95	94.38	123.20
28	p	304	NEX	C30-C31-C32	-9.95	94.38	123.20
28	7	304	NEX	C30-C31-C32	-9.94	94.39	123.20
28	G	304	NEX	C30-C31-C32	-9.94	94.40	123.20
28	9	319	NEX	C30-C31-C32	-9.94	94.40	123.20
28	y	304	NEX	C30-C31-C32	-9.94	94.41	123.20
28	g	304	NEX	C30-C31-C32	-9.94	94.41	123.20
28	l	303	NEX	C30-C31-C32	-9.93	94.42	123.20
28	2	304	NEX	C30-C31-C32	-9.93	94.43	123.20
28	4	303	NEX	C30-C31-C32	-9.93	94.44	123.20
24	7	305	CHL	C1B-CHB-C4A	9.74	127.59	121.32
31	S	614	8CT	C33-C32-C31	-9.41	115.85	124.83
24	n	309	CHL	C1B-CHB-C4A	9.35	127.34	121.32
31	s	415	8CT	C33-C32-C31	-9.34	115.91	124.83
31	c	615	8CT	C33-C32-C31	-9.34	115.91	124.83
24	p	305	CHL	C1B-CHB-C4A	9.33	127.33	121.32
31	C	615	8CT	C33-C32-C31	-9.32	115.94	124.83
24	s	414	CHL	O2D-CGD-CBD	9.25	121.11	110.95
24	3	317	CHL	O2D-CGD-CBD	9.17	121.02	110.95
24	S	613	CHL	O2D-CGD-CBD	9.17	121.02	110.95
24	Y	309	CHL	C1B-CHB-C4A	9.11	127.19	121.32
31	a	608	8CT	C33-C32-C31	-9.08	116.16	124.83
24	6	317	CHL	O2D-CGD-CBD	9.04	120.88	110.95
31	A	608	8CT	C33-C32-C31	-9.04	116.20	124.83
24	7	311	CHL	O2D-CGD-CBD	9.02	120.86	110.95
24	r	302	CHL	O2D-CGD-CBD	9.02	120.86	110.95
24	l	312	CHL	O2D-CGD-CBD	9.00	120.83	110.95
24	R	601	CHL	O2D-CGD-CBD	8.95	120.78	110.95
24	4	312	CHL	O2D-CGD-CBD	8.95	120.78	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	n	305	CHL	O2D-CGD-CBD	8.94	120.77	110.95
24	q	308	CHL	O2D-CGD-CBD	8.92	120.75	110.95
24	N	312	CHL	O2D-CGD-CBD	8.90	120.73	110.95
24	4	305	CHL	O2D-CGD-CBD	8.88	120.71	110.95
24	1	305	CHL	O2D-CGD-CBD	8.87	120.70	110.95
24	7	306	CHL	C1B-CHB-C4A	8.87	127.03	121.32
24	n	312	CHL	O2D-CGD-CBD	8.85	120.67	110.95
28	N	303	NEX	O24-C25-C24	8.85	121.78	113.49
28	3	318	NEX	O24-C25-C24	8.84	121.78	113.49
24	R	606	CHL	O2D-CGD-CBD	8.84	120.66	110.95
28	s	401	NEX	O24-C25-C24	8.84	121.77	113.49
28	6	303	NEX	O24-C25-C24	8.84	121.77	113.49
28	3	318	NEX	C38-C25-C26	-8.83	107.77	122.30
28	N	303	NEX	C38-C25-C26	-8.83	107.77	122.30
28	r	301	NEX	C38-C25-C26	-8.83	107.77	122.30
28	6	303	NEX	C38-C25-C26	-8.83	107.78	122.30
28	r	301	NEX	O24-C25-C24	8.82	121.75	113.49
28	n	303	NEX	C38-C25-C26	-8.81	107.80	122.30
28	n	303	NEX	O24-C25-C24	8.81	121.75	113.49
24	r	303	CHL	O2D-CGD-CBD	8.81	120.63	110.95
28	s	401	NEX	C38-C25-C26	-8.81	107.80	122.30
31	B	617	8CT	C33-C32-C31	-8.81	116.42	124.83
24	7	305	CHL	O2D-CGD-CBD	8.80	120.61	110.95
24	8	308	CHL	O2D-CGD-CBD	8.79	120.61	110.95
24	p	306	CHL	C1B-CHB-C4A	8.79	126.97	121.32
24	7	306	CHL	O2D-CGD-CBD	8.78	120.59	110.95
24	R	602	CHL	O2D-CGD-CBD	8.76	120.57	110.95
24	Y	304	CHL	C1B-CHB-C4A	8.76	126.96	121.32
24	r	307	CHL	O2D-CGD-CBD	8.75	120.56	110.95
24	8	307	CHL	O2D-CGD-CBD	8.74	120.55	110.95
24	p	306	CHL	O2D-CGD-CBD	8.73	120.54	110.95
24	1	304	CHL	O2D-CGD-CBD	8.72	120.53	110.95
24	G	313	CHL	O2D-CGD-CBD	8.71	120.52	110.95
24	p	305	CHL	O2D-CGD-CBD	8.71	120.52	110.95
31	c	614	8CT	C33-C32-C31	-8.68	116.54	124.83
24	Y	304	CHL	O2D-CGD-CBD	8.68	120.48	110.95
24	N	309	CHL	O2D-CGD-CBD	8.67	120.47	110.95
24	5	313	CHL	O2D-CGD-CBD	8.67	120.47	110.95
24	y	305	CHL	C1B-CHB-C4A	8.66	126.89	121.32
24	4	304	CHL	O2D-CGD-CBD	8.66	120.46	110.95
24	7	309	CHL	O2D-CGD-CBD	8.66	120.46	110.95
24	2	313	CHL	O2D-CGD-CBD	8.65	120.46	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	6	305	CHL	O2D-CGD-CBD	8.65	120.45	110.95
24	n	310	CHL	O2D-CGD-CBD	8.64	120.44	110.95
24	3	310	CHL	O2D-CGD-CBD	8.61	120.41	110.95
24	p	309	CHL	O2D-CGD-CBD	8.60	120.40	110.95
24	6	310	CHL	O2D-CGD-CBD	8.60	120.39	110.95
24	3	305	CHL	O2D-CGD-CBD	8.59	120.39	110.95
24	g	313	CHL	O2D-CGD-CBD	8.58	120.37	110.95
24	9	317	CHL	O2D-CGD-CBD	8.57	120.36	110.95
24	N	310	CHL	O2D-CGD-CBD	8.57	120.36	110.95
24	G	318	CHL	O2D-CGD-CBD	8.56	120.36	110.95
24	n	309	CHL	O2D-CGD-CBD	8.53	120.32	110.95
31	C	614	8CT	C33-C32-C31	-8.53	116.69	124.83
24	9	308	CHL	O2D-CGD-CBD	8.53	120.32	110.95
24	R	608	CHL	O2D-CGD-CBD	8.52	120.31	110.95
24	p	318	CHL	O2D-CGD-CBD	8.52	120.31	110.95
24	N	305	CHL	O2D-CGD-CBD	8.51	120.30	110.95
24	4	308	CHL	O2D-CGD-CBD	8.51	120.30	110.95
24	1	309	CHL	O2D-CGD-CBD	8.51	120.30	110.95
24	S	608	CHL	O2D-CGD-CBD	8.51	120.30	110.95
24	Y	319	CHL	O2D-CGD-CBD	8.51	120.29	110.95
24	y	318	CHL	O2D-CGD-CBD	8.50	120.29	110.95
24	S	602	CHL	O2D-CGD-CBD	8.50	120.28	110.95
24	Y	317	CHL	O2D-CGD-CBD	8.49	120.28	110.95
24	9	305	CHL	O2D-CGD-CBD	8.49	120.28	110.95
24	s	403	CHL	O2D-CGD-CBD	8.49	120.27	110.95
24	4	310	CHL	O2D-CGD-CBD	8.48	120.27	110.95
24	7	318	CHL	O2D-CGD-CBD	8.48	120.27	110.95
24	p	312	CHL	C1B-CHB-C4A	8.48	126.78	121.32
24	3	312	CHL	O2D-CGD-CBD	8.48	120.27	110.95
24	g	318	CHL	O2D-CGD-CBD	8.48	120.27	110.95
24	u	310	CHL	O2D-CGD-CBD	8.48	120.26	110.95
24	s	409	CHL	O2D-CGD-CBD	8.48	120.26	110.95
24	u	309	CHL	O2D-CGD-CBD	8.48	120.26	110.95
24	u	318	CHL	O2D-CGD-CBD	8.47	120.26	110.95
24	1	308	CHL	O2D-CGD-CBD	8.47	120.25	110.95
24	8	303	CHL	O2D-CGD-CBD	8.47	120.25	110.95
24	4	309	CHL	O2D-CGD-CBD	8.47	120.25	110.95
24	y	305	CHL	O2D-CGD-CBD	8.46	120.25	110.95
24	7	312	CHL	C1B-CHB-C4A	8.46	126.76	121.32
24	R	605	CHL	C1B-CHB-C4A	8.45	126.76	121.32
24	r	309	CHL	O2D-CGD-CBD	8.45	120.23	110.95
24	R	605	CHL	O2D-CGD-CBD	8.44	120.22	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	q	316	CHL	O2D-CGD-CBD	8.44	120.22	110.95
24	y	306	CHL	O2D-CGD-CBD	8.44	120.22	110.95
24	6	312	CHL	O2D-CGD-CBD	8.44	120.22	110.95
24	Y	305	CHL	O2D-CGD-CBD	8.43	120.21	110.95
24	7	310	CHL	O2D-CGD-CBD	8.43	120.21	110.95
24	1	310	CHL	O2D-CGD-CBD	8.43	120.20	110.95
24	8	315	CHL	O2D-CGD-CBD	8.42	120.20	110.95
24	q	307	CHL	O2D-CGD-CBD	8.42	120.19	110.95
24	3	309	CHL	O2D-CGD-CBD	8.41	120.19	110.95
24	g	310	CHL	O2D-CGD-CBD	8.41	120.19	110.95
24	G	311	CHL	O2D-CGD-CBD	8.41	120.19	110.95
24	8	309	CHL	C1B-CHB-C4A	8.41	126.73	121.32
24	9	309	CHL	O2D-CGD-CBD	8.41	120.19	110.95
24	u	311	CHL	O2D-CGD-CBD	8.40	120.18	110.95
24	p	310	CHL	O2D-CGD-CBD	8.40	120.17	110.95
24	8	304	CHL	O2D-CGD-CBD	8.39	120.17	110.95
24	q	309	CHL	O2D-CGD-CBD	8.39	120.17	110.95
24	6	309	CHL	O2D-CGD-CBD	8.39	120.17	110.95
24	2	311	CHL	O2D-CGD-CBD	8.39	120.16	110.95
24	2	318	CHL	O2D-CGD-CBD	8.38	120.16	110.95
24	r	306	CHL	O2D-CGD-CBD	8.38	120.15	110.95
31	V	401	8CT	C33-C32-C31	-8.36	116.85	124.83
24	n	317	CHL	O2D-CGD-CBD	8.36	120.13	110.95
24	G	309	CHL	O2D-CGD-CBD	8.36	120.13	110.95
24	5	311	CHL	O2D-CGD-CBD	8.36	120.13	110.95
24	5	318	CHL	O2D-CGD-CBD	8.35	120.12	110.95
24	q	303	CHL	O2D-CGD-CBD	8.35	120.12	110.95
24	u	306	CHL	O2D-CGD-CBD	8.35	120.12	110.95
31	v	401	8CT	C33-C32-C31	-8.34	116.87	124.83
24	G	306	CHL	O2D-CGD-CBD	8.33	120.10	110.95
31	b	617	8CT	C33-C32-C31	-8.33	116.88	124.83
24	q	304	CHL	O2D-CGD-CBD	8.33	120.10	110.95
24	9	310	CHL	O2D-CGD-CBD	8.31	120.08	110.95
24	N	317	CHL	O2D-CGD-CBD	8.31	120.08	110.95
24	N	308	CHL	O2D-CGD-CBD	8.30	120.07	110.95
24	g	309	CHL	O2D-CGD-CBD	8.29	120.06	110.95
24	g	306	CHL	O2D-CGD-CBD	8.29	120.05	110.95
24	S	601	CHL	O2D-CGD-CBD	8.28	120.05	110.95
24	y	311	CHL	O2D-CGD-CBD	8.26	120.03	110.95
24	y	311	CHL	C1B-CHB-C4A	8.26	126.64	121.32
24	G	310	CHL	O2D-CGD-CBD	8.25	120.01	110.95
31	D	410	8CT	C33-C32-C31	-8.24	116.96	124.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	p	311	CHL	O2D-CGD-CBD	8.22	119.98	110.95
24	s	402	CHL	O2D-CGD-CBD	8.22	119.98	110.95
24	2	306	CHL	O2D-CGD-CBD	8.22	119.97	110.95
24	S	605	CHL	O2D-CGD-CBD	8.21	119.97	110.95
24	8	310	CHL	O2D-CGD-CBD	8.21	119.97	110.95
24	u	305	CHL	O2D-CGD-CBD	8.21	119.97	110.95
24	y	310	CHL	C1B-CHB-C4A	8.21	126.60	121.32
31	d	410	8CT	C33-C32-C31	-8.20	117.00	124.83
24	7	313	CHL	O2D-CGD-CBD	8.20	119.96	110.95
24	5	306	CHL	O2D-CGD-CBD	8.20	119.96	110.95
24	9	304	CHL	O2D-CGD-CBD	8.19	119.95	110.95
24	Y	310	CHL	C1B-CHB-C4A	8.18	126.58	121.32
24	p	313	CHL	O2D-CGD-CBD	8.17	119.93	110.95
24	s	406	CHL	O2D-CGD-CBD	8.16	119.92	110.95
24	3	308	CHL	O2D-CGD-CBD	8.16	119.92	110.95
24	6	308	CHL	O2D-CGD-CBD	8.15	119.90	110.95
24	7	306	CHL	CHA-C1A-C2A	-8.15	114.17	133.31
24	6	304	CHL	O2D-CGD-CBD	8.15	119.90	110.95
24	n	309	CHL	CHA-C1A-C2A	-8.14	114.19	133.31
24	q	311	CHL	O2D-CGD-CBD	8.14	119.89	110.95
24	u	313	CHL	O2D-CGD-CBD	8.14	119.89	110.95
24	Y	310	CHL	O2D-CGD-CBD	8.14	119.89	110.95
24	Y	309	CHL	CHA-C1A-C2A	-8.14	114.20	133.31
24	9	312	CHL	O2D-CGD-CBD	8.13	119.88	110.95
24	2	310	CHL	O2D-CGD-CBD	8.12	119.87	110.95
24	S	606	CHL	O2D-CGD-CBD	8.12	119.86	110.95
24	p	306	CHL	CHA-C1A-C2A	-8.10	114.29	133.31
24	5	310	CHL	O2D-CGD-CBD	8.08	119.83	110.95
24	s	407	CHL	O2D-CGD-CBD	8.08	119.82	110.95
24	y	309	CHL	O2D-CGD-CBD	8.08	119.82	110.95
24	Y	309	CHL	O2D-CGD-CBD	8.07	119.81	110.95
24	Y	308	CHL	O2D-CGD-CBD	8.07	119.81	110.95
24	4	311	CHL	O2D-CGD-CBD	8.06	119.81	110.95
24	y	310	CHL	O2D-CGD-CBD	8.06	119.80	110.95
24	5	305	CHL	O2D-CGD-CBD	8.05	119.80	110.95
31	C	613	8CT	C33-C32-C31	-8.04	117.16	124.83
24	7	305	CHL	CHA-C1A-C2A	-8.03	114.45	133.31
24	p	305	CHL	CHA-C1A-C2A	-8.02	114.48	133.31
24	2	305	CHL	O2D-CGD-CBD	8.01	119.75	110.95
24	y	310	CHL	CHA-C1A-C2A	-8.01	114.50	133.31
24	3	304	CHL	O2D-CGD-CBD	8.01	119.75	110.95
24	Y	304	CHL	CHA-C1A-C2A	-8.00	114.52	133.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	y	305	CHL	CHA-C1A-C2A	-7.99	114.54	133.31
24	G	305	CHL	O2D-CGD-CBD	7.98	119.72	110.95
24	l	311	CHL	O2D-CGD-CBD	7.98	119.72	110.95
24	g	305	CHL	O2D-CGD-CBD	7.96	119.70	110.95
24	8	309	CHL	CHA-C1A-C2A	-7.95	114.64	133.31
24	g	306	CHL	CHA-C1A-C2A	-7.93	114.68	133.31
24	N	309	CHL	CHA-C1A-C2A	-7.93	114.69	133.31
24	r	303	CHL	C1B-CHB-C4A	7.92	126.42	121.32
24	q	308	CHL	CHA-C1A-C2A	-7.92	114.71	133.31
24	n	308	CHL	O2D-CGD-CBD	7.91	119.63	110.95
24	7	312	CHL	CHA-C1A-C2A	-7.90	114.75	133.31
24	p	312	CHL	CHA-C1A-C2A	-7.89	114.78	133.31
24	8	308	CHL	CHA-C1A-C2A	-7.87	114.82	133.31
24	q	310	CHL	CHA-C1A-C2A	-7.87	114.84	133.31
24	R	602	CHL	C1B-CHB-C4A	7.86	126.38	121.32
24	2	309	CHL	O2D-CGD-CBD	7.84	119.56	110.95
24	n	304	CHL	O2D-CGD-CBD	7.83	119.55	110.95
31	c	613	8CT	C33-C32-C31	-7.83	117.36	124.83
24	N	304	CHL	O2D-CGD-CBD	7.82	119.53	110.95
24	N	309	CHL	C1B-CHB-C4A	7.80	126.34	121.32
24	S	607	CHL	O2D-CGD-CBD	7.80	119.52	110.95
24	y	311	CHL	CHA-C1A-C2A	-7.78	115.05	133.31
24	y	313	CHL	O2D-CGD-CBD	7.78	119.49	110.95
24	q	310	CHL	O2D-CGD-CBD	7.78	119.49	110.95
24	S	602	CHL	CHA-C1A-C2A	-7.77	115.06	133.31
24	S	608	CHL	CHA-C1A-C2A	-7.76	115.09	133.31
24	8	309	CHL	O2D-CGD-CBD	7.76	119.47	110.95
24	l	317	CHL	O2D-CGD-CBD	7.75	119.46	110.95
24	4	317	CHL	O2D-CGD-CBD	7.74	119.45	110.95
24	q	304	CHL	CHA-C1A-C2A	-7.74	115.15	133.31
31	B	617	8CT	C14-C13-C12	-7.73	116.43	127.28
24	Y	312	CHL	O2D-CGD-CBD	7.73	119.44	110.95
24	5	309	CHL	O2D-CGD-CBD	7.72	119.42	110.95
24	Y	310	CHL	CHA-C1A-C2A	-7.71	115.20	133.31
24	g	311	CHL	O2D-CGD-CBD	7.70	119.41	110.95
24	q	311	CHL	CHA-C1A-C2A	-7.69	115.25	133.31
24	q	310	CHL	C1B-CHB-C4A	7.69	126.27	121.32
24	Y	305	CHL	CHA-C1A-C2A	-7.68	115.27	133.31
24	y	306	CHL	CHA-C1A-C2A	-7.68	115.27	133.31
24	s	403	CHL	CHA-C1A-C2A	-7.68	115.28	133.31
24	G	306	CHL	CHA-C1A-C2A	-7.68	115.28	133.31
24	R	602	CHL	CHA-C1A-C2A	-7.67	115.29	133.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	r	303	CHL	CHA-C1A-C2A	-7.66	115.31	133.31
24	1	311	CHL	CHA-C1A-C2A	-7.66	115.32	133.31
31	X	601	8CT	C33-C32-C31	-7.65	117.53	124.83
24	s	409	CHL	CHA-C1A-C2A	-7.63	115.38	133.31
24	8	310	CHL	CHA-C1A-C2A	-7.63	115.39	133.31
31	b	617	8CT	C14-C13-C12	-7.63	116.58	127.28
24	u	312	CHL	O2D-CGD-CBD	7.63	119.33	110.95
24	5	306	CHL	C1B-CHB-C4A	7.63	126.23	121.32
24	2	312	CHL	O2D-CGD-CBD	7.62	119.32	110.95
24	R	607	CHL	CHA-C1A-C2A	-7.62	115.43	133.31
24	8	304	CHL	CHA-C1A-C2A	-7.61	115.44	133.31
24	s	408	CHL	O2D-CGD-CBD	7.61	119.30	110.95
24	Y	312	CHL	CHA-C1A-C2A	-7.60	115.45	133.31
24	2	306	CHL	C1B-CHB-C4A	7.60	126.21	121.32
24	y	312	CHL	CHA-C1A-C2A	-7.60	115.47	133.31
24	Y	311	CHL	CHA-C1A-C2A	-7.59	115.48	133.31
24	3	311	CHL	O2D-CGD-CBD	7.59	119.28	110.95
24	r	308	CHL	CHA-C1A-C2A	-7.58	115.52	133.31
24	6	311	CHL	O2D-CGD-CBD	7.57	119.27	110.95
24	9	311	CHL	O2D-CGD-CBD	7.57	119.26	110.95
24	5	312	CHL	O2D-CGD-CBD	7.57	119.26	110.95
31	x	601	8CT	C33-C32-C31	-7.56	117.62	124.83
24	n	311	CHL	O2D-CGD-CBD	7.55	119.25	110.95
24	n	312	CHL	CHA-C1A-C2A	-7.54	115.61	133.31
24	N	312	CHL	CHA-C1A-C2A	-7.53	115.62	133.31
24	4	311	CHL	CHA-C1A-C2A	-7.51	115.67	133.31
24	5	306	CHL	CHA-C1A-C2A	-7.51	115.68	133.31
24	5	312	CHL	CHA-C1A-C2A	-7.50	115.69	133.31
24	R	608	CHL	CHA-C1A-C2A	-7.49	115.72	133.31
24	n	311	CHL	CHA-C1A-C2A	-7.49	115.72	133.31
24	2	306	CHL	CHA-C1A-C2A	-7.49	115.73	133.31
24	7	313	CHL	CHA-C1A-C2A	-7.49	115.73	133.31
24	r	309	CHL	CHA-C1A-C2A	-7.49	115.73	133.31
24	p	313	CHL	CHA-C1A-C2A	-7.47	115.77	133.31
24	N	311	CHL	O2D-CGD-CBD	7.47	119.15	110.95
24	y	313	CHL	CHA-C1A-C2A	-7.47	115.78	133.31
24	g	306	CHL	C1B-CHB-C4A	7.46	126.12	121.32
24	9	305	CHL	CHA-C1A-C2A	-7.45	115.81	133.31
24	N	305	CHL	CHA-C1A-C2A	-7.45	115.82	133.31
24	Y	319	CHL	CHA-C1A-C2A	-7.45	115.82	133.31
24	2	312	CHL	CHA-C1A-C2A	-7.44	115.83	133.31
24	u	306	CHL	CHA-C1A-C2A	-7.42	115.89	133.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	p	312	CHL	O2D-CGD-CBD	7.41	119.09	110.95
24	R	606	CHL	CHA-C1A-C2A	-7.41	115.91	133.31
31	s	416	8CT	C04-C03-C02	-7.41	112.52	122.64
24	r	308	CHL	O2D-CGD-CBD	7.39	119.07	110.95
24	n	305	CHL	CHA-C1A-C2A	-7.39	115.96	133.31
24	6	305	CHL	CHA-C1A-C2A	-7.38	115.99	133.31
24	R	607	CHL	O2D-CGD-CBD	7.37	119.05	110.95
24	1	305	CHL	CHA-C1A-C2A	-7.37	116.00	133.31
24	q	309	CHL	CHA-C1A-C2A	-7.37	116.00	133.31
24	6	311	CHL	CHA-C1A-C2A	-7.37	116.01	133.31
31	c	615	8CT	C24-C25-C26	-7.36	116.95	127.28
24	N	311	CHL	CHA-C1A-C2A	-7.36	116.03	133.31
24	4	305	CHL	CHA-C1A-C2A	-7.35	116.06	133.31
24	S	601	CHL	CHA-C1A-C2A	-7.33	116.09	133.31
31	C	615	8CT	C24-C25-C26	-7.32	117.01	127.28
31	S	615	8CT	C04-C03-C02	-7.32	112.64	122.64
24	r	307	CHL	CHA-C1A-C2A	-7.31	116.15	133.31
24	3	305	CHL	CHA-C1A-C2A	-7.30	116.17	133.31
24	g	312	CHL	O2D-CGD-CBD	7.27	118.94	110.95
24	S	607	CHL	CHA-C1A-C2A	-7.27	116.24	133.31
24	S	605	CHL	CHA-C1A-C2A	-7.27	116.24	133.31
27	r	316	XAT	C38-C25-C26	-7.27	110.34	122.30
27	R	615	XAT	C38-C25-C26	-7.26	110.35	122.30
24	s	402	CHL	CHA-C1A-C2A	-7.25	116.28	133.31
24	G	312	CHL	O2D-CGD-CBD	7.25	118.91	110.95
24	s	406	CHL	CHA-C1A-C2A	-7.24	116.30	133.31
24	7	309	CHL	C4D-ND-C1D	7.24	110.71	105.22
24	N	317	CHL	C4D-ND-C1D	7.24	110.71	105.22
24	n	317	CHL	C4D-ND-C1D	7.23	110.71	105.22
25	C	611	CLA	C4A-NA-C1A	7.23	109.98	106.68
24	g	312	CHL	CHA-C1A-C2A	-7.22	116.36	133.31
24	7	312	CHL	O2D-CGD-CBD	7.22	118.88	110.95
25	b	616	CLA	C4A-NA-C1A	7.21	109.97	106.68
24	s	407	CHL	CHA-C1A-C2A	-7.21	116.38	133.31
24	S	602	CHL	C1B-CHB-C4A	7.21	125.96	121.32
25	B	604	CLA	C4A-NA-C1A	7.21	109.97	106.68
24	S	608	CHL	C1B-CHB-C4A	7.21	125.96	121.32
24	3	311	CHL	CHA-C1A-C2A	-7.20	116.40	133.31
24	S	606	CHL	CHA-C1A-C2A	-7.20	116.41	133.31
25	B	616	CLA	C4A-NA-C1A	7.19	109.96	106.68
24	q	304	CHL	C1B-CHB-C4A	7.19	125.94	121.32
25	p	315	CLA	C4A-NA-C1A	7.18	109.96	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	315	CLA	C4A-NA-C1A	7.18	109.95	106.68
25	b	604	CLA	C4A-NA-C1A	7.15	109.94	106.68
25	y	316	CLA	C4A-NA-C1A	7.14	109.94	106.68
24	G	312	CHL	CHA-C1A-C2A	-7.12	116.59	133.31
24	p	309	CHL	C4D-ND-C1D	7.12	110.62	105.22
28	u	304	NEX	C27-C28-C29	7.12	136.57	125.53
24	s	408	CHL	CHA-C1A-C2A	-7.11	116.61	133.31
28	p	304	NEX	C27-C28-C29	7.10	136.55	125.53
25	c	611	CLA	C4A-NA-C1A	7.10	109.92	106.68
28	2	304	NEX	C27-C28-C29	7.10	136.55	125.53
24	u	318	CHL	C4D-ND-C1D	7.10	110.61	105.22
28	5	304	NEX	C27-C28-C29	7.10	136.54	125.53
28	G	304	NEX	C27-C28-C29	7.10	136.54	125.53
24	4	310	CHL	CHA-C1A-C2A	-7.09	116.67	133.31
24	6	309	CHL	CHA-C1A-C2A	-7.08	116.68	133.31
28	9	319	NEX	C27-C28-C29	7.08	136.51	125.53
28	4	303	NEX	C27-C28-C29	7.08	136.51	125.53
28	R	616	NEX	C27-C28-C29	7.07	136.51	125.53
24	1	310	CHL	CHA-C1A-C2A	-7.07	116.70	133.31
24	7	311	CHL	CHA-C1A-C2A	-7.07	116.71	133.31
24	8	304	CHL	C1B-CHB-C4A	7.06	125.87	121.32
28	r	317	NEX	C27-C28-C29	7.06	136.49	125.53
28	S	617	NEX	C27-C28-C29	7.06	136.49	125.53
28	7	304	NEX	C27-C28-C29	7.06	136.49	125.53
28	g	304	NEX	C27-C28-C29	7.06	136.48	125.53
24	1	304	CHL	C4D-ND-C1D	7.06	110.58	105.22
28	1	303	NEX	C27-C28-C29	7.06	136.48	125.53
28	y	304	NEX	C27-C28-C29	7.06	136.48	125.53
28	y	304	NEX	C35-C34-C33	-7.05	117.40	127.28
28	G	304	NEX	C35-C34-C33	-7.04	117.40	127.28
28	u	304	NEX	C35-C34-C33	-7.04	117.40	127.28
24	G	309	CHL	C4D-ND-C1D	7.04	110.56	105.22
24	4	304	CHL	C4D-ND-C1D	7.04	110.56	105.22
24	3	309	CHL	CHA-C1A-C2A	-7.03	116.79	133.31
24	5	305	CHL	CHA-C1A-C2A	-7.03	116.79	133.31
28	r	317	NEX	C35-C34-C33	-7.03	117.42	127.28
24	G	310	CHL	CHA-C1A-C2A	-7.03	116.80	133.31
28	1	303	NEX	C35-C34-C33	-7.03	117.42	127.28
28	9	319	NEX	C35-C34-C33	-7.02	117.43	127.28
24	p	311	CHL	CHA-C1A-C2A	-7.02	116.82	133.31
24	9	317	CHL	C4D-ND-C1D	7.02	110.55	105.22
24	g	309	CHL	C4D-ND-C1D	7.02	110.55	105.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	4	303	NEX	C35-C34-C33	-7.01	117.44	127.28
25	c	601	CLA	C4A-NA-C1A	7.01	109.88	106.68
28	7	304	NEX	C35-C34-C33	-7.01	117.45	127.28
25	7	315	CLA	C4A-NA-C1A	7.01	109.88	106.68
28	R	616	NEX	C35-C34-C33	-7.00	117.45	127.28
28	p	304	NEX	C35-C34-C33	-7.00	117.45	127.28
28	S	617	NEX	C35-C34-C33	-7.00	117.46	127.28
25	p	317	CLA	C4A-NA-C1A	6.99	109.87	106.68
28	g	304	NEX	C35-C34-C33	-6.99	117.47	127.28
24	1	312	CHL	CHA-C1A-C2A	-6.99	116.91	133.31
28	2	304	NEX	C35-C34-C33	-6.99	117.48	127.28
25	c	607	CLA	C4A-NA-C1A	6.99	109.87	106.68
28	5	304	NEX	C35-C34-C33	-6.98	117.49	127.28
24	3	304	CHL	CHA-C1A-C2A	-6.97	116.94	133.31
25	c	604	CLA	C4A-NA-C1A	6.97	109.86	106.68
25	C	607	CLA	C4A-NA-C1A	6.96	109.86	106.68
25	c	602	CLA	C4A-NA-C1A	6.96	109.85	106.68
31	x	601	8CT	C14-C13-C12	-6.96	117.52	127.28
25	C	612	CLA	C4A-NA-C1A	6.95	109.85	106.68
24	g	310	CHL	CHA-C1A-C2A	-6.94	117.00	133.31
24	2	305	CHL	CHA-C1A-C2A	-6.93	117.03	133.31
24	y	312	CHL	O2D-CGD-CBD	6.93	118.56	110.95
24	4	312	CHL	CHA-C1A-C2A	-6.93	117.03	133.31
24	Y	311	CHL	O2D-CGD-CBD	6.93	118.56	110.95
24	9	308	CHL	C4D-ND-C1D	6.93	110.48	105.22
25	g	316	CLA	C4A-NA-C1A	6.93	109.84	106.68
25	b	606	CLA	C4A-NA-C1A	6.92	109.84	106.68
25	B	606	CLA	C4A-NA-C1A	6.90	109.83	106.68
25	a	603	CLA	C4A-NA-C1A	6.90	109.83	106.68
31	X	601	8CT	C14-C13-C12	-6.90	117.60	127.28
24	7	310	CHL	CHA-C1A-C2A	-6.90	117.11	133.31
25	5	316	CLA	C4A-NA-C1A	6.90	109.83	106.68
24	N	308	CHL	CHA-C1A-C2A	-6.89	117.12	133.31
24	4	317	CHL	C4D-ND-C1D	6.89	110.45	105.22
24	G	305	CHL	CHA-C1A-C2A	-6.89	117.13	133.31
25	C	602	CLA	C4A-NA-C1A	6.88	109.82	106.68
24	g	305	CHL	CHA-C1A-C2A	-6.88	117.15	133.31
24	G	311	CHL	CHA-C1A-C2A	-6.88	117.15	133.31
31	a	608	8CT	C30-C29-C28	-6.88	113.87	124.58
24	N	310	CHL	CHA-C1A-C2A	-6.88	117.16	133.31
25	p	316	CLA	C4A-NA-C1A	6.88	109.82	106.68
25	b	611	CLA	C4A-NA-C1A	6.87	109.81	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	s	403	CHL	C1B-CHB-C4A	6.87	125.74	121.32
24	n	310	CHL	CHA-C1A-C2A	-6.87	117.18	133.31
24	p	310	CHL	CHA-C1A-C2A	-6.87	117.18	133.31
24	5	311	CHL	CHA-C1A-C2A	-6.87	117.19	133.31
31	A	608	8CT	C30-C29-C28	-6.86	113.91	124.58
24	2	311	CHL	CHA-C1A-C2A	-6.85	117.22	133.31
24	u	311	CHL	CHA-C1A-C2A	-6.85	117.23	133.31
25	c	612	CLA	C4A-NA-C1A	6.84	109.80	106.68
25	A	603	CLA	C4A-NA-C1A	6.84	109.80	106.68
24	9	309	CHL	CHA-C1A-C2A	-6.84	117.25	133.31
25	b	609	CLA	C4A-NA-C1A	6.84	109.80	106.68
25	q	314	CLA	C4A-NA-C1A	6.83	109.80	106.68
28	9	319	NEX	C35-C15-C14	6.83	137.50	123.52
25	B	611	CLA	C4A-NA-C1A	6.83	109.80	106.68
25	C	604	CLA	C4A-NA-C1A	6.83	109.80	106.68
24	y	309	CHL	CHA-C1A-C2A	-6.83	117.27	133.31
31	A	608	8CT	C14-C13-C12	-6.83	117.70	127.28
31	t	101	8CT	C30-C31-C32	-6.83	113.07	121.47
25	r	313	CLA	C4A-NA-C1A	6.82	109.79	106.68
28	p	304	NEX	C35-C15-C14	6.82	137.47	123.52
31	T	101	8CT	C30-C31-C32	-6.82	113.08	121.47
24	1	317	CHL	C4D-ND-C1D	6.82	110.39	105.22
25	2	316	CLA	C4A-NA-C1A	6.81	109.79	106.68
28	5	304	NEX	C35-C15-C14	6.81	137.46	123.52
28	r	317	NEX	C35-C15-C14	6.81	137.45	123.52
28	S	617	NEX	C35-C15-C14	6.81	137.45	123.52
28	u	304	NEX	C35-C15-C14	6.81	137.45	123.52
25	u	315	CLA	C4A-NA-C1A	6.81	109.78	106.68
25	7	307	CLA	C4A-NA-C1A	6.81	109.78	106.68
28	1	303	NEX	C35-C15-C14	6.81	137.45	123.52
24	5	318	CHL	C4D-ND-C1D	6.81	110.39	105.22
28	g	304	NEX	C35-C15-C14	6.81	137.45	123.52
28	2	304	NEX	C35-C15-C14	6.80	137.44	123.52
24	3	308	CHL	C4D-ND-C1D	6.80	110.38	105.22
25	8	313	CLA	C4A-NA-C1A	6.79	109.78	106.68
25	s	412	CLA	C4A-NA-C1A	6.79	109.78	106.68
24	u	313	CHL	C4D-ND-C1D	6.79	110.37	105.22
24	g	311	CHL	CHA-C1A-C2A	-6.79	117.36	133.31
25	7	317	CLA	C4A-NA-C1A	6.79	109.78	106.68
24	6	308	CHL	C4D-ND-C1D	6.79	110.37	105.22
28	R	616	NEX	C35-C15-C14	6.79	137.41	123.52
24	u	309	CHL	C4D-ND-C1D	6.79	110.37	105.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	r	304	CLA	C4A-NA-C1A	6.78	109.77	106.68
28	7	304	NEX	C35-C15-C14	6.78	137.39	123.52
25	d	405	CLA	C4A-NA-C1A	6.78	109.77	106.68
25	7	316	CLA	C4A-NA-C1A	6.78	109.77	106.68
28	y	304	NEX	C35-C15-C14	6.78	137.38	123.52
24	9	312	CHL	C4D-ND-C1D	6.77	110.36	105.22
24	4	308	CHL	C4D-ND-C1D	6.77	110.36	105.22
28	G	304	NEX	C35-C15-C14	6.77	137.37	123.52
25	G	316	CLA	C4A-NA-C1A	6.77	109.77	106.68
28	4	303	NEX	C35-C15-C14	6.77	137.37	123.52
25	5	315	CLA	C4A-NA-C1A	6.76	109.77	106.68
25	b	605	CLA	C4A-NA-C1A	6.76	109.77	106.68
25	6	315	CLA	C4A-NA-C1A	6.76	109.76	106.68
24	1	308	CHL	C4D-ND-C1D	6.76	110.35	105.22
25	2	315	CLA	C4A-NA-C1A	6.75	109.76	106.68
25	p	307	CLA	C4A-NA-C1A	6.75	109.76	106.68
25	D	405	CLA	C4A-NA-C1A	6.75	109.76	106.68
25	9	314	CLA	C4A-NA-C1A	6.75	109.76	106.68
25	b	607	CLA	C4A-NA-C1A	6.75	109.76	106.68
31	a	608	8CT	C14-C13-C12	-6.74	117.82	127.28
25	4	315	CLA	C4A-NA-C1A	6.73	109.75	106.68
24	2	318	CHL	C4D-ND-C1D	6.73	110.33	105.22
24	8	315	CHL	C4D-ND-C1D	6.73	110.33	105.22
24	Y	308	CHL	CHA-C1A-C2A	-6.73	117.52	133.31
25	C	601	CLA	C4A-NA-C1A	6.72	109.75	106.68
24	q	316	CHL	C4D-ND-C1D	6.72	110.32	105.22
25	r	310	CLA	C4A-NA-C1A	6.72	109.75	106.68
31	s	415	8CT	C18-C17-C16	-6.72	117.86	127.28
25	R	603	CLA	C4A-NA-C1A	6.72	109.74	106.68
24	9	310	CHL	CHA-C1A-C2A	-6.71	117.54	133.31
25	B	607	CLA	C4A-NA-C1A	6.71	109.74	106.68
25	B	609	CLA	C4A-NA-C1A	6.71	109.74	106.68
25	3	315	CLA	C4A-NA-C1A	6.71	109.74	106.68
25	d	404	CLA	C4A-NA-C1A	6.70	109.74	106.68
25	a	607	CLA	C4A-NA-C1A	6.70	109.74	106.68
31	S	614	8CT	C18-C17-C16	-6.70	117.88	127.28
25	R	609	CLA	C4A-NA-C1A	6.69	109.73	106.68
25	u	317	CLA	C4A-NA-C1A	6.69	109.73	106.68
24	4	309	CHL	CHA-C1A-C2A	-6.68	117.61	133.31
25	B	601	CLA	C4A-NA-C1A	6.68	109.72	106.68
25	s	411	CLA	C4A-NA-C1A	6.68	109.72	106.68
24	3	310	CHL	CHA-C1A-C2A	-6.68	117.64	133.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	9	304	CHL	CHA-C1A-C2A	-6.68	117.64	133.31
25	n	306	CLA	C4A-NA-C1A	6.67	109.72	106.68
24	6	312	CHL	CHA-C1A-C2A	-6.67	117.64	133.31
24	G	313	CHL	CHA-C1A-C2A	-6.67	117.65	133.31
25	1	315	CLA	C4A-NA-C1A	6.67	109.72	106.68
25	b	601	CLA	C4A-NA-C1A	6.67	109.72	106.68
25	u	307	CLA	C4A-NA-C1A	6.66	109.72	106.68
27	R	615	XAT	C18-C5-C6	-6.66	111.34	122.30
25	S	611	CLA	C4A-NA-C1A	6.66	109.72	106.68
25	G	317	CLA	C4A-NA-C1A	6.66	109.72	106.68
25	C	605	CLA	C4A-NA-C1A	6.66	109.72	106.68
24	Y	305	CHL	C1B-CHB-C4A	6.66	125.60	121.32
24	u	310	CHL	CHA-C1A-C2A	-6.65	117.69	133.31
25	Y	307	CLA	C4A-NA-C1A	6.65	109.71	106.68
25	n	315	CLA	C4A-NA-C1A	6.65	109.71	106.68
31	C	613	8CT	C14-C13-C12	-6.65	117.96	127.28
24	3	312	CHL	CHA-C1A-C2A	-6.65	117.70	133.31
25	9	315	CLA	C4A-NA-C1A	6.65	109.71	106.68
25	b	608	CLA	C4A-NA-C1A	6.64	109.71	106.68
24	6	304	CHL	CHA-C1A-C2A	-6.64	117.71	133.31
24	g	313	CHL	CHA-C1A-C2A	-6.64	117.71	133.31
25	q	305	CLA	C4A-NA-C1A	6.64	109.71	106.68
24	5	309	CHL	C4D-ND-C1D	6.64	110.26	105.22
31	c	613	8CT	C14-C13-C12	-6.64	117.97	127.28
24	y	306	CHL	C1B-CHB-C4A	6.64	125.59	121.32
24	u	313	CHL	CHA-C1A-C2A	-6.64	117.73	133.31
24	9	312	CHL	CHA-C1A-C2A	-6.63	117.73	133.31
25	5	317	CLA	C4A-NA-C1A	6.63	109.71	106.68
27	r	316	XAT	C18-C5-C6	-6.63	111.38	122.30
25	g	317	CLA	C4A-NA-C1A	6.63	109.70	106.68
25	A	607	CLA	C4A-NA-C1A	6.63	109.70	106.68
25	C	608	CLA	C4A-NA-C1A	6.62	109.70	106.68
24	G	313	CHL	C4D-ND-C1D	6.61	110.24	105.22
25	N	306	CLA	C4A-NA-C1A	6.61	109.70	106.68
25	S	616	CLA	C4A-NA-C1A	6.61	109.69	106.68
25	y	308	CLA	C4A-NA-C1A	6.61	109.69	106.68
25	4	306	CLA	C4A-NA-C1A	6.60	109.69	106.68
24	s	409	CHL	C1B-CHB-C4A	6.60	125.57	121.32
25	Y	306	CLA	C4A-NA-C1A	6.60	109.69	106.68
25	Y	316	CLA	C4A-NA-C1A	6.60	109.69	106.68
25	c	605	CLA	C4A-NA-C1A	6.60	109.69	106.68
25	5	307	CLA	C4A-NA-C1A	6.60	109.69	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	1	309	CHL	CHA-C1A-C2A	-6.60	117.82	133.31
24	g	313	CHL	C4D-ND-C1D	6.60	110.22	105.22
25	R	604	CLA	C4A-NA-C1A	6.59	109.69	106.68
25	b	602	CLA	C4A-NA-C1A	6.59	109.69	106.68
24	s	408	CHL	OBD-CAD-CBD	6.59	135.50	125.82
25	n	314	CLA	C4A-NA-C1A	6.59	109.68	106.68
25	9	306	CLA	C4A-NA-C1A	6.58	109.68	106.68
24	8	303	CHL	C4D-ND-C1D	6.58	110.22	105.22
25	B	605	CLA	C4A-NA-C1A	6.58	109.68	106.68
25	4	314	CLA	C4A-NA-C1A	6.58	109.68	106.68
25	9	307	CLA	C4A-NA-C1A	6.58	109.68	106.68
25	N	315	CLA	C4A-NA-C1A	6.58	109.68	106.68
25	B	602	CLA	C4A-NA-C1A	6.57	109.67	106.68
25	9	316	CLA	C4A-NA-C1A	6.56	109.67	106.68
31	T	101	8CT	C14-C13-C12	-6.56	118.07	127.28
25	A	610	CLA	C4A-NA-C1A	6.56	109.67	106.68
25	6	307	CLA	C4A-NA-C1A	6.56	109.67	106.68
25	1	313	CLA	C4A-NA-C1A	6.56	109.67	106.68
25	1	314	CLA	C4A-NA-C1A	6.56	109.67	106.68
25	r	314	CLA	C4A-NA-C1A	6.56	109.67	106.68
31	t	101	8CT	C14-C13-C12	-6.56	118.08	127.28
25	q	312	CLA	C4A-NA-C1A	6.56	109.67	106.68
24	6	310	CHL	C4D-ND-C1D	6.56	110.19	105.22
25	u	316	CLA	C4A-NA-C1A	6.56	109.67	106.68
25	r	312	CLA	C4A-NA-C1A	6.56	109.67	106.68
25	2	308	CLA	C4A-NA-C1A	6.55	109.67	106.68
24	n	308	CHL	C4D-ND-C1D	6.55	110.19	105.22
24	u	305	CHL	C4D-ND-C1D	6.54	110.19	105.22
25	s	413	CLA	C4A-NA-C1A	6.54	109.66	106.68
25	S	610	CLA	C4A-NA-C1A	6.54	109.66	106.68
24	2	309	CHL	C4D-ND-C1D	6.54	110.18	105.22
24	8	307	CHL	CHA-C1A-C2A	-6.54	117.96	133.31
24	6	310	CHL	CHA-C1A-C2A	-6.54	117.96	133.31
25	8	305	CLA	C4A-NA-C1A	6.53	109.66	106.68
25	c	609	CLA	C4A-NA-C1A	6.53	109.66	106.68
25	3	307	CLA	C4A-NA-C1A	6.53	109.66	106.68
24	6	312	CHL	C4D-ND-C1D	6.53	110.17	105.22
24	R	607	CHL	C1B-CHB-C4A	6.53	125.52	121.32
25	n	313	CLA	C4A-NA-C1A	6.53	109.66	106.68
25	n	307	CLA	C4A-NA-C1A	6.52	109.66	106.68
25	y	317	CLA	C4A-NA-C1A	6.52	109.66	106.68
24	q	303	CHL	C4D-ND-C1D	6.52	110.17	105.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	8	311	CLA	C4A-NA-C1A	6.52	109.65	106.68
25	s	417	CLA	C4A-NA-C1A	6.52	109.65	106.68
25	R	613	CLA	C4A-NA-C1A	6.52	109.65	106.68
25	C	616	CLA	C4A-NA-C1A	6.52	109.65	106.68
25	3	316	CLA	C4A-NA-C1A	6.51	109.65	106.68
24	r	308	CHL	C1B-CHB-C4A	6.51	125.51	121.32
24	n	304	CHL	C4D-ND-C1D	6.51	110.16	105.22
25	c	616	CLA	C4A-NA-C1A	6.51	109.65	106.68
25	C	609	CLA	C4A-NA-C1A	6.51	109.65	106.68
25	N	313	CLA	C4A-NA-C1A	6.49	109.64	106.68
25	y	307	CLA	C4A-NA-C1A	6.49	109.64	106.68
24	9	311	CHL	CHA-C1A-C2A	-6.49	118.07	133.31
25	B	608	CLA	C4A-NA-C1A	6.49	109.64	106.68
25	B	610	CLA	C4A-NA-C1A	6.49	109.64	106.68
25	c	608	CLA	C4A-NA-C1A	6.49	109.64	106.68
31	S	614	8CT	C14-C13-C12	-6.49	118.18	127.28
25	g	314	CLA	C4A-NA-C1A	6.49	109.64	106.68
25	p	314	CLA	C4A-NA-C1A	6.48	109.64	106.68
24	9	310	CHL	C4D-ND-C1D	6.48	110.14	105.22
25	8	312	CLA	C4A-NA-C1A	6.48	109.64	106.68
25	N	307	CLA	C4A-NA-C1A	6.48	109.63	106.68
24	N	304	CHL	C4D-ND-C1D	6.48	110.13	105.22
28	p	304	NEX	C11-C12-C13	-6.48	108.61	126.36
25	9	313	CLA	C4A-NA-C1A	6.47	109.63	106.68
25	6	316	CLA	C4A-NA-C1A	6.47	109.63	106.68
24	3	312	CHL	C4D-ND-C1D	6.47	110.13	105.22
25	1	306	CLA	C4A-NA-C1A	6.47	109.63	106.68
25	s	410	CLA	C4A-NA-C1A	6.47	109.63	106.68
24	R	601	CHL	C4D-ND-C1D	6.47	110.13	105.22
25	n	316	CLA	C4A-NA-C1A	6.47	109.63	106.68
28	r	317	NEX	C11-C12-C13	-6.47	108.63	126.36
28	g	304	NEX	C11-C12-C13	-6.47	108.63	126.36
25	N	314	CLA	C4A-NA-C1A	6.47	109.63	106.68
25	r	305	CLA	C4A-NA-C1A	6.47	109.63	106.68
28	5	304	NEX	C11-C12-C13	-6.47	108.64	126.36
28	7	304	NEX	C11-C12-C13	-6.47	108.64	126.36
28	u	304	NEX	C11-C12-C13	-6.46	108.64	126.36
25	a	610	CLA	C4A-NA-C1A	6.46	109.63	106.68
28	2	304	NEX	C11-C12-C13	-6.46	108.65	126.36
25	2	317	CLA	C4A-NA-C1A	6.46	109.63	106.68
25	s	405	CLA	C4A-NA-C1A	6.46	109.63	106.68
24	3	310	CHL	C4D-ND-C1D	6.46	110.12	105.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	D	404	CLA	C4A-NA-C1A	6.46	109.62	106.68
28	R	616	NEX	C11-C12-C13	-6.46	108.66	126.36
28	S	617	NEX	C11-C12-C13	-6.46	108.66	126.36
28	4	303	NEX	C11-C12-C13	-6.46	108.66	126.36
25	S	604	CLA	C4A-NA-C1A	6.46	109.62	106.68
25	5	308	CLA	C4A-NA-C1A	6.46	109.62	106.68
28	y	304	NEX	C11-C12-C13	-6.45	108.67	126.36
28	G	304	NEX	C11-C12-C13	-6.45	108.67	126.36
28	1	303	NEX	C11-C12-C13	-6.45	108.68	126.36
28	9	319	NEX	C11-C12-C13	-6.45	108.68	126.36
31	s	415	8CT	C14-C13-C12	-6.45	118.23	127.28
25	Y	313	CLA	C4A-NA-C1A	6.45	109.62	106.68
24	u	312	CHL	CHA-C1A-C2A	-6.44	118.18	133.31
25	B	615	CLA	C4A-NA-C1A	6.44	109.62	106.68
25	1	316	CLA	C4A-NA-C1A	6.44	109.62	106.68
25	2	307	CLA	C4A-NA-C1A	6.43	109.61	106.68
25	S	612	CLA	C4A-NA-C1A	6.43	109.61	106.68
25	G	307	CLA	C4A-NA-C1A	6.43	109.61	106.68
25	N	316	CLA	C4A-NA-C1A	6.43	109.61	106.68
29	4	301	0UR	C14-C15-C16	-6.43	118.26	127.28
25	C	603	CLA	C4A-NA-C1A	6.43	109.61	106.68
25	q	315	CLA	C4A-NA-C1A	6.43	109.61	106.68
25	b	610	CLA	C4A-NA-C1A	6.43	109.61	106.68
24	r	302	CHL	C4D-ND-C1D	6.43	110.10	105.22
29	1	301	0UR	C14-C15-C16	-6.43	118.27	127.28
25	R	612	CLA	C4A-NA-C1A	6.42	109.61	106.68
25	G	314	CLA	C4A-NA-C1A	6.42	109.61	106.68
24	q	303	CHL	CHA-C1A-C2A	-6.42	118.23	133.31
25	g	308	CLA	C4A-NA-C1A	6.42	109.61	106.68
24	q	307	CHL	CHA-C1A-C2A	-6.42	118.23	133.31
25	4	313	CLA	C4A-NA-C1A	6.42	109.61	106.68
25	b	603	CLA	C4A-NA-C1A	6.42	109.61	106.68
31	B	617	8CT	C35-C30-C29	-6.41	105.45	112.83
25	c	603	CLA	C4A-NA-C1A	6.41	109.60	106.68
31	b	617	8CT	C35-C30-C29	-6.41	105.46	112.83
25	u	308	CLA	C4A-NA-C1A	6.41	109.60	106.68
25	b	614	CLA	C4A-NA-C1A	6.40	109.60	106.68
25	B	612	CLA	C4A-NA-C1A	6.40	109.60	106.68
25	R	611	CLA	C4A-NA-C1A	6.40	109.60	106.68
25	y	314	CLA	C4A-NA-C1A	6.39	109.60	106.68
25	5	314	CLA	C4A-NA-C1A	6.38	109.59	106.68
25	b	615	CLA	C4A-NA-C1A	6.38	109.59	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	g	307	CLA	C4A-NA-C1A	6.38	109.59	106.68
25	g	315	CLA	C4A-NA-C1A	6.38	109.59	106.68
25	s	404	CLA	C4A-NA-C1A	6.37	109.59	106.68
25	7	314	CLA	C4A-NA-C1A	6.37	109.58	106.68
24	u	311	CHL	C4D-ND-C1D	6.37	110.05	105.22
25	B	603	CLA	C4A-NA-C1A	6.37	109.58	106.68
25	8	306	CLA	C4A-NA-C1A	6.37	109.58	106.68
25	7	308	CLA	C4A-NA-C1A	6.37	109.58	106.68
25	B	614	CLA	C4A-NA-C1A	6.36	109.58	106.68
27	R	615	XAT	O4-C5-C4	6.35	119.44	113.49
25	C	606	CLA	C4A-NA-C1A	6.35	109.57	106.68
25	4	316	CLA	C4A-NA-C1A	6.35	109.57	106.68
25	6	314	CLA	C4A-NA-C1A	6.35	109.57	106.68
24	8	303	CHL	CHA-C1A-C2A	-6.34	118.43	133.31
25	G	315	CLA	C4A-NA-C1A	6.33	109.57	106.68
25	u	314	CLA	C4A-NA-C1A	6.33	109.57	106.68
25	q	313	CLA	C4A-NA-C1A	6.33	109.57	106.68
24	N	304	CHL	CHA-C1A-C2A	-6.33	118.44	133.31
25	S	609	CLA	C4A-NA-C1A	6.33	109.56	106.68
25	3	306	CLA	C4A-NA-C1A	6.32	109.56	106.68
25	c	606	CLA	C4A-NA-C1A	6.32	109.56	106.68
25	R	610	CLA	C4A-NA-C1A	6.31	109.56	106.68
25	q	306	CLA	C4A-NA-C1A	6.31	109.56	106.68
25	p	308	CLA	C4A-NA-C1A	6.31	109.56	106.68
25	6	313	CLA	C4A-NA-C1A	6.30	109.56	106.68
24	g	311	CHL	C4D-ND-C1D	6.30	110.00	105.22
24	u	312	CHL	C4D-ND-C1D	6.30	110.00	105.22
24	1	309	CHL	C4D-ND-C1D	6.30	110.00	105.22
25	2	314	CLA	C4A-NA-C1A	6.30	109.55	106.68
25	y	315	CLA	C4A-NA-C1A	6.29	109.55	106.68
25	S	603	CLA	C4A-NA-C1A	6.28	109.55	106.68
24	4	312	CHL	C4D-ND-C1D	6.28	109.99	105.22
25	b	613	CLA	C4A-NA-C1A	6.28	109.54	106.68
25	Y	314	CLA	C4A-NA-C1A	6.28	109.54	106.68
25	6	306	CLA	C4A-NA-C1A	6.28	109.54	106.68
25	4	307	CLA	C4A-NA-C1A	6.27	109.54	106.68
25	G	308	CLA	C4A-NA-C1A	6.27	109.54	106.68
31	x	601	8CT	C30-C29-C28	-6.27	114.83	124.58
25	C	610	CLA	C4A-NA-C1A	6.26	109.54	106.68
24	r	302	CHL	CHA-C1A-C2A	-6.26	118.62	133.31
31	S	614	8CT	C04-C03-C02	-6.26	114.09	122.64
24	1	312	CHL	C4D-ND-C1D	6.25	109.96	105.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	N	310	CHL	C4D-ND-C1D	6.25	109.96	105.22
24	n	304	CHL	CHA-C1A-C2A	-6.25	118.63	133.31
28	7	304	NEX	C38-C25-C26	-6.25	112.02	122.30
28	4	303	NEX	C38-C25-C26	-6.25	112.02	122.30
24	9	311	CHL	C4D-ND-C1D	6.25	109.96	105.22
25	8	314	CLA	C4A-NA-C1A	6.25	109.53	106.68
24	4	309	CHL	C4D-ND-C1D	6.24	109.96	105.22
24	n	310	CHL	C4D-ND-C1D	6.24	109.96	105.22
25	A	604	CLA	C4A-NA-C1A	6.24	109.53	106.68
24	G	306	CHL	C1B-CHB-C4A	6.24	125.34	121.32
24	u	310	CHL	C4D-ND-C1D	6.24	109.95	105.22
28	G	304	NEX	C38-C25-C26	-6.24	112.04	122.30
28	S	617	NEX	C38-C25-C26	-6.23	112.04	122.30
25	r	311	CLA	C4A-NA-C1A	6.23	109.52	106.68
28	u	304	NEX	C38-C25-C26	-6.23	112.05	122.30
28	5	304	NEX	C38-C25-C26	-6.23	112.05	122.30
31	X	601	8CT	C30-C29-C28	-6.23	114.89	124.58
28	p	304	NEX	C38-C25-C26	-6.23	112.05	122.30
24	R	601	CHL	CHA-C1A-C2A	-6.22	118.69	133.31
24	u	305	CHL	CHA-C1A-C2A	-6.22	118.70	133.31
28	2	304	NEX	C38-C25-C26	-6.22	112.07	122.30
25	3	313	CLA	C4A-NA-C1A	6.22	109.52	106.68
28	9	319	NEX	C38-C25-C26	-6.21	112.08	122.30
28	y	304	NEX	C38-C25-C26	-6.21	112.08	122.30
28	g	304	NEX	C38-C25-C26	-6.21	112.08	122.30
24	6	317	CHL	C4D-ND-C1D	6.21	109.93	105.22
31	s	415	8CT	C04-C03-C02	-6.20	114.16	122.64
28	1	303	NEX	C38-C25-C26	-6.20	112.10	122.30
31	X	601	8CT	C18-C17-C16	-6.19	118.59	127.28
31	b	617	8CT	C19-C20-C21	-6.19	118.59	127.28
28	R	616	NEX	C38-C25-C26	-6.19	112.11	122.30
25	c	610	CLA	C4A-NA-C1A	6.19	109.50	106.68
28	r	317	NEX	C38-C25-C26	-6.18	112.13	122.30
24	q	307	CHL	C4D-ND-C1D	6.18	109.91	105.22
24	y	309	CHL	C4D-ND-C1D	6.17	109.91	105.22
24	2	309	CHL	CHA-C1A-C2A	-6.17	118.81	133.31
25	B	613	CLA	C4A-NA-C1A	6.17	109.49	106.68
24	6	304	CHL	C4D-ND-C1D	6.17	109.90	105.22
31	V	401	8CT	C10-C11-C12	-6.16	117.13	126.23
25	b	612	CLA	C4A-NA-C1A	6.15	109.49	106.68
24	Y	308	CHL	C4D-ND-C1D	6.15	109.89	105.22
25	1	307	CLA	C4A-NA-C1A	6.15	109.48	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	3	314	CLA	C4A-NA-C1A	6.15	109.48	106.68
24	3	317	CHL	C4D-ND-C1D	6.14	109.88	105.22
31	B	617	8CT	C19-C20-C21	-6.14	118.67	127.28
24	n	308	CHL	CHA-C1A-C2A	-6.13	118.90	133.31
24	G	310	CHL	C4D-ND-C1D	6.13	109.87	105.22
24	g	310	CHL	C4D-ND-C1D	6.13	109.87	105.22
25	A	605	CLA	C4A-NA-C1A	6.12	109.47	106.68
31	v	401	8CT	C10-C11-C12	-6.11	117.20	126.23
24	N	308	CHL	C4D-ND-C1D	6.10	109.85	105.22
29	4	301	0UR	C10-C11-C12	-6.10	118.72	127.28
24	6	305	CHL	C1B-CHB-C4A	6.09	125.24	121.32
24	y	312	CHL	C1B-CHB-C4A	6.09	125.24	121.32
24	7	312	CHL	OBD-CAD-CBD	6.08	134.75	125.82
27	r	316	XAT	O4-C5-C4	6.08	119.19	113.49
24	7	310	CHL	C4D-ND-C1D	6.08	109.84	105.22
24	3	311	CHL	OBD-CAD-CBD	6.08	134.75	125.82
25	a	605	CLA	C4A-NA-C1A	6.08	109.45	106.68
24	G	311	CHL	C4D-ND-C1D	6.08	109.83	105.22
25	a	604	CLA	C4A-NA-C1A	6.08	109.45	106.68
24	2	311	CHL	C4D-ND-C1D	6.07	109.83	105.22
24	5	311	CHL	C4D-ND-C1D	6.07	109.83	105.22
24	p	310	CHL	C4D-ND-C1D	6.07	109.83	105.22
31	x	601	8CT	C18-C17-C16	-6.07	118.77	127.28
24	8	307	CHL	C4D-ND-C1D	6.07	109.82	105.22
24	5	309	CHL	CHA-C1A-C2A	-6.06	119.07	133.31
24	Y	311	CHL	C1B-CHB-C4A	6.06	125.22	121.32
24	7	318	CHL	C4D-ND-C1D	6.03	109.80	105.22
24	5	309	CHL	C1A-CHA-C4D	-6.03	108.92	118.98
24	9	309	CHL	C4D-ND-C1D	6.03	109.79	105.22
24	p	318	CHL	C4D-ND-C1D	6.01	109.78	105.22
24	q	307	CHL	C1A-CHA-C4D	-6.00	108.96	118.98
24	s	408	CHL	OBD-CAD-C3D	-6.00	118.53	127.89
24	2	313	CHL	C4D-ND-C1D	5.98	109.76	105.22
24	8	307	CHL	C1A-CHA-C4D	-5.98	109.00	118.98
24	1	308	CHL	CHA-C1A-C2A	-5.98	119.27	133.31
24	4	308	CHL	CHA-C1A-C2A	-5.98	119.27	133.31
24	9	304	CHL	C4D-ND-C1D	5.96	109.75	105.22
24	3	309	CHL	C4D-ND-C1D	5.96	109.74	105.22
24	5	313	CHL	C4D-ND-C1D	5.96	109.74	105.22
29	1	301	0UR	C10-C11-C12	-5.95	118.93	127.28
31	S	614	8CT	C30-C31-C32	-5.95	114.15	121.47
24	G	305	CHL	C4D-ND-C1D	5.95	109.73	105.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	2	309	CHL	C1A-CHA-C4D	-5.94	109.07	118.98
24	6	308	CHL	C1A-CHA-C4D	-5.94	109.07	118.98
24	q	308	CHL	C1B-CHB-C4A	5.94	125.14	121.32
24	g	305	CHL	C4D-ND-C1D	5.93	109.72	105.22
24	6	309	CHL	C4D-ND-C1D	5.93	109.72	105.22
24	y	309	CHL	C1A-CHA-C4D	-5.92	109.10	118.98
31	s	415	8CT	C30-C31-C32	-5.92	114.18	121.47
31	s	416	8CT	C01-C02-C03	-5.91	118.03	124.48
24	Y	308	CHL	C1A-CHA-C4D	-5.91	109.13	118.98
24	u	310	CHL	C1A-CHA-C4D	-5.90	109.14	118.98
24	4	308	CHL	C1A-CHA-C4D	-5.90	109.14	118.98
24	6	308	CHL	CHA-C1A-C2A	-5.90	119.46	133.31
24	S	605	CHL	C4D-ND-C1D	5.90	109.69	105.22
24	3	308	CHL	C1A-CHA-C4D	-5.90	109.14	118.98
31	B	617	8CT	C18-C17-C16	-5.89	119.01	127.28
24	4	317	CHL	C1A-CHA-C4D	-5.89	109.15	118.98
24	g	309	CHL	C1A-CHA-C4D	-5.89	109.16	118.98
24	r	308	CHL	C1A-CHA-C4D	-5.88	109.17	118.98
31	T	101	8CT	C01-C02-C03	-5.88	118.07	124.48
24	s	406	CHL	C4D-ND-C1D	5.88	109.68	105.22
24	1	317	CHL	C1A-CHA-C4D	-5.88	109.18	118.98
24	Y	310	CHL	OBD-CAD-CBD	5.86	134.43	125.82
24	1	310	CHL	C4D-ND-C1D	5.86	109.66	105.22
24	u	309	CHL	CHA-C1A-C2A	-5.86	119.56	133.31
24	9	309	CHL	C1A-CHA-C4D	-5.85	109.21	118.98
31	C	614	8CT	C14-C13-C12	-5.85	119.07	127.28
24	R	607	CHL	C1A-CHA-C4D	-5.85	109.22	118.98
24	3	308	CHL	CHA-C1A-C2A	-5.85	119.57	133.31
24	4	310	CHL	C4D-ND-C1D	5.85	109.66	105.22
24	1	308	CHL	C1A-CHA-C4D	-5.85	109.22	118.98
24	G	309	CHL	C1A-CHA-C4D	-5.85	109.22	118.98
24	1	311	CHL	C1B-CHB-C4A	5.85	125.08	121.32
24	1	309	CHL	C1A-CHA-C4D	-5.84	109.24	118.98
24	g	318	CHL	C4D-ND-C1D	5.84	109.65	105.22
24	r	309	CHL	C1B-CHB-C4A	5.84	125.08	121.32
24	q	308	CHL	C1A-CHA-C4D	-5.84	109.24	118.98
24	r	306	CHL	C4D-ND-C1D	5.83	109.65	105.22
24	G	312	CHL	C4D-ND-C1D	5.83	109.64	105.22
24	8	308	CHL	C1A-CHA-C4D	-5.83	109.26	118.98
24	n	317	CHL	C1A-CHA-C4D	-5.82	109.27	118.98
31	c	614	8CT	C14-C13-C12	-5.82	119.11	127.28
24	2	305	CHL	C4D-ND-C1D	5.82	109.64	105.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	4	309	CHL	C1A-CHA-C4D	-5.82	109.27	118.98
24	9	308	CHL	C1A-CHA-C4D	-5.82	109.28	118.98
24	6	311	CHL	OBD-CAD-CBD	5.82	134.36	125.82
24	u	309	CHL	C1A-CHA-C4D	-5.82	109.28	118.98
24	N	317	CHL	C1A-CHA-C4D	-5.81	109.28	118.98
31	t	101	8CT	C01-C02-C03	-5.81	118.14	124.48
24	G	310	CHL	C1A-CHA-C4D	-5.81	109.29	118.98
24	N	311	CHL	C1A-CHA-C4D	-5.81	109.29	118.98
31	T	101	8CT	C18-C17-C16	-5.80	119.14	127.28
24	p	312	CHL	OBD-CAD-CBD	5.80	134.34	125.82
24	g	310	CHL	C1A-CHA-C4D	-5.80	109.31	118.98
31	t	101	8CT	C18-C17-C16	-5.80	119.15	127.28
24	8	315	CHL	C1A-CHA-C4D	-5.79	109.32	118.98
24	S	606	CHL	C4D-ND-C1D	5.79	109.61	105.22
24	u	305	CHL	C1A-CHA-C4D	-5.79	109.33	118.98
24	u	312	CHL	C1A-CHA-C4D	-5.78	109.33	118.98
24	y	313	CHL	C4D-ND-C1D	5.78	109.61	105.22
24	9	308	CHL	CHA-C1A-C2A	-5.78	119.73	133.31
31	b	617	8CT	C18-C17-C16	-5.78	119.17	127.28
24	3	304	CHL	C4D-ND-C1D	5.78	109.61	105.22
24	s	407	CHL	C4D-ND-C1D	5.78	109.61	105.22
24	7	309	CHL	C1A-CHA-C4D	-5.77	109.35	118.98
24	p	309	CHL	C1A-CHA-C4D	-5.77	109.35	118.98
31	S	615	8CT	C01-C02-C03	-5.77	118.19	124.48
24	u	318	CHL	C1A-CHA-C4D	-5.77	109.36	118.98
24	G	318	CHL	C4D-ND-C1D	5.76	109.59	105.22
24	2	305	CHL	C1A-CHA-C4D	-5.76	109.37	118.98
24	7	313	CHL	C4D-ND-C1D	5.76	109.59	105.22
24	9	311	CHL	C1A-CHA-C4D	-5.76	109.37	118.98
24	9	317	CHL	C1A-CHA-C4D	-5.76	109.37	118.98
24	y	310	CHL	C1A-CHA-C4D	-5.76	109.38	118.98
24	s	403	CHL	C1A-CHA-C4D	-5.76	109.38	118.98
24	p	312	CHL	C1A-CHA-C4D	-5.75	109.39	118.98
24	Y	309	CHL	C1A-CHA-C4D	-5.75	109.39	118.98
24	n	311	CHL	C1A-CHA-C4D	-5.75	109.39	118.98
24	S	602	CHL	C1A-CHA-C4D	-5.75	109.39	118.98
27	R	615	XAT	O24-C25-C38	5.75	121.47	115.05
24	r	303	CHL	C1A-CHA-C4D	-5.75	109.40	118.98
24	p	309	CHL	CHA-C1A-C2A	-5.74	119.83	133.31
24	n	304	CHL	C1A-CHA-C4D	-5.74	109.41	118.98
24	G	305	CHL	C1A-CHA-C4D	-5.74	109.41	118.98
24	7	311	CHL	C4D-ND-C1D	5.74	109.57	105.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	3	317	CHL	C1A-CHA-C4D	-5.74	109.41	118.98
35	d	403	PHO	C4D-CHA-CBD	-5.73	105.71	108.45
27	r	316	XAT	O24-C25-C38	5.73	121.45	115.05
24	3	311	CHL	C1A-CHA-C4D	-5.73	109.42	118.98
24	q	316	CHL	C1A-CHA-C4D	-5.73	109.42	118.98
24	5	318	CHL	C1A-CHA-C4D	-5.73	109.43	118.98
24	q	309	CHL	C1A-CHA-C4D	-5.73	109.43	118.98
24	g	305	CHL	C1A-CHA-C4D	-5.73	109.43	118.98
24	p	310	CHL	C1A-CHA-C4D	-5.73	109.43	118.98
24	R	607	CHL	OBD-CAD-CBD	5.73	134.23	125.82
24	7	310	CHL	C1A-CHA-C4D	-5.72	109.43	118.98
24	7	312	CHL	C1A-CHA-C4D	-5.72	109.43	118.98
24	p	311	CHL	C4D-ND-C1D	5.72	109.56	105.22
24	5	305	CHL	C1A-CHA-C4D	-5.71	109.45	118.98
24	Y	319	CHL	C1A-CHA-C4D	-5.71	109.46	118.98
24	9	311	CHL	OBD-CAD-CBD	5.71	134.20	125.82
35	a	606	PHO	C4D-CHA-CBD	-5.71	105.72	108.45
24	N	304	CHL	C1A-CHA-C4D	-5.71	109.46	118.98
24	R	602	CHL	C1A-CHA-C4D	-5.70	109.47	118.98
24	2	318	CHL	C1A-CHA-C4D	-5.70	109.47	118.98
24	n	309	CHL	C1A-CHA-C4D	-5.70	109.47	118.98
24	Y	310	CHL	C1A-CHA-C4D	-5.70	109.47	118.98
24	N	305	CHL	C1B-CHB-C4A	5.70	124.99	121.32
24	9	304	CHL	C1A-CHA-C4D	-5.70	109.47	118.98
24	8	308	CHL	C1B-CHB-C4A	5.70	124.99	121.32
24	6	311	CHL	C1A-CHA-C4D	-5.70	109.47	118.98
24	6	317	CHL	C1A-CHA-C4D	-5.70	109.47	118.98
24	8	303	CHL	C1A-CHA-C4D	-5.70	109.48	118.98
24	n	310	CHL	C1A-CHA-C4D	-5.70	109.48	118.98
31	t	101	8CT	C24-C25-C26	-5.70	119.29	127.28
24	r	309	CHL	C4D-ND-C1D	5.70	109.54	105.22
35	D	403	PHO	C4D-CHA-CBD	-5.69	105.72	108.45
24	7	318	CHL	C1A-CHA-C4D	-5.69	109.48	118.98
24	Y	304	CHL	C1A-CHA-C4D	-5.69	109.48	118.98
24	s	408	CHL	C1A-CHA-C4D	-5.69	109.48	118.98
24	2	310	CHL	C1A-CHA-C4D	-5.69	109.49	118.98
24	q	303	CHL	C1A-CHA-C4D	-5.69	109.49	118.98
24	5	305	CHL	C4D-ND-C1D	5.69	109.54	105.22
24	N	310	CHL	C1A-CHA-C4D	-5.69	109.49	118.98
24	S	607	CHL	C1A-CHA-C4D	-5.68	109.50	118.98
24	2	312	CHL	C1A-CHA-C4D	-5.68	109.50	118.98
24	7	309	CHL	CHA-C1A-C2A	-5.68	119.96	133.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	2	311	CHL	C1A-CHA-C4D	-5.68	109.50	118.98
24	Y	312	CHL	C4D-ND-C1D	5.68	109.53	105.22
24	p	313	CHL	C4D-ND-C1D	5.68	109.53	105.22
24	5	310	CHL	C1A-CHA-C4D	-5.68	109.51	118.98
24	g	312	CHL	C4D-ND-C1D	5.68	109.53	105.22
24	s	402	CHL	C4D-ND-C1D	5.68	109.53	105.22
24	G	318	CHL	C1A-CHA-C4D	-5.68	109.51	118.98
24	4	305	CHL	C1A-CHA-C4D	-5.67	109.52	118.98
24	p	318	CHL	C1A-CHA-C4D	-5.67	109.52	118.98
24	N	309	CHL	C1A-CHA-C4D	-5.67	109.52	118.98
24	g	318	CHL	C1A-CHA-C4D	-5.67	109.53	118.98
24	6	310	CHL	C1A-CHA-C4D	-5.67	109.53	118.98
24	y	311	CHL	C1A-CHA-C4D	-5.66	109.53	118.98
24	y	305	CHL	C1A-CHA-C4D	-5.66	109.54	118.98
24	5	312	CHL	C1A-CHA-C4D	-5.66	109.54	118.98
24	4	310	CHL	C1A-CHA-C4D	-5.66	109.54	118.98
24	1	305	CHL	C1A-CHA-C4D	-5.65	109.55	118.98
31	d	410	8CT	C14-C13-C12	-5.65	119.35	127.28
24	3	310	CHL	C1A-CHA-C4D	-5.65	109.56	118.98
24	2	310	CHL	C4D-ND-C1D	5.64	109.50	105.22
24	5	311	CHL	C1A-CHA-C4D	-5.64	109.57	118.98
24	r	308	CHL	OBD-CAD-CBD	5.64	134.09	125.82
24	Y	312	CHL	C1A-CHA-C4D	-5.63	109.58	118.98
24	5	313	CHL	C1A-CHA-C4D	-5.63	109.59	118.98
24	g	306	CHL	C1A-CHA-C4D	-5.63	109.59	118.98
24	3	305	CHL	C4D-ND-C1D	5.63	109.49	105.22
24	q	310	CHL	C1A-CHA-C4D	-5.62	109.61	118.98
24	y	313	CHL	C1A-CHA-C4D	-5.62	109.61	118.98
24	1	310	CHL	C1A-CHA-C4D	-5.62	109.61	118.98
24	R	608	CHL	C4D-ND-C1D	5.62	109.48	105.22
24	r	306	CHL	C1A-CHA-C4D	-5.62	109.61	118.98
24	1	311	CHL	C1A-CHA-C4D	-5.61	109.61	118.98
24	4	311	CHL	C1A-CHA-C4D	-5.61	109.61	118.98
24	R	608	CHL	C1B-CHB-C4A	5.61	124.93	121.32
24	9	310	CHL	C1A-CHA-C4D	-5.61	109.62	118.98
24	2	313	CHL	C1A-CHA-C4D	-5.61	109.63	118.98
24	1	304	CHL	C1A-CHA-C4D	-5.60	109.63	118.98
24	G	306	CHL	C1A-CHA-C4D	-5.60	109.63	118.98
35	A	606	PHO	C4D-CHA-CBD	-5.60	105.77	108.45
24	3	311	CHL	C4D-ND-C1D	5.60	109.47	105.22
24	p	305	CHL	C1A-CHA-C4D	-5.60	109.64	118.98
24	7	305	CHL	C1A-CHA-C4D	-5.60	109.64	118.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Y	317	CHL	C1A-CHA-C4D	-5.60	109.64	118.98
28	r	317	NEX	O24-C26-C27	-5.59	100.86	116.88
24	6	305	CHL	C1A-CHA-C4D	-5.59	109.66	118.98
24	Y	311	CHL	C1A-CHA-C4D	-5.59	109.66	118.98
24	3	305	CHL	C1A-CHA-C4D	-5.58	109.66	118.98
24	4	304	CHL	C1A-CHA-C4D	-5.58	109.66	118.98
24	8	309	CHL	C1A-CHA-C4D	-5.58	109.67	118.98
24	u	311	CHL	C1A-CHA-C4D	-5.58	109.67	118.98
24	s	402	CHL	OBD-CAD-CBD	5.58	134.01	125.82
28	u	304	NEX	O24-C26-C27	-5.58	100.89	116.88
28	R	616	NEX	O24-C26-C27	-5.58	100.90	116.88
28	1	303	NEX	O24-C26-C27	-5.57	100.91	116.88
28	9	319	NEX	O24-C26-C27	-5.57	100.91	116.88
24	r	302	CHL	C1A-CHA-C4D	-5.57	109.69	118.98
24	N	308	CHL	C1A-CHA-C4D	-5.57	109.69	118.98
24	N	312	CHL	C4D-ND-C1D	5.57	109.45	105.22
28	S	617	NEX	O24-C26-C27	-5.57	100.92	116.88
28	5	304	NEX	O24-C26-C27	-5.57	100.92	116.88
24	R	608	CHL	C1A-CHA-C4D	-5.57	109.69	118.98
28	G	304	NEX	O24-C26-C27	-5.57	100.93	116.88
24	n	308	CHL	C1A-CHA-C4D	-5.56	109.70	118.98
28	y	304	NEX	O24-C26-C27	-5.56	100.94	116.88
36	A	611	BCT	O2-C-O1	5.56	133.91	119.68
28	2	304	NEX	O24-C26-C27	-5.56	100.94	116.88
28	p	304	NEX	O24-C26-C27	-5.56	100.94	116.88
24	R	605	CHL	C1A-CHA-C4D	-5.56	109.70	118.98
24	y	318	CHL	C1A-CHA-C4D	-5.56	109.70	118.98
24	R	606	CHL	C1A-CHA-C4D	-5.56	109.71	118.98
28	g	304	NEX	O24-C26-C27	-5.56	100.95	116.88
24	y	312	CHL	C1A-CHA-C4D	-5.56	109.71	118.98
24	g	313	CHL	C1A-CHA-C4D	-5.56	109.71	118.98
24	G	312	CHL	C1A-CHA-C4D	-5.56	109.71	118.98
24	r	309	CHL	C1A-CHA-C4D	-5.56	109.71	118.98
28	7	304	NEX	O24-C26-C27	-5.55	100.96	116.88
24	r	307	CHL	C4D-ND-C1D	5.55	109.43	105.22
24	S	601	CHL	OBD-CAD-CBD	5.55	133.97	125.82
24	R	601	CHL	C1A-CHA-C4D	-5.55	109.73	118.98
24	n	312	CHL	C4D-ND-C1D	5.55	109.43	105.22
28	4	303	NEX	O24-C26-C27	-5.55	100.99	116.88
24	3	305	CHL	C1B-CHB-C4A	5.55	124.89	121.32
24	g	309	CHL	CHA-C1A-C2A	-5.54	120.30	133.31
24	q	304	CHL	C1A-CHA-C4D	-5.54	109.74	118.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	S	601	CHL	C4D-ND-C1D	5.53	109.42	105.22
31	v	401	8CT	C19-C20-C21	-5.53	119.52	127.28
24	9	305	CHL	C1A-CHA-C4D	-5.53	109.75	118.98
24	9	312	CHL	OBD-CAD-CBD	5.53	133.94	125.82
36	a	611	BCT	O2-C-O1	5.53	133.82	119.68
24	q	309	CHL	C4D-ND-C1D	5.53	109.41	105.22
24	6	304	CHL	C1A-CHA-C4D	-5.53	109.76	118.98
31	V	401	8CT	C19-C20-C21	-5.53	119.53	127.28
24	S	605	CHL	C1A-CHA-C4D	-5.53	109.76	118.98
24	9	312	CHL	C1A-CHA-C4D	-5.52	109.76	118.98
24	S	613	CHL	C1A-CHA-C4D	-5.52	109.77	118.98
24	8	304	CHL	C1A-CHA-C4D	-5.52	109.77	118.98
29	5	301	0UR	C14-C15-C16	-5.52	119.54	127.28
24	g	312	CHL	C1A-CHA-C4D	-5.52	109.78	118.98
29	2	301	0UR	C14-C15-C16	-5.51	119.54	127.28
24	S	601	CHL	C1A-CHA-C4D	-5.51	109.78	118.98
31	a	608	8CT	C18-C17-C16	-5.51	119.55	127.28
24	p	311	CHL	C1A-CHA-C4D	-5.51	109.79	118.98
24	s	409	CHL	C1A-CHA-C4D	-5.51	109.79	118.98
31	T	101	8CT	C24-C25-C26	-5.51	119.55	127.28
24	s	408	CHL	C4D-ND-C1D	5.51	109.40	105.22
24	u	306	CHL	C1A-CHA-C4D	-5.51	109.80	118.98
24	3	304	CHL	C1A-CHA-C4D	-5.50	109.80	118.98
24	G	309	CHL	CHA-C1A-C2A	-5.50	120.38	133.31
24	r	307	CHL	C1A-CHA-C4D	-5.50	109.80	118.98
24	G	313	CHL	C1A-CHA-C4D	-5.50	109.81	118.98
24	s	406	CHL	C1A-CHA-C4D	-5.50	109.81	118.98
24	s	402	CHL	C1A-CHA-C4D	-5.50	109.81	118.98
24	S	608	CHL	C1A-CHA-C4D	-5.50	109.81	118.98
24	n	305	CHL	C4D-ND-C1D	5.50	109.39	105.22
24	3	309	CHL	C1A-CHA-C4D	-5.50	109.81	118.98
24	n	305	CHL	C1A-CHA-C4D	-5.49	109.81	118.98
24	s	414	CHL	C1A-CHA-C4D	-5.49	109.82	118.98
24	6	305	CHL	C4D-ND-C1D	5.49	109.39	105.22
24	1	312	CHL	C1A-CHA-C4D	-5.49	109.82	118.98
24	5	310	CHL	C4D-ND-C1D	5.49	109.38	105.22
24	N	305	CHL	C4D-ND-C1D	5.48	109.38	105.22
24	6	309	CHL	C1A-CHA-C4D	-5.48	109.84	118.98
24	u	312	CHL	OBD-CAD-CBD	5.48	133.86	125.82
24	6	312	CHL	C1A-CHA-C4D	-5.48	109.84	118.98
24	G	311	CHL	C1A-CHA-C4D	-5.47	109.85	118.98
24	7	311	CHL	C1A-CHA-C4D	-5.47	109.86	118.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	3	312	CHL	C1A-CHA-C4D	-5.47	109.86	118.98
24	N	305	CHL	C1A-CHA-C4D	-5.47	109.86	118.98
24	8	304	CHL	C4D-ND-C1D	5.46	109.36	105.22
24	S	606	CHL	C1A-CHA-C4D	-5.45	109.89	118.98
24	u	313	CHL	C1A-CHA-C4D	-5.45	109.89	118.98
31	A	608	8CT	C18-C17-C16	-5.45	119.63	127.28
24	Y	317	CHL	C4D-ND-C1D	5.45	109.36	105.22
24	8	310	CHL	C4D-ND-C1D	5.45	109.35	105.22
24	q	311	CHL	C4D-ND-C1D	5.45	109.35	105.22
24	6	311	CHL	C4D-ND-C1D	5.45	109.35	105.22
24	Y	304	CHL	OBD-CAD-CBD	5.45	133.82	125.82
24	p	306	CHL	C1A-CHA-C4D	-5.45	109.89	118.98
24	q	311	CHL	C1A-CHA-C4D	-5.44	109.90	118.98
24	7	313	CHL	C1A-CHA-C4D	-5.44	109.90	118.98
24	2	306	CHL	C1A-CHA-C4D	-5.43	109.92	118.98
24	7	306	CHL	C1A-CHA-C4D	-5.43	109.92	118.98
24	s	407	CHL	C1A-CHA-C4D	-5.43	109.92	118.98
24	4	312	CHL	C1A-CHA-C4D	-5.43	109.92	118.98
24	n	312	CHL	C1A-CHA-C4D	-5.43	109.92	118.98
24	8	308	CHL	C4D-ND-C1D	5.43	109.34	105.22
24	g	311	CHL	C1A-CHA-C4D	-5.43	109.93	118.98
24	y	305	CHL	OBD-CAD-CBD	5.42	133.78	125.82
24	5	312	CHL	C1B-CHB-C4A	5.42	124.81	121.32
24	p	313	CHL	C1A-CHA-C4D	-5.41	109.95	118.98
24	8	310	CHL	C1A-CHA-C4D	-5.41	109.95	118.98
24	Y	310	CHL	C4D-ND-C1D	5.41	109.32	105.22
31	v	401	8CT	C01-C02-C03	-5.41	118.58	124.48
24	R	606	CHL	C4D-ND-C1D	5.41	109.32	105.22
31	C	613	8CT	C18-C17-C16	-5.40	119.70	127.28
24	s	409	CHL	C4D-ND-C1D	5.40	109.32	105.22
31	C	615	8CT	C01-C02-C03	-5.40	118.59	124.48
24	q	311	CHL	C1B-CHB-C4A	5.40	124.79	121.32
24	5	306	CHL	C1A-CHA-C4D	-5.39	109.98	118.98
24	N	312	CHL	C1A-CHA-C4D	-5.39	110.00	118.98
24	9	305	CHL	C4D-ND-C1D	5.38	109.30	105.22
24	Y	319	CHL	C4D-ND-C1D	5.38	109.30	105.22
31	c	613	8CT	C18-C17-C16	-5.37	119.74	127.28
31	V	401	8CT	C01-C02-C03	-5.37	118.63	124.48
24	N	311	CHL	C4D-ND-C1D	5.37	109.29	105.22
24	u	306	CHL	C4D-ND-C1D	5.37	109.29	105.22
24	Y	310	CHL	OBD-CAD-C3D	-5.36	119.54	127.89
24	q	308	CHL	C4D-ND-C1D	5.36	109.28	105.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	c	614	8CT	C18-C17-C16	-5.35	119.78	127.28
24	y	311	CHL	C4D-ND-C1D	5.35	109.28	105.22
24	N	311	CHL	OBD-CAD-CBD	5.34	133.66	125.82
24	5	312	CHL	OBD-CAD-CBD	5.34	133.65	125.82
24	y	306	CHL	C1A-CHA-C4D	-5.33	110.08	118.98
24	Y	305	CHL	C1A-CHA-C4D	-5.33	110.09	118.98
24	y	318	CHL	C4D-ND-C1D	5.33	109.26	105.22
24	4	311	CHL	C4D-ND-C1D	5.33	109.26	105.22
24	2	312	CHL	C4D-ND-C1D	5.33	109.26	105.22
31	C	614	8CT	C18-C17-C16	-5.31	119.84	127.28
24	2	312	CHL	OBD-CAD-CBD	5.30	133.60	125.82
31	C	613	8CT	C35-C30-C29	-5.30	106.73	112.83
24	n	311	CHL	OBD-CAD-CBD	5.30	133.60	125.82
24	G	306	CHL	C4D-ND-C1D	5.29	109.24	105.22
24	3	311	CHL	OBD-CAD-C3D	-5.29	119.64	127.89
24	s	414	CHL	C4D-ND-C1D	5.29	109.23	105.22
31	x	601	8CT	C01-C02-C03	-5.29	118.72	124.48
24	q	304	CHL	C4D-ND-C1D	5.29	109.23	105.22
24	7	312	CHL	OBD-CAD-C3D	-5.28	119.65	127.89
31	C	615	8CT	C19-C20-C21	-5.28	119.87	127.28
31	c	615	8CT	C01-C02-C03	-5.26	118.75	124.48
31	D	410	8CT	C14-C13-C12	-5.26	119.91	127.28
24	R	606	CHL	C1B-CHB-C4A	5.25	124.70	121.32
24	r	309	CHL	OBD-CAD-CBD	5.24	133.52	125.82
24	S	607	CHL	OBD-CAD-CBD	5.23	133.50	125.82
24	9	312	CHL	OBD-CAD-C3D	-5.22	119.74	127.89
24	n	305	CHL	C1B-CHB-C4A	5.22	124.68	121.32
24	n	311	CHL	C4D-ND-C1D	5.21	109.18	105.22
24	S	613	CHL	C4D-ND-C1D	5.21	109.17	105.22
24	5	312	CHL	C4D-ND-C1D	5.20	109.17	105.22
24	u	313	CHL	OBD-CAD-CBD	5.20	133.46	125.82
31	c	615	8CT	C19-C20-C21	-5.20	119.98	127.28
24	S	607	CHL	C4D-ND-C1D	5.20	109.17	105.22
24	S	608	CHL	C4D-ND-C1D	5.20	109.16	105.22
31	X	601	8CT	C01-C02-C03	-5.19	118.82	124.48
24	2	306	CHL	C4D-ND-C1D	5.18	109.15	105.22
24	q	310	CHL	OBD-CAD-CBD	5.18	133.43	125.82
24	R	608	CHL	OBD-CAD-CBD	5.18	133.42	125.82
24	N	309	CHL	OBD-CAD-CBD	5.17	133.42	125.82
24	y	312	CHL	OBD-CAD-CBD	5.17	133.41	125.82
24	4	305	CHL	C4D-ND-C1D	5.16	109.14	105.22
24	Y	319	CHL	C1B-CHB-C4A	5.16	124.64	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Y	311	CHL	OBD-CAD-CBD	5.16	133.40	125.82
24	p	305	CHL	OBD-CAD-CBD	5.16	133.40	125.82
24	5	306	CHL	C4D-ND-C1D	5.16	109.13	105.22
24	Y	312	CHL	C1B-CHB-C4A	5.16	124.64	121.32
29	2	301	0UR	C10-C11-C12	-5.15	120.06	127.28
24	1	311	CHL	C4D-ND-C1D	5.14	109.12	105.22
24	7	305	CHL	OBD-CAD-CBD	5.14	133.37	125.82
27	r	316	XAT	O24-C25-C24	5.14	118.31	113.49
29	5	301	0UR	C10-C11-C12	-5.14	120.07	127.28
31	C	614	8CT	C07-C02-C03	-5.14	115.76	122.70
24	R	607	CHL	C4D-ND-C1D	5.13	109.11	105.22
24	1	305	CHL	C4D-ND-C1D	5.13	109.11	105.22
28	r	301	NEX	O24-C25-C38	5.11	120.76	115.05
31	T	101	8CT	C19-C20-C21	-5.11	120.11	127.28
24	2	312	CHL	C1B-CHB-C4A	5.11	124.61	121.32
28	N	303	NEX	O24-C25-C38	5.11	120.76	115.05
31	t	101	8CT	C19-C20-C21	-5.11	120.12	127.28
28	n	303	NEX	O24-C25-C38	5.11	120.75	115.05
31	C	615	8CT	C14-C13-C12	-5.10	120.12	127.28
28	2	304	NEX	C15-C35-C34	5.10	133.96	123.52
28	9	319	NEX	C15-C35-C34	5.10	133.95	123.52
28	5	304	NEX	C15-C35-C34	5.10	133.95	123.52
28	3	318	NEX	O24-C25-C38	5.10	120.75	115.05
31	c	613	8CT	C35-C30-C29	-5.10	106.96	112.83
28	p	304	NEX	C15-C35-C34	5.10	133.95	123.52
31	D	410	8CT	C10-C11-C12	-5.10	118.69	126.23
24	g	312	CHL	OBD-CAD-CBD	5.09	133.30	125.82
31	a	608	8CT	C01-C02-C03	-5.09	118.93	124.48
28	S	617	NEX	C15-C35-C34	5.08	133.91	123.52
24	8	309	CHL	OBD-CAD-CBD	5.08	133.28	125.82
31	A	608	8CT	C01-C02-C03	-5.08	118.94	124.48
24	4	311	CHL	OBD-CAD-CBD	5.08	133.28	125.82
24	r	308	CHL	C4D-ND-C1D	5.08	109.07	105.22
28	s	401	NEX	O24-C25-C38	5.07	120.72	115.05
28	R	616	NEX	C15-C35-C34	5.07	133.89	123.52
28	1	303	NEX	C15-C35-C34	5.07	133.89	123.52
28	g	304	NEX	C15-C35-C34	5.07	133.89	123.52
28	6	303	NEX	O24-C25-C38	5.07	120.71	115.05
31	c	614	8CT	C07-C02-C03	-5.07	115.86	122.70
28	u	304	NEX	C15-C35-C34	5.07	133.88	123.52
28	4	303	NEX	C15-C35-C34	5.06	133.87	123.52
28	r	317	NEX	C15-C35-C34	5.06	133.87	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	7	304	NEX	C15-C35-C34	5.05	133.85	123.52
24	s	402	CHL	OBD-CAD-C3D	-5.04	120.02	127.89
24	y	312	CHL	C4D-ND-C1D	5.04	109.05	105.22
28	G	304	NEX	C15-C35-C34	5.04	133.83	123.52
24	s	403	CHL	OBD-CAD-CBD	5.04	133.22	125.82
28	y	304	NEX	C15-C35-C34	5.04	133.83	123.52
28	6	303	NEX	C35-C34-C33	-5.03	120.22	127.28
31	c	614	8CT	C30-C29-C28	-5.03	116.76	124.58
28	N	303	NEX	C35-C34-C33	-5.03	120.23	127.28
24	9	311	CHL	OBD-CAD-C3D	-5.03	120.05	127.89
24	9	305	CHL	C1B-CHB-C4A	5.02	124.56	121.32
24	q	310	CHL	C4D-ND-C1D	5.02	109.03	105.22
24	6	311	CHL	OBD-CAD-C3D	-5.02	120.06	127.89
24	p	312	CHL	OBD-CAD-C3D	-5.02	120.06	127.89
28	3	318	NEX	C27-C28-C29	-5.01	117.75	125.53
28	r	301	NEX	C35-C34-C33	-5.01	120.25	127.28
24	1	311	CHL	OBD-CAD-CBD	5.01	133.18	125.82
31	d	410	8CT	C10-C11-C12	-5.01	118.82	126.23
24	S	602	CHL	C4D-ND-C1D	5.01	109.02	105.22
24	S	602	CHL	OBD-CAD-CBD	5.01	133.17	125.82
24	G	312	CHL	OBD-CAD-CBD	5.01	133.17	125.82
24	y	318	CHL	C1B-CHB-C4A	5.00	124.54	121.32
24	S	601	CHL	OBD-CAD-C3D	-5.00	120.09	127.89
28	s	401	NEX	C27-C28-C29	-5.00	117.77	125.53
24	8	310	CHL	C1B-CHB-C4A	5.00	124.54	121.32
31	s	415	8CT	C19-C20-C21	-5.00	120.27	127.28
24	s	403	CHL	C4D-ND-C1D	4.99	109.01	105.22
28	6	303	NEX	C27-C28-C29	-4.99	117.78	125.53
24	g	306	CHL	C4D-ND-C1D	4.99	109.00	105.22
28	3	318	NEX	C35-C34-C33	-4.99	120.28	127.28
28	s	401	NEX	C35-C34-C33	-4.99	120.28	127.28
28	r	301	NEX	C27-C28-C29	-4.98	117.80	125.53
27	R	615	XAT	O24-C25-C24	4.98	118.16	113.49
24	Y	317	CHL	C1B-CHB-C4A	4.98	124.53	121.32
28	g	304	NEX	O24-C25-C38	4.97	120.61	115.05
28	N	303	NEX	C27-C28-C29	-4.97	117.81	125.53
24	u	313	CHL	OBD-CAD-C3D	-4.97	120.14	127.89
28	n	303	NEX	C27-C28-C29	-4.97	117.82	125.53
31	C	614	8CT	C30-C29-C28	-4.96	116.85	124.58
28	n	303	NEX	C35-C34-C33	-4.96	120.33	127.28
28	r	317	NEX	O24-C25-C38	4.95	120.58	115.05
29	u	301	0UR	C9-C8-C7	-4.95	120.34	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	R	616	NEX	O24-C25-C38	4.95	120.58	115.05
28	y	304	NEX	O24-C25-C38	4.94	120.57	115.05
28	1	303	NEX	O24-C25-C38	4.94	120.56	115.05
31	S	614	8CT	C19-C20-C21	-4.94	120.36	127.28
28	7	304	NEX	O24-C25-C38	4.93	120.56	115.05
28	4	303	NEX	O24-C25-C38	4.93	120.56	115.05
24	y	310	CHL	C4D-ND-C1D	4.92	108.96	105.22
28	p	304	NEX	O24-C25-C38	4.92	120.55	115.05
24	N	309	CHL	C4D-ND-C1D	4.91	108.95	105.22
29	G	301	0UR	C19-C18-C17	-4.91	116.94	124.58
28	5	304	NEX	O24-C25-C38	4.91	120.54	115.05
28	S	617	NEX	O24-C25-C38	4.91	120.53	115.05
28	4	303	NEX	C15-C14-C13	-4.91	120.39	127.28
24	8	309	CHL	C4D-ND-C1D	4.91	108.94	105.22
24	r	303	CHL	OBD-CAD-CBD	4.91	133.03	125.82
24	Y	304	CHL	OBD-CAD-C3D	-4.90	120.24	127.89
28	2	304	NEX	C15-C14-C13	-4.90	120.40	127.28
24	Y	311	CHL	C4D-ND-C1D	4.90	108.94	105.22
29	N	301	0UR	C10-C11-C12	-4.90	120.41	127.28
28	y	304	NEX	C15-C14-C13	-4.90	120.41	127.28
28	9	319	NEX	O24-C25-C38	4.89	120.52	115.05
28	G	304	NEX	C15-C14-C13	-4.89	120.42	127.28
24	R	602	CHL	OBD-CAD-CBD	4.89	133.00	125.82
31	V	401	8CT	C18-C17-C16	-4.88	120.43	127.28
24	R	605	CHL	OBD-CAD-CBD	4.88	132.98	125.82
28	9	319	NEX	C15-C14-C13	-4.88	120.44	127.28
31	B	617	8CT	C24-C25-C26	-4.88	120.44	127.28
28	u	304	NEX	O24-C25-C38	4.88	120.50	115.05
28	S	617	NEX	C15-C14-C13	-4.88	120.44	127.28
28	R	616	NEX	C15-C14-C13	-4.88	120.44	127.28
29	n	301	0UR	C10-C11-C12	-4.87	120.44	127.28
28	G	304	NEX	O24-C25-C38	4.87	120.49	115.05
24	Y	305	CHL	C4D-ND-C1D	4.87	108.91	105.22
28	5	304	NEX	C15-C14-C13	-4.87	120.45	127.28
28	2	304	NEX	O24-C25-C38	4.87	120.49	115.05
28	7	304	NEX	C15-C14-C13	-4.87	120.45	127.28
24	y	305	CHL	OBD-CAD-C3D	-4.87	120.30	127.89
24	y	306	CHL	C4D-ND-C1D	4.87	108.91	105.22
28	p	304	NEX	C15-C14-C13	-4.86	120.46	127.28
28	r	317	NEX	C15-C14-C13	-4.86	120.46	127.28
24	1	305	CHL	OBD-CAD-CBD	4.85	132.95	125.82
28	1	303	NEX	C15-C14-C13	-4.85	120.47	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	4	305	CHL	OBD-CAD-CBD	4.85	132.94	125.82
24	r	303	CHL	C4D-ND-C1D	4.85	108.90	105.22
28	u	304	NEX	C15-C14-C13	-4.84	120.49	127.28
24	y	311	CHL	OBD-CAD-CBD	4.84	132.93	125.82
28	g	304	NEX	C15-C14-C13	-4.84	120.49	127.28
24	r	307	CHL	OBD-CAD-CBD	4.83	132.91	125.82
24	R	602	CHL	C4D-ND-C1D	4.83	108.88	105.22
31	c	615	8CT	C14-C13-C12	-4.83	120.51	127.28
31	C	614	8CT	C10-C11-C12	-4.81	119.11	126.23
31	c	614	8CT	C10-C11-C12	-4.81	119.11	126.23
29	G	301	0UR	C10-C11-C12	-4.81	120.53	127.28
24	9	317	CHL	C1B-CHB-C4A	-4.81	118.23	121.32
24	n	309	CHL	OBD-CAD-CBD	4.80	132.87	125.82
24	4	317	CHL	OBD-CAD-CBD	4.80	132.87	125.82
24	R	607	CHL	OBD-CAD-C3D	-4.80	120.40	127.89
24	q	309	CHL	C1B-CHB-C4A	4.80	124.41	121.32
24	n	311	CHL	C1B-CHB-C4A	4.79	124.41	121.32
29	u	301	0UR	C10-C11-C12	-4.79	120.56	127.28
33	W	201	LMG	O7-C10-C11	4.79	121.84	111.48
24	y	313	CHL	OBD-CAD-CBD	4.79	132.85	125.82
31	s	415	8CT	C35-C30-C29	-4.79	107.32	112.83
31	s	416	8CT	C39-C16-C17	-4.78	115.08	122.82
24	4	311	CHL	C1B-CHB-C4A	4.77	124.39	121.32
24	p	310	CHL	OBD-CAD-CBD	4.77	132.82	125.82
24	1	308	CHL	OBD-CAD-CBD	4.77	132.82	125.82
31	B	617	8CT	C29-C28-C26	-4.77	116.07	126.32
24	u	312	CHL	OBD-CAD-C3D	-4.77	120.46	127.89
24	R	606	CHL	OBD-CAD-CBD	4.77	132.82	125.82
24	1	317	CHL	OBD-CAD-CBD	4.77	132.82	125.82
31	S	615	8CT	C39-C16-C17	-4.77	115.10	122.82
24	S	605	CHL	OBD-CAD-CBD	4.76	132.81	125.82
24	R	605	CHL	C4D-ND-C1D	4.76	108.83	105.22
24	Y	312	CHL	OBD-CAD-CBD	4.75	132.80	125.82
24	7	312	CHL	C4D-ND-C1D	4.75	108.83	105.22
24	y	310	CHL	OBD-CAD-CBD	4.75	132.79	125.82
24	9	310	CHL	OBD-CAD-CBD	4.75	132.79	125.82
24	r	306	CHL	OBD-CAD-CBD	4.75	132.79	125.82
33	w	201	LMG	O7-C10-C11	4.75	121.75	111.48
24	4	308	CHL	OBD-CAD-CBD	4.74	132.79	125.82
24	6	317	CHL	OBD-CAD-CBD	4.74	132.78	125.82
31	b	617	8CT	C24-C25-C26	-4.74	120.63	127.28
24	8	315	CHL	OBD-CAD-CBD	4.74	132.78	125.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	3	317	CHL	OBD-CAD-CBD	4.74	132.78	125.82
24	r	309	CHL	OBD-CAD-C3D	-4.74	120.50	127.89
24	1	309	CHL	OBD-CAD-CBD	4.74	132.78	125.82
29	9	301	0UR	C10-C11-C12	-4.74	120.64	127.28
24	2	305	CHL	OBD-CAD-CBD	4.74	132.77	125.82
28	9	319	NEX	C31-C30-C29	-4.73	120.64	127.28
28	u	304	NEX	C31-C30-C29	-4.73	120.64	127.28
39	D	406	PL9	C7-C3-C4	4.73	120.80	116.91
24	7	310	CHL	OBD-CAD-CBD	4.73	132.76	125.82
31	S	615	8CT	C30-C31-C32	-4.73	115.65	121.47
28	5	304	NEX	C31-C30-C29	-4.73	120.65	127.28
28	p	304	NEX	C31-C30-C29	-4.73	120.65	127.28
29	g	301	0UR	C10-C11-C12	-4.72	120.65	127.28
24	g	309	CHL	OBD-CAD-CBD	4.72	132.75	125.82
31	S	614	8CT	C35-C30-C29	-4.72	107.40	112.83
31	C	613	8CT	C07-C02-C03	-4.72	116.33	122.70
24	p	312	CHL	C4D-ND-C1D	4.71	108.80	105.22
24	5	305	CHL	OBD-CAD-CBD	4.71	132.74	125.82
31	v	401	8CT	C18-C17-C16	-4.71	120.67	127.28
24	q	316	CHL	OBD-CAD-CBD	4.71	132.73	125.82
28	7	304	NEX	C31-C30-C29	-4.71	120.68	127.28
24	n	317	CHL	OBD-CAD-CBD	4.71	132.73	125.82
28	y	304	NEX	C31-C30-C29	-4.71	120.68	127.28
24	4	309	CHL	OBD-CAD-CBD	4.71	132.73	125.82
24	5	312	CHL	OBD-CAD-C3D	-4.71	120.55	127.89
28	S	617	NEX	C31-C30-C29	-4.70	120.68	127.28
29	6	301	0UR	C10-C11-C12	-4.70	120.68	127.28
28	4	303	NEX	C31-C30-C29	-4.70	120.69	127.28
24	y	312	CHL	OBD-CAD-C3D	-4.70	120.56	127.89
24	N	317	CHL	C1A-CHA-CBD	4.70	144.39	132.36
24	s	406	CHL	OBD-CAD-CBD	4.69	132.71	125.82
31	C	613	8CT	C24-C25-C26	-4.69	120.70	127.28
28	G	304	NEX	C31-C30-C29	-4.69	120.70	127.28
24	r	308	CHL	OBD-CAD-C3D	-4.69	120.58	127.89
28	R	616	NEX	C31-C30-C29	-4.69	120.71	127.28
24	n	309	CHL	C4D-ND-C1D	4.69	108.78	105.22
28	1	303	NEX	C31-C30-C29	-4.69	120.71	127.28
24	R	608	CHL	OBD-CAD-C3D	-4.68	120.58	127.89
24	y	305	CHL	C4D-ND-C1D	4.68	108.77	105.22
39	d	406	PL9	C7-C3-C4	4.68	120.77	116.91
24	N	317	CHL	OBD-CAD-CBD	4.68	132.70	125.82
24	q	310	CHL	OBD-CAD-C3D	-4.68	120.59	127.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	r	317	NEX	C31-C30-C29	-4.68	120.71	127.28
24	2	306	CHL	OBD-CAD-CBD	4.68	132.69	125.82
28	2	304	NEX	C31-C30-C29	-4.68	120.72	127.28
24	Y	309	CHL	C4D-ND-C1D	4.68	108.77	105.22
24	n	317	CHL	C1A-CHA-CBD	4.68	144.34	132.36
31	V	401	8CT	C07-C02-C03	-4.67	116.39	122.70
27	r	316	XAT	O4-C5-C18	4.67	120.27	115.05
31	s	416	8CT	C30-C31-C32	-4.67	115.72	121.47
24	6	304	CHL	OBD-CAD-CBD	4.67	132.68	125.82
31	c	613	8CT	C07-C02-C03	-4.67	116.39	122.70
24	4	317	CHL	C1A-CHA-CBD	4.67	144.32	132.36
24	5	306	CHL	OBD-CAD-CBD	4.67	132.67	125.82
27	R	615	XAT	O4-C5-C18	4.67	120.26	115.05
24	p	305	CHL	C4D-ND-C1D	4.66	108.76	105.22
31	b	617	8CT	C29-C28-C26	-4.66	116.29	126.32
28	g	304	NEX	C31-C30-C29	-4.66	120.74	127.28
24	g	309	CHL	C1A-CHA-CBD	4.66	144.31	132.36
24	u	311	CHL	OBD-CAD-CBD	4.66	132.67	125.82
24	6	309	CHL	OBD-CAD-CBD	4.66	132.66	125.82
24	Y	311	CHL	OBD-CAD-C3D	-4.66	120.62	127.89
24	7	309	CHL	C1B-CHB-C4A	-4.66	118.33	121.32
24	5	309	CHL	C1A-CHA-CBD	4.65	144.28	132.36
31	v	401	8CT	C07-C02-C03	-4.65	116.42	122.70
24	q	304	CHL	OBD-CAD-CBD	4.65	132.65	125.82
24	3	309	CHL	OBD-CAD-CBD	4.65	132.65	125.82
24	Y	308	CHL	OBD-CAD-CBD	4.65	132.65	125.82
24	u	310	CHL	OBD-CAD-CBD	4.65	132.65	125.82
24	3	304	CHL	OBD-CAD-CBD	4.65	132.64	125.82
24	1	317	CHL	C1A-CHA-CBD	4.65	144.26	132.36
24	G	309	CHL	C1A-CHA-CBD	4.64	144.25	132.36
24	Y	309	CHL	OBD-CAD-CBD	4.64	132.63	125.82
24	7	305	CHL	C4D-ND-C1D	4.63	108.74	105.22
29	g	301	0UR	C19-C18-C17	-4.63	117.37	124.58
24	q	308	CHL	OBD-CAD-CBD	4.63	132.62	125.82
24	3	308	CHL	OBD-CAD-CBD	4.63	132.62	125.82
24	9	309	CHL	OBD-CAD-CBD	4.63	132.62	125.82
24	Y	304	CHL	C4D-ND-C1D	4.63	108.73	105.22
24	G	311	CHL	OBD-CAD-CBD	4.62	132.61	125.82
24	y	309	CHL	OBD-CAD-CBD	4.62	132.61	125.82
24	2	312	CHL	OBD-CAD-C3D	-4.62	120.68	127.89
24	8	315	CHL	C1A-CHA-CBD	4.62	144.20	132.36
24	8	304	CHL	OBD-CAD-CBD	4.62	132.60	125.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	r	317	NEX	C38-C25-C24	-4.62	109.06	114.24
31	c	615	8CT	C04-C03-C02	-4.61	116.33	122.64
31	c	613	8CT	C24-C25-C26	-4.61	120.82	127.28
24	N	309	CHL	OBD-CAD-C3D	-4.61	120.71	127.89
24	q	316	CHL	C1A-CHA-CBD	4.61	144.16	132.36
31	c	615	8CT	C18-C17-C16	-4.61	120.82	127.28
28	g	304	NEX	C38-C25-C24	-4.60	109.07	114.24
31	c	614	8CT	C01-C02-C03	-4.60	119.46	124.48
29	8	301	0UR	C10-C11-C12	-4.60	120.82	127.28
24	p	306	CHL	C4D-ND-C1D	4.60	108.71	105.22
24	9	308	CHL	C1A-CHA-CBD	4.60	144.13	132.36
31	C	614	8CT	C01-C02-C03	-4.60	119.47	124.48
24	u	305	CHL	OBD-CAD-CBD	4.59	132.57	125.82
24	u	318	CHL	OBD-CAD-CBD	4.59	132.56	125.82
28	1	303	NEX	C38-C25-C24	-4.59	109.08	114.24
24	7	306	CHL	C4D-ND-C1D	4.59	108.70	105.22
24	G	309	CHL	OBD-CAD-CBD	4.59	132.55	125.82
24	g	312	CHL	OBD-CAD-C3D	-4.59	120.74	127.89
24	G	313	CHL	OBD-CAD-CBD	4.58	132.55	125.82
28	R	616	NEX	C38-C25-C24	-4.58	109.10	114.24
24	3	310	CHL	OBD-CAD-CBD	4.58	132.54	125.82
28	4	303	NEX	C38-C25-C24	-4.58	109.10	114.24
24	2	309	CHL	C1A-CHA-CBD	4.57	144.07	132.36
28	G	304	NEX	C38-C25-C24	-4.57	109.11	114.24
24	4	308	CHL	C1A-CHA-CBD	4.57	144.07	132.36
24	6	308	CHL	C1A-CHA-CBD	4.57	144.07	132.36
28	y	304	NEX	C38-C25-C24	-4.57	109.11	114.24
28	p	304	NEX	C38-C25-C24	-4.57	109.11	114.24
24	4	310	CHL	OBD-CAD-CBD	4.56	132.52	125.82
24	u	312	CHL	C1A-CHA-CBD	4.56	144.05	132.36
24	9	308	CHL	OBD-CAD-CBD	4.56	132.52	125.82
24	2	318	CHL	OBD-CAD-CBD	4.56	132.52	125.82
24	g	311	CHL	OBD-CAD-CBD	4.56	132.52	125.82
24	g	313	CHL	OBD-CAD-CBD	4.56	132.52	125.82
24	S	607	CHL	OBD-CAD-C3D	-4.56	120.78	127.89
24	7	309	CHL	C1A-CHA-CBD	4.56	144.03	132.36
24	N	311	CHL	OBD-CAD-C3D	-4.56	120.78	127.89
24	n	312	CHL	OBD-CAD-CBD	4.56	132.51	125.82
24	g	310	CHL	OBD-CAD-CBD	4.55	132.51	125.82
24	u	309	CHL	C1A-CHA-CBD	4.55	144.02	132.36
24	g	318	CHL	OBD-CAD-CBD	4.55	132.50	125.82
31	d	410	8CT	C18-C17-C16	-4.55	120.89	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	7	304	NEX	C38-C25-C24	-4.55	109.13	114.24
24	9	317	CHL	OBD-CAD-CBD	4.55	132.50	125.82
24	6	308	CHL	OBD-CAD-CBD	4.55	132.50	125.82
24	3	308	CHL	C1A-CHA-CBD	4.54	144.00	132.36
26	9	303	OIE	C20-C3-C4	-4.54	118.44	124.72
24	s	403	CHL	OBD-CAD-C3D	-4.54	120.81	127.89
24	p	309	CHL	C1A-CHA-CBD	4.54	143.98	132.36
28	5	304	NEX	C38-C25-C24	-4.54	109.14	114.24
24	8	309	CHL	OBD-CAD-C3D	-4.54	120.82	127.89
24	1	310	CHL	OBD-CAD-CBD	4.53	132.48	125.82
29	9	301	OUR	C9-C8-C7	-4.53	120.92	127.28
31	b	617	8CT	C01-C02-C03	-4.53	119.54	124.48
24	S	606	CHL	OBD-CAD-CBD	4.53	132.47	125.82
24	6	310	CHL	OBD-CAD-CBD	4.53	132.47	125.82
24	1	308	CHL	C1A-CHA-CBD	4.53	143.95	132.36
24	u	309	CHL	OBD-CAD-CBD	4.53	132.47	125.82
31	B	617	8CT	C01-C02-C03	-4.52	119.55	124.48
28	S	617	NEX	C38-C25-C24	-4.52	109.16	114.24
24	G	318	CHL	OBD-CAD-CBD	4.52	132.46	125.82
24	9	311	CHL	C1A-CHA-CBD	4.52	143.94	132.36
24	n	311	CHL	OBD-CAD-C3D	-4.52	120.84	127.89
28	u	304	NEX	C38-C25-C24	-4.52	109.17	114.24
24	n	304	CHL	OBD-CAD-CBD	4.52	132.45	125.82
24	u	318	CHL	C1A-CHA-CBD	4.52	143.93	132.36
24	N	304	CHL	OBD-CAD-CBD	4.51	132.45	125.82
24	9	317	CHL	C1A-CHA-CBD	4.51	143.92	132.36
24	4	304	CHL	OBD-CAD-CBD	4.51	132.44	125.82
28	2	304	NEX	C38-C25-C24	-4.51	109.18	114.24
28	9	319	NEX	C38-C25-C24	-4.51	109.18	114.24
24	q	307	CHL	C1A-CHA-CBD	4.51	143.90	132.36
31	d	410	8CT	C19-C20-C21	-4.50	120.96	127.28
29	q	301	OUR	C10-C11-C12	-4.50	120.96	127.28
24	4	311	CHL	OBD-CAD-C3D	-4.50	120.87	127.89
24	G	312	CHL	OBD-CAD-C3D	-4.50	120.88	127.89
24	5	318	CHL	OBD-CAD-CBD	4.49	132.42	125.82
26	3	303	OIE	C10-C9-C8	4.49	132.71	123.52
24	S	602	CHL	OBD-CAD-C3D	-4.49	120.89	127.89
24	u	318	CHL	C1B-CHB-C4A	-4.49	118.44	121.32
24	8	303	CHL	OBD-CAD-CBD	4.49	132.41	125.82
31	S	614	8CT	C27-C26-C28	4.49	124.94	118.09
31	s	415	8CT	C27-C26-C28	4.49	124.94	118.09
24	p	313	CHL	C1B-CHB-C4A	4.49	124.21	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	Y	318	LHG	O7-C7-C8	4.48	121.18	111.48
24	r	307	CHL	C1B-CHB-C4A	4.48	124.21	121.32
24	y	313	CHL	OBD-CAD-C3D	-4.48	120.90	127.89
33	B	619	LMG	O7-C10-C11	4.48	121.18	111.48
24	2	309	CHL	OBD-CAD-CBD	4.48	132.40	125.82
31	C	615	8CT	C18-C17-C16	-4.48	121.00	127.28
24	Y	312	CHL	OBD-CAD-C3D	-4.48	120.91	127.89
30	d	408	LHG	O7-C7-C8	4.48	121.17	111.48
24	Y	319	CHL	OBD-CAD-CBD	4.48	132.39	125.82
31	C	614	8CT	C04-C03-C02	-4.47	116.53	122.64
24	1	311	CHL	OBD-CAD-C3D	-4.47	120.92	127.89
24	p	309	CHL	C1B-CHB-C4A	-4.46	118.45	121.32
24	5	309	CHL	OBD-CAD-CBD	4.46	132.38	125.82
24	G	310	CHL	OBD-CAD-CBD	4.46	132.37	125.82
24	1	304	CHL	OBD-CAD-CBD	4.46	132.37	125.82
31	c	614	8CT	C04-C03-C02	-4.46	116.55	122.64
24	4	312	CHL	OBD-CAD-CBD	4.46	132.36	125.82
24	q	309	CHL	OBD-CAD-CBD	4.45	132.36	125.82
24	9	310	CHL	OBD-CAD-C3D	-4.45	120.95	127.89
24	N	312	CHL	OBD-CAD-CBD	4.45	132.36	125.82
24	s	407	CHL	OBD-CAD-CBD	4.45	132.35	125.82
24	y	311	CHL	OBD-CAD-C3D	-4.44	120.96	127.89
24	9	304	CHL	OBD-CAD-CBD	4.44	132.34	125.82
29	y	301	0UR	C19-C18-C17	-4.44	117.67	124.58
24	7	313	CHL	C1B-CHB-C4A	4.43	124.17	121.32
24	p	310	CHL	OBD-CAD-C3D	-4.43	120.99	127.89
24	5	318	CHL	C1A-CHA-CBD	4.43	143.69	132.36
31	C	615	8CT	C04-C03-C02	-4.42	116.59	122.64
24	p	309	CHL	OBD-CAD-CBD	4.42	132.31	125.82
24	8	307	CHL	C1A-CHA-CBD	4.42	143.68	132.36
31	s	415	8CT	C07-C02-C03	-4.42	116.73	122.70
24	n	310	CHL	OBD-CAD-CBD	4.41	132.30	125.82
29	Y	301	0UR	C19-C18-C17	-4.41	117.71	124.58
24	q	303	CHL	OBD-CAD-CBD	4.41	132.30	125.82
27	R	615	XAT	C6-C7-C8	-4.41	116.67	125.99
24	1	304	CHL	C1A-CHA-CBD	4.41	143.65	132.36
24	4	304	CHL	C1A-CHA-CBD	4.41	143.65	132.36
31	v	401	8CT	C04-C03-C02	-4.41	116.61	122.64
31	C	614	8CT	C19-C20-C21	-4.41	121.10	127.28
24	1	305	CHL	OBD-CAD-C3D	-4.40	121.03	127.89
24	2	318	CHL	C1A-CHA-CBD	4.40	143.62	132.36
24	8	308	CHL	OBD-CAD-CBD	4.40	132.28	125.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Y	308	CHL	C1A-CHA-CBD	4.40	143.62	132.36
24	u	311	CHL	OBD-CAD-C3D	-4.39	121.04	127.89
24	n	304	CHL	C1A-CHA-CBD	4.39	143.61	132.36
24	u	305	CHL	C1A-CHA-CBD	4.39	143.60	132.36
24	l	312	CHL	OBD-CAD-CBD	4.39	132.26	125.82
24	r	308	CHL	C1A-CHA-CBD	4.39	143.60	132.36
24	y	309	CHL	C1A-CHA-CBD	4.39	143.59	132.36
31	D	410	8CT	C18-C17-C16	-4.38	121.13	127.28
24	7	310	CHL	OBD-CAD-C3D	-4.38	121.05	127.89
24	l	309	CHL	OBD-CAD-C3D	-4.38	121.06	127.89
24	q	304	CHL	OBD-CAD-C3D	-4.38	121.06	127.89
30	y	319	LHG	O7-C7-C8	4.38	120.95	111.48
24	5	310	CHL	OBD-CAD-CBD	4.37	132.24	125.82
31	V	401	8CT	C04-C03-C02	-4.37	116.66	122.64
29	3	301	0UR	C10-C11-C12	-4.37	121.15	127.28
24	2	310	CHL	OBD-CAD-CBD	4.37	132.24	125.82
24	r	302	CHL	OBD-CAD-CBD	4.37	132.24	125.82
24	N	310	CHL	OBD-CAD-CBD	4.37	132.23	125.82
24	R	601	CHL	OBD-CAD-CBD	4.37	132.23	125.82
24	4	309	CHL	OBD-CAD-C3D	-4.36	121.08	127.89
24	4	305	CHL	OBD-CAD-C3D	-4.36	121.09	127.89
24	g	312	CHL	C1B-CHB-C4A	4.36	124.13	121.32
24	R	607	CHL	C1A-CHA-CBD	4.36	143.53	132.36
31	C	613	8CT	C01-C02-C03	-4.36	119.73	124.48
24	7	309	CHL	OBD-CAD-CBD	4.36	132.22	125.82
24	8	304	CHL	OBD-CAD-C3D	-4.35	121.10	127.89
24	g	313	CHL	OBD-CAD-C3D	-4.35	121.11	127.89
24	p	305	CHL	OBD-CAD-C3D	-4.35	121.11	127.89
31	X	601	8CT	C10-C11-C12	-4.34	119.81	126.23
24	N	304	CHL	C1A-CHA-CBD	4.34	143.48	132.36
24	G	313	CHL	OBD-CAD-C3D	-4.34	121.12	127.89
31	c	614	8CT	C19-C20-C21	-4.34	121.19	127.28
29	7	301	0UR	C19-C18-C17	-4.33	117.83	124.58
30	5	319	LHG	O7-C7-C8	4.33	120.86	111.48
24	6	312	CHL	OBD-CAD-CBD	4.33	132.18	125.82
24	u	310	CHL	C1A-CHA-CBD	4.33	143.46	132.36
24	3	317	CHL	OBD-CAD-C3D	-4.33	121.14	127.89
31	S	615	8CT	C07-C02-C03	-4.33	116.86	122.70
24	n	308	CHL	C1A-CHA-CBD	4.33	143.44	132.36
24	7	305	CHL	OBD-CAD-C3D	-4.32	121.15	127.89
24	n	312	CHL	OBD-CAD-C3D	-4.32	121.16	127.89
37	C	620	DGD	O2G-C1B-C2B	4.32	120.82	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	x	601	8CT	C25-C24-C23	-4.32	110.69	123.20
27	r	316	XAT	C6-C7-C8	-4.31	116.87	125.99
24	2	306	CHL	OBD-CAD-C3D	-4.31	121.16	127.89
31	X	601	8CT	C25-C24-C23	-4.31	110.71	123.20
31	D	410	8CT	C19-C20-C21	-4.31	121.23	127.28
24	6	317	CHL	OBD-CAD-C3D	-4.31	121.17	127.89
24	u	306	CHL	C1B-CHB-C4A	4.30	124.09	121.32
29	3	301	0UR	C9-C8-C7	-4.29	121.26	127.28
30	2	319	LHG	O7-C7-C8	4.29	120.77	111.48
31	S	614	8CT	C07-C02-C03	-4.28	116.92	122.70
29	Y	301	0UR	C34-C27-C1	-4.28	119.11	124.45
24	G	305	CHL	OBD-CAD-CBD	4.28	132.11	125.82
24	1	308	CHL	OBD-CAD-C3D	-4.28	121.21	127.89
24	N	308	CHL	OBD-CAD-CBD	4.28	132.10	125.82
29	N	301	0UR	C9-C8-C7	-4.28	121.28	127.28
24	5	313	CHL	OBD-CAD-CBD	4.28	132.10	125.82
24	N	311	CHL	C1A-CHA-CBD	4.28	143.31	132.36
24	7	318	CHL	C1A-CHA-CBD	4.28	143.31	132.36
24	6	309	CHL	OBD-CAD-C3D	-4.28	121.22	127.89
24	r	302	CHL	C1A-CHA-CBD	4.28	143.31	132.36
24	5	306	CHL	OBD-CAD-C3D	-4.28	121.22	127.89
27	R	615	XAT	C26-C27-C28	-4.27	116.96	125.99
24	7	311	CHL	OBD-CAD-CBD	4.27	132.10	125.82
24	p	311	CHL	OBD-CAD-CBD	4.27	132.09	125.82
24	p	318	CHL	C1A-CHA-CBD	4.27	143.30	132.36
24	3	309	CHL	OBD-CAD-C3D	-4.27	121.23	127.89
24	2	311	CHL	OBD-CAD-CBD	4.27	132.09	125.82
24	n	308	CHL	OBD-CAD-CBD	4.27	132.09	125.82
26	u	303	0IE	C9-C10-C11	4.27	132.25	123.52
26	3	303	0IE	C20-C3-C4	-4.26	118.82	124.72
24	9	309	CHL	C1A-CHA-CBD	4.26	143.28	132.36
29	n	301	0UR	C9-C8-C7	-4.26	121.30	127.28
33	i	101	LMG	O7-C10-C11	4.26	120.69	111.48
24	G	311	CHL	OBD-CAD-C3D	-4.26	121.25	127.89
24	4	317	CHL	OBD-CAD-C3D	-4.25	121.26	127.89
24	p	318	CHL	OBD-CAD-CBD	4.25	132.06	125.82
24	g	309	CHL	C1B-CHB-C4A	-4.25	118.59	121.32
24	g	305	CHL	OBD-CAD-CBD	4.25	132.05	125.82
24	g	310	CHL	OBD-CAD-C3D	-4.24	121.27	127.89
24	9	304	CHL	C1A-CHA-CBD	4.24	143.22	132.36
24	8	303	CHL	C1A-CHA-CBD	4.24	143.22	132.36
24	r	306	CHL	OBD-CAD-C3D	-4.24	121.28	127.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	d	401	LMG	O7-C10-C11	4.24	120.65	111.48
24	2	310	CHL	C1A-CHA-CBD	4.24	143.21	132.36
24	R	601	CHL	C1A-CHA-CBD	4.23	143.20	132.36
24	4	308	CHL	OBD-CAD-C3D	-4.23	121.29	127.89
24	1	317	CHL	OBD-CAD-C3D	-4.23	121.30	127.89
24	N	312	CHL	C1B-CHB-C4A	4.22	124.04	121.32
24	3	310	CHL	OBD-CAD-C3D	-4.22	121.30	127.89
24	R	605	CHL	OBD-CAD-C3D	-4.22	121.31	127.89
24	S	605	CHL	OBD-CAD-C3D	-4.22	121.31	127.89
29	y	301	OUR	C34-C27-C1	-4.22	119.19	124.45
24	r	307	CHL	OBD-CAD-C3D	-4.21	121.32	127.89
30	D	408	LHG	O7-C7-C8	4.21	120.59	111.48
24	r	303	CHL	OBD-CAD-C3D	-4.21	121.32	127.89
24	G	305	CHL	C1A-CHA-CBD	4.21	143.15	132.36
24	n	311	CHL	C1A-CHA-CBD	4.21	143.15	132.36
24	Y	305	CHL	OBD-CAD-CBD	4.21	132.00	125.82
24	5	310	CHL	C1A-CHA-CBD	4.21	143.14	132.36
24	N	312	CHL	OBD-CAD-C3D	-4.21	121.33	127.89
27	r	316	XAT	C26-C27-C28	-4.21	117.10	125.99
24	7	318	CHL	OBD-CAD-CBD	4.21	132.00	125.82
24	q	303	CHL	C1A-CHA-CBD	4.21	143.13	132.36
24	2	305	CHL	C1A-CHA-CBD	4.20	143.12	132.36
31	C	615	8CT	C07-C02-C03	-4.20	117.03	122.70
31	x	601	8CT	C10-C11-C12	-4.20	120.02	126.23
24	y	313	CHL	C1B-CHB-C4A	4.20	124.02	121.32
24	g	305	CHL	C1A-CHA-CBD	4.20	143.11	132.36
24	5	311	CHL	OBD-CAD-CBD	4.20	131.99	125.82
24	u	306	CHL	OBD-CAD-CBD	4.20	131.99	125.82
24	3	311	CHL	C1A-CHA-CBD	4.20	143.11	132.36
24	g	306	CHL	OBD-CAD-CBD	4.20	131.98	125.82
24	G	310	CHL	OBD-CAD-C3D	-4.20	121.35	127.89
24	9	305	CHL	OBD-CAD-CBD	4.19	131.98	125.82
24	6	317	CHL	C1A-CHA-CBD	4.19	143.10	132.36
24	6	310	CHL	OBD-CAD-C3D	-4.19	121.35	127.89
31	s	416	8CT	C07-C02-C03	-4.19	117.04	122.70
24	3	317	CHL	C1A-CHA-CBD	4.19	143.09	132.36
24	s	406	CHL	OBD-CAD-C3D	-4.19	121.36	127.89
24	g	309	CHL	OBD-CAD-C3D	-4.19	121.36	127.89
24	G	309	CHL	C1B-CHB-C4A	-4.19	118.63	121.32
24	7	312	CHL	C1A-CHA-CBD	4.18	143.08	132.36
24	s	408	CHL	C1A-CHA-CBD	4.18	143.08	132.36
24	y	306	CHL	OBD-CAD-CBD	4.18	131.96	125.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	5	305	CHL	OBD-CAD-C3D	-4.18	121.37	127.89
24	2	318	CHL	OBD-CAD-C3D	-4.18	121.37	127.89
24	p	312	CHL	C1A-CHA-CBD	4.18	143.06	132.36
24	2	313	CHL	OBD-CAD-CBD	4.18	131.96	125.82
31	d	410	8CT	C01-C02-C03	-4.18	119.92	124.48
24	3	312	CHL	OBD-CAD-CBD	4.18	131.95	125.82
33	m	101	LMG	O7-C10-C11	4.18	120.51	111.48
31	c	615	8CT	C07-C02-C03	-4.17	117.06	122.70
24	R	602	CHL	OBD-CAD-C3D	-4.17	121.38	127.89
24	u	310	CHL	OBD-CAD-C3D	-4.17	121.39	127.89
24	g	311	CHL	OBD-CAD-C3D	-4.17	121.39	127.89
24	2	305	CHL	OBD-CAD-C3D	-4.17	121.39	127.89
24	5	318	CHL	OBD-CAD-C3D	-4.16	121.40	127.89
31	c	613	8CT	C01-C02-C03	-4.16	119.94	124.48
24	S	607	CHL	C1A-CHA-CBD	4.16	143.02	132.36
29	u	301	0UR	C19-C18-C17	-4.16	118.10	124.58
24	4	312	CHL	OBD-CAD-C3D	-4.16	121.40	127.89
31	s	416	8CT	C28-C26-C25	4.16	125.55	119.01
24	9	309	CHL	OBD-CAD-C3D	-4.16	121.41	127.89
31	S	615	8CT	C14-C13-C12	-4.16	121.45	127.28
24	g	318	CHL	C1A-CHA-CBD	4.16	143.00	132.36
24	5	305	CHL	C1A-CHA-CBD	4.15	143.00	132.36
24	8	315	CHL	OBD-CAD-C3D	-4.15	121.41	127.89
31	C	613	8CT	C04-C03-C02	-4.15	116.97	122.64
24	6	304	CHL	C1A-CHA-CBD	4.15	142.98	132.36
24	r	303	CHL	C1A-CHA-CBD	4.14	142.97	132.36
24	G	318	CHL	C1A-CHA-CBD	4.14	142.97	132.36
29	p	301	0UR	C19-C18-C17	-4.14	118.14	124.58
24	g	310	CHL	C1A-CHA-CBD	4.14	142.96	132.36
24	6	311	CHL	C1A-CHA-CBD	4.14	142.95	132.36
24	1	309	CHL	C1A-CHA-CBD	4.13	142.94	132.36
24	g	318	CHL	OBD-CAD-C3D	-4.13	121.45	127.89
27	R	615	XAT	C35-C34-C33	-4.13	121.48	127.28
24	9	310	CHL	C1A-CHA-CBD	4.13	142.94	132.36
24	4	309	CHL	C1A-CHA-CBD	4.13	142.94	132.36
24	1	312	CHL	OBD-CAD-C3D	-4.13	121.45	127.89
24	n	310	CHL	C1A-CHA-CBD	4.13	142.94	132.36
29	q	301	0UR	C9-C8-C7	-4.13	121.49	127.28
33	B	619	LMG	C8-O7-C10	-4.13	107.92	117.80
31	a	608	8CT	C10-C11-C12	-4.13	120.13	126.23
31	A	608	8CT	C10-C11-C12	-4.13	120.13	126.23
24	n	312	CHL	C1B-CHB-C4A	4.12	123.97	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	8	310	CHL	OBD-CAD-CBD	4.12	131.87	125.82
24	N	310	CHL	C1A-CHA-CBD	4.12	142.91	132.36
24	n	310	CHL	OBD-CAD-C3D	-4.12	121.46	127.89
24	6	310	CHL	C1A-CHA-CBD	4.12	142.91	132.36
29	6	301	OUR	C9-C8-C7	-4.12	121.50	127.28
33	C	618	LMG	O7-C10-C11	4.12	120.39	111.48
24	G	306	CHL	OBD-CAD-CBD	4.11	131.86	125.82
24	N	310	CHL	OBD-CAD-C3D	-4.11	121.48	127.89
24	q	307	CHL	OBD-CAD-CBD	4.11	131.85	125.82
24	G	318	CHL	OBD-CAD-C3D	-4.11	121.48	127.89
24	R	606	CHL	OBD-CAD-C3D	-4.11	121.49	127.89
24	4	304	CHL	OBD-CAD-C3D	-4.11	121.49	127.89
24	8	307	CHL	OBD-CAD-CBD	4.11	131.85	125.82
24	G	312	CHL	C1A-CHA-CBD	4.10	142.87	132.36
33	D	401	LMG	O7-C10-C11	4.10	120.36	111.48
24	R	602	CHL	C1A-CHA-CBD	4.10	142.87	132.36
24	6	312	CHL	OBD-CAD-C3D	-4.10	121.49	127.89
24	1	310	CHL	OBD-CAD-C3D	-4.10	121.49	127.89
24	6	304	CHL	OBD-CAD-C3D	-4.10	121.49	127.89
24	q	308	CHL	OBD-CAD-C3D	-4.10	121.49	127.89
24	G	310	CHL	C1A-CHA-CBD	4.10	142.87	132.36
24	q	309	CHL	C1A-CHA-CBD	4.10	142.87	132.36
24	s	403	CHL	C1A-CHA-CBD	4.10	142.87	132.36
24	G	309	CHL	OBD-CAD-C3D	-4.10	121.50	127.89
24	r	306	CHL	C1A-CHA-CBD	4.10	142.85	132.36
24	3	308	CHL	OBD-CAD-C3D	-4.10	121.50	127.89
24	2	312	CHL	C1A-CHA-CBD	4.09	142.84	132.36
24	3	310	CHL	C1A-CHA-CBD	4.09	142.84	132.36
24	u	318	CHL	OBD-CAD-C3D	-4.09	121.51	127.89
24	y	309	CHL	OBD-CAD-C3D	-4.09	121.51	127.89
24	4	310	CHL	C1A-CHA-CBD	4.09	142.83	132.36
24	5	312	CHL	C1A-CHA-CBD	4.09	142.83	132.36
29	N	301	OUR	C5-C4-C3	-4.09	122.03	126.92
24	R	606	CHL	C1A-CHA-CBD	4.09	142.82	132.36
24	Y	319	CHL	C1A-CHA-CBD	4.08	142.82	132.36
24	q	311	CHL	OBD-CAD-CBD	4.08	131.81	125.82
24	u	311	CHL	C1A-CHA-CBD	4.08	142.80	132.36
24	4	310	CHL	OBD-CAD-C3D	-4.07	121.54	127.89
24	2	311	CHL	C1A-CHA-CBD	4.07	142.79	132.36
24	q	316	CHL	OBD-CAD-C3D	-4.07	121.54	127.89
24	1	310	CHL	C1A-CHA-CBD	4.07	142.79	132.36
24	Y	311	CHL	C1A-CHA-CBD	4.07	142.79	132.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	q	309	CHL	OBD-CAD-C3D	-4.07	121.54	127.89
24	8	303	CHL	OBD-CAD-C3D	-4.07	121.54	127.89
28	r	317	NEX	C11-C10-C9	-4.07	121.57	127.28
24	y	310	CHL	OBD-CAD-C3D	-4.07	121.55	127.89
28	R	616	NEX	C11-C10-C9	-4.07	121.58	127.28
24	Y	308	CHL	OBD-CAD-C3D	-4.06	121.55	127.89
24	3	304	CHL	OBD-CAD-C3D	-4.06	121.55	127.89
24	g	312	CHL	C1A-CHA-CBD	4.06	142.76	132.36
24	n	317	CHL	OBD-CAD-C3D	-4.06	121.56	127.89
26	9	303	OIE	C10-C9-C8	4.06	131.82	123.52
24	9	317	CHL	OBD-CAD-C3D	-4.06	121.56	127.89
30	7	319	LHG	O7-C7-C8	4.05	120.25	111.48
37	c	619	DGD	O2G-C1B-C2B	4.05	120.25	111.48
31	s	416	8CT	C29-C28-C26	-4.05	117.60	126.32
26	G	303	OIE	C10-C9-C8	4.05	131.81	123.52
24	5	311	CHL	C1A-CHA-CBD	4.05	142.74	132.36
27	r	316	XAT	C35-C34-C33	-4.05	121.60	127.28
24	S	606	CHL	OBD-CAD-C3D	-4.05	121.58	127.89
24	6	308	CHL	OBD-CAD-C3D	-4.05	121.58	127.89
24	p	311	CHL	C1A-CHA-CBD	4.05	142.72	132.36
24	3	304	CHL	C1A-CHA-CBD	4.04	142.72	132.36
24	Y	319	CHL	OBD-CAD-C3D	-4.04	121.58	127.89
31	D	410	8CT	C01-C02-C03	-4.04	120.07	124.48
32	a	609	SQD	O9-S-O7	-4.04	100.68	113.82
24	p	309	CHL	OBD-CAD-C3D	-4.04	121.59	127.89
24	r	307	CHL	C1A-CHA-CBD	4.04	142.71	132.36
30	a	612	LHG	O7-C7-C8	4.04	120.22	111.48
24	y	312	CHL	C1A-CHA-CBD	4.04	142.70	132.36
31	D	410	8CT	C24-C25-C26	-4.04	121.61	127.28
24	S	602	CHL	C1A-CHA-CBD	4.04	142.69	132.36
28	1	303	NEX	C11-C10-C9	-4.04	121.62	127.28
28	G	304	NEX	C11-C10-C9	-4.04	121.62	127.28
29	G	301	O0UR	C9-C8-C7	-4.04	121.62	127.28
24	S	607	CHL	C1B-CHB-C4A	4.03	123.92	121.32
24	N	308	CHL	C1A-CHA-CBD	4.03	142.69	132.36
24	S	613	CHL	OBD-CAD-CBD	4.03	131.74	125.82
31	S	615	8CT	C28-C26-C25	4.03	125.35	119.01
24	9	308	CHL	OBD-CAD-C3D	-4.03	121.60	127.89
31	c	613	8CT	C10-C11-C12	-4.03	120.27	126.23
24	2	309	CHL	OBD-CAD-C3D	-4.03	121.61	127.89
24	p	310	CHL	C1A-CHA-CBD	4.03	142.68	132.36
24	5	313	CHL	OBD-CAD-C3D	-4.03	121.61	127.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Y	310	CHL	C1A-CHA-CBD	4.03	142.68	132.36
28	y	304	NEX	C11-C10-C9	-4.03	121.63	127.28
30	A	612	LHG	O7-C7-C8	4.03	120.19	111.48
31	d	410	8CT	C24-C25-C26	-4.03	121.63	127.28
24	4	305	CHL	C1A-CHA-CBD	4.02	142.66	132.36
31	t	101	8CT	C07-C02-C03	-4.02	117.27	122.70
30	p	319	LHG	O7-C7-C8	4.02	120.18	111.48
24	n	309	CHL	OBD-CAD-C3D	-4.02	121.62	127.89
24	N	317	CHL	OBD-CAD-C3D	-4.02	121.62	127.89
30	G	319	LHG	O7-C7-C8	4.02	120.18	111.48
31	A	608	8CT	C19-C20-C21	-4.02	121.64	127.28
30	C	617	LHG	O7-C7-C8	4.02	120.18	111.48
24	Y	317	CHL	C1A-CHA-CBD	4.02	142.66	132.36
24	7	310	CHL	C1A-CHA-CBD	4.02	142.66	132.36
31	s	416	8CT	C14-C13-C12	-4.02	121.64	127.28
29	q	301	0UR	C19-C18-C17	-4.02	118.33	124.58
29	p	301	0UR	C34-C27-C1	-4.02	119.44	124.45
24	y	318	CHL	C1A-CHA-CBD	4.02	142.65	132.36
26	p	302	0IE	C4-C3-C2	-4.02	116.66	120.16
28	g	304	NEX	C11-C10-C9	-4.01	121.65	127.28
29	3	301	0UR	C19-C18-C17	-4.01	118.33	124.58
29	8	301	0UR	C9-C8-C7	-4.01	121.65	127.28
24	y	310	CHL	C1A-CHA-CBD	4.01	142.63	132.36
24	q	303	CHL	OBD-CAD-C3D	-4.01	121.64	127.89
24	1	305	CHL	C1A-CHA-CBD	4.01	142.62	132.36
26	g	303	0IE	C10-C9-C8	4.01	131.72	123.52
28	N	303	NEX	C11-C10-C9	-4.01	121.66	127.28
24	u	305	CHL	OBD-CAD-C3D	-4.01	121.64	127.89
29	n	301	0UR	C5-C4-C3	-4.00	122.13	126.92
31	a	608	8CT	C19-C20-C21	-4.00	121.66	127.28
24	n	309	CHL	C1A-CHA-CBD	4.00	142.61	132.36
24	1	304	CHL	OBD-CAD-C3D	-4.00	121.65	127.89
24	5	309	CHL	OBD-CAD-C3D	-4.00	121.65	127.89
31	d	410	8CT	C35-C30-C29	-4.00	108.22	112.83
24	s	414	CHL	OBD-CAD-CBD	4.00	131.70	125.82
24	Y	309	CHL	C1A-CHA-CBD	4.00	142.61	132.36
28	n	303	NEX	C11-C10-C9	-4.00	121.67	127.28
31	c	613	8CT	C04-C03-C02	-4.00	117.17	122.64
24	4	311	CHL	C1A-CHA-CBD	4.00	142.60	132.36
28	4	303	NEX	C11-C10-C9	-4.00	121.67	127.28
28	7	304	NEX	C11-C10-C9	-4.00	121.67	127.28
30	c	617	LHG	O7-C7-C8	4.00	120.13	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	8	309	CHL	C1A-CHA-CBD	4.00	142.59	132.36
28	p	304	NEX	C11-C10-C9	-3.99	121.68	127.28
30	g	319	LHG	O7-C7-C8	3.99	120.12	111.48
28	5	304	NEX	C11-C10-C9	-3.99	121.68	127.28
24	N	309	CHL	C1A-CHA-CBD	3.99	142.59	132.36
24	5	313	CHL	C1A-CHA-CBD	3.99	142.59	132.36
28	3	318	NEX	C11-C10-C9	-3.99	121.68	127.28
24	p	313	CHL	OBD-CAD-CBD	3.99	131.68	125.82
24	S	613	CHL	C1A-CHA-CBD	3.99	142.58	132.36
31	x	601	8CT	C18-C19-C20	-3.99	115.36	123.52
24	s	409	CHL	OBD-CAD-CBD	3.99	131.68	125.82
29	g	301	0UR	C9-C8-C7	-3.99	121.69	127.28
29	u	301	0UR	C14-C15-C16	-3.99	121.69	127.28
24	q	310	CHL	C1A-CHA-CBD	3.98	142.56	132.36
24	3	312	CHL	OBD-CAD-C3D	-3.98	121.68	127.89
29	8	301	0UR	C19-C18-C17	-3.98	118.38	124.58
24	6	309	CHL	C1A-CHA-CBD	3.98	142.56	132.36
28	6	303	NEX	C11-C10-C9	-3.98	121.69	127.28
24	S	605	CHL	C1A-CHA-CBD	3.98	142.56	132.36
29	Y	301	0UR	C10-C11-C12	-3.98	121.69	127.28
24	2	313	CHL	C1A-CHA-CBD	3.98	142.56	132.36
37	C	619	DGD	O2G-C1B-C2B	3.98	120.09	111.48
24	7	313	CHL	OBD-CAD-CBD	3.98	131.66	125.82
24	g	311	CHL	C1A-CHA-CBD	3.98	142.55	132.36
28	r	301	NEX	C11-C10-C9	-3.98	121.70	127.28
29	7	301	0UR	C10-C11-C12	-3.98	121.70	127.28
24	u	309	CHL	OBD-CAD-C3D	-3.97	121.69	127.89
26	y	303	0IE	C10-C9-C8	3.97	131.65	123.52
28	s	401	NEX	C11-C10-C9	-3.97	121.71	127.28
24	3	309	CHL	C1A-CHA-CBD	3.97	142.53	132.36
24	s	414	CHL	C1A-CHA-CBD	3.97	142.53	132.36
24	s	406	CHL	C1A-CHA-CBD	3.97	142.53	132.36
31	S	615	8CT	C29-C28-C26	-3.97	117.79	126.32
24	7	311	CHL	C1A-CHA-CBD	3.97	142.52	132.36
24	G	311	CHL	C1A-CHA-CBD	3.97	142.52	132.36
28	S	617	NEX	C11-C10-C9	-3.97	121.72	127.28
31	s	415	8CT	C01-C02-C03	-3.96	120.16	124.48
30	9	318	LHG	O7-C7-C8	3.96	120.06	111.48
29	y	301	0UR	C10-C11-C12	-3.96	121.72	127.28
24	s	407	CHL	OBD-CAD-C3D	-3.96	121.71	127.89
24	n	305	CHL	OBD-CAD-CBD	3.96	131.64	125.82
31	T	101	8CT	C07-C02-C03	-3.96	117.35	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	g	313	CHL	C1A-CHA-CBD	3.96	142.50	132.36
24	R	601	CHL	OBD-CAD-C3D	-3.96	121.72	127.89
24	7	309	CHL	OBD-CAD-C3D	-3.96	121.72	127.89
24	2	311	CHL	OBD-CAD-C3D	-3.96	121.72	127.89
28	9	319	NEX	C11-C10-C9	-3.96	121.73	127.28
24	r	302	CHL	OBD-CAD-C3D	-3.96	121.72	127.89
24	2	313	CHL	OBD-CAD-C3D	-3.95	121.72	127.89
26	7	302	0IE	C4-C3-C2	-3.95	116.72	120.16
31	C	613	8CT	C10-C11-C12	-3.95	120.39	126.23
24	y	305	CHL	C1A-CHA-CBD	3.95	142.48	132.36
24	Y	309	CHL	OBD-CAD-C3D	-3.95	121.73	127.89
28	2	304	NEX	C11-C10-C9	-3.95	121.74	127.28
24	n	304	CHL	OBD-CAD-C3D	-3.95	121.73	127.89
24	N	308	CHL	OBD-CAD-C3D	-3.95	121.73	127.89
24	9	305	CHL	OBD-CAD-C3D	-3.95	121.73	127.89
24	6	312	CHL	C1A-CHA-CBD	3.95	142.47	132.36
24	p	305	CHL	C1A-CHA-CBD	3.94	142.46	132.36
24	S	613	CHL	C1B-CHB-C4A	3.94	123.86	121.32
24	7	311	CHL	OBD-CAD-C3D	-3.94	121.74	127.89
24	1	311	CHL	C1A-CHA-CBD	3.94	142.46	132.36
28	u	304	NEX	C11-C10-C9	-3.94	121.75	127.28
24	9	312	CHL	C1A-CHA-CBD	3.94	142.45	132.36
24	Y	304	CHL	C1A-CHA-CBD	3.94	142.45	132.36
24	y	311	CHL	C1A-CHA-CBD	3.94	142.45	132.36
31	T	101	8CT	C29-C28-C26	-3.94	117.85	126.32
24	5	311	CHL	OBD-CAD-C3D	-3.94	121.75	127.89
24	7	305	CHL	C1A-CHA-CBD	3.94	142.44	132.36
29	9	301	0UR	C19-C18-C17	-3.94	118.45	124.58
29	7	301	0UR	C34-C27-C1	-3.93	119.54	124.45
24	R	608	CHL	C1A-CHA-CBD	3.93	142.44	132.36
24	8	308	CHL	OBD-CAD-C3D	-3.93	121.76	127.89
24	N	304	CHL	OBD-CAD-C3D	-3.93	121.76	127.89
24	S	606	CHL	C1A-CHA-CBD	3.93	142.42	132.36
31	s	415	8CT	C28-C26-C25	-3.93	112.83	119.01
30	1	318	LHG	O7-C7-C8	3.93	119.98	111.48
24	3	312	CHL	C1A-CHA-CBD	3.93	142.42	132.36
31	S	614	8CT	C28-C26-C25	-3.93	112.83	119.01
31	X	601	8CT	C18-C19-C20	-3.92	115.49	123.52
37	c	618	DGD	O2G-C1B-C2B	3.92	119.97	111.48
32	b	618	SQD	O47-C7-C8	3.92	119.97	111.48
24	u	306	CHL	OBD-CAD-C3D	-3.92	121.78	127.89
24	n	305	CHL	C1A-CHA-CBD	3.92	142.40	132.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	1	308	CHL	C1B-CHB-C4A	-3.92	118.80	121.32
24	q	308	CHL	C1A-CHA-CBD	3.92	142.40	132.36
33	D	411	LMG	O7-C10-C11	3.92	119.96	111.48
30	4	318	LHG	O7-C7-C8	3.92	119.96	111.48
29	p	301	0UR	C10-C11-C12	-3.92	121.78	127.28
24	8	308	CHL	C1A-CHA-CBD	3.92	142.39	132.36
31	D	410	8CT	C35-C30-C29	-3.92	108.32	112.83
24	s	402	CHL	C1A-CHA-CBD	3.92	142.39	132.36
24	G	313	CHL	C1A-CHA-CBD	3.92	142.39	132.36
24	r	309	CHL	C1A-CHA-CBD	3.92	142.39	132.36
24	4	308	CHL	C1B-CHB-C4A	-3.91	118.81	121.32
24	y	313	CHL	C1A-CHA-CBD	3.91	142.37	132.36
32	B	618	SQD	O47-C7-C8	3.91	119.93	111.48
24	S	601	CHL	C1A-CHA-CBD	3.91	142.36	132.36
24	S	608	CHL	OBD-CAD-CBD	3.90	131.55	125.82
24	p	306	CHL	OBD-CAD-CBD	3.90	131.55	125.82
24	p	311	CHL	OBD-CAD-C3D	-3.90	121.81	127.89
24	N	305	CHL	OBD-CAD-CBD	3.90	131.55	125.82
24	s	407	CHL	C1A-CHA-CBD	3.90	142.34	132.36
32	B	618	SQD	O9-S-O7	-3.90	101.14	113.82
24	1	312	CHL	C1A-CHA-CBD	3.90	142.34	132.36
32	b	618	SQD	O9-S-O7	-3.89	101.16	113.82
31	c	615	8CT	C29-C28-C26	-3.89	117.95	126.32
26	5	303	0IE	C9-C10-C11	3.89	131.48	123.52
24	R	605	CHL	C1A-CHA-CBD	3.89	142.31	132.36
24	6	305	CHL	C1A-CHA-CBD	3.89	142.31	132.36
24	q	311	CHL	OBD-CAD-C3D	-3.89	121.83	127.89
24	3	305	CHL	C1A-CHA-CBD	3.88	142.31	132.36
31	t	101	8CT	C29-C28-C26	-3.88	117.97	126.32
24	1	304	CHL	C1B-CHB-C4A	-3.88	118.83	121.32
24	4	312	CHL	C1A-CHA-CBD	3.88	142.28	132.36
29	9	301	0UR	C14-C15-C16	-3.87	121.84	127.28
24	6	311	CHL	C1B-CHB-C4A	3.87	123.81	121.32
32	D	409	SQD	O9-S-O7	-3.87	101.22	113.82
24	9	308	CHL	C1B-CHB-C4A	-3.87	118.83	121.32
32	d	409	SQD	O9-S-O7	-3.86	101.25	113.82
24	7	306	CHL	C1-C2-C3	-3.86	119.87	126.20
24	Y	312	CHL	C1A-CHA-CBD	3.86	142.25	132.36
24	s	409	CHL	C1A-CHA-CBD	3.86	142.24	132.36
24	8	310	CHL	OBD-CAD-C3D	-3.86	121.87	127.89
24	s	402	CHL	OMC-CMC-C2C	-3.86	118.42	125.12
26	Y	303	0IE	C10-C9-C8	3.86	131.41	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	9	305	CHL	C1A-CHA-CBD	3.86	142.24	132.36
29	6	301	OUR	C14-C15-C16	-3.86	121.87	127.28
31	S	614	8CT	C01-C02-C03	-3.86	120.28	124.48
24	9	304	CHL	OBD-CAD-C3D	-3.86	121.88	127.89
30	N	318	LHG	O7-C7-C8	3.85	119.82	111.48
24	y	318	CHL	OBD-CAD-CBD	3.85	131.47	125.82
24	Y	305	CHL	OBD-CAD-C3D	-3.85	121.89	127.89
24	N	305	CHL	C1A-CHA-CBD	3.84	142.21	132.36
24	p	318	CHL	OBD-CAD-C3D	-3.84	121.90	127.89
26	6	302	OIE	C10-C9-C8	3.84	131.38	123.52
24	u	313	CHL	C1A-CHA-CBD	3.84	142.19	132.36
30	d	407	LHG	O7-C7-C8	3.84	119.79	111.48
24	G	306	CHL	C1A-CHA-CBD	3.84	142.18	132.36
24	u	306	CHL	C1A-CHA-CBD	3.83	142.18	132.36
24	N	311	CHL	C1B-CHB-C4A	3.83	123.79	121.32
24	S	608	CHL	C1A-CHA-CBD	3.83	142.18	132.36
24	y	306	CHL	OBD-CAD-C3D	-3.83	121.92	127.89
30	n	318	LHG	O7-C7-C8	3.83	119.77	111.48
24	p	306	CHL	C1-C2-C3	-3.83	119.92	126.20
31	C	615	8CT	C29-C28-C26	-3.83	118.09	126.32
24	7	306	CHL	OBD-CAD-CBD	3.83	131.44	125.82
32	A	609	SQD	O9-S-O7	-3.82	101.39	113.82
24	2	310	CHL	OBD-CAD-C3D	-3.82	121.93	127.89
31	T	101	8CT	C10-C11-C12	-3.82	120.59	126.23
24	2	306	CHL	C1A-CHA-CBD	3.82	142.13	132.36
26	2	303	OIE	C9-C10-C11	3.82	131.33	123.52
32	A	609	SQD	O47-C7-C8	3.81	119.73	111.48
26	9	302	OIE	C10-C9-C8	3.81	131.32	123.52
24	5	310	CHL	OBD-CAD-C3D	-3.81	121.95	127.89
26	1	302	OIE	C10-C9-C8	3.81	131.32	123.52
24	s	414	CHL	C1B-CHB-C4A	3.81	123.77	121.32
24	g	306	CHL	C1A-CHA-CBD	3.81	142.12	132.36
26	3	302	OIE	C10-C9-C8	3.80	131.30	123.52
26	7	302	OIE	C10-C9-C8	3.80	131.30	123.52
26	4	302	OIE	C10-C9-C8	3.80	131.30	123.52
24	7	312	CHL	OMC-CMC-C2C	-3.80	118.52	125.12
24	7	318	CHL	OBD-CAD-C3D	-3.80	121.97	127.89
24	6	305	CHL	OBD-CAD-CBD	3.80	131.40	125.82
30	D	407	LHG	O7-C7-C8	3.80	119.69	111.48
24	5	306	CHL	C1A-CHA-CBD	3.78	142.04	132.36
29	1	301	OUR	C9-C8-C7	-3.78	121.98	127.28
30	A	601	LHG	O7-C7-C8	3.78	119.65	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	y	306	CHL	C1A-CHA-CBD	3.77	142.02	132.36
24	n	305	CHL	OBD-CAD-C3D	-3.77	122.01	127.89
24	p	313	CHL	C1A-CHA-CBD	3.77	142.01	132.36
24	n	308	CHL	OBD-CAD-C3D	-3.77	122.02	127.89
32	a	609	SQD	O47-C7-C8	3.77	119.63	111.48
24	7	313	CHL	C1A-CHA-CBD	3.76	142.00	132.36
26	p	302	0IE	C10-C9-C8	3.76	131.21	123.52
24	3	305	CHL	OBD-CAD-CBD	3.76	131.34	125.82
24	Y	317	CHL	OBD-CAD-CBD	3.76	131.34	125.82
24	7	313	CHL	OBD-CAD-C3D	-3.75	122.04	127.89
24	g	305	CHL	OBD-CAD-C3D	-3.75	122.04	127.89
24	Y	305	CHL	C1A-CHA-CBD	3.75	141.96	132.36
24	S	601	CHL	C1B-CHB-C4A	3.75	123.73	121.32
24	q	311	CHL	C1A-CHA-CBD	3.75	141.95	132.36
24	p	306	CHL	C1A-CHA-CBD	3.74	141.95	132.36
39	D	406	PL9	C7-C3-C2	-3.74	118.98	123.39
24	G	305	CHL	OBD-CAD-C3D	-3.74	122.06	127.89
24	8	310	CHL	C1A-CHA-CBD	3.74	141.94	132.36
31	t	101	8CT	C10-C11-C12	-3.74	120.70	126.23
29	G	301	0UR	C34-C27-C1	-3.74	119.79	124.45
24	p	313	CHL	OBD-CAD-C3D	-3.73	122.07	127.89
24	7	306	CHL	C1A-CHA-CBD	3.72	141.90	132.36
29	5	301	0UR	C34-C27-C1	-3.72	119.81	124.45
24	q	304	CHL	C1A-CHA-CBD	3.72	141.88	132.36
24	N	305	CHL	OBD-CAD-C3D	-3.72	122.09	127.89
31	C	613	8CT	C29-C28-C26	-3.72	118.33	126.32
24	8	304	CHL	C1A-CHA-CBD	3.72	141.88	132.36
24	4	304	CHL	C1B-CHB-C4A	-3.72	118.93	121.32
29	4	301	0UR	C9-C8-C7	-3.71	122.07	127.28
26	7	303	0IE	C10-C9-C8	3.71	131.12	123.52
39	d	406	PL9	C7-C3-C2	-3.71	119.01	123.39
29	g	301	0UR	C34-C27-C1	-3.71	119.82	124.45
24	y	306	CHL	C1-C2-C3	-3.70	120.13	126.20
24	1	305	CHL	C1B-CHB-C4A	3.70	123.70	121.32
29	2	301	0UR	C34-C27-C1	-3.70	119.84	124.45
32	b	618	SQD	O5-C5-C4	3.70	116.36	109.70
29	Y	301	0UR	O44-C45-C46	3.69	120.67	111.55
24	G	306	CHL	OBD-CAD-C3D	-3.69	122.13	127.89
24	8	307	CHL	OBD-CAD-C3D	-3.69	122.14	127.89
26	p	303	0IE	C10-C9-C8	3.69	131.06	123.52
31	c	613	8CT	C29-C28-C26	-3.69	118.40	126.32
30	a	601	LHG	O7-C7-C8	3.68	119.45	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	a	609	SQD	O7-S-C6	3.68	112.25	106.76
32	B	618	SQD	O5-C5-C4	3.68	116.33	109.70
24	g	306	CHL	OBD-CAD-C3D	-3.68	122.15	127.89
31	s	416	8CT	C25-C24-C23	-3.68	112.54	123.20
26	g	302	0IE	C10-C9-C8	3.68	131.05	123.52
31	c	614	8CT	C35-C30-C29	-3.68	108.60	112.83
29	y	301	0UR	O44-C45-C46	3.68	120.62	111.55
24	N	312	CHL	C1A-CHA-CBD	3.67	141.77	132.36
29	u	301	0UR	C34-C27-C1	-3.67	119.87	124.45
31	C	613	8CT	C30-C31-C32	-3.67	116.95	121.47
31	S	615	8CT	C25-C24-C23	-3.67	112.57	123.20
24	s	414	CHL	OBD-CAD-C3D	-3.67	122.17	127.89
24	n	312	CHL	C1A-CHA-CBD	3.66	141.74	132.36
31	c	613	8CT	C19-C20-C21	-3.66	122.14	127.28
24	5	310	CHL	C1B-CHB-C4A	3.66	123.68	121.32
29	q	301	0UR	C34-C27-C1	-3.66	119.89	124.45
26	5	302	0IE	C10-C9-C8	3.65	130.99	123.52
24	7	305	CHL	CBC-CAC-C3C	-3.65	107.65	112.87
29	6	301	0UR	C5-C4-C3	-3.64	122.56	126.92
26	n	302	0IE	C10-C9-C8	3.64	130.97	123.52
24	S	613	CHL	OBD-CAD-C3D	-3.64	122.22	127.89
24	5	318	CHL	C1B-CHB-C4A	-3.64	118.98	121.32
29	N	301	0UR	C19-C18-C17	-3.63	118.92	124.58
28	s	401	NEX	C15-C14-C13	-3.63	122.18	127.28
31	B	617	8CT	C30-C31-C32	-3.63	117.00	121.47
29	8	301	0UR	C34-C27-C1	-3.63	119.92	124.45
24	6	305	CHL	OBD-CAD-C3D	-3.63	122.23	127.89
24	s	409	CHL	OBD-CAD-C3D	-3.63	122.23	127.89
24	Y	305	CHL	C1-C2-C3	-3.62	120.26	126.20
28	6	303	NEX	C15-C14-C13	-3.62	122.20	127.28
24	q	303	CHL	CBC-CAC-C3C	-3.62	107.69	112.87
28	n	303	NEX	C15-C14-C13	-3.62	122.20	127.28
26	G	302	0IE	C10-C9-C8	3.62	130.92	123.52
26	N	302	0IE	C4-C3-C2	-3.61	117.01	120.16
26	2	302	0IE	C10-C9-C8	3.61	130.91	123.52
26	N	302	0IE	C10-C9-C8	3.61	130.91	123.52
24	S	601	CHL	OMC-CMC-C2C	-3.61	118.85	125.12
24	4	317	CHL	C1B-CHB-C4A	-3.61	119.00	121.32
24	q	307	CHL	OBD-CAD-C3D	-3.61	122.26	127.89
28	N	303	NEX	C15-C14-C13	-3.61	122.22	127.28
26	R	614	0IE	C10-C9-C8	3.60	130.89	123.52
24	3	305	CHL	OBD-CAD-C3D	-3.59	122.29	127.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	1	317	CHL	C1B-CHB-C4A	-3.59	119.02	121.32
24	u	309	CHL	C1B-CHB-C4A	-3.58	119.02	121.32
24	8	303	CHL	CBC-CAC-C3C	-3.58	107.74	112.87
24	7	312	CHL	CBC-CAC-C3C	-3.58	107.75	112.87
28	r	301	NEX	C15-C14-C13	-3.58	122.26	127.28
29	4	301	0UR	C34-C27-C1	-3.58	119.99	124.45
24	Y	304	CHL	C1-C2-C3	-3.58	120.34	126.20
28	3	318	NEX	C15-C14-C13	-3.58	122.26	127.28
29	9	301	0UR	C34-C27-C1	-3.58	119.99	124.45
24	p	306	CHL	OBD-CAD-C3D	-3.57	122.33	127.89
26	q	302	0IE	C9-C10-C11	3.57	130.81	123.52
24	q	316	CHL	CAA-C2A-C3A	-3.56	108.06	116.23
31	S	615	8CT	C10-C11-C12	-3.56	120.97	126.23
29	y	301	0UR	C9-C8-C7	-3.55	122.29	127.28
24	G	312	CHL	C1-C2-C3	-3.55	121.01	126.76
31	a	608	8CT	C07-C02-C03	-3.55	117.91	122.70
31	b	617	8CT	C07-C02-C03	-3.55	117.91	122.70
29	1	301	0UR	C34-C27-C1	-3.55	120.03	124.45
31	b	617	8CT	C30-C31-C32	-3.55	117.11	121.47
31	C	613	8CT	C19-C20-C21	-3.54	122.31	127.28
31	c	613	8CT	C30-C31-C32	-3.54	117.11	121.47
26	r	315	0IE	C10-C9-C8	3.54	130.76	123.52
24	4	305	CHL	C1B-CHB-C4A	3.54	123.60	121.32
24	7	306	CHL	OBD-CAD-C3D	-3.53	122.38	127.89
26	8	302	0IE	C9-C10-C11	3.53	130.75	123.52
31	C	614	8CT	C35-C30-C29	-3.53	108.76	112.83
31	x	601	8CT	C07-C02-C03	-3.53	117.93	122.70
31	b	617	8CT	C10-C11-C12	-3.53	121.01	126.23
29	Y	301	0UR	C9-C8-C7	-3.53	122.33	127.28
29	n	301	0UR	C19-C18-C17	-3.52	119.09	124.58
29	n	301	0UR	C34-C27-C1	-3.52	120.06	124.45
24	S	608	CHL	OBD-CAD-C3D	-3.52	122.40	127.89
31	A	608	8CT	C07-C02-C03	-3.52	117.94	122.70
26	G	303	0IE	C20-C3-C4	-3.50	119.88	124.72
33	m	101	LMG	C8-O7-C10	-3.50	109.41	117.80
24	R	607	CHL	CMD-C2D-C3D	-3.50	117.69	124.68
31	s	416	8CT	C27-C26-C25	-3.50	117.14	122.82
24	y	305	CHL	C1-C2-C3	-3.50	120.46	126.20
24	9	311	CHL	CBC-CAC-C3C	-3.50	107.87	112.87
31	B	617	8CT	C07-C02-C03	-3.49	117.99	122.70
24	g	312	CHL	C1-C2-C3	-3.49	121.12	126.76
26	p	303	0IE	C23-C16-C15	-3.49	117.17	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	q	301	0UR	C5-C4-C3	-3.48	122.75	126.92
26	Y	303	0IE	C23-C16-C15	-3.48	117.18	122.82
26	y	303	0IE	C23-C16-C15	-3.48	117.19	122.82
28	s	401	NEX	C24-C23-C22	-3.47	104.29	110.79
26	u	303	0IE	C23-C16-C15	-3.47	117.19	122.82
26	7	303	0IE	C23-C16-C15	-3.47	117.19	122.82
28	r	301	NEX	C24-C23-C22	-3.47	104.30	110.79
24	3	308	CHL	C1B-CHB-C4A	-3.47	119.09	121.32
29	n	301	0UR	C14-C15-C16	-3.47	122.42	127.28
24	6	308	CHL	C1B-CHB-C4A	-3.47	119.09	121.32
31	A	608	8CT	C18-C19-C20	-3.47	116.43	123.52
31	S	614	8CT	C40-C12-C11	3.47	123.38	118.09
26	9	303	0IE	C9-C10-C11	3.47	130.61	123.52
24	u	313	CHL	CMD-C2D-C3D	-3.46	117.76	124.68
24	3	311	CHL	CMD-C2D-C3D	-3.46	117.76	124.68
27	R	615	XAT	C10-C11-C12	-3.46	113.17	123.20
28	N	303	NEX	C24-C23-C22	-3.46	104.31	110.79
28	6	303	NEX	C24-C23-C22	-3.46	104.32	110.79
24	g	306	CHL	C1-C2-C3	-3.46	120.53	126.20
24	y	312	CHL	C1-C2-C3	-3.46	121.16	126.76
24	p	312	CHL	CBC-CAC-C3C	-3.46	107.92	112.87
28	3	318	NEX	C24-C23-C22	-3.46	104.32	110.79
35	d	403	PHO	C2B-C1B-NB	-3.46	106.93	109.43
28	n	303	NEX	C24-C23-C22	-3.46	104.33	110.79
24	p	305	CHL	CBC-CAC-C3C	-3.45	107.93	112.87
24	8	315	CHL	CAA-C2A-C3A	-3.45	108.31	116.23
25	C	609	CLA	C3B-C4B-NB	-3.45	107.45	110.53
24	3	309	CHL	C1-C2-C3	-3.45	121.18	126.76
31	B	617	8CT	C10-C11-C12	-3.45	121.13	126.23
35	A	606	PHO	C2B-C1B-NB	-3.45	106.94	109.43
29	N	301	0UR	C34-C27-C1	-3.44	120.15	124.45
31	s	415	8CT	C40-C12-C11	3.44	123.35	118.09
31	S	615	8CT	C27-C26-C25	-3.44	117.24	122.82
24	Y	304	CHL	CBC-CAC-C3C	-3.44	107.94	112.87
24	G	312	CHL	C1B-CHB-C4A	3.44	123.54	121.32
25	b	611	CLA	C1-C2-C3	-3.44	120.56	126.20
26	u	303	0IE	C10-C9-C8	3.44	130.56	123.52
25	c	601	CLA	O2D-CGD-O1D	-3.43	117.16	123.85
24	r	308	CHL	CMD-C2D-C3D	-3.43	117.83	124.68
35	D	403	PHO	C2B-C1B-NB	-3.43	106.95	109.43
31	a	608	8CT	C18-C19-C20	-3.43	116.50	123.52
25	C	601	CLA	O2D-CGD-O1D	-3.43	117.18	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	g	313	CHL	CMD-C2D-C3D	-3.43	117.84	124.68
26	q	302	OIE	C20-C3-C4	-3.43	119.98	124.72
24	G	306	CHL	C1-C2-C3	-3.42	120.59	126.20
29	N	301	OUR	C14-C15-C16	-3.42	122.48	127.28
24	y	318	CHL	OBD-CAD-C3D	-3.41	122.57	127.89
26	8	302	OIE	C20-C3-C4	-3.41	120.00	124.72
24	S	605	CHL	C1B-CHB-C4A	3.41	123.52	121.32
26	u	302	OIE	C9-C10-C11	3.41	130.50	123.52
29	N	301	OUR	C28-C19-C18	-3.41	108.90	112.83
26	g	303	OIE	C20-C3-C4	-3.40	120.01	124.72
25	B	611	CLA	C1-C2-C3	-3.40	120.62	126.20
24	6	311	CHL	CMD-C2D-C3D	-3.40	117.88	124.68
24	Y	311	CHL	C1-C2-C3	-3.40	121.26	126.76
31	D	410	8CT	C05-C04-C03	3.40	115.38	110.44
24	6	309	CHL	C1-C2-C3	-3.40	121.27	126.76
35	a	606	PHO	C2B-C1B-NB	-3.40	106.97	109.43
24	2	318	CHL	C1B-CHB-C4A	-3.40	119.14	121.32
24	9	317	CHL	CMD-C2D-C3D	-3.39	117.90	124.68
26	3	303	OIE	C6-C7-C8	3.39	124.35	119.01
24	y	305	CHL	CBC-CAC-C3C	-3.39	108.02	112.87
24	N	317	CHL	CMD-C2D-C3D	-3.39	117.91	124.68
24	n	317	CHL	CMD-C2D-C3D	-3.39	117.91	124.68
33	D	411	LMG	C8-O7-C10	-3.39	109.69	117.80
26	n	302	OIE	C4-C3-C2	-3.39	117.21	120.16
24	u	306	CHL	C1-C2-C3	-3.39	120.65	126.20
24	u	305	CHL	CMD-C2D-C3D	-3.39	117.92	124.68
24	G	313	CHL	CMD-C2D-C3D	-3.38	117.92	124.68
24	9	305	CHL	C1-C2-C3	-3.38	120.65	126.20
31	b	617	8CT	C14-C15-C16	-3.38	117.09	126.36
26	3	303	OIE	C23-C16-C15	-3.38	117.33	122.82
24	u	318	CHL	CMD-C2D-C3D	-3.38	117.93	124.68
27	r	316	XAT	C10-C11-C12	-3.38	113.41	123.20
31	d	410	8CT	C05-C04-C03	3.38	115.35	110.44
31	s	415	8CT	C25-C24-C23	-3.37	113.42	123.20
29	6	301	OUR	C19-C18-C17	-3.37	119.33	124.58
25	c	609	CLA	C3B-C4B-NB	-3.37	107.52	110.53
29	3	301	OUR	C14-C15-C16	-3.37	122.55	127.28
31	B	617	8CT	C04-C03-C02	-3.37	118.03	122.64
24	1	309	CHL	CMD-C2D-C3D	-3.37	117.95	124.68
24	4	309	CHL	CMD-C2D-C3D	-3.36	117.97	124.68
26	G	302	OIE	C23-C16-C15	-3.36	117.38	122.82
31	V	401	8CT	C35-C30-C29	-3.36	108.97	112.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	8	301	0UR	C5-C4-C3	-3.35	122.91	126.92
31	B	617	8CT	C14-C15-C16	-3.35	117.17	126.36
24	9	312	CHL	CMD-C2D-C3D	-3.35	117.99	124.68
31	b	617	8CT	C04-C03-C02	-3.35	118.06	122.64
24	s	403	CHL	C1-C2-C3	-3.35	120.71	126.20
26	r	315	0IE	C9-C10-C11	3.35	130.38	123.52
24	q	304	CHL	C1-C2-C3	-3.35	120.71	126.20
31	S	614	8CT	C25-C24-C23	-3.35	113.50	123.20
26	g	302	0IE	C23-C16-C15	-3.35	117.39	122.82
24	Y	317	CHL	OBD-CAD-C3D	-3.35	122.67	127.89
29	q	301	0UR	C28-C19-C18	-3.35	108.98	112.83
26	u	303	0IE	C20-C3-C4	-3.34	120.10	124.72
25	c	616	CLA	O2D-CGD-O1D	-3.34	117.35	123.85
29	n	301	0UR	C28-C19-C18	-3.34	108.99	112.83
24	q	308	CHL	CMD-C2D-C3D	-3.34	118.02	124.68
25	D	405	CLA	O2D-CGD-O1D	-3.34	117.36	123.85
25	C	616	CLA	O2D-CGD-O1D	-3.33	117.36	123.85
26	9	303	0IE	C6-C7-C8	3.33	124.25	119.01
24	8	308	CHL	CMD-C2D-C3D	-3.33	118.03	124.68
31	c	615	8CT	C19-C18-C17	-3.33	116.71	123.52
24	p	312	CHL	OMC-CMC-C2C	-3.33	119.34	125.12
26	9	302	0IE	C23-C16-C15	-3.33	117.43	122.82
26	9	303	0IE	C23-C16-C15	-3.32	117.43	122.82
31	d	410	8CT	C30-C29-C28	-3.32	119.41	124.58
26	y	302	0IE	C9-C10-C11	3.32	130.32	123.52
24	7	311	CHL	CBC-CAC-C3C	-3.32	108.12	112.87
26	Y	302	0IE	C9-C10-C11	3.32	130.31	123.52
26	5	302	0IE	C23-C16-C15	-3.32	117.44	122.82
31	C	615	8CT	C24-C23-C21	-3.32	117.27	126.36
25	d	405	CLA	O2D-CGD-O1D	-3.31	117.40	123.85
29	g	301	0UR	O44-C45-C46	3.31	119.72	111.55
24	9	304	CHL	CMD-C2D-C3D	-3.31	118.06	124.68
31	c	615	8CT	C24-C23-C21	-3.31	117.29	126.36
26	g	303	0IE	C23-C16-C15	-3.31	117.46	122.82
25	A	607	CLA	O2D-CGD-O1D	-3.31	117.41	123.85
31	D	410	8CT	C30-C29-C28	-3.31	119.43	124.58
26	u	302	0IE	C23-C16-C15	-3.31	117.46	122.82
24	p	305	CHL	C1-C2-C3	-3.31	120.78	126.20
31	s	415	8CT	C39-C16-C15	3.30	123.14	118.09
31	T	101	8CT	C18-C19-C20	-3.30	116.76	123.52
26	G	303	0IE	C23-C16-C15	-3.30	117.47	122.82
25	B	609	CLA	O2D-CGD-O1D	-3.30	117.42	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	607	CLA	O2D-CGD-O1D	-3.30	117.42	123.85
32	D	409	SQD	O9-S-C6	3.30	111.68	106.76
29	G	301	0UR	O44-C45-C46	3.30	119.69	111.55
29	8	301	0UR	C28-C19-C18	-3.30	109.03	112.83
26	2	302	0IE	C23-C16-C15	-3.30	117.47	122.82
32	d	409	SQD	O9-S-C6	3.30	111.68	106.76
24	7	305	CHL	C1-C2-C3	-3.29	120.80	126.20
26	p	303	0IE	C20-C3-C4	-3.29	120.17	124.72
31	v	401	8CT	C35-C30-C29	-3.29	109.04	112.83
26	n	302	0IE	C23-C16-C15	-3.29	117.48	122.82
31	a	608	8CT	C30-C31-C32	-3.29	117.42	121.47
24	s	403	CHL	CBC-CAC-C3C	-3.29	108.16	112.87
26	6	302	0IE	C4-C3-C2	-3.29	117.29	120.16
32	d	409	SQD	O7-S-C6	3.29	111.67	106.76
24	s	408	CHL	C1B-CHB-C4A	3.29	123.44	121.32
31	C	614	8CT	C05-C04-C03	3.29	115.22	110.44
29	4	301	0UR	O44-C45-C46	3.29	119.66	111.55
32	d	409	SQD	O47-C7-C8	3.29	118.59	111.48
24	y	306	CHL	CBC-CAC-C3C	-3.29	108.17	112.87
24	3	312	CHL	CMD-C2D-C3D	-3.29	118.11	124.68
25	7	317	CLA	O2D-CGD-O1D	-3.29	117.45	123.85
24	g	311	CHL	C1-C2-C3	-3.28	120.81	126.20
26	5	303	0IE	C23-C16-C15	-3.28	117.50	122.82
25	b	609	CLA	O2D-CGD-O1D	-3.28	117.46	123.85
31	C	615	8CT	C19-C18-C17	-3.28	116.81	123.52
25	D	404	CLA	O2D-CGD-O1D	-3.28	117.47	123.85
31	C	614	8CT	C25-C24-C23	-3.28	113.70	123.20
29	6	301	0UR	C34-C27-C1	-3.28	120.36	124.45
26	R	614	0IE	C9-C10-C11	3.27	130.22	123.52
24	9	317	CHL	CAA-C2A-C3A	-3.27	108.72	116.23
26	r	315	0IE	C23-C16-C15	-3.27	117.51	122.82
31	A	608	8CT	C30-C31-C32	-3.27	117.44	121.47
26	G	302	0IE	C9-C10-C11	3.27	130.22	123.52
24	p	305	CHL	CMD-C2D-C3D	-3.27	118.14	124.68
24	S	602	CHL	C1-C2-C3	-3.27	120.83	126.20
31	S	614	8CT	C39-C16-C15	3.27	123.09	118.09
24	N	317	CHL	CAA-C2A-C3A	-3.27	108.73	116.23
24	3	317	CHL	CMD-C2D-C3D	-3.27	118.15	124.68
31	x	601	8CT	C14-C15-C16	-3.27	117.39	126.36
26	2	303	0IE	C23-C16-C15	-3.27	117.52	122.82
31	t	101	8CT	C18-C19-C20	-3.27	116.83	123.52
26	R	614	0IE	C23-C16-C15	-3.27	117.52	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	c	619	DGD	O1G-C1A-C2A	3.27	121.80	111.83
31	c	614	8CT	C05-C04-C03	3.27	115.18	110.44
26	y	302	0IE	C23-C16-C15	-3.27	117.52	122.82
24	u	310	CHL	CMD-C2D-C3D	-3.27	118.16	124.68
26	g	302	0IE	C9-C10-C11	3.27	130.20	123.52
24	n	317	CHL	CAA-C2A-C3A	-3.26	108.75	116.23
31	c	614	8CT	C25-C24-C23	-3.26	113.75	123.20
24	Y	310	CHL	O2A-CGA-CBA	3.26	121.78	111.83
25	d	404	CLA	O2D-CGD-O1D	-3.26	117.50	123.85
31	X	601	8CT	C14-C15-C16	-3.26	117.42	126.36
26	u	302	0IE	C10-C9-C8	3.26	130.19	123.52
29	q	301	0UR	C43-C3-C4	-3.26	121.18	125.03
24	4	311	CHL	CMD-C2D-C3D	-3.26	118.17	124.68
24	6	312	CHL	CMD-C2D-C3D	-3.26	118.17	124.68
24	g	310	CHL	CMD-C2D-C3D	-3.26	118.17	124.68
24	p	311	CHL	CBC-CAC-C3C	-3.26	108.21	112.87
29	3	301	0UR	C34-C27-C1	-3.26	120.39	124.45
24	6	317	CHL	CMD-C2D-C3D	-3.26	118.18	124.68
26	Y	302	0IE	C23-C16-C15	-3.26	117.54	122.82
26	3	302	0IE	C23-C16-C15	-3.25	117.54	122.82
24	Y	305	CHL	CBC-CAC-C3C	-3.25	108.21	112.87
24	g	309	CHL	CMD-C2D-C3D	-3.25	118.19	124.68
24	G	310	CHL	CMD-C2D-C3D	-3.25	118.19	124.68
27	r	316	XAT	C24-C23-C22	-3.24	104.72	110.79
26	4	302	0IE	C23-C16-C15	-3.24	117.56	122.82
24	g	306	CHL	CMD-C2D-C3D	-3.24	118.20	124.68
29	3	301	0UR	C48-C47-C46	-3.24	119.17	125.92
32	D	409	SQD	O7-S-C6	3.24	111.59	106.76
26	6	302	0IE	C23-C16-C15	-3.24	117.57	122.82
26	p	302	0IE	C23-C16-C15	-3.24	117.57	122.82
26	7	302	0IE	C23-C16-C15	-3.24	117.57	122.82
25	c	608	CLA	O2D-CGD-O1D	-3.24	117.54	123.85
24	5	313	CHL	CMD-C2D-C3D	-3.24	118.21	124.68
27	R	615	XAT	C24-C23-C22	-3.24	104.74	110.79
24	y	310	CHL	CMD-C2D-C3D	-3.23	118.22	124.68
26	1	302	0IE	C23-C16-C15	-3.23	117.58	122.82
24	g	313	CHL	C1-C2-C3	-3.23	120.90	126.20
24	u	318	CHL	CAA-C2A-C3A	-3.23	108.82	116.23
26	N	302	0IE	C23-C16-C15	-3.23	117.58	122.82
24	y	309	CHL	CMD-C2D-C3D	-3.23	118.23	124.68
25	A	604	CLA	C3B-C4B-NB	-3.23	107.65	110.53
24	5	305	CHL	CMD-C2D-C3D	-3.23	118.23	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	n	309	CHL	CMD-C2D-C3D	-3.23	118.23	124.68
24	p	309	CHL	CMD-C2D-C3D	-3.23	118.23	124.68
24	7	309	CHL	CMD-C2D-C3D	-3.23	118.23	124.68
24	G	306	CHL	CMD-C2D-C3D	-3.23	118.23	124.68
24	G	309	CHL	CMD-C2D-C3D	-3.22	118.24	124.68
24	y	313	CHL	CMD-C2D-C3D	-3.22	118.24	124.68
24	9	309	CHL	CMD-C2D-C3D	-3.22	118.24	124.68
25	C	608	CLA	O2D-CGD-O1D	-3.22	117.57	123.85
25	p	315	CLA	O2D-CGD-O1D	-3.22	117.57	123.85
24	p	306	CHL	OMC-CMC-C2C	-3.22	119.52	125.12
25	a	604	CLA	C3B-C4B-NB	-3.22	107.66	110.53
31	s	416	8CT	C10-C11-C12	-3.22	121.47	126.23
24	1	311	CHL	CMD-C2D-C3D	-3.22	118.25	124.68
32	D	409	SQD	O47-C7-C8	3.22	118.45	111.48
24	N	312	CHL	CMD-C2D-C3D	-3.22	118.25	124.68
24	8	315	CHL	CMD-C2D-C3D	-3.22	118.25	124.68
24	8	304	CHL	C1-C2-C3	-3.22	120.93	126.20
25	B	607	CLA	O2D-CGD-O1D	-3.22	117.59	123.85
24	n	312	CHL	CMD-C2D-C3D	-3.22	118.26	124.68
24	7	305	CHL	CMD-C2D-C3D	-3.21	118.26	124.68
24	G	313	CHL	C1-C2-C3	-3.21	120.93	126.20
25	7	315	CLA	O2D-CGD-O1D	-3.21	117.59	123.85
24	G	311	CHL	C1-C2-C3	-3.21	120.93	126.20
24	S	608	CHL	CMD-C2D-C3D	-3.21	118.27	124.68
24	4	317	CHL	CMD-C2D-C3D	-3.21	118.27	124.68
24	2	305	CHL	CMD-C2D-C3D	-3.21	118.28	124.68
24	n	311	CHL	CMD-C2D-C3D	-3.21	118.28	124.68
26	5	302	0IE	C20-C3-C4	-3.21	120.29	124.72
24	2	313	CHL	CMD-C2D-C3D	-3.21	118.28	124.68
24	S	602	CHL	CBC-CAC-C3C	-3.21	108.28	112.87
24	s	406	CHL	C1B-CHB-C4A	3.21	123.39	121.32
26	q	302	0IE	C23-C16-C15	-3.21	117.62	122.82
24	3	308	CHL	CMD-C2D-C3D	-3.21	118.28	124.68
29	p	301	0UR	C48-C47-C46	-3.20	119.25	125.92
24	s	402	CHL	CMD-C2D-C3D	-3.20	118.28	124.68
26	2	302	0IE	C20-C3-C4	-3.20	120.29	124.72
24	Y	308	CHL	CMD-C2D-C3D	-3.20	118.28	124.68
29	1	301	0UR	O44-C45-C46	3.20	119.45	111.55
29	8	301	0UR	C43-C3-C4	-3.20	121.25	125.03
24	6	304	CHL	CMD-C2D-C3D	-3.20	118.29	124.68
24	Y	312	CHL	CMD-C2D-C3D	-3.20	118.29	124.68
26	8	302	0IE	C23-C16-C15	-3.20	117.63	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Y	302	0IE	C10-C9-C8	3.20	130.06	123.52
32	a	609	SQD	C44-O6-C1	3.20	120.65	113.80
24	N	311	CHL	CMD-C2D-C3D	-3.20	118.29	124.68
26	9	302	0IE	C4-C3-C2	-3.20	117.38	120.16
24	5	312	CHL	CMD-C2D-C3D	-3.20	118.30	124.68
31	X	601	8CT	C07-C02-C03	-3.19	118.39	122.70
24	1	304	CHL	CMD-C2D-C3D	-3.19	118.30	124.68
24	s	409	CHL	CMD-C2D-C3D	-3.19	118.31	124.68
29	6	301	0UR	C48-C47-C46	-3.19	119.28	125.92
29	2	301	0UR	C9-C8-C7	-3.19	122.81	127.28
26	n	302	0IE	C9-C10-C11	3.19	130.04	123.52
24	q	303	CHL	CMD-C2D-C3D	-3.19	118.31	124.68
24	N	308	CHL	CMD-C2D-C3D	-3.19	118.32	124.68
24	7	313	CHL	CMD-C2D-C3D	-3.19	118.32	124.68
29	2	301	0UR	C48-C47-C46	-3.19	119.29	125.92
24	S	601	CHL	CMD-C2D-C3D	-3.19	118.32	124.68
24	n	304	CHL	CMD-C2D-C3D	-3.19	118.32	124.68
35	A	606	PHO	O1D-CGD-CBD	3.18	129.55	124.72
24	9	308	CHL	CMD-C2D-C3D	-3.18	118.32	124.68
24	y	311	CHL	O2A-CGA-CBA	3.18	121.54	111.83
24	2	312	CHL	CMD-C2D-C3D	-3.18	118.32	124.68
24	G	311	CHL	CMD-C2D-C3D	-3.18	118.32	124.68
26	4	302	0IE	C20-C3-C4	-3.18	120.32	124.72
24	1	317	CHL	CMD-C2D-C3D	-3.18	118.33	124.68
26	u	303	0IE	C13-C12-C11	3.18	124.01	119.01
31	x	601	8CT	C11-C10-C03	-3.18	118.50	127.00
25	b	612	CLA	C3B-C4B-NB	-3.18	107.69	110.53
26	y	302	0IE	C10-C9-C8	3.18	130.02	123.52
24	g	305	CHL	C1-C2-C3	-3.18	120.99	126.20
25	b	607	CLA	O2D-CGD-O1D	-3.18	117.67	123.85
24	3	304	CHL	CMD-C2D-C3D	-3.17	118.34	124.68
24	7	306	CHL	OMC-CMC-C2C	-3.17	119.61	125.12
29	N	301	0UR	C43-C3-C4	-3.17	121.28	125.03
24	n	317	CHL	C1B-CHB-C4A	-3.17	119.28	121.32
29	5	301	0UR	C48-C47-C46	-3.17	119.31	125.92
29	n	301	0UR	C48-C47-C46	-3.17	119.31	125.92
24	7	310	CHL	CMD-C2D-C3D	-3.17	118.34	124.68
26	N	302	0IE	C9-C10-C11	3.17	130.01	123.52
35	d	403	PHO	O1D-CGD-CBD	3.17	129.53	124.72
24	G	305	CHL	C1-C2-C3	-3.17	121.00	126.20
24	3	310	CHL	CMD-C2D-C3D	-3.17	118.35	124.68
24	Y	309	CHL	CMD-C2D-C3D	-3.17	118.35	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	t	101	8CT	C11-C10-C03	-3.17	118.54	127.00
24	Y	319	CHL	CMD-C2D-C3D	-3.16	118.36	124.68
31	B	617	8CT	C11-C10-C03	-3.16	118.55	127.00
26	p	303	0IE	C9-C10-C11	3.16	129.99	123.52
29	N	301	0UR	C48-C47-C46	-3.16	119.33	125.92
24	p	313	CHL	CMD-C2D-C3D	-3.16	118.36	124.68
31	b	617	8CT	C11-C10-C03	-3.16	118.55	127.00
26	4	302	0IE	C9-C10-C11	3.16	129.99	123.52
24	N	310	CHL	CMD-C2D-C3D	-3.16	118.37	124.68
24	8	303	CHL	CMD-C2D-C3D	-3.16	118.37	124.68
31	T	101	8CT	C11-C10-C03	-3.16	118.56	127.00
29	7	301	0UR	C48-C47-C46	-3.16	119.34	125.92
24	9	305	CHL	OMC-CMC-C2C	-3.16	119.64	125.12
24	S	606	CHL	CMD-C2D-C3D	-3.16	118.37	124.68
24	6	308	CHL	CMD-C2D-C3D	-3.16	118.37	124.68
24	9	311	CHL	CMD-C2D-C3D	-3.16	118.38	124.68
24	u	309	CHL	CMD-C2D-C3D	-3.16	118.38	124.68
26	2	303	0IE	C10-C9-C8	3.16	129.98	123.52
26	1	302	0IE	C20-C3-C4	-3.16	120.36	124.72
24	N	304	CHL	CMD-C2D-C3D	-3.16	118.38	124.68
24	N	309	CHL	CMD-C2D-C3D	-3.16	118.38	124.68
31	X	601	8CT	C11-C10-C03	-3.15	118.57	127.00
24	6	310	CHL	CMD-C2D-C3D	-3.15	118.38	124.68
32	B	618	SQD	O9-S-C6	3.15	111.46	106.76
24	S	605	CHL	CMD-C2D-C3D	-3.15	118.39	124.68
26	1	302	0IE	C9-C10-C11	3.15	129.97	123.52
24	S	613	CHL	CAA-C2A-C3A	-3.15	109.00	116.23
31	a	608	8CT	C11-C10-C03	-3.15	118.58	127.00
24	3	317	CHL	O1D-CGD-CBD	-3.15	119.95	124.72
24	s	406	CHL	CBC-CAC-C3C	-3.15	108.36	112.87
24	u	312	CHL	CMD-C2D-C3D	-3.15	118.39	124.68
35	D	403	PHO	O1D-CGD-CBD	3.15	129.50	124.72
25	b	613	CLA	C3B-C4B-NB	-3.15	107.72	110.53
31	c	613	8CT	C05-C04-C03	3.15	115.01	110.44
31	V	401	8CT	C18-C19-C20	-3.15	117.08	123.52
35	d	403	PHO	CMB-C2B-C3B	3.15	130.97	124.68
24	5	309	CHL	C1B-CHB-C4A	-3.15	119.30	121.32
24	G	305	CHL	CBC-CAC-C3C	-3.15	108.37	112.87
24	N	305	CHL	C1-C2-C3	-3.15	121.04	126.20
31	s	415	8CT	C30-C29-C28	3.14	129.47	124.58
25	2	308	CLA	O2D-CGD-O1D	-3.14	117.73	123.85
24	N	317	CHL	C1B-CHB-C4A	-3.14	119.30	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	q	316	CHL	CMD-C2D-C3D	-3.14	118.41	124.68
25	p	317	CLA	O2D-CGD-O1D	-3.14	117.73	123.85
24	s	406	CHL	CMD-C2D-C3D	-3.14	118.41	124.68
32	b	618	SQD	O9-S-C6	3.14	111.44	106.76
24	g	311	CHL	CMD-C2D-C3D	-3.14	118.41	124.68
31	v	401	8CT	C18-C19-C20	-3.14	117.10	123.52
24	s	403	CHL	OMC-CMC-C2C	-3.14	119.67	125.12
25	R	612	CLA	O2D-CGD-O1D	-3.14	117.74	123.85
25	S	604	CLA	O2D-CGD-O1D	-3.13	117.75	123.85
25	b	604	CLA	O2D-CGD-O1D	-3.13	117.75	123.85
29	5	301	0UR	C9-C8-C7	-3.13	122.89	127.28
25	B	602	CLA	O2D-CGD-O1D	-3.13	117.76	123.85
25	B	615	CLA	C3B-C4B-NB	-3.13	107.74	110.53
24	s	407	CHL	CMD-C2D-C3D	-3.13	118.43	124.68
25	B	612	CLA	C3B-C4B-NB	-3.13	107.74	110.53
33	i	101	LMG	C8-O7-C10	-3.13	110.31	117.80
26	Y	302	0IE	C20-C3-C4	-3.13	120.40	124.72
25	5	308	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
29	3	301	0UR	O44-C45-C46	3.12	119.26	111.55
29	5	301	0UR	O44-C45-C46	3.12	119.25	111.55
25	6	307	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
24	4	308	CHL	CMD-C2D-C3D	-3.12	118.45	124.68
24	Y	319	CHL	O2A-CGA-CBA	3.12	121.34	111.83
24	N	312	CHL	C1-C2-C3	-3.12	121.09	126.20
24	5	318	CHL	CAA-C2A-C3A	-3.12	109.08	116.23
31	b	617	8CT	C01-C02-C07	3.12	120.25	113.60
25	B	604	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
25	B	613	CLA	C3B-C4B-NB	-3.12	107.75	110.53
29	p	301	0UR	C5-C4-C3	-3.12	123.19	126.92
24	1	308	CHL	CMD-C2D-C3D	-3.12	118.46	124.68
24	5	309	CHL	CMD-C2D-C3D	-3.12	118.46	124.68
25	r	313	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
31	C	615	8CT	C11-C10-C03	-3.11	118.68	127.00
31	c	615	8CT	C30-C29-C28	-3.11	119.73	124.58
26	y	302	0IE	C20-C3-C4	-3.11	120.42	124.72
24	9	310	CHL	CMD-C2D-C3D	-3.11	118.47	124.68
24	u	311	CHL	CMD-C2D-C3D	-3.11	118.47	124.68
31	a	608	8CT	C25-C24-C23	-3.11	114.19	123.20
25	s	405	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
29	3	301	0UR	C5-C4-C3	-3.11	123.20	126.92
24	2	311	CHL	CMD-C2D-C3D	-3.11	118.47	124.68
29	2	301	0UR	O44-C45-C46	3.11	119.22	111.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	w	201	LMG	O8-C28-C29	3.11	121.31	111.83
24	n	310	CHL	CMD-C2D-C3D	-3.11	118.47	124.68
29	q	301	0UR	O44-C45-C46	3.11	119.22	111.55
26	5	303	0IE	C10-C9-C8	3.10	129.87	123.52
31	A	608	8CT	C11-C10-C03	-3.10	118.71	127.00
24	p	310	CHL	CMD-C2D-C3D	-3.10	118.48	124.68
24	G	305	CHL	CMD-C2D-C3D	-3.10	118.48	124.68
24	Y	312	CHL	C1-C2-C3	-3.10	121.11	126.20
25	b	602	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
26	9	302	0IE	C9-C10-C11	3.10	129.86	123.52
24	q	309	CHL	O2A-CGA-CBA	3.10	121.29	111.83
24	2	318	CHL	CAA-C2A-C3A	-3.10	109.12	116.23
29	9	301	0UR	O44-C45-C46	3.10	119.20	111.55
24	R	605	CHL	CMD-C2D-C3D	-3.10	118.49	124.68
31	S	614	8CT	C30-C29-C28	3.10	129.40	124.58
24	4	317	CHL	CAA-C2A-C3A	-3.10	109.13	116.23
24	r	306	CHL	CMD-C2D-C3D	-3.10	118.49	124.68
29	6	301	0UR	O44-C45-C46	3.10	119.19	111.55
24	8	303	CHL	C1B-CHB-C4A	-3.10	119.33	121.32
31	s	415	8CT	C29-C28-C26	3.10	132.99	126.32
24	s	414	CHL	CAA-C2A-C3A	-3.10	109.13	116.23
35	D	403	PHO	O2D-CGD-O1D	-3.10	117.82	123.85
24	n	312	CHL	C1-C2-C3	-3.10	121.12	126.20
24	2	309	CHL	CMD-C2D-C3D	-3.10	118.50	124.68
32	B	618	SQD	O6-C1-C2	3.09	112.97	108.27
24	6	309	CHL	CMD-C2D-C3D	-3.09	118.50	124.68
25	S	616	CLA	C3B-C4B-NB	-3.09	107.77	110.53
25	c	605	CLA	C3B-C4B-NB	-3.09	107.77	110.53
33	W	201	LMG	C8-O7-C10	-3.09	110.39	117.80
31	c	615	8CT	C11-C10-C03	-3.09	118.74	127.00
31	S	614	8CT	C29-C28-C26	3.09	132.97	126.32
29	5	301	0UR	C43-C3-C4	-3.09	121.38	125.03
35	D	403	PHO	CMB-C2B-C3B	3.09	130.86	124.68
24	1	317	CHL	CAA-C2A-C3A	-3.09	109.14	116.23
32	b	618	SQD	O6-C1-C2	3.09	112.97	108.27
35	d	403	PHO	O2D-CGD-O1D	-3.09	117.83	123.85
29	G	301	0UR	C48-C47-C46	-3.09	119.49	125.92
24	3	309	CHL	CMD-C2D-C3D	-3.09	118.51	124.68
24	n	305	CHL	C1-C2-C3	-3.09	121.14	126.20
24	S	602	CHL	OMC-CMC-C2C	-3.09	119.76	125.12
25	q	312	CLA	C3B-C4B-NB	-3.09	107.77	110.53
31	A	608	8CT	C25-C24-C23	-3.09	114.26	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	q	303	CHL	C1-C2-C3	-3.09	121.14	126.20
29	g	301	0UR	C48-C47-C46	-3.09	119.49	125.92
24	8	303	CHL	C1-C2-C3	-3.08	121.14	126.20
24	S	613	CHL	CBC-CAC-C3C	-3.08	108.46	112.87
31	C	615	8CT	C30-C29-C28	-3.08	119.78	124.58
29	q	301	0UR	C14-C15-C16	-3.08	122.96	127.28
24	p	311	CHL	CMD-C2D-C3D	-3.08	118.53	124.68
24	2	318	CHL	CMD-C2D-C3D	-3.08	118.53	124.68
24	5	318	CHL	CMD-C2D-C3D	-3.08	118.53	124.68
24	n	308	CHL	CMD-C2D-C3D	-3.08	118.53	124.68
24	8	310	CHL	CMD-C2D-C3D	-3.08	118.54	124.68
24	4	312	CHL	CMD-C2D-C3D	-3.08	118.54	124.68
24	7	311	CHL	O1D-CGD-CBD	-3.07	120.06	124.72
24	g	318	CHL	CAA-C2A-C3A	-3.07	109.18	116.23
29	G	301	0UR	C14-C15-C16	-3.07	122.97	127.28
31	V	401	8CT	C29-C28-C26	-3.07	119.72	126.32
29	n	301	0UR	C43-C3-C4	-3.07	121.41	125.03
29	8	301	0UR	O44-C45-C46	3.07	119.13	111.55
26	u	303	0IE	C6-C7-C8	3.07	123.84	119.01
24	g	305	CHL	CBC-CAC-C3C	-3.07	108.48	112.87
24	6	317	CHL	O1D-CGD-CBD	-3.07	120.07	124.72
31	s	416	8CT	C39-C16-C15	3.07	122.77	118.09
29	u	301	0UR	O44-C45-C46	3.07	119.12	111.55
24	4	304	CHL	CAA-C2A-C3A	-3.07	109.20	116.23
24	8	309	CHL	CMD-C2D-C3D	-3.07	118.56	124.68
31	B	617	8CT	C01-C02-C07	3.07	120.13	113.60
24	q	311	CHL	CMD-C2D-C3D	-3.07	118.56	124.68
25	b	615	CLA	C3B-C4B-NB	-3.06	107.80	110.53
35	a	606	PHO	O1D-CGD-CBD	3.06	129.37	124.72
24	4	304	CHL	CMD-C2D-C3D	-3.06	118.56	124.68
24	1	304	CHL	CAA-C2A-C3A	-3.06	109.20	116.23
24	6	305	CHL	CMD-C2D-C3D	-3.06	118.56	124.68
25	b	605	CLA	C3B-C4B-NB	-3.06	107.80	110.53
39	d	406	PL9	C7-C8-C9	-3.06	121.56	126.83
25	b	614	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
25	4	314	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
24	4	305	CHL	CMD-C2D-C3D	-3.06	118.57	124.68
25	b	615	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
24	s	414	CHL	CBC-CAC-C3C	-3.06	108.50	112.87
24	g	305	CHL	CMD-C2D-C3D	-3.06	118.57	124.68
24	q	310	CHL	CMD-C2D-C3D	-3.06	118.57	124.68
39	D	406	PL9	C7-C8-C9	-3.06	121.56	126.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	y	313	CHL	CBC-CAC-C3C	-3.06	108.50	112.87
24	y	313	CHL	C1-C2-C3	-3.06	121.19	126.20
25	s	417	CLA	C3B-C4B-NB	-3.06	107.80	110.53
26	N	302	0IE	C20-C3-C2	3.05	122.02	115.01
26	3	303	0IE	C21-C7-C8	-3.05	117.87	122.82
24	G	318	CHL	CAA-C2A-C3A	-3.05	109.23	116.23
33	C	618	LMG	O8-C28-C29	3.05	121.14	111.83
24	q	304	CHL	CMD-C2D-C3D	-3.05	118.58	124.68
25	1	314	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
24	S	605	CHL	CBC-CAC-C3C	-3.05	108.51	112.87
24	q	307	CHL	CMD-C2D-C3D	-3.05	118.59	124.68
24	5	311	CHL	CMD-C2D-C3D	-3.05	118.59	124.68
24	Y	312	CHL	CBC-CAC-C3C	-3.05	108.51	112.87
24	R	601	CHL	CMD-C2D-C3D	-3.05	118.59	124.68
29	p	301	0UR	C9-C8-C7	-3.05	123.00	127.28
25	B	605	CLA	C3B-C4B-NB	-3.04	107.81	110.53
29	4	301	0UR	C36-C28-C19	3.04	114.16	109.55
24	r	302	CHL	CMD-C2D-C3D	-3.04	118.60	124.68
31	C	614	8CT	C01-C02-C07	3.04	120.09	113.60
26	9	303	0IE	C21-C7-C8	-3.04	117.89	122.82
24	7	311	CHL	CMD-C2D-C3D	-3.04	118.60	124.68
25	y	317	CLA	O2D-CGD-O1D	-3.04	117.92	123.85
33	i	101	LMG	O8-C28-C29	3.04	121.11	111.83
31	S	615	8CT	C39-C16-C15	3.04	122.73	118.09
24	8	304	CHL	CMD-C2D-C3D	-3.04	118.61	124.68
25	B	614	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
25	B	615	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
24	3	305	CHL	CMD-C2D-C3D	-3.04	118.61	124.68
24	2	310	CHL	C1B-CHB-C4A	3.04	123.28	121.32
25	9	316	CLA	C3B-C4B-NB	-3.04	107.82	110.53
25	C	605	CLA	C3B-C4B-NB	-3.04	107.82	110.53
26	7	303	0IE	C9-C10-C11	3.04	129.73	123.52
32	A	609	SQD	O9-S-C6	3.04	111.29	106.76
24	Y	319	CHL	O1D-CGD-CBD	-3.04	120.12	124.72
25	Y	316	CLA	O2D-CGD-O1D	-3.03	117.94	123.85
26	n	302	0IE	C20-C3-C2	3.03	121.98	115.01
29	2	301	0UR	C43-C3-C4	-3.03	121.45	125.03
24	1	312	CHL	CMD-C2D-C3D	-3.03	118.62	124.68
24	s	414	CHL	O1D-CGD-CBD	-3.03	120.12	124.72
31	x	601	8CT	C19-C20-C21	-3.03	123.03	127.28
25	B	610	CLA	C3B-C4B-NB	-3.03	107.82	110.53
24	G	311	CHL	O2A-CGA-CBA	3.03	121.08	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	G	318	CHL	CMD-C2D-C3D	-3.03	118.63	124.68
31	c	614	8CT	C01-C02-C07	3.03	120.06	113.60
24	5	306	CHL	OMC-CMC-C2C	-3.03	119.86	125.12
25	8	311	CLA	C3B-C4B-NB	-3.03	107.83	110.53
24	g	318	CHL	CMD-C2D-C3D	-3.03	118.63	124.68
25	C	612	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
25	b	610	CLA	C3B-C4B-NB	-3.02	107.83	110.53
24	R	602	CHL	CMD-C2D-C3D	-3.02	118.64	124.68
25	4	315	CLA	O2D-CGD-O1D	-3.02	117.96	123.85
24	Y	319	CHL	C1-C2-C3	-3.02	121.25	126.20
25	d	405	CLA	C3B-C4B-NB	-3.02	107.83	110.53
24	8	307	CHL	CMD-C2D-C3D	-3.02	118.65	124.68
24	r	302	CHL	O1D-CGD-CBD	-3.02	120.14	124.72
24	q	311	CHL	C1-C2-C3	-3.02	121.25	126.20
25	R	613	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
24	G	312	CHL	CMD-C2D-C3D	-3.02	118.65	124.68
24	q	309	CHL	C1-C2-C3	-3.02	121.25	126.20
24	Y	304	CHL	CMD-C2D-C3D	-3.02	118.65	124.68
24	g	312	CHL	CMD-C2D-C3D	-3.02	118.65	124.68
31	c	614	8CT	C30-C31-C32	-3.02	117.75	121.47
24	S	607	CHL	CMD-C2D-C3D	-3.02	118.66	124.68
25	b	607	CLA	C3B-C4B-NB	-3.02	107.84	110.53
25	3	313	CLA	C3B-C4B-NB	-3.01	107.84	110.53
24	y	311	CHL	CMD-C2D-C3D	-3.01	118.66	124.68
29	9	301	0UR	C5-C4-C3	-3.01	123.32	126.92
29	2	301	0UR	C36-C28-C19	3.01	114.11	109.55
29	p	301	0UR	O44-C45-C46	3.01	118.98	111.55
25	r	314	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
29	7	301	0UR	O44-C45-C46	3.01	118.98	111.55
24	R	601	CHL	O1D-CGD-CBD	-3.01	120.16	124.72
26	p	303	0IE	C6-C7-C8	3.01	123.74	119.01
24	8	310	CHL	C1-C2-C3	-3.01	121.27	126.20
24	N	311	CHL	CBC-CAC-C3C	-3.01	108.57	112.87
29	u	301	0UR	C5-C4-C3	-3.01	123.32	126.92
24	q	309	CHL	CMD-C2D-C3D	-3.01	118.67	124.68
24	g	311	CHL	O2A-CGA-CBA	3.01	121.00	111.83
25	8	314	CLA	O2D-CGD-O1D	-3.01	118.00	123.85
25	C	611	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
29	g	301	0UR	C14-C15-C16	-3.00	123.07	127.28
31	v	401	8CT	C29-C28-C26	-3.00	119.87	126.32
25	B	604	CLA	C1-C2-C3	-3.00	121.28	126.20
26	3	303	0IE	C9-C10-C11	3.00	129.66	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	y	305	CHL	CMD-C2D-C3D	-3.00	118.69	124.68
29	8	301	0UR	C14-C15-C16	-3.00	123.07	127.28
24	r	303	CHL	CMD-C2D-C3D	-3.00	118.69	124.68
26	p	302	0IE	C9-C10-C11	3.00	129.66	123.52
25	9	314	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
25	B	612	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
32	B	618	SQD	O7-S-C6	3.00	111.23	106.76
26	7	302	0IE	C9-C10-C11	3.00	129.65	123.52
37	C	619	DGD	C2G-O2G-C1B	-3.00	110.62	117.80
25	c	607	CLA	O2D-CGD-O1D	-3.00	118.02	123.85
25	Y	316	CLA	C3B-C4B-NB	-3.00	107.86	110.53
33	d	411	LMG	O7-C10-C11	2.99	117.96	111.48
25	3	307	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
24	2	306	CHL	OMC-CMC-C2C	-2.99	119.92	125.12
25	a	605	CLA	C3B-C4B-NB	-2.99	107.86	110.53
29	5	301	0UR	C36-C28-C19	2.99	114.08	109.55
26	u	303	0IE	C22-C12-C11	-2.99	117.97	122.82
29	7	301	0UR	C9-C8-C7	-2.99	123.08	127.28
26	3	302	0IE	C4-C3-C2	-2.99	117.56	120.16
30	d	408	LHG	C5-O7-C7	-2.99	110.65	117.80
31	C	615	8CT	C10-C11-C12	-2.99	121.82	126.23
29	1	301	0UR	C36-C28-C19	2.99	114.07	109.55
31	A	608	8CT	C35-C30-C29	-2.99	109.39	112.83
25	C	607	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
24	n	305	CHL	O1D-CGD-CBD	-2.98	120.20	124.72
26	G	303	0IE	C6-C7-C8	2.98	123.70	119.01
25	c	608	CLA	C3B-C4B-NB	-2.98	107.87	110.53
26	Y	302	0IE	C20-C3-C2	2.98	121.86	115.01
24	s	408	CHL	CMD-C2D-C3D	-2.98	118.72	124.68
31	C	613	8CT	C11-C10-C03	-2.98	119.03	127.00
25	r	304	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
31	X	601	8CT	C19-C20-C21	-2.98	123.10	127.28
24	Y	317	CHL	CBC-CAC-C3C	-2.98	108.61	112.87
29	1	301	0UR	C48-C47-C46	-2.98	119.72	125.92
25	b	604	CLA	C1-C2-C3	-2.98	121.32	126.20
29	9	301	0UR	C48-C47-C46	-2.98	119.72	125.92
31	c	613	8CT	C11-C10-C03	-2.98	119.05	127.00
31	c	615	8CT	C10-C11-C12	-2.98	121.83	126.23
33	d	401	LMG	C8-O7-C10	-2.98	110.67	117.80
31	c	614	8CT	C18-C19-C20	-2.98	117.43	123.52
25	5	314	CLA	O2D-CGD-O1D	-2.98	118.06	123.85
24	5	313	CHL	O1D-CGD-CBD	-2.98	120.21	124.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	607	CLA	C3B-C4B-NB	-2.98	107.87	110.53
26	g	303	0IE	C6-C7-C8	2.97	123.69	119.01
24	1	310	CHL	CMD-C2D-C3D	-2.97	118.74	124.68
24	4	312	CHL	O1D-CGD-CBD	-2.97	120.22	124.72
24	2	310	CHL	CAA-C2A-C3A	-2.97	109.42	116.23
31	C	613	8CT	C05-C04-C03	2.97	114.75	110.44
25	C	608	CLA	C3B-C4B-NB	-2.97	107.88	110.53
24	y	312	CHL	O2A-CGA-CBA	2.97	120.89	111.83
25	N	313	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
31	t	101	8CT	C04-C03-C02	-2.97	118.58	122.64
31	a	608	8CT	C04-C03-C02	-2.97	118.58	122.64
25	2	314	CLA	C3B-C4B-NB	-2.97	107.88	110.53
24	1	305	CHL	CMD-C2D-C3D	-2.97	118.75	124.68
25	3	316	CLA	C3B-C4B-NB	-2.97	107.88	110.53
24	7	318	CHL	CAA-C2A-C3A	-2.97	109.43	116.23
25	1	315	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
24	s	407	CHL	C1B-CHB-C4A	2.97	123.23	121.32
26	4	302	0IE	C20-C3-C2	2.97	121.82	115.01
32	b	618	SQD	O7-S-C6	2.97	111.18	106.76
24	1	304	CHL	O1D-CGD-CBD	-2.97	120.23	124.72
24	N	309	CHL	O1D-CGD-CBD	-2.97	120.23	124.72
24	R	608	CHL	O1D-CGD-CBD	-2.96	120.23	124.72
24	7	318	CHL	CMD-C2D-C3D	-2.96	118.76	124.68
31	a	608	8CT	C35-C30-C29	-2.96	109.42	112.83
26	1	302	0IE	C20-C3-C2	2.96	121.81	115.01
24	p	318	CHL	CMD-C2D-C3D	-2.96	118.76	124.68
24	3	317	CHL	CAA-C2A-C3A	-2.96	109.44	116.23
24	6	317	CHL	CAA-C2A-C3A	-2.96	109.44	116.23
25	u	315	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
24	S	613	CHL	O1D-CGD-CBD	-2.96	120.23	124.72
25	y	308	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
24	R	608	CHL	CMD-C2D-C3D	-2.96	118.77	124.68
24	4	310	CHL	CMD-C2D-C3D	-2.96	118.77	124.68
25	c	612	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
24	g	306	CHL	C4-C3-C5	2.96	120.36	115.23
26	9	303	0IE	C13-C12-C11	2.96	123.66	119.01
26	7	303	0IE	C6-C7-C8	2.96	123.66	119.01
25	D	405	CLA	C3B-C4B-NB	-2.96	107.89	110.53
24	y	318	CHL	CMD-C2D-C3D	-2.95	118.78	124.68
24	p	312	CHL	CMD-C2D-C3D	-2.95	118.78	124.68
25	2	314	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
29	u	301	0UR	C48-C47-C46	-2.95	119.77	125.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	n	301	0UR	O44-C45-C46	2.95	118.84	111.55
24	q	308	CHL	O1D-CGD-CBD	-2.95	120.24	124.72
31	C	614	8CT	C30-C31-C32	-2.95	117.83	121.47
24	N	312	CHL	O1D-CGD-CBD	-2.95	120.25	124.72
24	q	309	CHL	O1D-CGD-CBD	-2.95	120.25	124.72
24	s	414	CHL	CMD-C2D-C3D	-2.95	118.78	124.68
31	C	614	8CT	C18-C19-C20	-2.95	117.48	123.52
24	9	305	CHL	CMD-C2D-C3D	-2.95	118.78	124.68
25	A	605	CLA	C3B-C4B-NB	-2.95	107.89	110.53
26	5	302	0IE	C9-C10-C11	2.95	129.55	123.52
31	A	608	8CT	C04-C03-C02	-2.95	118.61	122.64
24	2	313	CHL	O1D-CGD-CBD	-2.95	120.25	124.72
24	6	304	CHL	CBC-CAC-C3C	-2.95	108.65	112.87
24	u	312	CHL	CBC-CAC-C3C	-2.95	108.65	112.87
25	B	611	CLA	C3B-C4B-NB	-2.95	107.90	110.53
24	1	312	CHL	O1D-CGD-CBD	-2.95	120.25	124.72
24	N	305	CHL	O1D-CGD-CBD	-2.95	120.25	124.72
24	1	317	CHL	CBC-CAC-C3C	-2.95	108.66	112.87
37	C	620	DGD	O6D-C1D-C2D	-2.95	104.32	110.37
25	R	603	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
24	G	311	CHL	CBC-CAC-C3C	-2.94	108.66	112.87
25	6	316	CLA	C3B-C4B-NB	-2.94	107.90	110.53
25	u	315	CLA	C3B-C4B-NB	-2.94	107.90	110.53
25	r	312	CLA	C3B-C4B-NB	-2.94	107.90	110.53
25	5	314	CLA	C3B-C4B-NB	-2.94	107.90	110.53
33	w	201	LMG	C8-O7-C10	-2.94	110.76	117.80
26	8	302	0IE	C20-C3-C2	2.94	121.76	115.01
24	Y	311	CHL	O2A-CGA-CBA	2.94	120.80	111.83
25	Y	315	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
25	R	611	CLA	C3B-C4B-NB	-2.94	107.91	110.53
24	8	307	CHL	O1D-CGD-CBD	-2.94	120.27	124.72
25	C	605	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
24	4	304	CHL	O1D-CGD-CBD	-2.94	120.27	124.72
37	C	620	DGD	O1G-C1A-C2A	2.94	120.79	111.83
24	G	313	CHL	O1D-CGD-CBD	-2.93	120.27	124.72
25	b	611	CLA	C3B-C4B-NB	-2.93	107.91	110.53
24	5	310	CHL	CAA-C2A-C3A	-2.93	109.50	116.23
26	G	302	0IE	C4-C3-C2	-2.93	117.61	120.16
24	5	313	CHL	CBC-CAC-C3C	-2.93	108.67	112.87
24	G	306	CHL	C4-C3-C5	2.93	120.32	115.23
24	Y	317	CHL	CMD-C2D-C3D	-2.93	118.83	124.68
31	d	410	8CT	C07-C02-C03	-2.93	118.75	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	s	403	CHL	O2A-CGA-CBA	2.93	120.77	111.83
25	n	313	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
24	n	310	CHL	O2A-CGA-CBA	2.93	120.76	111.83
26	q	302	0IE	C20-C3-C2	2.93	121.73	115.01
31	v	401	8CT	C14-C13-C12	-2.93	123.17	127.28
24	2	313	CHL	CBC-CAC-C3C	-2.93	108.68	112.87
25	a	605	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
24	y	306	CHL	C4-C3-C5	2.92	120.31	115.23
25	c	605	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
25	p	314	CLA	C3B-C4B-NB	-2.92	107.92	110.53
25	q	305	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
26	g	302	0IE	C4-C3-C2	-2.92	117.61	120.16
39	D	406	PL9	C27-C28-C29	-2.92	120.94	127.62
24	S	613	CHL	CMD-C2D-C3D	-2.92	118.85	124.68
26	G	303	0IE	C21-C7-C8	-2.92	118.09	122.82
31	D	410	8CT	C30-C31-C32	-2.92	117.88	121.47
25	y	316	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
25	C	616	CLA	C3B-C4B-NB	-2.92	107.93	110.53
24	r	309	CHL	O1D-CGD-CBD	-2.92	120.30	124.72
26	g	303	0IE	C21-C7-C8	-2.92	118.09	122.82
24	S	602	CHL	O2A-CGA-CBA	2.92	120.72	111.83
31	c	613	8CT	C01-C02-C07	2.91	119.81	113.60
26	y	302	0IE	C20-C3-C2	2.91	121.70	115.01
24	n	312	CHL	O1D-CGD-CBD	-2.91	120.30	124.72
24	g	318	CHL	CBC-CAC-C3C	-2.91	108.70	112.87
30	a	601	LHG	O8-C23-C24	2.91	120.72	111.83
25	b	601	CLA	C3B-C4B-NB	-2.91	107.93	110.53
31	D	410	8CT	C07-C02-C03	-2.91	118.77	122.70
24	G	318	CHL	CBC-CAC-C3C	-2.91	108.71	112.87
25	B	601	CLA	C3B-C4B-NB	-2.91	107.93	110.53
25	c	603	CLA	C3B-C4B-NB	-2.91	107.93	110.53
24	p	318	CHL	CAA-C2A-C3A	-2.91	109.56	116.23
24	7	312	CHL	CMD-C2D-C3D	-2.91	118.87	124.68
24	u	306	CHL	CMD-C2D-C3D	-2.91	118.87	124.68
29	N	301	0UR	O44-C45-C46	2.91	118.73	111.55
25	c	611	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
39	d	406	PL9	C27-C28-C29	-2.91	120.97	127.62
25	q	315	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
24	N	310	CHL	O2A-CGA-CBA	2.91	120.70	111.83
24	8	309	CHL	O2A-CGA-CBA	2.91	120.69	111.83
25	y	317	CLA	C3B-C4B-NB	-2.90	107.94	110.53
26	g	302	0IE	C20-C3-C4	-2.90	120.70	124.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	3	305	CHL	OMC-CMC-C2C	-2.90	120.08	125.12
26	u	303	0IE	C21-C7-C8	-2.90	118.11	122.82
29	7	301	0UR	C5-C4-C3	-2.90	123.45	126.92
24	7	310	CHL	O1D-CGD-CBD	-2.90	120.32	124.72
25	A	610	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
26	2	302	0IE	C20-C3-C2	2.90	121.67	115.01
26	g	302	0IE	C20-C3-C2	2.90	121.67	115.01
24	g	313	CHL	O1D-CGD-CBD	-2.90	120.32	124.72
25	g	317	CLA	C3B-C4B-NB	-2.90	107.94	110.53
24	y	311	CHL	C1-C2-C3	-2.90	121.44	126.20
24	3	310	CHL	O1D-CGD-CBD	-2.90	120.33	124.72
24	n	311	CHL	O2A-CGA-CBA	2.90	120.67	111.83
24	8	308	CHL	O1D-CGD-CBD	-2.90	120.33	124.72
24	N	311	CHL	O2A-CGA-CBA	2.90	120.67	111.83
26	2	302	0IE	C9-C10-C11	2.90	129.45	123.52
25	Y	307	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
25	C	610	CLA	O2D-CGD-O1D	-2.89	118.21	123.85
24	2	310	CHL	CMD-C2D-C3D	-2.89	118.90	124.68
24	6	305	CHL	O1D-CGD-CBD	-2.89	120.33	124.72
25	u	317	CLA	C3B-C4B-NB	-2.89	107.95	110.53
29	y	301	0UR	C48-C47-C46	-2.89	119.89	125.92
24	p	310	CHL	OMC-CMC-C2C	-2.89	120.09	125.12
25	2	315	CLA	C3B-C4B-NB	-2.89	107.95	110.53
25	3	315	CLA	C3B-C4B-NB	-2.89	107.95	110.53
25	4	313	CLA	C3B-C4B-NB	-2.89	107.95	110.53
26	G	302	0IE	C20-C3-C2	2.89	121.65	115.01
25	b	612	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
25	A	605	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
25	b	611	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
24	9	308	CHL	O1D-CGD-CBD	-2.89	120.34	124.72
24	n	309	CHL	O1D-CGD-CBD	-2.89	120.34	124.72
24	r	309	CHL	CMD-C2D-C3D	-2.89	118.91	124.68
25	N	316	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
29	5	301	0UR	C5-C4-C3	-2.89	123.46	126.92
25	3	313	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
24	2	318	CHL	CBC-CAC-C3C	-2.89	108.73	112.87
26	5	302	0IE	C20-C3-C2	2.89	121.64	115.01
24	p	310	CHL	O1D-CGD-CBD	-2.89	120.34	124.72
25	4	307	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
24	4	317	CHL	CBC-CAC-C3C	-2.89	108.74	112.87
26	p	303	0IE	C21-C7-C8	-2.89	118.14	122.82
24	Y	310	CHL	C1-C2-C3	-2.89	121.47	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	5	315	CLA	C3B-C4B-NB	-2.89	107.95	110.53
25	2	317	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
24	q	310	CHL	O2A-CGA-CBA	2.89	120.64	111.83
25	S	612	CLA	C3B-C4B-NB	-2.89	107.95	110.53
30	y	319	LHG	O8-C23-C24	2.88	120.63	111.83
24	8	304	CHL	CBC-CAC-C3C	-2.88	108.74	112.87
25	n	313	CLA	C3B-C4B-NB	-2.88	107.95	110.53
24	1	305	CHL	O1D-CGD-CBD	-2.88	120.35	124.72
29	4	301	OUR	C48-C47-C46	-2.88	119.92	125.92
26	G	302	OIE	C20-C3-C4	-2.88	120.73	124.72
25	a	610	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
24	g	313	CHL	O2A-CGA-CBA	2.88	120.62	111.83
25	6	313	CLA	C3B-C4B-NB	-2.88	107.96	110.53
24	5	318	CHL	CBC-CAC-C3C	-2.88	108.75	112.87
24	q	304	CHL	CBC-CAC-C3C	-2.88	108.75	112.87
32	A	609	SQD	O7-S-C6	2.88	111.06	106.76
25	c	616	CLA	C3B-C4B-NB	-2.88	107.96	110.53
24	5	310	CHL	CMD-C2D-C3D	-2.88	118.93	124.68
25	n	316	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
33	D	401	LMG	C8-O7-C10	-2.88	110.91	117.80
24	N	310	CHL	C1-C2-C3	-2.88	121.48	126.20
26	r	315	OIE	C4-C3-C2	-2.87	117.66	120.16
25	6	315	CLA	C3B-C4B-NB	-2.87	107.96	110.53
24	y	312	CHL	CMD-C2D-C3D	-2.87	118.94	124.68
25	c	603	CLA	O2D-CGD-O1D	-2.87	118.25	123.85
24	4	305	CHL	O1D-CGD-CBD	-2.87	120.36	124.72
24	G	313	CHL	O2A-CGA-CBA	2.87	120.60	111.83
25	s	413	CLA	C3B-C4B-NB	-2.87	107.97	110.53
25	5	317	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
25	C	603	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
24	Y	311	CHL	CMD-C2D-C3D	-2.87	118.94	124.68
24	q	303	CHL	O2A-CGA-CBA	2.87	120.59	111.83
37	c	618	DGD	C2G-O2G-C1B	-2.87	110.93	117.80
25	N	313	CLA	C3B-C4B-NB	-2.87	107.97	110.53
26	3	302	OIE	C9-C10-C11	2.87	129.39	123.52
25	g	308	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
24	n	311	CHL	CBC-CAC-C3C	-2.87	108.77	112.87
24	Y	310	CHL	CMD-C2D-C3D	-2.87	118.95	124.68
25	g	317	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
25	S	611	CLA	C3B-C4B-NB	-2.87	107.97	110.53
31	V	401	8CT	C14-C13-C12	-2.87	123.26	127.28
25	1	314	CLA	C3B-C4B-NB	-2.87	107.97	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	6	302	0IE	C20-C3-C2	2.87	121.59	115.01
26	7	303	0IE	C21-C7-C8	-2.87	118.17	122.82
26	p	302	0IE	C20-C3-C2	2.87	121.59	115.01
25	b	603	CLA	O2D-CGD-O1D	-2.86	118.27	123.85
25	R	604	CLA	CAA-C2A-C3A	-2.86	109.66	116.23
30	Y	318	LHG	O8-C23-C24	2.86	120.57	111.83
25	b	606	CLA	C3B-C4B-NB	-2.86	107.97	110.53
25	s	412	CLA	C3B-C4B-NB	-2.86	107.97	110.53
24	y	312	CHL	CBC-CAC-C3C	-2.86	108.77	112.87
25	9	313	CLA	C3B-C4B-NB	-2.86	107.97	110.53
25	y	307	CLA	C3B-C4B-NB	-2.86	107.97	110.53
25	G	317	CLA	C3B-C4B-NB	-2.86	107.98	110.53
29	4	301	0UR	C18-C17-C16	-2.86	120.17	126.32
37	C	619	DGD	O1G-C1A-C2A	2.86	120.55	111.83
29	1	301	0UR	C43-C3-C4	-2.86	121.66	125.03
25	c	606	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
25	G	316	CLA	C3B-C4B-NB	-2.86	107.98	110.53
25	9	307	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
29	Y	301	0UR	C48-C47-C46	-2.86	119.97	125.92
24	8	303	CHL	O2A-CGA-CBA	2.86	120.54	111.83
25	G	307	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
25	n	307	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
24	s	402	CHL	C1B-CHB-C4A	2.86	123.16	121.32
24	3	305	CHL	O1D-CGD-CBD	-2.86	120.39	124.72
25	B	611	CLA	O2D-CGD-O1D	-2.85	118.29	123.85
24	n	304	CHL	C1-C2-C3	-2.85	121.52	126.20
24	6	310	CHL	O1D-CGD-CBD	-2.85	120.39	124.72
25	C	603	CLA	C3B-C4B-NB	-2.85	107.98	110.53
25	G	317	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
25	C	606	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
24	q	307	CHL	O1D-CGD-CBD	-2.85	120.40	124.72
35	A	606	PHO	O2D-CGD-O1D	-2.85	118.30	123.85
26	R	614	0IE	C4-C3-C2	-2.85	117.67	120.16
24	4	308	CHL	O1D-CGD-CBD	-2.85	120.40	124.72
24	y	318	CHL	CBC-CAC-C3C	-2.85	108.79	112.87
25	1	307	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
33	W	201	LMG	O8-C28-C29	2.85	120.52	111.83
24	S	606	CHL	C1B-CHB-C4A	2.85	123.16	121.32
24	7	305	CHL	O1D-CGD-CBD	-2.85	120.40	124.72
37	c	618	DGD	O1G-C1A-C2A	2.85	120.52	111.83
25	G	308	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
24	Y	311	CHL	CBC-CAC-C3C	-2.85	108.80	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	r	308	CHL	O2A-CGA-CBA	2.85	120.52	111.83
28	u	304	NEX	C26-C27-C28	2.85	132.01	125.99
25	S	609	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
25	8	313	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
25	8	305	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
24	R	606	CHL	CMD-C2D-C3D	-2.84	119.00	124.68
25	l	313	CLA	C3B-C4B-NB	-2.84	107.99	110.53
31	d	410	8CT	C30-C31-C32	-2.84	117.97	121.47
25	N	306	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
25	c	612	CLA	C3B-C4B-NB	-2.84	107.99	110.53
26	9	303	0IE	C22-C12-C11	-2.84	118.21	122.82
25	q	314	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
28	p	304	NEX	C26-C27-C28	2.84	132.00	125.99
25	c	610	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
24	R	607	CHL	O2A-CGA-CBA	2.84	120.50	111.83
30	A	601	LHG	O8-C23-C24	2.84	120.49	111.83
33	C	618	LMG	C8-O7-C10	-2.84	111.00	117.80
24	N	308	CHL	O1D-CGD-CBD	-2.84	120.42	124.72
25	b	616	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
24	q	310	CHL	CBC-CAC-C3C	-2.84	108.81	112.87
24	7	310	CHL	OMC-CMC-C2C	-2.84	120.19	125.12
31	S	615	8CT	C19-C18-C17	-2.84	117.71	123.52
25	l	316	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
24	Y	304	CHL	O1D-CGD-CBD	-2.84	120.42	124.72
26	6	302	0IE	C9-C10-C11	2.84	129.32	123.52
25	B	616	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
25	n	306	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
25	9	314	CLA	C3B-C4B-NB	-2.84	108.00	110.53
26	7	302	0IE	C20-C3-C2	2.84	121.52	115.01
25	N	307	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
25	4	316	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
28	G	304	NEX	C26-C27-C28	2.83	131.98	125.99
24	y	313	CHL	O2A-CGA-CBA	2.83	120.47	111.83
28	5	304	NEX	C26-C27-C28	2.83	131.98	125.99
25	7	307	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
25	9	315	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
25	u	308	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
25	b	606	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
25	p	307	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
25	s	410	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
24	q	304	CHL	O2A-CGA-CBA	2.83	120.47	111.83
25	6	313	CLA	O2D-CGD-O1D	-2.83	118.34	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	p	305	CHL	O1D-CGD-CBD	-2.83	120.43	124.72
24	7	306	CHL	O1D-CGD-CBD	-2.83	120.43	124.72
25	C	612	CLA	C3B-C4B-NB	-2.83	108.01	110.53
28	R	616	NEX	C26-C27-C28	2.83	131.97	125.99
24	R	606	CHL	O2A-CGA-CBA	2.83	120.45	111.83
26	n	302	0IE	C20-C3-C4	-2.83	120.81	124.72
24	n	310	CHL	O1D-CGD-CBD	-2.83	120.44	124.72
26	p	303	0IE	C22-C12-C11	-2.83	118.24	122.82
24	s	406	CHL	O1D-CGD-CBD	-2.82	120.44	124.72
31	X	601	8CT	C05-C04-C03	2.82	114.54	110.44
24	y	311	CHL	O1D-CGD-CBD	-2.82	120.44	124.72
25	u	316	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
25	u	314	CLA	C3B-C4B-NB	-2.82	108.01	110.53
24	2	306	CHL	CMD-C2D-C3D	-2.82	119.04	124.68
29	1	301	0UR	C5-C4-C3	-2.82	123.54	126.92
31	d	410	8CT	C01-C02-C07	2.82	119.62	113.60
24	9	304	CHL	CBC-CAC-C3C	-2.82	108.83	112.87
25	6	315	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
32	a	609	SQD	O9-S-C6	2.82	110.97	106.76
24	1	309	CHL	O1D-CGD-CBD	-2.82	120.44	124.72
28	2	304	NEX	C26-C27-C28	2.82	131.96	125.99
25	B	601	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
26	G	302	0IE	C21-C7-C8	-2.82	118.25	122.82
29	q	301	0UR	C48-C47-C46	-2.82	120.05	125.92
29	4	301	0UR	C14-C13-C12	-2.82	118.63	126.36
25	6	314	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
24	G	311	CHL	O1D-CGD-CBD	-2.82	120.45	124.72
28	r	317	NEX	C26-C27-C28	2.82	131.96	125.99
31	B	617	8CT	C24-C23-C21	-2.82	118.63	126.36
24	p	305	CHL	O2A-CGA-CBA	2.82	120.43	111.83
24	u	309	CHL	O1D-CGD-CBD	-2.82	120.45	124.72
25	8	312	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
28	g	304	NEX	C26-C27-C28	2.82	131.95	125.99
24	Y	305	CHL	C4-C3-C5	2.82	120.12	115.23
25	4	314	CLA	C3B-C4B-NB	-2.82	108.01	110.53
24	2	311	CHL	O1D-CGD-CBD	-2.82	120.45	124.72
25	B	606	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
25	B	603	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
24	3	304	CHL	CBC-CAC-C3C	-2.82	108.84	112.87
31	v	401	8CT	C30-C29-C28	-2.82	120.20	124.58
26	4	302	0IE	C21-C7-C8	-2.82	118.25	122.82
24	S	605	CHL	O1D-CGD-CBD	-2.82	120.45	124.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	1	303	NEX	C26-C27-C28	2.82	131.94	125.99
24	q	316	CHL	O1D-CGD-CBD	-2.82	120.45	124.72
35	D	403	PHO	C1-C2-C3	-2.81	121.58	126.20
24	r	307	CHL	CMD-C2D-C3D	-2.81	119.06	124.68
28	9	319	NEX	C26-C27-C28	2.81	131.94	125.99
25	B	606	CLA	C3B-C4B-NB	-2.81	108.02	110.53
25	7	314	CLA	C3B-C4B-NB	-2.81	108.02	110.53
35	a	606	PHO	CMB-C2B-C3B	2.81	130.31	124.68
35	a	606	PHO	O2D-CGD-O1D	-2.81	118.37	123.85
24	1	308	CHL	O1D-CGD-CBD	-2.81	120.46	124.72
24	Y	317	CHL	CAA-C2A-C3A	-2.81	109.78	116.23
24	4	310	CHL	O1D-CGD-CBD	-2.81	120.46	124.72
26	1	302	OIE	C21-C7-C8	-2.81	118.26	122.82
24	u	306	CHL	OMC-CMC-C2C	-2.81	120.24	125.12
25	g	316	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
25	s	413	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
24	n	310	CHL	C1-C2-C3	-2.81	121.59	126.20
24	5	311	CHL	O1D-CGD-CBD	-2.81	120.46	124.72
24	N	310	CHL	O1D-CGD-CBD	-2.81	120.46	124.72
25	C	602	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
25	C	604	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
24	R	605	CHL	O1D-CGD-CBD	-2.81	120.46	124.72
24	8	304	CHL	O2A-CGA-CBA	2.81	120.40	111.83
25	S	612	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
31	s	416	8CT	C19-C18-C17	-2.81	117.78	123.52
25	C	602	CLA	C3B-C4B-NB	-2.81	108.02	110.53
25	c	610	CLA	C3B-C4B-NB	-2.81	108.02	110.53
28	4	303	NEX	C26-C27-C28	2.81	131.93	125.99
28	y	304	NEX	C26-C27-C28	2.81	131.93	125.99
25	7	308	CLA	O2D-CGD-O1D	-2.81	118.39	123.85
28	7	304	NEX	C26-C27-C28	2.81	131.93	125.99
26	p	302	OIE	C21-C7-C8	-2.81	118.27	122.82
24	S	606	CHL	O1D-CGD-CBD	-2.81	120.47	124.72
25	Y	306	CLA	C3B-C4B-NB	-2.80	108.03	110.53
25	Y	313	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
29	8	301	OUR	C48-C47-C46	-2.80	120.08	125.92
28	S	617	NEX	C26-C27-C28	2.80	131.92	125.99
25	3	314	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
31	T	101	8CT	C04-C03-C02	-2.80	118.81	122.64
29	1	301	OUR	C18-C17-C16	-2.80	120.30	126.32
26	8	302	OIE	C10-C9-C8	2.80	129.25	123.52
24	N	304	CHL	C1-C2-C3	-2.80	121.61	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	u	307	CLA	C3B-C4B-NB	-2.80	108.03	110.53
25	7	315	CLA	C3B-C4B-NB	-2.80	108.03	110.53
24	3	312	CHL	O1D-CGD-CBD	-2.80	120.47	124.72
24	6	305	CHL	OMC-CMC-C2C	-2.80	120.26	125.12
26	g	302	0IE	C21-C7-C8	-2.80	118.28	122.82
25	g	307	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
25	C	610	CLA	C3B-C4B-NB	-2.80	108.03	110.53
24	8	309	CHL	CBC-CAC-C3C	-2.80	108.86	112.87
33	D	411	LMG	O8-C28-C29	2.80	120.37	111.83
25	q	312	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
35	d	403	PHO	C1-C2-C3	-2.80	121.61	126.20
35	A	606	PHO	CMB-C2B-C3B	2.80	130.28	124.68
25	R	610	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
25	S	603	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
25	r	311	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
25	3	306	CLA	C3B-C4B-NB	-2.80	108.03	110.53
25	9	306	CLA	C3B-C4B-NB	-2.80	108.03	110.53
25	g	316	CLA	C3B-C4B-NB	-2.80	108.03	110.53
25	l	315	CLA	C3B-C4B-NB	-2.80	108.03	110.53
25	p	308	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
25	q	313	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
24	y	306	CHL	O2A-CGA-CBA	2.80	120.36	111.83
24	u	310	CHL	O1D-CGD-CBD	-2.80	120.48	124.72
24	4	311	CHL	CBC-CAC-C3C	-2.80	108.87	112.87
25	2	316	CLA	C3B-C4B-NB	-2.80	108.03	110.53
25	y	316	CLA	C3B-C4B-NB	-2.79	108.04	110.53
25	p	315	CLA	C3B-C4B-NB	-2.79	108.04	110.53
25	S	611	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
24	r	307	CHL	O2A-CGA-CBA	2.79	120.35	111.83
25	N	315	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
25	c	602	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
25	r	305	CLA	CAA-C2A-C3A	-2.79	109.83	116.23
24	S	602	CHL	C4-C3-C5	2.79	120.07	115.23
25	s	404	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
24	9	309	CHL	O1D-CGD-CBD	-2.79	120.50	124.72
27	r	316	XAT	C31-C30-C29	-2.79	123.37	127.28
25	b	601	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
24	q	311	CHL	CMA-C3A-C4A	-2.79	108.61	114.61
24	y	318	CHL	CAA-C2A-C3A	-2.79	109.84	116.23
24	4	309	CHL	O1D-CGD-CBD	-2.79	120.50	124.72
25	y	314	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
31	S	615	8CT	C19-C20-C21	-2.79	123.37	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	p	306	CHL	O1D-CGD-CBD	-2.79	120.50	124.72
26	Y	302	0IE	C4-C3-C2	-2.79	117.73	120.16
26	5	302	0IE	C21-C7-C8	-2.78	118.31	122.82
24	r	303	CHL	O1D-CGD-CBD	-2.78	120.50	124.72
25	u	317	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
24	7	305	CHL	O2A-CGA-CBA	2.78	120.32	111.83
25	a	607	CLA	C3B-C4B-NB	-2.78	108.05	110.53
24	G	318	CHL	CMB-C2B-C3B	2.78	130.24	124.68
24	G	309	CHL	O1D-CGD-CBD	-2.78	120.50	124.72
24	Y	312	CHL	O2A-CGA-CBA	2.78	120.31	111.83
25	3	315	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
25	9	313	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
26	q	302	0IE	C10-C9-C8	2.78	129.21	123.52
25	4	306	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
25	g	314	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
30	d	408	LHG	O8-C23-C24	2.78	120.31	111.83
24	S	608	CHL	O1D-CGD-CBD	-2.78	120.51	124.72
25	2	307	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
25	C	604	CLA	C3B-C4B-NB	-2.78	108.05	110.53
29	6	301	0UR	C28-C19-C18	-2.78	109.63	112.83
24	Y	310	CHL	C4-C3-C5	2.78	120.05	115.23
25	p	315	CLA	CHB-C4A-NA	2.78	128.41	124.40
25	A	603	CLA	C3B-C4B-NB	-2.78	108.05	110.53
24	s	403	CHL	C4-C3-C5	2.78	120.05	115.23
24	G	306	CHL	O2A-CGA-CBA	2.78	120.30	111.83
29	2	301	0UR	C5-C4-C3	-2.78	123.60	126.92
25	c	604	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
26	y	303	0IE	C21-C7-C8	-2.77	118.32	122.82
24	s	407	CHL	O1D-CGD-CBD	-2.77	120.52	124.72
24	q	304	CHL	OMC-CMC-C2C	-2.77	120.30	125.12
25	q	306	CLA	C1-C2-C3	-2.77	122.27	126.76
24	g	318	CHL	CMB-C2B-C3B	2.77	130.23	124.68
25	G	315	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
24	g	309	CHL	O1D-CGD-CBD	-2.77	120.52	124.72
24	G	305	CHL	O2A-CGA-CBA	2.77	120.29	111.83
26	7	302	0IE	C21-C7-C8	-2.77	118.32	122.82
24	1	310	CHL	O1D-CGD-CBD	-2.77	120.52	124.72
24	7	313	CHL	O1D-CGD-CBD	-2.77	120.52	124.72
25	a	603	CLA	C3B-C4B-NB	-2.77	108.06	110.53
25	p	314	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
24	g	305	CHL	O2A-CGA-CBA	2.77	120.28	111.83
25	G	314	CLA	C3B-C4B-NB	-2.77	108.06	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	5	303	0IE	C22-C12-C11	-2.77	118.33	122.82
24	Y	305	CHL	O2A-CGA-CBA	2.77	120.28	111.83
24	Y	312	CHL	CMB-C2B-C3B	2.77	130.22	124.68
24	p	318	CHL	O1D-CGD-CBD	-2.77	120.53	124.72
25	n	314	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
29	u	301	0UR	C43-C3-C4	-2.77	121.77	125.03
25	R	609	CLA	C3B-C4B-NB	-2.77	108.06	110.53
25	n	315	CLA	C3B-C4B-NB	-2.77	108.06	110.53
29	1	301	0UR	C14-C13-C12	-2.77	118.78	126.36
24	7	318	CHL	O1D-CGD-CBD	-2.77	120.53	124.72
26	3	302	0IE	C20-C3-C2	2.77	121.36	115.01
24	6	312	CHL	O1D-CGD-CBD	-2.76	120.53	124.72
24	9	304	CHL	C1-C2-C3	-2.76	121.67	126.20
25	N	315	CLA	C3B-C4B-NB	-2.76	108.06	110.53
24	y	311	CHL	C4-C3-C5	2.76	120.02	115.23
24	8	315	CHL	O1D-CGD-CBD	-2.76	120.53	124.72
24	7	309	CHL	O1D-CGD-CBD	-2.76	120.53	124.72
25	1	316	CLA	C3B-C4B-NB	-2.76	108.06	110.53
24	8	304	CHL	OMC-CMC-C2C	-2.76	120.33	125.12
26	4	302	0IE	C6-C7-C8	2.76	123.35	119.01
26	y	303	0IE	C6-C7-C8	2.76	123.35	119.01
24	R	606	CHL	O1D-CGD-CBD	-2.76	120.54	124.72
25	N	314	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
29	6	301	0UR	C43-C3-C4	-2.76	121.77	125.03
25	9	316	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
25	n	315	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
25	a	604	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
26	Y	303	0IE	C21-C7-C8	-2.76	118.34	122.82
25	y	314	CLA	C3B-C4B-NB	-2.76	108.07	110.53
25	7	317	CLA	C3B-C4B-NB	-2.76	108.07	110.53
25	A	604	CLA	C1-C2-C3	-2.76	121.67	126.20
27	R	615	XAT	C15-C14-C13	-2.76	123.41	127.28
25	y	315	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
25	G	316	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
24	6	309	CHL	O2A-CGA-CBA	2.76	120.25	111.83
26	5	303	0IE	C13-C12-C11	2.76	123.35	119.01
24	8	310	CHL	C4-C3-C5	2.76	120.02	115.23
24	5	306	CHL	CMD-C2D-C3D	-2.76	119.17	124.68
25	5	307	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
25	7	314	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
25	G	314	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
25	u	314	CLA	O2D-CGD-O1D	-2.76	118.48	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	n	305	CHL	C4-C3-C5	2.76	120.01	115.23
24	q	311	CHL	C4-C3-C5	2.76	120.01	115.23
24	s	409	CHL	O1D-CGD-CBD	-2.76	120.54	124.72
25	9	315	CLA	C3B-C4B-NB	-2.76	108.07	110.53
25	5	307	CLA	C3B-C4B-NB	-2.76	108.07	110.53
31	b	617	8CT	C24-C23-C21	-2.76	118.80	126.36
25	Y	314	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
25	b	608	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
24	8	310	CHL	CMA-C3A-C4A	-2.76	108.67	114.61
29	4	301	0UR	C43-C3-C4	-2.76	121.78	125.03
24	3	309	CHL	O2A-CGA-CBA	2.76	120.24	111.83
24	g	306	CHL	O2A-CGA-CBA	2.76	120.24	111.83
24	3	309	CHL	O1D-CGD-CBD	-2.76	120.55	124.72
24	p	313	CHL	O1D-CGD-CBD	-2.76	120.55	124.72
25	3	316	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
25	5	315	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
25	3	307	CLA	C3B-C4B-NB	-2.75	108.07	110.53
25	B	608	CLA	C3B-C4B-NB	-2.75	108.07	110.53
24	g	312	CHL	O2A-CGA-CBA	2.75	120.23	111.83
26	2	302	0IE	C21-C7-C8	-2.75	118.36	122.82
24	7	306	CHL	CMD-C2D-C3D	-2.75	119.18	124.68
24	2	310	CHL	O1D-CGD-CBD	-2.75	120.55	124.72
26	2	303	0IE	C22-C12-C11	-2.75	118.36	122.82
24	Y	309	CHL	CBC-CAC-C3C	-2.75	108.93	112.87
25	6	307	CLA	C3B-C4B-NB	-2.75	108.07	110.53
24	G	312	CHL	O2A-CGA-CBA	2.75	120.23	111.83
33	d	401	LMG	O8-C28-C29	2.75	120.23	111.83
24	N	305	CHL	C4-C3-C5	2.75	120.00	115.23
25	7	315	CLA	CHB-C4A-NA	2.75	128.37	124.40
25	A	607	CLA	C3B-C4B-NB	-2.75	108.07	110.53
25	8	311	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
30	n	318	LHG	O8-C23-C24	2.75	120.22	111.83
24	y	310	CHL	CBC-CAC-C3C	-2.75	108.94	112.87
25	s	412	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
25	u	316	CLA	C3B-C4B-NB	-2.75	108.08	110.53
25	a	604	CLA	C1-C2-C3	-2.75	121.69	126.20
30	D	407	LHG	O8-C23-C24	2.75	120.21	111.83
24	Y	305	CHL	OMC-CMC-C2C	-2.75	120.35	125.12
30	N	318	LHG	O8-C23-C24	2.75	120.21	111.83
27	R	615	XAT	C31-C30-C29	-2.75	123.43	127.28
25	9	306	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
33	m	101	LMG	O8-C28-C29	2.74	120.20	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	r	306	CHL	O1D-CGD-CBD	-2.74	120.56	124.72
26	9	302	0IE	C21-C7-C8	-2.74	118.37	122.82
24	r	307	CHL	O1D-CGD-CBD	-2.74	120.56	124.72
24	u	311	CHL	O1D-CGD-CBD	-2.74	120.56	124.72
25	5	316	CLA	C3B-C4B-NB	-2.74	108.08	110.53
24	R	602	CHL	O1D-CGD-CBD	-2.74	120.56	124.72
25	q	305	CLA	C3B-C4B-NB	-2.74	108.08	110.53
31	V	401	8CT	C30-C29-C28	-2.74	120.31	124.58
25	8	306	CLA	C1-C2-C3	-2.74	122.33	126.76
24	9	304	CHL	O2A-CGA-CBA	2.74	120.19	111.83
25	S	603	CLA	C3B-C4B-NB	-2.74	108.08	110.53
25	g	314	CLA	C3B-C4B-NB	-2.74	108.08	110.53
25	1	306	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
25	A	604	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
24	5	310	CHL	O1D-CGD-CBD	-2.74	120.57	124.72
25	6	316	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
31	x	601	8CT	C04-C03-C02	-2.74	118.89	122.64
26	1	302	0IE	C6-C7-C8	2.74	123.32	119.01
24	y	313	CHL	CMB-C2B-C3B	2.74	130.15	124.68
33	B	619	LMG	O8-C28-C29	2.74	120.18	111.83
24	Y	312	CHL	CMA-C3A-C4A	-2.74	108.71	114.61
29	7	301	0UR	C43-C3-C4	-2.74	121.80	125.03
26	5	303	0IE	C21-C7-C8	-2.74	118.38	122.82
26	G	302	0IE	C6-C7-C8	2.74	123.31	119.01
26	8	302	0IE	C23-C16-C17	2.73	122.27	118.09
31	v	401	8CT	C25-C24-C23	-2.73	115.28	123.20
25	2	307	CLA	C3B-C4B-NB	-2.73	108.09	110.53
24	4	312	CHL	CBC-CAC-C3C	-2.73	108.96	112.87
29	4	301	0UR	C5-C4-C3	-2.73	123.65	126.92
25	p	317	CLA	C3B-C4B-NB	-2.73	108.09	110.53
24	n	304	CHL	C4-C3-C5	2.73	119.97	115.23
26	u	302	0IE	C20-C3-C4	-2.73	120.94	124.72
26	3	303	0IE	C22-C12-C11	-2.73	118.39	122.82
25	N	306	CLA	C3B-C4B-NB	-2.73	108.09	110.53
26	q	302	0IE	C23-C16-C17	2.73	122.26	118.09
25	5	316	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
25	6	306	CLA	C3B-C4B-NB	-2.73	108.09	110.53
25	n	306	CLA	C3B-C4B-NB	-2.73	108.09	110.53
26	7	303	0IE	C22-C12-C11	-2.73	118.40	122.82
24	1	312	CHL	CBC-CAC-C3C	-2.73	108.97	112.87
25	b	608	CLA	C3B-C4B-NB	-2.73	108.09	110.53
25	7	316	CLA	C3B-C4B-NB	-2.73	108.09	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	4	311	CHL	O1D-CGD-CBD	-2.73	120.59	124.72
26	2	303	OIE	C21-C7-C8	-2.73	118.40	122.82
25	2	315	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
26	p	302	OIE	C6-C7-C8	2.73	123.30	119.01
25	c	602	CLA	C3B-C4B-NB	-2.73	108.10	110.53
24	Y	305	CHL	CMD-C2D-C3D	-2.73	119.23	124.68
24	r	309	CHL	CMA-C3A-C4A	-2.73	108.74	114.61
26	g	302	OIE	C6-C7-C8	2.73	123.30	119.01
25	6	306	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
24	9	305	CHL	O1D-CGD-CBD	-2.73	120.59	124.72
26	9	302	OIE	C20-C3-C2	2.73	121.27	115.01
24	R	608	CHL	CMA-C3A-C4A	-2.72	108.74	114.61
24	p	311	CHL	O1D-CGD-CBD	-2.72	120.59	124.72
24	Y	310	CHL	O1D-CGD-CBD	-2.72	120.59	124.72
25	R	604	CLA	C3B-C4B-NB	-2.72	108.10	110.53
30	A	612	LHG	O8-C23-C24	2.72	120.14	111.83
24	y	305	CHL	O1D-CGD-CBD	-2.72	120.59	124.72
25	g	315	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
25	3	306	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
26	Y	303	OIE	C6-C7-C8	2.72	123.29	119.01
25	u	307	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
25	Y	313	CLA	CMB-C2B-C1B	-2.72	121.28	125.42
29	Y	301	OUR	C15-C14-C13	-2.72	115.32	123.20
31	V	401	8CT	C25-C24-C23	-2.72	115.32	123.20
25	B	610	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
25	8	305	CLA	C3B-C4B-NB	-2.72	108.10	110.53
26	N	302	OIE	C20-C3-C4	-2.72	120.96	124.72
25	Y	306	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
24	s	403	CHL	O1D-CGD-CBD	-2.72	120.60	124.72
24	7	306	CHL	O2A-CGA-CBA	2.72	120.11	111.83
24	9	310	CHL	O1D-CGD-CBD	-2.72	120.61	124.72
26	5	302	OIE	C6-C7-C8	2.72	123.28	119.01
30	p	319	LHG	O8-C23-C24	2.71	120.11	111.83
24	S	606	CHL	CBC-CAC-C3C	-2.71	108.99	112.87
24	p	309	CHL	O1D-CGD-CBD	-2.71	120.61	124.72
25	Y	315	CLA	C3B-C4B-NB	-2.71	108.11	110.53
25	4	316	CLA	C3B-C4B-NB	-2.71	108.11	110.53
24	Y	309	CHL	O1D-CGD-CBD	-2.71	120.61	124.72
33	d	411	LMG	C7-O1-C1	-2.71	107.98	113.80
30	9	318	LHG	O8-C23-C24	2.71	120.11	111.83
24	6	309	CHL	O1D-CGD-CBD	-2.71	120.61	124.72
25	8	314	CLA	C3B-C4B-NB	-2.71	108.11	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	S	614	8CT	C01-C02-C07	2.71	119.38	113.60
25	p	316	CLA	C3B-C4B-NB	-2.71	108.11	110.53
24	q	311	CHL	CMB-C2B-C3B	2.71	130.10	124.68
30	2	319	LHG	O8-C23-C24	2.71	120.10	111.83
25	1	313	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
26	N	302	0IE	C21-C7-C8	-2.71	118.43	122.82
31	c	614	8CT	C24-C25-C26	-2.71	123.48	127.28
30	5	319	LHG	O8-C23-C24	2.71	120.09	111.83
25	B	608	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
25	A	603	CLA	CMB-C2B-C1B	-2.71	121.30	125.42
26	2	303	0IE	C13-C12-C11	2.71	123.27	119.01
25	b	606	CLA	C1-C2-C3	-2.71	121.76	126.20
25	a	603	CLA	CMB-C2B-C1B	-2.71	121.30	125.42
24	7	318	CHL	CBC-CAC-C3C	-2.71	109.00	112.87
25	C	609	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
25	4	315	CLA	C3B-C4B-NB	-2.71	108.11	110.53
24	7	311	CHL	C1B-CHB-C4A	2.71	123.06	121.32
25	2	316	CLA	O2D-CGD-O1D	-2.70	118.58	123.85
25	u	308	CLA	C3B-C4B-NB	-2.70	108.12	110.53
25	b	610	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
25	N	313	CLA	C1-C2-C3	-2.70	121.77	126.20
24	G	305	CHL	C4-C3-C5	2.70	119.92	115.23
25	q	315	CLA	C3B-C4B-NB	-2.70	108.12	110.53
24	4	305	CHL	CBC-CAC-C3C	-2.70	109.00	112.87
24	S	602	CHL	O1D-CGD-CBD	-2.70	120.63	124.72
25	q	313	CLA	C1-C2-C3	-2.70	121.77	126.20
25	b	613	CLA	C1-C2-C3	-2.70	121.77	126.20
25	c	604	CLA	C3B-C4B-NB	-2.70	108.12	110.53
26	6	302	0IE	C21-C7-C8	-2.70	118.44	122.82
26	n	302	0IE	C21-C7-C8	-2.70	118.44	122.82
24	p	306	CHL	O2A-CGA-CBA	2.70	120.07	111.83
24	g	311	CHL	CBC-CAC-C3C	-2.70	109.01	112.87
30	g	319	LHG	O8-C23-C24	2.70	120.06	111.83
24	u	305	CHL	O2A-CGA-CBA	2.70	120.06	111.83
30	D	408	LHG	O8-C23-C24	2.70	120.06	111.83
26	3	303	0IE	C13-C12-C11	2.70	123.25	119.01
24	y	306	CHL	OMC-CMC-C2C	-2.70	120.44	125.12
24	y	305	CHL	C4-C3-C5	2.70	119.91	115.23
25	R	611	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
24	6	304	CHL	O1D-CGD-CBD	-2.70	120.63	124.72
24	y	313	CHL	O1D-CGD-CBD	-2.70	120.63	124.72
30	7	319	LHG	O8-C23-C24	2.69	120.05	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	G	303	0IE	C22-C12-C11	-2.69	118.45	122.82
24	G	311	CHL	C4-C3-C5	2.69	119.90	115.23
25	c	607	CLA	C3B-C4B-NB	-2.69	108.13	110.53
24	6	305	CHL	O2A-CGA-CBA	2.69	120.04	111.83
24	q	303	CHL	C1B-CHB-C4A	-2.69	119.59	121.32
31	D	410	8CT	C01-C02-C07	2.69	119.33	113.60
26	p	303	0IE	C13-C12-C11	2.69	123.24	119.01
24	n	308	CHL	CBC-CAC-C3C	-2.69	109.02	112.87
25	A	603	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
24	1	308	CHL	CBC-CAC-C3C	-2.69	109.02	112.87
29	9	301	0UR	C43-C3-C4	-2.69	121.86	125.03
26	7	302	0IE	C6-C7-C8	2.69	123.24	119.01
24	y	310	CHL	O1D-CGD-CBD	-2.69	120.65	124.72
25	R	609	CLA	O2D-CGD-O1D	-2.69	118.62	123.85
24	n	305	CHL	CMD-C2D-C3D	-2.69	119.31	124.68
24	8	310	CHL	CMB-C2B-C3B	2.69	130.05	124.68
24	g	305	CHL	C4-C3-C5	2.69	119.89	115.23
24	g	311	CHL	C4-C3-C5	2.69	119.89	115.23
24	n	308	CHL	C1B-CHB-C4A	-2.69	119.59	121.32
24	1	311	CHL	O1D-CGD-CBD	-2.69	120.65	124.72
24	S	601	CHL	O1D-CGD-CBD	-2.69	120.65	124.72
25	9	313	CLA	C1-C2-C3	-2.69	121.80	126.20
24	1	311	CHL	CBC-CAC-C3C	-2.69	109.03	112.87
24	G	318	CHL	O2D-CGD-O1D	-2.69	118.62	123.85
24	N	304	CHL	C4-C3-C5	2.69	119.89	115.23
30	a	612	LHG	O8-C23-C24	2.69	120.02	111.83
25	Y	315	CLA	CHB-C4A-NA	2.69	128.28	124.40
25	y	307	CLA	O2D-CGD-O1D	-2.68	118.62	123.85
33	d	411	LMG	C8-O7-C10	-2.68	111.37	117.80
24	8	310	CHL	O1D-CGD-CBD	-2.68	120.65	124.72
24	p	306	CHL	CMD-C2D-C3D	-2.68	119.32	124.68
24	N	317	CHL	O1D-CGD-CBD	-2.68	120.65	124.72
33	D	401	LMG	O8-C28-C29	2.68	120.02	111.83
29	y	301	0UR	C15-C14-C13	-2.68	115.43	123.20
24	y	306	CHL	CMD-C2D-C3D	-2.68	119.32	124.68
26	R	614	0IE	C21-C7-C8	-2.68	118.47	122.82
25	c	607	CLA	CHB-C4A-NA	2.68	128.27	124.40
25	s	404	CLA	C3B-C4B-NB	-2.68	108.14	110.53
24	s	407	CHL	CBC-CAC-C3C	-2.68	109.03	112.87
24	6	308	CHL	O1D-CGD-CBD	-2.68	120.66	124.72
31	d	410	8CT	C11-C10-C03	-2.68	119.84	127.00
24	1	305	CHL	CBC-CAC-C3C	-2.68	109.04	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	s	416	8CT	C19-C20-C21	-2.68	123.52	127.28
24	u	306	CHL	O2A-CGA-CBA	2.68	120.00	111.83
25	r	312	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
24	q	309	CHL	CBC-CAC-C3C	-2.68	109.04	112.87
25	r	310	CLA	C3B-C4B-NB	-2.68	108.14	110.53
24	8	310	CHL	O2A-CGA-CBA	2.68	120.00	111.83
25	4	313	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
25	g	307	CLA	C3B-C4B-NB	-2.68	108.14	110.53
26	1	302	0IE	C4-C3-C2	-2.68	117.83	120.16
30	d	407	LHG	O8-C23-C24	2.68	120.00	111.83
25	B	612	CLA	C1-C2-C3	-2.68	121.81	126.20
25	1	307	CLA	C3B-C4B-NB	-2.68	108.14	110.53
39	D	406	PL9	C22-C23-C24	-2.68	121.50	127.62
26	G	303	0IE	C9-C10-C11	2.68	128.99	123.52
26	r	315	0IE	C21-C7-C8	-2.68	118.48	122.82
25	9	307	CLA	C3B-C4B-NB	-2.68	108.14	110.53
26	g	302	0IE	C22-C12-C11	-2.67	118.48	122.82
26	6	302	0IE	C23-C16-C17	2.67	122.17	118.09
26	6	302	0IE	C6-C7-C8	2.67	123.21	119.01
26	g	303	0IE	C22-C12-C11	-2.67	118.48	122.82
31	V	401	8CT	C24-C25-C26	-2.67	123.53	127.28
25	Y	307	CLA	C3B-C4B-NB	-2.67	108.15	110.53
25	B	606	CLA	C1-C2-C3	-2.67	121.82	126.20
25	6	314	CLA	C3B-C4B-NB	-2.67	108.15	110.53
24	u	306	CHL	C4-C3-C5	2.67	119.86	115.23
24	q	311	CHL	O1D-CGD-CBD	-2.67	120.68	124.72
24	p	318	CHL	CBC-CAC-C3C	-2.67	109.05	112.87
26	G	302	0IE	C22-C12-C11	-2.67	118.49	122.82
24	3	308	CHL	O1D-CGD-CBD	-2.67	120.68	124.72
31	A	608	8CT	C27-C26-C28	2.67	122.16	118.09
25	C	607	CLA	CHB-C4A-NA	2.67	128.25	124.40
37	C	619	DGD	C1E-O6E-C5E	-2.67	108.51	113.72
31	x	601	8CT	C05-C04-C03	2.67	114.31	110.44
31	a	608	8CT	C27-C26-C28	2.67	122.16	118.09
24	N	312	CHL	O2A-CGA-CBA	2.67	119.96	111.83
31	C	613	8CT	C01-C02-C07	2.67	119.28	113.60
24	Y	304	CHL	C4-C3-C5	2.67	119.85	115.23
24	3	304	CHL	O1D-CGD-CBD	-2.66	120.68	124.72
24	3	317	CHL	CMA-C3A-C2A	-2.66	110.12	116.23
24	6	304	CHL	O2A-CGA-CBA	2.66	119.95	111.83
24	g	310	CHL	O1D-CGD-CBD	-2.66	120.69	124.72
24	u	306	CHL	O1D-CGD-CBD	-2.66	120.69	124.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	6	306	CLA	CAA-C2A-C3A	-2.66	110.12	116.23
26	9	302	0IE	C6-C7-C8	2.66	123.20	119.01
39	d	406	PL9	C22-C23-C24	-2.66	121.53	127.62
24	n	312	CHL	O2A-CGA-CBA	2.66	119.95	111.83
24	Y	308	CHL	O1D-CGD-CBD	-2.66	120.69	124.72
31	S	614	8CT	C10-C11-C12	2.66	130.17	126.23
25	S	609	CLA	C3B-C4B-NB	-2.66	108.15	110.53
25	5	317	CLA	C3B-C4B-NB	-2.66	108.15	110.53
25	s	410	CLA	C3B-C4B-NB	-2.66	108.15	110.53
26	2	302	0IE	C6-C7-C8	2.66	123.19	119.01
31	D	410	8CT	C11-C10-C03	-2.66	119.89	127.00
24	g	318	CHL	O2D-CGD-O1D	-2.66	118.67	123.85
29	u	301	0UR	C28-C19-C18	-2.66	109.77	112.83
26	3	302	0IE	C21-C7-C8	-2.66	118.51	122.82
26	8	302	0IE	C21-C7-C8	-2.66	118.51	122.82
25	c	609	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
25	6	313	CLA	CAA-C2A-C3A	-2.66	110.13	116.23
25	u	314	CLA	C1-C2-C3	-2.66	121.84	126.20
25	3	313	CLA	CAA-C2A-C3A	-2.66	110.13	116.23
28	N	303	NEX	C31-C30-C29	-2.66	123.55	127.28
25	r	310	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
25	4	307	CLA	C3B-C4B-NB	-2.66	108.16	110.53
24	G	306	CHL	O1D-CGD-CBD	-2.66	120.69	124.72
24	8	303	CHL	O1D-CGD-CBD	-2.66	120.69	124.72
24	y	313	CHL	OMC-CMC-C2C	-2.66	120.51	125.12
24	7	306	CHL	CBC-CAC-C3C	-2.66	109.07	112.87
25	y	316	CLA	CHB-C4A-NA	2.66	128.23	124.40
24	N	305	CHL	CMD-C2D-C3D	-2.66	119.38	124.68
24	n	317	CHL	O1D-CGD-CBD	-2.65	120.70	124.72
24	y	309	CHL	O1D-CGD-CBD	-2.65	120.70	124.72
24	p	306	CHL	CBC-CAC-C3C	-2.65	109.07	112.87
24	3	304	CHL	O2A-CGA-CBA	2.65	119.93	111.83
28	6	303	NEX	C31-C30-C29	-2.65	123.56	127.28
24	Y	317	CHL	OMC-CMC-C2C	-2.65	120.51	125.12
24	q	311	CHL	O2A-CGA-CBA	2.65	119.92	111.83
24	9	317	CHL	O1D-CGD-CBD	-2.65	120.70	124.72
24	8	310	CHL	CBC-CAC-C3C	-2.65	109.08	112.87
25	2	308	CLA	C3B-C4B-NB	-2.65	108.16	110.53
24	s	402	CHL	O1D-CGD-CBD	-2.65	120.70	124.72
24	3	305	CHL	O2A-CGA-CBA	2.65	119.92	111.83
24	u	318	CHL	O1D-CGD-CBD	-2.65	120.70	124.72
25	D	404	CLA	C3B-C4B-NB	-2.65	108.17	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	9	303	0IE	C4-C5-C6	2.65	130.87	123.20
25	8	312	CLA	C1-C2-C3	-2.65	121.86	126.20
25	n	307	CLA	C3B-C4B-NB	-2.65	108.17	110.53
28	r	301	NEX	C31-C30-C29	-2.65	123.56	127.28
25	p	308	CLA	C1-C2-C3	-2.65	122.48	126.76
25	u	317	CLA	C1-C2-C3	-2.65	121.86	126.20
30	G	319	LHG	O8-C23-C24	2.65	119.90	111.83
24	y	313	CHL	CMA-C3A-C4A	-2.64	108.91	114.61
24	G	306	CHL	OMC-CMC-C2C	-2.64	120.53	125.12
26	4	302	0IE	C4-C3-C2	-2.64	117.86	120.16
25	C	607	CLA	C3B-C4B-NB	-2.64	108.17	110.53
24	7	309	CHL	CBC-CAC-C3C	-2.64	109.09	112.87
31	s	415	8CT	C10-C11-C12	2.64	130.14	126.23
26	u	302	0IE	C20-C3-C2	2.64	121.07	115.01
31	s	415	8CT	C01-C02-C07	2.64	119.22	113.60
24	S	607	CHL	O1D-CGD-CBD	-2.64	120.72	124.72
26	2	303	0IE	C6-C7-C8	2.64	123.16	119.01
37	C	620	DGD	C2G-O2G-C1B	-2.64	111.48	117.80
25	Y	313	CLA	C3B-C4B-NB	-2.64	108.17	110.53
24	u	305	CHL	O1D-CGD-CBD	-2.64	120.72	124.72
26	3	302	0IE	C23-C16-C17	2.64	122.12	118.09
24	8	303	CHL	C4-C3-C5	2.64	119.80	115.23
29	G	301	0UR	C4-C3-C2	-2.64	117.86	120.16
25	B	613	CLA	C1-C2-C3	-2.64	121.88	126.20
24	9	305	CHL	C4-C3-C5	2.64	119.80	115.23
31	C	614	8CT	C11-C10-C03	-2.64	119.96	127.00
25	G	307	CLA	C3B-C4B-NB	-2.63	108.18	110.53
29	p	301	0UR	C43-C3-C4	-2.63	121.92	125.03
24	N	310	CHL	CBC-CAC-C3C	-2.63	109.10	112.87
28	s	401	NEX	C31-C30-C29	-2.63	123.58	127.28
25	s	417	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
24	Y	317	CHL	O1D-CGD-CBD	-2.63	120.73	124.72
25	R	612	CLA	C3B-C4B-NB	-2.63	108.18	110.53
24	q	304	CHL	C4-C3-C5	2.63	119.80	115.23
25	b	605	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
25	p	307	CLA	C3B-C4B-NB	-2.63	108.18	110.53
25	b	612	CLA	C1-C2-C3	-2.63	121.88	126.20
24	9	305	CHL	O2A-CGA-CBA	2.63	119.86	111.83
24	S	613	CHL	O2D-CGD-O1D	-2.63	118.72	123.85
25	5	308	CLA	C3B-C4B-NB	-2.63	108.18	110.53
28	3	318	NEX	C31-C30-C29	-2.63	123.59	127.28
25	a	603	CLA	O2D-CGD-O1D	-2.63	118.73	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	8	306	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
24	6	305	CHL	CBC-CAC-C3C	-2.63	109.11	112.87
26	3	302	0IE	C20-C3-C4	-2.63	121.08	124.72
26	y	302	0IE	C4-C3-C2	-2.63	117.87	120.16
24	6	317	CHL	CMA-C3A-C2A	-2.63	110.20	116.23
29	Y	301	0UR	C4-C5-C6	-2.63	115.59	123.20
26	y	302	0IE	C22-C12-C11	-2.63	118.56	122.82
26	y	302	0IE	C21-C7-C8	-2.63	118.56	122.82
25	u	308	CLA	C1-C2-C3	-2.63	122.51	126.76
25	1	313	CLA	CHB-C4A-NA	2.63	128.19	124.40
25	C	609	CLA	CHB-C4A-NA	2.63	128.19	124.40
24	y	318	CHL	O1D-CGD-CBD	-2.63	120.74	124.72
26	Y	302	0IE	C21-C7-C8	-2.63	118.56	122.82
24	5	305	CHL	O1D-CGD-CBD	-2.63	120.74	124.72
25	c	609	CLA	CHB-C4A-NA	2.62	128.19	124.40
24	Y	319	CHL	CBC-CAC-C3C	-2.62	109.11	112.87
26	3	302	0IE	C6-C7-C8	2.62	123.14	119.01
24	2	306	CHL	CMB-C2B-C3B	2.62	129.93	124.68
31	C	614	8CT	C06-C07-C02	-2.62	109.38	114.06
24	s	414	CHL	O2D-CGD-O1D	-2.62	118.74	123.85
29	y	301	0UR	C4-C5-C6	-2.62	115.60	123.20
26	q	302	0IE	C21-C7-C8	-2.62	118.57	122.82
28	n	303	NEX	C31-C30-C29	-2.62	123.60	127.28
24	2	306	CHL	O1D-CGD-CBD	-2.62	120.75	124.72
24	g	306	CHL	O1D-CGD-CBD	-2.62	120.75	124.72
24	Y	312	CHL	OMC-CMC-C2C	-2.62	120.57	125.12
31	c	614	8CT	C11-C10-C03	-2.62	120.00	127.00
31	C	614	8CT	C24-C25-C26	-2.62	123.60	127.28
29	9	301	0UR	C28-C19-C18	-2.62	109.81	112.83
24	9	312	CHL	O1D-CGD-CBD	-2.62	120.75	124.72
24	q	311	CHL	CBC-CAC-C3C	-2.62	109.12	112.87
25	b	614	CLA	C3B-C4B-NB	-2.62	108.19	110.53
24	Y	305	CHL	O1D-CGD-CBD	-2.62	120.75	124.72
25	q	314	CLA	C3B-C4B-NB	-2.62	108.19	110.53
24	4	308	CHL	CBC-CAC-C3C	-2.62	109.12	112.87
26	g	303	0IE	C9-C10-C11	2.62	128.88	123.52
25	3	306	CLA	CAA-C2A-C3A	-2.62	110.23	116.23
24	y	318	CHL	OMC-CMC-C2C	-2.62	120.58	125.12
24	n	304	CHL	O2A-CGA-CBA	2.62	119.81	111.83
24	N	317	CHL	C4D-CHA-CBD	-2.62	106.33	108.97
24	q	303	CHL	O1D-CGD-CBD	-2.62	120.76	124.72
24	Y	312	CHL	O1D-CGD-CBD	-2.62	120.76	124.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	S	616	CLA	O2D-CGD-O1D	-2.61	118.76	123.85
24	9	304	CHL	C4-C3-C5	2.61	119.77	115.23
25	d	404	CLA	C3B-C4B-NB	-2.61	108.20	110.53
24	Y	304	CHL	O2A-CGA-CBA	2.61	119.81	111.83
25	a	607	CLA	CHB-C4A-NA	2.61	128.17	124.40
25	6	314	CLA	CAA-C2A-C3A	-2.61	110.24	116.23
26	Y	302	0IE	C22-C12-C11	-2.61	118.58	122.82
26	5	303	0IE	C6-C7-C8	2.61	123.12	119.01
24	s	414	CHL	OMC-CMC-C2C	-2.61	120.58	125.12
25	r	313	CLA	CHB-C4A-NA	2.61	128.17	124.40
37	c	619	DGD	C2G-O2G-C1B	-2.61	111.55	117.80
25	r	305	CLA	C3B-C4B-NB	-2.61	108.20	110.53
25	b	616	CLA	CHB-C4A-NA	2.61	128.17	124.40
24	8	304	CHL	O1D-CGD-CBD	-2.61	120.77	124.72
25	c	603	CLA	CMB-C2B-C1B	-2.61	121.45	125.42
31	v	401	8CT	C24-C25-C26	-2.61	123.62	127.28
25	y	308	CLA	C3B-C4B-NB	-2.61	108.20	110.53
26	6	302	0IE	C20-C3-C4	-2.61	121.11	124.72
24	r	303	CHL	CBC-CAC-C3C	-2.61	109.14	112.87
24	5	306	CHL	CMB-C2B-C3B	2.61	129.89	124.68
26	5	303	0IE	C20-C3-C4	-2.61	121.11	124.72
32	A	609	SQD	C44-O6-C1	2.61	119.39	113.80
25	7	307	CLA	C3B-C4B-NB	-2.61	108.20	110.53
24	q	303	CHL	C4-C3-C5	2.61	119.75	115.23
25	B	616	CLA	CHB-C4A-NA	2.61	128.16	124.40
26	2	302	0IE	C22-C12-C11	-2.61	118.59	122.82
25	q	306	CLA	O2D-CGD-O1D	-2.61	118.78	123.85
24	u	313	CHL	O1D-CGD-CBD	-2.61	120.77	124.72
31	T	101	8CT	C05-C04-C03	2.60	114.22	110.44
24	N	312	CHL	CBC-CAC-C3C	-2.60	109.15	112.87
25	r	305	CLA	O2D-CGD-O1D	-2.60	118.78	123.85
25	n	307	CLA	C1-C2-C3	-2.60	122.55	126.76
24	y	305	CHL	O2A-CGA-CBA	2.60	119.77	111.83
25	C	603	CLA	CMB-C2B-C1B	-2.60	121.46	125.42
24	p	306	CHL	CMB-C2B-C3B	2.60	129.88	124.68
31	C	613	8CT	C18-C19-C20	-2.60	118.20	123.52
24	5	311	CHL	CBC-CAC-C3C	-2.60	109.15	112.87
25	B	614	CLA	C3B-C4B-NB	-2.60	108.21	110.53
25	R	603	CLA	CHB-C4A-NA	2.60	128.15	124.40
25	r	304	CLA	CHB-C4A-NA	2.60	128.15	124.40
24	N	304	CHL	O2A-CGA-CBA	2.60	119.75	111.83
29	G	301	0UR	C4-C5-C6	-2.60	115.68	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	V	401	8CT	C30-C31-C32	-2.60	118.27	121.47
24	r	308	CHL	O1D-CGD-CBD	-2.60	120.79	124.72
24	S	613	CHL	OMC-CMC-C2C	-2.60	120.61	125.12
33	C	618	LMG	C1-O6-C5	-2.59	108.65	113.72
25	B	605	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
24	u	305	CHL	C4-C3-C5	2.59	119.73	115.23
24	5	306	CHL	O1D-CGD-CBD	-2.59	120.79	124.72
24	u	305	CHL	C1-C2-C3	-2.59	121.95	126.20
25	s	411	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
25	C	611	CLA	C3B-C4B-NB	-2.59	108.22	110.53
33	d	411	LMG	O8-C28-C29	2.59	119.74	111.83
24	p	305	CHL	C4-C3-C5	2.59	119.73	115.23
24	N	310	CHL	C4-C3-C5	2.59	119.72	115.23
31	c	614	8CT	C06-C07-C02	-2.59	109.44	114.06
24	R	606	CHL	O2D-CGD-O1D	-2.59	118.81	123.85
25	n	313	CLA	C1-C2-C3	-2.59	121.95	126.20
24	n	308	CHL	O1D-CGD-CBD	-2.59	120.80	124.72
25	A	607	CLA	CHB-C4A-NA	2.59	128.13	124.40
24	R	602	CHL	CBC-CAC-C3C	-2.59	109.17	112.87
24	3	305	CHL	CBC-CAC-C3C	-2.59	109.17	112.87
26	R	614	0IE	C6-C7-C8	2.59	123.08	119.01
24	8	304	CHL	C4-C3-C5	2.59	119.72	115.23
24	2	309	CHL	C1B-CHB-C4A	-2.59	119.66	121.32
24	8	308	CHL	CMB-C2B-C3B	2.59	129.85	124.68
24	2	311	CHL	CBC-CAC-C3C	-2.58	109.17	112.87
25	7	316	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
31	X	601	8CT	C01-C02-C07	2.58	119.10	113.60
24	n	305	CHL	O2A-CGA-CBA	2.58	119.71	111.83
24	y	306	CHL	O1D-CGD-CBD	-2.58	120.81	124.72
24	G	310	CHL	O1D-CGD-CBD	-2.58	120.81	124.72
24	g	305	CHL	O1D-CGD-CBD	-2.58	120.81	124.72
25	2	317	CLA	C3B-C4B-NB	-2.58	108.23	110.53
24	q	308	CHL	CMB-C2B-C3B	2.58	129.84	124.68
24	G	305	CHL	O1D-CGD-CBD	-2.58	120.81	124.72
24	q	304	CHL	O1D-CGD-CBD	-2.58	120.81	124.72
26	5	302	0IE	C22-C12-C11	-2.58	118.64	122.82
24	g	306	CHL	OMC-CMC-C2C	-2.58	120.64	125.12
25	4	307	CLA	CAA-C2A-C3A	-2.58	110.31	116.23
25	2	308	CLA	CHB-C4A-NA	2.58	128.12	124.40
24	4	304	CHL	CBC-CAC-C3C	-2.58	109.18	112.87
26	3	302	0IE	C22-C12-C11	-2.58	118.64	122.82
25	c	606	CLA	C3B-C4B-NB	-2.58	108.23	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	n	310	CHL	C4-C3-C5	2.58	119.70	115.23
24	6	317	CHL	CBC-CAC-C3C	-2.58	109.18	112.87
24	n	304	CHL	CMB-C2B-C3B	2.58	129.83	124.68
25	8	311	CLA	C1-C2-C3	-2.58	121.98	126.20
25	B	607	CLA	CHB-C4A-NA	2.57	128.12	124.40
24	2	305	CHL	O1D-CGD-CBD	-2.57	120.82	124.72
32	B	618	SQD	O48-C23-C24	2.57	119.68	111.83
31	c	613	8CT	C18-C19-C20	-2.57	118.25	123.52
25	D	405	CLA	CHB-C4A-NA	2.57	128.11	124.40
26	n	302	0IE	C6-C7-C8	2.57	123.06	119.01
26	2	303	0IE	C20-C3-C4	-2.57	121.16	124.72
25	B	616	CLA	C3B-C4B-NB	-2.57	108.23	110.53
24	7	305	CHL	C4-C3-C5	2.57	119.69	115.23
24	p	310	CHL	CMB-C2B-C3B	2.57	129.82	124.68
25	R	604	CLA	CHB-C4A-NA	2.57	128.11	124.40
26	R	614	0IE	C22-C12-C11	-2.57	118.65	122.82
24	1	305	CHL	CMB-C2B-C3B	2.57	129.82	124.68
31	v	401	8CT	C30-C31-C32	-2.57	118.30	121.47
31	C	613	8CT	C14-C15-C16	-2.57	119.31	126.36
24	4	312	CHL	CMB-C2B-C3B	2.57	129.82	124.68
24	s	408	CHL	CMB-C2B-C3B	2.57	129.82	124.68
24	S	607	CHL	CMB-C2B-C3B	2.57	129.82	124.68
24	N	304	CHL	CMB-C2B-C3B	2.57	129.82	124.68
26	r	315	0IE	C20-C3-C2	2.57	120.91	115.01
24	7	306	CHL	CMB-C2B-C3B	2.57	129.82	124.68
25	9	314	CLA	CHB-C4A-NA	2.57	128.11	124.40
26	r	315	0IE	C22-C12-C11	-2.57	118.66	122.82
24	s	403	CHL	CMA-C3A-C4A	-2.57	109.08	114.61
25	1	314	CLA	CAA-C2A-C3A	-2.57	110.34	116.23
24	R	602	CHL	O2D-CGD-O1D	-2.57	118.85	123.85
29	g	301	0UR	C43-C3-C4	-2.57	122.00	125.03
39	d	406	PL9	C40-C39-C41	2.56	119.68	115.23
25	4	314	CLA	CAA-C2A-C3A	-2.56	110.35	116.23
25	2	308	CLA	C1-C2-C3	-2.56	122.61	126.76
32	d	409	SQD	O48-C23-C24	2.56	119.65	111.83
27	r	316	XAT	C35-C15-C14	-2.56	118.27	123.52
25	5	316	CLA	CHB-C4A-NA	2.56	128.10	124.40
25	6	315	CLA	CHB-C4A-NA	2.56	128.10	124.40
24	n	312	CHL	CBC-CAC-C3C	-2.56	109.20	112.87
24	p	318	CHL	CMB-C2B-C3B	2.56	129.81	124.68
28	3	318	NEX	C26-C27-C28	-2.56	120.57	125.99
25	a	607	CLA	C1-C2-C3	-2.56	122.00	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	b	618	SQD	O48-C23-C24	2.56	119.65	111.83
26	9	302	OIE	C22-C12-C11	-2.56	118.67	122.82
24	7	318	CHL	CMB-C2B-C3B	2.56	129.80	124.68
25	9	307	CLA	C1-C2-C3	-2.56	122.62	126.76
24	r	303	CHL	O2D-CGD-O1D	-2.56	118.86	123.85
24	8	307	CHL	CBC-CAC-C3C	-2.56	109.21	112.87
28	6	303	NEX	C26-C27-C28	-2.56	120.58	125.99
25	4	313	CLA	CHB-C4A-NA	2.56	128.09	124.40
24	N	305	CHL	O2A-CGA-CBA	2.56	119.64	111.83
25	G	308	CLA	C3B-C4B-NB	-2.56	108.25	110.53
25	8	313	CLA	C3B-C4B-NB	-2.56	108.25	110.53
24	4	305	CHL	CMB-C2B-C3B	2.56	129.79	124.68
24	u	313	CHL	CMB-C2B-C3B	2.56	129.79	124.68
25	b	613	CLA	O2D-CGD-O1D	-2.56	118.87	123.85
25	r	312	CLA	CHB-C4A-NA	2.56	128.09	124.40
32	a	609	SQD	O6-C1-C2	2.56	112.15	108.27
24	7	311	CHL	CMB-C2B-C3B	2.56	129.79	124.68
25	5	308	CLA	CHB-C4A-NA	2.55	128.09	124.40
24	u	318	CHL	CMB-C2B-C3B	2.55	129.79	124.68
26	4	302	OIE	C22-C12-C11	-2.55	118.68	122.82
24	9	317	CHL	CMB-C2B-C3B	2.55	129.79	124.68
25	l	307	CLA	CAA-C2A-C3A	-2.55	110.37	116.23
28	r	301	NEX	C26-C27-C28	-2.55	120.59	125.99
25	c	611	CLA	C3B-C4B-NB	-2.55	108.25	110.53
25	b	616	CLA	C3B-C4B-NB	-2.55	108.25	110.53
24	r	307	CHL	O2D-CGD-O1D	-2.55	118.88	123.85
24	n	317	CHL	C4D-CHA-CBD	-2.55	106.39	108.97
26	N	302	OIE	C6-C7-C8	2.55	123.02	119.01
31	x	601	8CT	C01-C02-C07	2.55	119.03	113.60
25	y	314	CLA	CMB-C2B-C1B	-2.55	121.54	125.42
26	6	302	OIE	C22-C12-C11	-2.55	118.69	122.82
24	p	311	CHL	CMB-C2B-C3B	2.55	129.78	124.68
24	2	310	CHL	CMB-C2B-C3B	2.55	129.77	124.68
26	Y	303	OIE	C9-C10-C11	2.55	128.73	123.52
25	u	315	CLA	CHB-C4A-NA	2.55	128.08	124.40
29	g	301	OUR	C4-C5-C6	-2.55	115.82	123.20
25	b	611	CLA	CHB-C4A-NA	2.55	128.07	124.40
24	5	310	CHL	CMB-C2B-C3B	2.55	129.77	124.68
24	R	606	CHL	CBC-CAC-C3C	-2.55	109.23	112.87
24	2	312	CHL	CMB-C2B-C3B	2.55	129.77	124.68
24	s	408	CHL	O1D-CGD-CBD	-2.55	120.86	124.72
25	N	313	CLA	CHB-C4A-NA	2.55	128.07	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	611	CLA	CHB-C4A-NA	2.55	128.07	124.40
25	S	610	CLA	C3B-C4B-NB	-2.55	108.26	110.53
30	4	318	LHG	O8-C23-C24	2.55	119.59	111.83
25	5	308	CLA	C1-C2-C3	-2.54	122.64	126.76
24	p	309	CHL	CBC-CAC-C3C	-2.54	109.23	112.87
26	7	303	0IE	C20-C3-C4	-2.54	121.20	124.72
25	R	610	CLA	C3B-C4B-NB	-2.54	108.26	110.53
24	n	305	CHL	OMC-CMC-C2C	-2.54	120.70	125.12
25	N	307	CLA	C1-C2-C3	-2.54	122.65	126.76
28	s	401	NEX	C26-C27-C28	-2.54	120.62	125.99
29	G	301	0UR	C10-C9-C8	-2.54	118.32	123.52
31	A	608	8CT	C01-C02-C07	2.54	119.02	113.60
24	3	311	CHL	C1B-CHB-C4A	2.54	122.96	121.32
25	b	606	CLA	CHB-C4A-NA	2.54	128.07	124.40
25	b	607	CLA	CHB-C4A-NA	2.54	128.07	124.40
31	a	608	8CT	C01-C02-C07	2.54	119.02	113.60
24	6	311	CHL	CMB-C2B-C3B	2.54	129.76	124.68
24	3	308	CHL	CMB-C2B-C3B	2.54	129.76	124.68
24	1	312	CHL	CMB-C2B-C3B	2.54	129.76	124.68
25	c	601	CLA	C3B-C4B-NB	-2.54	108.26	110.53
25	2	316	CLA	CHB-C4A-NA	2.54	128.06	124.40
25	B	601	CLA	CHB-C4A-NA	2.54	128.06	124.40
24	s	408	CHL	CBC-CAC-C3C	-2.54	109.24	112.87
26	u	302	0IE	C21-C7-C8	-2.54	118.70	122.82
24	u	310	CHL	OMC-CMC-C2C	-2.54	120.71	125.12
24	l	312	CHL	O2D-CGD-O1D	-2.54	118.91	123.85
28	n	303	NEX	C26-C27-C28	-2.54	120.63	125.99
25	g	308	CLA	C3B-C4B-NB	-2.54	108.27	110.53
25	g	316	CLA	CHB-C4A-NA	2.54	128.06	124.40
25	q	312	CLA	CHB-C4A-NA	2.54	128.06	124.40
25	S	611	CLA	CHB-C4A-NA	2.54	128.06	124.40
24	9	312	CHL	CMB-C2B-C3B	2.54	129.75	124.68
24	n	308	CHL	CMB-C2B-C3B	2.54	129.75	124.68
24	n	311	CHL	O1D-CGD-CBD	-2.53	120.88	124.72
25	C	608	CLA	CHB-C4A-NA	2.53	128.06	124.40
24	G	313	CHL	CMB-C2B-C3B	2.53	129.75	124.68
26	u	302	0IE	C22-C12-C11	-2.53	118.71	122.82
26	Y	303	0IE	C20-C3-C4	-2.53	121.22	124.72
24	n	310	CHL	CBC-CAC-C3C	-2.53	109.25	112.87
26	n	302	0IE	C22-C12-C11	-2.53	118.71	122.82
25	N	314	CLA	C1-C2-C3	-2.53	122.05	126.20
25	r	311	CLA	C3B-C4B-NB	-2.53	108.27	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	s	412	CLA	CHB-C4A-NA	2.53	128.05	124.40
25	p	315	CLA	O2D-CGD-CBD	2.53	115.66	111.23
24	q	316	CHL	C4D-CHA-CBD	-2.53	106.42	108.97
25	2	315	CLA	CHB-C4A-NA	2.53	128.05	124.40
25	A	607	CLA	C1-C2-C3	-2.53	122.05	126.20
25	S	610	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
25	p	316	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
29	8	301	0UR	C15-C14-C13	-2.53	115.87	123.20
24	N	308	CHL	CBC-CAC-C3C	-2.53	109.25	112.87
24	5	318	CHL	O1D-CGD-CBD	-2.53	120.89	124.72
26	N	302	0IE	C22-C12-C11	-2.53	118.72	122.82
24	2	318	CHL	O2D-CGD-O1D	-2.53	118.93	123.85
25	R	612	CLA	CHB-C4A-NA	2.53	128.05	124.40
32	a	609	SQD	O8-S-C6	2.53	110.85	105.97
26	1	302	0IE	C22-C12-C11	-2.53	118.72	122.82
24	4	305	CHL	O2D-CGD-O1D	-2.53	118.93	123.85
32	D	409	SQD	O48-C23-C24	2.53	119.54	111.83
24	5	309	CHL	CBC-CAC-C3C	-2.53	109.25	112.87
25	q	312	CLA	C1-C2-C3	-2.53	122.06	126.20
25	R	604	CLA	O2D-CGD-O1D	-2.53	118.93	123.85
25	3	315	CLA	CHB-C4A-NA	2.53	128.05	124.40
29	G	301	0UR	C43-C3-C4	-2.53	122.05	125.03
24	u	305	CHL	CBC-CAC-C3C	-2.53	109.26	112.87
25	5	317	CLA	CHB-C4A-NA	2.53	128.04	124.40
25	d	405	CLA	CHB-C4A-NA	2.53	128.04	124.40
28	N	303	NEX	C26-C27-C28	-2.53	120.65	125.99
25	C	612	CLA	CHB-C4A-NA	2.53	128.04	124.40
24	R	607	CHL	O1D-CGD-CBD	-2.52	120.89	124.72
24	3	317	CHL	CBC-CAC-C3C	-2.52	109.26	112.87
31	c	613	8CT	C14-C15-C16	-2.52	119.44	126.36
24	Y	319	CHL	C4-C3-C5	2.52	119.61	115.23
24	9	317	CHL	O2D-CGD-O1D	-2.52	118.94	123.85
24	S	602	CHL	CMA-C3A-C4A	-2.52	109.17	114.61
25	A	610	CLA	C3B-C4B-NB	-2.52	108.28	110.53
24	s	414	CHL	CMB-C2B-C3B	2.52	129.72	124.68
25	n	313	CLA	CHB-C4A-NA	2.52	128.04	124.40
25	p	317	CLA	CHB-C4A-NA	2.52	128.04	124.40
25	q	314	CLA	CHB-C4A-NA	2.52	128.04	124.40
25	B	611	CLA	CHB-C4A-NA	2.52	128.04	124.40
24	3	311	CHL	CMB-C2B-C3B	2.52	129.72	124.68
26	R	614	0IE	C20-C3-C2	2.52	120.80	115.01
24	1	305	CHL	OMC-CMC-C2C	-2.52	120.75	125.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	7	303	0IE	C13-C12-C11	2.52	122.97	119.01
25	7	308	CLA	C1-C2-C3	-2.52	122.69	126.76
28	n	303	NEX	O24-C25-C26	-2.52	56.93	58.93
25	a	610	CLA	C3B-C4B-NB	-2.52	108.28	110.53
25	5	315	CLA	CHB-C4A-NA	2.52	128.03	124.40
24	p	313	CHL	CMB-C2B-C3B	2.52	129.72	124.68
32	A	609	SQD	O5-C5-C4	2.52	114.23	109.70
32	A	609	SQD	O48-C23-C24	2.52	119.51	111.83
25	p	314	CLA	C1-C2-C3	-2.52	122.07	126.20
24	7	306	CHL	C4-C3-C5	2.52	119.60	115.23
24	p	306	CHL	C4-C3-C5	2.52	119.60	115.23
31	t	101	8CT	C05-C04-C03	2.52	114.09	110.44
25	G	316	CLA	CHB-C4A-NA	2.52	128.03	124.40
24	5	312	CHL	CMB-C2B-C3B	2.52	129.71	124.68
25	7	314	CLA	C1-C2-C3	-2.52	122.08	126.20
30	1	318	LHG	O8-C23-C24	2.52	119.50	111.83
27	r	316	XAT	C15-C14-C13	-2.51	123.75	127.28
25	G	317	CLA	CHB-C4A-NA	2.51	128.03	124.40
28	6	303	NEX	O24-C25-C26	-2.51	56.94	58.93
24	1	305	CHL	O2D-CGD-O1D	-2.51	118.95	123.85
28	s	401	NEX	O24-C25-C26	-2.51	56.94	58.93
31	c	614	8CT	C27-C26-C28	2.51	121.93	118.09
24	S	601	CHL	CBC-CAC-C3C	-2.51	109.28	112.87
25	6	307	CLA	CHB-C4A-NA	2.51	128.03	124.40
25	c	611	CLA	CHB-C4A-NA	2.51	128.03	124.40
26	r	315	0IE	C6-C7-C8	2.51	122.96	119.01
24	G	309	CHL	CBC-CAC-C3C	-2.51	109.28	112.87
26	Y	303	0IE	C22-C12-C11	-2.51	118.75	122.82
24	q	309	CHL	C4-C3-C5	2.51	119.59	115.23
25	G	315	CLA	C1-C2-C3	-2.51	122.08	126.20
28	N	303	NEX	O24-C25-C26	-2.51	56.94	58.93
24	q	304	CHL	CMB-C2B-C3B	2.51	129.70	124.68
25	b	603	CLA	CMB-C2B-C1B	-2.51	121.60	125.42
24	7	313	CHL	CMB-C2B-C3B	2.51	129.70	124.68
24	2	318	CHL	O1D-CGD-CBD	-2.51	120.92	124.72
26	y	303	0IE	C22-C12-C11	-2.51	118.75	122.82
24	2	318	CHL	CMB-C2B-C3B	2.51	129.70	124.68
24	p	306	CHL	O2D-CGD-O1D	-2.51	118.96	123.85
25	b	608	CLA	CHB-C4A-NA	2.51	128.02	124.40
25	c	601	CLA	CHB-C4A-NA	2.51	128.02	124.40
25	c	612	CLA	CHB-C4A-NA	2.51	128.02	124.40
24	5	318	CHL	CMB-C2B-C3B	2.51	129.70	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	6	308	CHL	CMB-C2B-C3B	2.51	129.70	124.68
25	C	601	CLA	C3B-C4B-NB	-2.51	108.29	110.53
25	y	315	CLA	C3B-C4B-NB	-2.51	108.29	110.53
25	8	311	CLA	CHB-C4A-NA	2.51	128.02	124.40
25	n	307	CLA	CHB-C4A-NA	2.51	128.02	124.40
24	N	310	CHL	CMB-C2B-C3B	2.51	129.69	124.68
25	b	612	CLA	CMB-C2B-C1B	-2.51	121.60	125.42
24	2	312	CHL	O1D-CGD-CBD	-2.51	120.92	124.72
25	3	307	CLA	CHB-C4A-NA	2.51	128.02	124.40
25	4	314	CLA	CHB-C4A-NA	2.51	128.02	124.40
25	N	316	CLA	C3B-C4B-NB	-2.51	108.29	110.53
25	C	606	CLA	C3B-C4B-NB	-2.51	108.29	110.53
25	G	308	CLA	C1-C2-C3	-2.51	122.71	126.76
29	4	301	OUR	C10-C9-C8	-2.51	118.39	123.52
26	q	302	OIE	C22-C12-C11	-2.51	118.75	122.82
24	2	309	CHL	O1D-CGD-CBD	-2.51	120.92	124.72
24	y	318	CHL	O2D-CGD-O1D	-2.51	118.97	123.85
25	d	404	CLA	CHB-C4A-NA	2.51	128.02	124.40
25	r	305	CLA	CHB-C4A-NA	2.51	128.02	124.40
24	9	304	CHL	O1D-CGD-CBD	-2.51	120.92	124.72
25	B	613	CLA	O2D-CGD-O1D	-2.51	118.97	123.85
25	s	410	CLA	O2A-CGA-O1A	-2.51	117.36	123.63
24	y	318	CHL	CMB-C2B-C3B	2.50	129.69	124.68
25	l	313	CLA	C1-C2-C3	-2.50	122.09	126.20
25	n	314	CLA	C1-C2-C3	-2.50	122.09	126.20
24	g	313	CHL	CMB-C2B-C3B	2.50	129.69	124.68
25	r	305	CLA	CMA-C3A-C2A	-2.50	110.49	116.23
24	y	306	CHL	O2D-CGD-O1D	-2.50	118.98	123.85
24	7	306	CHL	O2D-CGD-O1D	-2.50	118.98	123.85
26	y	302	OIE	C23-C16-C17	2.50	121.91	118.09
25	s	411	CLA	C3B-C4B-NB	-2.50	108.30	110.53
25	Y	306	CLA	CHB-C4A-NA	2.50	128.01	124.40
25	B	606	CLA	CHB-C4A-NA	2.50	128.01	124.40
24	8	304	CHL	CMB-C2B-C3B	2.50	129.68	124.68
25	N	306	CLA	CHB-C4A-NA	2.50	128.01	124.40
25	g	317	CLA	CHB-C4A-NA	2.50	128.01	124.40
26	u	302	OIE	C4-C3-C2	-2.50	117.98	120.16
27	R	615	XAT	C19-C9-C8	2.50	121.91	118.09
27	R	615	XAT	C35-C15-C14	-2.50	118.41	123.52
24	7	305	CHL	O2D-CGD-O1D	-2.50	118.98	123.85
25	4	315	CLA	CHB-C4A-NA	2.50	128.01	124.40
24	G	309	CHL	CMB-C2B-C3B	2.50	129.68	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	N	311	CHL	O1D-CGD-CBD	-2.50	120.93	124.72
24	y	312	CHL	CMB-C2B-C3B	2.50	129.68	124.68
25	7	308	CLA	C3B-C4B-NB	-2.50	108.30	110.53
25	n	315	CLA	CHB-C4A-NA	2.50	128.00	124.40
25	n	316	CLA	C3B-C4B-NB	-2.50	108.30	110.53
24	5	318	CHL	O2D-CGD-O1D	-2.50	118.99	123.85
25	b	601	CLA	CHB-C4A-NA	2.50	128.00	124.40
25	C	608	CLA	CMB-C2B-C1B	-2.49	121.62	125.42
24	N	304	CHL	CBC-CAC-C3C	-2.49	109.30	112.87
25	b	609	CLA	O2D-CGD-CBD	2.49	115.59	111.23
25	B	608	CLA	CHB-C4A-NA	2.49	128.00	124.40
24	Y	317	CHL	O2D-CGD-O1D	-2.49	118.99	123.85
24	S	607	CHL	CBC-CAC-C3C	-2.49	109.30	112.87
24	R	606	CHL	CMB-C2B-C3B	2.49	129.67	124.68
25	7	315	CLA	O2D-CGD-CBD	2.49	115.59	111.23
25	g	315	CLA	C1-C2-C3	-2.49	122.11	126.20
24	N	309	CHL	OMC-CMC-C2C	-2.49	120.79	125.12
24	p	309	CHL	O2D-CGD-O1D	-2.49	119.00	123.85
25	n	314	CLA	C3B-C4B-NB	-2.49	108.31	110.53
25	1	315	CLA	CHB-C4A-NA	2.49	128.00	124.40
24	S	613	CHL	CMB-C2B-C3B	2.49	129.66	124.68
28	3	318	NEX	O24-C25-C26	-2.49	56.95	58.93
25	g	315	CLA	C3B-C4B-NB	-2.49	108.31	110.53
24	6	309	CHL	CBC-CAC-C3C	-2.49	109.31	112.87
25	1	314	CLA	CHB-C4A-NA	2.49	128.00	124.40
25	7	317	CLA	CHB-C4A-NA	2.49	128.00	124.40
24	r	302	CHL	O2D-CGD-O1D	-2.49	119.00	123.85
26	Y	302	0IE	C23-C16-C17	2.49	121.89	118.09
24	4	312	CHL	O2D-CGD-O1D	-2.49	119.00	123.85
24	Y	317	CHL	CMB-C2B-C3B	2.49	129.66	124.68
31	T	101	8CT	C01-C02-C07	2.49	118.90	113.60
25	6	316	CLA	CHB-C4A-NA	2.49	127.99	124.40
25	S	609	CLA	O2A-CGA-O1A	-2.49	117.40	123.63
24	q	308	CHL	O2D-CGD-O1D	-2.49	119.00	123.85
24	2	309	CHL	CBC-CAC-C3C	-2.49	109.31	112.87
24	n	317	CHL	CMB-C2B-C3B	2.49	129.65	124.68
24	7	309	CHL	O2D-CGD-O1D	-2.49	119.01	123.85
27	r	316	XAT	C19-C9-C8	2.49	121.89	118.09
29	q	301	0UR	C15-C14-C13	-2.49	116.00	123.20
26	Y	302	0IE	C6-C7-C8	2.49	122.92	119.01
24	N	317	CHL	CMB-C2B-C3B	2.49	129.65	124.68
24	6	312	CHL	CMB-C2B-C3B	2.49	129.65	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	7	310	CHL	CMB-C2B-C3B	2.49	129.65	124.68
25	7	316	CLA	CHB-C4A-NA	2.49	127.99	124.40
24	s	402	CHL	CMB-C2B-C3B	2.49	129.65	124.68
24	N	305	CHL	OMC-CMC-C2C	-2.49	120.81	125.12
24	R	605	CHL	CBC-CAC-C3C	-2.49	109.31	112.87
25	8	313	CLA	CHB-C4A-NA	2.48	127.99	124.40
25	B	609	CLA	O2D-CGD-CBD	2.48	115.57	111.23
25	R	611	CLA	CHB-C4A-NA	2.48	127.98	124.40
25	n	306	CLA	CHB-C4A-NA	2.48	127.98	124.40
24	N	317	CHL	CBC-CAC-C3C	-2.48	109.32	112.87
24	G	313	CHL	C4-C3-C5	2.48	119.54	115.23
24	g	309	CHL	CMB-C2B-C3B	2.48	129.64	124.68
24	u	311	CHL	CMB-C2B-C3B	2.48	129.64	124.68
25	c	608	CLA	CMB-C2B-C1B	-2.48	121.64	125.42
24	Y	311	CHL	OMC-CMC-C2C	-2.48	120.81	125.12
24	n	305	CHL	O2D-CGD-O1D	-2.48	119.02	123.85
26	g	302	OIE	C13-C12-C11	2.48	122.91	119.01
26	y	302	OIE	C6-C7-C8	2.48	122.91	119.01
24	N	304	CHL	O1D-CGD-CBD	-2.48	120.96	124.72
25	B	604	CLA	CHB-C4A-NA	2.48	127.98	124.40
37	c	618	DGD	C1E-O6E-C5E	-2.48	108.88	113.72
24	n	310	CHL	CMB-C2B-C3B	2.48	129.64	124.68
24	g	311	CHL	O1D-CGD-CBD	-2.48	120.96	124.72
25	C	605	CLA	CHB-C4A-NA	2.48	127.98	124.40
39	D	406	PL9	C40-C39-C41	2.48	119.53	115.23
24	3	317	CHL	O2D-CGD-O1D	-2.48	119.03	123.85
31	t	101	8CT	C01-C02-C07	2.48	118.88	113.60
24	N	312	CHL	O2D-CGD-O1D	-2.48	119.03	123.85
24	n	312	CHL	O2D-CGD-O1D	-2.48	119.03	123.85
26	7	302	OIE	C22-C12-C11	-2.48	118.80	122.82
24	p	309	CHL	CMB-C2B-C3B	2.48	129.63	124.68
25	p	316	CLA	CHB-C4A-NA	2.48	127.97	124.40
24	9	311	CHL	CMB-C2B-C3B	2.48	129.63	124.68
29	g	301	OUR	C5-C4-C3	-2.48	123.96	126.92
25	3	316	CLA	CHB-C4A-NA	2.48	127.97	124.40
25	c	604	CLA	CHB-C4A-NA	2.48	127.97	124.40
24	3	309	CHL	CBC-CAC-C3C	-2.48	109.33	112.87
25	y	317	CLA	CHB-C4A-NA	2.48	127.97	124.40
25	b	605	CLA	CHB-C4A-NA	2.48	127.97	124.40
24	S	608	CHL	CMA-C3A-C4A	-2.47	109.28	114.61
24	Y	311	CHL	CMB-C2B-C3B	2.47	129.63	124.68
24	8	307	CHL	CMB-C2B-C3B	2.47	129.63	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	s	417	CLA	CHB-C4A-NA	2.47	127.97	124.40
24	u	312	CHL	CMB-C2B-C3B	2.47	129.63	124.68
24	8	315	CHL	CBC-CAC-C3C	-2.47	109.33	112.87
24	5	311	CHL	CMB-C2B-C3B	2.47	129.62	124.68
24	R	607	CHL	CMB-C2B-C3B	2.47	129.62	124.68
24	3	312	CHL	CMB-C2B-C3B	2.47	129.62	124.68
29	6	301	0UR	C18-C17-C16	-2.47	121.01	126.32
24	u	318	CHL	O2D-CGD-O1D	-2.47	119.04	123.85
24	r	302	CHL	CMB-C2B-C3B	2.47	129.62	124.68
25	7	307	CLA	CHB-C4A-NA	2.47	127.97	124.40
26	8	302	0IE	C22-C12-C11	-2.47	118.81	122.82
24	Y	305	CHL	O2D-CGD-O1D	-2.47	119.04	123.85
24	6	317	CHL	O2D-CGD-O1D	-2.47	119.04	123.85
24	r	308	CHL	CMB-C2B-C3B	2.47	129.62	124.68
24	1	304	CHL	CBC-CAC-C3C	-2.47	109.34	112.87
29	g	301	0UR	C4-C3-C2	-2.47	118.01	120.16
25	p	307	CLA	CHB-C4A-NA	2.47	127.97	124.40
25	y	307	CLA	CHB-C4A-NA	2.47	127.96	124.40
24	1	308	CHL	CMB-C2B-C3B	2.47	129.62	124.68
24	8	315	CHL	CMB-C2B-C3B	2.47	129.62	124.68
24	G	306	CHL	CBC-CAC-C3C	-2.47	109.34	112.87
24	5	309	CHL	O1D-CGD-CBD	-2.47	120.98	124.72
24	4	304	CHL	CMB-C2B-C3B	2.47	129.62	124.68
25	9	315	CLA	CHB-C4A-NA	2.47	127.96	124.40
25	Y	307	CLA	CHB-C4A-NA	2.47	127.96	124.40
24	9	310	CHL	CMB-C2B-C3B	2.47	129.62	124.68
26	G	302	0IE	C13-C12-C11	2.47	122.89	119.01
25	N	307	CLA	C3B-C4B-NB	-2.47	108.33	110.53
26	p	302	0IE	C22-C12-C11	-2.47	118.82	122.82
28	r	301	NEX	O24-C25-C26	-2.47	56.97	58.93
24	8	315	CHL	C4D-CHA-CBD	-2.47	106.48	108.97
26	r	315	0IE	C13-C12-C11	2.47	122.89	119.01
24	g	306	CHL	CBC-CAC-C3C	-2.47	109.34	112.87
25	A	603	CLA	CHB-C4A-NA	2.47	127.96	124.40
24	2	311	CHL	CMB-C2B-C3B	2.47	129.61	124.68
24	p	305	CHL	O2D-CGD-O1D	-2.47	119.05	123.85
24	u	309	CHL	CMB-C2B-C3B	2.47	129.61	124.68
25	y	308	CLA	C1-C2-C3	-2.47	122.77	126.76
24	8	303	CHL	O2D-CGD-O1D	-2.47	119.05	123.85
25	C	604	CLA	CHB-C4A-NA	2.46	127.96	124.40
24	5	310	CHL	CBC-CAC-C3C	-2.46	109.35	112.87
24	4	308	CHL	CMB-C2B-C3B	2.46	129.60	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	X	601	8CT	C22-C21-C23	2.46	121.85	118.09
24	r	307	CHL	CMB-C2B-C3B	2.46	129.60	124.68
24	R	601	CHL	O2D-CGD-O1D	-2.46	119.06	123.85
25	R	609	CLA	CHB-C4A-NA	2.46	127.95	124.40
24	2	310	CHL	CBC-CAC-C3C	-2.46	109.35	112.87
25	B	610	CLA	CHB-C4A-NA	2.46	127.95	124.40
25	a	603	CLA	CHB-C4A-NA	2.46	127.95	124.40
24	s	409	CHL	CMA-C3A-C4A	-2.46	109.31	114.61
31	C	614	8CT	C27-C26-C28	2.46	121.85	118.09
25	u	307	CLA	CHB-C4A-NA	2.46	127.95	124.40
24	8	308	CHL	O2D-CGD-O1D	-2.46	119.06	123.85
24	R	608	CHL	CMB-C2B-C3B	2.46	129.60	124.68
24	7	309	CHL	CMB-C2B-C3B	2.46	129.60	124.68
25	4	306	CLA	C3B-C4B-NB	-2.46	108.33	110.53
24	8	304	CHL	O2D-CGD-O1D	-2.46	119.06	123.85
25	r	310	CLA	CHB-C4A-NA	2.46	127.95	124.40
24	s	414	CHL	CMA-C3A-C2A	-2.46	110.59	116.23
25	9	307	CLA	CHB-C4A-NA	2.46	127.95	124.40
25	B	605	CLA	CHB-C4A-NA	2.46	127.95	124.40
25	B	612	CLA	CMB-C2B-C1B	-2.46	121.68	125.42
26	y	302	0IE	C13-C12-C11	2.46	122.87	119.01
25	2	317	CLA	CHB-C4A-NA	2.46	127.94	124.40
25	c	616	CLA	CHB-C4A-NA	2.46	127.94	124.40
24	7	311	CHL	O2D-CGD-O1D	-2.46	119.07	123.85
24	N	312	CHL	CMB-C2B-C3B	2.45	129.59	124.68
24	Y	308	CHL	CBC-CAC-C3C	-2.45	109.36	112.87
24	9	308	CHL	CMB-C2B-C3B	2.45	129.59	124.68
25	N	307	CLA	CHB-C4A-NA	2.45	127.94	124.40
25	B	603	CLA	CMB-C2B-C1B	-2.45	121.69	125.42
24	6	312	CHL	CBC-CAC-C3C	-2.45	109.36	112.87
25	y	314	CLA	O2A-CGA-O1A	-2.45	117.50	123.63
31	x	601	8CT	C27-C26-C28	2.45	121.83	118.09
25	Y	313	CLA	O2A-CGA-O1A	-2.45	117.50	123.63
31	X	601	8CT	C27-C26-C28	2.45	121.83	118.09
25	c	606	CLA	CMB-C2B-C1B	-2.45	121.69	125.42
24	6	317	CHL	CMB-C2B-C3B	2.45	129.58	124.68
25	C	616	CLA	CHB-C4A-NA	2.45	127.94	124.40
24	5	305	CHL	CBC-CAC-C3C	-2.45	109.37	112.87
24	5	312	CHL	O1D-CGD-CBD	-2.45	121.01	124.72
24	S	602	CHL	O2D-CGD-O1D	-2.45	119.08	123.85
25	c	602	CLA	CHB-C4A-NA	2.45	127.93	124.40
25	p	308	CLA	C3B-C4B-NB	-2.45	108.34	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	R	601	CHL	CMB-C2B-C3B	2.45	129.58	124.68
26	9	303	0IE	C20-C3-C2	2.45	120.63	115.01
25	C	610	CLA	CHB-C4A-NA	2.45	127.93	124.40
24	3	310	CHL	CMB-C2B-C3B	2.45	129.57	124.68
24	6	310	CHL	CMB-C2B-C3B	2.45	129.57	124.68
24	S	613	CHL	CMA-C3A-C2A	-2.45	110.62	116.23
25	Y	314	CLA	C3B-C4B-NB	-2.45	108.34	110.53
25	p	314	CLA	CHB-C4A-NA	2.45	127.93	124.40
24	3	317	CHL	CMB-C2B-C3B	2.45	129.57	124.68
25	c	610	CLA	CHB-C4A-NA	2.45	127.93	124.40
24	q	304	CHL	O2D-CGD-O1D	-2.44	119.09	123.85
25	S	616	CLA	CHB-C4A-NA	2.44	127.93	124.40
25	9	306	CLA	CHB-C4A-NA	2.44	127.93	124.40
25	C	602	CLA	CHB-C4A-NA	2.44	127.93	124.40
25	6	313	CLA	CHB-C4A-NA	2.44	127.93	124.40
25	b	604	CLA	CHB-C4A-NA	2.44	127.93	124.40
26	Y	302	0IE	C13-C12-C11	2.44	122.85	119.01
25	4	306	CLA	CHB-C4A-NA	2.44	127.93	124.40
25	4	316	CLA	CHB-C4A-NA	2.44	127.93	124.40
24	u	305	CHL	C1B-CHB-C4A	-2.44	119.75	121.32
25	Y	316	CLA	CHB-C4A-NA	2.44	127.93	124.40
24	g	313	CHL	C4-C3-C5	2.44	119.47	115.23
24	r	306	CHL	CBC-CAC-C3C	-2.44	109.38	112.87
30	c	617	LHG	O8-C23-C24	2.44	119.28	111.83
26	2	302	0IE	C4-C3-C2	-2.44	118.03	120.16
25	1	316	CLA	CHB-C4A-NA	2.44	127.92	124.40
25	S	604	CLA	CHB-C4A-NA	2.44	127.92	124.40
25	5	314	CLA	CHB-C4A-NA	2.44	127.92	124.40
24	G	318	CHL	O1D-CGD-CBD	-2.44	121.02	124.72
24	8	310	CHL	OMC-CMC-C2C	-2.44	120.88	125.12
24	n	317	CHL	CBC-CAC-C3C	-2.44	109.38	112.87
30	C	617	LHG	O8-C23-C24	2.44	119.28	111.83
24	2	305	CHL	CBC-CAC-C3C	-2.44	109.38	112.87
24	Y	304	CHL	O2D-CGD-O1D	-2.44	119.10	123.85
24	9	309	CHL	OMC-CMC-C2C	-2.44	120.88	125.12
24	n	312	CHL	CMB-C2B-C3B	2.44	129.56	124.68
24	S	601	CHL	CMB-C2B-C3B	2.44	129.56	124.68
24	4	305	CHL	OMC-CMC-C2C	-2.44	120.88	125.12
24	y	311	CHL	CMB-C2B-C3B	2.44	129.56	124.68
29	g	301	0UR	C10-C9-C8	-2.44	118.53	123.52
24	n	304	CHL	CBC-CAC-C3C	-2.44	109.38	112.87
29	1	301	0UR	C10-C9-C8	-2.44	118.53	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	3	313	CLA	CHB-C4A-NA	2.44	127.92	124.40
24	q	307	CHL	CMB-C2B-C3B	2.44	129.55	124.68
25	1	306	CLA	CHB-C4A-NA	2.44	127.92	124.40
25	7	314	CLA	CHB-C4A-NA	2.44	127.92	124.40
26	R	614	0IE	C13-C12-C11	2.44	122.84	119.01
24	n	304	CHL	O1D-CGD-CBD	-2.44	121.03	124.72
25	g	314	CLA	CHB-C4A-NA	2.44	127.92	124.40
25	G	314	CLA	CHB-C4A-NA	2.44	127.91	124.40
24	1	304	CHL	CMB-C2B-C3B	2.43	129.55	124.68
25	S	604	CLA	C3B-C4B-NB	-2.43	108.36	110.53
24	r	309	CHL	CMB-C2B-C3B	2.43	129.55	124.68
25	9	313	CLA	CHB-C4A-NA	2.43	127.91	124.40
25	u	316	CLA	CHB-C4A-NA	2.43	127.91	124.40
32	a	609	SQD	O5-C5-C4	2.43	114.08	109.70
25	C	606	CLA	CMB-C2B-C1B	-2.43	121.72	125.42
25	s	405	CLA	CHB-C4A-NA	2.43	127.91	124.40
26	9	302	0IE	C20-C3-C4	-2.43	121.36	124.72
26	4	302	0IE	C23-C16-C17	2.43	121.80	118.09
24	4	317	CHL	CMB-C2B-C3B	2.43	129.54	124.68
25	D	404	CLA	CHB-C4A-NA	2.43	127.91	124.40
25	3	314	CLA	CAA-C2A-C3A	-2.43	110.65	116.23
26	1	302	0IE	C23-C16-C17	2.43	121.80	118.09
24	1	317	CHL	CMB-C2B-C3B	2.43	129.54	124.68
24	s	403	CHL	O2D-CGD-O1D	-2.43	119.12	123.85
25	b	602	CLA	C3B-C4B-NB	-2.43	108.36	110.53
24	3	311	CHL	O1D-CGD-CBD	-2.43	121.04	124.72
24	6	311	CHL	O1D-CGD-CBD	-2.43	121.04	124.72
24	y	310	CHL	CMB-C2B-C3B	2.43	129.54	124.68
24	n	310	CHL	O2D-CGD-O1D	-2.43	119.12	123.85
24	q	310	CHL	CMA-C3A-C4A	-2.43	109.38	114.61
25	6	314	CLA	CHB-C4A-NA	2.43	127.91	124.40
25	b	615	CLA	CHB-C4A-NA	2.43	127.91	124.40
25	c	605	CLA	CHB-C4A-NA	2.43	127.91	124.40
39	d	406	PL9	C20-C19-C21	2.43	119.44	115.23
24	q	303	CHL	O2D-CGD-O1D	-2.43	119.12	123.85
25	n	314	CLA	CHB-C4A-NA	2.43	127.91	124.40
25	b	602	CLA	CHB-C4A-NA	2.43	127.91	124.40
25	c	608	CLA	CHB-C4A-NA	2.43	127.91	124.40
31	x	601	8CT	C22-C21-C23	2.43	121.80	118.09
25	4	313	CLA	C1-C2-C3	-2.43	122.22	126.20
26	y	303	0IE	C9-C10-C11	2.43	128.49	123.52
24	u	312	CHL	O1D-CGD-CBD	-2.43	121.04	124.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	G	309	CHL	C4D-CHA-CBD	-2.43	106.52	108.97
31	v	401	8CT	C11-C10-C03	-2.43	120.51	127.00
29	7	301	0UR	C15-C14-C13	-2.43	116.17	123.20
24	y	306	CHL	CMB-C2B-C3B	2.43	129.53	124.68
31	c	613	8CT	C25-C24-C23	-2.43	116.17	123.20
24	G	305	CHL	CMB-C2B-C3B	2.43	129.53	124.68
25	B	615	CLA	CHB-C4A-NA	2.43	127.90	124.40
25	y	308	CLA	CHB-C4A-NA	2.43	127.90	124.40
24	n	305	CHL	CMB-C2B-C3B	2.43	129.53	124.68
29	p	301	0UR	C15-C14-C13	-2.43	116.17	123.20
24	g	310	CHL	O2D-CGD-O1D	-2.43	119.12	123.85
25	B	602	CLA	C3B-C4B-NB	-2.43	108.36	110.53
26	3	303	0IE	C4-C5-C6	2.43	130.23	123.20
25	Y	307	CLA	C1-C2-C3	-2.43	122.84	126.76
24	8	308	CHL	CBC-CAC-C3C	-2.42	109.40	112.87
31	s	416	8CT	C01-C02-C07	2.42	118.77	113.60
31	S	614	8CT	C40-C12-C13	-2.42	118.89	122.82
24	9	305	CHL	O2D-CGD-O1D	-2.42	119.13	123.85
35	a	606	PHO	C1-C2-C3	-2.42	122.22	126.20
24	q	310	CHL	O1D-CGD-CBD	-2.42	121.05	124.72
25	N	315	CLA	CHB-C4A-NA	2.42	127.90	124.40
25	A	605	CLA	CHB-C4A-NA	2.42	127.90	124.40
24	9	304	CHL	O2D-CGD-O1D	-2.42	119.13	123.85
25	A	610	CLA	CAA-C2A-C3A	-2.42	110.67	116.23
25	a	610	CLA	CAA-C2A-C3A	-2.42	110.67	116.23
35	A	606	PHO	C1-C2-C3	-2.42	122.23	126.20
24	N	311	CHL	CMB-C2B-C3B	2.42	129.53	124.68
24	Y	309	CHL	CMB-C2B-C3B	2.42	129.52	124.68
24	u	306	CHL	CBC-CAC-C3C	-2.42	109.41	112.87
24	N	308	CHL	CMB-C2B-C3B	2.42	129.52	124.68
24	r	307	CHL	CBC-CAC-C3C	-2.42	109.41	112.87
24	R	602	CHL	OMC-CMC-C2C	-2.42	120.92	125.12
25	b	613	CLA	CHB-C4A-NA	2.42	127.89	124.40
24	n	309	CHL	CBC-CAC-C3C	-2.42	109.41	112.87
31	v	401	8CT	C01-C02-C07	2.42	118.76	113.60
24	Y	310	CHL	CMB-C2B-C3B	2.42	129.52	124.68
24	y	309	CHL	CBC-CAC-C3C	-2.42	109.41	112.87
27	r	316	XAT	C4-C3-C2	-2.42	106.26	110.79
26	G	303	0IE	C20-C3-C2	2.42	120.56	115.01
24	4	317	CHL	C4D-CHA-CBD	-2.42	106.53	108.97
24	s	402	CHL	CBC-CAC-C3C	-2.42	109.41	112.87
33	B	619	LMG	O7-C10-O9	-2.42	118.05	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	N	302	0IE	C23-C16-C17	2.42	121.78	118.09
24	N	305	CHL	CMB-C2B-C3B	2.42	129.51	124.68
24	q	311	CHL	OMC-CMC-C2C	-2.42	120.92	125.12
31	V	401	8CT	C11-C10-C03	-2.42	120.54	127.00
25	r	311	CLA	CMB-C2B-C1B	-2.42	121.74	125.42
26	p	302	0IE	C5-C4-C3	2.42	129.81	126.92
24	l	310	CHL	CBC-CAC-C3C	-2.42	109.41	112.87
25	g	308	CLA	CHB-C4A-NA	2.42	127.89	124.40
24	q	307	CHL	CBC-CAC-C3C	-2.42	109.41	112.87
24	q	308	CHL	OMC-CMC-C2C	-2.42	120.92	125.12
25	b	610	CLA	CHB-C4A-NA	2.42	127.89	124.40
24	s	409	CHL	CBC-CAC-C3C	-2.42	109.41	112.87
25	C	601	CLA	CHB-C4A-NA	2.41	127.88	124.40
26	g	303	0IE	C20-C3-C2	2.41	120.55	115.01
24	g	318	CHL	O1D-CGD-CBD	-2.41	121.06	124.72
24	R	605	CHL	CMB-C2B-C3B	2.41	129.50	124.68
24	g	305	CHL	CMB-C2B-C3B	2.41	129.50	124.68
25	A	610	CLA	CHB-C4A-NA	2.41	127.88	124.40
24	2	305	CHL	CMB-C2B-C3B	2.41	129.50	124.68
31	S	615	8CT	C18-C19-C20	-2.41	118.58	123.52
39	D	406	PL9	C20-C19-C21	2.41	119.41	115.23
24	S	605	CHL	CMB-C2B-C3B	2.41	129.50	124.68
24	9	305	CHL	CBC-CAC-C3C	-2.41	109.42	112.87
24	q	316	CHL	CBC-CAC-C3C	-2.41	109.42	112.87
24	g	309	CHL	C4D-CHA-CBD	-2.41	106.54	108.97
26	7	302	0IE	C5-C4-C3	2.41	129.80	126.92
25	l	306	CLA	C3B-C4B-NB	-2.41	108.38	110.53
26	9	303	0IE	C17-C16-C15	2.41	122.80	119.01
24	y	305	CHL	O2D-CGD-O1D	-2.41	119.16	123.85
24	g	310	CHL	CMB-C2B-C3B	2.41	129.50	124.68
29	G	301	0UR	C15-C14-C13	-2.41	116.22	123.20
24	G	311	CHL	CMB-C2B-C3B	2.41	129.50	124.68
24	5	313	CHL	CMB-C2B-C3B	2.41	129.50	124.68
26	y	303	0IE	C20-C3-C4	-2.41	121.39	124.72
24	g	309	CHL	CBC-CAC-C3C	-2.41	109.43	112.87
25	u	314	CLA	CHB-C4A-NA	2.41	127.87	124.40
25	a	605	CLA	CHB-C4A-NA	2.41	127.87	124.40
31	c	613	8CT	C30-C29-C28	-2.41	120.83	124.58
26	5	302	0IE	C4-C3-C2	-2.41	118.06	120.16
25	g	308	CLA	C1-C2-C3	-2.41	122.87	126.76
25	C	604	CLA	C1-C2-C3	-2.41	122.25	126.20
25	C	601	CLA	CMB-C2B-C1B	-2.41	121.75	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	N	314	CLA	CHB-C4A-NA	2.41	127.87	124.40
26	2	302	0IE	C13-C12-C11	2.41	122.79	119.01
25	c	601	CLA	CMB-C2B-C1B	-2.41	121.76	125.42
25	3	313	CLA	CMA-C3A-C2A	-2.40	110.72	116.23
24	r	303	CHL	OMC-CMC-C2C	-2.40	120.94	125.12
29	G	301	0UR	C5-C4-C3	-2.40	124.04	126.92
24	p	318	CHL	O2D-CGD-O1D	-2.40	119.17	123.85
24	n	317	CHL	O2D-CGD-O1D	-2.40	119.17	123.85
25	B	603	CLA	C3B-C4B-NB	-2.40	108.39	110.53
25	b	603	CLA	C3B-C4B-NB	-2.40	108.39	110.53
25	s	405	CLA	C3B-C4B-NB	-2.40	108.39	110.53
24	3	310	CHL	CBC-CAC-C3C	-2.40	109.43	112.87
24	9	309	CHL	CMB-C2B-C3B	2.40	129.48	124.68
26	G	303	0IE	C13-C12-C11	2.40	122.79	119.01
25	u	317	CLA	CHB-C4A-NA	2.40	127.87	124.40
25	b	614	CLA	CHB-C4A-NA	2.40	127.87	124.40
24	2	313	CHL	CMB-C2B-C3B	2.40	129.48	124.68
24	r	306	CHL	CMB-C2B-C3B	2.40	129.48	124.68
25	Y	307	CLA	CMB-C2B-C1B	-2.40	121.76	125.42
25	s	410	CLA	CHB-C4A-NA	2.40	127.86	124.40
24	p	312	CHL	CMB-C2B-C3B	2.40	129.48	124.68
24	g	312	CHL	CBC-CAC-C3C	-2.40	109.44	112.87
25	B	613	CLA	CHB-C4A-NA	2.40	127.86	124.40
25	8	306	CLA	C3B-C4B-NB	-2.40	108.39	110.53
24	N	310	CHL	O2D-CGD-O1D	-2.40	119.18	123.85
24	8	309	CHL	O1D-CGD-CBD	-2.40	121.08	124.72
24	G	310	CHL	O2D-CGD-O1D	-2.40	119.18	123.85
24	8	307	CHL	O2D-CGD-O1D	-2.40	119.18	123.85
25	8	311	CLA	O2A-CGA-O1A	-2.40	117.63	123.63
24	N	308	CHL	CMA-C3A-C4A	-2.40	109.44	114.61
24	N	305	CHL	CBC-CAC-C3C	-2.40	109.44	112.87
31	s	415	8CT	C40-C12-C13	-2.40	118.93	122.82
24	3	312	CHL	CBC-CAC-C3C	-2.40	109.44	112.87
31	C	615	8CT	C01-C02-C07	2.40	118.70	113.60
24	q	316	CHL	CMB-C2B-C3B	2.40	129.47	124.68
25	q	315	CLA	CHB-C4A-NA	2.39	127.86	124.40
24	y	312	CHL	OMC-CMC-C2C	-2.39	120.96	125.12
37	c	619	DGD	O1G-C1A-O1A	-2.39	117.64	123.63
25	a	610	CLA	CHB-C4A-NA	2.39	127.85	124.40
25	c	603	CLA	CHB-C4A-NA	2.39	127.85	124.40
29	n	301	0UR	C18-C17-C16	-2.39	121.18	126.32
24	S	608	CHL	O2D-CGD-O1D	-2.39	119.19	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	g	311	CHL	CMB-C2B-C3B	2.39	129.47	124.68
24	S	602	CHL	CMB-C2B-C3B	2.39	129.46	124.68
26	5	302	0IE	C13-C12-C11	2.39	122.77	119.01
24	u	310	CHL	CMB-C2B-C3B	2.39	129.46	124.68
24	Y	305	CHL	CMB-C2B-C3B	2.39	129.46	124.68
24	g	306	CHL	O2D-CGD-O1D	-2.39	119.19	123.85
24	r	308	CHL	CBC-CAC-C3C	-2.39	109.45	112.87
25	Y	313	CLA	CHB-C4A-NA	2.39	127.85	124.40
24	5	305	CHL	CMB-C2B-C3B	2.39	129.46	124.68
24	G	306	CHL	O2D-CGD-O1D	-2.39	119.19	123.85
24	s	409	CHL	O2D-CGD-O1D	-2.39	119.19	123.85
33	D	401	LMG	O6-C1-C2	-2.39	105.46	110.37
25	G	315	CLA	C3B-C4B-NB	-2.39	108.40	110.53
33	d	401	LMG	O6-C1-C2	-2.39	105.46	110.37
25	A	604	CLA	CHB-C4A-NA	2.39	127.85	124.40
25	a	604	CLA	CHB-C4A-NA	2.39	127.85	124.40
24	u	306	CHL	O2D-CGD-O1D	-2.39	119.20	123.85
24	3	311	CHL	CBC-CAC-C3C	-2.39	109.45	112.87
25	u	308	CLA	CHB-C4A-NA	2.39	127.85	124.40
24	1	317	CHL	C4D-CHA-CBD	-2.39	106.56	108.97
25	y	314	CLA	CHB-C4A-NA	2.39	127.84	124.40
24	G	313	CHL	O2D-CGD-O1D	-2.39	119.20	123.85
24	7	313	CHL	CMA-C3A-C4A	-2.39	109.47	114.61
24	6	311	CHL	CBC-CAC-C3C	-2.39	109.46	112.87
24	7	318	CHL	O2D-CGD-O1D	-2.39	119.20	123.85
31	X	601	8CT	C04-C03-C02	-2.38	119.38	122.64
25	c	604	CLA	C1-C2-C3	-2.38	122.29	126.20
32	D	409	SQD	O5-C5-C4	2.38	114.00	109.70
25	2	314	CLA	CHB-C4A-NA	2.38	127.84	124.40
25	S	609	CLA	CHB-C4A-NA	2.38	127.84	124.40
24	n	311	CHL	CMB-C2B-C3B	2.38	129.45	124.68
29	6	301	0UR	C10-C9-C8	-2.38	118.64	123.52
24	n	305	CHL	CBC-CAC-C3C	-2.38	109.46	112.87
31	S	615	8CT	C01-C02-C07	2.38	118.68	113.60
24	s	406	CHL	CMB-C2B-C3B	2.38	129.45	124.68
24	R	607	CHL	CBC-CAC-C3C	-2.38	109.46	112.87
24	6	305	CHL	O2D-CGD-O1D	-2.38	119.21	123.85
24	6	310	CHL	O2D-CGD-O1D	-2.38	119.21	123.85
24	9	311	CHL	O1D-CGD-CBD	-2.38	121.11	124.72
25	G	308	CLA	CHB-C4A-NA	2.38	127.84	124.40
25	N	314	CLA	C3B-C4B-NB	-2.38	108.40	110.53
24	6	305	CHL	CMB-C2B-C3B	2.38	129.44	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	4	307	CLA	CHB-C4A-NA	2.38	127.84	124.40
25	8	314	CLA	CHB-C4A-NA	2.38	127.83	124.40
31	D	410	8CT	C19-C18-C17	-2.38	118.65	123.52
24	3	305	CHL	O2D-CGD-O1D	-2.38	119.22	123.85
24	r	306	CHL	OMC-CMC-C2C	-2.38	120.99	125.12
24	S	608	CHL	CMB-C2B-C3B	2.38	129.44	124.68
32	d	409	SQD	O5-C5-C4	2.38	113.98	109.70
24	1	311	CHL	CMB-C2B-C3B	2.38	129.43	124.68
25	5	307	CLA	CHB-C4A-NA	2.38	127.83	124.40
24	g	310	CHL	CBC-CAC-C3C	-2.38	109.47	112.87
24	p	313	CHL	CMA-C3A-C4A	-2.38	109.49	114.61
29	8	301	0UR	C4-C5-C6	-2.38	116.31	123.20
24	9	308	CHL	CBC-CAC-C3C	-2.38	109.47	112.87
24	u	309	CHL	CBC-CAC-C3C	-2.38	109.47	112.87
24	6	309	CHL	O2D-CGD-O1D	-2.38	119.22	123.85
26	r	315	0IE	C20-C3-C4	-2.38	121.44	124.72
24	q	309	CHL	CMB-C2B-C3B	2.37	129.43	124.68
24	8	309	CHL	CMA-C3A-C4A	-2.37	109.50	114.61
24	2	306	CHL	CMA-C3A-C4A	-2.37	109.50	114.61
25	8	305	CLA	CHB-C4A-NA	2.37	127.83	124.40
24	5	306	CHL	CMA-C3A-C4A	-2.37	109.50	114.61
31	s	416	8CT	C18-C19-C20	-2.37	118.67	123.52
25	B	614	CLA	CHB-C4A-NA	2.37	127.82	124.40
24	R	605	CHL	CMA-C3A-C4A	-2.37	109.50	114.61
25	y	308	CLA	CMB-C2B-C1B	-2.37	121.81	125.42
24	1	317	CHL	O1D-CGD-CBD	-2.37	121.13	124.72
25	s	411	CLA	CHB-C4A-NA	2.37	127.82	124.40
37	C	620	DGD	O1G-C1A-O1A	-2.37	117.70	123.63
24	7	312	CHL	CMB-C2B-C3B	2.37	129.41	124.68
24	N	312	CHL	C4-C3-C5	2.37	119.34	115.23
29	g	301	0UR	C15-C14-C13	-2.37	116.34	123.20
24	N	309	CHL	CBC-CAC-C3C	-2.37	109.48	112.87
24	4	310	CHL	CBC-CAC-C3C	-2.37	109.48	112.87
24	6	310	CHL	CBC-CAC-C3C	-2.37	109.48	112.87
24	p	311	CHL	C1B-CHB-C4A	2.37	122.84	121.32
25	r	311	CLA	CHB-C4A-NA	2.37	127.81	124.40
24	1	304	CHL	O2D-CGD-O1D	-2.37	119.24	123.85
25	b	609	CLA	CHB-C4A-NA	2.37	127.81	124.40
25	C	610	CLA	C1-C2-C3	-2.36	122.32	126.20
26	8	302	0IE	C6-C7-C8	2.36	122.73	119.01
25	9	316	CLA	CHB-C4A-NA	2.36	127.81	124.40
24	5	306	CHL	O2D-CGD-O1D	-2.36	119.25	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	6	312	CHL	O2D-CGD-O1D	-2.36	119.25	123.85
24	s	409	CHL	CMB-C2B-C3B	2.36	129.40	124.68
29	N	301	0UR	C18-C17-C16	-2.36	121.24	126.32
25	q	305	CLA	CHB-C4A-NA	2.36	127.81	124.40
25	r	304	CLA	C3B-C4B-NB	-2.36	108.42	110.53
25	6	306	CLA	CHB-C4A-NA	2.36	127.81	124.40
24	G	312	CHL	CBC-CAC-C3C	-2.36	109.49	112.87
24	n	309	CHL	CMB-C2B-C3B	2.36	129.40	124.68
24	s	403	CHL	CMB-C2B-C3B	2.36	129.40	124.68
24	9	308	CHL	C4D-CHA-CBD	-2.36	106.59	108.97
24	u	310	CHL	O2D-CGD-O1D	-2.36	119.25	123.85
24	4	309	CHL	O2D-CGD-O1D	-2.36	119.25	123.85
24	u	311	CHL	O2D-CGD-O1D	-2.36	119.25	123.85
24	5	309	CHL	CMB-C2B-C3B	2.36	129.40	124.68
24	8	315	CHL	O2D-CGD-O1D	-2.36	119.26	123.85
25	b	610	CLA	C1-C2-C3	-2.36	122.33	126.20
25	3	306	CLA	CHB-C4A-NA	2.36	127.80	124.40
24	2	309	CHL	CMB-C2B-C3B	2.36	129.40	124.68
31	d	410	8CT	C29-C28-C26	-2.36	121.25	126.32
25	B	612	CLA	CHB-C4A-NA	2.36	127.80	124.40
24	1	309	CHL	O2D-CGD-O1D	-2.36	119.26	123.85
25	B	610	CLA	C1-C2-C3	-2.36	122.33	126.20
24	3	312	CHL	O2D-CGD-O1D	-2.36	119.26	123.85
26	q	302	0IE	C6-C7-C8	2.36	122.72	119.01
29	9	301	0UR	C18-C17-C16	-2.36	121.26	126.32
25	B	602	CLA	CHB-C4A-NA	2.36	127.80	124.40
28	N	303	NEX	C39-C29-C30	-2.36	119.00	122.82
24	4	311	CHL	CMB-C2B-C3B	2.36	129.39	124.68
24	n	312	CHL	C4-C3-C5	2.36	119.32	115.23
24	6	309	CHL	OMC-CMC-C2C	-2.36	121.03	125.12
24	N	317	CHL	O2D-CGD-O1D	-2.36	119.26	123.85
24	3	309	CHL	O2D-CGD-O1D	-2.35	119.27	123.85
32	b	618	SQD	C3-C4-C5	2.35	114.50	110.23
31	V	401	8CT	C01-C02-C07	2.35	118.62	113.60
24	S	608	CHL	CBC-CAC-C3C	-2.35	109.50	112.87
25	q	312	CLA	O2A-CGA-O1A	-2.35	117.74	123.63
25	g	314	CLA	C1-C2-C3	-2.35	122.34	126.20
31	B	617	8CT	C18-C19-C20	-2.35	118.70	123.52
25	p	315	CLA	C1-C2-C3	-2.35	122.34	126.20
25	7	308	CLA	CHB-C4A-NA	2.35	127.80	124.40
24	3	305	CHL	CMB-C2B-C3B	2.35	129.38	124.68
24	4	309	CHL	CMB-C2B-C3B	2.35	129.38	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	9	302	0IE	C13-C12-C11	2.35	122.71	119.01
24	4	317	CHL	O1D-CGD-CBD	-2.35	121.16	124.72
24	R	606	CHL	CMA-C3A-C4A	-2.35	109.54	114.61
24	3	310	CHL	O2D-CGD-O1D	-2.35	119.27	123.85
24	2	306	CHL	O2D-CGD-O1D	-2.35	119.27	123.85
24	4	304	CHL	O2D-CGD-O1D	-2.35	119.27	123.85
24	4	310	CHL	O2D-CGD-O1D	-2.35	119.27	123.85
25	C	603	CLA	CHB-C4A-NA	2.35	127.79	124.40
28	6	303	NEX	C39-C29-C30	-2.35	119.01	122.82
24	1	310	CHL	O2D-CGD-O1D	-2.35	119.27	123.85
25	c	610	CLA	C1-C2-C3	-2.35	122.35	126.20
24	8	308	CHL	OMC-CMC-C2C	-2.35	121.04	125.12
25	s	413	CLA	CHB-C4A-NA	2.35	127.79	124.40
26	4	302	0IE	C13-C12-C11	2.35	122.70	119.01
25	S	610	CLA	CHB-C4A-NA	2.35	127.79	124.40
25	g	315	CLA	CHB-C4A-NA	2.35	127.79	124.40
29	7	301	0UR	C10-C9-C8	-2.35	118.72	123.52
25	5	314	CLA	O2A-CGA-O1A	-2.35	117.76	123.63
25	N	316	CLA	CHB-C4A-NA	2.35	127.79	124.40
25	b	612	CLA	O2A-CGA-O1A	-2.35	117.76	123.63
24	2	311	CHL	CMA-C3A-C4A	-2.35	109.56	114.61
26	p	303	0IE	C20-C3-C2	2.35	120.40	115.01
28	r	301	NEX	C39-C29-C30	-2.35	119.02	122.82
29	3	301	0UR	C43-C3-C4	-2.35	122.26	125.03
24	R	602	CHL	CMA-C3A-C4A	-2.35	109.56	114.61
24	y	311	CHL	CMA-C3A-C4A	-2.35	109.56	114.61
24	G	306	CHL	CMB-C2B-C3B	2.35	129.37	124.68
26	r	315	0IE	C23-C16-C17	2.35	121.67	118.09
25	B	610	CLA	O2A-CGA-O1A	-2.35	117.76	123.63
24	1	310	CHL	CMB-C2B-C3B	2.34	129.37	124.68
32	A	609	SQD	C1-O5-C5	2.34	118.30	113.72
25	R	603	CLA	C3B-C4B-NB	-2.34	108.44	110.53
24	9	317	CHL	CBC-CAC-C3C	-2.34	109.52	112.87
31	C	613	8CT	C25-C24-C23	-2.34	116.41	123.20
26	g	303	0IE	C13-C12-C11	2.34	122.69	119.01
26	u	303	0IE	C4-C5-C6	2.34	129.99	123.20
25	n	316	CLA	CHB-C4A-NA	2.34	127.78	124.40
24	1	308	CHL	O2D-CGD-O1D	-2.34	119.29	123.85
24	r	306	CHL	O2D-CGD-O1D	-2.34	119.29	123.85
28	s	401	NEX	C39-C29-C30	-2.34	119.02	122.82
24	r	307	CHL	CMA-C3A-C4A	-2.34	109.56	114.61
27	R	615	XAT	C4-C3-C2	-2.34	106.41	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	n	304	CHL	C1B-CHB-C4A	-2.34	119.82	121.32
25	r	313	CLA	C3B-C4B-NB	-2.34	108.44	110.53
24	u	318	CHL	CBC-CAC-C3C	-2.34	109.52	112.87
25	R	610	CLA	CHB-C4A-NA	2.34	127.78	124.40
25	2	307	CLA	CHB-C4A-NA	2.34	127.78	124.40
24	2	313	CHL	O2D-CGD-O1D	-2.34	119.29	123.85
24	3	309	CHL	OMC-CMC-C2C	-2.34	121.06	125.12
24	u	309	CHL	O2D-CGD-O1D	-2.34	119.29	123.85
24	Y	319	CHL	CMB-C2B-C3B	2.34	129.36	124.68
29	5	301	0UR	C18-C17-C16	-2.34	121.29	126.32
24	G	310	CHL	CBC-CAC-C3C	-2.34	109.53	112.87
28	n	303	NEX	C39-C29-C30	-2.34	119.03	122.82
24	4	308	CHL	O2D-CGD-O1D	-2.34	119.30	123.85
24	n	312	CHL	CMA-C3A-C4A	-2.34	109.57	114.61
24	G	310	CHL	CMB-C2B-C3B	2.34	129.35	124.68
24	4	310	CHL	CMB-C2B-C3B	2.34	129.35	124.68
24	5	311	CHL	CMA-C3A-C4A	-2.34	109.58	114.61
24	N	309	CHL	O2D-CGD-O1D	-2.34	119.30	123.85
24	g	313	CHL	O2D-CGD-O1D	-2.34	119.30	123.85
24	S	601	CHL	O2D-CGD-O1D	-2.34	119.30	123.85
24	2	312	CHL	CBC-CAC-C3C	-2.34	109.53	112.87
25	2	314	CLA	O2A-CGA-O1A	-2.34	117.79	123.63
24	6	308	CHL	CBC-CAC-C3C	-2.33	109.53	112.87
25	B	609	CLA	C3B-C4B-NB	-2.33	108.45	110.53
31	c	615	8CT	C01-C02-C07	2.33	118.57	113.60
28	3	318	NEX	C39-C29-C30	-2.33	119.03	122.82
24	u	313	CHL	O2D-CGD-O1D	-2.33	119.31	123.85
24	u	312	CHL	C4D-CHA-CBD	-2.33	106.62	108.97
24	u	305	CHL	O2D-CGD-O1D	-2.33	119.31	123.85
24	s	402	CHL	O2D-CGD-O1D	-2.33	119.31	123.85
24	r	303	CHL	CMA-C3A-C4A	-2.33	109.59	114.61
31	c	615	8CT	C13-C14-C15	-2.33	116.45	123.20
25	C	606	CLA	CHB-C4A-NA	2.33	127.76	124.40
24	1	309	CHL	CMB-C2B-C3B	2.33	129.34	124.68
24	S	606	CHL	CMB-C2B-C3B	2.33	129.34	124.68
24	R	605	CHL	O2D-CGD-O1D	-2.33	119.31	123.85
26	p	302	0IE	C23-C16-C17	2.33	121.65	118.09
24	7	309	CHL	C4D-CHA-CBD	-2.33	106.62	108.97
24	9	310	CHL	O2D-CGD-O1D	-2.33	119.31	123.85
24	N	305	CHL	CMA-C3A-C4A	-2.33	109.59	114.61
24	5	313	CHL	O2D-CGD-O1D	-2.33	119.32	123.85
25	b	612	CLA	CHB-C4A-NA	2.33	127.76	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	9	309	CHL	O2D-CGD-O1D	-2.33	119.32	123.85
25	1	307	CLA	CHB-C4A-NA	2.33	127.76	124.40
25	c	606	CLA	CHB-C4A-NA	2.33	127.76	124.40
24	q	316	CHL	O2D-CGD-O1D	-2.33	119.32	123.85
25	B	609	CLA	CHB-C4A-NA	2.33	127.76	124.40
25	G	314	CLA	C1-C2-C3	-2.33	122.39	126.20
26	9	302	0IE	C5-C4-C3	2.33	129.70	126.92
28	n	303	NEX	C35-C15-C14	-2.33	118.76	123.52
24	G	318	CHL	OMC-CMC-C2C	-2.33	121.08	125.12
29	p	301	0UR	C23-C24-C25	-2.32	108.50	113.59
24	Y	312	CHL	C4-C3-C5	2.32	119.26	115.23
25	q	313	CLA	C3B-C4B-NB	-2.32	108.45	110.53
24	g	313	CHL	CBC-CAC-C3C	-2.32	109.55	112.87
24	y	313	CHL	C4-C3-C5	2.32	119.26	115.23
24	g	318	CHL	OMC-CMC-C2C	-2.32	121.09	125.12
26	N	302	0IE	C5-C4-C3	2.32	129.70	126.92
29	u	301	0UR	C18-C17-C16	-2.32	121.33	126.32
25	D	404	CLA	C1-C2-C3	-2.32	122.39	126.20
26	7	303	0IE	C20-C3-C2	2.32	120.34	115.01
25	A	603	CLA	CMB-C2B-C3B	2.32	132.01	126.55
25	p	317	CLA	O2D-CGD-CBD	2.32	115.29	111.23
24	G	312	CHL	O1D-CGD-CBD	-2.32	121.20	124.72
29	8	301	0UR	C10-C9-C8	-2.32	118.77	123.52
24	N	309	CHL	CMB-C2B-C3B	2.32	129.32	124.68
25	G	307	CLA	CHB-C4A-NA	2.32	127.75	124.40
29	y	301	0UR	C28-C19-C18	-2.32	110.16	112.83
25	b	604	CLA	O2A-CGA-O1A	-2.32	117.83	123.63
28	6	303	NEX	C35-C15-C14	-2.32	118.78	123.52
25	g	307	CLA	CHB-C4A-NA	2.32	127.74	124.40
24	g	312	CHL	O1D-CGD-CBD	-2.32	121.21	124.72
24	9	312	CHL	O2D-CGD-O1D	-2.32	119.34	123.85
29	y	301	0UR	C10-C9-C8	-2.32	118.78	123.52
25	b	610	CLA	O2A-CGA-O1A	-2.32	117.83	123.63
25	a	603	CLA	CMB-C2B-C3B	2.31	132.00	126.55
24	N	312	CHL	OMC-CMC-C2C	-2.31	121.10	125.12
24	Y	308	CHL	CMB-C2B-C3B	2.31	129.31	124.68
24	s	407	CHL	CMB-C2B-C3B	2.31	129.31	124.68
25	7	315	CLA	C1-C2-C3	-2.31	122.41	126.20
25	7	317	CLA	O2D-CGD-CBD	2.31	115.28	111.23
24	5	305	CHL	OMC-CMC-C2C	-2.31	121.10	125.12
24	s	406	CHL	CMA-C3A-C4A	-2.31	109.62	114.61
24	n	309	CHL	O2D-CGD-O1D	-2.31	119.34	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	s	401	NEX	C35-C15-C14	-2.31	118.79	123.52
24	9	308	CHL	O2D-CGD-O1D	-2.31	119.35	123.85
27	r	316	XAT	C30-C31-C32	-2.31	116.50	123.20
25	y	307	CLA	C1-C2-C3	-2.31	122.41	126.20
24	N	312	CHL	CMA-C3A-C4A	-2.31	109.63	114.61
29	5	301	0UR	C10-C9-C8	-2.31	118.79	123.52
25	s	404	CLA	CHB-C4A-NA	2.31	127.73	124.40
24	Y	310	CHL	CMA-C3A-C4A	-2.31	109.63	114.61
24	y	309	CHL	CMB-C2B-C3B	2.31	129.30	124.68
25	b	609	CLA	C3B-C4B-NB	-2.31	108.47	110.53
26	R	614	0IE	C23-C16-C17	2.31	121.62	118.09
26	7	302	0IE	C23-C16-C17	2.31	121.62	118.09
24	G	312	CHL	C5-C3-C4	2.31	119.90	114.59
25	6	313	CLA	CMA-C3A-C2A	-2.31	110.94	116.23
31	A	608	8CT	C05-C04-C03	2.31	113.79	110.44
31	a	608	8CT	C05-C04-C03	2.31	113.79	110.44
26	R	614	0IE	C20-C3-C4	-2.31	121.53	124.72
24	s	403	CHL	CMD-C2D-C3D	-2.31	120.07	124.68
25	C	611	CLA	CMB-C2B-C1B	-2.31	121.91	125.42
25	8	312	CLA	CHB-C4A-NA	2.31	127.73	124.40
33	w	201	LMG	O7-C10-O9	-2.31	118.31	123.70
24	G	311	CHL	O2D-CGD-O1D	-2.31	119.36	123.85
24	u	305	CHL	CMB-C2B-C3B	2.31	129.29	124.68
24	r	303	CHL	CMB-C2B-C3B	2.31	129.29	124.68
29	2	301	0UR	C18-C17-C16	-2.31	121.36	126.32
24	q	308	CHL	CBC-CAC-C3C	-2.31	109.57	112.87
24	9	310	CHL	CBC-CAC-C3C	-2.30	109.57	112.87
24	4	309	CHL	CBC-CAC-C3C	-2.30	109.57	112.87
25	G	315	CLA	CHB-C4A-NA	2.30	127.73	124.40
24	G	309	CHL	O2D-CGD-O1D	-2.30	119.36	123.85
26	1	302	0IE	C13-C12-C11	2.30	122.63	119.01
28	N	303	NEX	C35-C15-C14	-2.30	118.81	123.52
29	Y	301	0UR	C10-C9-C8	-2.30	118.81	123.52
24	Y	319	CHL	CMA-C3A-C4A	-2.30	109.65	114.61
28	r	301	NEX	C35-C15-C14	-2.30	118.81	123.52
25	p	308	CLA	CHB-C4A-NA	2.30	127.72	124.40
24	q	309	CHL	CMA-C3A-C4A	-2.30	109.65	114.61
25	N	313	CLA	O2A-CGA-O1A	-2.30	117.87	123.63
24	5	312	CHL	CBC-CAC-C3C	-2.30	109.58	112.87
24	8	310	CHL	O2D-CGD-O1D	-2.30	119.37	123.85
31	d	410	8CT	C19-C18-C17	-2.30	118.81	123.52
24	p	306	CHL	CMA-C3A-C4A	-2.30	109.66	114.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	D	410	8CT	C29-C28-C26	-2.30	121.38	126.32
25	B	603	CLA	CHB-C4A-NA	2.30	127.72	124.40
24	R	602	CHL	CMB-C2B-C3B	2.30	129.28	124.68
25	B	612	CLA	O2A-CGA-O1A	-2.30	117.88	123.63
25	q	306	CLA	C3B-C4B-NB	-2.30	108.48	110.53
31	C	615	8CT	C04-C03-C10	2.30	121.88	115.65
25	q	313	CLA	CHB-C4A-NA	2.30	127.71	124.40
27	R	615	XAT	C30-C31-C32	-2.30	116.55	123.20
25	c	611	CLA	CMB-C2B-C1B	-2.30	121.92	125.42
24	2	306	CHL	CBC-CAC-C3C	-2.30	109.59	112.87
31	C	613	8CT	C40-C12-C13	-2.29	119.10	122.82
24	S	605	CHL	CMA-C3A-C4A	-2.29	109.67	114.61
24	g	306	CHL	CMB-C2B-C3B	2.29	129.27	124.68
24	2	311	CHL	O2D-CGD-O1D	-2.29	119.39	123.85
24	4	317	CHL	O2D-CGD-O1D	-2.29	119.39	123.85
26	6	302	0IE	C13-C12-C11	2.29	122.61	119.01
25	D	404	CLA	CAA-CBA-CGA	-2.29	106.70	113.21
28	3	318	NEX	C35-C15-C14	-2.29	118.83	123.52
29	p	301	0UR	C10-C9-C8	-2.29	118.83	123.52
31	c	613	8CT	C40-C12-C13	-2.29	119.11	122.82
25	B	604	CLA	O2A-CGA-O1A	-2.29	117.90	123.63
32	B	618	SQD	C3-C4-C5	2.29	114.38	110.23
24	g	312	CHL	C5-C3-C4	2.29	119.86	114.59
29	2	301	0UR	C10-C9-C8	-2.29	118.83	123.52
24	3	308	CHL	CBC-CAC-C3C	-2.29	109.60	112.87
26	u	303	0IE	C17-C16-C15	2.29	122.61	119.01
33	D	411	LMG	O1-C1-C2	2.29	111.75	108.27
25	R	604	CLA	CMA-C3A-C2A	-2.29	110.98	116.23
25	S	612	CLA	CHB-C4A-NA	2.29	127.70	124.40
24	1	309	CHL	CBC-CAC-C3C	-2.29	109.60	112.87
24	y	311	CHL	OMC-CMC-C2C	-2.28	121.15	125.12
29	Y	301	0UR	C28-C19-C18	-2.28	110.20	112.83
24	4	309	CHL	OMC-CMC-C2C	-2.28	121.15	125.12
24	q	307	CHL	O2D-CGD-O1D	-2.28	119.40	123.85
24	7	313	CHL	CBC-CAC-C3C	-2.28	109.60	112.87
24	4	312	CHL	OMC-CMC-C2C	-2.28	121.16	125.12
28	r	317	NEX	C31-C32-C33	-2.28	120.10	126.36
39	D	406	PL9	C37-C38-C39	-2.28	122.40	127.62
39	d	406	PL9	C37-C38-C39	-2.28	122.40	127.62
24	7	306	CHL	CMA-C3A-C4A	-2.28	109.69	114.61
24	1	317	CHL	O2D-CGD-O1D	-2.28	119.41	123.85
24	p	309	CHL	C4D-CHA-CBD	-2.28	106.67	108.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	3	308	CHL	O2D-CGD-O1D	-2.28	119.41	123.85
24	5	311	CHL	O2D-CGD-O1D	-2.28	119.41	123.85
30	d	408	LHG	O7-C7-O9	-2.28	118.37	123.70
25	C	605	CLA	CMB-C2B-C1B	-2.28	121.95	125.42
25	B	611	CLA	O2A-CGA-O1A	-2.28	117.92	123.63
24	q	303	CHL	CMB-C2B-C3B	2.28	129.24	124.68
25	S	603	CLA	CHB-C4A-NA	2.28	127.69	124.40
24	5	306	CHL	CBC-CAC-C3C	-2.28	109.61	112.87
29	9	301	OUR	C4-C3-C2	-2.28	118.17	120.16
24	y	306	CHL	CAC-C3C-C4C	2.28	129.89	124.03
25	d	404	CLA	CAA-CBA-CGA	-2.28	106.74	113.21
39	d	406	PL9	O1-C4-C3	-2.28	118.33	120.73
24	n	312	CHL	OMC-CMC-C2C	-2.28	121.16	125.12
24	S	602	CHL	CMD-C2D-C3D	-2.28	120.13	124.68
26	3	302	OIE	C13-C12-C11	2.28	122.59	119.01
25	B	602	CLA	O2D-CGD-CBD	2.28	115.21	111.23
25	R	613	CLA	C3B-C4B-NB	-2.28	108.50	110.53
24	s	408	CHL	OMC-CMC-C2C	-2.28	121.17	125.12
24	7	305	CHL	CMA-C3A-C4A	-2.28	109.71	114.61
33	W	201	LMG	O7-C10-O9	-2.28	118.38	123.70
24	6	304	CHL	OMC-CMC-C2C	-2.28	121.17	125.12
24	p	311	CHL	O2D-CGD-O1D	-2.27	119.42	123.85
24	q	311	CHL	O2D-CGD-O1D	-2.27	119.42	123.85
24	8	303	CHL	CMB-C2B-C3B	2.27	129.23	124.68
24	u	311	CHL	CBC-CAC-C3C	-2.27	109.62	112.87
24	n	304	CHL	O2D-CGD-O1D	-2.27	119.42	123.85
24	y	310	CHL	CMA-C3A-C4A	-2.27	109.71	114.61
24	g	309	CHL	O2D-CGD-O1D	-2.27	119.42	123.85
24	Y	310	CHL	OMC-CMC-C2C	-2.27	121.17	125.12
26	p	303	OIE	C17-C16-C15	2.27	122.58	119.01
31	a	608	8CT	C28-C26-C25	-2.27	115.44	119.01
24	n	305	CHL	CMA-C3A-C4A	-2.27	109.72	114.61
24	2	305	CHL	O2D-CGD-O1D	-2.27	119.43	123.85
31	s	416	8CT	C11-C10-C03	-2.27	120.94	127.00
28	R	616	NEX	C31-C32-C33	-2.27	120.14	126.36
25	c	605	CLA	CMB-C2B-C1B	-2.27	121.97	125.42
24	N	305	CHL	O2D-CGD-O1D	-2.27	119.43	123.85
25	r	314	CLA	CHB-C4A-NA	2.27	127.67	124.40
24	Y	305	CHL	CAC-C3C-C4C	2.27	129.86	124.03
25	4	307	CLA	CMA-C3A-C2A	-2.27	111.03	116.23
25	b	611	CLA	O2A-CGA-O1A	-2.27	117.96	123.63
25	R	613	CLA	CHB-C4A-NA	2.27	127.67	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	6	308	CHL	O2D-CGD-O1D	-2.27	119.44	123.85
26	N	302	0IE	C13-C12-C11	2.26	122.57	119.01
26	n	302	0IE	C13-C12-C11	2.26	122.57	119.01
25	C	601	CLA	C1-C2-C3	-2.26	122.49	126.20
24	9	311	CHL	C4D-CHA-CBD	-2.26	106.68	108.97
25	B	606	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
24	6	309	CHL	CMA-C3A-C4A	-2.26	109.73	114.61
29	7	301	0UR	C23-C24-C25	-2.26	108.63	113.59
25	8	312	CLA	C3B-C4B-NB	-2.26	108.51	110.53
24	8	309	CHL	O2D-CGD-O1D	-2.26	119.44	123.85
25	R	610	CLA	CMB-C2B-C1B	-2.26	121.97	125.42
26	n	302	0IE	C23-C16-C17	2.26	121.54	118.09
24	4	304	CHL	C4D-CHA-CBD	-2.26	106.69	108.97
24	6	309	CHL	C1B-CHB-C4A	2.26	122.78	121.32
25	3	314	CLA	CHB-C4A-NA	2.26	127.66	124.40
25	d	404	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
25	b	606	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
26	q	302	0IE	C13-C12-C11	2.26	122.56	119.01
25	1	307	CLA	CMA-C3A-C2A	-2.26	111.05	116.23
28	u	304	NEX	C31-C32-C33	-2.26	120.17	126.36
28	5	304	NEX	C31-C32-C33	-2.26	120.17	126.36
27	R	615	XAT	C38-C25-C24	2.26	116.78	114.24
28	N	303	NEX	C30-C31-C32	-2.26	116.66	123.20
29	q	301	0UR	C4-C5-C6	-2.26	116.66	123.20
26	2	303	0IE	C20-C3-C2	2.26	120.19	115.01
25	7	314	CLA	O2A-CGA-O1A	-2.26	117.98	123.63
26	7	303	0IE	C17-C16-C15	2.26	122.56	119.01
25	B	609	CLA	C1-C2-C3	-2.26	122.50	126.20
29	N	301	0UR	C10-C9-C8	-2.26	118.90	123.52
24	G	312	CHL	CMB-C2B-C3B	2.26	129.19	124.68
29	q	301	0UR	C10-C9-C8	-2.26	118.90	123.52
24	6	304	CHL	CMB-C2B-C3B	2.26	129.19	124.68
24	5	305	CHL	O2D-CGD-O1D	-2.25	119.46	123.85
28	S	617	NEX	C31-C32-C33	-2.25	120.18	126.36
25	c	609	CLA	C1-C2-C3	-2.25	122.50	126.20
24	q	310	CHL	O2D-CGD-O1D	-2.25	119.46	123.85
25	b	603	CLA	CHB-C4A-NA	2.25	127.65	124.40
24	R	608	CHL	O2D-CGD-O1D	-2.25	119.46	123.85
24	6	304	CHL	O2D-CGD-O1D	-2.25	119.46	123.85
29	n	301	0UR	C10-C9-C8	-2.25	118.91	123.52
28	p	304	NEX	C31-C32-C33	-2.25	120.19	126.36
24	n	310	CHL	CMA-C3A-C4A	-2.25	109.76	114.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	s	409	CHL	O2A-CGA-CBA	2.25	120.64	112.14
25	R	609	CLA	C1-C2-C3	-2.25	122.51	126.20
31	D	410	8CT	C25-C24-C23	-2.25	116.68	123.20
25	b	602	CLA	O2D-CGD-CBD	2.25	115.16	111.23
24	r	309	CHL	O2D-CGD-O1D	-2.25	119.47	123.85
24	G	305	CHL	O2D-CGD-O1D	-2.25	119.47	123.85
28	9	319	NEX	C31-C32-C33	-2.25	120.20	126.36
24	7	310	CHL	O2D-CGD-O1D	-2.25	119.47	123.85
24	u	309	CHL	C4D-CHA-CBD	-2.25	106.70	108.97
24	Y	309	CHL	CMA-C3A-C4A	-2.25	109.77	114.61
28	G	304	NEX	C31-C32-C33	-2.25	120.20	126.36
28	g	304	NEX	C31-C32-C33	-2.25	120.20	126.36
25	r	310	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
24	S	608	CHL	O2A-CGA-CBA	2.25	120.63	112.14
33	i	101	LMG	C1-O6-C5	-2.25	109.33	113.72
28	r	301	NEX	C30-C31-C32	-2.25	116.69	123.20
29	6	301	0UR	C29-C30-C31	-2.25	107.85	111.18
31	A	608	8CT	C28-C26-C25	-2.25	115.47	119.01
28	7	304	NEX	C31-C32-C33	-2.25	120.20	126.36
28	6	303	NEX	C30-C31-C32	-2.25	116.69	123.20
24	Y	317	CHL	CMA-C3A-C2A	-2.25	111.08	116.23
29	u	301	0UR	C4-C5-C6	-2.25	116.69	123.20
24	g	310	CHL	OMC-CMC-C2C	-2.25	121.22	125.12
28	3	318	NEX	C30-C31-C32	-2.24	116.70	123.20
31	D	410	8CT	C18-C19-C20	-2.24	118.93	123.52
24	N	309	CHL	CMA-C3A-C4A	-2.24	109.78	114.61
24	y	309	CHL	O2D-CGD-O1D	-2.24	119.48	123.85
24	g	306	CHL	CMA-C3A-C4A	-2.24	109.78	114.61
28	4	303	NEX	C31-C32-C33	-2.24	120.22	126.36
24	1	312	CHL	OMC-CMC-C2C	-2.24	121.23	125.12
25	D	405	CLA	C1-C2-C3	-2.24	122.53	126.20
29	Y	301	0UR	C23-C24-C25	-2.24	108.68	113.59
28	s	401	NEX	C30-C31-C32	-2.24	116.71	123.20
24	p	310	CHL	O2D-CGD-O1D	-2.24	119.49	123.85
26	u	302	0IE	C13-C12-C11	2.24	122.53	119.01
24	G	318	CHL	C1B-CHB-C4A	2.24	122.76	121.32
25	1	313	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
28	1	303	NEX	C31-C32-C33	-2.24	120.22	126.36
28	y	304	NEX	C31-C32-C33	-2.24	120.22	126.36
28	2	304	NEX	C31-C32-C33	-2.24	120.23	126.36
25	c	608	CLA	O2D-CGD-CBD	2.24	115.14	111.23
25	c	603	CLA	CMB-C2B-C3B	2.24	131.81	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	C	617	LHG	C26-C25-C24	2.24	121.35	113.13
25	b	609	CLA	C1-C2-C3	-2.24	122.53	126.20
24	l	304	CHL	C4D-CHA-CBD	-2.24	106.71	108.97
25	p	314	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
24	g	305	CHL	O2D-CGD-O1D	-2.24	119.50	123.85
24	Y	310	CHL	C1-O2A-CGA	2.24	122.06	116.65
24	G	305	CHL	CMA-C3A-C4A	-2.24	109.80	114.61
24	9	317	CHL	C4D-CHA-CBD	-2.23	106.71	108.97
24	u	318	CHL	C4D-CHA-CBD	-2.23	106.71	108.97
26	n	302	0IE	C5-C4-C3	2.23	129.59	126.92
24	6	309	CHL	C5-C3-C4	2.23	119.73	114.59
24	3	305	CHL	CMA-C3A-C4A	-2.23	109.80	114.61
25	B	604	CLA	C3B-C4B-NB	-2.23	108.54	110.53
25	c	609	CLA	O1D-CGD-CBD	2.23	128.92	124.52
24	N	304	CHL	O2D-CGD-O1D	-2.23	119.50	123.85
25	y	307	CLA	O2A-CGA-O1A	-2.23	118.04	123.63
24	Y	308	CHL	O2D-CGD-O1D	-2.23	119.50	123.85
25	A	607	CLA	CMB-C2B-C1B	-2.23	122.02	125.42
28	n	303	NEX	C30-C31-C32	-2.23	116.73	123.20
26	5	303	0IE	C20-C3-C2	2.23	120.13	115.01
24	g	312	CHL	CMB-C2B-C3B	2.23	129.14	124.68
25	C	609	CLA	O1D-CGD-CBD	2.23	128.92	124.52
24	5	311	CHL	O2A-CGA-CBA	2.23	120.57	112.14
24	u	306	CHL	CMB-C2B-C3B	2.23	129.14	124.68
24	p	312	CHL	O1D-CGD-CBD	-2.23	121.34	124.72
30	c	617	LHG	C26-C25-C24	2.23	121.32	113.13
24	Y	310	CHL	O2D-CGD-O1D	-2.23	119.51	123.85
24	p	305	CHL	CMA-C3A-C4A	-2.23	109.81	114.61
25	D	404	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
39	D	406	PL9	O2-C1-C6	2.23	124.03	120.48
25	C	603	CLA	CMB-C2B-C3B	2.23	131.79	126.55
25	R	609	CLA	O2A-CGA-O1A	-2.23	118.06	123.63
31	T	101	8CT	C24-C23-C21	-2.23	120.25	126.36
24	N	310	CHL	CMA-C3A-C4A	-2.23	109.81	114.61
39	D	406	PL9	O1-C4-C3	-2.23	118.38	120.73
25	c	601	CLA	C1-C2-C3	-2.23	122.55	126.20
31	c	613	8CT	C06-C07-C02	-2.23	110.08	114.06
24	y	318	CHL	CMA-C3A-C2A	-2.23	111.12	116.23
24	9	304	CHL	CMB-C2B-C3B	2.23	129.13	124.68
24	2	309	CHL	O2D-CGD-O1D	-2.23	119.52	123.85
26	u	302	0IE	C6-C7-C8	2.23	122.51	119.01
24	N	308	CHL	O2D-CGD-O1D	-2.23	119.52	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	7	313	CHL	O2D-CGD-O1D	-2.23	119.52	123.85
25	b	606	CLA	CMB-C2B-C1B	-2.23	122.03	125.42
27	r	316	XAT	C20-C13-C12	2.23	121.49	118.09
26	8	302	0IE	C13-C12-C11	2.22	122.51	119.01
25	C	609	CLA	C1-C2-C3	-2.22	122.55	126.20
24	Y	305	CHL	CMA-C3A-C4A	-2.22	109.82	114.61
24	y	311	CHL	O2D-CGD-O1D	-2.22	119.52	123.85
24	6	309	CHL	CMB-C2B-C3B	2.22	129.12	124.68
24	N	311	CHL	CMA-C3A-C4A	-2.22	109.82	114.61
24	2	311	CHL	O2A-CGA-CBA	2.22	120.53	112.14
24	p	313	CHL	O2D-CGD-O1D	-2.22	119.52	123.85
24	G	306	CHL	CMA-C3A-C4A	-2.22	109.82	114.61
25	Y	306	CLA	C1-C2-C3	-2.22	122.56	126.20
26	y	303	0IE	C13-C12-C11	2.22	122.50	119.01
25	B	607	CLA	O2D-CGD-CBD	2.22	115.11	111.23
24	R	607	CHL	OMC-CMC-C2C	-2.22	121.27	125.12
24	R	607	CHL	CMA-C3A-C4A	-2.22	109.83	114.61
31	C	615	8CT	C13-C14-C15	-2.22	116.77	123.20
24	1	311	CHL	CMA-C3A-C4A	-2.22	109.83	114.61
24	4	309	CHL	C1B-CHB-C4A	2.22	122.75	121.32
26	Y	303	0IE	C13-C12-C11	2.22	122.50	119.01
25	b	607	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
39	d	406	PL9	O2-C1-C6	2.22	124.01	120.48
24	8	304	CHL	CMA-C3A-C4A	-2.22	109.84	114.61
24	n	311	CHL	CMA-C3A-C4A	-2.22	109.84	114.61
32	D	409	SQD	C44-O6-C1	2.21	118.54	113.80
24	q	307	CHL	CMA-C3A-C4A	-2.21	109.84	114.61
24	S	608	CHL	OMC-CMC-C2C	-2.21	121.28	125.12
25	C	612	CLA	C1-C2-C3	-2.21	122.57	126.20
33	d	401	LMG	O7-C10-O9	-2.21	118.53	123.70
25	B	606	CLA	CMB-C2B-C1B	-2.21	122.05	125.42
25	G	314	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
24	p	311	CHL	CMA-C3A-C4A	-2.21	109.85	114.61
25	b	605	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
24	p	313	CHL	CBC-CAC-C3C	-2.21	109.71	112.87
33	w	201	LMG	O8-C28-O10	-2.21	118.10	123.63
26	8	302	0IE	C4-C3-C2	-2.21	118.23	120.16
24	1	309	CHL	OMC-CMC-C2C	-2.21	121.28	125.12
25	u	314	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
25	Y	314	CLA	CHB-C4A-NA	2.21	127.59	124.40
25	8	306	CLA	CHB-C4A-NA	2.21	127.59	124.40
24	y	306	CHL	CMA-C3A-C4A	-2.21	109.85	114.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	C	615	8CT	C40-C12-C13	-2.21	119.24	122.82
24	y	310	CHL	O2D-CGD-O1D	-2.21	119.55	123.85
24	r	308	CHL	OMC-CMC-C2C	-2.21	121.29	125.12
25	Y	313	CLA	CMB-C2B-C3B	2.21	131.74	126.55
24	3	309	CHL	C5-C3-C4	2.21	119.67	114.59
31	d	410	8CT	C14-C15-C16	-2.21	120.31	126.36
26	2	303	0IE	C23-C16-C17	2.21	121.46	118.09
25	4	313	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
24	y	306	CHL	C6-C5-C3	-2.21	108.09	113.47
24	6	305	CHL	CMA-C3A-C4A	-2.20	109.86	114.61
24	q	304	CHL	CMA-C3A-C4A	-2.20	109.86	114.61
24	n	308	CHL	O2D-CGD-O1D	-2.20	119.56	123.85
24	q	304	CHL	CAC-C3C-C4C	2.20	129.69	124.03
24	8	307	CHL	OMC-CMC-C2C	-2.20	121.30	125.12
24	n	317	CHL	OMC-CMC-C2C	-2.20	121.30	125.12
25	3	314	CLA	C3B-C4B-NB	-2.20	108.56	110.53
24	g	311	CHL	CMA-C3A-C4A	-2.20	109.87	114.61
24	p	312	CHL	O2D-CGD-O1D	-2.20	119.56	123.85
31	t	101	8CT	C24-C23-C21	-2.20	120.33	126.36
24	3	304	CHL	O2D-CGD-O1D	-2.20	119.56	123.85
25	Y	306	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
24	G	310	CHL	OMC-CMC-C2C	-2.20	121.30	125.12
24	u	313	CHL	CMA-C3A-C4A	-2.20	109.87	114.61
31	d	410	8CT	C25-C24-C23	-2.20	116.83	123.20
25	B	609	CLA	O2A-CGA-O1A	-2.20	118.13	123.63
26	9	303	0IE	C15-C14-C13	2.20	129.56	123.20
24	Y	319	CHL	O2D-CGD-O1D	-2.20	119.58	123.85
25	9	313	CLA	O2A-CGA-O1A	-2.20	118.14	123.63
25	d	405	CLA	C1-C2-C3	-2.19	122.60	126.20
24	3	309	CHL	CMA-C3A-C4A	-2.19	109.88	114.61
24	2	310	CHL	O2D-CGD-O1D	-2.19	119.58	123.85
24	3	309	CHL	CMB-C2B-C3B	2.19	129.07	124.68
27	R	615	XAT	C20-C13-C12	2.19	121.44	118.09
25	8	305	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
25	a	607	CLA	CMB-C2B-C1B	-2.19	122.08	125.42
24	S	605	CHL	O2D-CGD-O1D	-2.19	119.58	123.85
24	Y	309	CHL	O2D-CGD-O1D	-2.19	119.58	123.85
24	y	312	CHL	C5-C3-C4	2.19	119.63	114.59
25	q	306	CLA	CHB-C4A-NA	2.19	127.56	124.40
31	v	401	8CT	C27-C26-C28	2.19	121.44	118.09
30	Y	318	LHG	C5-O7-C7	-2.19	112.55	117.80
26	7	302	0IE	C13-C12-C11	2.19	122.46	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	q	309	CHL	O2D-CGD-O1D	-2.19	119.58	123.85
25	B	605	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
24	7	312	CHL	CAC-C3C-C4C	2.19	129.66	124.03
29	9	301	0UR	C4-C5-C6	-2.19	116.85	123.20
25	b	604	CLA	C3B-C4B-NB	-2.19	108.58	110.53
25	y	315	CLA	CHB-C4A-NA	2.19	127.56	124.40
24	7	311	CHL	CMA-C3A-C4A	-2.19	109.90	114.61
24	9	304	CHL	OMC-CMC-C2C	-2.19	121.32	125.12
24	5	309	CHL	O2D-CGD-O1D	-2.18	119.59	123.85
32	A	609	SQD	O8-S-C6	2.18	110.19	105.97
24	8	304	CHL	CAC-C3C-C4C	2.18	129.65	124.03
24	7	312	CHL	O2D-CGD-O1D	-2.18	119.60	123.85
25	7	307	CLA	C1-C2-C3	-2.18	122.62	126.20
32	a	609	SQD	O48-C23-C24	2.18	118.49	111.83
24	3	304	CHL	CMB-C2B-C3B	2.18	129.04	124.68
31	S	615	8CT	C11-C10-C03	-2.18	121.17	127.00
31	V	401	8CT	C27-C26-C28	2.18	121.42	118.09
24	9	312	CHL	CBC-CAC-C3C	-2.18	109.75	112.87
26	g	302	0IE	C23-C16-C17	2.18	121.42	118.09
25	g	314	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
24	5	310	CHL	O2D-CGD-O1D	-2.18	119.60	123.85
24	4	311	CHL	O2D-CGD-O1D	-2.18	119.60	123.85
31	C	613	8CT	C06-C07-C02	-2.18	110.17	114.06
25	u	308	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
28	6	303	NEX	C17-C1-C6	-2.18	108.52	110.47
24	2	305	CHL	OMC-CMC-C2C	-2.18	121.34	125.12
25	c	602	CLA	C1-C2-C3	-2.18	122.63	126.20
25	p	307	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
33	m	101	LMG	O7-C10-O9	-2.18	118.62	123.70
26	u	302	0IE	C5-C4-C3	2.18	129.52	126.92
25	p	307	CLA	C1-C2-C3	-2.17	122.63	126.20
24	4	311	CHL	CMA-C3A-C4A	-2.17	109.93	114.61
29	4	301	0UR	C34-C27-C26	2.17	118.42	114.42
24	Y	305	CHL	C6-C5-C3	-2.17	108.17	113.47
25	B	607	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
25	b	607	CLA	O2D-CGD-CBD	2.17	115.03	111.23
31	V	401	8CT	C13-C14-C15	-2.17	116.91	123.20
24	g	311	CHL	O2D-CGD-O1D	-2.17	119.62	123.85
31	c	614	8CT	C10-C03-C02	-2.17	116.55	121.56
24	Y	309	CHL	O2A-CGA-CBA	2.17	120.34	112.14
24	y	318	CHL	CMA-C3A-C4A	-2.17	109.93	114.61
25	r	314	CLA	C3B-C4B-NB	-2.17	108.59	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	b	617	8CT	C18-C19-C20	-2.17	119.08	123.52
33	D	401	LMG	O7-C10-O9	-2.17	118.63	123.70
29	G	301	0UR	C22-C16-C17	2.17	121.40	118.09
24	G	311	CHL	CMA-C3A-C4A	-2.17	109.94	114.61
25	r	310	CLA	C1-C2-C3	-2.17	122.64	126.20
25	y	308	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
24	u	312	CHL	O2D-CGD-O1D	-2.17	119.63	123.85
25	C	608	CLA	O2D-CGD-CBD	2.17	115.02	111.23
32	d	409	SQD	C44-O6-C1	2.17	118.44	113.80
32	A	609	SQD	O6-C1-C2	2.17	111.56	108.27
24	9	311	CHL	O2D-CGD-O1D	-2.17	119.63	123.85
29	6	301	0UR	C4-C5-C6	-2.17	116.92	123.20
24	2	312	CHL	OMC-CMC-C2C	-2.17	121.36	125.12
24	y	310	CHL	O2A-CGA-CBA	2.17	120.33	112.14
24	Y	310	CHL	O2A-CGA-O1A	-2.17	118.21	123.63
29	y	301	0UR	C23-C24-C25	-2.17	108.84	113.59
28	s	401	NEX	C17-C1-C6	-2.17	108.53	110.47
24	r	302	CHL	CBC-CAC-C3C	-2.17	109.77	112.87
24	Y	311	CHL	C5-C3-C4	2.17	119.57	114.59
24	1	311	CHL	O2D-CGD-O1D	-2.17	119.63	123.85
31	B	617	8CT	C40-C12-C13	-2.17	119.31	122.82
24	n	309	CHL	CMA-C3A-C4A	-2.17	109.95	114.61
25	7	307	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
25	c	612	CLA	C1-C2-C3	-2.16	122.65	126.20
25	y	315	CLA	C1-C2-C3	-2.16	122.65	126.20
25	b	609	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
24	s	406	CHL	O2D-CGD-O1D	-2.16	119.64	123.85
29	6	301	0UR	C15-C14-C13	-2.16	116.94	123.20
25	n	313	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
24	4	317	CHL	OMC-CMC-C2C	-2.16	121.37	125.12
31	v	401	8CT	C13-C14-C15	-2.16	116.94	123.20
28	n	303	NEX	C17-C1-C6	-2.16	108.54	110.47
24	2	309	CHL	CMA-C3A-C4A	-2.16	109.96	114.61
31	d	410	8CT	C18-C19-C20	-2.16	119.11	123.52
24	4	308	CHL	C4D-CHA-CBD	-2.16	106.79	108.97
26	q	302	0IE	C4-C3-C2	-2.16	118.28	120.16
24	s	409	CHL	OMC-CMC-C2C	-2.16	121.38	125.12
24	5	318	CHL	CMA-C3A-C4A	-2.16	109.97	114.61
24	R	605	CHL	CAA-C2A-C3A	-2.15	111.29	116.23
24	g	310	CHL	O2A-CGA-CBA	2.15	120.28	112.14
25	a	605	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
25	Y	307	CLA	O2A-CGA-O1A	-2.15	118.24	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	G	301	0UR	C20-C7-C6	2.15	121.38	118.09
24	g	312	CHL	CAA-CBA-CGA	-2.15	107.09	113.21
25	a	607	CLA	O2D-CGD-CBD	2.15	115.00	111.23
24	s	407	CHL	O2D-CGD-O1D	-2.15	119.66	123.85
26	9	303	0IE	C19-C18-C17	2.15	127.93	124.58
24	2	309	CHL	OMC-CMC-C2C	-2.15	121.38	125.12
31	C	614	8CT	C10-C03-C02	-2.15	116.60	121.56
24	g	305	CHL	CMA-C3A-C4A	-2.15	109.97	114.61
31	x	601	8CT	C35-C30-C29	-2.15	110.35	112.83
24	S	606	CHL	O2D-CGD-O1D	-2.15	119.66	123.85
29	u	301	0UR	C9-C10-C11	-2.15	119.12	123.52
25	q	305	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
25	A	607	CLA	O2D-CGD-CBD	2.15	114.99	111.23
24	s	402	CHL	CMA-C3A-C4A	-2.15	109.98	114.61
26	p	302	0IE	C20-C3-C4	-2.15	121.75	124.72
24	3	317	CHL	OMC-CMC-C2C	-2.15	121.39	125.12
24	9	312	CHL	CMA-C3A-C4A	-2.15	109.98	114.61
25	G	308	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
25	g	308	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
24	5	309	CHL	C4D-CHA-CBD	-2.15	106.80	108.97
24	2	318	CHL	CMA-C3A-C4A	-2.15	109.98	114.61
24	1	317	CHL	OMC-CMC-C2C	-2.15	121.39	125.12
37	C	619	DGD	O5D-C6D-C5D	2.15	114.26	109.42
29	u	301	0UR	C4-C3-C2	-2.15	118.29	120.16
24	u	313	CHL	CBC-CAC-C3C	-2.15	109.80	112.87
36	a	611	BCT	O3-C-O1	-2.15	114.19	119.68
28	3	318	NEX	C17-C1-C6	-2.15	108.55	110.47
28	N	303	NEX	C17-C1-C6	-2.15	108.55	110.47
24	3	311	CHL	O2D-CGD-O1D	-2.15	119.67	123.85
24	G	310	CHL	O2A-CGA-CBA	2.15	120.25	112.14
24	N	317	CHL	OMC-CMC-C2C	-2.15	121.39	125.12
29	g	301	0UR	C22-C16-C17	2.15	121.36	118.09
24	q	308	CHL	CMA-C3A-C4A	-2.14	109.99	114.61
24	Y	317	CHL	CMA-C3A-C4A	-2.14	109.99	114.61
24	5	309	CHL	CMA-C3A-C4A	-2.14	109.99	114.61
25	b	608	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
25	b	613	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
26	p	302	0IE	C13-C12-C11	2.14	122.38	119.01
25	B	604	CLA	CAA-CBA-CGA	-2.14	107.13	113.21
26	7	302	0IE	C20-C3-C4	-2.14	121.76	124.72
29	8	301	0UR	C18-C17-C16	-2.14	121.72	126.32
31	C	615	8CT	C27-C26-C25	-2.14	119.35	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	314	CLA	C1-C2-C3	-2.14	122.69	126.20
25	5	317	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
25	G	317	CLA	CMB-C2B-C1B	-2.14	122.16	125.42
24	6	311	CHL	O2D-CGD-O1D	-2.14	119.69	123.85
24	5	309	CHL	OMC-CMC-C2C	-2.14	121.41	125.12
31	c	615	8CT	C27-C26-C25	-2.14	119.35	122.82
25	u	307	CLA	C1-C2-C3	-2.14	122.70	126.20
24	n	312	CHL	CAC-C3C-C4C	2.14	129.52	124.03
29	3	301	0UR	C15-C14-C13	-2.14	117.01	123.20
24	8	308	CHL	CMA-C3A-C4A	-2.14	110.01	114.61
24	r	308	CHL	CMA-C3A-C4A	-2.13	110.01	114.61
25	c	616	CLA	O2D-CGD-CBD	2.13	114.96	111.23
29	N	301	0UR	C15-C14-C13	-2.13	117.03	123.20
26	7	302	0IE	C14-C15-C16	2.13	130.27	127.28
24	N	312	CHL	CAC-C3C-C4C	2.13	129.51	124.03
24	8	315	CHL	C1B-CHB-C4A	-2.13	119.95	121.32
25	3	314	CLA	CMB-C2B-C1B	-2.13	122.18	125.42
25	S	609	CLA	C1-C2-C3	-2.13	122.71	126.20
26	p	302	0IE	C14-C15-C16	2.13	130.26	127.28
25	y	317	CLA	CMB-C2B-C1B	-2.13	122.18	125.42
24	1	308	CHL	C4D-CHA-CBD	-2.13	106.82	108.97
25	C	616	CLA	O2D-CGD-CBD	2.13	114.95	111.23
25	y	314	CLA	CMB-C2B-C3B	2.13	131.55	126.55
25	r	311	CLA	CMB-C2B-C3B	2.12	131.55	126.55
29	2	301	0UR	C33-C32-C31	-2.12	118.33	123.36
29	q	301	0UR	C18-C17-C16	-2.12	121.76	126.32
39	D	406	PL9	C12-C13-C14	-2.12	122.76	127.62
32	b	618	SQD	O8-S-C6	2.12	110.07	105.97
24	5	312	CHL	O2D-CGD-O1D	-2.12	119.72	123.85
31	b	617	8CT	C40-C12-C13	-2.12	119.38	122.82
25	c	601	CLA	CMB-C2B-C3B	2.12	131.53	126.55
25	q	306	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
25	b	604	CLA	CAA-CBA-CGA	-2.12	107.19	113.21
25	C	604	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
24	7	310	CHL	CBC-CAC-C3C	-2.12	109.84	112.87
25	R	613	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
24	q	307	CHL	OMC-CMC-C2C	-2.12	121.44	125.12
36	A	611	BCT	O3-C-O1	-2.12	114.26	119.68
24	9	305	CHL	CMA-C3A-C4A	-2.12	110.05	114.61
26	G	303	0IE	C23-C16-C17	2.12	121.32	118.09
25	C	601	CLA	CMB-C2B-C3B	2.12	131.53	126.55
25	c	604	CLA	O2A-CGA-O1A	-2.12	118.33	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	6	308	CHL	CMA-C3A-C4A	-2.12	110.05	114.61
25	C	610	CLA	CMB-C2B-C1B	-2.11	122.20	125.42
24	p	312	CHL	CAC-C3C-C4C	2.11	129.47	124.03
24	n	309	CHL	OMC-CMC-C2C	-2.11	121.45	125.12
31	C	614	8CT	C13-C14-C15	-2.11	117.07	123.20
31	c	615	8CT	C40-C12-C13	-2.11	119.39	122.82
24	Y	304	CHL	C6-C5-C3	-2.11	108.32	113.47
25	8	306	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
31	t	101	8CT	C13-C14-C15	-2.11	117.08	123.20
27	r	316	XAT	C38-C25-C24	2.11	116.61	114.24
24	7	312	CHL	O1D-CGD-CBD	-2.11	121.52	124.72
25	s	410	CLA	C1-C2-C3	-2.11	122.74	126.20
24	u	305	CHL	OMC-CMC-C2C	-2.11	121.46	125.12
29	n	301	0UR	C15-C14-C13	-2.11	117.09	123.20
25	B	602	CLA	CMB-C2B-C1B	-2.11	122.21	125.42
24	R	601	CHL	CMA-C3A-C4A	-2.11	110.07	114.61
24	G	310	CHL	CMA-C3A-C4A	-2.11	110.07	114.61
25	r	314	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
28	r	301	NEX	C17-C1-C6	-2.11	108.58	110.47
25	Y	316	CLA	CMB-C2B-C1B	-2.11	122.21	125.42
25	b	603	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
24	2	312	CHL	O2D-CGD-O1D	-2.11	119.75	123.85
29	1	301	0UR	C34-C27-C26	2.11	118.30	114.42
31	s	415	8CT	C39-C16-C17	-2.11	119.40	122.82
25	B	613	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
25	A	605	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
25	2	317	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
29	2	301	0UR	C22-C16-C15	-2.11	119.40	122.82
24	9	304	CHL	CMA-C3A-C4A	-2.11	110.07	114.61
39	d	406	PL9	C12-C13-C14	-2.11	122.80	127.62
25	B	608	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
25	Y	307	CLA	CMB-C2B-C3B	2.10	131.50	126.55
25	C	605	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
25	4	306	CLA	CMB-C2B-C1B	-2.10	122.22	125.42
24	S	607	CHL	O2D-CGD-O1D	-2.10	119.75	123.85
29	Y	301	0UR	C22-C16-C17	2.10	121.30	118.09
29	1	301	0UR	C22-C16-C15	-2.10	119.41	122.82
24	9	305	CHL	CMB-C2B-C3B	2.10	128.88	124.68
24	S	607	CHL	OMC-CMC-C2C	-2.10	121.47	125.12
31	c	614	8CT	C13-C14-C15	-2.10	117.11	123.20
24	5	312	CHL	OMC-CMC-C2C	-2.10	121.47	125.12
24	2	305	CHL	CMA-C3A-C4A	-2.10	110.08	114.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	s	402	CHL	CAC-C3C-C4C	2.10	129.43	124.03
24	g	310	CHL	CMA-C3A-C4A	-2.10	110.08	114.61
25	g	317	CLA	CMB-C2B-C1B	-2.10	122.22	125.42
24	R	608	CHL	O2A-CGA-CBA	2.10	120.64	114.00
25	n	307	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
29	5	301	0UR	C33-C32-C31	-2.10	118.39	123.36
24	G	313	CHL	CBC-CAC-C3C	-2.10	109.87	112.87
26	g	303	0IE	C23-C16-C17	2.10	121.29	118.09
25	B	603	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
25	q	306	CLA	CMB-C2B-C1B	-2.10	122.23	125.42
28	N	303	NEX	C28-C29-C30	2.10	122.31	119.01
24	u	306	CHL	CMA-C3A-C4A	-2.10	110.09	114.61
24	8	310	CHL	CAC-C3C-C4C	2.10	129.42	124.03
24	u	310	CHL	CMA-C3A-C4A	-2.09	110.10	114.61
24	2	309	CHL	C4D-CHA-CBD	-2.09	106.86	108.97
25	9	306	CLA	C1-C2-C3	-2.09	122.77	126.20
25	b	603	CLA	C1-C2-C3	-2.09	122.77	126.20
31	T	101	8CT	C13-C14-C15	-2.09	117.14	123.20
24	N	311	CHL	OMC-CMC-C2C	-2.09	121.49	125.12
24	5	318	CHL	OMC-CMC-C2C	-2.09	121.49	125.12
25	d	404	CLA	C1-C2-C3	-2.09	122.77	126.20
24	3	308	CHL	C4D-CHA-CBD	-2.09	106.86	108.97
25	C	602	CLA	C1-C2-C3	-2.09	122.77	126.20
24	6	308	CHL	C4D-CHA-CBD	-2.09	106.86	108.97
26	3	303	0IE	C20-C3-C2	2.09	119.81	115.01
24	y	312	CHL	O2D-CGD-O1D	-2.09	119.78	123.85
31	c	613	8CT	C37-C35-C30	-2.09	106.38	109.55
28	r	301	NEX	C28-C29-C30	2.09	122.29	119.01
24	q	311	CHL	CAC-C3C-C4C	2.09	129.40	124.03
26	y	303	0IE	C20-C3-C2	2.09	119.80	115.01
24	n	308	CHL	C4D-CHA-CBD	-2.09	106.86	108.97
24	s	403	CHL	CAC-C3C-C4C	2.09	129.39	124.03
26	5	303	0IE	C23-C16-C17	2.09	121.28	118.09
24	2	318	CHL	OMC-CMC-C2C	-2.09	121.50	125.12
24	8	308	CHL	CAC-C3C-C4C	2.09	129.39	124.03
31	c	615	8CT	C04-C03-C10	2.09	121.31	115.65
25	b	602	CLA	CMB-C2B-C1B	-2.09	122.24	125.42
24	p	312	CHL	O2A-CGA-CBA	2.09	120.02	112.14
24	1	309	CHL	CMA-C3A-C4A	-2.08	110.12	114.61
24	4	309	CHL	CMA-C3A-C4A	-2.08	110.12	114.61
24	r	302	CHL	CMA-C3A-C4A	-2.08	110.12	114.61
25	c	610	CLA	CMB-C2B-C1B	-2.08	122.25	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	u	305	CHL	CMA-C3A-C4A	-2.08	110.12	114.61
29	g	301	0UR	C28-C19-C18	-2.08	110.43	112.83
25	c	609	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
24	q	308	CHL	CAC-C3C-C4C	2.08	129.39	124.03
28	6	303	NEX	C28-C29-C30	2.08	122.29	119.01
29	y	301	0UR	C22-C16-C17	2.08	121.27	118.09
25	N	307	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
24	y	309	CHL	OMC-CMC-C2C	-2.08	121.50	125.12
24	r	302	CHL	OMC-CMC-C2C	-2.08	121.50	125.12
24	S	608	CHL	CAC-C3C-C4C	2.08	129.38	124.03
24	2	313	CHL	CAA-C2A-C3A	-2.08	111.46	116.23
25	9	314	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
29	3	301	0UR	C10-C9-C8	-2.08	119.26	123.52
31	S	614	8CT	C39-C16-C17	-2.08	119.44	122.82
35	d	403	PHO	O2A-CGA-O1A	-2.08	118.42	123.63
25	b	612	CLA	CMB-C2B-C3B	2.08	131.44	126.55
25	u	315	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
29	4	301	0UR	C22-C16-C15	-2.08	119.45	122.82
24	S	601	CHL	CMA-C3A-C4A	-2.08	110.13	114.61
24	9	309	CHL	CBC-CAC-C3C	-2.08	109.90	112.87
24	r	309	CHL	O2A-CGA-CBA	2.08	120.57	114.00
37	c	618	DGD	O5D-C6D-C5D	2.08	114.11	109.42
33	W	201	LMG	C4-C3-C2	-2.08	107.18	110.83
30	5	319	LHG	C5-O7-C7	-2.08	112.82	117.80
24	p	310	CHL	CBC-CAC-C3C	-2.08	109.90	112.87
28	n	303	NEX	C28-C29-C30	2.08	122.28	119.01
25	D	404	CLA	O2D-CGD-CBD	2.08	114.86	111.23
24	1	312	CHL	CMA-C3A-C4A	-2.08	110.14	114.61
25	1	306	CLA	CMB-C2B-C1B	-2.08	122.26	125.42
24	Y	312	CHL	O2D-CGD-O1D	-2.08	119.81	123.85
24	s	408	CHL	O2A-CGA-CBA	2.08	120.56	114.00
25	y	308	CLA	CMB-C2B-C3B	2.08	131.43	126.55
25	p	317	CLA	C1-C2-C3	-2.08	122.80	126.20
25	b	608	CLA	CMB-C2B-C1B	-2.08	122.26	125.42
29	g	301	0UR	C20-C7-C6	2.07	121.26	118.09
24	r	306	CHL	CMA-C3A-C4A	-2.07	110.14	114.61
25	8	306	CLA	CMB-C2B-C1B	-2.07	122.26	125.42
26	u	302	0IE	C23-C16-C17	2.07	121.25	118.09
24	5	306	CHL	O2A-CGA-CBA	2.07	119.97	112.14
24	G	318	CHL	CMA-C3A-C2A	-2.07	111.48	116.23
25	N	306	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
25	c	603	CLA	C1-C2-C3	-2.07	122.80	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	B	618	SQD	O8-S-C6	2.07	109.97	105.97
24	1	312	CHL	C1B-CHB-C4A	2.07	122.66	121.32
24	S	602	CHL	CAC-C3C-C4C	2.07	129.36	124.03
27	R	615	XAT	O4-C5-C6	-2.07	57.29	58.93
24	R	601	CHL	OMC-CMC-C2C	-2.07	121.52	125.12
29	1	301	0UR	C21-C12-C11	-2.07	119.46	122.82
24	8	307	CHL	CMA-C3A-C4A	-2.07	110.15	114.61
24	5	318	CHL	C4D-CHA-CBD	-2.07	106.88	108.97
30	1	318	LHG	C26-C25-C24	2.07	120.73	113.13
24	2	306	CHL	O2A-CGA-CBA	2.07	119.96	112.14
29	p	301	0UR	C4-C5-C6	-2.07	117.21	123.20
31	X	601	8CT	C35-C30-C29	-2.07	110.45	112.83
25	B	603	CLA	C1-C2-C3	-2.07	122.81	126.20
24	S	601	CHL	CAC-C3C-C4C	2.07	129.35	124.03
32	b	618	SQD	C4-C3-C2	2.07	114.46	110.83
29	5	301	0UR	C22-C16-C15	-2.07	119.47	122.82
24	7	312	CHL	O2A-CGA-CBA	2.07	119.95	112.14
24	Y	311	CHL	O1D-CGD-CBD	-2.07	121.59	124.72
24	N	309	CHL	CAC-C3C-C4C	2.07	129.34	124.03
30	4	318	LHG	C26-C25-C24	2.07	120.72	113.13
24	u	310	CHL	CBC-CAC-C3C	-2.07	109.92	112.87
24	s	408	CHL	O2D-CGD-O1D	-2.07	119.83	123.85
25	C	603	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
25	c	610	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
25	d	404	CLA	O2D-CGD-CBD	2.07	114.84	111.23
25	8	305	CLA	C1-C2-C3	-2.07	122.81	126.20
24	5	305	CHL	CMA-C3A-C4A	-2.07	110.16	114.61
28	s	401	NEX	C28-C29-C30	2.06	122.26	119.01
24	9	312	CHL	CAC-C3C-C4C	2.06	129.34	124.03
24	p	305	CHL	CAC-C3C-C4C	2.06	129.34	124.03
24	5	306	CHL	CAC-C3C-C4C	2.06	129.34	124.03
25	C	609	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
24	2	306	CHL	CAC-C3C-C4C	2.06	129.33	124.03
25	B	608	CLA	CMB-C2B-C1B	-2.06	122.28	125.42
24	Y	312	CHL	CAC-C3C-C4C	2.06	129.33	124.03
24	n	309	CHL	CAC-C3C-C4C	2.06	129.33	124.03
37	c	619	DGD	O3D-C3D-C2D	-2.06	105.52	110.38
25	c	603	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
24	9	310	CHL	CMA-C3A-C4A	-2.06	110.17	114.61
24	Y	308	CHL	OMC-CMC-C2C	-2.06	121.54	125.12
24	s	409	CHL	CAC-C3C-C4C	2.06	129.33	124.03
25	A	604	CLA	CHB-C1B-NB	2.06	127.14	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	y	311	CHL	O2A-CGA-O1A	-2.06	118.48	123.63
24	Y	311	CHL	O2D-CGD-O1D	-2.06	119.84	123.85
31	D	410	8CT	C27-C26-C28	2.06	121.23	118.09
33	W	201	LMG	O8-C28-O10	-2.06	118.48	123.63
24	g	312	CHL	O2D-CGD-O1D	-2.06	119.84	123.85
24	S	606	CHL	OMC-CMC-C2C	-2.06	121.55	125.12
28	3	318	NEX	C28-C29-C30	2.06	122.25	119.01
25	g	307	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
24	S	607	CHL	CAC-C3C-C4C	2.06	129.31	124.03
24	s	407	CHL	OMC-CMC-C2C	-2.06	121.55	125.12
24	R	601	CHL	CBC-CAC-C3C	-2.06	109.93	112.87
24	G	312	CHL	CMA-C3A-C4A	-2.05	110.18	114.61
25	5	308	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
25	A	603	CLA	O1D-CGD-CBD	2.05	128.57	124.52
24	5	313	CHL	CAA-C2A-C3A	-2.05	111.52	116.23
29	3	301	0UR	C4-C5-C6	-2.05	117.25	123.20
29	g	301	0UR	C23-C24-C25	-2.05	109.09	113.59
24	y	310	CHL	CAC-C3C-C4C	2.05	129.31	124.03
29	G	301	0UR	C28-C19-C18	-2.05	110.47	112.83
32	d	409	SQD	O47-C7-O49	-2.05	118.91	123.70
24	g	318	CHL	CMA-C3A-C2A	-2.05	111.52	116.23
24	S	607	CHL	O2A-CGA-CBA	2.05	120.48	114.00
24	1	308	CHL	CMA-C3A-C4A	-2.05	110.19	114.61
24	4	310	CHL	C1B-CHB-C4A	2.05	122.64	121.32
24	9	305	CHL	CAC-C3C-C4C	2.05	129.31	124.03
24	n	308	CHL	CMA-C3A-C4A	-2.05	110.19	114.61
29	5	301	0UR	C4-C5-C6	-2.05	117.25	123.20
25	C	602	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
25	b	606	CLA	CMB-C2B-C3B	2.05	131.37	126.55
24	1	305	CHL	O2A-CGA-CBA	2.05	120.48	114.00
24	u	313	CHL	CAC-C3C-C4C	2.05	129.30	124.03
24	R	605	CHL	CMA-C3A-C2A	-2.05	111.53	116.23
24	R	605	CHL	CAC-C3C-C4C	2.05	129.30	124.03
24	2	318	CHL	CMA-C3A-C2A	-2.05	111.54	116.23
29	2	301	0UR	C4-C5-C6	-2.05	117.27	123.20
24	u	306	CHL	CAC-C3C-C4C	2.05	129.29	124.03
25	c	611	CLA	CMB-C2B-C3B	2.05	131.36	126.55
24	y	311	CHL	CBC-CAC-C3C	-2.05	109.94	112.87
25	n	306	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
30	a	612	LHG	C26-C25-C24	2.05	120.64	113.13
24	6	305	CHL	CAC-C3C-C4C	2.05	129.29	124.03
24	y	313	CHL	CAC-C3C-C4C	2.05	129.29	124.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	610	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
24	9	309	CHL	CMA-C3A-C4A	-2.04	110.20	114.61
25	6	306	CLA	CMA-C3A-C2A	-2.04	111.54	116.23
25	9	316	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
24	u	311	CHL	CMA-C3A-C4A	-2.04	110.21	114.61
25	3	306	CLA	CMA-C3A-C2A	-2.04	111.54	116.23
25	C	611	CLA	CMB-C2B-C3B	2.04	131.36	126.55
24	n	311	CHL	O2D-CGD-O1D	-2.04	119.87	123.85
24	Y	317	CHL	CAC-C3C-C4C	2.04	129.28	124.03
24	G	312	CHL	O2D-CGD-O1D	-2.04	119.87	123.85
30	A	612	LHG	C26-C25-C24	2.04	120.63	113.13
25	b	603	CLA	CMB-C2B-C3B	2.04	131.35	126.55
24	n	311	CHL	OMC-CMC-C2C	-2.04	121.58	125.12
24	y	313	CHL	O2D-CGD-O1D	-2.04	119.88	123.85
25	B	614	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
25	a	604	CLA	CHB-C1B-NB	2.04	127.11	124.05
25	G	307	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
25	c	602	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
31	D	410	8CT	C14-C15-C16	-2.04	120.77	126.36
24	2	318	CHL	C4D-CHA-CBD	-2.04	106.91	108.97
24	S	605	CHL	OMC-CMC-C2C	-2.04	121.58	125.12
25	c	601	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
25	R	610	CLA	CMB-C2B-C3B	2.04	131.34	126.55
24	G	306	CHL	CAC-C3C-C4C	2.04	129.27	124.03
26	Y	303	0IE	C20-C3-C2	2.04	119.69	115.01
24	g	306	CHL	CAC-C3C-C4C	2.04	129.27	124.03
24	s	408	CHL	CAC-C3C-C4C	2.04	129.27	124.03
25	c	612	CLA	CAA-C2A-C3A	-2.04	107.50	113.00
24	9	311	CHL	O2A-CGA-CBA	2.04	119.83	112.14
29	y	301	0UR	C14-C15-C16	-2.04	124.42	127.28
24	Y	304	CHL	CAC-C3C-C4C	2.04	129.26	124.03
24	4	312	CHL	CAC-C3C-C4C	2.04	129.26	124.03
25	r	313	CLA	O2A-CGA-O1A	-2.04	118.10	123.33
25	C	608	CLA	O2A-CGA-O1A	-2.04	118.54	123.63
24	y	311	CHL	C1-O2A-CGA	2.04	121.58	116.65
25	8	312	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
24	R	602	CHL	O2A-CGA-CBA	2.03	119.83	112.14
24	5	318	CHL	CMA-C3A-C2A	-2.03	111.56	116.23
25	c	608	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
24	4	308	CHL	OMC-CMC-C2C	-2.03	121.59	125.12
25	d	405	CLA	O2D-CGD-CBD	2.03	114.79	111.23
25	A	603	CLA	CAA-CBA-CGA	-2.03	107.43	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	612	CLA	CHB-C1B-NB	2.03	127.10	124.05
26	l	302	0IE	C14-C15-C16	2.03	130.13	127.28
24	q	309	CHL	C1-O2A-CGA	2.03	121.57	116.65
24	Y	309	CHL	CAC-C3C-C4C	2.03	129.26	124.03
24	g	313	CHL	CMA-C3A-C4A	-2.03	110.23	114.61
24	S	605	CHL	CAC-C3C-C4C	2.03	129.25	124.03
24	p	310	CHL	CAC-C3C-C4C	2.03	129.25	124.03
32	B	618	SQD	C4-C3-C2	2.03	114.40	110.83
24	u	312	CHL	O2A-CGA-CBA	2.03	119.82	112.14
25	q	313	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
24	3	304	CHL	OMC-CMC-C2C	-2.03	121.59	125.12
29	4	301	0UR	C21-C12-C11	-2.03	119.52	122.82
24	g	309	CHL	CMA-C3A-C4A	-2.03	110.23	114.61
24	y	312	CHL	O1D-CGD-CBD	-2.03	121.64	124.72
24	3	308	CHL	CMA-C3A-C4A	-2.03	110.23	114.61
24	r	303	CHL	O2A-CGA-CBA	2.03	119.81	112.14
37	c	618	DGD	O6D-C5D-C4D	-2.03	106.04	109.70
25	N	314	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
25	b	616	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
35	D	403	PHO	O2A-CGA-O1A	-2.03	118.55	123.63
29	7	301	0UR	C4-C5-C6	-2.03	117.32	123.20
25	a	610	CLA	CMB-C2B-C1B	-2.03	122.33	125.42
25	C	606	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
25	g	317	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
24	l	312	CHL	CAC-C3C-C4C	2.03	129.25	124.03
29	G	301	0UR	C23-C24-C25	-2.03	109.14	113.59
24	n	317	CHL	C3D-C4D-ND	-2.03	109.69	112.94
25	B	606	CLA	CMB-C2B-C3B	2.03	131.32	126.55
25	c	601	CLA	O2D-CGD-CBD	2.03	114.77	111.23
24	7	310	CHL	CAC-C3C-C4C	2.03	129.24	124.03
25	N	306	CLA	C1-C2-C3	-2.03	122.88	126.20
24	u	311	CHL	OMC-CMC-C2C	-2.03	121.60	125.12
24	u	318	CHL	OMC-CMC-C2C	-2.03	121.60	125.12
25	B	612	CLA	CMB-C2B-C3B	2.02	131.31	126.55
24	S	607	CHL	CMA-C3A-C4A	-2.02	110.25	114.61
24	g	312	CHL	CMA-C3A-C4A	-2.02	110.25	114.61
24	l	310	CHL	C1B-CHB-C4A	2.02	122.62	121.32
24	N	311	CHL	O2D-CGD-O1D	-2.02	119.91	123.85
24	G	309	CHL	CMA-C3A-C4A	-2.02	110.25	114.61
25	c	605	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
24	9	317	CHL	OMC-CMC-C2C	-2.02	121.61	125.12
25	u	314	CLA	CMB-C2B-C1B	-2.02	122.34	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	607	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
24	5	305	CHL	CAC-C3C-C4C	2.02	129.23	124.03
32	D	409	SQD	O47-C7-O49	-2.02	118.98	123.70
23	E	201	HEM	C4D-ND-C1D	2.02	107.60	105.21
24	9	310	CHL	OMC-CMC-C2C	-2.02	121.61	125.12
25	A	603	CLA	C1-C2-C3	-2.02	122.89	126.20
25	q	305	CLA	C1-C2-C3	-2.02	122.89	126.20
32	B	618	SQD	C44-O6-C1	2.02	118.13	113.80
25	8	314	CLA	CMB-C2B-C1B	-2.02	122.34	125.42
24	Y	319	CHL	C1-O2A-CGA	2.02	121.54	116.65
24	p	309	CHL	CMA-C3A-C4A	-2.02	110.26	114.61
24	y	318	CHL	CAC-C3C-C4C	2.02	129.22	124.03
25	b	615	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
24	q	309	CHL	OMC-CMC-C2C	-2.02	121.61	125.12
25	2	308	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
29	4	301	OUR	C4-C5-C6	-2.02	117.35	123.20
39	D	406	PL9	C32-C33-C34	-2.02	123.01	127.62
24	3	305	CHL	CAC-C3C-C4C	2.02	129.22	124.03
25	B	615	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
24	5	313	CHL	CAC-C3C-C4C	2.02	129.21	124.03
24	s	406	CHL	CAC-C3C-C4C	2.02	129.21	124.03
25	D	405	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
25	D	405	CLA	O2D-CGD-CBD	2.02	114.75	111.23
24	4	312	CHL	CMA-C3A-C4A	-2.02	110.27	114.61
25	n	314	CLA	O2A-CGA-O1A	-2.02	118.59	123.63
25	c	606	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
25	d	405	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
25	u	315	CLA	C1-C2-C3	-2.01	122.90	126.20
25	S	612	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
30	2	319	LHG	C5-O7-C7	-2.01	112.98	117.80
30	y	319	LHG	C5-O7-C7	-2.01	112.98	117.80
25	s	413	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
24	s	406	CHL	OMC-CMC-C2C	-2.01	121.62	125.12
24	2	312	CHL	O2A-CGA-CBA	2.01	120.36	114.00
29	u	301	OUR	C14-C13-C12	-2.01	120.84	126.36
24	G	312	CHL	CAA-CBA-CGA	-2.01	107.49	113.21
24	2	310	CHL	CAC-C3C-C4C	2.01	129.20	124.03
24	1	312	CHL	O2A-CGA-CBA	2.01	120.36	114.00
25	B	603	CLA	CMB-C2B-C3B	2.01	131.28	126.55
24	G	310	CHL	CAC-C3C-C4C	2.01	129.20	124.03
24	7	318	CHL	CMA-C3A-C2A	-2.01	111.62	116.23
24	4	312	CHL	O2A-CGA-CBA	2.01	120.35	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	S	615	8CT	C15-C16-C17	2.01	122.17	119.01
27	r	316	XAT	O4-C5-C6	-2.01	57.34	58.93
24	N	304	CHL	C1B-CHB-C4A	-2.01	120.03	121.32
24	7	305	CHL	CAC-C3C-C4C	2.01	129.20	124.03
25	5	315	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
25	c	616	CLA	CMB-C2B-C1B	-2.01	122.36	125.42
24	G	305	CHL	OMC-CMC-C2C	-2.01	121.63	125.12
25	A	610	CLA	O2D-CGD-CBD	2.01	114.74	111.23
24	5	313	CHL	CMA-C3A-C2A	-2.01	111.62	116.23
24	4	308	CHL	CMA-C3A-C4A	-2.01	110.28	114.61
25	a	603	CLA	CAA-CBA-CGA	-2.01	107.51	113.21
25	9	314	CLA	C1-C2-C3	-2.01	122.91	126.20
24	3	304	CHL	CMA-C3A-C4A	-2.01	110.29	114.61
27	R	615	XAT	O24-C25-C26	-2.01	57.34	58.93
25	n	306	CLA	C1-C2-C3	-2.01	122.91	126.20
24	8	303	CHL	CMA-C3A-C4A	-2.01	110.29	114.61
32	b	618	SQD	C44-O6-C1	2.01	118.10	113.80
25	a	603	CLA	O1D-CGD-CBD	2.01	128.47	124.52
25	r	305	CLA	O1D-CGD-CBD	2.01	128.47	124.52
39	D	406	PL9	O2-C1-C2	-2.00	117.27	121.83
29	q	301	0UR	C29-C30-C31	-2.00	108.21	111.18
39	d	406	PL9	O2-C1-C2	-2.00	117.27	121.83
24	2	313	CHL	CAC-C3C-C4C	2.00	129.18	124.03
24	5	312	CHL	O2A-CGA-CBA	2.00	120.33	114.00
25	b	614	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
24	9	309	CHL	O2A-CGA-CBA	2.00	120.33	114.00
24	6	304	CHL	CMA-C3A-C4A	-2.00	110.30	114.61
29	Y	301	0UR	C14-C15-C16	-2.00	124.47	127.28
24	r	306	CHL	CAC-C3C-C4C	2.00	129.18	124.03
32	a	609	SQD	C4-C3-C2	2.00	114.34	110.83
24	5	310	CHL	CAC-C3C-C4C	2.00	129.17	124.03
28	p	304	NEX	C24-C23-C22	-2.00	107.05	110.79
24	g	310	CHL	CAC-C3C-C4C	2.00	129.17	124.03
24	Y	310	CHL	CBC-CAC-C3C	-2.00	110.01	112.87
25	A	607	CLA	CMB-C2B-C3B	2.00	131.25	126.55
26	4	302	0IE	C14-C15-C16	2.00	130.08	127.28

All (718) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	R	601	CHL	NA
24	R	601	CHL	NC

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Mol	Chain	Res	Type	Atom
24	R	601	CHL	ND
24	R	602	CHL	NA
24	R	602	CHL	NC
24	R	602	CHL	ND
24	R	605	CHL	NA
24	R	605	CHL	NC
24	R	605	CHL	ND
24	R	606	CHL	NA
24	R	606	CHL	NC
24	R	606	CHL	ND
24	R	607	CHL	NA
24	R	607	CHL	NC
24	R	607	CHL	ND
24	R	608	CHL	NA
24	R	608	CHL	NC
24	R	608	CHL	ND
24	1	304	CHL	NA
24	1	304	CHL	NC
24	1	304	CHL	ND
24	1	305	CHL	NA
24	1	305	CHL	NC
24	1	305	CHL	ND
24	1	308	CHL	NA
24	1	308	CHL	NC
24	1	308	CHL	ND
24	1	309	CHL	NA
24	1	309	CHL	NC
24	1	309	CHL	ND
24	1	310	CHL	NA
24	1	310	CHL	NC
24	1	310	CHL	ND
24	1	311	CHL	NA
24	1	311	CHL	NC
24	1	311	CHL	ND
24	1	312	CHL	NA
24	1	312	CHL	NC
24	1	312	CHL	ND
24	1	317	CHL	NA
24	1	317	CHL	NC
24	1	317	CHL	ND
24	2	305	CHL	NA
24	2	305	CHL	NC

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Mol	Chain	Res	Type	Atom
24	2	305	CHL	ND
24	2	306	CHL	NA
24	2	306	CHL	NC
24	2	306	CHL	ND
24	2	309	CHL	NA
24	2	309	CHL	NC
24	2	309	CHL	ND
24	2	310	CHL	NA
24	2	310	CHL	NC
24	2	310	CHL	ND
24	2	311	CHL	NA
24	2	311	CHL	NC
24	2	311	CHL	ND
24	2	312	CHL	NA
24	2	312	CHL	NC
24	2	312	CHL	ND
24	2	313	CHL	NA
24	2	313	CHL	NC
24	2	313	CHL	ND
24	2	318	CHL	NA
24	2	318	CHL	NC
24	2	318	CHL	ND
24	3	304	CHL	NA
24	3	304	CHL	NC
24	3	304	CHL	ND
24	3	305	CHL	NA
24	3	305	CHL	NC
24	3	305	CHL	ND
24	3	308	CHL	NA
24	3	308	CHL	NC
24	3	308	CHL	ND
24	3	309	CHL	NA
24	3	309	CHL	NC
24	3	309	CHL	ND
24	3	310	CHL	NA
24	3	310	CHL	NC
24	3	310	CHL	ND
24	3	311	CHL	NA
24	3	311	CHL	NC
24	3	311	CHL	ND
24	3	312	CHL	NA
24	3	312	CHL	NC

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Mol	Chain	Res	Type	Atom
24	3	312	CHL	ND
24	3	317	CHL	NA
24	3	317	CHL	NC
24	3	317	CHL	ND
24	S	601	CHL	NA
24	S	601	CHL	NC
24	S	601	CHL	ND
24	S	602	CHL	NA
24	S	602	CHL	NC
24	S	602	CHL	ND
24	S	605	CHL	NA
24	S	605	CHL	NC
24	S	605	CHL	ND
24	S	606	CHL	NA
24	S	606	CHL	NC
24	S	606	CHL	ND
24	S	607	CHL	NA
24	S	607	CHL	NC
24	S	607	CHL	ND
24	S	608	CHL	NA
24	S	608	CHL	NC
24	S	608	CHL	ND
24	S	613	CHL	NA
24	S	613	CHL	NC
24	S	613	CHL	ND
24	G	305	CHL	NA
24	G	305	CHL	NC
24	G	305	CHL	ND
24	G	306	CHL	NA
24	G	306	CHL	NC
24	G	306	CHL	ND
24	G	309	CHL	NA
24	G	309	CHL	NC
24	G	309	CHL	ND
24	G	310	CHL	NA
24	G	310	CHL	NC
24	G	310	CHL	ND
24	G	311	CHL	NA
24	G	311	CHL	NC
24	G	311	CHL	ND
24	G	312	CHL	NA
24	G	312	CHL	NC

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Mol	Chain	Res	Type	Atom
24	G	312	CHL	ND
24	G	313	CHL	NA
24	G	313	CHL	NC
24	G	313	CHL	ND
24	G	318	CHL	NA
24	G	318	CHL	NC
24	G	318	CHL	ND
24	9	304	CHL	NA
24	9	304	CHL	NC
24	9	304	CHL	ND
24	9	305	CHL	NA
24	9	305	CHL	NC
24	9	305	CHL	ND
24	9	308	CHL	NA
24	9	308	CHL	NC
24	9	308	CHL	ND
24	9	309	CHL	NA
24	9	309	CHL	NC
24	9	309	CHL	ND
24	9	310	CHL	NA
24	9	310	CHL	NC
24	9	310	CHL	ND
24	9	311	CHL	NA
24	9	311	CHL	NC
24	9	311	CHL	ND
24	9	312	CHL	NA
24	9	312	CHL	NC
24	9	312	CHL	ND
24	9	317	CHL	NA
24	9	317	CHL	NC
24	9	317	CHL	ND
24	N	304	CHL	NA
24	N	304	CHL	NC
24	N	304	CHL	ND
24	N	305	CHL	NA
24	N	305	CHL	NC
24	N	305	CHL	ND
24	N	308	CHL	NA
24	N	308	CHL	NC
24	N	308	CHL	ND
24	N	309	CHL	NA
24	N	309	CHL	NC

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Mol	Chain	Res	Type	Atom
24	N	309	CHL	ND
24	N	310	CHL	NA
24	N	310	CHL	NC
24	N	310	CHL	ND
24	N	311	CHL	NA
24	N	311	CHL	NC
24	N	311	CHL	ND
24	N	312	CHL	NA
24	N	312	CHL	NC
24	N	312	CHL	ND
24	N	317	CHL	NA
24	N	317	CHL	NC
24	N	317	CHL	ND
24	Y	304	CHL	NA
24	Y	304	CHL	NC
24	Y	304	CHL	ND
24	Y	305	CHL	NA
24	Y	305	CHL	NC
24	Y	305	CHL	ND
24	Y	308	CHL	NA
24	Y	308	CHL	NC
24	Y	308	CHL	ND
24	Y	309	CHL	NA
24	Y	309	CHL	NC
24	Y	309	CHL	ND
24	Y	310	CHL	NA
24	Y	310	CHL	NC
24	Y	310	CHL	ND
24	Y	311	CHL	NA
24	Y	311	CHL	NC
24	Y	311	CHL	ND
24	Y	312	CHL	NA
24	Y	312	CHL	NC
24	Y	312	CHL	ND
24	Y	317	CHL	NA
24	Y	317	CHL	NC
24	Y	317	CHL	ND
24	Y	319	CHL	NA
24	Y	319	CHL	NC
24	Y	319	CHL	ND
24	8	303	CHL	NA
24	8	303	CHL	NC

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Mol	Chain	Res	Type	Atom
24	8	303	CHL	ND
24	8	304	CHL	NA
24	8	304	CHL	NC
24	8	304	CHL	ND
24	8	307	CHL	NA
24	8	307	CHL	NC
24	8	307	CHL	ND
24	8	308	CHL	NA
24	8	308	CHL	NC
24	8	308	CHL	ND
24	8	309	CHL	NA
24	8	309	CHL	NC
24	8	309	CHL	ND
24	8	310	CHL	NA
24	8	310	CHL	NC
24	8	310	CHL	ND
24	8	315	CHL	NA
24	8	315	CHL	NC
24	8	315	CHL	ND
24	4	304	CHL	NA
24	4	304	CHL	NC
24	4	304	CHL	ND
24	4	305	CHL	NA
24	4	305	CHL	NC
24	4	305	CHL	ND
24	4	308	CHL	NA
24	4	308	CHL	NC
24	4	308	CHL	ND
24	4	309	CHL	NA
24	4	309	CHL	NC
24	4	309	CHL	ND
24	4	310	CHL	NA
24	4	310	CHL	NC
24	4	310	CHL	ND
24	4	311	CHL	NA
24	4	311	CHL	NC
24	4	311	CHL	ND
24	4	312	CHL	NA
24	4	312	CHL	NC
24	4	312	CHL	ND
24	4	317	CHL	NA
24	4	317	CHL	NC

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Mol	Chain	Res	Type	Atom
24	4	317	CHL	ND
24	5	305	CHL	NA
24	5	305	CHL	NC
24	5	305	CHL	ND
24	5	306	CHL	NA
24	5	306	CHL	NC
24	5	306	CHL	ND
24	5	309	CHL	NA
24	5	309	CHL	NC
24	5	309	CHL	ND
24	5	310	CHL	NA
24	5	310	CHL	NC
24	5	310	CHL	ND
24	5	311	CHL	NA
24	5	311	CHL	NC
24	5	311	CHL	ND
24	5	312	CHL	NA
24	5	312	CHL	NC
24	5	312	CHL	ND
24	5	313	CHL	NA
24	5	313	CHL	NC
24	5	313	CHL	ND
24	5	318	CHL	NA
24	5	318	CHL	NC
24	5	318	CHL	ND
24	6	304	CHL	NA
24	6	304	CHL	NC
24	6	304	CHL	ND
24	6	305	CHL	NA
24	6	305	CHL	NC
24	6	305	CHL	ND
24	6	308	CHL	NA
24	6	308	CHL	NC
24	6	308	CHL	ND
24	6	309	CHL	NA
24	6	309	CHL	NC
24	6	309	CHL	ND
24	6	310	CHL	NA
24	6	310	CHL	NC
24	6	310	CHL	ND
24	6	311	CHL	NA
24	6	311	CHL	NC

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Mol	Chain	Res	Type	Atom
24	6	311	CHL	ND
24	6	312	CHL	NA
24	6	312	CHL	NC
24	6	312	CHL	ND
24	6	317	CHL	NA
24	6	317	CHL	NC
24	6	317	CHL	ND
24	g	305	CHL	NA
24	g	305	CHL	NC
24	g	305	CHL	ND
24	g	306	CHL	NA
24	g	306	CHL	NC
24	g	306	CHL	ND
24	g	309	CHL	NA
24	g	309	CHL	NC
24	g	309	CHL	ND
24	g	310	CHL	NA
24	g	310	CHL	NC
24	g	310	CHL	ND
24	g	311	CHL	NA
24	g	311	CHL	NC
24	g	311	CHL	ND
24	g	312	CHL	NA
24	g	312	CHL	NC
24	g	312	CHL	ND
24	g	313	CHL	NA
24	g	313	CHL	NC
24	g	313	CHL	ND
24	g	318	CHL	NA
24	g	318	CHL	NC
24	g	318	CHL	ND
24	u	305	CHL	NA
24	u	305	CHL	NC
24	u	305	CHL	ND
24	u	306	CHL	NA
24	u	306	CHL	NC
24	u	306	CHL	ND
24	u	309	CHL	NA
24	u	309	CHL	NC
24	u	309	CHL	ND
24	u	310	CHL	NA
24	u	310	CHL	NC

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Mol	Chain	Res	Type	Atom
24	u	310	CHL	ND
24	u	311	CHL	NA
24	u	311	CHL	NC
24	u	311	CHL	ND
24	u	312	CHL	NA
24	u	312	CHL	NC
24	u	312	CHL	ND
24	u	313	CHL	NA
24	u	313	CHL	NC
24	u	313	CHL	ND
24	u	318	CHL	NA
24	u	318	CHL	NC
24	u	318	CHL	ND
24	n	304	CHL	NA
24	n	304	CHL	NC
24	n	304	CHL	ND
24	n	305	CHL	NA
24	n	305	CHL	NC
24	n	305	CHL	ND
24	n	308	CHL	NA
24	n	308	CHL	NC
24	n	308	CHL	ND
24	n	309	CHL	NA
24	n	309	CHL	NC
24	n	309	CHL	ND
24	n	310	CHL	NA
24	n	310	CHL	NC
24	n	310	CHL	ND
24	n	311	CHL	NA
24	n	311	CHL	NC
24	n	311	CHL	ND
24	n	312	CHL	NA
24	n	312	CHL	NC
24	n	312	CHL	ND
24	n	317	CHL	NA
24	n	317	CHL	NC
24	n	317	CHL	ND
24	y	305	CHL	NA
24	y	305	CHL	NC
24	y	305	CHL	ND
24	y	306	CHL	NA
24	y	306	CHL	NC

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Mol	Chain	Res	Type	Atom
24	y	306	CHL	ND
24	y	309	CHL	NA
24	y	309	CHL	NC
24	y	309	CHL	ND
24	y	310	CHL	NA
24	y	310	CHL	NC
24	y	310	CHL	ND
24	y	311	CHL	NA
24	y	311	CHL	NC
24	y	311	CHL	ND
24	y	312	CHL	NA
24	y	312	CHL	NC
24	y	312	CHL	ND
24	y	313	CHL	NA
24	y	313	CHL	NC
24	y	313	CHL	ND
24	y	318	CHL	NA
24	y	318	CHL	NC
24	y	318	CHL	ND
24	p	305	CHL	NA
24	p	305	CHL	NC
24	p	305	CHL	ND
24	p	306	CHL	NA
24	p	306	CHL	NC
24	p	306	CHL	ND
24	p	309	CHL	NA
24	p	309	CHL	NC
24	p	309	CHL	ND
24	p	310	CHL	NA
24	p	310	CHL	NC
24	p	310	CHL	ND
24	p	311	CHL	NA
24	p	311	CHL	NC
24	p	311	CHL	ND
24	p	312	CHL	NA
24	p	312	CHL	NC
24	p	312	CHL	ND
24	p	313	CHL	NA
24	p	313	CHL	NC
24	p	313	CHL	ND
24	p	318	CHL	NA
24	p	318	CHL	NC

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Mol	Chain	Res	Type	Atom
24	p	318	CHL	ND
24	q	303	CHL	NA
24	q	303	CHL	NC
24	q	303	CHL	ND
24	q	304	CHL	NA
24	q	304	CHL	NC
24	q	304	CHL	ND
24	q	307	CHL	NA
24	q	307	CHL	NC
24	q	307	CHL	ND
24	q	308	CHL	NA
24	q	308	CHL	NC
24	q	308	CHL	ND
24	q	309	CHL	NA
24	q	309	CHL	NC
24	q	309	CHL	ND
24	q	310	CHL	NA
24	q	310	CHL	NC
24	q	310	CHL	ND
24	q	311	CHL	NA
24	q	311	CHL	NC
24	q	311	CHL	ND
24	q	316	CHL	NA
24	q	316	CHL	NC
24	q	316	CHL	ND
24	s	402	CHL	NA
24	s	402	CHL	NC
24	s	402	CHL	ND
24	s	403	CHL	NA
24	s	403	CHL	NC
24	s	403	CHL	ND
24	s	406	CHL	NA
24	s	406	CHL	NC
24	s	406	CHL	ND
24	s	407	CHL	NA
24	s	407	CHL	NC
24	s	407	CHL	ND
24	s	408	CHL	NA
24	s	408	CHL	NC
24	s	408	CHL	ND
24	s	409	CHL	NA
24	s	409	CHL	NC

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Mol	Chain	Res	Type	Atom
24	s	409	CHL	ND
24	s	414	CHL	NA
24	s	414	CHL	NC
24	s	414	CHL	ND
24	r	302	CHL	NA
24	r	302	CHL	NC
24	r	302	CHL	ND
24	r	303	CHL	NA
24	r	303	CHL	NC
24	r	303	CHL	ND
24	r	306	CHL	NA
24	r	306	CHL	NC
24	r	306	CHL	ND
24	r	307	CHL	NA
24	r	307	CHL	NC
24	r	307	CHL	ND
24	r	308	CHL	NA
24	r	308	CHL	NC
24	r	308	CHL	ND
24	r	309	CHL	NA
24	r	309	CHL	NC
24	r	309	CHL	ND
24	7	305	CHL	NA
24	7	305	CHL	NC
24	7	305	CHL	ND
24	7	306	CHL	NA
24	7	306	CHL	NC
24	7	306	CHL	ND
24	7	309	CHL	NA
24	7	309	CHL	NC
24	7	309	CHL	ND
24	7	310	CHL	NA
24	7	310	CHL	NC
24	7	310	CHL	ND
24	7	311	CHL	NA
24	7	311	CHL	NC
24	7	311	CHL	ND
24	7	312	CHL	NA
24	7	312	CHL	NC
24	7	312	CHL	ND
24	7	313	CHL	NA
24	7	313	CHL	NC

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Mol	Chain	Res	Type	Atom
24	7	313	CHL	ND
24	7	318	CHL	NA
24	7	318	CHL	NC
24	7	318	CHL	ND
25	R	603	CLA	ND
25	R	604	CLA	ND
25	R	609	CLA	ND
25	R	610	CLA	ND
25	R	611	CLA	ND
25	R	612	CLA	ND
25	R	613	CLA	ND
25	1	306	CLA	ND
25	1	307	CLA	ND
25	1	313	CLA	ND
25	1	314	CLA	ND
25	1	315	CLA	ND
25	1	316	CLA	ND
25	2	307	CLA	ND
25	2	308	CLA	ND
25	2	314	CLA	ND
25	2	315	CLA	ND
25	2	316	CLA	ND
25	2	317	CLA	ND
25	3	306	CLA	ND
25	3	307	CLA	ND
25	3	313	CLA	ND
25	3	314	CLA	ND
25	3	315	CLA	ND
25	3	316	CLA	ND
25	S	603	CLA	ND
25	S	604	CLA	ND
25	S	609	CLA	ND
25	S	610	CLA	ND
25	S	611	CLA	ND
25	S	612	CLA	ND
25	S	616	CLA	ND
25	G	307	CLA	ND
25	G	308	CLA	ND
25	G	314	CLA	ND
25	G	315	CLA	ND
25	G	316	CLA	ND
25	G	317	CLA	ND

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Mol	Chain	Res	Type	Atom
25	9	306	CLA	ND
25	9	307	CLA	ND
25	9	313	CLA	ND
25	9	314	CLA	ND
25	9	315	CLA	ND
25	9	316	CLA	ND
25	N	306	CLA	ND
25	N	307	CLA	ND
25	N	313	CLA	ND
25	N	314	CLA	ND
25	N	315	CLA	ND
25	N	316	CLA	ND
25	Y	306	CLA	ND
25	Y	307	CLA	ND
25	Y	313	CLA	ND
25	Y	314	CLA	ND
25	Y	315	CLA	ND
25	Y	316	CLA	ND
25	8	305	CLA	ND
25	8	306	CLA	ND
25	8	311	CLA	ND
25	8	312	CLA	ND
25	8	313	CLA	ND
25	8	314	CLA	ND
25	B	601	CLA	ND
25	B	602	CLA	ND
25	B	603	CLA	ND
25	B	604	CLA	ND
25	B	605	CLA	ND
25	B	606	CLA	ND
25	B	607	CLA	ND
25	B	608	CLA	ND
25	B	609	CLA	ND
25	B	610	CLA	ND
25	B	611	CLA	ND
25	B	612	CLA	ND
25	B	613	CLA	ND
25	B	614	CLA	ND
25	B	615	CLA	ND
25	B	616	CLA	ND
25	A	603	CLA	ND
25	A	604	CLA	ND

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Mol	Chain	Res	Type	Atom
25	A	605	CLA	ND
25	A	607	CLA	ND
25	A	610	CLA	ND
25	C	601	CLA	ND
25	C	602	CLA	ND
25	C	603	CLA	ND
25	C	604	CLA	ND
25	C	605	CLA	ND
25	C	606	CLA	ND
25	C	607	CLA	ND
25	C	608	CLA	ND
25	C	609	CLA	ND
25	C	610	CLA	ND
25	C	611	CLA	ND
25	C	612	CLA	ND
25	C	616	CLA	ND
25	D	404	CLA	ND
25	D	405	CLA	ND
25	4	306	CLA	ND
25	4	307	CLA	ND
25	4	313	CLA	ND
25	4	314	CLA	ND
25	4	315	CLA	ND
25	4	316	CLA	ND
25	5	307	CLA	ND
25	5	308	CLA	ND
25	5	314	CLA	ND
25	5	315	CLA	ND
25	5	316	CLA	ND
25	5	317	CLA	ND
25	6	306	CLA	ND
25	6	307	CLA	ND
25	6	313	CLA	ND
25	6	314	CLA	ND
25	6	315	CLA	ND
25	6	316	CLA	ND
25	g	307	CLA	ND
25	g	308	CLA	ND
25	g	314	CLA	ND
25	g	315	CLA	ND
25	g	316	CLA	ND
25	g	317	CLA	ND

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Mol	Chain	Res	Type	Atom
25	u	307	CLA	ND
25	u	308	CLA	ND
25	u	314	CLA	ND
25	u	315	CLA	ND
25	u	316	CLA	ND
25	u	317	CLA	ND
25	n	306	CLA	ND
25	n	307	CLA	ND
25	n	313	CLA	ND
25	n	314	CLA	ND
25	n	315	CLA	ND
25	n	316	CLA	ND
25	y	307	CLA	ND
25	y	308	CLA	ND
25	y	314	CLA	ND
25	y	315	CLA	ND
25	y	316	CLA	ND
25	y	317	CLA	ND
25	p	307	CLA	ND
25	p	308	CLA	ND
25	p	314	CLA	ND
25	p	315	CLA	ND
25	p	316	CLA	ND
25	p	317	CLA	ND
25	q	305	CLA	ND
25	q	306	CLA	ND
25	q	312	CLA	ND
25	q	313	CLA	ND
25	q	314	CLA	ND
25	q	315	CLA	ND
25	b	601	CLA	ND
25	b	602	CLA	ND
25	b	603	CLA	ND
25	b	604	CLA	ND
25	b	605	CLA	ND
25	b	606	CLA	ND
25	b	607	CLA	ND
25	b	608	CLA	ND
25	b	609	CLA	ND
25	b	610	CLA	ND
25	b	611	CLA	ND
25	b	612	CLA	ND

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Mol	Chain	Res	Type	Atom
25	b	613	CLA	ND
25	b	614	CLA	ND
25	b	615	CLA	ND
25	b	616	CLA	ND
25	a	603	CLA	ND
25	a	604	CLA	ND
25	a	605	CLA	ND
25	a	607	CLA	ND
25	a	610	CLA	ND
25	c	601	CLA	ND
25	c	602	CLA	ND
25	c	603	CLA	ND
25	c	604	CLA	ND
25	c	605	CLA	ND
25	c	606	CLA	ND
25	c	607	CLA	ND
25	c	608	CLA	ND
25	c	609	CLA	ND
25	c	610	CLA	ND
25	c	611	CLA	ND
25	c	612	CLA	ND
25	c	616	CLA	ND
25	d	404	CLA	ND
25	d	405	CLA	ND
25	s	404	CLA	ND
25	s	405	CLA	ND
25	s	410	CLA	ND
25	s	411	CLA	ND
25	s	412	CLA	ND
25	s	413	CLA	ND
25	s	417	CLA	ND
25	r	304	CLA	ND
25	r	305	CLA	ND
25	r	310	CLA	ND
25	r	311	CLA	ND
25	r	312	CLA	ND
25	r	313	CLA	ND
25	r	314	CLA	ND
25	7	307	CLA	ND
25	7	308	CLA	ND
25	7	314	CLA	ND
25	7	315	CLA	ND

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Mol	Chain	Res	Type	Atom
25	7	316	CLA	ND
25	7	317	CLA	ND

All (4267) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	R	601	CHL	C1C-C2C-CMC-OMC
24	R	601	CHL	C3C-C2C-CMC-OMC
24	R	606	CHL	C1A-C2A-CAA-CBA
24	R	607	CHL	C1C-C2C-CMC-OMC
24	R	607	CHL	C3C-C2C-CMC-OMC
24	R	608	CHL	C4C-C3C-CAC-CBC
24	1	305	CHL	C1C-C2C-CMC-OMC
24	1	312	CHL	C1C-C2C-CMC-OMC
24	1	312	CHL	CHA-CBD-CGD-O1D
24	1	317	CHL	CAD-CBD-CGD-O1D
24	1	317	CHL	CAD-CBD-CGD-O2D
24	2	305	CHL	C1C-C2C-CMC-OMC
24	2	305	CHL	C3C-C2C-CMC-OMC
24	2	306	CHL	C1C-C2C-CMC-OMC
24	2	306	CHL	C3C-C2C-CMC-OMC
24	2	306	CHL	CHA-CBD-CGD-O2D
24	2	312	CHL	C1C-C2C-CMC-OMC
24	2	312	CHL	C3C-C2C-CMC-OMC
24	2	312	CHL	CBD-CGD-O2D-CED
24	2	318	CHL	CAD-CBD-CGD-O1D
24	2	318	CHL	CAD-CBD-CGD-O2D
24	3	304	CHL	C1A-C2A-CAA-CBA
24	3	304	CHL	C3A-C2A-CAA-CBA
24	3	304	CHL	CHA-CBD-CGD-O1D
24	3	304	CHL	CHA-CBD-CGD-O2D
24	3	305	CHL	C1C-C2C-CMC-OMC
24	3	305	CHL	C3C-C2C-CMC-OMC
24	3	310	CHL	C1A-C2A-CAA-CBA
24	3	317	CHL	C1C-C2C-CMC-OMC
24	S	601	CHL	C1C-C2C-CMC-OMC
24	S	601	CHL	C3C-C2C-CMC-OMC
24	S	602	CHL	C1C-C2C-CMC-OMC
24	S	602	CHL	C3C-C2C-CMC-OMC
24	S	606	CHL	C1A-C2A-CAA-CBA
24	S	606	CHL	CHA-CBD-CGD-O1D
24	S	607	CHL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	S	608	CHL	C1C-C2C-CMC-OMC
24	S	608	CHL	C3C-C2C-CMC-OMC
24	S	608	CHL	C4C-C3C-CAC-CBC
24	S	613	CHL	C1C-C2C-CMC-OMC
24	S	613	CHL	C3C-C2C-CMC-OMC
24	G	305	CHL	C3A-C2A-CAA-CBA
24	G	306	CHL	C1C-C2C-CMC-OMC
24	G	306	CHL	C3C-C2C-CMC-OMC
24	G	306	CHL	C6-C7-C8-C9
24	G	311	CHL	C1A-C2A-CAA-CBA
24	G	311	CHL	CHA-CBD-CGD-O1D
24	G	311	CHL	CHA-CBD-CGD-O2D
24	G	311	CHL	CBD-CGD-O2D-CED
24	G	312	CHL	CBD-CGD-O2D-CED
24	G	313	CHL	C4C-C3C-CAC-CBC
24	G	318	CHL	C1C-C2C-CMC-OMC
24	G	318	CHL	C3C-C2C-CMC-OMC
24	G	318	CHL	CAD-CBD-CGD-O1D
24	G	318	CHL	CAD-CBD-CGD-O2D
24	9	304	CHL	C1C-C2C-CMC-OMC
24	9	304	CHL	C3C-C2C-CMC-OMC
24	9	305	CHL	C1C-C2C-CMC-OMC
24	9	305	CHL	C3C-C2C-CMC-OMC
24	9	309	CHL	C1C-C2C-CMC-OMC
24	9	310	CHL	C1A-C2A-CAA-CBA
24	9	310	CHL	C3A-C2A-CAA-CBA
24	9	312	CHL	CBD-CGD-O2D-CED
24	9	317	CHL	CAD-CBD-CGD-O1D
24	9	317	CHL	CAD-CBD-CGD-O2D
24	N	305	CHL	C1C-C2C-CMC-OMC
24	N	305	CHL	C3C-C2C-CMC-OMC
24	N	309	CHL	C1C-C2C-CMC-OMC
24	N	309	CHL	C3C-C2C-CMC-OMC
24	N	310	CHL	C1A-C2A-CAA-CBA
24	N	310	CHL	CHA-CBD-CGD-O1D
24	N	311	CHL	CBD-CGD-O2D-CED
24	N	312	CHL	C1C-C2C-CMC-OMC
24	N	312	CHL	C3C-C2C-CMC-OMC
24	Y	308	CHL	C1C-C2C-CMC-OMC
24	Y	308	CHL	C3C-C2C-CMC-OMC
24	Y	310	CHL	C1A-C2A-CAA-CBA
24	Y	310	CHL	C1C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
24	Y	310	CHL	C3C-C2C-CMC-OMC
24	Y	311	CHL	C1C-C2C-CMC-OMC
24	Y	311	CHL	C3C-C2C-CMC-OMC
24	Y	312	CHL	C1C-C2C-CMC-OMC
24	Y	312	CHL	C3C-C2C-CMC-OMC
24	Y	312	CHL	C6-C7-C8-C9
24	Y	317	CHL	C1C-C2C-CMC-OMC
24	Y	317	CHL	C3C-C2C-CMC-OMC
24	Y	319	CHL	C1A-C2A-CAA-CBA
24	8	303	CHL	C3A-C2A-CAA-CBA
24	8	303	CHL	C2-C3-C5-C6
24	8	303	CHL	C4-C3-C5-C6
24	8	304	CHL	C1C-C2C-CMC-OMC
24	8	304	CHL	C3C-C2C-CMC-OMC
24	8	304	CHL	CHA-CBD-CGD-O2D
24	8	307	CHL	C1C-C2C-CMC-OMC
24	8	310	CHL	C1C-C2C-CMC-OMC
24	8	310	CHL	C3C-C2C-CMC-OMC
24	8	310	CHL	C4C-C3C-CAC-CBC
24	8	310	CHL	CHA-CBD-CGD-O1D
24	4	312	CHL	C1C-C2C-CMC-OMC
24	4	312	CHL	C3C-C2C-CMC-OMC
24	4	317	CHL	CAD-CBD-CGD-O1D
24	4	317	CHL	CAD-CBD-CGD-O2D
24	5	305	CHL	C1C-C2C-CMC-OMC
24	5	305	CHL	C3C-C2C-CMC-OMC
24	5	306	CHL	C1C-C2C-CMC-OMC
24	5	306	CHL	C3C-C2C-CMC-OMC
24	5	306	CHL	CHA-CBD-CGD-O2D
24	5	312	CHL	C1C-C2C-CMC-OMC
24	5	312	CHL	C3C-C2C-CMC-OMC
24	5	312	CHL	CBD-CGD-O2D-CED
24	5	318	CHL	CAD-CBD-CGD-O1D
24	5	318	CHL	CAD-CBD-CGD-O2D
24	6	304	CHL	C1A-C2A-CAA-CBA
24	6	304	CHL	C3A-C2A-CAA-CBA
24	6	304	CHL	C1C-C2C-CMC-OMC
24	6	304	CHL	C3C-C2C-CMC-OMC
24	6	305	CHL	C1C-C2C-CMC-OMC
24	6	305	CHL	C3C-C2C-CMC-OMC
24	6	310	CHL	C1A-C2A-CAA-CBA
24	g	305	CHL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	g	306	CHL	C1C-C2C-CMC-OMC
24	g	306	CHL	C3C-C2C-CMC-OMC
24	g	311	CHL	C1A-C2A-CAA-CBA
24	g	312	CHL	CBD-CGD-O2D-CED
24	g	318	CHL	C1C-C2C-CMC-OMC
24	g	318	CHL	C3C-C2C-CMC-OMC
24	g	318	CHL	CAD-CBD-CGD-O1D
24	g	318	CHL	CAD-CBD-CGD-O2D
24	u	306	CHL	C1C-C2C-CMC-OMC
24	u	306	CHL	C3C-C2C-CMC-OMC
24	u	310	CHL	C1C-C2C-CMC-OMC
24	u	310	CHL	C3C-C2C-CMC-OMC
24	u	311	CHL	C1A-C2A-CAA-CBA
24	u	318	CHL	CAD-CBD-CGD-O1D
24	u	318	CHL	CAD-CBD-CGD-O2D
24	n	305	CHL	C1C-C2C-CMC-OMC
24	n	305	CHL	C3C-C2C-CMC-OMC
24	n	310	CHL	C1A-C2A-CAA-CBA
24	n	311	CHL	CBD-CGD-O2D-CED
24	n	312	CHL	C1C-C2C-CMC-OMC
24	n	312	CHL	C3C-C2C-CMC-OMC
24	n	317	CHL	C1C-C2C-CMC-OMC
24	y	305	CHL	C11-C12-C13-C14
24	y	309	CHL	C1C-C2C-CMC-OMC
24	y	309	CHL	C3C-C2C-CMC-OMC
24	y	311	CHL	C1A-C2A-CAA-CBA
24	y	311	CHL	C1C-C2C-CMC-OMC
24	y	311	CHL	C3C-C2C-CMC-OMC
24	y	312	CHL	C1C-C2C-CMC-OMC
24	y	312	CHL	C3C-C2C-CMC-OMC
24	y	313	CHL	C1C-C2C-CMC-OMC
24	y	313	CHL	C3C-C2C-CMC-OMC
24	y	313	CHL	C6-C7-C8-C9
24	y	318	CHL	C1C-C2C-CMC-OMC
24	y	318	CHL	C3C-C2C-CMC-OMC
24	p	306	CHL	C1C-C2C-CMC-OMC
24	p	306	CHL	CHA-CBD-CGD-O2D
24	p	309	CHL	CHA-CBD-CGD-O1D
24	p	309	CHL	CHA-CBD-CGD-O2D
24	p	310	CHL	C1C-C2C-CMC-OMC
24	p	310	CHL	C3C-C2C-CMC-OMC
24	p	311	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	p	312	CHL	C1C-C2C-CMC-OMC
24	p	312	CHL	C3C-C2C-CMC-OMC
24	p	312	CHL	CBD-CGD-O2D-CED
24	p	313	CHL	C4C-C3C-CAC-CBC
24	q	303	CHL	C3A-C2A-CAA-CBA
24	q	303	CHL	C2-C3-C5-C6
24	q	303	CHL	C4-C3-C5-C6
24	q	304	CHL	C1C-C2C-CMC-OMC
24	q	304	CHL	C3C-C2C-CMC-OMC
24	q	309	CHL	C1A-C2A-CAA-CBA
24	q	311	CHL	C1C-C2C-CMC-OMC
24	q	311	CHL	C3C-C2C-CMC-OMC
24	q	311	CHL	C4C-C3C-CAC-CBC
24	q	311	CHL	CHA-CBD-CGD-O1D
24	s	402	CHL	C1C-C2C-CMC-OMC
24	s	402	CHL	C3C-C2C-CMC-OMC
24	s	403	CHL	C1C-C2C-CMC-OMC
24	s	403	CHL	C3C-C2C-CMC-OMC
24	s	407	CHL	C1A-C2A-CAA-CBA
24	s	407	CHL	CHA-CBD-CGD-O1D
24	s	408	CHL	C3A-C2A-CAA-CBA
24	s	409	CHL	C1C-C2C-CMC-OMC
24	s	409	CHL	C3C-C2C-CMC-OMC
24	s	409	CHL	C4C-C3C-CAC-CBC
24	s	414	CHL	C1C-C2C-CMC-OMC
24	s	414	CHL	C3C-C2C-CMC-OMC
24	r	302	CHL	C1C-C2C-CMC-OMC
24	r	302	CHL	C3C-C2C-CMC-OMC
24	r	306	CHL	C1C-C2C-CMC-OMC
24	r	306	CHL	C3C-C2C-CMC-OMC
24	r	307	CHL	C1A-C2A-CAA-CBA
24	r	308	CHL	C1C-C2C-CMC-OMC
24	r	309	CHL	C4C-C3C-CAC-CBC
24	7	306	CHL	C1C-C2C-CMC-OMC
24	7	306	CHL	CHA-CBD-CGD-O2D
24	7	309	CHL	CHA-CBD-CGD-O1D
24	7	309	CHL	CHA-CBD-CGD-O2D
24	7	310	CHL	C1C-C2C-CMC-OMC
24	7	310	CHL	C3C-C2C-CMC-OMC
24	7	311	CHL	C1A-C2A-CAA-CBA
24	7	312	CHL	C1C-C2C-CMC-OMC
24	7	312	CHL	C3C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
24	7	312	CHL	CBD-CGD-O2D-CED
24	7	313	CHL	C4C-C3C-CAC-CBC
25	R	603	CLA	CHA-CBD-CGD-O1D
25	R	603	CLA	CHA-CBD-CGD-O2D
25	R	611	CLA	CHA-CBD-CGD-O1D
25	R	611	CLA	CHA-CBD-CGD-O2D
25	R	611	CLA	CBD-CGD-O2D-CED
25	R	613	CLA	C3A-C2A-CAA-CBA
25	1	306	CLA	CAA-CBA-CGA-O1A
25	1	306	CLA	CAD-CBD-CGD-O1D
25	1	306	CLA	CAD-CBD-CGD-O2D
25	1	306	CLA	CBD-CGD-O2D-CED
25	1	307	CLA	CHA-CBD-CGD-O1D
25	1	307	CLA	CHA-CBD-CGD-O2D
25	1	313	CLA	CBD-CGD-O2D-CED
25	1	315	CLA	CHA-CBD-CGD-O1D
25	1	315	CLA	CHA-CBD-CGD-O2D
25	2	307	CLA	CHA-CBD-CGD-O2D
25	2	307	CLA	CBD-CGD-O2D-CED
25	2	308	CLA	CAD-CBD-CGD-O1D
25	2	308	CLA	CAD-CBD-CGD-O2D
25	2	314	CLA	CBD-CGD-O2D-CED
25	2	316	CLA	CHA-CBD-CGD-O1D
25	2	316	CLA	CHA-CBD-CGD-O2D
25	3	306	CLA	CBD-CGD-O2D-CED
25	3	307	CLA	CAD-CBD-CGD-O1D
25	3	307	CLA	CAD-CBD-CGD-O2D
25	3	307	CLA	CBD-CGD-O2D-CED
25	3	315	CLA	CHA-CBD-CGD-O2D
25	S	603	CLA	CHA-CBD-CGD-O2D
25	S	611	CLA	CHA-CBD-CGD-O1D
25	S	611	CLA	CHA-CBD-CGD-O2D
25	S	612	CLA	CBD-CGD-O2D-CED
25	S	616	CLA	C1A-C2A-CAA-CBA
25	G	307	CLA	CHA-CBD-CGD-O1D
25	G	307	CLA	CHA-CBD-CGD-O2D
25	G	308	CLA	CAD-CBD-CGD-O1D
25	G	308	CLA	CAD-CBD-CGD-O2D
25	G	314	CLA	CBD-CGD-O2D-CED
25	G	315	CLA	CBD-CGD-O2D-CED
25	G	316	CLA	CHA-CBD-CGD-O1D
25	G	316	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
25	9	306	CLA	CBD-CGD-O2D-CED
25	9	307	CLA	C1A-C2A-CAA-CBA
25	9	307	CLA	C3A-C2A-CAA-CBA
25	9	313	CLA	CBD-CGD-O2D-CED
25	9	314	CLA	CBD-CGD-O2D-CED
25	9	315	CLA	CHA-CBD-CGD-O1D
25	9	315	CLA	CHA-CBD-CGD-O2D
25	9	316	CLA	C4B-C3B-CAB-CBB
25	9	316	CLA	CBD-CGD-O2D-CED
25	N	306	CLA	CHA-CBD-CGD-O1D
25	N	306	CLA	CHA-CBD-CGD-O2D
25	N	315	CLA	CHA-CBD-CGD-O2D
25	Y	307	CLA	CAD-CBD-CGD-O1D
25	Y	307	CLA	CAD-CBD-CGD-O2D
25	Y	315	CLA	CHA-CBD-CGD-O1D
25	Y	315	CLA	CHA-CBD-CGD-O2D
25	8	305	CLA	CHA-CBD-CGD-O1D
25	8	305	CLA	CHA-CBD-CGD-O2D
25	8	313	CLA	CHA-CBD-CGD-O1D
25	8	313	CLA	CHA-CBD-CGD-O2D
25	B	601	CLA	C1A-C2A-CAA-CBA
25	B	601	CLA	C3A-C2A-CAA-CBA
25	B	601	CLA	C4B-C3B-CAB-CBB
25	B	601	CLA	CAD-CBD-CGD-O1D
25	B	601	CLA	CAD-CBD-CGD-O2D
25	B	601	CLA	CBD-CGD-O2D-CED
25	B	604	CLA	C6-C7-C8-C9
25	B	605	CLA	CAD-CBD-CGD-O1D
25	B	605	CLA	CAD-CBD-CGD-O2D
25	B	605	CLA	CBD-CGD-O2D-CED
25	B	608	CLA	CBD-CGD-O2D-CED
25	B	614	CLA	CBD-CGD-O2D-CED
25	B	616	CLA	CHA-CBD-CGD-O1D
25	B	616	CLA	CHA-CBD-CGD-O2D
25	B	616	CLA	CBD-CGD-O2D-CED
25	A	604	CLA	C1A-C2A-CAA-CBA
25	C	601	CLA	CAD-CBD-CGD-O1D
25	C	601	CLA	CAD-CBD-CGD-O2D
25	C	601	CLA	C14-C13-C15-C16
25	C	602	CLA	CAD-CBD-CGD-O2D
25	C	605	CLA	CAD-CBD-CGD-O2D
25	C	606	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	C	606	CLA	CAD-CBD-CGD-O2D
25	C	606	CLA	CBD-CGD-O2D-CED
25	C	607	CLA	CHA-CBD-CGD-O1D
25	C	607	CLA	CHA-CBD-CGD-O2D
25	C	608	CLA	CHA-CBD-CGD-O1D
25	C	608	CLA	CHA-CBD-CGD-O2D
25	C	612	CLA	C1A-C2A-CAA-CBA
25	C	612	CLA	C3A-C2A-CAA-CBA
25	D	404	CLA	C1A-C2A-CAA-CBA
25	D	405	CLA	C1A-C2A-CAA-CBA
25	D	405	CLA	C3A-C2A-CAA-CBA
25	4	306	CLA	CAA-CBA-CGA-O1A
25	4	306	CLA	CAD-CBD-CGD-O1D
25	4	306	CLA	CAD-CBD-CGD-O2D
25	4	306	CLA	CBD-CGD-O2D-CED
25	4	307	CLA	CHA-CBD-CGD-O1D
25	4	307	CLA	CHA-CBD-CGD-O2D
25	4	313	CLA	CBD-CGD-O2D-CED
25	4	315	CLA	CHA-CBD-CGD-O1D
25	4	315	CLA	CHA-CBD-CGD-O2D
25	5	307	CLA	CHA-CBD-CGD-O2D
25	5	307	CLA	CBD-CGD-O2D-CED
25	5	308	CLA	CAD-CBD-CGD-O1D
25	5	308	CLA	CAD-CBD-CGD-O2D
25	5	314	CLA	CBD-CGD-O2D-CED
25	5	316	CLA	CHA-CBD-CGD-O1D
25	5	316	CLA	CHA-CBD-CGD-O2D
25	6	306	CLA	CBD-CGD-O2D-CED
25	6	307	CLA	CAD-CBD-CGD-O1D
25	6	307	CLA	CAD-CBD-CGD-O2D
25	6	315	CLA	CHA-CBD-CGD-O2D
25	g	307	CLA	CHA-CBD-CGD-O1D
25	g	307	CLA	CHA-CBD-CGD-O2D
25	g	308	CLA	CAD-CBD-CGD-O1D
25	g	308	CLA	CAD-CBD-CGD-O2D
25	g	315	CLA	CBD-CGD-O2D-CED
25	g	316	CLA	CHA-CBD-CGD-O1D
25	g	316	CLA	CHA-CBD-CGD-O2D
25	g	317	CLA	CBD-CGD-O2D-CED
25	u	308	CLA	C1A-C2A-CAA-CBA
25	u	308	CLA	C3A-C2A-CAA-CBA
25	u	314	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	u	315	CLA	CBD-CGD-O2D-CED
25	u	316	CLA	CHA-CBD-CGD-O1D
25	u	316	CLA	CHA-CBD-CGD-O2D
25	n	306	CLA	CHA-CBD-CGD-O1D
25	n	306	CLA	CHA-CBD-CGD-O2D
25	y	308	CLA	CAD-CBD-CGD-O1D
25	y	308	CLA	CAD-CBD-CGD-O2D
25	y	316	CLA	CHA-CBD-CGD-O1D
25	y	316	CLA	CHA-CBD-CGD-O2D
25	p	307	CLA	CHA-CBD-CGD-O1D
25	p	307	CLA	CHA-CBD-CGD-O2D
25	p	308	CLA	C1A-C2A-CAA-CBA
25	p	308	CLA	C3A-C2A-CAA-CBA
25	p	314	CLA	CBD-CGD-O2D-CED
25	p	315	CLA	CHA-CBD-CGD-O1D
25	p	315	CLA	CHA-CBD-CGD-O2D
25	p	316	CLA	CHA-CBD-CGD-O1D
25	p	316	CLA	CHA-CBD-CGD-O2D
25	q	305	CLA	CHA-CBD-CGD-O1D
25	q	305	CLA	CHA-CBD-CGD-O2D
25	q	314	CLA	CHA-CBD-CGD-O1D
25	q	314	CLA	CHA-CBD-CGD-O2D
25	q	315	CLA	CBD-CGD-O2D-CED
25	b	601	CLA	C1A-C2A-CAA-CBA
25	b	601	CLA	C3A-C2A-CAA-CBA
25	b	601	CLA	CAD-CBD-CGD-O1D
25	b	601	CLA	CAD-CBD-CGD-O2D
25	b	601	CLA	CBD-CGD-O2D-CED
25	b	604	CLA	C6-C7-C8-C9
25	b	605	CLA	CAD-CBD-CGD-O1D
25	b	605	CLA	CAD-CBD-CGD-O2D
25	b	605	CLA	CBD-CGD-O2D-CED
25	b	608	CLA	CBD-CGD-O2D-CED
25	b	609	CLA	C11-C10-C8-C9
25	b	614	CLA	CBD-CGD-O2D-CED
25	b	616	CLA	CHA-CBD-CGD-O1D
25	b	616	CLA	CHA-CBD-CGD-O2D
25	b	616	CLA	CBD-CGD-O2D-CED
25	a	604	CLA	C1A-C2A-CAA-CBA
25	c	601	CLA	CAD-CBD-CGD-O1D
25	c	601	CLA	CAD-CBD-CGD-O2D
25	c	601	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	c	602	CLA	CAD-CBD-CGD-O2D
25	c	605	CLA	CAD-CBD-CGD-O2D
25	c	606	CLA	CAD-CBD-CGD-O1D
25	c	606	CLA	CAD-CBD-CGD-O2D
25	c	606	CLA	CBD-CGD-O2D-CED
25	c	607	CLA	CHA-CBD-CGD-O1D
25	c	607	CLA	CHA-CBD-CGD-O2D
25	c	608	CLA	CHA-CBD-CGD-O1D
25	c	608	CLA	CHA-CBD-CGD-O2D
25	c	612	CLA	C1A-C2A-CAA-CBA
25	c	612	CLA	C3A-C2A-CAA-CBA
25	d	405	CLA	C1A-C2A-CAA-CBA
25	d	405	CLA	C3A-C2A-CAA-CBA
25	s	404	CLA	CHA-CBD-CGD-O2D
25	s	404	CLA	CBD-CGD-O2D-CED
25	s	412	CLA	CHA-CBD-CGD-O1D
25	s	412	CLA	CHA-CBD-CGD-O2D
25	s	413	CLA	CBD-CGD-O2D-CED
25	s	417	CLA	C1A-C2A-CAA-CBA
25	r	304	CLA	CHA-CBD-CGD-O1D
25	r	304	CLA	CHA-CBD-CGD-O2D
25	r	310	CLA	CBD-CGD-O2D-CED
25	r	312	CLA	CHA-CBD-CGD-O1D
25	r	312	CLA	CHA-CBD-CGD-O2D
25	r	314	CLA	C3A-C2A-CAA-CBA
25	7	307	CLA	CHA-CBD-CGD-O1D
25	7	307	CLA	CHA-CBD-CGD-O2D
25	7	308	CLA	C1A-C2A-CAA-CBA
25	7	308	CLA	C3A-C2A-CAA-CBA
25	7	314	CLA	CBD-CGD-O2D-CED
25	7	315	CLA	CHA-CBD-CGD-O1D
25	7	315	CLA	CHA-CBD-CGD-O2D
25	7	316	CLA	CHA-CBD-CGD-O1D
25	7	316	CLA	CHA-CBD-CGD-O2D
26	R	614	0IE	O1-C2-C3-C20
26	9	303	0IE	C14-C15-C16-C23
26	r	315	0IE	O1-C2-C3-C20
28	R	616	NEX	O24-C26-C27-C28
28	1	303	NEX	O24-C26-C27-C28
28	2	304	NEX	O24-C26-C27-C28
28	3	318	NEX	O24-C26-C27-C28
28	S	617	NEX	O24-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
28	G	304	NEX	O24-C26-C27-C28
28	9	319	NEX	O24-C26-C27-C28
28	N	303	NEX	O24-C26-C27-C28
28	4	303	NEX	O24-C26-C27-C28
28	5	304	NEX	O24-C26-C27-C28
28	6	303	NEX	O24-C26-C27-C28
28	g	304	NEX	O24-C26-C27-C28
28	u	304	NEX	O24-C26-C27-C28
28	n	303	NEX	O24-C26-C27-C28
28	y	304	NEX	O24-C26-C27-C28
28	p	304	NEX	O24-C26-C27-C28
28	s	401	NEX	O24-C26-C27-C28
28	r	301	NEX	O24-C26-C27-C28
28	r	317	NEX	O24-C26-C27-C28
28	7	304	NEX	O24-C26-C27-C28
29	1	301	0UR	C17-C18-C19-C28
29	1	301	0UR	C17-C18-C19-C32
29	2	301	0UR	O42-C2-C3-C43
29	2	301	0UR	C5-C6-C7-C8
29	2	301	0UR	C17-C18-C19-C28
29	2	301	0UR	C17-C18-C19-C32
29	3	301	0UR	O42-C2-C3-C43
29	G	301	0UR	O42-C2-C3-C43
29	G	301	0UR	C5-C6-C7-C8
29	9	301	0UR	O42-C2-C3-C43
29	9	301	0UR	C5-C6-C7-C8
29	N	301	0UR	O42-C2-C3-C43
29	Y	301	0UR	O42-C2-C3-C43
29	4	301	0UR	C17-C18-C19-C28
29	4	301	0UR	C17-C18-C19-C32
29	5	301	0UR	O42-C2-C3-C43
29	5	301	0UR	C5-C6-C7-C8
29	5	301	0UR	C17-C18-C19-C28
29	5	301	0UR	C17-C18-C19-C32
29	6	301	0UR	O42-C2-C3-C43
29	g	301	0UR	O42-C2-C3-C43
29	g	301	0UR	C5-C6-C7-C8
29	u	301	0UR	O42-C2-C3-C43
29	n	301	0UR	O42-C2-C3-C43
29	y	301	0UR	O42-C2-C3-C43
29	p	301	0UR	O42-C2-C3-C43
29	7	301	0UR	O42-C2-C3-C43

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Mol	Chain	Res	Type	Atoms
30	1	318	LHG	O1-C1-C2-C3
30	1	318	LHG	C4-O6-P-O3
30	1	318	LHG	C4-O6-P-O4
30	1	318	LHG	C4-O6-P-O5
30	1	318	LHG	O7-C5-C6-O8
30	2	319	LHG	C1-C2-C3-O3
30	2	319	LHG	C3-O3-P-O4
30	2	319	LHG	C3-O3-P-O5
30	2	319	LHG	C3-O3-P-O6
30	G	319	LHG	O1-C1-C2-C3
30	G	319	LHG	C3-O3-P-O4
30	G	319	LHG	C3-O3-P-O6
30	G	319	LHG	C4-O6-P-O3
30	G	319	LHG	C4-O6-P-O4
30	G	319	LHG	C4-O6-P-O5
30	9	318	LHG	C1-C2-C3-O3
30	9	318	LHG	O2-C2-C3-O3
30	9	318	LHG	C3-O3-P-O4
30	9	318	LHG	C3-O3-P-O6
30	N	318	LHG	O1-C1-C2-O2
30	N	318	LHG	O2-C2-C3-O3
30	Y	318	LHG	C1-C2-C3-O3
30	Y	318	LHG	O10-C23-O8-C6
30	Y	318	LHG	C24-C23-O8-C6
30	A	601	LHG	C4-O6-P-O3
30	A	601	LHG	C4-O6-P-O4
30	A	601	LHG	C4-O6-P-O5
30	A	612	LHG	C3-O3-P-O5
30	C	617	LHG	C3-O3-P-O5
30	C	617	LHG	C4-O6-P-O3
30	C	617	LHG	C4-O6-P-O5
30	C	617	LHG	C8-C7-O7-C5
30	D	407	LHG	O1-C1-C2-C3
30	D	407	LHG	C1-C2-C3-O3
30	D	407	LHG	O2-C2-C3-O3
30	D	407	LHG	C3-O3-P-O4
30	D	407	LHG	C3-O3-P-O5
30	D	407	LHG	C3-O3-P-O6
30	D	407	LHG	C4-O6-P-O3
30	D	407	LHG	C4-O6-P-O5
30	D	408	LHG	C3-O3-P-O5
30	D	408	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
30	D	408	LHG	C4-O6-P-O5
30	4	318	LHG	O1-C1-C2-C3
30	4	318	LHG	C3-O3-P-O6
30	4	318	LHG	C4-O6-P-O3
30	4	318	LHG	C4-O6-P-O4
30	4	318	LHG	O7-C5-C6-O8
30	5	319	LHG	C1-C2-C3-O3
30	5	319	LHG	C3-O3-P-O4
30	5	319	LHG	C3-O3-P-O5
30	5	319	LHG	C3-O3-P-O6
30	g	319	LHG	O1-C1-C2-C3
30	g	319	LHG	C3-O3-P-O4
30	g	319	LHG	C3-O3-P-O6
30	g	319	LHG	C4-O6-P-O3
30	g	319	LHG	C4-O6-P-O5
30	n	318	LHG	O2-C2-C3-O3
30	y	319	LHG	C1-C2-C3-O3
30	y	319	LHG	O10-C23-O8-C6
30	y	319	LHG	C24-C23-O8-C6
30	p	319	LHG	O1-C1-C2-C3
30	p	319	LHG	C1-C2-C3-O3
30	p	319	LHG	C3-O3-P-O4
30	p	319	LHG	C3-O3-P-O6
30	p	319	LHG	C4-O6-P-O3
30	p	319	LHG	C4-O6-P-O4
30	p	319	LHG	C4-O6-P-O5
30	a	601	LHG	C1-C2-C3-O3
30	a	601	LHG	C4-O6-P-O3
30	a	601	LHG	C4-O6-P-O4
30	a	601	LHG	C4-O6-P-O5
30	a	612	LHG	C3-O3-P-O5
30	c	617	LHG	C3-O3-P-O5
30	c	617	LHG	C4-O6-P-O3
30	c	617	LHG	C4-O6-P-O5
30	c	617	LHG	C8-C7-O7-C5
30	d	407	LHG	O1-C1-C2-C3
30	d	407	LHG	C1-C2-C3-O3
30	d	407	LHG	C3-O3-P-O4
30	d	407	LHG	C3-O3-P-O5
30	d	407	LHG	C3-O3-P-O6
30	d	407	LHG	C4-O6-P-O3
30	d	407	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
30	d	408	LHG	C3-O3-P-O5
30	d	408	LHG	C3-O3-P-O6
30	d	408	LHG	C4-O6-P-O5
30	7	319	LHG	O1-C1-C2-C3
30	7	319	LHG	C1-C2-C3-O3
30	7	319	LHG	C3-O3-P-O4
30	7	319	LHG	C3-O3-P-O6
30	7	319	LHG	C4-O6-P-O3
30	7	319	LHG	C4-O6-P-O4
30	7	319	LHG	C4-O6-P-O5
31	S	615	8CT	C28-C29-C30-C31
31	S	615	8CT	C28-C29-C30-C35
31	X	601	8CT	C14-C15-C16-C17
31	X	601	8CT	C14-C15-C16-C39
31	X	601	8CT	C18-C19-C20-C21
31	V	401	8CT	C02-C03-C10-C11
31	V	401	8CT	C10-C11-C12-C13
31	V	401	8CT	C10-C11-C12-C40
31	V	401	8CT	C20-C21-C23-C24
31	V	401	8CT	C22-C21-C23-C24
31	V	401	8CT	C25-C26-C28-C29
31	V	401	8CT	C27-C26-C28-C29
31	V	401	8CT	C28-C29-C30-C31
31	T	101	8CT	C16-C17-C18-C19
31	T	101	8CT	C25-C26-C28-C29
31	T	101	8CT	C27-C26-C28-C29
31	T	101	8CT	C28-C29-C30-C31
31	T	101	8CT	C28-C29-C30-C35
31	B	617	8CT	C14-C15-C16-C39
31	B	617	8CT	C20-C21-C23-C24
31	B	617	8CT	C28-C29-C30-C31
31	B	617	8CT	C28-C29-C30-C35
31	A	608	8CT	C16-C17-C18-C19
31	A	608	8CT	C18-C19-C20-C21
31	C	613	8CT	C14-C15-C16-C17
31	C	613	8CT	C14-C15-C16-C39
31	C	613	8CT	C16-C17-C18-C19
31	C	613	8CT	C28-C29-C30-C31
31	C	614	8CT	C20-C21-C23-C24
31	C	614	8CT	C22-C21-C23-C24
31	C	614	8CT	C25-C26-C28-C29
31	C	614	8CT	C27-C26-C28-C29

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Mol	Chain	Res	Type	Atoms
31	C	614	8CT	C28-C29-C30-C31
31	C	614	8CT	C28-C29-C30-C35
31	C	615	8CT	C20-C21-C23-C24
31	C	615	8CT	C22-C21-C23-C24
31	C	615	8CT	C25-C26-C28-C29
31	C	615	8CT	C27-C26-C28-C29
31	D	410	8CT	C02-C03-C10-C11
31	D	410	8CT	C25-C26-C28-C29
31	D	410	8CT	C27-C26-C28-C29
31	D	410	8CT	C28-C29-C30-C31
31	x	601	8CT	C14-C15-C16-C17
31	x	601	8CT	C14-C15-C16-C39
31	x	601	8CT	C18-C19-C20-C21
31	v	401	8CT	C02-C03-C10-C11
31	v	401	8CT	C10-C11-C12-C13
31	v	401	8CT	C10-C11-C12-C40
31	v	401	8CT	C20-C21-C23-C24
31	v	401	8CT	C22-C21-C23-C24
31	v	401	8CT	C25-C26-C28-C29
31	v	401	8CT	C27-C26-C28-C29
31	v	401	8CT	C28-C29-C30-C31
31	t	101	8CT	C16-C17-C18-C19
31	t	101	8CT	C25-C26-C28-C29
31	t	101	8CT	C27-C26-C28-C29
31	t	101	8CT	C28-C29-C30-C31
31	t	101	8CT	C28-C29-C30-C35
31	b	617	8CT	C14-C15-C16-C39
31	b	617	8CT	C20-C21-C23-C24
31	b	617	8CT	C22-C21-C23-C24
31	b	617	8CT	C28-C29-C30-C31
31	b	617	8CT	C28-C29-C30-C35
31	a	608	8CT	C16-C17-C18-C19
31	a	608	8CT	C18-C19-C20-C21
31	c	613	8CT	C14-C15-C16-C17
31	c	613	8CT	C14-C15-C16-C39
31	c	613	8CT	C28-C29-C30-C31
31	c	614	8CT	C20-C21-C23-C24
31	c	614	8CT	C22-C21-C23-C24
31	c	614	8CT	C25-C26-C28-C29
31	c	614	8CT	C27-C26-C28-C29
31	c	614	8CT	C28-C29-C30-C31
31	c	614	8CT	C28-C29-C30-C35

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Mol	Chain	Res	Type	Atoms
31	c	615	8CT	C10-C11-C12-C13
31	c	615	8CT	C10-C11-C12-C40
31	c	615	8CT	C20-C21-C23-C24
31	c	615	8CT	C22-C21-C23-C24
31	c	615	8CT	C25-C26-C28-C29
31	c	615	8CT	C27-C26-C28-C29
31	d	410	8CT	C02-C03-C10-C11
31	d	410	8CT	C25-C26-C28-C29
31	d	410	8CT	C27-C26-C28-C29
31	d	410	8CT	C28-C29-C30-C31
31	s	416	8CT	C28-C29-C30-C31
31	s	416	8CT	C28-C29-C30-C35
32	A	609	SQD	C5-C6-S-O7
32	A	609	SQD	C5-C6-S-O8
32	A	609	SQD	C5-C6-S-O9
33	B	619	LMG	C2-C1-O1-C7
33	B	619	LMG	O6-C1-O1-C7
33	D	411	LMG	C2-C1-O1-C7
33	W	201	LMG	O6-C1-O1-C7
33	w	201	LMG	C2-C1-O1-C7
37	C	620	DGD	C2D-C1D-O3G-C3G
37	C	620	DGD	O6D-C1D-O3G-C3G
39	D	406	PL9	C7-C8-C9-C11
39	D	406	PL9	C12-C13-C14-C16
39	d	406	PL9	C7-C8-C9-C11
39	d	406	PL9	C12-C13-C14-C16
25	1	306	CLA	O1D-CGD-O2D-CED
25	2	307	CLA	O1D-CGD-O2D-CED
25	S	603	CLA	O1D-CGD-O2D-CED
25	S	612	CLA	O1D-CGD-O2D-CED
25	9	306	CLA	O1D-CGD-O2D-CED
25	8	314	CLA	O1D-CGD-O2D-CED
25	4	306	CLA	O1D-CGD-O2D-CED
25	5	307	CLA	O1D-CGD-O2D-CED
25	6	315	CLA	O1D-CGD-O2D-CED
25	u	307	CLA	O1D-CGD-O2D-CED
25	s	404	CLA	O1D-CGD-O2D-CED
25	s	413	CLA	O1D-CGD-O2D-CED
25	3	315	CLA	O1D-CGD-O2D-CED
25	9	313	CLA	O1D-CGD-O2D-CED
25	u	314	CLA	O1D-CGD-O2D-CED
25	n	307	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	p	307	CLA	O1D-CGD-O2D-CED
25	p	314	CLA	O1D-CGD-O2D-CED
25	7	314	CLA	O1D-CGD-O2D-CED
24	R	607	CHL	CBD-CGD-O2D-CED
24	1	311	CHL	CBD-CGD-O2D-CED
24	1	317	CHL	CBD-CGD-O2D-CED
24	3	311	CHL	CBD-CGD-O2D-CED
24	S	607	CHL	CBD-CGD-O2D-CED
24	9	311	CHL	CBD-CGD-O2D-CED
24	Y	311	CHL	CBD-CGD-O2D-CED
24	8	309	CHL	CBD-CGD-O2D-CED
24	8	310	CHL	CBD-CGD-O2D-CED
24	4	311	CHL	CBD-CGD-O2D-CED
24	4	317	CHL	CBD-CGD-O2D-CED
24	6	311	CHL	CBD-CGD-O2D-CED
24	g	311	CHL	CBD-CGD-O2D-CED
24	u	313	CHL	CBD-CGD-O2D-CED
24	y	312	CHL	CBD-CGD-O2D-CED
24	p	313	CHL	CBD-CGD-O2D-CED
24	q	310	CHL	CBD-CGD-O2D-CED
24	q	311	CHL	CBD-CGD-O2D-CED
24	s	408	CHL	CBD-CGD-O2D-CED
24	r	308	CHL	CBD-CGD-O2D-CED
25	R	609	CLA	CBD-CGD-O2D-CED
25	R	610	CLA	CBD-CGD-O2D-CED
25	1	314	CLA	CBD-CGD-O2D-CED
25	3	313	CLA	CBD-CGD-O2D-CED
25	3	314	CLA	CBD-CGD-O2D-CED
25	3	315	CLA	CBD-CGD-O2D-CED
25	S	603	CLA	CBD-CGD-O2D-CED
25	S	611	CLA	CBD-CGD-O2D-CED
25	G	307	CLA	CBD-CGD-O2D-CED
25	N	307	CLA	CBD-CGD-O2D-CED
25	N	313	CLA	CBD-CGD-O2D-CED
25	Y	306	CLA	CBD-CGD-O2D-CED
25	Y	307	CLA	CBD-CGD-O2D-CED
25	8	314	CLA	CBD-CGD-O2D-CED
25	C	611	CLA	CBD-CGD-O2D-CED
25	4	307	CLA	CBD-CGD-O2D-CED
25	6	313	CLA	CBD-CGD-O2D-CED
25	6	315	CLA	CBD-CGD-O2D-CED
25	g	307	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	g	314	CLA	CBD-CGD-O2D-CED
25	u	307	CLA	CBD-CGD-O2D-CED
25	u	317	CLA	CBD-CGD-O2D-CED
25	n	307	CLA	CBD-CGD-O2D-CED
25	n	313	CLA	CBD-CGD-O2D-CED
25	y	307	CLA	CBD-CGD-O2D-CED
25	p	307	CLA	CBD-CGD-O2D-CED
25	b	606	CLA	CBD-CGD-O2D-CED
25	c	611	CLA	CBD-CGD-O2D-CED
25	s	412	CLA	CBD-CGD-O2D-CED
25	r	311	CLA	CBD-CGD-O2D-CED
25	r	312	CLA	CBD-CGD-O2D-CED
25	7	307	CLA	CBD-CGD-O2D-CED
25	A	603	CLA	O1A-CGA-O2A-C1
25	a	603	CLA	O1A-CGA-O2A-C1
30	D	408	LHG	O10-C23-O8-C6
30	d	408	LHG	O10-C23-O8-C6
25	3	306	CLA	O1D-CGD-O2D-CED
25	6	306	CLA	O1D-CGD-O2D-CED
25	q	315	CLA	O1D-CGD-O2D-CED
37	C	620	DGD	C4E-C5E-C6E-O5E
25	A	603	CLA	CBA-CGA-O2A-C1
25	a	603	CLA	CBA-CGA-O2A-C1
30	D	408	LHG	C24-C23-O8-C6
30	d	408	LHG	C24-C23-O8-C6
24	u	312	CHL	CBD-CGD-O2D-CED
25	4	314	CLA	CBD-CGD-O2D-CED
25	c	612	CLA	O1A-CGA-O2A-C1
30	p	319	LHG	O10-C23-O8-C6
30	7	319	LHG	O10-C23-O8-C6
37	c	619	DGD	C4E-C5E-C6E-O5E
24	2	312	CHL	O1D-CGD-O2D-CED
24	Y	311	CHL	O1D-CGD-O2D-CED
24	y	312	CHL	O1D-CGD-O2D-CED
24	p	312	CHL	O1D-CGD-O2D-CED
25	R	611	CLA	O1D-CGD-O2D-CED
25	1	313	CLA	O1D-CGD-O2D-CED
25	2	314	CLA	O1D-CGD-O2D-CED
25	G	314	CLA	O1D-CGD-O2D-CED
25	9	314	CLA	O1D-CGD-O2D-CED
25	N	307	CLA	O1D-CGD-O2D-CED
25	B	605	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	B	608	CLA	O1D-CGD-O2D-CED
25	g	315	CLA	O1D-CGD-O2D-CED
25	g	317	CLA	O1D-CGD-O2D-CED
25	u	315	CLA	O1D-CGD-O2D-CED
25	b	605	CLA	O1D-CGD-O2D-CED
25	r	312	CLA	O1D-CGD-O2D-CED
25	7	307	CLA	O1D-CGD-O2D-CED
24	G	311	CHL	O1D-CGD-O2D-CED
24	G	312	CHL	O1D-CGD-O2D-CED
24	5	312	CHL	O1D-CGD-O2D-CED
24	g	312	CHL	O1D-CGD-O2D-CED
24	7	312	CHL	O1D-CGD-O2D-CED
25	G	315	CLA	O1D-CGD-O2D-CED
25	9	316	CLA	O1D-CGD-O2D-CED
25	B	601	CLA	O1D-CGD-O2D-CED
25	B	614	CLA	O1D-CGD-O2D-CED
25	B	616	CLA	O1D-CGD-O2D-CED
25	4	313	CLA	O1D-CGD-O2D-CED
25	5	314	CLA	O1D-CGD-O2D-CED
25	b	601	CLA	O1D-CGD-O2D-CED
25	b	608	CLA	O1D-CGD-O2D-CED
25	b	614	CLA	O1D-CGD-O2D-CED
25	b	616	CLA	O1D-CGD-O2D-CED
25	c	606	CLA	O1D-CGD-O2D-CED
24	5	311	CHL	CBD-CGD-O2D-CED
25	1	307	CLA	CBD-CGD-O2D-CED
30	9	318	LHG	O9-C7-O7-C5
29	9	301	OUR	O57-C45-O44-C43
24	Y	310	CHL	C3-C5-C6-C7
24	p	305	CHL	C3-C5-C6-C7
24	7	305	CHL	C3-C5-C6-C7
25	2	315	CLA	C3-C5-C6-C7
25	G	315	CLA	C3-C5-C6-C7
25	9	314	CLA	C3-C5-C6-C7
25	N	314	CLA	C3-C5-C6-C7
25	Y	314	CLA	C3-C5-C6-C7
25	8	312	CLA	C3-C5-C6-C7
25	B	612	CLA	C3-C5-C6-C7
25	B	614	CLA	C3-C5-C6-C7
25	C	611	CLA	C3-C5-C6-C7
25	C	612	CLA	C3-C5-C6-C7
25	5	315	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
25	g	315	CLA	C3-C5-C6-C7
25	u	315	CLA	C3-C5-C6-C7
25	y	315	CLA	C3-C5-C6-C7
25	q	313	CLA	C3-C5-C6-C7
25	b	602	CLA	C3-C5-C6-C7
25	b	608	CLA	C3-C5-C6-C7
25	b	612	CLA	C3-C5-C6-C7
25	b	614	CLA	C3-C5-C6-C7
25	c	611	CLA	C3-C5-C6-C7
35	A	606	PHO	C3-C5-C6-C7
35	a	606	PHO	C3-C5-C6-C7
29	9	301	0UR	C46-C45-O44-C43
29	u	301	0UR	C46-C45-O44-C43
25	N	307	CLA	CBA-CGA-O2A-C1
25	A	604	CLA	CBA-CGA-O2A-C1
25	n	307	CLA	CBA-CGA-O2A-C1
25	a	604	CLA	CBA-CGA-O2A-C1
30	N	318	LHG	C24-C23-O8-C6
30	n	318	LHG	C24-C23-O8-C6
30	p	319	LHG	C24-C23-O8-C6
30	7	319	LHG	C24-C23-O8-C6
33	B	619	LMG	C29-C28-O8-C9
24	R	608	CHL	CBD-CGD-O2D-CED
24	2	311	CHL	CBD-CGD-O2D-CED
24	3	304	CHL	CBD-CGD-O2D-CED
24	S	606	CHL	CBD-CGD-O2D-CED
24	N	305	CHL	CBD-CGD-O2D-CED
24	6	304	CHL	CBD-CGD-O2D-CED
24	n	308	CHL	CBD-CGD-O2D-CED
24	s	403	CHL	CBD-CGD-O2D-CED
24	s	407	CHL	CBD-CGD-O2D-CED
24	r	309	CHL	CBD-CGD-O2D-CED
24	7	313	CHL	CBD-CGD-O2D-CED
25	1	315	CLA	CBD-CGD-O2D-CED
25	2	317	CLA	CBD-CGD-O2D-CED
25	S	616	CLA	CBD-CGD-O2D-CED
25	N	315	CLA	CBD-CGD-O2D-CED
25	B	606	CLA	CBD-CGD-O2D-CED
25	B	607	CLA	CBD-CGD-O2D-CED
25	A	610	CLA	CBD-CGD-O2D-CED
25	C	601	CLA	CBD-CGD-O2D-CED
25	C	603	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	5	317	CLA	CBD-CGD-O2D-CED
25	6	307	CLA	CBD-CGD-O2D-CED
25	6	314	CLA	CBD-CGD-O2D-CED
25	n	315	CLA	CBD-CGD-O2D-CED
25	p	315	CLA	CBD-CGD-O2D-CED
25	q	313	CLA	CBD-CGD-O2D-CED
25	b	607	CLA	CBD-CGD-O2D-CED
25	b	613	CLA	CBD-CGD-O2D-CED
25	a	603	CLA	CBD-CGD-O2D-CED
25	a	610	CLA	CBD-CGD-O2D-CED
25	c	601	CLA	CBD-CGD-O2D-CED
25	c	603	CLA	CBD-CGD-O2D-CED
25	7	315	CLA	CBD-CGD-O2D-CED
30	9	318	LHG	C8-C7-O7-C5
24	9	312	CHL	O1D-CGD-O2D-CED
24	N	311	CHL	O1D-CGD-O2D-CED
24	n	311	CHL	O1D-CGD-O2D-CED
25	3	307	CLA	O1D-CGD-O2D-CED
25	C	606	CLA	O1D-CGD-O2D-CED
25	C	612	CLA	O1A-CGA-O2A-C1
25	3	313	CLA	O1D-CGD-O2D-CED
25	r	310	CLA	O1D-CGD-O2D-CED
25	B	603	CLA	C4-C3-C5-C6
25	B	613	CLA	C4-C3-C5-C6
25	B	614	CLA	C4-C3-C5-C6
25	C	603	CLA	C4-C3-C5-C6
25	u	315	CLA	C4-C3-C5-C6
25	b	603	CLA	C4-C3-C5-C6
25	b	613	CLA	C4-C3-C5-C6
25	b	614	CLA	C4-C3-C5-C6
35	D	403	PHO	C4-C3-C5-C6
35	d	403	PHO	C4-C3-C5-C6
25	B	603	CLA	C2-C3-C5-C6
25	B	614	CLA	C2-C3-C5-C6
25	u	315	CLA	C2-C3-C5-C6
25	b	603	CLA	C2-C3-C5-C6
35	D	403	PHO	C2-C3-C5-C6
35	d	403	PHO	C2-C3-C5-C6
24	2	305	CHL	CBD-CGD-O2D-CED
24	2	306	CHL	CBD-CGD-O2D-CED
24	5	305	CHL	CBD-CGD-O2D-CED
24	n	305	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	B	613	CLA	CBD-CGD-O2D-CED
25	A	603	CLA	CBD-CGD-O2D-CED
24	3	311	CHL	O1D-CGD-O2D-CED
24	8	309	CHL	O1D-CGD-O2D-CED
24	g	311	CHL	O1D-CGD-O2D-CED
24	u	313	CHL	O1D-CGD-O2D-CED
24	q	310	CHL	O1D-CGD-O2D-CED
25	6	313	CLA	O1D-CGD-O2D-CED
25	g	307	CLA	O1D-CGD-O2D-CED
25	u	317	CLA	O1D-CGD-O2D-CED
24	G	312	CHL	C2A-CAA-CBA-CGA
24	9	309	CHL	C2A-CAA-CBA-CGA
24	g	312	CHL	C2A-CAA-CBA-CGA
24	u	310	CHL	C2A-CAA-CBA-CGA
24	n	311	CHL	C2A-CAA-CBA-CGA
25	8	305	CLA	C2A-CAA-CBA-CGA
25	B	607	CLA	C2A-CAA-CBA-CGA
25	q	305	CLA	C2A-CAA-CBA-CGA
25	b	607	CLA	C2A-CAA-CBA-CGA
33	D	411	LMG	O10-C28-O8-C9
24	8	304	CHL	C3-C5-C6-C7
24	g	306	CHL	C3-C5-C6-C7
24	y	306	CHL	C3-C5-C6-C7
24	y	311	CHL	C3-C5-C6-C7
24	q	304	CHL	C3-C5-C6-C7
25	B	602	CLA	C3-C5-C6-C7
25	B	608	CLA	C3-C5-C6-C7
25	B	609	CLA	C3-C5-C6-C7
25	c	612	CLA	C3-C5-C6-C7
25	9	314	CLA	CBA-CGA-O2A-C1
25	B	606	CLA	CBA-CGA-O2A-C1
25	C	612	CLA	CBA-CGA-O2A-C1
25	p	315	CLA	CBA-CGA-O2A-C1
25	b	606	CLA	CBA-CGA-O2A-C1
25	c	604	CLA	CBA-CGA-O2A-C1
25	c	612	CLA	CBA-CGA-O2A-C1
30	G	319	LHG	C24-C23-O8-C6
30	C	617	LHG	C24-C25-C26-C27
30	D	407	LHG	C24-C25-C26-C27
30	g	319	LHG	C24-C25-C26-C27
30	y	319	LHG	C24-C25-C26-C27
30	c	617	LHG	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
30	d	407	LHG	C24-C25-C26-C27
30	7	319	LHG	C24-C25-C26-C27
37	C	620	DGD	O6E-C5E-C6E-O5E
30	Y	318	LHG	C24-C25-C26-C27
30	p	319	LHG	C24-C25-C26-C27
30	D	408	LHG	C24-C25-C26-C27
30	5	319	LHG	C24-C25-C26-C27
37	c	619	DGD	O6E-C5E-C6E-O5E
31	C	614	8CT	C12-C13-C14-C15
31	C	615	8CT	C16-C17-C18-C19
31	C	615	8CT	C23-C24-C25-C26
31	c	613	8CT	C16-C17-C18-C19
31	c	614	8CT	C12-C13-C14-C15
31	c	615	8CT	C16-C17-C18-C19
25	B	606	CLA	O1A-CGA-O2A-C1
25	A	604	CLA	O1A-CGA-O2A-C1
25	b	606	CLA	O1A-CGA-O2A-C1
30	G	319	LHG	O10-C23-O8-C6
30	N	318	LHG	O10-C23-O8-C6
30	g	319	LHG	O10-C23-O8-C6
30	n	318	LHG	O10-C23-O8-C6
32	a	609	SQD	O10-C23-O48-C46
30	C	617	LHG	O9-C7-O7-C5
30	c	617	LHG	O9-C7-O7-C5
32	D	409	SQD	O49-C7-O47-C45
32	d	409	SQD	O49-C7-O47-C45
24	6	311	CHL	O1D-CGD-O2D-CED
30	1	318	LHG	C24-C25-C26-C27
30	G	319	LHG	C24-C25-C26-C27
30	4	318	LHG	C24-C25-C26-C27
30	2	319	LHG	C24-C25-C26-C27
30	9	318	LHG	C24-C25-C26-C27
30	N	318	LHG	C24-C25-C26-C27
30	A	612	LHG	C24-C25-C26-C27
30	n	318	LHG	C24-C25-C26-C27
30	a	612	LHG	C24-C25-C26-C27
29	1	301	0UR	O57-C45-O44-C43
29	2	301	0UR	O57-C45-O44-C43
29	3	301	0UR	O57-C45-O44-C43
29	G	301	0UR	O57-C45-O44-C43
29	N	301	0UR	O57-C45-O44-C43
29	Y	301	0UR	O57-C45-O44-C43

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Mol	Chain	Res	Type	Atoms
29	8	301	0UR	O57-C45-O44-C43
29	4	301	0UR	O57-C45-O44-C43
29	5	301	0UR	O57-C45-O44-C43
29	6	301	0UR	O57-C45-O44-C43
29	g	301	0UR	O57-C45-O44-C43
29	u	301	0UR	O57-C45-O44-C43
29	n	301	0UR	O57-C45-O44-C43
29	y	301	0UR	O57-C45-O44-C43
29	p	301	0UR	O57-C45-O44-C43
29	q	301	0UR	O57-C45-O44-C43
29	7	301	0UR	O57-C45-O44-C43
24	s	408	CHL	O1D-CGD-O2D-CED
25	G	307	CLA	O1D-CGD-O2D-CED
25	g	314	CLA	O1D-CGD-O2D-CED
24	G	306	CHL	C3-C5-C6-C7
24	Y	305	CHL	C3-C5-C6-C7
24	n	305	CHL	C3-C5-C6-C7
25	n	314	CLA	C3-C5-C6-C7
25	b	609	CLA	C3-C5-C6-C7
24	1	310	CHL	CBD-CGD-O2D-CED
24	S	602	CHL	CBD-CGD-O2D-CED
24	G	306	CHL	CBD-CGD-O2D-CED
24	9	305	CHL	CBD-CGD-O2D-CED
24	5	306	CHL	CBD-CGD-O2D-CED
24	5	309	CHL	CBD-CGD-O2D-CED
24	u	306	CHL	CBD-CGD-O2D-CED
24	y	313	CHL	CBD-CGD-O2D-CED
24	s	402	CHL	CBD-CGD-O2D-CED
25	G	317	CLA	CBD-CGD-O2D-CED
25	s	410	CLA	CBD-CGD-O2D-CED
25	s	417	CLA	CBD-CGD-O2D-CED
33	d	411	LMG	C29-C30-C31-C32
29	1	301	0UR	C46-C45-O44-C43
29	2	301	0UR	C46-C45-O44-C43
29	3	301	0UR	C46-C45-O44-C43
29	G	301	0UR	C46-C45-O44-C43
29	N	301	0UR	C46-C45-O44-C43
29	Y	301	0UR	C46-C45-O44-C43
29	8	301	0UR	C46-C45-O44-C43
29	4	301	0UR	C46-C45-O44-C43
29	5	301	0UR	C46-C45-O44-C43
29	6	301	0UR	C46-C45-O44-C43

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Mol	Chain	Res	Type	Atoms
29	g	301	0UR	C46-C45-O44-C43
29	n	301	0UR	C46-C45-O44-C43
29	y	301	0UR	C46-C45-O44-C43
29	p	301	0UR	C46-C45-O44-C43
29	q	301	0UR	C46-C45-O44-C43
29	7	301	0UR	C46-C45-O44-C43
30	2	319	LHG	O2-C2-C3-O3
30	Y	318	LHG	O2-C2-C3-O3
30	5	319	LHG	O2-C2-C3-O3
30	y	319	LHG	O2-C2-C3-O3
30	p	319	LHG	O2-C2-C3-O3
30	d	407	LHG	O2-C2-C3-O3
30	d	408	LHG	O2-C2-C3-O3
30	7	319	LHG	O2-C2-C3-O3
24	r	308	CHL	O1D-CGD-O2D-CED
25	R	609	CLA	O1D-CGD-O2D-CED
25	R	610	CLA	O1D-CGD-O2D-CED
25	Y	306	CLA	O1D-CGD-O2D-CED
25	C	611	CLA	O1D-CGD-O2D-CED
25	y	307	CLA	O1D-CGD-O2D-CED
25	c	611	CLA	O1D-CGD-O2D-CED
25	C	604	CLA	CBA-CGA-O2A-C1
25	7	315	CLA	CBA-CGA-O2A-C1
30	9	318	LHG	C24-C23-O8-C6
33	D	411	LMG	C29-C28-O8-C9
33	m	101	LMG	C29-C28-O8-C9
25	N	307	CLA	O1A-CGA-O2A-C1
25	n	307	CLA	O1A-CGA-O2A-C1
25	a	604	CLA	O1A-CGA-O2A-C1
33	B	619	LMG	O10-C28-O8-C9
24	R	607	CHL	O1D-CGD-O2D-CED
24	1	317	CHL	O1D-CGD-O2D-CED
24	4	317	CHL	O1D-CGD-O2D-CED
29	2	301	0UR	O44-C45-C46-C47
29	9	301	0UR	O44-C45-C46-C47
29	5	301	0UR	O44-C45-C46-C47
29	u	301	0UR	O44-C45-C46-C47
29	p	301	0UR	O44-C45-C46-C47
29	7	301	0UR	O44-C45-C46-C47
24	N	304	CHL	CBD-CGD-O2D-CED
24	Y	312	CHL	CBD-CGD-O2D-CED
24	4	310	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	4	312	CHL	CBD-CGD-O2D-CED
24	g	306	CHL	CBD-CGD-O2D-CED
24	n	304	CHL	CBD-CGD-O2D-CED
24	y	310	CHL	CBD-CGD-O2D-CED
25	B	609	CLA	CBD-CGD-O2D-CED
25	4	315	CLA	CBD-CGD-O2D-CED
25	y	308	CLA	CBD-CGD-O2D-CED
32	D	409	SQD	C8-C7-O47-C45
32	d	409	SQD	C8-C7-O47-C45
24	S	607	CHL	O1D-CGD-O2D-CED
25	1	314	CLA	O1D-CGD-O2D-CED
25	r	311	CLA	O1D-CGD-O2D-CED
33	w	201	LMG	C15-C16-C17-C18
24	1	309	CHL	CBD-CGD-O2D-CED
24	1	312	CHL	CBD-CGD-O2D-CED
24	3	305	CHL	CBD-CGD-O2D-CED
24	S	601	CHL	CBD-CGD-O2D-CED
24	Y	309	CHL	CBD-CGD-O2D-CED
24	6	305	CHL	CBD-CGD-O2D-CED
24	g	313	CHL	CBD-CGD-O2D-CED
24	g	318	CHL	CBD-CGD-O2D-CED
24	p	305	CHL	CBD-CGD-O2D-CED
24	q	303	CHL	CBD-CGD-O2D-CED
25	R	613	CLA	CBD-CGD-O2D-CED
25	S	609	CLA	CBD-CGD-O2D-CED
25	9	307	CLA	CBD-CGD-O2D-CED
25	8	312	CLA	CBD-CGD-O2D-CED
25	D	405	CLA	CBD-CGD-O2D-CED
25	b	609	CLA	CBD-CGD-O2D-CED
24	9	311	CHL	O1D-CGD-O2D-CED
25	S	611	CLA	O1D-CGD-O2D-CED
25	n	313	CLA	O1D-CGD-O2D-CED
25	b	606	CLA	O1D-CGD-O2D-CED
25	s	412	CLA	O1D-CGD-O2D-CED
25	u	315	CLA	CBA-CGA-O2A-C1
30	g	319	LHG	C24-C23-O8-C6
25	c	603	CLA	C4-C3-C5-C6
39	D	406	PL9	C20-C19-C21-C22
39	d	406	PL9	C20-C19-C21-C22
25	B	613	CLA	C2-C3-C5-C6
25	b	613	CLA	C2-C3-C5-C6
25	b	614	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	9	314	CLA	O1A-CGA-O2A-C1
25	C	604	CLA	O1A-CGA-O2A-C1
25	p	315	CLA	O1A-CGA-O2A-C1
25	7	315	CLA	O1A-CGA-O2A-C1
33	m	101	LMG	O10-C28-O8-C9
24	2	309	CHL	CBD-CGD-O2D-CED
24	G	313	CHL	CBD-CGD-O2D-CED
24	G	318	CHL	CBD-CGD-O2D-CED
24	Y	308	CHL	CBD-CGD-O2D-CED
24	8	304	CHL	CBD-CGD-O2D-CED
24	q	304	CHL	CBD-CGD-O2D-CED
25	C	602	CLA	CBD-CGD-O2D-CED
25	b	610	CLA	CBD-CGD-O2D-CED
25	c	602	CLA	CBD-CGD-O2D-CED
25	3	314	CLA	O1D-CGD-O2D-CED
37	C	619	DGD	C4E-C5E-C6E-O5E
24	y	310	CHL	C2A-CAA-CBA-CGA
25	Y	307	CLA	C2A-CAA-CBA-CGA
25	b	601	CLA	C2A-CAA-CBA-CGA
29	1	301	0UR	O44-C45-C46-C47
29	3	301	0UR	O44-C45-C46-C47
29	G	301	0UR	O44-C45-C46-C47
29	4	301	0UR	O44-C45-C46-C47
29	6	301	0UR	O44-C45-C46-C47
29	g	301	0UR	O44-C45-C46-C47
24	8	310	CHL	O1D-CGD-O2D-CED
25	Y	307	CLA	O1D-CGD-O2D-CED
25	4	307	CLA	O1D-CGD-O2D-CED
25	c	604	CLA	O1A-CGA-O2A-C1
30	9	318	LHG	O10-C23-O8-C6
33	C	618	LMG	O6-C1-O1-C7
37	C	619	DGD	O6D-C1D-O3G-C3G
37	c	618	DGD	O6D-C1D-O3G-C3G
33	w	201	LMG	O6-C5-C6-O5
33	d	411	LMG	O6-C5-C6-O5
24	1	311	CHL	O1D-CGD-O2D-CED
24	4	311	CHL	O1D-CGD-O2D-CED
24	u	312	CHL	O1D-CGD-O2D-CED
24	q	311	CHL	O1D-CGD-O2D-CED
25	N	313	CLA	O1D-CGD-O2D-CED
25	Y	307	CLA	CBA-CGA-O2A-C1
33	D	411	LMG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
24	R	605	CHL	CBD-CGD-O2D-CED
24	2	310	CHL	CBD-CGD-O2D-CED
24	3	309	CHL	CBD-CGD-O2D-CED
24	S	605	CHL	CBD-CGD-O2D-CED
24	G	305	CHL	CBD-CGD-O2D-CED
24	N	310	CHL	CBD-CGD-O2D-CED
24	Y	304	CHL	CBD-CGD-O2D-CED
24	8	303	CHL	CBD-CGD-O2D-CED
24	4	309	CHL	CBD-CGD-O2D-CED
24	5	310	CHL	CBD-CGD-O2D-CED
24	6	308	CHL	CBD-CGD-O2D-CED
24	6	312	CHL	CBD-CGD-O2D-CED
24	g	305	CHL	CBD-CGD-O2D-CED
24	u	305	CHL	CBD-CGD-O2D-CED
24	y	309	CHL	CBD-CGD-O2D-CED
24	s	406	CHL	CBD-CGD-O2D-CED
24	r	307	CHL	CBD-CGD-O2D-CED
25	R	603	CLA	CBD-CGD-O2D-CED
25	2	308	CLA	CBD-CGD-O2D-CED
25	B	604	CLA	CBD-CGD-O2D-CED
25	B	610	CLA	CBD-CGD-O2D-CED
25	5	308	CLA	CBD-CGD-O2D-CED
25	6	316	CLA	CBD-CGD-O2D-CED
25	u	308	CLA	CBD-CGD-O2D-CED
25	n	306	CLA	CBD-CGD-O2D-CED
25	b	604	CLA	CBD-CGD-O2D-CED
25	c	604	CLA	CBD-CGD-O2D-CED
25	d	405	CLA	CBD-CGD-O2D-CED
25	s	411	CLA	CBD-CGD-O2D-CED
25	r	304	CLA	CBD-CGD-O2D-CED
25	r	314	CLA	CBD-CGD-O2D-CED
37	C	619	DGD	O6E-C5E-C6E-O5E
25	u	315	CLA	O1A-CGA-O2A-C1
24	p	313	CHL	O1D-CGD-O2D-CED
24	R	606	CHL	CBD-CGD-O2D-CED
25	Y	313	CLA	CBD-CGD-O2D-CED
25	C	604	CLA	CBD-CGD-O2D-CED
39	d	406	PL9	C47-C48-C49-C51
30	d	408	LHG	C24-C25-C26-C27
37	c	618	DGD	C4E-C5E-C6E-O5E
30	2	319	LHG	C12-C13-C14-C15
30	d	408	LHG	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
33	C	618	LMG	C14-C15-C16-C17
33	d	401	LMG	C11-C12-C13-C14
37	C	619	DGD	C5B-C6B-C7B-C8B
31	X	601	8CT	C16-C17-C18-C19
31	T	101	8CT	C18-C19-C20-C21
31	B	617	8CT	C16-C17-C18-C19
31	x	601	8CT	C16-C17-C18-C19
31	t	101	8CT	C18-C19-C20-C21
31	b	617	8CT	C16-C17-C18-C19
31	c	615	8CT	C23-C24-C25-C26
30	N	318	LHG	C1-C2-C3-O3
30	A	601	LHG	C1-C2-C3-O3
30	D	408	LHG	C1-C2-C3-O3
30	n	318	LHG	C1-C2-C3-O3
30	d	408	LHG	C1-C2-C3-O3
25	l	307	CLA	O1D-CGD-O2D-CED
24	G	311	CHL	CBA-CGA-O2A-C1
24	9	305	CHL	CBA-CGA-O2A-C1
24	N	305	CHL	CBA-CGA-O2A-C1
24	Y	310	CHL	CBA-CGA-O2A-C1
24	g	311	CHL	CBA-CGA-O2A-C1
24	u	306	CHL	CBA-CGA-O2A-C1
25	Y	314	CLA	CBA-CGA-O2A-C1
25	C	605	CLA	CBA-CGA-O2A-C1
25	C	610	CLA	CBA-CGA-O2A-C1
25	D	405	CLA	CBA-CGA-O2A-C1
25	y	308	CLA	CBA-CGA-O2A-C1
25	y	315	CLA	CBA-CGA-O2A-C1
25	c	610	CLA	CBA-CGA-O2A-C1
25	d	405	CLA	CBA-CGA-O2A-C1
30	D	407	LHG	C24-C23-O8-C6
30	d	407	LHG	C24-C23-O8-C6
32	a	609	SQD	C24-C23-O48-C46
33	W	201	LMG	C29-C28-O8-C9
33	w	201	LMG	C29-C28-O8-C9
33	B	619	LMG	C13-C14-C15-C16
33	m	101	LMG	C29-C30-C31-C32
24	u	311	CHL	CBD-CGD-O2D-CED
24	n	312	CHL	CBD-CGD-O2D-CED
24	7	305	CHL	CBD-CGD-O2D-CED
25	S	610	CLA	CBD-CGD-O2D-CED
33	d	411	LMG	C4-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
33	C	618	LMG	C12-C13-C14-C15
33	C	618	LMG	C29-C30-C31-C32
37	C	620	DGD	C6B-C7B-C8B-C9B
37	c	618	DGD	C5B-C6B-C7B-C8B
24	5	311	CHL	O1D-CGD-O2D-CED
25	4	314	CLA	O1D-CGD-O2D-CED
25	c	603	CLA	O1D-CGD-O2D-CED
24	g	311	CHL	O1A-CGA-O2A-C1
25	C	603	CLA	O1D-CGD-O2D-CED
25	9	314	CLA	C4-C3-C5-C6
25	B	612	CLA	C4-C3-C5-C6
25	b	612	CLA	C4-C3-C5-C6
25	9	314	CLA	C2-C3-C5-C6
25	B	612	CLA	C2-C3-C5-C6
25	C	603	CLA	C2-C3-C5-C6
25	b	612	CLA	C2-C3-C5-C6
25	c	603	CLA	C2-C3-C5-C6
39	d	406	PL9	C12-C11-C9-C8
39	D	406	PL9	C47-C48-C49-C51
25	c	610	CLA	C3-C5-C6-C7
24	9	310	CHL	CBD-CGD-O2D-CED
24	G	306	CHL	C11-C12-C13-C14
24	9	305	CHL	C14-C13-C15-C16
24	Y	305	CHL	C6-C7-C8-C9
24	Y	305	CHL	C11-C12-C13-C14
24	Y	312	CHL	C11-C12-C13-C14
24	8	304	CHL	C6-C7-C8-C9
24	g	306	CHL	C11-C12-C13-C14
24	u	306	CHL	C14-C13-C15-C16
24	n	305	CHL	C6-C7-C8-C9
24	y	306	CHL	C6-C7-C8-C9
24	y	306	CHL	C11-C12-C13-C14
24	y	313	CHL	C11-C12-C13-C14
24	p	305	CHL	C11-C12-C13-C14
24	p	306	CHL	C6-C7-C8-C9
24	p	306	CHL	C11-C12-C13-C14
24	q	304	CHL	C6-C7-C8-C9
24	7	305	CHL	C11-C12-C13-C14
24	7	306	CHL	C6-C7-C8-C9
24	7	306	CHL	C11-C12-C13-C14
25	B	603	CLA	C11-C12-C13-C14
25	B	604	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
25	B	605	CLA	C14-C13-C15-C16
25	B	609	CLA	C11-C10-C8-C9
25	A	604	CLA	C14-C13-C15-C16
25	C	608	CLA	C11-C12-C13-C14
25	p	315	CLA	C6-C7-C8-C9
25	b	603	CLA	C11-C12-C13-C14
25	b	605	CLA	C14-C13-C15-C16
25	a	604	CLA	C14-C13-C15-C16
25	c	608	CLA	C11-C12-C13-C14
35	A	606	PHO	C14-C13-C15-C16
30	5	319	LHG	C12-C13-C14-C15
33	D	401	LMG	C14-C15-C16-C17
33	m	101	LMG	C13-C14-C15-C16
37	c	619	DGD	C6B-C7B-C8B-C9B
24	n	308	CHL	O1D-CGD-O2D-CED
24	7	313	CHL	O1D-CGD-O2D-CED
25	5	317	CLA	O1D-CGD-O2D-CED
25	6	307	CLA	O1D-CGD-O2D-CED
32	a	609	SQD	C2-C1-O6-C44
37	C	619	DGD	C2D-C1D-O3G-C3G
37	c	618	DGD	C2D-C1D-O3G-C3G
30	5	319	LHG	C14-C15-C16-C17
33	D	411	LMG	C28-C29-C30-C31
25	q	313	CLA	O1D-CGD-O2D-CED
29	1	301	0UR	O57-C45-C46-C47
29	9	301	0UR	O57-C45-C46-C47
29	4	301	0UR	O57-C45-C46-C47
24	2	318	CHL	CBD-CGD-O2D-CED
24	n	317	CHL	CBD-CGD-O2D-CED
24	2	311	CHL	O1D-CGD-O2D-CED
25	2	317	CLA	O1D-CGD-O2D-CED
25	B	606	CLA	O1D-CGD-O2D-CED
25	p	315	CLA	O1D-CGD-O2D-CED
29	1	301	0UR	C5-C6-C7-C20
29	2	301	0UR	C5-C6-C7-C20
29	2	301	0UR	C22-C16-C17-C18
29	G	301	0UR	C5-C6-C7-C20
29	9	301	0UR	C5-C6-C7-C20
29	8	301	0UR	C5-C6-C7-C20
29	4	301	0UR	C5-C6-C7-C20
29	5	301	0UR	C5-C6-C7-C20
29	5	301	0UR	C22-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
29	6	301	0UR	C5-C6-C7-C20
29	g	301	0UR	C5-C6-C7-C20
29	n	301	0UR	C5-C6-C7-C20
29	q	301	0UR	C5-C6-C7-C20
31	S	615	8CT	C22-C21-C23-C24
31	X	601	8CT	C10-C11-C12-C40
31	T	101	8CT	C10-C11-C12-C40
31	T	101	8CT	C14-C15-C16-C39
31	B	617	8CT	C22-C21-C23-C24
31	B	617	8CT	C27-C26-C28-C29
31	A	608	8CT	C10-C11-C12-C40
31	A	608	8CT	C14-C15-C16-C39
31	C	614	8CT	C10-C11-C12-C40
31	C	615	8CT	C14-C15-C16-C39
31	x	601	8CT	C10-C11-C12-C40
31	t	101	8CT	C10-C11-C12-C40
31	b	617	8CT	C27-C26-C28-C29
31	a	608	8CT	C10-C11-C12-C40
31	a	608	8CT	C14-C15-C16-C39
31	c	614	8CT	C10-C11-C12-C40
31	c	615	8CT	C14-C15-C16-C39
31	s	416	8CT	C22-C21-C23-C24
37	c	618	DGD	O6E-C5E-C6E-O5E
29	2	301	0UR	C15-C16-C17-C18
29	5	301	0UR	C15-C16-C17-C18
31	X	601	8CT	C10-C11-C12-C13
31	T	101	8CT	C10-C11-C12-C13
31	T	101	8CT	C14-C15-C16-C17
31	B	617	8CT	C14-C15-C16-C17
31	A	608	8CT	C10-C11-C12-C13
31	A	608	8CT	C14-C15-C16-C17
31	C	614	8CT	C10-C11-C12-C13
31	C	615	8CT	C14-C15-C16-C17
31	x	601	8CT	C10-C11-C12-C13
31	t	101	8CT	C10-C11-C12-C13
31	t	101	8CT	C14-C15-C16-C17
31	b	617	8CT	C10-C11-C12-C13
31	b	617	8CT	C14-C15-C16-C17
31	a	608	8CT	C10-C11-C12-C13
31	a	608	8CT	C14-C15-C16-C17
31	c	614	8CT	C10-C11-C12-C13
31	c	615	8CT	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
24	S	605	CHL	C2A-CAA-CBA-CGA
24	Y	309	CHL	C2A-CAA-CBA-CGA
24	u	306	CHL	C2A-CAA-CBA-CGA
25	B	610	CLA	C2A-CAA-CBA-CGA
25	y	308	CLA	C2A-CAA-CBA-CGA
33	B	619	LMG	C29-C30-C31-C32
37	C	620	DGD	C2B-C3B-C4B-C5B
29	8	301	0UR	O44-C45-C46-C47
29	n	301	0UR	O44-C45-C46-C47
29	q	301	0UR	O44-C45-C46-C47
25	C	610	CLA	O1A-CGA-O2A-C1
25	c	610	CLA	O1A-CGA-O2A-C1
24	u	309	CHL	CBD-CGD-O2D-CED
24	y	305	CHL	CBD-CGD-O2D-CED
25	B	602	CLA	CBD-CGD-O2D-CED
25	C	611	CLA	CBA-CGA-O2A-C1
25	c	605	CLA	CBA-CGA-O2A-C1
29	2	301	0UR	O57-C45-C46-C47
29	5	301	0UR	O57-C45-C46-C47
29	6	301	0UR	O57-C45-C46-C47
29	7	301	0UR	O57-C45-C46-C47
25	u	307	CLA	C5-C6-C7-C8
25	c	603	CLA	C15-C16-C17-C18
24	S	606	CHL	O1D-CGD-O2D-CED
24	N	305	CHL	O1D-CGD-O2D-CED
24	6	304	CHL	O1D-CGD-O2D-CED
25	S	616	CLA	O1D-CGD-O2D-CED
25	N	315	CLA	O1D-CGD-O2D-CED
25	B	607	CLA	O1D-CGD-O2D-CED
25	6	314	CLA	O1D-CGD-O2D-CED
25	b	607	CLA	O1D-CGD-O2D-CED
25	a	610	CLA	O1D-CGD-O2D-CED
24	3	312	CHL	CBD-CGD-O2D-CED
24	N	312	CHL	CBD-CGD-O2D-CED
24	6	309	CHL	CBD-CGD-O2D-CED
24	n	310	CHL	CBD-CGD-O2D-CED
24	G	305	CHL	C15-C16-C17-C18
24	G	313	CHL	C5-C6-C7-C8
24	9	304	CHL	C13-C15-C16-C17
24	g	306	CHL	C8-C10-C11-C12
24	g	313	CHL	C5-C6-C7-C8
24	y	305	CHL	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
24	7	306	CHL	C10-C11-C12-C13
25	B	609	CLA	C8-C10-C11-C12
25	b	603	CLA	C13-C15-C16-C17
25	7	315	CLA	O1D-CGD-O2D-CED
24	s	407	CHL	O1D-CGD-O2D-CED
24	Y	305	CHL	C10-C11-C12-C13
24	g	305	CHL	C15-C16-C17-C18
25	B	603	CLA	C13-C15-C16-C17
24	3	308	CHL	CBD-CGD-O2D-CED
24	9	304	CHL	CBD-CGD-O2D-CED
24	9	308	CHL	CBD-CGD-O2D-CED
25	N	306	CLA	CBD-CGD-O2D-CED
25	q	312	CLA	CBD-CGD-O2D-CED
33	m	101	LMG	C15-C16-C17-C18
24	u	305	CHL	C12-C13-C15-C16
25	8	312	CLA	C11-C10-C8-C7
25	y	315	CLA	C11-C10-C8-C7
25	q	313	CLA	C11-C10-C8-C7
25	c	611	CLA	CBA-CGA-O2A-C1
29	3	301	0UR	O57-C45-C46-C47
29	G	301	0UR	O57-C45-C46-C47
29	g	301	0UR	O57-C45-C46-C47
29	u	301	0UR	O57-C45-C46-C47
29	p	301	0UR	O57-C45-C46-C47
29	N	301	0UR	O44-C45-C46-C47
30	4	318	LHG	C14-C15-C16-C17
33	B	619	LMG	C15-C16-C17-C18
24	N	312	CHL	C5-C6-C7-C8
24	n	312	CHL	C5-C6-C7-C8
25	C	603	CLA	C15-C16-C17-C18
25	a	603	CLA	C15-C16-C17-C18
33	w	201	LMG	C4-C5-C6-O5
25	c	601	CLA	O1D-CGD-O2D-CED
30	y	319	LHG	C23-C24-C25-C26
31	V	401	8CT	C16-C17-C18-C19
31	A	608	8CT	C12-C13-C14-C15
31	C	614	8CT	C18-C19-C20-C21
31	v	401	8CT	C16-C17-C18-C19
31	v	401	8CT	C18-C19-C20-C21
31	a	608	8CT	C12-C13-C14-C15
31	c	614	8CT	C18-C19-C20-C21
24	u	318	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
37	C	619	DGD	C4D-C5D-C6D-O5D
24	3	304	CHL	O1D-CGD-O2D-CED
25	C	601	CLA	O1D-CGD-O2D-CED
25	b	613	CLA	O1D-CGD-O2D-CED
24	u	305	CHL	C13-C15-C16-C17
30	1	318	LHG	C14-C15-C16-C17
33	D	411	LMG	C12-C13-C14-C15
30	Y	318	LHG	C23-C24-C25-C26
30	p	319	LHG	C23-C24-C25-C26
33	i	101	LMG	C28-C29-C30-C31
24	G	311	CHL	O1A-CGA-O2A-C1
24	N	305	CHL	O1A-CGA-O2A-C1
24	Y	310	CHL	O1A-CGA-O2A-C1
24	u	306	CHL	O1A-CGA-O2A-C1
25	Y	314	CLA	O1A-CGA-O2A-C1
25	C	605	CLA	O1A-CGA-O2A-C1
25	c	605	CLA	O1A-CGA-O2A-C1
30	d	407	LHG	O10-C23-O8-C6
33	w	201	LMG	O10-C28-O8-C9
24	N	317	CHL	CBD-CGD-O2D-CED
24	5	318	CHL	CBD-CGD-O2D-CED
24	R	608	CHL	O1D-CGD-O2D-CED
24	r	309	CHL	O1D-CGD-O2D-CED
25	A	610	CLA	O1D-CGD-O2D-CED
24	G	306	CHL	C8-C10-C11-C12
24	g	305	CHL	C13-C15-C16-C17
25	B	611	CLA	C13-C15-C16-C17
25	D	405	CLA	C15-C16-C17-C18
24	R	601	CHL	C2A-CAA-CBA-CGA
24	S	607	CHL	C2A-CAA-CBA-CGA
24	N	311	CHL	C2A-CAA-CBA-CGA
24	Y	311	CHL	C2A-CAA-CBA-CGA
24	8	303	CHL	C2A-CAA-CBA-CGA
24	8	308	CHL	C2A-CAA-CBA-CGA
24	n	304	CHL	C2A-CAA-CBA-CGA
24	y	312	CHL	C2A-CAA-CBA-CGA
24	p	310	CHL	C2A-CAA-CBA-CGA
24	p	312	CHL	C2A-CAA-CBA-CGA
24	q	303	CHL	C2A-CAA-CBA-CGA
24	q	308	CHL	C2A-CAA-CBA-CGA
24	r	302	CHL	C2A-CAA-CBA-CGA
24	7	310	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
24	7	312	CHL	C2A-CAA-CBA-CGA
25	N	307	CLA	C2A-CAA-CBA-CGA
25	B	601	CLA	C2A-CAA-CBA-CGA
25	b	608	CLA	C2A-CAA-CBA-CGA
25	b	610	CLA	C2A-CAA-CBA-CGA
25	b	614	CLA	C2A-CAA-CBA-CGA
25	1	315	CLA	O1D-CGD-O2D-CED
24	G	305	CHL	C8-C10-C11-C12
24	9	304	CHL	C15-C16-C17-C18
24	9	305	CHL	C5-C6-C7-C8
24	N	305	CHL	C8-C10-C11-C12
24	u	306	CHL	C5-C6-C7-C8
24	p	306	CHL	C10-C11-C12-C13
24	7	306	CHL	C5-C6-C7-C8
25	C	604	CLA	C13-C15-C16-C17
25	b	612	CLA	C5-C6-C7-C8
25	c	604	CLA	C13-C15-C16-C17
25	d	405	CLA	C15-C16-C17-C18
30	Y	318	LHG	C7-C8-C9-C10
30	7	319	LHG	C23-C24-C25-C26
32	a	609	SQD	C7-C8-C9-C10
32	a	609	SQD	C23-C24-C25-C26
33	i	101	LMG	C10-C11-C12-C13
24	9	305	CHL	O1A-CGA-O2A-C1
25	D	405	CLA	O1A-CGA-O2A-C1
25	y	308	CLA	O1A-CGA-O2A-C1
25	y	315	CLA	O1A-CGA-O2A-C1
25	d	405	CLA	O1A-CGA-O2A-C1
33	W	201	LMG	O10-C28-O8-C9
25	C	609	CLA	C3-C5-C6-C7
25	c	609	CLA	C3-C5-C6-C7
24	4	304	CHL	CBD-CGD-O2D-CED
33	w	201	LMG	O6-C1-O1-C7
33	d	411	LMG	O6-C1-O1-C7
37	C	619	DGD	O6E-C1E-O5D-C6D
33	D	411	LMG	C14-C15-C16-C17
25	B	613	CLA	O1D-CGD-O2D-CED
25	a	603	CLA	O1D-CGD-O2D-CED
24	G	305	CHL	C13-C15-C16-C17
24	G	306	CHL	C5-C6-C7-C8
24	n	305	CHL	C8-C10-C11-C12
24	y	306	CHL	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
24	p	305	CHL	C8-C10-C11-C12
24	p	306	CHL	C5-C6-C7-C8
24	p	306	CHL	C8-C10-C11-C12
24	q	304	CHL	C8-C10-C11-C12
25	C	604	CLA	C15-C16-C17-C18
25	D	405	CLA	C5-C6-C7-C8
25	b	609	CLA	C8-C10-C11-C12
25	b	609	CLA	C15-C16-C17-C18
25	b	611	CLA	C13-C15-C16-C17
25	c	604	CLA	C15-C16-C17-C18
30	A	612	LHG	C31-C32-C33-C34
33	C	618	LMG	C33-C34-C35-C36
30	A	601	LHG	O2-C2-C3-O3
30	D	408	LHG	O2-C2-C3-O3
30	a	601	LHG	O2-C2-C3-O3
25	n	315	CLA	O1D-CGD-O2D-CED
25	B	604	CLA	CBA-CGA-O2A-C1
25	y	314	CLA	CBD-CGD-O2D-CED
25	Y	307	CLA	O1A-CGA-O2A-C1
30	D	407	LHG	O10-C23-O8-C6
24	1	311	CHL	C2A-CAA-CBA-CGA
24	S	602	CHL	C8-C10-C11-C12
24	s	403	CHL	C8-C10-C11-C12
25	8	314	CLA	C2A-CAA-CBA-CGA
30	y	319	LHG	C7-C8-C9-C10
33	C	618	LMG	C28-C29-C30-C31
24	8	304	CHL	C8-C10-C11-C12
24	y	305	CHL	C13-C15-C16-C17
24	7	305	CHL	C8-C10-C11-C12
25	B	608	CLA	C5-C6-C7-C8
25	a	603	CLA	C13-C15-C16-C17
24	2	305	CHL	O1D-CGD-O2D-CED
24	5	305	CHL	O1D-CGD-O2D-CED
24	R	602	CHL	CBA-CGA-O2A-C1
24	r	303	CHL	CBA-CGA-O2A-C1
24	5	309	CHL	O1D-CGD-O2D-CED
24	s	403	CHL	O1D-CGD-O2D-CED
25	G	317	CLA	O1D-CGD-O2D-CED
25	A	603	CLA	O1D-CGD-O2D-CED
25	s	410	CLA	O1D-CGD-O2D-CED
33	d	411	LMG	C12-C13-C14-C15
24	g	313	CHL	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
25	B	605	CLA	C5-C6-C7-C8
25	B	612	CLA	C5-C6-C7-C8
25	b	605	CLA	C5-C6-C7-C8
25	b	608	CLA	C5-C6-C7-C8
24	g	309	CHL	CBD-CGD-O2D-CED
30	A	601	LHG	C11-C12-C13-C14
30	a	612	LHG	C31-C32-C33-C34
24	1	310	CHL	O1D-CGD-O2D-CED
24	2	306	CHL	O1D-CGD-O2D-CED
24	G	313	CHL	C8-C10-C11-C12
24	g	305	CHL	C8-C10-C11-C12
24	y	313	CHL	C5-C6-C7-C8
24	7	305	CHL	C13-C15-C16-C17
25	B	607	CLA	C8-C10-C11-C12
25	B	613	CLA	C10-C11-C12-C13
25	A	603	CLA	C13-C15-C16-C17
24	8	310	CHL	CBA-CGA-O2A-C1
24	n	305	CHL	CBA-CGA-O2A-C1
24	q	311	CHL	CBA-CGA-O2A-C1
24	r	306	CHL	CBD-CGD-O2D-CED
25	3	316	CLA	CBD-CGD-O2D-CED
25	C	611	CLA	O1A-CGA-O2A-C1
24	u	306	CHL	O1D-CGD-O2D-CED
24	y	313	CHL	O1D-CGD-O2D-CED
25	s	417	CLA	O1D-CGD-O2D-CED
24	g	310	CHL	CBA-CGA-O2A-C1
24	p	305	CHL	C13-C15-C16-C17
25	b	604	CLA	C5-C6-C7-C8
25	b	607	CLA	C8-C10-C11-C12
25	b	613	CLA	C10-C11-C12-C13
24	Y	304	CHL	C3-C5-C6-C7
24	y	305	CHL	C3-C5-C6-C7
24	9	305	CHL	O1D-CGD-O2D-CED
24	3	311	CHL	C2A-CAA-CBA-CGA
24	4	311	CHL	C2A-CAA-CBA-CGA
24	5	305	CHL	C2A-CAA-CBA-CGA
33	D	401	LMG	C35-C36-C37-C38
33	D	411	LMG	C18-C19-C20-C21
31	V	401	8CT	C18-C19-C20-C21
31	T	101	8CT	C12-C13-C14-C15
31	B	617	8CT	C18-C19-C20-C21
31	C	615	8CT	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
31	t	101	8CT	C12-C13-C14-C15
31	b	617	8CT	C18-C19-C20-C21
31	c	615	8CT	C18-C19-C20-C21
24	7	305	CHL	C15-C16-C17-C18
25	c	610	CLA	C15-C16-C17-C18
24	R	607	CHL	C2A-CAA-CBA-CGA
24	2	312	CHL	C2A-CAA-CBA-CGA
24	9	305	CHL	C2A-CAA-CBA-CGA
24	N	304	CHL	C2A-CAA-CBA-CGA
24	8	309	CHL	C2A-CAA-CBA-CGA
24	5	312	CHL	C2A-CAA-CBA-CGA
24	6	309	CHL	C2A-CAA-CBA-CGA
24	n	309	CHL	C2A-CAA-CBA-CGA
24	s	402	CHL	C2A-CAA-CBA-CGA
24	s	406	CHL	C2A-CAA-CBA-CGA
24	s	408	CHL	C2A-CAA-CBA-CGA
25	B	608	CLA	C2A-CAA-CBA-CGA
25	B	614	CLA	C2A-CAA-CBA-CGA
24	5	306	CHL	O1D-CGD-O2D-CED
24	n	305	CHL	O1D-CGD-O2D-CED
24	y	311	CHL	CBA-CGA-O2A-C1
25	b	604	CLA	CBA-CGA-O2A-C1
24	Y	304	CHL	C15-C16-C17-C18
24	u	305	CHL	C15-C16-C17-C18
24	p	305	CHL	C15-C16-C17-C18
25	B	604	CLA	C5-C6-C7-C8
25	B	609	CLA	C15-C16-C17-C18
25	d	405	CLA	C5-C6-C7-C8
25	b	602	CLA	CBD-CGD-O2D-CED
37	C	619	DGD	O6D-C5D-C6D-O5D
33	D	401	LMG	C11-C12-C13-C14
24	G	306	CHL	O1D-CGD-O2D-CED
24	s	402	CHL	O1D-CGD-O2D-CED
24	9	305	CHL	C13-C15-C16-C17
24	g	306	CHL	C13-C15-C16-C17
25	b	609	CLA	C5-C6-C7-C8
30	a	601	LHG	C11-C12-C13-C14
24	u	306	CHL	C13-C15-C16-C17
25	B	609	CLA	C5-C6-C7-C8
25	C	610	CLA	C15-C16-C17-C18
24	y	310	CHL	O1D-CGD-O2D-CED
29	8	301	OUR	O57-C45-C46-C47

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Mol	Chain	Res	Type	Atoms
29	n	301	0UR	O57-C45-C46-C47
29	q	301	0UR	O57-C45-C46-C47
37	c	618	DGD	C2A-C1A-O1G-C1G
37	c	618	DGD	O6D-C5D-C6D-O5D
24	2	305	CHL	C2A-CAA-CBA-CGA
24	6	311	CHL	C2A-CAA-CBA-CGA
24	N	304	CHL	C4-C3-C5-C6
24	n	304	CHL	C4-C3-C5-C6
39	d	406	PL9	C47-C48-C49-C50
24	G	306	CHL	C10-C11-C12-C13
25	A	603	CLA	C15-C16-C17-C18
25	C	610	CLA	C3-C5-C6-C7
24	1	304	CHL	CBD-CGD-O2D-CED
32	A	609	SQD	C8-C7-O47-C45
33	m	101	LMG	C11-C10-O7-C8
35	a	606	PHO	C14-C13-C15-C16
24	S	602	CHL	O1D-CGD-O2D-CED
24	Y	309	CHL	O1D-CGD-O2D-CED
24	4	310	CHL	O1D-CGD-O2D-CED
24	4	312	CHL	O1D-CGD-O2D-CED
25	8	312	CLA	O1D-CGD-O2D-CED
25	4	315	CLA	O1D-CGD-O2D-CED
25	y	308	CLA	O1D-CGD-O2D-CED
33	m	101	LMG	O9-C10-O7-C8
32	D	409	SQD	C2-C1-O6-C44
32	d	409	SQD	C2-C1-O6-C44
33	C	618	LMG	C2-C1-O1-C7
33	i	101	LMG	C2-C1-O1-C7
33	d	411	LMG	C2-C1-O1-C7
37	C	619	DGD	C2E-C1E-O5D-C6D
37	c	618	DGD	C2E-C1E-O5D-C6D
29	Y	301	0UR	O44-C45-C46-C47
29	y	301	0UR	O44-C45-C46-C47
24	N	304	CHL	O1D-CGD-O2D-CED
25	R	613	CLA	O1D-CGD-O2D-CED
24	Y	312	CHL	O1D-CGD-O2D-CED
24	p	306	CHL	CBA-CGA-O2A-C1
35	D	403	PHO	CBA-CGA-O2A-C1
35	d	403	PHO	CBA-CGA-O2A-C1
24	G	313	CHL	C16-C17-C18-C20
24	Y	312	CHL	C16-C17-C18-C19
24	y	313	CHL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
25	b	615	CLA	C16-C17-C18-C19
24	n	309	CHL	CBD-CGD-O2D-CED
24	g	306	CHL	O1D-CGD-O2D-CED
25	9	307	CLA	O1D-CGD-O2D-CED
26	9	303	0IE	C22-C12-C13-C14
29	N	301	0UR	C5-C6-C7-C20
29	u	301	0UR	C5-C6-C7-C20
29	y	301	0UR	C5-C6-C7-C20
30	4	318	LHG	C5-C4-O6-P
31	S	615	8CT	C27-C26-C28-C29
31	X	601	8CT	C27-C26-C28-C29
31	B	617	8CT	C10-C11-C12-C40
31	C	613	8CT	C10-C11-C12-C40
31	C	614	8CT	C14-C15-C16-C39
31	x	601	8CT	C27-C26-C28-C29
31	t	101	8CT	C14-C15-C16-C39
31	b	617	8CT	C10-C11-C12-C40
31	c	613	8CT	C10-C11-C12-C40
31	c	614	8CT	C14-C15-C16-C39
31	d	410	8CT	C10-C11-C12-C40
31	s	416	8CT	C27-C26-C28-C29
29	8	301	0UR	C5-C6-C7-C8
29	4	301	0UR	C5-C6-C7-C8
29	6	301	0UR	C5-C6-C7-C8
29	n	301	0UR	C5-C6-C7-C8
31	S	615	8CT	C25-C26-C28-C29
31	B	617	8CT	C10-C11-C12-C13
31	C	613	8CT	C10-C11-C12-C13
31	C	614	8CT	C14-C15-C16-C17
31	c	613	8CT	C10-C11-C12-C13
31	c	614	8CT	C14-C15-C16-C17
31	d	410	8CT	C10-C11-C12-C13
31	s	416	8CT	C25-C26-C28-C29
25	c	611	CLA	O1A-CGA-O2A-C1
24	n	304	CHL	O1D-CGD-O2D-CED
24	2	311	CHL	C2A-CAA-CBA-CGA
24	3	309	CHL	C2A-CAA-CBA-CGA
24	S	601	CHL	C2A-CAA-CBA-CGA
24	G	310	CHL	C2A-CAA-CBA-CGA
24	N	305	CHL	C2A-CAA-CBA-CGA
24	N	309	CHL	C2A-CAA-CBA-CGA
24	5	311	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
24	u	312	CHL	C2A-CAA-CBA-CGA
24	y	306	CHL	C2A-CAA-CBA-CGA
24	r	308	CHL	C2A-CAA-CBA-CGA
24	p	312	CHL	CBA-CGA-O2A-C1
24	7	312	CHL	CBA-CGA-O2A-C1
24	g	306	CHL	C10-C11-C12-C13
30	2	319	LHG	O1-C1-C2-C3
30	9	318	LHG	O1-C1-C2-C3
30	N	318	LHG	O1-C1-C2-C3
30	C	617	LHG	O1-C1-C2-C3
30	n	318	LHG	O1-C1-C2-C3
30	c	617	LHG	O1-C1-C2-C3
30	d	408	LHG	O1-C1-C2-C3
24	S	601	CHL	O1D-CGD-O2D-CED
25	S	609	CLA	O1D-CGD-O2D-CED
24	q	309	CHL	CBA-CGA-O2A-C1
29	N	301	OUR	O57-C45-C46-C47
32	D	409	SQD	C44-C45-O47-C7
32	d	409	SQD	C44-C45-O47-C7
24	Y	304	CHL	C16-C17-C18-C19
24	g	313	CHL	C16-C17-C18-C20
25	B	608	CLA	C6-C7-C8-C10
25	B	615	CLA	C16-C17-C18-C19
25	b	615	CLA	C16-C17-C18-C20
37	C	620	DGD	C3A-C4A-C5A-C6A
24	1	312	CHL	O1D-CGD-O2D-CED
24	2	309	CHL	O1D-CGD-O2D-CED
25	B	609	CLA	O1D-CGD-O2D-CED
25	D	405	CLA	O1D-CGD-O2D-CED
35	D	403	PHO	C3-C5-C6-C7
35	d	403	PHO	C3-C5-C6-C7
25	A	604	CLA	C13-C15-C16-C17
25	a	607	CLA	C8-C10-C11-C12
26	9	303	OIE	C14-C15-C16-C17
33	D	411	LMG	C29-C30-C31-C32
32	D	409	SQD	O5-C1-O6-C44
32	d	409	SQD	O5-C1-O6-C44
33	i	101	LMG	O6-C1-O1-C7
37	c	618	DGD	O6E-C1E-O5D-C6D
24	G	310	CHL	CBA-CGA-O2A-C1
39	D	406	PL9	C12-C11-C9-C8
24	1	309	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	Y	308	CHL	O1D-CGD-O2D-CED
24	g	313	CHL	O1D-CGD-O2D-CED
25	C	602	CLA	O1D-CGD-O2D-CED
25	b	609	CLA	O1D-CGD-O2D-CED
25	c	602	CLA	O1D-CGD-O2D-CED
24	g	318	CHL	O1D-CGD-O2D-CED
24	y	309	CHL	O1D-CGD-O2D-CED
24	p	305	CHL	O1D-CGD-O2D-CED
25	b	610	CLA	O1D-CGD-O2D-CED
24	Y	319	CHL	CBA-CGA-O2A-C1
33	d	401	LMG	C35-C36-C37-C38
24	8	304	CHL	C5-C6-C7-C8
24	y	313	CHL	C8-C10-C11-C12
24	7	306	CHL	C8-C10-C11-C12
25	2	315	CLA	CBD-CGD-O2D-CED
30	D	407	LHG	C7-C8-C9-C10
25	y	317	CLA	C3-C5-C6-C7
33	D	411	LMG	C20-C21-C22-C23
24	q	303	CHL	O1D-CGD-O2D-CED
24	G	313	CHL	C16-C17-C18-C19
24	9	304	CHL	C16-C17-C18-C19
24	9	304	CHL	C16-C17-C18-C20
24	Y	312	CHL	C16-C17-C18-C20
24	g	313	CHL	C16-C17-C18-C19
24	p	305	CHL	C16-C17-C18-C20
24	7	305	CHL	C16-C17-C18-C20
25	B	602	CLA	C16-C17-C18-C19
25	B	602	CLA	C16-C17-C18-C20
25	B	606	CLA	C16-C17-C18-C20
25	C	602	CLA	C16-C17-C18-C19
25	b	602	CLA	C16-C17-C18-C19
25	b	602	CLA	C16-C17-C18-C20
25	b	606	CLA	C16-C17-C18-C20
25	b	609	CLA	C16-C17-C18-C19
24	3	305	CHL	O1D-CGD-O2D-CED
24	8	304	CHL	O1D-CGD-O2D-CED
24	6	305	CHL	O1D-CGD-O2D-CED
25	y	317	CLA	C6-C7-C8-C10
30	Y	318	LHG	C15-C16-C17-C18
30	A	601	LHG	C15-C16-C17-C18
32	B	618	SQD	C33-C34-C35-C36
33	D	411	LMG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
24	R	601	CHL	CBD-CGD-O2D-CED
24	p	310	CHL	CBD-CGD-O2D-CED
30	N	318	LHG	C14-C15-C16-C17
30	y	319	LHG	C14-C15-C16-C17
30	a	601	LHG	C15-C16-C17-C18
32	a	609	SQD	C12-C13-C14-C15
24	G	318	CHL	O1D-CGD-O2D-CED
25	6	316	CLA	O1D-CGD-O2D-CED
24	G	306	CHL	C13-C15-C16-C17
24	Y	312	CHL	C8-C10-C11-C12
24	q	304	CHL	C5-C6-C7-C8
30	2	319	LHG	C27-C28-C29-C30
30	5	319	LHG	C27-C28-C29-C30
30	p	319	LHG	C12-C13-C14-C15
32	b	618	SQD	C33-C34-C35-C36
32	a	609	SQD	C11-C10-C9-C8
24	n	305	CHL	O1A-CGA-O2A-C1
24	y	311	CHL	O1A-CGA-O2A-C1
24	7	306	CHL	CBA-CGA-O2A-C1
35	a	606	PHO	CBA-CGA-O2A-C1
30	g	319	LHG	C26-C27-C28-C29
30	p	319	LHG	C30-C31-C32-C33
30	7	319	LHG	C30-C31-C32-C33
32	B	618	SQD	C9-C10-C11-C12
32	b	618	SQD	C9-C10-C11-C12
30	G	319	LHG	O1-C1-C2-O2
30	n	318	LHG	O1-C1-C2-O2
30	p	319	LHG	O1-C1-C2-O2
25	Y	316	CLA	C6-C7-C8-C10
30	9	318	LHG	C14-C15-C16-C17
24	G	305	CHL	O1D-CGD-O2D-CED
24	6	308	CHL	O1D-CGD-O2D-CED
24	u	305	CHL	O1D-CGD-O2D-CED
24	q	304	CHL	O1D-CGD-O2D-CED
25	B	610	CLA	O1D-CGD-O2D-CED
25	u	308	CLA	O1D-CGD-O2D-CED
25	d	405	CLA	O1D-CGD-O2D-CED
37	c	618	DGD	C4D-C5D-C6D-O5D
25	Y	306	CLA	C4B-C3B-CAB-CBB
25	u	316	CLA	C4B-C3B-CAB-CBB
25	y	307	CLA	C4B-C3B-CAB-CBB
25	b	601	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
24	G	305	CHL	C16-C17-C18-C19
24	G	305	CHL	C16-C17-C18-C20
24	Y	304	CHL	C16-C17-C18-C20
24	g	305	CHL	C16-C17-C18-C19
24	g	305	CHL	C16-C17-C18-C20
24	u	305	CHL	C16-C17-C18-C20
24	y	313	CHL	C16-C17-C18-C20
24	p	305	CHL	C16-C17-C18-C19
24	7	305	CHL	C16-C17-C18-C19
25	C	604	CLA	C16-C17-C18-C20
25	b	606	CLA	C16-C17-C18-C19
25	a	603	CLA	C16-C17-C18-C20
25	c	604	CLA	C16-C17-C18-C19
25	c	604	CLA	C16-C17-C18-C20
24	G	313	CHL	O1D-CGD-O2D-CED
24	5	310	CHL	O1D-CGD-O2D-CED
24	8	310	CHL	O1A-CGA-O2A-C1
24	Y	305	CHL	C2A-CAA-CBA-CGA
24	6	310	CHL	C2A-CAA-CBA-CGA
25	B	606	CLA	C2A-CAA-CBA-CGA
25	n	307	CLA	C2A-CAA-CBA-CGA
25	b	606	CLA	C2A-CAA-CBA-CGA
25	q	315	CLA	C2A-CAA-CBA-CGA
24	y	306	CHL	C13-C15-C16-C17
25	A	607	CLA	C8-C10-C11-C12
30	D	408	LHG	C8-C7-O7-C5
30	d	408	LHG	C8-C7-O7-C5
30	D	408	LHG	C9-C10-C11-C12
30	p	319	LHG	C28-C29-C30-C31
24	G	305	CHL	C6-C7-C8-C10
24	9	304	CHL	C12-C13-C15-C16
24	g	305	CHL	C6-C7-C8-C10
24	p	305	CHL	C12-C13-C15-C16
25	Y	314	CLA	C11-C10-C8-C7
25	C	603	CLA	C12-C13-C15-C16
25	C	604	CLA	C6-C7-C8-C10
25	c	603	CLA	C12-C13-C15-C16
25	c	604	CLA	C6-C7-C8-C10
30	5	319	LHG	C26-C27-C28-C29
30	7	319	LHG	C28-C29-C30-C31
32	b	618	SQD	C11-C12-C13-C14
33	d	401	LMG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
30	g	319	LHG	C23-C24-C25-C26
24	Y	312	CHL	C5-C6-C7-C8
24	u	305	CHL	C8-C10-C11-C12
25	g	317	CLA	C6-C7-C8-C10
30	2	319	LHG	C26-C27-C28-C29
30	n	318	LHG	C14-C15-C16-C17
32	a	609	SQD	C9-C10-C11-C12
24	q	311	CHL	O1A-CGA-O2A-C1
25	B	604	CLA	O1A-CGA-O2A-C1
24	R	606	CHL	C3A-C2A-CAA-CBA
24	3	310	CHL	C3A-C2A-CAA-CBA
24	S	606	CHL	C3A-C2A-CAA-CBA
24	G	311	CHL	C3A-C2A-CAA-CBA
24	N	310	CHL	C3A-C2A-CAA-CBA
24	Y	310	CHL	C3A-C2A-CAA-CBA
24	Y	319	CHL	C3A-C2A-CAA-CBA
24	6	310	CHL	C3A-C2A-CAA-CBA
24	g	311	CHL	C3A-C2A-CAA-CBA
24	u	310	CHL	C3A-C2A-CAA-CBA
24	u	311	CHL	C3A-C2A-CAA-CBA
24	n	310	CHL	C3A-C2A-CAA-CBA
24	y	311	CHL	C3A-C2A-CAA-CBA
24	p	311	CHL	C3A-C2A-CAA-CBA
24	q	309	CHL	C3A-C2A-CAA-CBA
24	s	407	CHL	C3A-C2A-CAA-CBA
24	r	307	CHL	C3A-C2A-CAA-CBA
24	7	311	CHL	C3A-C2A-CAA-CBA
25	S	616	CLA	C3A-C2A-CAA-CBA
25	A	603	CLA	C3A-C2A-CAA-CBA
25	D	404	CLA	C3A-C2A-CAA-CBA
25	a	603	CLA	C3A-C2A-CAA-CBA
25	s	417	CLA	C3A-C2A-CAA-CBA
24	2	310	CHL	O1D-CGD-O2D-CED
24	4	309	CHL	O1D-CGD-O2D-CED
24	g	305	CHL	O1D-CGD-O2D-CED
24	s	406	CHL	O1D-CGD-O2D-CED
25	r	314	CLA	O1D-CGD-O2D-CED
32	B	618	SQD	C11-C12-C13-C14
24	9	304	CHL	C8-C10-C11-C12
25	C	602	CLA	C5-C6-C7-C8
25	C	604	CLA	C5-C6-C7-C8
25	C	610	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
25	c	604	CLA	C5-C6-C7-C8
24	8	303	CHL	O1D-CGD-O2D-CED
25	2	308	CLA	O1D-CGD-O2D-CED
33	w	201	LMG	C10-C11-C12-C13
33	D	401	LMG	C17-C18-C19-C20
33	d	411	LMG	C17-C18-C19-C20
24	u	305	CHL	C16-C17-C18-C19
25	B	606	CLA	C16-C17-C18-C19
25	B	615	CLA	C16-C17-C18-C20
25	A	603	CLA	C16-C17-C18-C20
25	C	604	CLA	C16-C17-C18-C19
30	y	319	LHG	C27-C28-C29-C30
32	B	618	SQD	C12-C13-C14-C15
24	G	313	CHL	C13-C15-C16-C17
25	c	602	CLA	C5-C6-C7-C8
33	d	411	LMG	C16-C17-C18-C19
24	Y	305	CHL	CBA-CGA-O2A-C1
24	g	306	CHL	CBA-CGA-O2A-C1
25	B	608	CLA	CBA-CGA-O2A-C1
25	u	317	CLA	CBA-CGA-O2A-C1
25	b	608	CLA	CBA-CGA-O2A-C1
35	A	606	PHO	CBA-CGA-O2A-C1
30	A	601	LHG	C4-C5-C6-O8
30	a	601	LHG	C4-C5-C6-O8
30	Y	318	LHG	C27-C28-C29-C30
30	D	408	LHG	C25-C26-C27-C28
30	d	407	LHG	C30-C31-C32-C33
24	3	309	CHL	O1D-CGD-O2D-CED
24	6	312	CHL	O1D-CGD-O2D-CED
30	G	319	LHG	C26-C27-C28-C29
32	A	609	SQD	C9-C10-C11-C12
32	b	618	SQD	C12-C13-C14-C15
33	D	401	LMG	C15-C16-C17-C18
37	C	620	DGD	C2A-C3A-C4A-C5A
37	c	618	DGD	C3B-C4B-C5B-C6B
24	Y	319	CHL	O1A-CGA-O2A-C1
24	p	306	CHL	O1A-CGA-O2A-C1
24	q	309	CHL	O1A-CGA-O2A-C1
25	b	604	CLA	O1A-CGA-O2A-C1
35	d	403	PHO	O1A-CGA-O2A-C1
37	c	618	DGD	O1A-C1A-O1G-C1G
24	N	310	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	Y	304	CHL	O1D-CGD-O2D-CED
24	r	307	CHL	O1D-CGD-O2D-CED
25	R	603	CLA	O1D-CGD-O2D-CED
33	D	401	LMG	C37-C38-C39-C40
25	a	604	CLA	C13-C15-C16-C17
24	S	605	CHL	O1D-CGD-O2D-CED
25	c	604	CLA	O1D-CGD-O2D-CED
25	s	411	CLA	O1D-CGD-O2D-CED
25	r	304	CLA	O1D-CGD-O2D-CED
37	C	619	DGD	C3B-C4B-C5B-C6B
30	G	319	LHG	C23-C24-C25-C26
30	d	407	LHG	C7-C8-C9-C10
39	D	406	PL9	C47-C48-C49-C50
35	D	403	PHO	O1A-CGA-O2A-C1
25	9	316	CLA	C2B-C3B-CAB-CBB
25	B	601	CLA	C2B-C3B-CAB-CBB
25	B	607	CLA	C2B-C3B-CAB-CBB
25	b	607	CLA	C2B-C3B-CAB-CBB
31	S	614	8CT	C02-C03-C10-C11
31	S	615	8CT	C04-C03-C10-C11
31	X	601	8CT	C02-C03-C10-C11
31	C	615	8CT	C02-C03-C10-C11
31	x	601	8CT	C02-C03-C10-C11
31	d	410	8CT	C04-C03-C10-C11
31	s	416	8CT	C04-C03-C10-C11
24	9	309	CHL	CBD-CGD-O2D-CED
25	G	308	CLA	CBD-CGD-O2D-CED
33	w	201	LMG	C11-C10-O7-C8
37	C	619	DGD	C2A-C1A-O1G-C1G
30	2	319	LHG	C28-C29-C30-C31
30	5	319	LHG	C28-C29-C30-C31
37	C	620	DGD	CCB-CDB-CEB-CFB
24	9	311	CHL	CBA-CGA-O2A-C1
24	R	605	CHL	O1D-CGD-O2D-CED
25	5	308	CLA	O1D-CGD-O2D-CED
30	9	318	LHG	C26-C27-C28-C29
30	y	319	LHG	C15-C16-C17-C18
24	S	602	CHL	C2A-CAA-CBA-CGA
24	G	306	CHL	C2A-CAA-CBA-CGA
24	9	311	CHL	C2A-CAA-CBA-CGA
24	g	305	CHL	C2A-CAA-CBA-CGA
24	g	306	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
24	n	305	CHL	C2A-CAA-CBA-CGA
24	p	306	CHL	C2A-CAA-CBA-CGA
24	s	403	CHL	C2A-CAA-CBA-CGA
24	7	306	CHL	C2A-CAA-CBA-CGA
25	9	307	CLA	C2A-CAA-CBA-CGA
24	7	306	CHL	O1A-CGA-O2A-C1
35	a	606	PHO	O1A-CGA-O2A-C1
24	G	310	CHL	CBD-CGD-O2D-CED
30	D	407	LHG	C15-C16-C17-C18
33	D	411	LMG	C35-C36-C37-C38
30	2	319	LHG	C14-C15-C16-C17
30	D	408	LHG	O9-C7-O7-C5
25	C	607	CLA	C4-C3-C5-C6
25	c	607	CLA	C4-C3-C5-C6
25	c	610	CLA	C10-C11-C12-C13
24	N	304	CHL	C2-C3-C5-C6
24	n	304	CHL	C2-C3-C5-C6
37	C	620	DGD	CDB-CEB-CFB-CGB
25	G	317	CLA	C6-C7-C8-C10
30	9	318	LHG	C12-C13-C14-C15
30	9	318	LHG	C29-C30-C31-C32
30	a	601	LHG	C13-C14-C15-C16
37	c	619	DGD	CCB-CDB-CEB-CFB
24	R	606	CHL	O1D-CGD-O2D-CED
25	b	604	CLA	O1D-CGD-O2D-CED
24	y	306	CHL	CBA-CGA-O2A-C1
24	g	306	CHL	C6-C7-C8-C9
25	B	603	CLA	C14-C13-C15-C16
25	7	315	CLA	C6-C7-C8-C9
30	d	407	LHG	C15-C16-C17-C18
30	d	407	LHG	C31-C32-C33-C34
37	C	620	DGD	C8B-C9B-CAB-CBB
24	g	313	CHL	C13-C15-C16-C17
33	D	411	LMG	C34-C35-C36-C37
33	d	401	LMG	C37-C38-C39-C40
30	9	318	LHG	C15-C16-C17-C18
32	a	609	SQD	C13-C14-C15-C16
33	m	101	LMG	C2-C1-O1-C7
24	p	318	CHL	CBD-CGD-O2D-CED
25	C	612	CLA	CBD-CGD-O2D-CED
30	a	601	LHG	C7-C8-C9-C10
33	d	411	LMG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
32	a	609	SQD	C11-C12-C13-C14
30	p	319	LHG	C14-C15-C16-C17
24	p	306	CHL	C13-C15-C16-C17
24	G	306	CHL	CBA-CGA-O2A-C1
29	Y	301	0UR	O57-C45-C46-C47
29	y	301	0UR	O57-C45-C46-C47
31	X	601	8CT	C23-C24-C25-C26
25	a	603	CLA	C16-C17-C18-C19
24	r	302	CHL	CBD-CGD-O2D-CED
32	a	609	SQD	C8-C7-O47-C45
33	B	619	LMG	C11-C10-O7-C8
37	C	619	DGD	C2B-C1B-O2G-C2G
37	c	618	DGD	C2B-C1B-O2G-C2G
35	A	606	PHO	O1A-CGA-O2A-C1
30	l	318	LHG	C28-C29-C30-C31
25	d	405	CLA	C13-C15-C16-C17
30	d	408	LHG	O9-C7-O7-C5
37	C	619	DGD	O1B-C1B-O2G-C2G
37	c	618	DGD	O1B-C1B-O2G-C2G
30	4	318	LHG	C28-C29-C30-C31
37	c	619	DGD	CDB-CEB-CFB-CGB
33	d	401	LMG	C15-C16-C17-C18
25	D	405	CLA	C13-C15-C16-C17
29	Y	301	0UR	C5-C6-C7-C20
32	A	609	SQD	C7-C8-C9-C10
32	a	609	SQD	C24-C25-C26-C27
25	Y	316	CLA	C3-C5-C6-C7
25	B	607	CLA	C3-C5-C6-C7
31	B	617	8CT	C25-C26-C28-C29
31	b	617	8CT	C25-C26-C28-C29
24	q	310	CHL	C2A-CAA-CBA-CGA
25	b	608	CLA	C6-C7-C8-C10
25	c	602	CLA	C16-C17-C18-C19
25	c	603	CLA	C16-C17-C18-C20
37	c	619	DGD	C9B-CAB-CBB-CCB
25	C	604	CLA	O1D-CGD-O2D-CED
25	n	306	CLA	O1D-CGD-O2D-CED
25	5	315	CLA	CBD-CGD-O2D-CED
33	B	619	LMG	C17-C18-C19-C20
33	m	101	LMG	C18-C19-C20-C21
25	u	317	CLA	O1A-CGA-O2A-C1
25	b	608	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
24	Y	304	CHL	C8-C10-C11-C12
24	n	305	CHL	C5-C6-C7-C8
25	b	604	CLA	C8-C10-C11-C12
25	Y	313	CLA	O1D-CGD-O2D-CED
32	b	618	SQD	C10-C11-C12-C13
24	G	309	CHL	CBD-CGD-O2D-CED
25	8	312	CLA	C5-C6-C7-C8
24	y	305	CHL	C16-C17-C18-C20
25	A	603	CLA	C16-C17-C18-C19
24	Y	305	CHL	O1A-CGA-O2A-C1
24	g	306	CHL	O1A-CGA-O2A-C1
25	B	608	CLA	O1A-CGA-O2A-C1
30	G	319	LHG	C14-C15-C16-C17
30	d	408	LHG	C31-C32-C33-C34
32	B	618	SQD	C10-C11-C12-C13
24	7	306	CHL	C13-C15-C16-C17
25	B	604	CLA	O1D-CGD-O2D-CED
24	7	306	CHL	C3-C5-C6-C7
25	b	607	CLA	C3-C5-C6-C7
30	n	318	LHG	C12-C13-C14-C15
37	c	619	DGD	C8B-C9B-CAB-CBB
25	s	413	CLA	C6-C7-C8-C10
32	b	618	SQD	C14-C15-C16-C17
33	i	101	LMG	C17-C18-C19-C20
25	N	316	CLA	C2A-CAA-CBA-CGA
25	n	316	CLA	C2A-CAA-CBA-CGA
30	y	319	LHG	C11-C12-C13-C14
33	i	101	LMG	C37-C38-C39-C40
24	u	312	CHL	CBA-CGA-O2A-C1
37	C	620	DGD	C9B-CAB-CBB-CCB
30	A	601	LHG	C5-C4-O6-P
25	S	612	CLA	C6-C7-C8-C10
32	B	618	SQD	C14-C15-C16-C17
30	a	612	LHG	C12-C13-C14-C15
33	B	619	LMG	C18-C19-C20-C21
24	N	305	CHL	C3-C5-C6-C7
33	B	619	LMG	O9-C10-O7-C8
24	G	305	CHL	C2A-CAA-CBA-CGA
24	8	304	CHL	C2A-CAA-CBA-CGA
24	q	304	CHL	C2A-CAA-CBA-CGA
25	3	316	CLA	C2A-CAA-CBA-CGA
24	7	310	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	R	602	CHL	O1A-CGA-O2A-C1
24	g	310	CHL	O1A-CGA-O2A-C1
24	r	303	CHL	O1A-CGA-O2A-C1
30	p	319	LHG	C10-C11-C12-C13
37	c	619	DGD	C3A-C4A-C5A-C6A
25	a	607	CLA	C5-C6-C7-C8
35	A	606	PHO	C13-C15-C16-C17
37	C	620	DGD	C1B-C2B-C3B-C4B
24	u	311	CHL	O1D-CGD-O2D-CED
25	S	610	CLA	O1D-CGD-O2D-CED
30	A	612	LHG	C12-C13-C14-C15
30	p	319	LHG	C25-C26-C27-C28
24	7	305	CHL	O1D-CGD-O2D-CED
30	1	318	LHG	O1-C1-C2-O2
30	D	407	LHG	O1-C1-C2-O2
30	4	318	LHG	O1-C1-C2-O2
30	g	319	LHG	O1-C1-C2-O2
30	d	407	LHG	O1-C1-C2-O2
30	d	408	LHG	O1-C1-C2-O2
30	7	319	LHG	O1-C1-C2-O2
24	y	306	CHL	O1A-CGA-O2A-C1
37	C	619	DGD	O1A-C1A-O1G-C1G
25	R	613	CLA	C1A-C2A-CAA-CBA
25	1	313	CLA	C1A-C2A-CAA-CBA
25	S	609	CLA	C1A-C2A-CAA-CBA
25	N	313	CLA	C1A-C2A-CAA-CBA
25	A	603	CLA	C1A-C2A-CAA-CBA
25	4	313	CLA	C1A-C2A-CAA-CBA
25	n	313	CLA	C1A-C2A-CAA-CBA
25	a	603	CLA	C1A-C2A-CAA-CBA
25	s	410	CLA	C1A-C2A-CAA-CBA
25	r	313	CLA	C1A-C2A-CAA-CBA
25	r	314	CLA	C1A-C2A-CAA-CBA
24	9	310	CHL	O1D-CGD-O2D-CED
24	g	313	CHL	C15-C16-C17-C18
25	A	607	CLA	C5-C6-C7-C8
35	a	606	PHO	C13-C15-C16-C17
32	A	609	SQD	C11-C12-C13-C14
24	u	309	CHL	O1D-CGD-O2D-CED
33	D	411	LMG	C32-C33-C34-C35
24	Y	305	CHL	C13-C15-C16-C17
30	9	318	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
32	A	609	SQD	O49-C7-O47-C45
33	w	201	LMG	O9-C10-O7-C8
25	A	607	CLA	C3-C5-C6-C7
25	a	607	CLA	C3-C5-C6-C7
24	9	305	CHL	C12-C13-C15-C16
24	Y	304	CHL	C12-C13-C15-C16
24	Y	305	CHL	C12-C13-C15-C16
24	8	304	CHL	C6-C7-C8-C10
24	u	306	CHL	C12-C13-C15-C16
24	y	306	CHL	C11-C10-C8-C7
24	p	305	CHL	C11-C12-C13-C15
24	p	306	CHL	C6-C7-C8-C10
24	7	305	CHL	C11-C12-C13-C15
24	7	305	CHL	C12-C13-C15-C16
25	2	315	CLA	C6-C7-C8-C10
25	8	312	CLA	C6-C7-C8-C10
25	B	603	CLA	C6-C7-C8-C10
25	B	604	CLA	C12-C13-C15-C16
25	B	611	CLA	C12-C13-C15-C16
25	A	604	CLA	C12-C13-C15-C16
25	C	601	CLA	C12-C13-C15-C16
25	D	404	CLA	C11-C10-C8-C7
25	q	313	CLA	C6-C7-C8-C10
25	b	603	CLA	C6-C7-C8-C10
25	b	604	CLA	C12-C13-C15-C16
25	b	607	CLA	C11-C12-C13-C15
25	b	609	CLA	C12-C13-C15-C16
25	b	611	CLA	C12-C13-C15-C16
25	a	604	CLA	C12-C13-C15-C16
25	c	608	CLA	C11-C12-C13-C15
25	c	611	CLA	C11-C10-C8-C7
30	A	612	LHG	C11-C12-C13-C14
24	n	317	CHL	O1D-CGD-O2D-CED
24	y	306	CHL	C8-C10-C11-C12
25	C	610	CLA	C13-C15-C16-C17
39	D	406	PL9	C43-C44-C46-C47
24	G	306	CHL	O1A-CGA-O2A-C1
24	g	306	CHL	C5-C6-C7-C8
25	q	313	CLA	C5-C6-C7-C8
25	7	315	CLA	C8-C10-C11-C12
24	2	306	CHL	C2A-CAA-CBA-CGA
24	3	305	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
24	5	306	CHL	C2A-CAA-CBA-CGA
24	6	305	CHL	C2A-CAA-CBA-CGA
25	B	602	CLA	C2A-CAA-CBA-CGA
25	b	602	CLA	C2A-CAA-CBA-CGA
25	b	603	CLA	C2A-CAA-CBA-CGA
25	s	413	CLA	C2A-CAA-CBA-CGA
24	G	305	CHL	C11-C10-C8-C9
24	G	306	CHL	C14-C13-C15-C16
24	Y	305	CHL	C14-C13-C15-C16
24	g	306	CHL	C14-C13-C15-C16
24	y	306	CHL	C11-C10-C8-C9
25	B	602	CLA	C11-C12-C13-C14
25	B	603	CLA	C6-C7-C8-C9
25	B	609	CLA	C14-C13-C15-C16
25	B	611	CLA	C14-C13-C15-C16
25	B	614	CLA	C6-C7-C8-C9
25	D	404	CLA	C11-C10-C8-C9
25	5	315	CLA	C6-C7-C8-C9
25	q	313	CLA	C6-C7-C8-C9
25	b	603	CLA	C6-C7-C8-C9
25	b	603	CLA	C14-C13-C15-C16
25	b	607	CLA	C11-C12-C13-C14
25	b	611	CLA	C14-C13-C15-C16
25	b	614	CLA	C6-C7-C8-C9
25	c	607	CLA	C11-C10-C8-C9
25	c	611	CLA	C14-C13-C15-C16
25	d	404	CLA	C11-C10-C8-C9
30	A	601	LHG	C13-C14-C15-C16
33	d	411	LMG	C14-C15-C16-C17
33	B	619	LMG	C28-C29-C30-C31
31	x	601	8CT	C23-C24-C25-C26
30	g	319	LHG	C27-C28-C29-C30
24	n	310	CHL	O1D-CGD-O2D-CED
24	r	307	CHL	CBA-CGA-O2A-C1
25	9	316	CLA	CBA-CGA-O2A-C1
25	c	608	CLA	CBA-CGA-O2A-C1
25	D	404	CLA	C10-C11-C12-C13
24	2	318	CHL	O1D-CGD-O2D-CED
24	n	312	CHL	O1D-CGD-O2D-CED
25	B	602	CLA	O1D-CGD-O2D-CED
25	C	607	CLA	C10-C11-C12-C13
25	c	610	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
30	y	319	LHG	C12-C13-C14-C15
30	d	408	LHG	C9-C10-C11-C12
30	C	617	LHG	C4-C5-C6-O8
30	4	318	LHG	C4-C5-C6-O8
30	c	617	LHG	C4-C5-C6-O8
32	B	618	SQD	O6-C44-C45-C46
32	b	618	SQD	O6-C44-C45-C46
33	D	401	LMG	C7-C8-C9-O8
33	D	411	LMG	C7-C8-C9-O8
33	d	401	LMG	C7-C8-C9-O8
33	d	411	LMG	O1-C7-C8-C9
37	C	620	DGD	O1G-C1G-C2G-C3G
33	W	201	LMG	C11-C12-C13-C14
30	N	318	LHG	C12-C13-C14-C15
30	c	617	LHG	C9-C10-C11-C12
33	m	101	LMG	C17-C18-C19-C20
33	w	201	LMG	C18-C19-C20-C21
37	C	620	DGD	C6A-C7A-C8A-C9A
25	B	611	CLA	C10-C11-C12-C13
30	1	318	LHG	O2-C2-C3-O3
30	G	319	LHG	C15-C16-C17-C18
30	g	319	LHG	C15-C16-C17-C18
24	9	308	CHL	O1D-CGD-O2D-CED
24	N	310	CHL	CBA-CGA-O2A-C1
24	8	304	CHL	CBA-CGA-O2A-C1
25	B	613	CLA	CBA-CGA-O2A-C1
25	C	608	CLA	CBA-CGA-O2A-C1
25	p	317	CLA	CBA-CGA-O2A-C1
24	y	305	CHL	C16-C17-C18-C19
24	S	608	CHL	C2C-C3C-CAC-CBC
30	7	319	LHG	C25-C26-C27-C28
25	c	604	CLA	C8-C10-C11-C12
24	3	308	CHL	O1D-CGD-O2D-CED
24	6	309	CHL	O1D-CGD-O2D-CED
24	y	305	CHL	O1D-CGD-O2D-CED
30	C	617	LHG	C9-C10-C11-C12
24	3	312	CHL	O1D-CGD-O2D-CED
25	q	312	CLA	O1D-CGD-O2D-CED
24	R	601	CHL	CHA-CBD-CGD-O1D
24	R	606	CHL	CHA-CBD-CGD-O1D
24	R	606	CHL	CHA-CBD-CGD-O2D
24	1	305	CHL	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
24	1	305	CHL	CHA-CBD-CGD-O2D
24	1	308	CHL	CHA-CBD-CGD-O1D
24	1	312	CHL	CHA-CBD-CGD-O2D
24	2	306	CHL	CHA-CBD-CGD-O1D
24	3	305	CHL	CHA-CBD-CGD-O1D
24	3	305	CHL	CHA-CBD-CGD-O2D
24	3	311	CHL	CHA-CBD-CGD-O1D
24	3	311	CHL	CHA-CBD-CGD-O2D
24	S	602	CHL	CHA-CBD-CGD-O1D
24	S	602	CHL	CHA-CBD-CGD-O2D
24	S	606	CHL	CHA-CBD-CGD-O2D
24	S	607	CHL	CHA-CBD-CGD-O1D
24	G	306	CHL	CHA-CBD-CGD-O1D
24	G	306	CHL	CHA-CBD-CGD-O2D
24	9	305	CHL	CHA-CBD-CGD-O1D
24	9	305	CHL	CHA-CBD-CGD-O2D
24	N	305	CHL	CHA-CBD-CGD-O1D
24	N	305	CHL	CHA-CBD-CGD-O2D
24	N	310	CHL	CHA-CBD-CGD-O2D
24	Y	305	CHL	CHA-CBD-CGD-O1D
24	Y	305	CHL	CHA-CBD-CGD-O2D
24	8	304	CHL	CHA-CBD-CGD-O1D
24	8	310	CHL	CHA-CBD-CGD-O2D
24	4	305	CHL	CHA-CBD-CGD-O1D
24	4	305	CHL	CHA-CBD-CGD-O2D
24	4	309	CHL	CHA-CBD-CGD-O1D
24	4	309	CHL	CHA-CBD-CGD-O2D
24	4	312	CHL	CHA-CBD-CGD-O1D
24	4	312	CHL	CHA-CBD-CGD-O2D
24	5	306	CHL	CHA-CBD-CGD-O1D
24	6	304	CHL	CHA-CBD-CGD-O1D
24	6	304	CHL	CHA-CBD-CGD-O2D
24	6	305	CHL	CHA-CBD-CGD-O1D
24	6	305	CHL	CHA-CBD-CGD-O2D
24	6	311	CHL	CHA-CBD-CGD-O1D
24	6	311	CHL	CHA-CBD-CGD-O2D
24	g	306	CHL	CHA-CBD-CGD-O1D
24	g	306	CHL	CHA-CBD-CGD-O2D
24	u	306	CHL	CHA-CBD-CGD-O1D
24	u	306	CHL	CHA-CBD-CGD-O2D
24	n	310	CHL	CHA-CBD-CGD-O1D
24	n	310	CHL	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	y	306	CHL	CHA-CBD-CGD-O1D
24	y	306	CHL	CHA-CBD-CGD-O2D
24	p	305	CHL	CHA-CBD-CGD-O1D
24	p	306	CHL	CHA-CBD-CGD-O1D
24	q	304	CHL	CHA-CBD-CGD-O1D
24	q	304	CHL	CHA-CBD-CGD-O2D
24	q	311	CHL	CHA-CBD-CGD-O2D
24	s	403	CHL	CHA-CBD-CGD-O1D
24	s	403	CHL	CHA-CBD-CGD-O2D
24	s	407	CHL	CHA-CBD-CGD-O2D
24	r	307	CHL	CHA-CBD-CGD-O1D
24	r	307	CHL	CHA-CBD-CGD-O2D
24	7	305	CHL	CHA-CBD-CGD-O1D
24	7	306	CHL	CHA-CBD-CGD-O1D
25	B	612	CLA	C8-C10-C11-C12
30	a	612	LHG	C11-C12-C13-C14
28	S	617	NEX	C31-C32-C33-C40
28	9	319	NEX	C31-C32-C33-C40
28	5	304	NEX	C31-C32-C33-C40
28	u	304	NEX	C31-C32-C33-C40
28	p	304	NEX	C31-C32-C33-C40
29	l	301	0UR	C22-C16-C17-C18
29	4	301	0UR	C22-C16-C17-C18
31	C	615	8CT	C10-C11-C12-C40
30	g	319	LHG	C14-C15-C16-C17
25	C	603	CLA	C16-C17-C18-C20
29	4	301	0UR	C15-C16-C17-C18
29	q	301	0UR	C5-C6-C7-C8
31	C	615	8CT	C10-C11-C12-C13
31	D	410	8CT	C10-C11-C12-C13
25	c	602	CLA	C13-C15-C16-C17
25	c	607	CLA	C10-C11-C12-C13
25	G	308	CLA	C2A-CAA-CBA-CGA
25	B	603	CLA	C2A-CAA-CBA-CGA
25	B	605	CLA	C13-C15-C16-C17
30	N	318	LHG	C23-C24-C25-C26
30	G	319	LHG	C28-C29-C30-C31
25	N	306	CLA	O1D-CGD-O2D-CED
24	R	606	CHL	CBA-CGA-O2A-C1
24	n	310	CHL	CBA-CGA-O2A-C1
24	q	304	CHL	CBA-CGA-O2A-C1
25	b	613	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	s	413	CLA	CBA-CGA-O2A-C1
25	7	317	CLA	CBA-CGA-O2A-C1
30	D	407	LHG	C19-C20-C21-C22
24	Y	305	CHL	C8-C10-C11-C12
25	p	315	CLA	C5-C6-C7-C8
25	b	605	CLA	C13-C15-C16-C17
25	b	611	CLA	C10-C11-C12-C13
24	N	317	CHL	O1D-CGD-O2D-CED
24	1	305	CHL	C3C-C2C-CMC-OMC
24	1	312	CHL	C3C-C2C-CMC-OMC
24	1	317	CHL	C3C-C2C-CMC-OMC
24	3	304	CHL	C3C-C2C-CMC-OMC
24	3	311	CHL	C3C-C2C-CMC-OMC
24	3	317	CHL	C3C-C2C-CMC-OMC
24	9	309	CHL	C3C-C2C-CMC-OMC
24	N	311	CHL	C3C-C2C-CMC-OMC
24	N	317	CHL	C3C-C2C-CMC-OMC
24	8	307	CHL	C3C-C2C-CMC-OMC
24	4	305	CHL	C3C-C2C-CMC-OMC
24	4	309	CHL	C3C-C2C-CMC-OMC
24	4	317	CHL	C3C-C2C-CMC-OMC
24	n	311	CHL	C3C-C2C-CMC-OMC
24	n	317	CHL	C3C-C2C-CMC-OMC
24	p	306	CHL	C3C-C2C-CMC-OMC
24	r	308	CHL	C3C-C2C-CMC-OMC
24	7	306	CHL	C3C-C2C-CMC-OMC
31	D	410	8CT	C16-C17-C18-C19
31	c	613	8CT	C18-C19-C20-C21
30	y	319	LHG	C10-C11-C12-C13
30	A	612	LHG	C23-C24-C25-C26
30	n	318	LHG	C23-C24-C25-C26
24	9	304	CHL	O1D-CGD-O2D-CED
24	5	311	CHL	CBA-CGA-O2A-C1
24	N	312	CHL	O1D-CGD-O2D-CED
24	u	318	CHL	O1D-CGD-O2D-CED
30	A	612	LHG	O6-C4-C5-O7
30	p	319	LHG	O6-C4-C5-O7
30	7	319	LHG	O6-C4-C5-O7
25	7	315	CLA	C5-C6-C7-C8
25	y	314	CLA	O1D-CGD-O2D-CED
25	S	612	CLA	CBA-CGA-O2A-C1
25	9	307	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
30	a	601	LHG	C25-C26-C27-C28
37	C	619	DGD	C8B-C9B-CAB-CBB
25	B	606	CLA	C13-C15-C16-C17
25	C	611	CLA	C10-C11-C12-C13
25	Y	314	CLA	C4-C3-C5-C6
24	N	312	CHL	C2-C3-C5-C6
30	d	407	LHG	C14-C15-C16-C17
25	b	609	CLA	C16-C17-C18-C20
30	A	601	LHG	C25-C26-C27-C28
30	g	319	LHG	C12-C13-C14-C15
30	7	319	LHG	C10-C11-C12-C13
24	G	306	CHL	C15-C16-C17-C18
33	m	101	LMG	C10-C11-C12-C13
24	s	409	CHL	C2C-C3C-CAC-CBC
33	D	411	LMG	C15-C16-C17-C18
30	A	601	LHG	O7-C5-C6-O8
30	a	601	LHG	O7-C5-C6-O8
33	D	401	LMG	O7-C8-C9-O8
33	d	401	LMG	O7-C8-C9-O8
37	c	618	DGD	C8B-C9B-CAB-CBB
30	y	319	LHG	C17-C18-C19-C20
30	y	319	LHG	C11-C10-C9-C8
24	5	318	CHL	O1D-CGD-O2D-CED
24	g	309	CHL	O1D-CGD-O2D-CED
24	2	311	CHL	CBA-CGA-O2A-C1
24	G	311	CHL	CAA-CBA-CGA-O2A
33	D	411	LMG	C11-C12-C13-C14
24	p	311	CHL	C2A-CAA-CBA-CGA
30	d	407	LHG	C19-C20-C21-C22
24	4	304	CHL	O1D-CGD-O2D-CED
24	G	313	CHL	C15-C16-C17-C18
30	G	319	LHG	C27-C28-C29-C30
30	Y	318	LHG	C11-C10-C9-C8
30	9	318	LHG	C10-C11-C12-C13
24	r	307	CHL	O1A-CGA-O2A-C1
30	a	612	LHG	C23-C24-C25-C26
30	D	407	LHG	C14-C15-C16-C17
25	B	614	CLA	CBA-CGA-O2A-C1
25	C	606	CLA	CBA-CGA-O2A-C1
33	d	411	LMG	C21-C22-C23-C24
24	Y	309	CHL	CBA-CGA-O2A-C1
24	1	317	CHL	C1C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
24	3	304	CHL	C1C-C2C-CMC-OMC
24	3	311	CHL	C1C-C2C-CMC-OMC
24	N	311	CHL	C1C-C2C-CMC-OMC
24	N	317	CHL	C1C-C2C-CMC-OMC
24	4	305	CHL	C1C-C2C-CMC-OMC
24	4	309	CHL	C1C-C2C-CMC-OMC
24	4	317	CHL	C1C-C2C-CMC-OMC
24	2	313	CHL	CBD-CGD-O2D-CED
24	5	313	CHL	CBD-CGD-O2D-CED
33	W	201	LMG	C11-C10-O7-C8
30	1	318	LHG	C12-C13-C14-C15
25	B	604	CLA	C8-C10-C11-C12
25	b	615	CLA	C15-C16-C17-C18
25	9	316	CLA	O1A-CGA-O2A-C1
24	r	306	CHL	O1D-CGD-O2D-CED
24	q	304	CHL	C11-C12-C13-C14
30	4	318	LHG	C15-C16-C17-C18
37	c	619	DGD	C6A-C7A-C8A-C9A
30	g	319	LHG	C28-C29-C30-C31
30	C	617	LHG	C10-C11-C12-C13
30	c	617	LHG	C10-C11-C12-C13
25	N	314	CLA	C5-C6-C7-C8
25	B	603	CLA	C10-C11-C12-C13
25	b	612	CLA	C8-C10-C11-C12
26	9	303	OIE	C13-C14-C15-C16
25	B	609	CLA	C4-C3-C5-C6
39	d	406	PL9	C43-C44-C46-C47
24	3	309	CHL	CBA-CGA-O2A-C1
24	6	309	CHL	CBA-CGA-O2A-C1
25	b	614	CLA	CBA-CGA-O2A-C1
25	b	606	CLA	C13-C15-C16-C17
30	1	318	LHG	C15-C16-C17-C18
30	Y	318	LHG	C26-C27-C28-C29
30	C	617	LHG	O1-C1-C2-O2
24	p	312	CHL	O1A-CGA-O2A-C1
24	7	312	CHL	O1A-CGA-O2A-C1
24	G	313	CHL	C6-C7-C8-C9
24	G	313	CHL	C11-C12-C13-C14
24	Y	304	CHL	C14-C13-C15-C16
24	Y	305	CHL	C11-C10-C8-C9
24	g	305	CHL	C11-C10-C8-C9
24	y	306	CHL	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	2	315	CLA	C6-C7-C8-C9
25	8	312	CLA	C6-C7-C8-C9
25	B	604	CLA	C14-C13-C15-C16
25	C	607	CLA	C11-C10-C8-C9
25	C	611	CLA	C11-C10-C8-C9
25	C	611	CLA	C14-C13-C15-C16
25	y	315	CLA	C6-C7-C8-C9
25	b	602	CLA	C11-C12-C13-C14
25	b	604	CLA	C11-C12-C13-C14
25	b	604	CLA	C14-C13-C15-C16
25	b	609	CLA	C14-C13-C15-C16
25	c	611	CLA	C11-C10-C8-C9
32	A	609	SQD	C14-C15-C16-C17
25	3	316	CLA	O1D-CGD-O2D-CED
25	B	615	CLA	C15-C16-C17-C18
25	c	603	CLA	C8-C10-C11-C12
30	1	318	LHG	C5-C4-O6-P
30	C	617	LHG	C2-C3-O3-P
30	a	601	LHG	C5-C4-O6-P
30	c	617	LHG	C2-C3-O3-P
30	D	408	LHG	C10-C11-C12-C13
25	c	608	CLA	O1A-CGA-O2A-C1
25	R	604	CLA	C4B-C3B-CAB-CBB
25	1	314	CLA	C4B-C3B-CAB-CBB
25	2	307	CLA	C4B-C3B-CAB-CBB
25	S	604	CLA	C4B-C3B-CAB-CBB
25	S	616	CLA	C4B-C3B-CAB-CBB
25	9	315	CLA	C4B-C3B-CAB-CBB
25	B	607	CLA	C4B-C3B-CAB-CBB
25	4	314	CLA	C4B-C3B-CAB-CBB
25	5	307	CLA	C4B-C3B-CAB-CBB
25	u	315	CLA	C4B-C3B-CAB-CBB
25	p	315	CLA	C4B-C3B-CAB-CBB
25	b	607	CLA	C4B-C3B-CAB-CBB
25	s	405	CLA	C4B-C3B-CAB-CBB
25	s	417	CLA	C4B-C3B-CAB-CBB
25	r	305	CLA	C4B-C3B-CAB-CBB
25	7	315	CLA	C4B-C3B-CAB-CBB
25	7	317	CLA	C4B-C3B-CAB-CBB
25	C	601	CLA	C8-C10-C11-C12
25	b	603	CLA	C10-C11-C12-C13
25	s	413	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
24	S	608	CHL	C2A-CAA-CBA-CGA
25	S	612	CLA	C2A-CAA-CBA-CGA
25	C	601	CLA	C2A-CAA-CBA-CGA
30	Y	318	LHG	C10-C11-C12-C13
30	y	319	LHG	C26-C27-C28-C29
24	n	309	CHL	O1D-CGD-O2D-CED
33	W	201	LMG	C2-C1-O1-C7
25	C	602	CLA	C13-C15-C16-C17
32	A	609	SQD	C12-C13-C14-C15
24	g	306	CHL	C15-C16-C17-C18
24	y	306	CHL	C15-C16-C17-C18
30	l	318	LHG	O6-C4-C5-C6
30	a	612	LHG	O6-C4-C5-C6
33	w	201	LMG	C16-C17-C18-C19
25	S	612	CLA	C11-C10-C8-C7
24	G	310	CHL	O1A-CGA-O2A-C1
24	G	305	CHL	C11-C10-C8-C7
24	G	306	CHL	C12-C13-C15-C16
24	Y	305	CHL	C11-C10-C8-C7
24	Y	305	CHL	C11-C12-C13-C15
24	Y	312	CHL	C12-C13-C15-C16
24	g	305	CHL	C11-C10-C8-C7
24	g	306	CHL	C12-C13-C15-C16
24	g	313	CHL	C12-C13-C15-C16
24	y	305	CHL	C11-C12-C13-C15
24	y	306	CHL	C12-C13-C15-C16
24	y	313	CHL	C12-C13-C15-C16
24	p	306	CHL	C12-C13-C15-C16
24	q	304	CHL	C6-C7-C8-C10
25	B	602	CLA	C11-C12-C13-C15
25	B	604	CLA	C6-C7-C8-C10
25	B	609	CLA	C11-C10-C8-C7
25	B	609	CLA	C12-C13-C15-C16
25	B	614	CLA	C6-C7-C8-C10
25	C	611	CLA	C11-C10-C8-C7
25	5	315	CLA	C6-C7-C8-C10
25	y	315	CLA	C6-C7-C8-C10
25	b	602	CLA	C11-C12-C13-C15
25	b	604	CLA	C6-C7-C8-C10
25	b	609	CLA	C6-C7-C8-C10
25	b	609	CLA	C11-C10-C8-C7
25	b	614	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
25	c	601	CLA	C12-C13-C15-C16
25	d	404	CLA	C11-C10-C8-C7
25	y	315	CLA	C5-C6-C7-C8
24	8	304	CHL	C11-C12-C13-C14
30	d	408	LHG	C7-C8-C9-C10
33	W	201	LMG	C10-C11-C12-C13
30	G	319	LHG	C12-C13-C14-C15
30	D	408	LHG	C26-C27-C28-C29
25	p	317	CLA	C6-C7-C8-C10
29	Y	301	0UR	C46-C47-C48-C49
29	y	301	0UR	C46-C47-C48-C49
24	N	310	CHL	O1A-CGA-O2A-C1
24	8	304	CHL	O1A-CGA-O2A-C1
25	B	613	CLA	O1A-CGA-O2A-C1
25	C	608	CLA	O1A-CGA-O2A-C1
25	p	317	CLA	O1A-CGA-O2A-C1
24	Y	305	CHL	C15-C16-C17-C18
33	D	411	LMG	C36-C37-C38-C39
24	9	311	CHL	C3A-C2A-CAA-CBA
24	Y	304	CHL	C3A-C2A-CAA-CBA
24	u	312	CHL	C3A-C2A-CAA-CBA
24	y	305	CHL	C3A-C2A-CAA-CBA
24	p	305	CHL	C3A-C2A-CAA-CBA
24	s	402	CHL	C3A-C2A-CAA-CBA
24	7	305	CHL	C3A-C2A-CAA-CBA
25	R	612	CLA	C3A-C2A-CAA-CBA
25	8	306	CLA	C3A-C2A-CAA-CBA
25	q	306	CLA	C3A-C2A-CAA-CBA
25	r	313	CLA	C3A-C2A-CAA-CBA
39	D	406	PL9	C45-C44-C46-C47
39	d	406	PL9	C45-C44-C46-C47
25	B	604	CLA	C10-C11-C12-C13
25	B	612	CLA	C10-C11-C12-C13
25	C	604	CLA	C8-C10-C11-C12
24	G	313	CHL	C2-C3-C5-C6
24	g	313	CHL	C2-C3-C5-C6
24	n	312	CHL	C2-C3-C5-C6
30	A	601	LHG	C7-C8-C9-C10
33	m	101	LMG	O6-C1-O1-C7
24	R	606	CHL	O1A-CGA-O2A-C1
25	b	613	CLA	O1A-CGA-O2A-C1
24	y	313	CHL	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
29	p	301	0UR	C3-C4-C5-C6
31	B	617	8CT	C12-C13-C14-C15
31	C	613	8CT	C18-C19-C20-C21
31	b	617	8CT	C12-C13-C14-C15
31	d	410	8CT	C16-C17-C18-C19
25	p	315	CLA	C8-C10-C11-C12
28	R	616	NEX	C31-C32-C33-C40
28	1	303	NEX	C31-C32-C33-C40
28	2	304	NEX	C31-C32-C33-C40
28	G	304	NEX	C31-C32-C33-C40
28	4	303	NEX	C31-C32-C33-C40
28	g	304	NEX	C31-C32-C33-C40
28	y	304	NEX	C31-C32-C33-C40
28	r	317	NEX	C31-C32-C33-C40
28	7	304	NEX	C31-C32-C33-C40
24	9	305	CHL	C15-C16-C17-C18
24	q	304	CHL	O1A-CGA-O2A-C1
25	s	413	CLA	O1A-CGA-O2A-C1
25	b	602	CLA	O1D-CGD-O2D-CED
29	1	301	0UR	C5-C6-C7-C8
30	g	319	LHG	C10-C11-C12-C13
24	u	306	CHL	C15-C16-C17-C18
30	G	319	LHG	C10-C11-C12-C13
25	p	307	CLA	C2A-CAA-CBA-CGA
30	D	407	LHG	C32-C33-C34-C35
33	C	618	LMG	C16-C17-C18-C19
25	b	612	CLA	C10-C11-C12-C13
30	1	318	LHG	C4-C5-C6-O8
32	D	409	SQD	O6-C44-C45-C46
32	d	409	SQD	O6-C44-C45-C46
33	w	201	LMG	C7-C8-C9-O8
25	7	315	CLA	C3-C5-C6-C7
25	9	316	CLA	C6-C7-C8-C10
30	1	318	LHG	C23-C24-C25-C26
25	C	603	CLA	C16-C17-C18-C19
24	Y	312	CHL	C13-C15-C16-C17
25	b	605	CLA	C15-C16-C17-C18
25	c	611	CLA	C10-C11-C12-C13
25	2	315	CLA	O1D-CGD-O2D-CED
24	n	310	CHL	O1A-CGA-O2A-C1
25	7	317	CLA	O1A-CGA-O2A-C1
30	Y	318	LHG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
30	n	318	LHG	C15-C16-C17-C18
30	d	407	LHG	C12-C13-C14-C15
24	G	305	CHL	C1A-C2A-CAA-CBA
24	Y	304	CHL	C1A-C2A-CAA-CBA
24	8	303	CHL	C1A-C2A-CAA-CBA
24	g	305	CHL	C1A-C2A-CAA-CBA
24	y	305	CHL	C1A-C2A-CAA-CBA
24	q	303	CHL	C1A-C2A-CAA-CBA
25	C	603	CLA	C8-C10-C11-C12
30	n	318	LHG	C28-C29-C30-C31
37	c	619	DGD	C5B-C6B-C7B-C8B
24	G	313	CHL	C4-C3-C5-C6
24	N	312	CHL	C4-C3-C5-C6
24	g	313	CHL	C4-C3-C5-C6
25	b	605	CLA	C4-C3-C5-C6
25	c	607	CLA	C2-C3-C5-C6
25	b	604	CLA	C3-C5-C6-C7
24	l	304	CHL	O1D-CGD-O2D-CED
24	p	310	CHL	O1D-CGD-O2D-CED
24	N	308	CHL	CBD-CGD-O2D-CED
26	3	303	OIE	O1-C2-C30-C31
24	9	309	CHL	O1D-CGD-O2D-CED
30	5	319	LHG	C23-C24-C25-C26
25	B	609	CLA	C10-C11-C12-C13
30	G	319	LHG	O6-C4-C5-O7
30	A	612	LHG	C26-C27-C28-C29
25	S	616	CLA	C2B-C3B-CAB-CBB
25	4	314	CLA	C2B-C3B-CAB-CBB
25	6	315	CLA	C2B-C3B-CAB-CBB
25	u	315	CLA	C2B-C3B-CAB-CBB
25	s	417	CLA	C2B-C3B-CAB-CBB
25	7	317	CLA	C2B-C3B-CAB-CBB
31	D	410	8CT	C04-C03-C10-C11
31	s	415	8CT	C02-C03-C10-C11
33	d	411	LMG	C33-C34-C35-C36
32	B	618	SQD	C29-C30-C31-C32
25	B	605	CLA	C15-C16-C17-C18
24	7	318	CHL	CBD-CGD-O2D-CED
35	d	403	PHO	CBD-CGD-O2D-CED
33	W	201	LMG	C30-C31-C32-C33
30	n	318	LHG	C10-C11-C12-C13
32	a	609	SQD	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
37	C	620	DGD	C5A-C6A-C7A-C8A
33	d	411	LMG	C13-C14-C15-C16
25	B	608	CLA	C6-C7-C8-C9
25	b	608	CLA	C6-C7-C8-C9
25	c	602	CLA	C16-C17-C18-C20
25	c	603	CLA	C16-C17-C18-C19
30	n	318	LHG	O8-C23-C24-C25
32	A	609	SQD	O47-C7-C8-C9
25	c	601	CLA	C2A-CAA-CBA-CGA
30	C	617	LHG	O7-C5-C6-O8
30	c	617	LHG	O7-C5-C6-O8
30	d	408	LHG	O7-C5-C6-O8
32	D	409	SQD	O6-C44-C45-O47
33	B	619	LMG	O7-C8-C9-O8
33	D	411	LMG	O1-C7-C8-O7
33	W	201	LMG	O1-C7-C8-O7
33	m	101	LMG	O7-C8-C9-O8
33	w	201	LMG	O7-C8-C9-O8
37	C	620	DGD	O1G-C1G-C2G-O2G
25	g	308	CLA	CBD-CGD-O2D-CED
25	c	609	CLA	CBD-CGD-O2D-CED
24	R	601	CHL	O1D-CGD-O2D-CED
32	a	609	SQD	C26-C27-C28-C29
30	2	319	LHG	C23-C24-C25-C26
30	D	407	LHG	C23-C24-C25-C26
25	9	307	CLA	O1A-CGA-O2A-C1
24	n	312	CHL	C4-C3-C5-C6
25	C	607	CLA	C2-C3-C5-C6
30	9	318	LHG	C28-C29-C30-C31
25	C	602	CLA	C16-C17-C18-C20
30	N	318	LHG	C28-C29-C30-C31
30	p	319	LHG	C11-C10-C9-C8
33	d	411	LMG	C15-C16-C17-C18
25	8	305	CLA	CBA-CGA-O2A-C1
24	u	305	CHL	C3-C5-C6-C7
24	9	317	CHL	CBD-CGD-O2D-CED
24	Y	312	CHL	C14-C13-C15-C16
24	y	313	CHL	C14-C13-C15-C16
24	p	306	CHL	C14-C13-C15-C16
25	B	607	CLA	C11-C12-C13-C14
30	G	319	LHG	C25-C26-C27-C28
30	N	318	LHG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
30	c	617	LHG	C11-C10-C9-C8
25	S	612	CLA	O1A-CGA-O2A-C1
24	y	310	CHL	CBA-CGA-O2A-C1
30	g	319	LHG	C25-C26-C27-C28
30	7	319	LHG	C11-C10-C9-C8
33	i	101	LMG	C40-C41-C42-C43
25	2	317	CLA	O2A-C1-C2-C3
25	5	317	CLA	O2A-C1-C2-C3
24	G	310	CHL	O1D-CGD-O2D-CED
25	a	603	CLA	C2A-CAA-CBA-CGA
29	1	301	0UR	C46-C47-C48-C49
29	2	301	0UR	C46-C47-C48-C49
29	3	301	0UR	C46-C47-C48-C49
29	G	301	0UR	C46-C47-C48-C49
29	N	301	0UR	C46-C47-C48-C49
29	4	301	0UR	C46-C47-C48-C49
29	5	301	0UR	C46-C47-C48-C49
29	g	301	0UR	C46-C47-C48-C49
30	A	601	LHG	C10-C11-C12-C13
37	c	619	DGD	C2B-C3B-C4B-C5B
24	p	306	CHL	C15-C16-C17-C18
24	7	306	CHL	C15-C16-C17-C18
24	G	309	CHL	O1D-CGD-O2D-CED
24	p	318	CHL	O1D-CGD-O2D-CED
30	4	318	LHG	C23-C24-C25-C26
32	b	618	SQD	C7-C8-C9-C10
25	c	601	CLA	C8-C10-C11-C12
30	c	617	LHG	O1-C1-C2-O2
24	N	312	CHL	CBA-CGA-O2A-C1
25	c	606	CLA	CBA-CGA-O2A-C1
29	3	301	0UR	C3-C4-C5-C6
30	N	318	LHG	O8-C23-C24-C25
26	1	302	0IE	O1-C2-C3-C4
26	2	302	0IE	O1-C2-C3-C4
26	3	302	0IE	O1-C2-C3-C4
26	G	302	0IE	O1-C2-C3-C4
26	9	302	0IE	O1-C2-C3-C4
26	N	302	0IE	O1-C2-C3-C4
26	Y	302	0IE	O1-C2-C3-C4
26	8	302	0IE	O1-C2-C3-C4
26	4	302	0IE	O1-C2-C3-C4
26	5	302	0IE	O1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
26	6	302	0IE	O1-C2-C3-C4
26	g	302	0IE	O1-C2-C3-C4
26	u	302	0IE	O1-C2-C3-C4
26	n	302	0IE	O1-C2-C3-C4
26	y	302	0IE	O1-C2-C3-C4
26	p	302	0IE	O1-C2-C3-C4
26	q	302	0IE	O1-C2-C3-C4
26	7	302	0IE	O1-C2-C3-C4
29	1	301	0UR	O42-C2-C3-C4
29	2	301	0UR	O42-C2-C3-C4
29	G	301	0UR	O42-C2-C3-C4
29	9	301	0UR	O42-C2-C3-C4
29	Y	301	0UR	O42-C2-C3-C4
29	8	301	0UR	O42-C2-C3-C4
29	4	301	0UR	O42-C2-C3-C4
29	5	301	0UR	O42-C2-C3-C4
29	g	301	0UR	O42-C2-C3-C4
29	u	301	0UR	O42-C2-C3-C4
29	y	301	0UR	O42-C2-C3-C4
29	q	301	0UR	O42-C2-C3-C4
37	c	618	DGD	C3A-C4A-C5A-C6A
25	8	311	CLA	CBD-CGD-O2D-CED
30	N	318	LHG	C10-C11-C12-C13
30	A	601	LHG	C12-C13-C14-C15
30	5	319	LHG	C15-C16-C17-C18
30	a	601	LHG	C10-C11-C12-C13
25	B	614	CLA	O1A-CGA-O2A-C1
25	p	315	CLA	C3-C5-C6-C7
25	2	317	CLA	CBA-CGA-O2A-C1
32	B	618	SQD	C7-C8-C9-C10
32	b	618	SQD	C29-C30-C31-C32
30	4	318	LHG	C12-C13-C14-C15
30	G	319	LHG	O6-C4-C5-C6
30	A	612	LHG	O6-C4-C5-C6
30	4	318	LHG	O6-C4-C5-C6
30	p	319	LHG	O6-C4-C5-C6
30	7	319	LHG	O6-C4-C5-C6
29	n	301	0UR	C46-C47-C48-C49
25	G	308	CLA	O1D-CGD-O2D-CED
29	3	301	0UR	C5-C6-C7-C20
31	D	410	8CT	C10-C11-C12-C40
30	C	617	LHG	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
33	C	618	LMG	C30-C31-C32-C33
24	G	313	CHL	C12-C13-C15-C16
24	7	306	CHL	C6-C7-C8-C10
24	7	306	CHL	C12-C13-C15-C16
25	B	607	CLA	C11-C12-C13-C15
25	B	609	CLA	C6-C7-C8-C10
25	B	612	CLA	C11-C12-C13-C15
25	C	602	CLA	C12-C13-C15-C16
25	b	606	CLA	C11-C10-C8-C7
25	b	612	CLA	C11-C12-C13-C15
25	c	602	CLA	C12-C13-C15-C16
32	D	409	SQD	C7-C8-C9-C10
32	d	409	SQD	C12-C13-C14-C15
25	5	315	CLA	O1D-CGD-O2D-CED
29	1	301	0UR	C15-C16-C17-C18
29	N	301	0UR	C5-C6-C7-C8
29	u	301	0UR	C5-C6-C7-C8
24	r	302	CHL	O1D-CGD-O2D-CED
25	q	305	CLA	CBA-CGA-O2A-C1
30	a	612	LHG	C26-C27-C28-C29
37	C	619	DGD	C3A-C4A-C5A-C6A
33	D	411	LMG	C8-C7-O1-C1
37	C	619	DGD	C2G-C3G-O3G-C1D
37	C	619	DGD	C5D-C6D-O5D-C1E
37	c	618	DGD	C2G-C3G-O3G-C1D
37	c	618	DGD	C5D-C6D-O5D-C1E
30	d	407	LHG	C23-C24-C25-C26
24	1	305	CHL	C2A-CAA-CBA-CGA
24	s	409	CHL	C2A-CAA-CBA-CGA
25	9	316	CLA	C2A-CAA-CBA-CGA
25	A	603	CLA	C2A-CAA-CBA-CGA
25	u	308	CLA	C2A-CAA-CBA-CGA
25	c	605	CLA	C2A-CAA-CBA-CGA
30	D	408	LHG	C27-C28-C29-C30
32	B	618	SQD	O49-C7-O47-C45
30	a	601	LHG	C12-C13-C14-C15
25	B	605	CLA	C4-C3-C5-C6
25	b	609	CLA	C4-C3-C5-C6
24	Y	310	CHL	CAA-CBA-CGA-O2A
24	6	309	CHL	O1A-CGA-O2A-C1
25	C	606	CLA	O1A-CGA-O2A-C1
25	b	614	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	b	606	CLA	C3-C5-C6-C7
25	C	609	CLA	CBD-CGD-O2D-CED
24	3	309	CHL	O1A-CGA-O2A-C1
24	1	308	CHL	CBD-CGD-O2D-CED
25	Y	316	CLA	C11-C10-C8-C7
25	5	317	CLA	CBA-CGA-O2A-C1
30	G	319	LHG	C11-C10-C9-C8
33	W	201	LMG	O9-C10-O7-C8
30	9	318	LHG	O6-C4-C5-O7
30	a	612	LHG	O6-C4-C5-O7
30	5	319	LHG	C10-C11-C12-C13
32	A	609	SQD	C26-C27-C28-C29
33	D	411	LMG	O1-C7-C8-C9
37	C	619	DGD	O1G-C1G-C2G-C3G
37	C	620	DGD	C1G-C2G-C3G-O3G
24	9	304	CHL	C3-C5-C6-C7
29	6	301	OUR	C46-C47-C48-C49
37	C	620	DGD	C4D-C5D-C6D-O5D
24	R	602	CHL	C2A-CAA-CBA-CGA
24	r	303	CHL	C2A-CAA-CBA-CGA
37	c	619	DGD	C1B-C2B-C3B-C4B
25	B	607	CLA	C10-C11-C12-C13
25	b	615	CLA	C5-C6-C7-C8
32	B	618	SQD	O6-C44-C45-O47
32	d	409	SQD	O6-C44-C45-O47
37	C	619	DGD	O1G-C1G-C2G-O2G
37	C	620	DGD	O2G-C2G-C3G-O3G
25	y	317	CLA	C11-C10-C8-C7
24	g	313	CHL	C11-C12-C13-C14
24	u	305	CHL	C11-C12-C13-C14
24	7	306	CHL	C14-C13-C15-C16
25	B	612	CLA	C11-C12-C13-C14
25	C	602	CLA	C6-C7-C8-C9
25	C	602	CLA	C14-C13-C15-C16
24	8	310	CHL	C6-C7-C8-C9
24	q	311	CHL	C6-C7-C8-C9
30	D	407	LHG	C28-C29-C30-C31
33	w	201	LMG	C14-C15-C16-C17
32	b	618	SQD	O49-C7-O47-C45
33	d	411	LMG	C34-C35-C36-C37
24	N	312	CHL	O1A-CGA-O2A-C1
33	d	411	LMG	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
25	g	315	CLA	C5-C6-C7-C8
25	b	609	CLA	C10-C11-C12-C13
25	d	404	CLA	C10-C11-C12-C13
31	S	614	8CT	C26-C28-C29-C30
31	s	415	8CT	C26-C28-C29-C30
30	2	319	LHG	C10-C11-C12-C13
33	C	618	LMG	C13-C14-C15-C16
25	8	305	CLA	O1A-CGA-O2A-C1
25	c	606	CLA	O1A-CGA-O2A-C1
24	7	310	CHL	O1D-CGD-O2D-CED
29	7	301	0UR	C46-C47-C48-C49
32	D	409	SQD	C9-C10-C11-C12
33	D	411	LMG	C19-C20-C21-C22
25	G	308	CLA	CBA-CGA-O2A-C1
32	D	409	SQD	C27-C28-C29-C30
26	g	302	0IE	O1-C2-C3-C20
29	8	301	0UR	O42-C2-C3-C43
29	q	301	0UR	O42-C2-C3-C43
25	n	314	CLA	C5-C6-C7-C8
25	C	605	CLA	C2A-CAA-CBA-CGA
24	s	403	CHL	CBA-CGA-O2A-C1
33	B	619	LMG	C16-C17-C18-C19
37	c	618	DGD	C2B-C3B-C4B-C5B
25	c	601	CLA	C16-C17-C18-C20
24	u	310	CHL	CBD-CGD-O2D-CED
30	D	407	LHG	C12-C13-C14-C15
25	B	604	CLA	C3-C5-C6-C7
24	2	305	CHL	C4C-C3C-CAC-CBC
24	2	306	CHL	C4C-C3C-CAC-CBC
24	3	304	CHL	C4C-C3C-CAC-CBC
24	3	312	CHL	C4C-C3C-CAC-CBC
24	S	601	CHL	C4C-C3C-CAC-CBC
24	9	312	CHL	C4C-C3C-CAC-CBC
24	N	312	CHL	C4C-C3C-CAC-CBC
24	Y	312	CHL	C4C-C3C-CAC-CBC
24	5	305	CHL	C4C-C3C-CAC-CBC
24	5	306	CHL	C4C-C3C-CAC-CBC
24	6	312	CHL	C4C-C3C-CAC-CBC
24	g	313	CHL	C4C-C3C-CAC-CBC
24	u	313	CHL	C4C-C3C-CAC-CBC
24	n	312	CHL	C4C-C3C-CAC-CBC
24	y	305	CHL	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
24	y	313	CHL	C4C-C3C-CAC-CBC
24	p	309	CHL	C4C-C3C-CAC-CBC
24	s	402	CHL	C4C-C3C-CAC-CBC
24	7	309	CHL	C4C-C3C-CAC-CBC
25	c	608	CLA	C14-C13-C15-C16
25	b	607	CLA	C10-C11-C12-C13
25	c	612	CLA	CBD-CGD-O2D-CED
30	9	318	LHG	O1-C1-C2-O2
25	g	317	CLA	C3-C5-C6-C7
24	9	311	CHL	O1A-CGA-O2A-C1
25	R	612	CLA	C4B-C3B-CAB-CBB
25	1	315	CLA	C4B-C3B-CAB-CBB
25	2	315	CLA	C4B-C3B-CAB-CBB
25	3	315	CLA	C4B-C3B-CAB-CBB
25	9	313	CLA	C1A-C2A-CAA-CBA
25	9	314	CLA	C4B-C3B-CAB-CBB
25	8	306	CLA	C1A-C2A-CAA-CBA
25	A	605	CLA	C1A-C2A-CAA-CBA
25	C	601	CLA	C1A-C2A-CAA-CBA
25	4	315	CLA	C4B-C3B-CAB-CBB
25	5	315	CLA	C4B-C3B-CAB-CBB
25	6	315	CLA	C4B-C3B-CAB-CBB
25	6	316	CLA	C4B-C3B-CAB-CBB
25	u	314	CLA	C1A-C2A-CAA-CBA
25	p	317	CLA	C4B-C3B-CAB-CBB
25	a	605	CLA	C1A-C2A-CAA-CBA
25	c	601	CLA	C1A-C2A-CAA-CBA
25	r	313	CLA	C4B-C3B-CAB-CBB
26	3	302	0IE	O29-C20-C3-C2
26	9	302	0IE	O29-C20-C3-C2
26	6	302	0IE	O29-C20-C3-C2
26	u	302	0IE	O29-C20-C3-C2
26	u	303	0IE	O29-C20-C3-C2
26	p	302	0IE	O29-C20-C3-C2
26	p	303	0IE	O29-C20-C3-C2
26	7	302	0IE	O29-C20-C3-C2
26	7	303	0IE	O29-C20-C3-C4
26	7	303	0IE	O29-C20-C3-C2
24	2	313	CHL	O1D-CGD-O2D-CED
24	5	313	CHL	O1D-CGD-O2D-CED
25	C	612	CLA	O1D-CGD-O2D-CED
24	n	312	CHL	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	y	301	0UR	C5-C6-C7-C8
31	X	601	8CT	C25-C26-C28-C29
24	q	311	CHL	C2C-C3C-CAC-CBC
29	p	301	0UR	C46-C47-C48-C49
24	3	310	CHL	C2A-CAA-CBA-CGA
25	G	317	CLA	C2A-CAA-CBA-CGA
37	C	619	DGD	C2B-C3B-C4B-C5B
25	q	305	CLA	CBD-CGD-O2D-CED
33	D	401	LMG	C12-C13-C14-C15
25	2	315	CLA	C11-C12-C13-C15
25	Y	314	CLA	C6-C7-C8-C10
25	B	604	CLA	C11-C12-C13-C15
25	C	608	CLA	C6-C7-C8-C10
25	5	315	CLA	C11-C12-C13-C15
25	c	608	CLA	C6-C7-C8-C10
25	d	404	CLA	C11-C12-C13-C15
37	C	620	DGD	O6D-C5D-C6D-O5D
32	d	409	SQD	C9-C10-C11-C12
24	N	312	CHL	C6-C7-C8-C9
24	n	312	CHL	C6-C7-C8-C9
25	d	405	CLA	C16-C17-C18-C20
25	q	305	CLA	O1A-CGA-O2A-C1
24	S	602	CHL	CBA-CGA-O2A-C1
30	A	612	LHG	C27-C28-C29-C30
29	8	301	0UR	C46-C47-C48-C49
25	2	317	CLA	O1A-CGA-O2A-C1
24	8	310	CHL	C2C-C3C-CAC-CBC
24	S	601	CHL	C3A-C2A-CAA-CBA
24	y	313	CHL	C4-C3-C5-C6
25	A	604	CLA	C3A-C2A-CAA-CBA
25	a	604	CLA	C3A-C2A-CAA-CBA
25	C	601	CLA	C16-C17-C18-C20
25	D	405	CLA	C16-C17-C18-C20
24	2	311	CHL	CAA-CBA-CGA-O2A
24	u	312	CHL	O1A-CGA-O2A-C1
30	1	318	LHG	O6-C4-C5-O7
30	4	318	LHG	O6-C4-C5-O7
30	g	319	LHG	O6-C4-C5-O7
30	a	612	LHG	C14-C15-C16-C17
25	B	606	CLA	C3-C5-C6-C7
24	u	310	CHL	O1D-CGD-O2D-CED
24	7	318	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	g	317	CLA	C2A-CAA-CBA-CGA
25	7	307	CLA	C2A-CAA-CBA-CGA
24	g	306	CHL	C11-C10-C8-C9
25	8	312	CLA	C11-C10-C8-C9
25	y	315	CLA	C11-C10-C8-C9
25	q	313	CLA	C11-C10-C8-C9
25	b	609	CLA	C6-C7-C8-C9
25	b	612	CLA	C11-C12-C13-C14
25	c	602	CLA	C6-C7-C8-C9
25	c	602	CLA	C14-C13-C15-C16
24	s	403	CHL	O1A-CGA-O2A-C1
25	G	308	CLA	O1A-CGA-O2A-C1
30	n	318	LHG	C26-C27-C28-C29
33	d	411	LMG	C20-C21-C22-C23
29	6	301	0UR	C3-C4-C5-C6
31	d	410	8CT	C12-C13-C14-C15
35	d	403	PHO	O1D-CGD-O2D-CED
25	G	315	CLA	C5-C6-C7-C8
24	N	311	CHL	C1-C2-C3-C4
24	8	309	CHL	C1-C2-C3-C4
24	n	311	CHL	C1-C2-C3-C4
24	q	310	CHL	C1-C2-C3-C4
25	2	317	CLA	C1-C2-C3-C4
25	5	317	CLA	C1-C2-C3-C4
29	q	301	0UR	C46-C47-C48-C49
25	5	314	CLA	C3-C5-C6-C7
32	b	618	SQD	O6-C44-C45-O47
33	D	411	LMG	O7-C8-C9-O8
33	i	101	LMG	O7-C8-C9-O8
37	c	618	DGD	O1G-C1G-C2G-O2G
30	1	318	LHG	C11-C10-C9-C8
25	b	604	CLA	C10-C11-C12-C13
30	N	318	LHG	C26-C27-C28-C29
30	A	612	LHG	C14-C15-C16-C17
25	c	601	CLA	C16-C17-C18-C19
30	d	408	LHG	C4-C5-C6-O8
33	C	618	LMG	O1-C7-C8-C9
33	W	201	LMG	O1-C7-C8-C9
33	m	101	LMG	C7-C8-C9-O8
37	c	618	DGD	O1G-C1G-C2G-C3G
24	Y	317	CHL	CAD-CBD-CGD-O2D
24	y	318	CHL	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	p	318	CHL	CAD-CBD-CGD-O2D
24	7	318	CHL	CAD-CBD-CGD-O2D
25	D	405	CLA	CAD-CBD-CGD-O2D
25	d	405	CLA	CAD-CBD-CGD-O2D
24	1	308	CHL	O1D-CGD-O2D-CED
24	9	317	CHL	O1D-CGD-O2D-CED
24	n	312	CHL	O1A-CGA-O2A-C1
30	D	407	LHG	C31-C32-C33-C34
24	r	308	CHL	CBA-CGA-O2A-C1
32	D	409	SQD	C12-C13-C14-C15
25	2	314	CLA	C3-C5-C6-C7
25	g	308	CLA	C2A-CAA-CBA-CGA
25	u	317	CLA	C2A-CAA-CBA-CGA
25	B	615	CLA	C5-C6-C7-C8
24	S	602	CHL	O1A-CGA-O2A-C1
25	5	317	CLA	O1A-CGA-O2A-C1
25	8	311	CLA	O1D-CGD-O2D-CED
30	d	408	LHG	C27-C28-C29-C30
30	4	318	LHG	C27-C28-C29-C30
24	R	601	CHL	CHA-CBD-CGD-O2D
24	R	602	CHL	CHA-CBD-CGD-O1D
24	R	602	CHL	CHA-CBD-CGD-O2D
24	1	304	CHL	CHA-CBD-CGD-O2D
24	1	308	CHL	CHA-CBD-CGD-O2D
24	1	309	CHL	CHA-CBD-CGD-O1D
24	1	309	CHL	CHA-CBD-CGD-O2D
24	2	305	CHL	CHA-CBD-CGD-O1D
24	2	305	CHL	CHA-CBD-CGD-O2D
24	2	311	CHL	CHA-CBD-CGD-O1D
24	2	311	CHL	CHA-CBD-CGD-O2D
24	2	312	CHL	CHA-CBD-CGD-O2D
24	3	309	CHL	CHA-CBD-CGD-O1D
24	3	309	CHL	CHA-CBD-CGD-O2D
24	3	312	CHL	CHA-CBD-CGD-O1D
24	3	312	CHL	CHA-CBD-CGD-O2D
24	S	607	CHL	CHA-CBD-CGD-O2D
24	N	312	CHL	CHA-CBD-CGD-O1D
24	N	312	CHL	CHA-CBD-CGD-O2D
24	Y	304	CHL	CHA-CBD-CGD-O1D
24	Y	304	CHL	CHA-CBD-CGD-O2D
24	Y	317	CHL	CAD-CBD-CGD-O1D
24	8	308	CHL	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	4	304	CHL	CHA-CBD-CGD-O2D
24	4	308	CHL	CHA-CBD-CGD-O1D
24	4	308	CHL	CHA-CBD-CGD-O2D
24	5	305	CHL	CHA-CBD-CGD-O1D
24	5	305	CHL	CHA-CBD-CGD-O2D
24	5	311	CHL	CHA-CBD-CGD-O1D
24	5	311	CHL	CHA-CBD-CGD-O2D
24	6	309	CHL	CHA-CBD-CGD-O2D
24	g	310	CHL	CHA-CBD-CGD-O2D
24	g	311	CHL	CHA-CBD-CGD-O1D
24	g	311	CHL	CHA-CBD-CGD-O2D
24	g	312	CHL	CHA-CBD-CGD-O2D
24	u	305	CHL	CHA-CBD-CGD-O1D
24	u	305	CHL	CHA-CBD-CGD-O2D
24	u	311	CHL	CHA-CBD-CGD-O2D
24	n	305	CHL	CHA-CBD-CGD-O1D
24	n	305	CHL	CHA-CBD-CGD-O2D
24	n	312	CHL	CHA-CBD-CGD-O1D
24	n	312	CHL	CHA-CBD-CGD-O2D
24	n	317	CHL	CHA-CBD-CGD-O1D
24	n	317	CHL	CHA-CBD-CGD-O2D
24	y	318	CHL	CAD-CBD-CGD-O1D
24	p	305	CHL	CHA-CBD-CGD-O2D
24	p	313	CHL	CHA-CBD-CGD-O1D
24	p	313	CHL	CHA-CBD-CGD-O2D
24	p	318	CHL	CAD-CBD-CGD-O1D
24	q	308	CHL	CHA-CBD-CGD-O2D
24	s	408	CHL	CHA-CBD-CGD-O2D
24	r	302	CHL	CHA-CBD-CGD-O2D
24	r	303	CHL	CHA-CBD-CGD-O1D
24	r	303	CHL	CHA-CBD-CGD-O2D
24	7	305	CHL	CHA-CBD-CGD-O2D
24	7	318	CHL	CAD-CBD-CGD-O1D
25	R	609	CLA	CHA-CBD-CGD-O1D
25	2	307	CLA	CHA-CBD-CGD-O1D
25	3	306	CLA	CHA-CBD-CGD-O1D
25	3	306	CLA	CHA-CBD-CGD-O2D
25	3	315	CLA	CHA-CBD-CGD-O1D
25	S	603	CLA	CHA-CBD-CGD-O1D
25	9	306	CLA	CHA-CBD-CGD-O2D
25	N	315	CLA	CHA-CBD-CGD-O1D
25	8	306	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	8	306	CLA	CHA-CBD-CGD-O2D
25	B	614	CLA	CHA-CBD-CGD-O1D
25	C	602	CLA	CAD-CBD-CGD-O1D
25	C	605	CLA	CAD-CBD-CGD-O1D
25	D	405	CLA	CAD-CBD-CGD-O1D
25	5	307	CLA	CHA-CBD-CGD-O1D
25	6	306	CLA	CHA-CBD-CGD-O1D
25	6	306	CLA	CHA-CBD-CGD-O2D
25	6	315	CLA	CHA-CBD-CGD-O1D
25	n	315	CLA	CHA-CBD-CGD-O1D
25	n	315	CLA	CHA-CBD-CGD-O2D
25	p	308	CLA	CAD-CBD-CGD-O1D
25	q	306	CLA	CHA-CBD-CGD-O2D
25	c	602	CLA	CAD-CBD-CGD-O1D
25	c	605	CLA	CAD-CBD-CGD-O1D
25	d	405	CLA	CAD-CBD-CGD-O1D
25	s	404	CLA	CHA-CBD-CGD-O1D
25	7	308	CLA	CAD-CBD-CGD-O1D
29	2	301	0UR	C41-C2-C3-C4
29	G	301	0UR	C41-C2-C3-C4
29	Y	301	0UR	C41-C2-C3-C4
29	5	301	0UR	C41-C2-C3-C4
29	g	301	0UR	C41-C2-C3-C4
29	y	301	0UR	C41-C2-C3-C4
29	7	301	0UR	C3-C4-C5-C6
30	2	319	LHG	C4-O6-P-O5
30	Y	318	LHG	C4-O6-P-O5
30	A	601	LHG	C3-O3-P-O4
30	A	601	LHG	C3-O3-P-O5
30	A	601	LHG	C3-O3-P-O6
30	C	617	LHG	C3-O3-P-O6
30	C	617	LHG	C4-O6-P-O4
30	D	407	LHG	C4-O6-P-O4
30	D	408	LHG	C3-O3-P-O4
30	D	408	LHG	C4-O6-P-O3
30	4	318	LHG	C4-O6-P-O5
30	5	319	LHG	C4-O6-P-O5
30	g	319	LHG	C4-O6-P-O4
30	y	319	LHG	C4-O6-P-O5
30	a	601	LHG	C3-O3-P-O4
30	a	601	LHG	C3-O3-P-O5
30	a	601	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
30	c	617	LHG	C3-O3-P-O6
30	c	617	LHG	C4-O6-P-O4
30	d	407	LHG	C4-O6-P-O4
30	d	408	LHG	C3-O3-P-O4
30	d	408	LHG	C4-O6-P-O3
30	d	408	LHG	C4-O6-P-O4
31	C	614	8CT	C16-C17-C18-C19
31	c	614	8CT	C16-C17-C18-C19
32	A	609	SQD	C28-C29-C30-C31
25	y	315	CLA	C4-C3-C5-C6
25	c	610	CLA	C4-C3-C5-C6
25	1	314	CLA	C2B-C3B-CAB-CBB
25	3	315	CLA	C2B-C3B-CAB-CBB
25	S	604	CLA	C2B-C3B-CAB-CBB
25	9	314	CLA	C2B-C3B-CAB-CBB
25	4	315	CLA	C2B-C3B-CAB-CBB
25	u	316	CLA	C2B-C3B-CAB-CBB
25	y	307	CLA	C2B-C3B-CAB-CBB
25	p	317	CLA	C2B-C3B-CAB-CBB
25	b	601	CLA	C2B-C3B-CAB-CBB
25	r	313	CLA	C2B-C3B-CAB-CBB
31	A	608	8CT	C02-C03-C10-C11
31	a	608	8CT	C02-C03-C10-C11
25	8	305	CLA	CBD-CGD-O2D-CED
32	B	618	SQD	C8-C7-O47-C45
25	B	602	CLA	CAA-CBA-CGA-O2A
24	y	313	CHL	C2-C3-C5-C6
30	D	407	LHG	C17-C18-C19-C20
30	A	612	LHG	C2-C3-O3-P
30	a	612	LHG	C2-C3-O3-P
24	G	313	CHL	C2C-C3C-CAC-CBC
24	N	308	CHL	O1D-CGD-O2D-CED
25	g	308	CLA	O1D-CGD-O2D-CED
24	2	306	CHL	CBA-CGA-O2A-C1
24	5	306	CHL	CBA-CGA-O2A-C1
25	c	609	CLA	O1D-CGD-O2D-CED
24	5	311	CHL	CAA-CBA-CGA-O2A
26	9	303	0IE	C11-C12-C13-C14
30	a	601	LHG	C29-C30-C31-C32
30	a	612	LHG	C27-C28-C29-C30
25	q	306	CLA	C2A-CAA-CBA-CGA
30	2	319	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
33	C	618	LMG	C11-C12-C13-C14
37	C	619	DGD	C3G-C2G-O2G-C1B
37	c	619	DGD	C4D-C5D-C6D-O5D
31	S	614	8CT	C13-C14-C15-C16
31	S	615	8CT	C13-C14-C15-C16
31	s	415	8CT	C13-C14-C15-C16
31	s	416	8CT	C13-C14-C15-C16
24	g	311	CHL	CAA-CBA-CGA-O2A
33	m	101	LMG	C28-C29-C30-C31
33	d	401	LMG	C13-C14-C15-C16
30	a	601	LHG	C9-C10-C11-C12
33	B	619	LMG	O6-C5-C6-O5
32	A	609	SQD	C16-C17-C18-C19
30	g	319	LHG	O6-C4-C5-C6
25	u	317	CLA	C6-C7-C8-C10
24	r	308	CHL	O1A-CGA-O2A-C1
30	p	319	LHG	C31-C32-C33-C34
24	G	313	CHL	C14-C13-C15-C16
24	Y	304	CHL	C11-C12-C13-C14
24	g	313	CHL	C6-C7-C8-C9
24	g	313	CHL	C14-C13-C15-C16
25	G	315	CLA	C6-C7-C8-C9
25	B	609	CLA	C6-C7-C8-C9
25	C	601	CLA	C11-C12-C13-C14
25	D	405	CLA	C11-C10-C8-C9
25	g	315	CLA	C6-C7-C8-C9
25	y	315	CLA	C14-C13-C15-C16
25	p	315	CLA	C14-C13-C15-C16
25	7	315	CLA	C14-C13-C15-C16
24	g	306	CHL	C11-C10-C8-C7
24	g	306	CHL	C11-C12-C13-C15
25	G	315	CLA	C6-C7-C8-C10
25	B	606	CLA	C11-C10-C8-C7
25	C	608	CLA	C11-C12-C13-C15
25	D	404	CLA	C11-C12-C13-C15
25	g	315	CLA	C6-C7-C8-C10
25	p	315	CLA	C12-C13-C15-C16
25	7	315	CLA	C12-C13-C15-C16
24	5	311	CHL	O1A-CGA-O2A-C1
35	D	403	PHO	CBD-CGD-O2D-CED
24	4	305	CHL	C2A-CAA-CBA-CGA
25	C	601	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
25	b	602	CLA	CAA-CBA-CGA-O2A
32	a	609	SQD	O47-C7-C8-C9
30	D	407	LHG	C30-C31-C32-C33
33	C	618	LMG	C34-C35-C36-C37
30	7	319	LHG	C9-C10-C11-C12
25	B	609	CLA	C2-C3-C5-C6
25	B	609	CLA	C16-C17-C18-C20
25	C	602	CLA	C8-C10-C11-C12
30	D	408	LHG	C11-C10-C9-C8
33	C	618	LMG	O1-C7-C8-O7
33	d	411	LMG	O1-C7-C8-O7
24	q	309	CHL	CAA-CBA-CGA-O2A
24	2	311	CHL	O1A-CGA-O2A-C1
25	C	609	CLA	O1D-CGD-O2D-CED
32	b	618	SQD	C8-C7-O47-C45
24	Y	319	CHL	CAA-CBA-CGA-O2A
32	B	618	SQD	O47-C7-C8-C9
32	b	618	SQD	O47-C7-C8-C9
25	G	307	CLA	C2A-CAA-CBA-CGA
25	8	306	CLA	C2A-CAA-CBA-CGA
25	6	316	CLA	C2A-CAA-CBA-CGA
25	n	313	CLA	C2A-CAA-CBA-CGA
24	n	305	CHL	C11-C12-C13-C14
30	7	319	LHG	C31-C32-C33-C34
25	a	605	CLA	O2A-C1-C2-C3
32	D	409	SQD	C14-C15-C16-C17
37	C	619	DGD	C1B-C2B-C3B-C4B
37	c	618	DGD	C7B-C8B-C9B-CAB
30	D	408	LHG	C31-C32-C33-C34
33	C	618	LMG	C10-C11-C12-C13
24	n	311	CHL	C1C-C2C-CMC-OMC
37	C	619	DGD	C7B-C8B-C9B-CAB
31	x	601	8CT	C25-C26-C28-C29
24	y	311	CHL	CAA-CBA-CGA-O2A
32	D	409	SQD	O47-C7-C8-C9
24	u	305	CHL	C2A-CAA-CBA-CGA
25	p	317	CLA	C2A-CAA-CBA-CGA
25	7	317	CLA	C2A-CAA-CBA-CGA
31	D	410	8CT	C18-C19-C20-C21
37	c	618	DGD	C1B-C2B-C3B-C4B
32	d	409	SQD	O47-C7-C8-C9
35	D	403	PHO	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	n	306	CLA	C6-C7-C8-C9
30	d	407	LHG	C17-C18-C19-C20
24	r	309	CHL	C2C-C3C-CAC-CBC
25	B	607	CLA	C16-C17-C18-C20
25	7	314	CLA	C6-C7-C8-C9
24	Y	309	CHL	O1A-CGA-O2A-C1
25	2	315	CLA	C11-C12-C13-C14
25	B	606	CLA	C14-C13-C15-C16
25	5	315	CLA	C11-C12-C13-C14
25	c	608	CLA	C6-C7-C8-C9
25	d	404	CLA	C11-C12-C13-C14
25	d	405	CLA	C11-C10-C8-C9
35	d	403	PHO	C11-C12-C13-C14
33	i	101	LMG	C12-C13-C14-C15
24	3	310	CHL	O1D-CGD-O2D-CED
24	S	608	CHL	O1D-CGD-O2D-CED
25	3	316	CLA	C4B-C3B-CAB-CBB
25	8	305	CLA	C4B-C3B-CAB-CBB
25	B	605	CLA	C4B-C3B-CAB-CBB
25	u	307	CLA	C4B-C3B-CAB-CBB
25	n	306	CLA	C4B-C3B-CAB-CBB
25	q	305	CLA	C4B-C3B-CAB-CBB
25	b	605	CLA	C4B-C3B-CAB-CBB
25	r	312	CLA	C4B-C3B-CAB-CBB
25	R	611	CLA	CAA-CBA-CGA-O2A
24	3	310	CHL	CBD-CGD-O2D-CED
24	R	607	CHL	CBA-CGA-O2A-C1
25	b	606	CLA	C15-C16-C17-C18
25	c	607	CLA	C2A-CAA-CBA-CGA
25	c	612	CLA	C4-C3-C5-C6
29	u	301	OUR	C46-C47-C48-C49
30	d	407	LHG	C11-C12-C13-C14
32	b	618	SQD	C16-C17-C18-C19
24	R	608	CHL	C2C-C3C-CAC-CBC
24	N	309	CHL	O1D-CGD-O2D-CED
24	G	306	CHL	C11-C10-C8-C7
24	p	306	CHL	C11-C12-C13-C15
24	7	306	CHL	C11-C12-C13-C15
24	R	607	CHL	O1A-CGA-O2A-C1
24	p	313	CHL	C2C-C3C-CAC-CBC
24	q	309	CHL	O1D-CGD-O2D-CED
24	G	313	CHL	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	A	605	CLA	CBA-CGA-O2A-C1
29	9	301	0UR	C46-C47-C48-C49
33	B	619	LMG	C10-C11-C12-C13
25	B	612	CLA	C13-C15-C16-C17
25	g	316	CLA	CAA-CBA-CGA-O1A
24	G	305	CHL	C4-C3-C5-C6
24	9	309	CHL	C3A-C2A-CAA-CBA
25	6	316	CLA	C3A-C2A-CAA-CBA
25	u	315	CLA	C3A-C2A-CAA-CBA
25	C	607	CLA	C2A-CAA-CBA-CGA
25	g	307	CLA	C2A-CAA-CBA-CGA
25	p	308	CLA	C2A-CAA-CBA-CGA
24	7	313	CHL	C2C-C3C-CAC-CBC
25	B	606	CLA	C15-C16-C17-C18
28	R	616	NEX	C39-C29-C30-C31
28	1	303	NEX	C39-C29-C30-C31
28	2	304	NEX	C39-C29-C30-C31
28	3	318	NEX	C39-C29-C30-C31
28	S	617	NEX	C39-C29-C30-C31
28	G	304	NEX	C39-C29-C30-C31
28	9	319	NEX	C39-C29-C30-C31
28	N	303	NEX	C39-C29-C30-C31
28	4	303	NEX	C39-C29-C30-C31
28	5	304	NEX	C39-C29-C30-C31
28	6	303	NEX	C39-C29-C30-C31
28	g	304	NEX	C39-C29-C30-C31
28	u	304	NEX	C39-C29-C30-C31
28	n	303	NEX	C39-C29-C30-C31
28	y	304	NEX	C39-C29-C30-C31
28	p	304	NEX	C39-C29-C30-C31
28	s	401	NEX	C39-C29-C30-C31
28	r	301	NEX	C39-C29-C30-C31
28	r	317	NEX	C39-C29-C30-C31
28	7	304	NEX	C39-C29-C30-C31
31	S	614	8CT	C40-C12-C13-C14
31	S	614	8CT	C39-C16-C17-C18
31	S	615	8CT	C39-C16-C17-C18
31	S	615	8CT	C19-C20-C21-C22
31	S	615	8CT	C24-C25-C26-C27
31	s	415	8CT	C40-C12-C13-C14
31	s	415	8CT	C39-C16-C17-C18
31	s	416	8CT	C39-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
31	s	416	8CT	C19-C20-C21-C22
31	s	416	8CT	C24-C25-C26-C27
30	Y	318	LHG	C14-C15-C16-C17
24	9	309	CHL	CAA-CBA-CGA-O2A
24	g	310	CHL	O1D-CGD-O2D-CED
32	d	409	SQD	C14-C15-C16-C17
24	Y	305	CHL	C2-C1-O2A-CGA
24	8	303	CHL	C2-C1-O2A-CGA
24	g	311	CHL	C2-C1-O2A-CGA
25	G	308	CLA	C2-C1-O2A-CGA
25	c	603	CLA	C2-C1-O2A-CGA
31	C	614	8CT	C23-C24-C25-C26
31	D	410	8CT	C12-C13-C14-C15
33	i	101	LMG	C38-C39-C40-C41
25	c	603	CLA	C5-C6-C7-C8
24	u	310	CHL	CAA-CBA-CGA-O1A
25	G	316	CLA	CAA-CBA-CGA-O1A
25	9	315	CLA	CAA-CBA-CGA-O1A
33	D	401	LMG	C34-C35-C36-C37
29	Y	301	0UR	C5-C6-C7-C8
25	C	604	CLA	C4-C3-C5-C6
25	c	604	CLA	C4-C3-C5-C6
23	f	201	HEM	C3D-CAD-CBD-CGD
25	b	612	CLA	C13-C15-C16-C17
25	b	613	CLA	C5-C6-C7-C8
24	q	308	CHL	CAA-CBA-CGA-O2A
33	i	101	LMG	C7-C8-C9-O8
25	9	316	CLA	C11-C10-C8-C7
24	G	311	CHL	CAA-CBA-CGA-O1A
30	d	408	LHG	C28-C29-C30-C31
32	A	609	SQD	C13-C14-C15-C16
33	d	401	LMG	C18-C19-C20-C21
24	9	309	CHL	CAA-CBA-CGA-O1A
25	2	316	CLA	CAA-CBA-CGA-O1A
25	S	611	CLA	CAA-CBA-CGA-O1A
25	5	316	CLA	CAA-CBA-CGA-O1A
25	s	412	CLA	CAA-CBA-CGA-O1A
25	N	306	CLA	C6-C7-C8-C9
24	S	602	CHL	C6-C7-C8-C9
24	G	306	CHL	C11-C10-C8-C9
24	g	313	CHL	C11-C10-C8-C9
24	p	305	CHL	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
24	s	403	CHL	C6-C7-C8-C9
24	7	305	CHL	C11-C10-C8-C9
24	7	306	CHL	C11-C10-C8-C9
25	Y	314	CLA	C6-C7-C8-C9
25	Y	314	CLA	C11-C12-C13-C14
25	Y	314	CLA	C14-C13-C15-C16
25	u	315	CLA	C6-C7-C8-C9
25	b	606	CLA	C11-C10-C8-C9
25	b	606	CLA	C14-C13-C15-C16
25	c	601	CLA	C11-C12-C13-C14
35	A	606	PHO	C6-C7-C8-C9
35	D	403	PHO	C6-C7-C8-C9
35	D	403	PHO	C11-C12-C13-C14
35	a	606	PHO	C6-C7-C8-C9
35	d	403	PHO	C6-C7-C8-C9
33	d	401	LMG	C40-C41-C42-C43
25	y	317	CLA	CBA-CGA-O2A-C1
24	8	308	CHL	CAA-CBA-CGA-O2A
30	5	319	LHG	O8-C23-C24-C25
37	c	618	DGD	C1G-C2G-O2G-C1B
25	c	602	CLA	C8-C10-C11-C12
30	9	318	LHG	C30-C31-C32-C33
24	R	602	CHL	C1A-C2A-CAA-CBA
24	1	305	CHL	C1A-C2A-CAA-CBA
24	Y	305	CHL	C1A-C2A-CAA-CBA
24	4	305	CHL	C1A-C2A-CAA-CBA
24	u	310	CHL	C1A-C2A-CAA-CBA
24	y	306	CHL	C1A-C2A-CAA-CBA
24	p	305	CHL	C1A-C2A-CAA-CBA
24	s	402	CHL	C1A-C2A-CAA-CBA
24	r	303	CHL	C1A-C2A-CAA-CBA
37	c	619	DGD	O6D-C5D-C6D-O5D
25	A	607	CLA	C4-C3-C5-C6
25	a	607	CLA	C4-C3-C5-C6
25	q	306	CLA	CBA-CGA-O2A-C1
25	a	605	CLA	CBA-CGA-O2A-C1
24	g	310	CHL	CBD-CGD-O2D-CED
24	p	306	CHL	CBD-CGD-O2D-CED
30	9	318	LHG	O8-C23-C24-C25
30	1	318	LHG	C27-C28-C29-C30
24	G	311	CHL	C3-C5-C6-C7
32	B	618	SQD	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
24	r	309	CHL	CAA-CBA-CGA-O2A
25	R	611	CLA	CAA-CBA-CGA-O1A
25	2	316	CLA	CAA-CBA-CGA-O2A
25	S	611	CLA	CAA-CBA-CGA-O2A
25	s	412	CLA	CAA-CBA-CGA-O2A
25	c	612	CLA	O1D-CGD-O2D-CED
25	N	313	CLA	C2A-CAA-CBA-CGA
25	Y	316	CLA	C2A-CAA-CBA-CGA
25	y	314	CLA	C2A-CAA-CBA-CGA
24	6	310	CHL	O1D-CGD-O2D-CED
30	2	319	LHG	O8-C23-C24-C25
25	R	612	CLA	C1A-C2A-CAA-CBA
25	G	314	CLA	C1A-C2A-CAA-CBA
25	B	603	CLA	C1A-C2A-CAA-CBA
25	C	606	CLA	C1A-C2A-CAA-CBA
25	C	608	CLA	C1A-C2A-CAA-CBA
25	C	616	CLA	C1A-C2A-CAA-CBA
25	5	314	CLA	C1A-C2A-CAA-CBA
25	g	314	CLA	C1A-C2A-CAA-CBA
25	q	306	CLA	C1A-C2A-CAA-CBA
25	b	603	CLA	C1A-C2A-CAA-CBA
25	c	606	CLA	C1A-C2A-CAA-CBA
25	c	608	CLA	C1A-C2A-CAA-CBA
25	c	616	CLA	C1A-C2A-CAA-CBA
25	r	310	CLA	C1A-C2A-CAA-CBA
28	R	616	NEX	C28-C29-C30-C31
28	1	303	NEX	C28-C29-C30-C31
28	2	304	NEX	C28-C29-C30-C31
28	3	318	NEX	C28-C29-C30-C31
28	S	617	NEX	C28-C29-C30-C31
28	G	304	NEX	C28-C29-C30-C31
28	9	319	NEX	C28-C29-C30-C31
28	N	303	NEX	C28-C29-C30-C31
28	4	303	NEX	C28-C29-C30-C31
28	5	304	NEX	C28-C29-C30-C31
28	6	303	NEX	C28-C29-C30-C31
28	g	304	NEX	C28-C29-C30-C31
28	u	304	NEX	C28-C29-C30-C31
28	n	303	NEX	C28-C29-C30-C31
28	y	304	NEX	C28-C29-C30-C31
28	p	304	NEX	C28-C29-C30-C31
28	s	401	NEX	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
28	r	301	NEX	C28-C29-C30-C31
28	r	317	NEX	C28-C29-C30-C31
28	7	304	NEX	C28-C29-C30-C31
31	S	614	8CT	C11-C12-C13-C14
31	S	614	8CT	C15-C16-C17-C18
31	S	615	8CT	C15-C16-C17-C18
31	S	615	8CT	C24-C25-C26-C28
31	s	415	8CT	C11-C12-C13-C14
31	s	415	8CT	C15-C16-C17-C18
31	s	416	8CT	C15-C16-C17-C18
31	s	416	8CT	C24-C25-C26-C28
25	Y	316	CLA	CBA-CGA-O2A-C1
24	u	310	CHL	CAA-CBA-CGA-O2A
24	q	308	CHL	CAA-CBA-CGA-O1A
25	G	316	CLA	CAA-CBA-CGA-O2A
25	5	316	CLA	CAA-CBA-CGA-O2A
25	B	613	CLA	C5-C6-C7-C8
25	R	612	CLA	C2B-C3B-CAB-CBB
25	1	315	CLA	C2B-C3B-CAB-CBB
25	2	315	CLA	C2B-C3B-CAB-CBB
25	9	306	CLA	C2B-C3B-CAB-CBB
25	N	306	CLA	C2B-C3B-CAB-CBB
25	Y	306	CLA	C2B-C3B-CAB-CBB
25	8	305	CLA	C2B-C3B-CAB-CBB
25	B	605	CLA	C2B-C3B-CAB-CBB
25	5	315	CLA	C2B-C3B-CAB-CBB
25	6	316	CLA	C2B-C3B-CAB-CBB
25	u	307	CLA	C2B-C3B-CAB-CBB
25	n	306	CLA	C2B-C3B-CAB-CBB
25	q	305	CLA	C2B-C3B-CAB-CBB
25	b	605	CLA	C2B-C3B-CAB-CBB
25	s	405	CLA	C2B-C3B-CAB-CBB
25	r	305	CLA	C2B-C3B-CAB-CBB
25	r	312	CLA	C2B-C3B-CAB-CBB
31	T	101	8CT	C02-C03-C10-C11
31	C	613	8CT	C02-C03-C10-C11
31	C	614	8CT	C02-C03-C10-C11
31	t	101	8CT	C02-C03-C10-C11
31	c	613	8CT	C02-C03-C10-C11
31	c	614	8CT	C02-C03-C10-C11
31	c	615	8CT	C02-C03-C10-C11
30	4	318	LHG	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
25	n	315	CLA	CAA-CBA-CGA-O1A
25	q	314	CLA	CAA-CBA-CGA-O2A
25	8	306	CLA	CBA-CGA-O2A-C1
30	D	407	LHG	C2-C3-O3-P
30	5	319	LHG	C9-C10-C11-C12
33	m	101	LMG	C11-C12-C13-C14
25	C	608	CLA	C14-C13-C15-C16
24	R	608	CHL	CAA-CBA-CGA-O2A
25	y	316	CLA	CAA-CBA-CGA-O2A
24	G	306	CHL	C4-C3-C5-C6
24	Y	319	CHL	C4-C3-C5-C6
24	8	310	CHL	C4-C3-C5-C6
24	g	305	CHL	C4-C3-C5-C6
24	q	309	CHL	C4-C3-C5-C6
25	C	604	CLA	C2-C3-C5-C6
25	c	610	CLA	C2-C3-C5-C6
32	d	409	SQD	C27-C28-C29-C30
24	s	409	CHL	O1D-CGD-O2D-CED
24	N	311	CHL	O2A-C1-C2-C3
24	8	309	CHL	O2A-C1-C2-C3
24	n	311	CHL	O2A-C1-C2-C3
24	q	310	CHL	O2A-C1-C2-C3
24	8	308	CHL	CAA-CBA-CGA-O1A
24	r	309	CHL	CAA-CBA-CGA-O1A
25	9	315	CLA	CAA-CBA-CGA-O2A
25	6	316	CLA	CAA-CBA-CGA-O2A
25	u	316	CLA	CAA-CBA-CGA-O2A
25	r	312	CLA	CAA-CBA-CGA-O1A
24	G	306	CHL	C11-C12-C13-C15
24	Y	312	CHL	C11-C12-C13-C15
24	y	313	CHL	C11-C12-C13-C15
25	G	315	CLA	C11-C10-C8-C7
25	B	603	CLA	C11-C12-C13-C15
25	B	606	CLA	C12-C13-C15-C16
25	C	607	CLA	C6-C7-C8-C10
25	b	603	CLA	C11-C12-C13-C15
25	b	604	CLA	C11-C10-C8-C7
25	b	606	CLA	C12-C13-C15-C16
25	c	607	CLA	C6-C7-C8-C10
25	c	611	CLA	C11-C12-C13-C15
33	d	401	LMG	C36-C37-C38-C39
24	3	304	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
24	N	310	CHL	C2A-CAA-CBA-CGA
24	n	310	CHL	C2A-CAA-CBA-CGA
25	Y	313	CLA	C2A-CAA-CBA-CGA
25	y	317	CLA	C2A-CAA-CBA-CGA
25	s	410	CLA	C2A-CAA-CBA-CGA
30	A	612	LHG	O7-C5-C6-O8
30	a	612	LHG	O7-C5-C6-O8
25	N	315	CLA	CAA-CBA-CGA-O1A
33	d	411	LMG	C30-C31-C32-C33
30	g	319	LHG	C11-C10-C9-C8
32	d	409	SQD	C7-C8-C9-C10
25	g	316	CLA	CAA-CBA-CGA-O2A
30	2	319	LHG	C9-C10-C11-C12
24	5	305	CHL	C2C-C3C-CAC-CBC
24	y	310	CHL	O1A-CGA-O2A-C1
25	Y	315	CLA	CAA-CBA-CGA-O2A
25	8	313	CLA	CAA-CBA-CGA-O2A
24	q	311	CHL	C4-C3-C5-C6
25	R	613	CLA	CAA-CBA-CGA-O2A
25	Y	314	CLA	C2-C3-C5-C6
25	b	605	CLA	C2-C3-C5-C6
25	b	609	CLA	C2-C3-C5-C6
25	c	612	CLA	C2-C3-C5-C6
25	A	605	CLA	O1A-CGA-O2A-C1
25	q	305	CLA	O1D-CGD-O2D-CED
24	s	403	CHL	C2-C1-O2A-CGA
24	p	310	CHL	CAA-CBA-CGA-O2A
24	7	310	CHL	CAA-CBA-CGA-O2A
25	n	315	CLA	CAA-CBA-CGA-O2A
25	p	317	CLA	C11-C10-C8-C7
25	p	307	CLA	CBA-CGA-O2A-C1
25	N	315	CLA	CAA-CBA-CGA-O2A
33	m	101	LMG	C30-C31-C32-C33
31	c	614	8CT	C23-C24-C25-C26
25	C	603	CLA	C5-C6-C7-C8
25	C	607	CLA	C13-C15-C16-C17
25	b	602	CLA	C13-C15-C16-C17
33	m	101	LMG	O8-C28-C29-C30
25	7	314	CLA	C6-C7-C8-C10
33	C	618	LMG	C17-C18-C19-C20
25	y	316	CLA	CAA-CBA-CGA-O1A
25	s	404	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
25	r	312	CLA	CAA-CBA-CGA-O2A
25	q	306	CLA	O1A-CGA-O2A-C1
30	A	601	LHG	C26-C27-C28-C29
24	n	305	CHL	C4-C3-C5-C6
24	s	403	CHL	C4-C3-C5-C6
25	C	605	CLA	C4-C3-C5-C6
25	c	605	CLA	C4-C3-C5-C6
39	D	406	PL9	C40-C39-C41-C42
25	Y	314	CLA	C5-C6-C7-C8
25	Y	315	CLA	CAA-CBA-CGA-O1A
25	8	313	CLA	CAA-CBA-CGA-O1A
25	6	316	CLA	CAA-CBA-CGA-O1A
30	d	407	LHG	C2-C3-O3-P
25	B	605	CLA	C2-C3-C5-C6
25	c	604	CLA	C2-C3-C5-C6
24	6	310	CHL	CBD-CGD-O2D-CED
24	G	313	CHL	O1A-CGA-O2A-C1
25	a	605	CLA	O1A-CGA-O2A-C1
24	R	607	CHL	C2-C1-O2A-CGA
25	B	613	CLA	C3-C5-C6-C7
37	C	619	DGD	C5A-C6A-C7A-C8A
24	R	608	CHL	CAA-CBA-CGA-O1A
25	u	316	CLA	CAA-CBA-CGA-O1A
25	A	605	CLA	O2A-C1-C2-C3
25	8	306	CLA	O1A-CGA-O2A-C1
25	y	317	CLA	O1A-CGA-O2A-C1
33	i	101	LMG	C14-C15-C16-C17
30	G	319	LHG	O8-C23-C24-C25
30	1	318	LHG	C25-C26-C27-C28
25	R	612	CLA	CAA-CBA-CGA-O2A
25	q	314	CLA	CAA-CBA-CGA-O1A
25	Y	316	CLA	O1A-CGA-O2A-C1
25	p	307	CLA	O1A-CGA-O2A-C1
25	S	609	CLA	C2A-CAA-CBA-CGA
30	a	601	LHG	C19-C20-C21-C22
30	d	408	LHG	C10-C11-C12-C13
25	2	307	CLA	C2A-CAA-CBA-CGA
24	r	307	CHL	CAA-CBA-CGA-O2A
25	r	314	CLA	CAA-CBA-CGA-O2A
24	S	601	CHL	CAA-CBA-CGA-O2A
37	C	619	DGD	C1A-C2A-C3A-C4A
25	B	602	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
24	p	306	CHL	C3-C5-C6-C7
30	A	601	LHG	O6-C4-C5-O7
24	S	602	CHL	C4-C3-C5-C6
25	S	612	CLA	C4-C3-C5-C6
29	Y	301	0UR	C3-C4-C5-C6
30	c	617	LHG	O8-C23-C24-C25
24	s	403	CHL	C2-C3-C5-C6
24	8	310	CHL	C6-C7-C8-C10
24	S	608	CHL	CBD-CGD-O2D-CED
30	n	318	LHG	C27-C28-C29-C30
25	R	611	CLA	C4B-C3B-CAB-CBB
25	3	306	CLA	C4B-C3B-CAB-CBB
25	9	306	CLA	C4B-C3B-CAB-CBB
25	N	306	CLA	C4B-C3B-CAB-CBB
25	N	315	CLA	C4B-C3B-CAB-CBB
25	Y	315	CLA	C4B-C3B-CAB-CBB
25	B	616	CLA	C4B-C3B-CAB-CBB
25	A	605	CLA	C4B-C3B-CAB-CBB
25	6	306	CLA	C4B-C3B-CAB-CBB
25	6	307	CLA	C4B-C3B-CAB-CBB
25	g	316	CLA	C4B-C3B-CAB-CBB
25	y	316	CLA	C4B-C3B-CAB-CBB
25	b	616	CLA	C4B-C3B-CAB-CBB
29	N	301	0UR	O42-C2-C3-C4
29	n	301	0UR	O42-C2-C3-C4
29	p	301	0UR	O42-C2-C3-C4
29	7	301	0UR	O42-C2-C3-C4
25	b	609	CLA	C13-C15-C16-C17
24	6	310	CHL	CAA-CBA-CGA-O2A
30	C	617	LHG	O8-C23-C24-C25
30	g	319	LHG	O8-C23-C24-C25
30	y	319	LHG	C29-C30-C31-C32
30	p	319	LHG	C9-C10-C11-C12
24	p	306	CHL	O1D-CGD-O2D-CED
24	1	312	CHL	CAA-CBA-CGA-O2A
24	4	312	CHL	CAA-CBA-CGA-O2A
24	s	402	CHL	CAA-CBA-CGA-O2A
25	1	315	CLA	CAA-CBA-CGA-O2A
25	4	315	CLA	CAA-CBA-CGA-O2A
25	p	316	CLA	CAA-CBA-CGA-O1A
25	N	313	CLA	C6-C7-C8-C10
25	B	607	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
24	4	308	CHL	O1D-CGD-O2D-CED
24	1	310	CHL	CHA-CBD-CGD-O1D
24	1	310	CHL	CHA-CBD-CGD-O2D
24	3	308	CHL	CHA-CBD-CGD-O1D
24	3	308	CHL	CHA-CBD-CGD-O2D
24	S	601	CHL	CHA-CBD-CGD-O1D
24	S	601	CHL	CHA-CBD-CGD-O2D
24	G	312	CHL	CHA-CBD-CGD-O2D
24	9	304	CHL	CHA-CBD-CGD-O1D
24	9	304	CHL	CHA-CBD-CGD-O2D
24	N	304	CHL	CHA-CBD-CGD-O1D
24	N	304	CHL	CHA-CBD-CGD-O2D
24	N	317	CHL	CHA-CBD-CGD-O2D
24	Y	310	CHL	CHA-CBD-CGD-O2D
24	8	303	CHL	CHA-CBD-CGD-O1D
24	8	303	CHL	CHA-CBD-CGD-O2D
24	4	310	CHL	CHA-CBD-CGD-O1D
24	4	310	CHL	CHA-CBD-CGD-O2D
24	5	312	CHL	CHA-CBD-CGD-O2D
24	6	308	CHL	CHA-CBD-CGD-O1D
24	6	308	CHL	CHA-CBD-CGD-O2D
24	6	312	CHL	CHA-CBD-CGD-O1D
24	6	312	CHL	CHA-CBD-CGD-O2D
24	n	304	CHL	CHA-CBD-CGD-O1D
24	n	304	CHL	CHA-CBD-CGD-O2D
24	y	305	CHL	CHA-CBD-CGD-O1D
24	y	305	CHL	CHA-CBD-CGD-O2D
24	y	310	CHL	CHA-CBD-CGD-O2D
24	y	311	CHL	CHA-CBD-CGD-O1D
24	y	311	CHL	CHA-CBD-CGD-O2D
24	q	303	CHL	CHA-CBD-CGD-O1D
24	q	303	CHL	CHA-CBD-CGD-O2D
24	s	402	CHL	CHA-CBD-CGD-O1D
24	s	402	CHL	CHA-CBD-CGD-O2D
24	s	408	CHL	CHA-CBD-CGD-O1D
24	r	302	CHL	CHA-CBD-CGD-O1D
24	7	313	CHL	CHA-CBD-CGD-O1D
24	7	313	CHL	CHA-CBD-CGD-O2D
24	6	304	CHL	C2A-CAA-CBA-CGA
25	2	317	CLA	C2A-CAA-CBA-CGA
25	3	316	CLA	CAA-CBA-CGA-O2A
25	7	316	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
25	5	307	CLA	C2A-CAA-CBA-CGA
30	A	601	LHG	O6-C4-C5-C6
39	d	406	PL9	C40-C39-C41-C42
24	r	308	CHL	C2-C1-O2A-CGA
25	c	607	CLA	C13-C15-C16-C17
24	p	310	CHL	CAA-CBA-CGA-O1A
24	7	310	CHL	CAA-CBA-CGA-O1A
25	3	315	CLA	CAA-CBA-CGA-O2A
25	S	603	CLA	CAA-CBA-CGA-O2A
30	a	601	LHG	C16-C17-C18-C19
37	C	620	DGD	C4A-C5A-C6A-C7A
24	2	305	CHL	C2C-C3C-CAC-CBC
25	8	305	CLA	O1D-CGD-O2D-CED
25	C	604	CLA	C10-C11-C12-C13
25	C	609	CLA	C10-C11-C12-C13
25	c	609	CLA	C10-C11-C12-C13
24	G	305	CHL	C11-C12-C13-C15
24	3	304	CHL	C2-C1-O2A-CGA
25	1	315	CLA	CAA-CBA-CGA-O1A
25	S	616	CLA	CAA-CBA-CGA-O2A
25	4	315	CLA	CAA-CBA-CGA-O1A
25	6	315	CLA	CAA-CBA-CGA-O2A
33	i	101	LMG	C13-C14-C15-C16
30	A	601	LHG	C19-C20-C21-C22
24	6	304	CHL	C2-C1-O2A-CGA
25	7	314	CLA	O1A-CGA-O2A-C1
30	9	318	LHG	C9-C10-C11-C12
25	p	316	CLA	CAA-CBA-CGA-O2A
24	G	313	CHL	C11-C10-C8-C9
24	p	306	CHL	C11-C10-C8-C9
25	C	608	CLA	C6-C7-C8-C9
30	A	601	LHG	C16-C17-C18-C19
25	8	312	CLA	O1A-CGA-O2A-C1
25	p	314	CLA	O1A-CGA-O2A-C1
32	A	609	SQD	C15-C16-C17-C18
24	N	310	CHL	CAA-CBA-CGA-O2A
24	n	310	CHL	CAA-CBA-CGA-O2A
30	1	318	LHG	C9-C10-C11-C12
24	3	310	CHL	CAA-CBA-CGA-O2A
25	R	613	CLA	C2A-CAA-CBA-CGA
25	5	317	CLA	C2A-CAA-CBA-CGA
25	r	314	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
25	7	308	CLA	C2A-CAA-CBA-CGA
24	G	311	CHL	C2-C1-O2A-CGA
24	Y	312	CHL	C2-C1-O2A-CGA
24	n	312	CHL	C2-C1-O2A-CGA
24	y	306	CHL	C2-C1-O2A-CGA
24	y	313	CHL	C2-C1-O2A-CGA
24	p	306	CHL	C2-C1-O2A-CGA
24	q	303	CHL	C2-C1-O2A-CGA
25	C	603	CLA	C2-C1-O2A-CGA
25	g	308	CLA	C2-C1-O2A-CGA
24	q	311	CHL	C6-C7-C8-C10
25	n	313	CLA	C6-C7-C8-C10
33	B	619	LMG	C30-C31-C32-C33
24	N	304	CHL	C3A-C2A-CAA-CBA
24	u	305	CHL	C3A-C2A-CAA-CBA
24	n	304	CHL	C3A-C2A-CAA-CBA
25	9	314	CLA	C3A-C2A-CAA-CBA
25	B	608	CLA	C3A-C2A-CAA-CBA
25	C	612	CLA	C4-C3-C5-C6
25	n	316	CLA	C3A-C2A-CAA-CBA
25	d	404	CLA	C3A-C2A-CAA-CBA
24	n	309	CHL	CAA-CBA-CGA-O2A
25	s	404	CLA	CAA-CBA-CGA-O1A
25	7	316	CLA	CAA-CBA-CGA-O2A
30	5	319	LHG	O1-C1-C2-C3
30	p	319	LHG	C26-C27-C28-C29
30	n	318	LHG	O10-C23-C24-C25
24	S	601	CHL	CAA-CBA-CGA-O1A
25	r	313	CLA	CAA-CBA-CGA-O2A
24	5	306	CHL	O1A-CGA-O2A-C1
24	g	313	CHL	CBA-CGA-O2A-C1
37	C	619	DGD	C1G-C2G-O2G-C1B
37	c	618	DGD	C3G-C2G-O2G-C1B
24	1	305	CHL	CAA-CBA-CGA-O2A
24	1	312	CHL	CAA-CBA-CGA-O1A
24	N	309	CHL	CAA-CBA-CGA-O2A
24	6	310	CHL	CAA-CBA-CGA-O1A
25	s	417	CLA	CAA-CBA-CGA-O2A
37	c	619	DGD	CBB-CCB-CDB-CEB
24	2	313	CHL	C3C-C2C-CMC-OMC
24	3	312	CHL	C3C-C2C-CMC-OMC
24	G	310	CHL	C3C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
24	8	308	CHL	C3C-C2C-CMC-OMC
24	g	310	CHL	C3C-C2C-CMC-OMC
24	u	305	CHL	C3C-C2C-CMC-OMC
24	n	309	CHL	C3C-C2C-CMC-OMC
24	q	307	CHL	C3C-C2C-CMC-OMC
24	q	308	CHL	C3C-C2C-CMC-OMC
24	s	408	CHL	C3C-C2C-CMC-OMC
24	2	312	CHL	CAA-CBA-CGA-O2A
24	4	312	CHL	CAA-CBA-CGA-O1A
24	s	402	CHL	CAA-CBA-CGA-O1A
25	C	603	CLA	C10-C11-C12-C13
25	4	313	CLA	C2A-CAA-CBA-CGA
30	d	408	LHG	C32-C33-C34-C35
30	Y	318	LHG	C29-C30-C31-C32
24	5	312	CHL	CAA-CBA-CGA-O2A
25	S	603	CLA	CAA-CBA-CGA-O1A
30	2	319	LHG	O6-C4-C5-O7
30	5	319	LHG	O6-C4-C5-O7
24	g	313	CHL	O1A-CGA-O2A-C1
25	8	312	CLA	CBA-CGA-O2A-C1
25	R	612	CLA	CAA-CBA-CGA-O1A
25	6	315	CLA	CAA-CBA-CGA-O1A
25	r	313	CLA	CAA-CBA-CGA-O1A
24	N	309	CHL	CBD-CGD-O2D-CED
25	C	602	CLA	O1A-CGA-O2A-C1
25	b	602	CLA	C5-C6-C7-C8
25	R	604	CLA	O1D-CGD-O2D-CED
25	7	307	CLA	CBA-CGA-O2A-C1
25	7	314	CLA	CBA-CGA-O2A-C1
24	g	306	CHL	C4-C3-C5-C6
25	s	413	CLA	C4-C3-C5-C6
24	2	312	CHL	CAA-CBA-CGA-O1A
24	N	309	CHL	CAA-CBA-CGA-O1A
30	4	318	LHG	C9-C10-C11-C12
24	2	306	CHL	O1A-CGA-O2A-C1
24	R	606	CHL	C2-C1-O2A-CGA
25	S	616	CLA	CAA-CBA-CGA-O1A
25	R	604	CLA	CBD-CGD-O2D-CED
32	a	609	SQD	O47-C45-C46-O48
25	7	307	CLA	O1A-CGA-O2A-C1
24	G	305	CHL	C6-C7-C8-C9
24	g	305	CHL	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
25	B	606	CLA	C11-C10-C8-C9
25	C	604	CLA	C6-C7-C8-C9
25	b	607	CLA	C16-C17-C18-C20
30	y	319	LHG	O8-C23-C24-C25
24	Y	310	CHL	CAA-CBA-CGA-O1A
24	5	312	CHL	CAA-CBA-CGA-O1A
28	1	303	NEX	C31-C32-C33-C34
28	2	304	NEX	C31-C32-C33-C34
28	S	617	NEX	C31-C32-C33-C34
28	9	319	NEX	C31-C32-C33-C34
28	4	303	NEX	C31-C32-C33-C34
28	5	304	NEX	C31-C32-C33-C34
28	u	304	NEX	C31-C32-C33-C34
28	y	304	NEX	C31-C32-C33-C34
28	p	304	NEX	C31-C32-C33-C34
28	7	304	NEX	C31-C32-C33-C34
29	3	301	OUR	C5-C6-C7-C8
33	w	201	LMG	C11-C12-C13-C14
24	Y	305	CHL	CAA-CBA-CGA-O2A
25	S	612	CLA	C2-C3-C5-C6
24	1	305	CHL	CAA-CBA-CGA-O1A
24	S	605	CHL	CAA-CBA-CGA-O2A
24	4	305	CHL	CAA-CBA-CGA-O2A
25	3	315	CLA	CAA-CBA-CGA-O1A
25	3	316	CLA	CAA-CBA-CGA-O1A
25	r	311	CLA	CAA-CBA-CGA-O2A
25	9	306	CLA	C2A-CAA-CBA-CGA
25	u	307	CLA	C2A-CAA-CBA-CGA
24	Y	305	CHL	C6-C7-C8-C10
24	Y	312	CHL	C6-C7-C8-C10
24	g	305	CHL	C11-C12-C13-C15
24	y	306	CHL	C11-C12-C13-C15
24	y	313	CHL	C6-C7-C8-C10
25	2	315	CLA	C11-C10-C8-C7
25	C	604	CLA	C12-C13-C15-C16
25	5	315	CLA	C11-C10-C8-C7
25	d	404	CLA	C12-C13-C15-C16
25	g	317	CLA	C11-C10-C8-C7
25	b	613	CLA	C3-C5-C6-C7
24	3	312	CHL	C2C-C3C-CAC-CBC
30	a	612	LHG	C13-C14-C15-C16
24	3	310	CHL	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
25	s	417	CLA	CAA-CBA-CGA-O1A
25	R	604	CLA	C2B-C3B-CAB-CBB
25	R	611	CLA	C2B-C3B-CAB-CBB
25	2	307	CLA	C2B-C3B-CAB-CBB
25	3	306	CLA	C2B-C3B-CAB-CBB
25	9	315	CLA	C2B-C3B-CAB-CBB
25	N	315	CLA	C2B-C3B-CAB-CBB
25	Y	315	CLA	C2B-C3B-CAB-CBB
25	B	616	CLA	C2B-C3B-CAB-CBB
25	A	603	CLA	C2B-C3B-CAB-CBB
25	C	602	CLA	C2B-C3B-CAB-CBB
25	C	603	CLA	C2B-C3B-CAB-CBB
25	5	307	CLA	C2B-C3B-CAB-CBB
25	6	306	CLA	C2B-C3B-CAB-CBB
25	6	307	CLA	C2B-C3B-CAB-CBB
25	n	315	CLA	C2B-C3B-CAB-CBB
25	y	316	CLA	C2B-C3B-CAB-CBB
25	p	315	CLA	C2B-C3B-CAB-CBB
25	b	616	CLA	C2B-C3B-CAB-CBB
25	a	603	CLA	C2B-C3B-CAB-CBB
25	a	605	CLA	C2B-C3B-CAB-CBB
25	c	602	CLA	C2B-C3B-CAB-CBB
25	s	411	CLA	C2B-C3B-CAB-CBB
25	7	315	CLA	C2B-C3B-CAB-CBB
31	C	615	8CT	C04-C03-C10-C11
24	q	304	CHL	C10-C11-C12-C13
33	D	411	LMG	C21-C22-C23-C24
24	S	602	CHL	C2-C1-O2A-CGA
24	G	313	CHL	C2-C1-O2A-CGA
24	N	312	CHL	C2-C1-O2A-CGA
24	g	313	CHL	C2-C1-O2A-CGA
24	y	311	CHL	C2-C1-O2A-CGA
24	p	305	CHL	C2-C1-O2A-CGA
24	q	309	CHL	C2-C1-O2A-CGA
24	7	305	CHL	C2-C1-O2A-CGA
24	7	306	CHL	C2-C1-O2A-CGA
25	p	314	CLA	CBA-CGA-O2A-C1
30	1	318	LHG	C2-C3-O3-P
33	d	401	LMG	C39-C40-C41-C42
37	c	619	DGD	O6E-C1E-O5D-C6D
25	c	603	CLA	C10-C11-C12-C13
24	s	406	CHL	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
30	N	318	LHG	C27-C28-C29-C30
30	A	601	LHG	C9-C10-C11-C12
26	1	302	OIE	O1-C2-C3-C20
26	2	302	OIE	O1-C2-C3-C20
26	3	302	OIE	O1-C2-C3-C20
26	G	302	OIE	O1-C2-C3-C20
26	9	302	OIE	O1-C2-C3-C20
26	N	302	OIE	O1-C2-C3-C20
26	Y	302	OIE	O1-C2-C3-C20
26	8	302	OIE	O1-C2-C3-C20
26	4	302	OIE	O1-C2-C3-C20
26	5	302	OIE	O1-C2-C3-C20
26	6	302	OIE	O1-C2-C3-C20
26	u	302	OIE	O1-C2-C3-C20
26	n	302	OIE	O1-C2-C3-C20
26	y	302	OIE	O1-C2-C3-C20
26	p	302	OIE	O1-C2-C3-C20
26	q	302	OIE	O1-C2-C3-C20
26	7	302	OIE	O1-C2-C3-C20
29	1	301	OUR	O42-C2-C3-C43
29	4	301	OUR	O42-C2-C3-C43
25	B	612	CLA	CBA-CGA-O2A-C1
24	y	306	CHL	CAA-CBA-CGA-O2A
33	D	411	LMG	O7-C10-C11-C12
25	s	413	CLA	C2-C3-C5-C6
30	D	407	LHG	C11-C12-C13-C14
25	1	313	CLA	C2A-CAA-CBA-CGA
24	q	309	CHL	CBD-CGD-O2D-CED
25	c	602	CLA	O1A-CGA-O2A-C1
37	C	620	DGD	O2G-C1B-C2B-C3B
30	7	319	LHG	C26-C27-C28-C29
33	m	101	LMG	C16-C17-C18-C19
30	N	318	LHG	O10-C23-C24-C25
24	n	309	CHL	CAA-CBA-CGA-O1A
24	y	311	CHL	C5-C6-C7-C8
25	C	608	CLA	C12-C13-C15-C16
25	c	608	CLA	C12-C13-C15-C16
32	a	609	SQD	C4-C5-C6-S
30	a	601	LHG	C26-C27-C28-C29
30	D	407	LHG	C33-C34-C35-C36
30	p	319	LHG	C7-C8-C9-C10
25	B	606	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
25	y	315	CLA	C2-C3-C5-C6
24	n	305	CHL	C10-C11-C12-C13
25	B	607	CLA	C13-C15-C16-C17
37	c	618	DGD	C1A-C2A-C3A-C4A
24	G	305	CHL	C11-C12-C13-C14
25	9	314	CLA	C6-C7-C8-C9
25	D	404	CLA	C11-C12-C13-C14
25	b	614	CLA	CAA-CBA-CGA-O2A
33	B	619	LMG	C7-C8-C9-O8
33	C	618	LMG	C7-C8-C9-O8
25	R	609	CLA	C1A-C2A-CAA-CBA
25	R	613	CLA	C4B-C3B-CAB-CBB
25	2	314	CLA	C1A-C2A-CAA-CBA
25	S	604	CLA	C1A-C2A-CAA-CBA
25	G	316	CLA	C4B-C3B-CAB-CBB
25	Y	313	CLA	C1A-C2A-CAA-CBA
25	C	602	CLA	C4B-C3B-CAB-CBB
25	5	307	CLA	C1A-C2A-CAA-CBA
25	n	315	CLA	C4B-C3B-CAB-CBB
25	y	314	CLA	C1A-C2A-CAA-CBA
25	b	610	CLA	C4B-C3B-CAB-CBB
25	b	615	CLA	C4B-C3B-CAB-CBB
25	a	605	CLA	C4B-C3B-CAB-CBB
25	c	602	CLA	C4B-C3B-CAB-CBB
25	d	404	CLA	C1A-C2A-CAA-CBA
25	s	411	CLA	C4B-C3B-CAB-CBB
25	r	314	CLA	C4B-C3B-CAB-CBB
26	3	302	0IE	O29-C20-C3-C4
26	9	302	0IE	O29-C20-C3-C4
26	6	302	0IE	O29-C20-C3-C4
26	u	302	0IE	O29-C20-C3-C4
26	u	303	0IE	O29-C20-C3-C4
26	p	302	0IE	O29-C20-C3-C4
26	p	303	0IE	O29-C20-C3-C4
26	7	302	0IE	O29-C20-C3-C4
25	b	612	CLA	CBA-CGA-O2A-C1
30	9	318	LHG	C23-C24-C25-C26
24	s	402	CHL	C2C-C3C-CAC-CBC
37	C	620	DGD	O6E-C1E-O5D-C6D
25	b	606	CLA	CAA-CBA-CGA-O2A
30	Y	318	LHG	O8-C23-C24-C25
30	d	407	LHG	O7-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
28	R	616	NEX	C31-C32-C33-C34
28	G	304	NEX	C31-C32-C33-C34
28	g	304	NEX	C31-C32-C33-C34
28	r	317	NEX	C31-C32-C33-C34
29	N	301	0UR	C3-C4-C5-C6
29	y	301	0UR	C3-C4-C5-C6
24	s	409	CHL	CBD-CGD-O2D-CED
24	7	306	CHL	CBD-CGD-O2D-CED
24	9	304	CHL	O1A-CGA-O2A-C1
24	Y	310	CHL	C5-C6-C7-C8
30	Y	318	LHG	C28-C29-C30-C31
25	B	614	CLA	CAA-CBA-CGA-O2A
25	C	601	CLA	CAA-CBA-CGA-O2A
25	c	601	CLA	CAA-CBA-CGA-O2A
24	7	306	CHL	O1D-CGD-O2D-CED
30	5	319	LHG	C25-C26-C27-C28
30	y	319	LHG	C9-C10-C11-C12
30	y	319	LHG	C28-C29-C30-C31
25	c	604	CLA	C10-C11-C12-C13
33	i	101	LMG	C32-C33-C34-C35
25	4	313	CLA	C6-C7-C8-C10
30	D	408	LHG	O6-C4-C5-C6
30	D	407	LHG	O7-C7-C8-C9
25	9	306	CLA	C5-C6-C7-C8
25	r	311	CLA	CAA-CBA-CGA-O1A
39	d	406	PL9	C15-C14-C16-C17
24	3	309	CHL	C2-C1-O2A-CGA
24	G	306	CHL	C2-C1-O2A-CGA
24	N	310	CHL	C2-C1-O2A-CGA
24	Y	319	CHL	C2-C1-O2A-CGA
24	g	306	CHL	C2-C1-O2A-CGA
24	n	310	CHL	C2-C1-O2A-CGA
24	q	304	CHL	C2-C1-O2A-CGA
25	b	609	CLA	C2-C1-O2A-CGA
24	G	306	CHL	C6-C7-C8-C10
24	u	306	CHL	C11-C12-C13-C15
24	y	306	CHL	C6-C7-C8-C10
25	B	603	CLA	C12-C13-C15-C16
25	B	605	CLA	C12-C13-C15-C16
25	C	611	CLA	C11-C12-C13-C15
25	g	315	CLA	C11-C10-C8-C7
25	b	605	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	c	604	CLA	C12-C13-C15-C16
35	A	606	PHO	C12-C13-C15-C16
25	C	602	CLA	CBA-CGA-O2A-C1
24	G	306	CHL	C2-C3-C5-C6
25	A	607	CLA	C2-C3-C5-C6
25	a	607	CLA	C2-C3-C5-C6
24	4	305	CHL	CAA-CBA-CGA-O1A
30	A	612	LHG	C29-C30-C31-C32
24	s	406	CHL	CAA-CBA-CGA-O1A
25	B	602	CLA	C5-C6-C7-C8
30	4	318	LHG	C25-C26-C27-C28
25	B	612	CLA	C2A-CAA-CBA-CGA
25	b	612	CLA	C2A-CAA-CBA-CGA
25	c	607	CLA	C15-C16-C17-C18
24	S	605	CHL	CAA-CBA-CGA-O1A
33	D	411	LMG	O9-C10-C11-C12
39	D	406	PL9	C34-C36-C37-C38
24	9	304	CHL	CBA-CGA-O2A-C1
24	Y	304	CHL	C13-C15-C16-C17
25	b	607	CLA	C13-C15-C16-C17
24	N	305	CHL	C11-C12-C13-C14
25	C	616	CLA	C3A-C2A-CAA-CBA
25	c	616	CLA	C3A-C2A-CAA-CBA
32	a	609	SQD	C29-C30-C31-C32
24	G	305	CHL	C2-C3-C5-C6
33	w	201	LMG	C12-C13-C14-C15
37	C	620	DGD	O1B-C1B-C2B-C3B
25	G	317	CLA	O1A-CGA-O2A-C1
25	G	317	CLA	CBA-CGA-O2A-C1
25	c	602	CLA	CBA-CGA-O2A-C1
30	7	319	LHG	C7-C8-C9-C10
24	r	308	CHL	CAA-CBA-CGA-O2A
25	C	605	CLA	CAA-CBA-CGA-O2A
25	c	605	CLA	CAA-CBA-CGA-O2A
24	u	313	CHL	C2C-C3C-CAC-CBC
24	Y	305	CHL	CAA-CBA-CGA-O1A
30	y	319	LHG	C31-C32-C33-C34
30	Y	318	LHG	C31-C32-C33-C34
25	a	604	CLA	C2A-CAA-CBA-CGA
24	N	305	CHL	C11-C10-C8-C9
25	C	607	CLA	C6-C7-C8-C9
25	c	604	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
25	c	607	CLA	C6-C7-C8-C9
30	n	318	LHG	C11-C12-C13-C14
30	a	601	LHG	C14-C15-C16-C17
25	C	610	CLA	C4-C3-C5-C6
25	b	606	CLA	CAA-CBA-CGA-O1A
25	C	610	CLA	C2-C3-C5-C6
24	y	306	CHL	CAA-CBA-CGA-O1A
30	D	407	LHG	O9-C7-C8-C9
25	n	306	CLA	CAA-CBA-CGA-O2A
28	3	318	NEX	C11-C12-C13-C14
28	N	303	NEX	C11-C12-C13-C14
28	6	303	NEX	C11-C12-C13-C14
28	n	303	NEX	C11-C12-C13-C14
28	s	401	NEX	C11-C12-C13-C14
28	r	301	NEX	C11-C12-C13-C14
30	Y	318	LHG	O10-C23-C24-C25
30	d	407	LHG	O9-C7-C8-C9
32	a	609	SQD	O49-C7-C8-C9
25	C	607	CLA	C15-C16-C17-C18
25	C	610	CLA	C8-C10-C11-C12
37	c	619	DGD	C5D-C6D-O5D-C1E
25	B	612	CLA	O1A-CGA-O2A-C1
25	r	310	CLA	O1A-CGA-O2A-C1
30	y	319	LHG	O10-C23-C24-C25
24	R	607	CHL	CAA-CBA-CGA-O2A
33	B	619	LMG	O8-C28-C29-C30
30	Y	318	LHG	C11-C12-C13-C14
25	B	606	CLA	CAA-CBA-CGA-O1A
30	D	408	LHG	C7-C8-C9-C10
24	2	309	CHL	CAD-CBD-CGD-O2D
24	5	309	CHL	CAD-CBD-CGD-O2D
24	q	316	CHL	CAD-CBD-CGD-O2D
25	Y	313	CLA	CAD-CBD-CGD-O2D
25	C	609	CLA	CAD-CBD-CGD-O2D
25	y	314	CLA	CAD-CBD-CGD-O2D
25	p	308	CLA	CAD-CBD-CGD-O2D
25	c	609	CLA	CAD-CBD-CGD-O2D
25	d	404	CLA	CAD-CBD-CGD-O2D
25	s	410	CLA	CAD-CBD-CGD-O2D
25	7	308	CLA	CAD-CBD-CGD-O2D
30	2	319	LHG	C25-C26-C27-C28
24	R	606	CHL	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
24	3	305	CHL	CAA-CBA-CGA-O2A
25	R	603	CLA	CAA-CBA-CGA-O2A
25	B	614	CLA	CAA-CBA-CGA-O1A
25	C	601	CLA	CAA-CBA-CGA-O1A
25	C	602	CLA	C10-C11-C12-C13
30	5	319	LHG	O6-C4-C5-C6
24	g	313	CHL	C2C-C3C-CAC-CBC
37	c	618	DGD	C5A-C6A-C7A-C8A
24	S	602	CHL	CAA-CBA-CGA-O2A
24	S	601	CHL	C1A-C2A-CAA-CBA
24	9	309	CHL	C1A-C2A-CAA-CBA
24	7	305	CHL	C1A-C2A-CAA-CBA
30	d	407	LHG	C9-C10-C11-C12
24	g	310	CHL	C2A-CAA-CBA-CGA
24	q	309	CHL	C3-C5-C6-C7
24	s	407	CHL	CAA-CBA-CGA-O2A
25	c	601	CLA	CAA-CBA-CGA-O1A
33	B	619	LMG	O10-C28-C29-C30
24	3	309	CHL	CAA-CBA-CGA-O2A
24	G	310	CHL	CAA-CBA-CGA-O2A
24	6	309	CHL	CAA-CBA-CGA-O2A
24	p	306	CHL	CAA-CBA-CGA-O2A
24	7	306	CHL	CAA-CBA-CGA-O2A
25	a	607	CLA	C11-C12-C13-C15
24	4	308	CHL	CBD-CGD-O2D-CED
24	g	306	CHL	CAA-CBA-CGA-O2A
25	b	612	CLA	O1A-CGA-O2A-C1
24	S	606	CHL	CAA-CBA-CGA-O1A
24	S	606	CHL	CAA-CBA-CGA-O2A
25	b	614	CLA	CAA-CBA-CGA-O1A
24	r	307	CHL	C2-C1-O2A-CGA

There are no ring outliers.

435 monomers are involved in 1342 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	9	315	CLA	4	0
25	q	312	CLA	2	0
37	c	618	DGD	4	0
39	d	406	PL9	2	0
25	N	307	CLA	4	0
25	7	314	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	b	615	CLA	7	0
24	n	312	CHL	2	0
24	G	318	CHL	1	0
30	4	318	LHG	3	0
25	2	314	CLA	1	0
24	5	309	CHL	1	0
25	6	307	CLA	2	0
25	u	315	CLA	4	0
30	D	407	LHG	7	0
25	C	611	CLA	5	0
24	n	309	CHL	1	0
24	s	402	CHL	3	0
24	7	310	CHL	14	0
28	g	304	NEX	15	0
25	C	605	CLA	1	0
25	c	609	CLA	3	0
24	N	312	CHL	4	0
32	D	409	SQD	1	0
24	8	308	CHL	3	0
25	B	615	CLA	8	0
24	Y	311	CHL	4	0
25	b	612	CLA	8	0
24	g	312	CHL	3	0
25	3	306	CLA	1	0
26	9	302	0IE	2	0
24	N	308	CHL	3	0
23	f	201	HEM	3	0
25	A	603	CLA	5	0
24	y	311	CHL	1	0
25	y	316	CLA	3	0
27	r	316	XAT	8	0
24	N	309	CHL	1	0
24	y	313	CHL	6	0
24	9	308	CHL	1	0
30	1	318	LHG	3	0
25	C	616	CLA	2	0
25	7	308	CLA	15	0
25	c	601	CLA	3	0
25	a	603	CLA	5	0
24	9	317	CHL	1	0
24	4	304	CHL	2	0
33	m	101	LMG	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	p	315	CLA	2	0
24	y	306	CHL	2	0
24	8	304	CHL	6	0
24	R	605	CHL	3	0
24	9	305	CHL	6	0
25	2	315	CLA	1	0
24	s	408	CHL	1	0
25	p	308	CLA	12	0
24	q	304	CHL	4	0
24	3	317	CHL	2	0
24	S	606	CHL	2	0
24	3	308	CHL	2	0
25	a	605	CLA	1	0
28	4	303	NEX	21	0
24	q	308	CHL	3	0
25	b	603	CLA	4	0
25	b	604	CLA	10	0
24	r	306	CHL	3	0
25	R	603	CLA	1	0
24	4	305	CHL	1	0
26	y	303	0IE	1	0
25	1	315	CLA	2	0
33	B	619	LMG	5	0
25	5	316	CLA	2	0
29	8	301	0UR	1	0
24	g	309	CHL	2	0
25	y	307	CLA	2	0
30	y	319	LHG	2	0
25	g	315	CLA	3	0
24	2	312	CHL	2	0
37	c	619	DGD	4	0
25	a	604	CLA	6	0
24	4	311	CHL	5	0
25	4	314	CLA	1	0
24	7	313	CHL	3	0
25	d	405	CLA	6	0
25	B	611	CLA	5	0
24	n	305	CHL	5	0
25	7	317	CLA	4	0
25	p	307	CLA	2	0
26	9	303	0IE	1	0
25	1	316	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	s	410	CLA	4	0
32	b	618	SQD	5	0
24	8	307	CHL	1	0
25	8	313	CLA	1	0
28	r	301	NEX	6	0
30	n	318	LHG	4	0
26	7	302	0IE	2	0
25	C	609	CLA	2	0
28	5	304	NEX	10	0
25	g	317	CLA	1	0
25	B	614	CLA	3	0
25	C	601	CLA	4	0
26	3	302	0IE	2	0
37	C	619	DGD	5	0
24	q	303	CHL	3	0
25	q	305	CLA	2	0
29	4	301	0UR	1	0
24	q	307	CHL	1	0
25	b	606	CLA	9	0
25	p	314	CLA	2	0
24	Y	304	CHL	5	0
29	p	301	0UR	1	0
24	S	602	CHL	5	0
24	y	305	CHL	8	0
28	R	616	NEX	6	0
25	Y	316	CLA	2	0
24	5	305	CHL	6	0
25	b	605	CLA	4	0
26	u	302	0IE	1	0
24	9	310	CHL	2	0
24	9	312	CHL	3	0
24	9	304	CHL	6	0
25	G	307	CLA	2	0
25	B	613	CLA	5	0
25	4	316	CLA	2	0
25	c	610	CLA	4	0
30	9	318	LHG	6	0
25	1	314	CLA	1	0
25	d	404	CLA	4	0
28	u	304	NEX	9	0
25	D	405	CLA	5	0
24	5	312	CHL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	c	604	CLA	3	0
25	G	315	CLA	3	0
24	g	318	CHL	2	0
24	u	312	CHL	4	0
35	a	606	PHO	4	0
28	2	304	NEX	9	0
25	b	616	CLA	3	0
25	S	609	CLA	4	0
25	c	611	CLA	3	0
25	C	607	CLA	2	0
25	s	412	CLA	3	0
24	1	317	CHL	2	0
30	A	612	LHG	2	0
25	n	315	CLA	2	0
31	V	401	8CT	1	0
25	Y	314	CLA	1	0
24	G	310	CHL	3	0
23	E	201	HEM	2	0
24	3	311	CHL	6	0
24	8	310	CHL	6	0
25	r	304	CLA	1	0
30	7	319	LHG	3	0
25	5	308	CLA	5	0
30	D	408	LHG	6	0
25	9	316	CLA	4	0
24	q	310	CHL	6	0
24	8	309	CHL	5	0
24	g	313	CHL	6	0
33	D	401	LMG	3	0
29	q	301	0UR	1	0
29	G	301	0UR	1	0
24	n	311	CHL	4	0
24	4	308	CHL	1	0
25	b	610	CLA	3	0
24	y	310	CHL	1	0
25	Y	315	CLA	1	0
25	8	311	CLA	2	0
25	R	612	CLA	7	0
24	p	312	CHL	5	0
25	n	306	CLA	2	0
25	9	307	CLA	4	0
28	r	317	NEX	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	8	303	CHL	3	0
25	5	314	CLA	2	0
25	y	314	CLA	2	0
25	p	316	CLA	2	0
25	3	307	CLA	2	0
24	1	312	CHL	4	0
33	C	618	LMG	6	0
24	4	317	CHL	2	0
24	s	406	CHL	2	0
24	p	309	CHL	3	0
25	9	314	CLA	3	0
24	1	304	CHL	3	0
24	S	601	CHL	1	0
24	7	311	CHL	2	0
24	9	311	CHL	4	0
24	1	305	CHL	2	0
24	g	305	CHL	4	0
24	s	409	CHL	2	0
25	r	314	CLA	1	0
25	n	307	CLA	4	0
25	n	316	CLA	4	0
25	c	605	CLA	2	0
24	s	414	CHL	2	0
25	g	308	CLA	6	0
24	7	306	CHL	4	0
29	u	301	0UR	1	0
25	S	612	CLA	1	0
25	B	605	CLA	6	0
24	G	313	CHL	10	0
24	Y	312	CHL	7	0
25	b	607	CLA	3	0
25	s	411	CLA	3	0
29	9	301	0UR	1	0
24	G	305	CHL	4	0
25	b	613	CLA	5	0
25	q	313	CLA	1	0
25	q	306	CLA	5	0
24	p	311	CHL	2	0
24	S	605	CHL	2	0
28	p	304	NEX	27	0
25	2	308	CLA	5	0
28	N	303	NEX	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	2	313	CHL	3	0
24	Y	309	CHL	2	0
25	2	317	CLA	2	0
28	3	318	NEX	22	0
25	B	612	CLA	8	0
30	d	407	LHG	7	0
25	a	607	CLA	2	0
25	S	611	CLA	1	0
24	4	310	CHL	3	0
25	1	307	CLA	9	0
25	5	317	CLA	2	0
24	G	309	CHL	2	0
24	6	308	CHL	1	0
29	2	301	OUR	1	0
24	n	308	CHL	3	0
24	R	608	CHL	2	0
30	a	601	LHG	5	0
30	g	319	LHG	2	0
25	y	315	CLA	3	0
24	5	313	CHL	4	0
25	A	607	CLA	2	0
24	u	313	CHL	1	0
25	9	313	CLA	2	0
35	A	606	PHO	4	0
28	G	304	NEX	32	0
24	6	305	CHL	1	0
25	G	308	CLA	16	0
25	B	604	CLA	12	0
25	b	602	CLA	8	0
26	6	302	OIE	2	0
24	u	306	CHL	4	0
35	d	403	PHO	6	0
24	y	312	CHL	4	0
28	n	303	NEX	7	0
25	4	307	CLA	16	0
24	r	308	CHL	3	0
25	A	604	CLA	5	0
25	C	610	CLA	4	0
28	s	401	NEX	21	0
25	g	314	CLA	2	0
31	v	401	8CT	1	0
25	9	306	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	G	306	CHL	6	0
24	r	307	CHL	4	0
24	6	310	CHL	2	0
30	d	408	LHG	4	0
26	R	614	OIE	1	0
25	R	604	CLA	7	0
24	6	317	CHL	2	0
24	r	309	CHL	2	0
25	c	607	CLA	3	0
30	a	612	LHG	2	0
24	1	311	CHL	7	0
24	g	310	CHL	6	0
24	1	310	CHL	3	0
24	r	302	CHL	3	0
32	a	609	SQD	4	0
25	C	612	CLA	2	0
32	d	409	SQD	1	0
25	7	307	CLA	2	0
25	D	404	CLA	5	0
25	c	612	CLA	4	0
25	b	601	CLA	1	0
35	D	403	PHO	6	0
25	4	313	CLA	2	0
25	G	317	CLA	2	0
24	7	305	CHL	6	0
25	B	606	CLA	8	0
25	B	603	CLA	3	0
24	p	313	CHL	3	0
24	G	311	CHL	4	0
25	q	314	CLA	1	0
24	g	311	CHL	3	0
25	8	305	CLA	2	0
33	W	201	LMG	2	0
24	3	309	CHL	19	0
27	R	615	XAT	16	0
25	R	610	CLA	1	0
24	q	311	CHL	6	0
25	B	616	CLA	3	0
24	3	310	CHL	1	0
26	p	302	OIE	2	0
24	Y	308	CHL	3	0
24	y	318	CHL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	u	310	CHL	4	0
25	B	608	CLA	6	0
24	p	305	CHL	7	0
24	s	403	CHL	3	0
26	r	315	0IE	1	0
25	g	316	CLA	2	0
39	D	406	PL9	2	0
24	n	304	CHL	4	0
24	u	305	CHL	5	0
24	Y	305	CHL	2	0
24	g	306	CHL	3	0
24	y	309	CHL	2	0
26	2	303	0IE	1	0
24	N	305	CHL	2	0
30	5	319	LHG	2	0
24	n	310	CHL	2	0
25	c	603	CLA	3	0
25	8	306	CLA	4	0
28	6	303	NEX	21	0
25	4	315	CLA	2	0
30	2	319	LHG	2	0
24	2	305	CHL	5	0
25	u	308	CLA	1	0
29	n	301	0UR	1	0
25	N	313	CLA	1	0
33	D	411	LMG	5	0
24	S	607	CHL	2	0
25	N	306	CLA	1	0
25	u	317	CLA	5	0
37	C	620	DGD	2	0
24	Y	317	CHL	2	0
25	r	311	CLA	1	0
25	G	316	CLA	3	0
24	6	311	CHL	9	0
25	1	313	CLA	2	0
25	u	307	CLA	2	0
28	S	617	NEX	24	0
25	C	604	CLA	4	0
24	6	304	CHL	3	0
25	b	614	CLA	3	0
29	6	301	0UR	1	0
30	N	318	LHG	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	Y	306	CLA	2	0
25	r	310	CLA	1	0
26	Y	302	0IE	1	0
33	d	401	LMG	3	0
25	7	315	CLA	2	0
25	C	602	CLA	2	0
24	2	309	CHL	1	0
28	y	304	NEX	4	0
25	c	616	CLA	2	0
25	R	609	CLA	1	0
25	3	315	CLA	1	0
25	N	315	CLA	3	0
30	G	319	LHG	1	0
24	N	304	CHL	5	0
25	Y	313	CLA	2	0
24	1	309	CHL	5	0
24	5	311	CHL	1	0
25	8	312	CLA	1	0
25	N	316	CLA	4	0
31	C	613	8CT	1	0
25	G	314	CLA	2	0
24	R	607	CHL	3	0
24	R	602	CHL	4	0
24	s	407	CHL	2	0
24	p	310	CHL	12	0
25	6	316	CLA	3	0
30	A	601	LHG	6	0
25	b	609	CLA	4	0
25	B	602	CLA	7	0
25	p	317	CLA	5	0
28	1	303	NEX	22	0
24	R	601	CHL	3	0
24	S	613	CHL	2	0
30	p	319	LHG	3	0
25	B	607	CLA	4	0
29	Y	301	0UR	1	0
24	4	309	CHL	7	0
33	i	101	LMG	3	0
24	u	311	CHL	1	0
25	B	610	CLA	2	0
25	c	608	CLA	3	0
25	u	314	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	B	618	SQD	4	0
25	g	307	CLA	2	0
25	q	315	CLA	1	0
25	b	611	CLA	3	0
24	7	312	CHL	6	0
24	Y	310	CHL	1	0
26	y	302	0IE	1	0
25	6	306	CLA	1	0
24	3	304	CHL	1	0
24	7	318	CHL	2	0
24	u	318	CHL	1	0
25	r	313	CLA	5	0
25	7	316	CLA	3	0
25	u	316	CLA	4	0
25	c	602	CLA	2	0
25	s	413	CLA	1	0
24	N	311	CHL	4	0
24	r	303	CHL	5	0
25	3	316	CLA	2	0
24	p	318	CHL	3	0
25	B	609	CLA	3	0
25	2	316	CLA	1	0
31	c	613	8CT	1	0
24	p	306	CHL	4	0
25	y	308	CLA	1	0
24	3	305	CHL	1	0
25	B	601	CLA	1	0
25	r	305	CLA	9	0
25	S	616	CLA	4	0
25	A	605	CLA	1	0
25	y	317	CLA	2	0
33	w	201	LMG	6	0
25	C	603	CLA	5	0
24	6	309	CHL	20	0
24	u	309	CHL	2	0
24	N	310	CHL	2	0
25	8	314	CLA	2	0
25	6	315	CLA	1	0
28	7	304	NEX	32	0
24	R	606	CHL	2	0
24	S	608	CHL	1	0
32	A	609	SQD	2	0

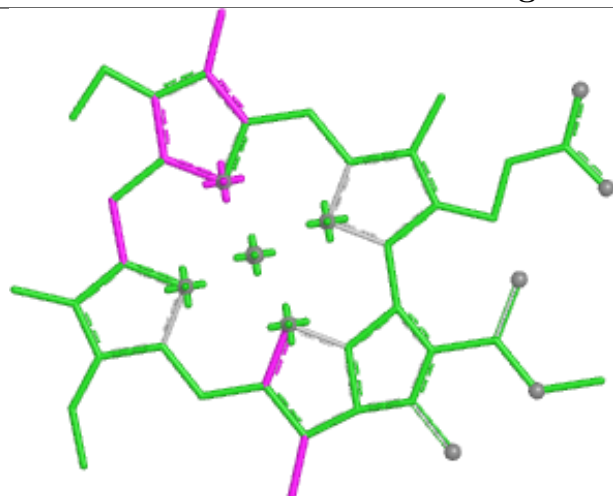
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	5	315	CLA	1	0
24	G	312	CHL	12	0
28	9	319	NEX	6	0
24	4	312	CHL	3	0
25	s	417	CLA	4	0
33	d	411	LMG	5	0
24	9	309	CHL	3	0
29	y	301	OUR	1	0
25	b	608	CLA	5	0

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.

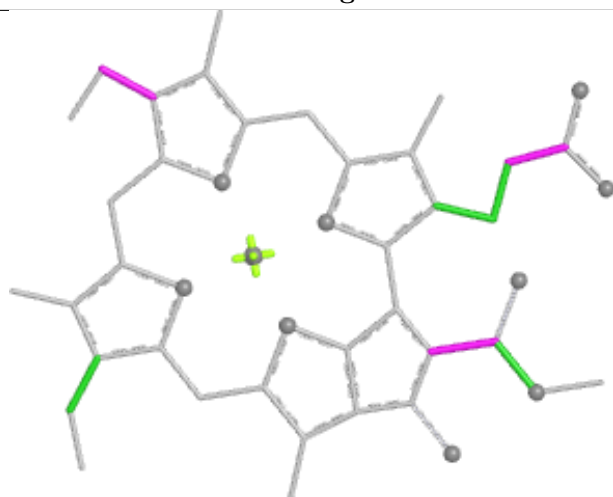
Ligand CLA 9 315



Bond lengths



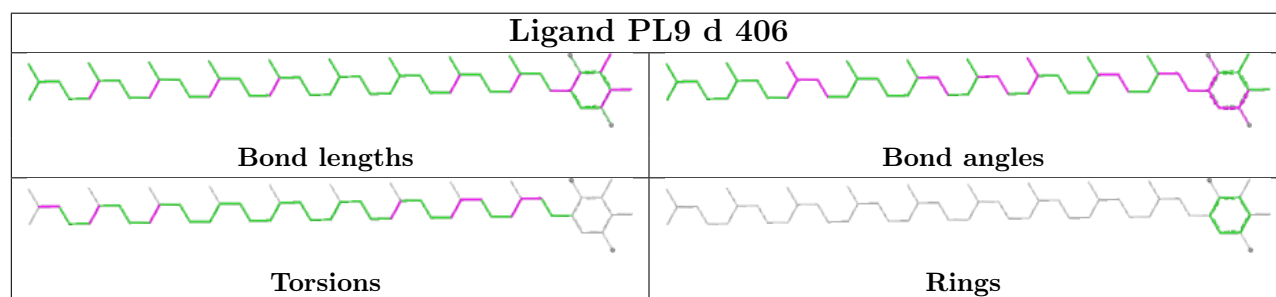
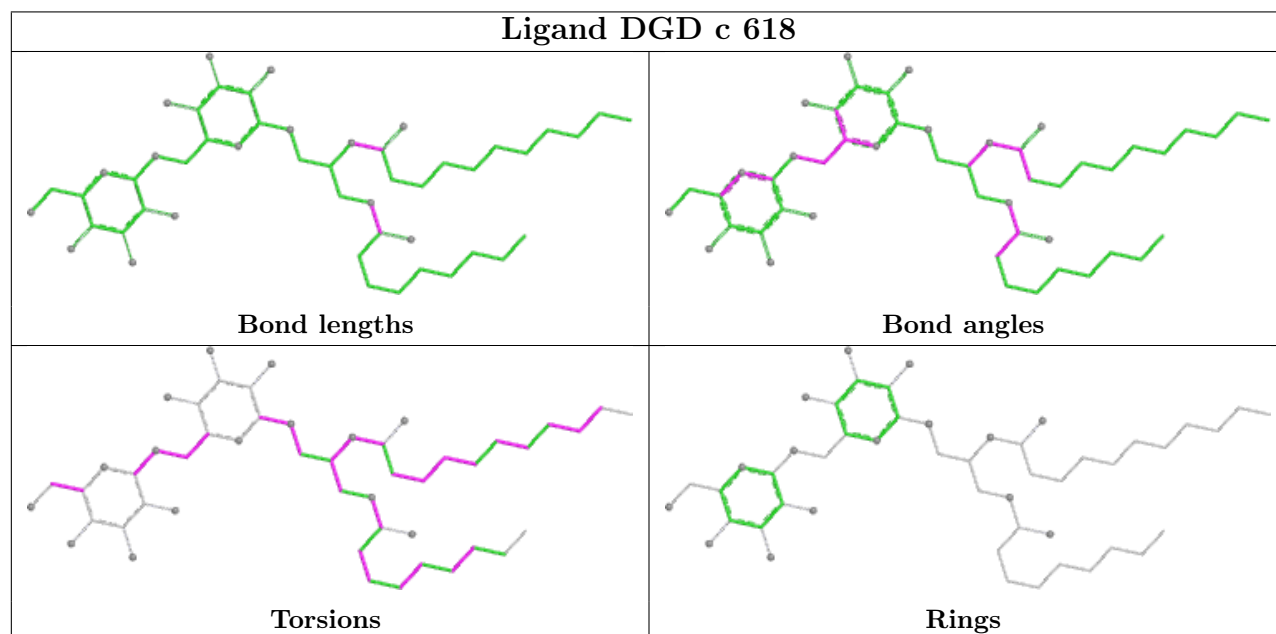
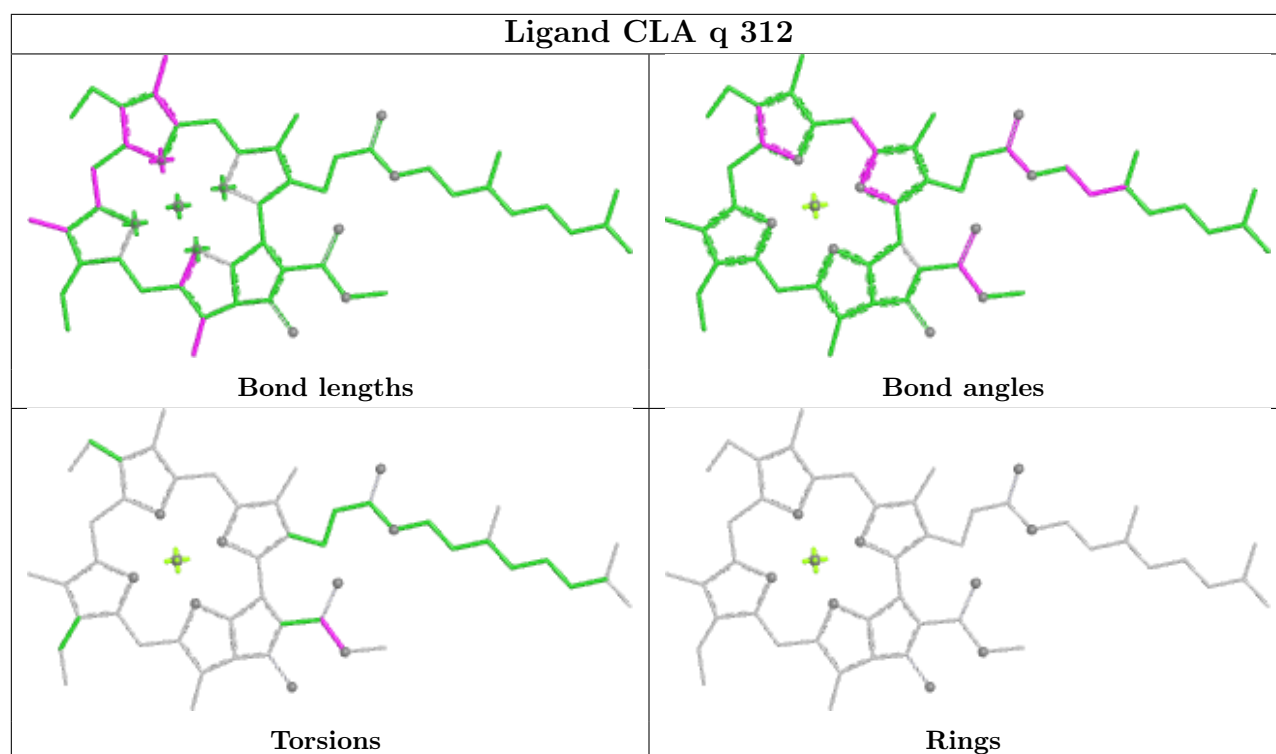
Bond angles

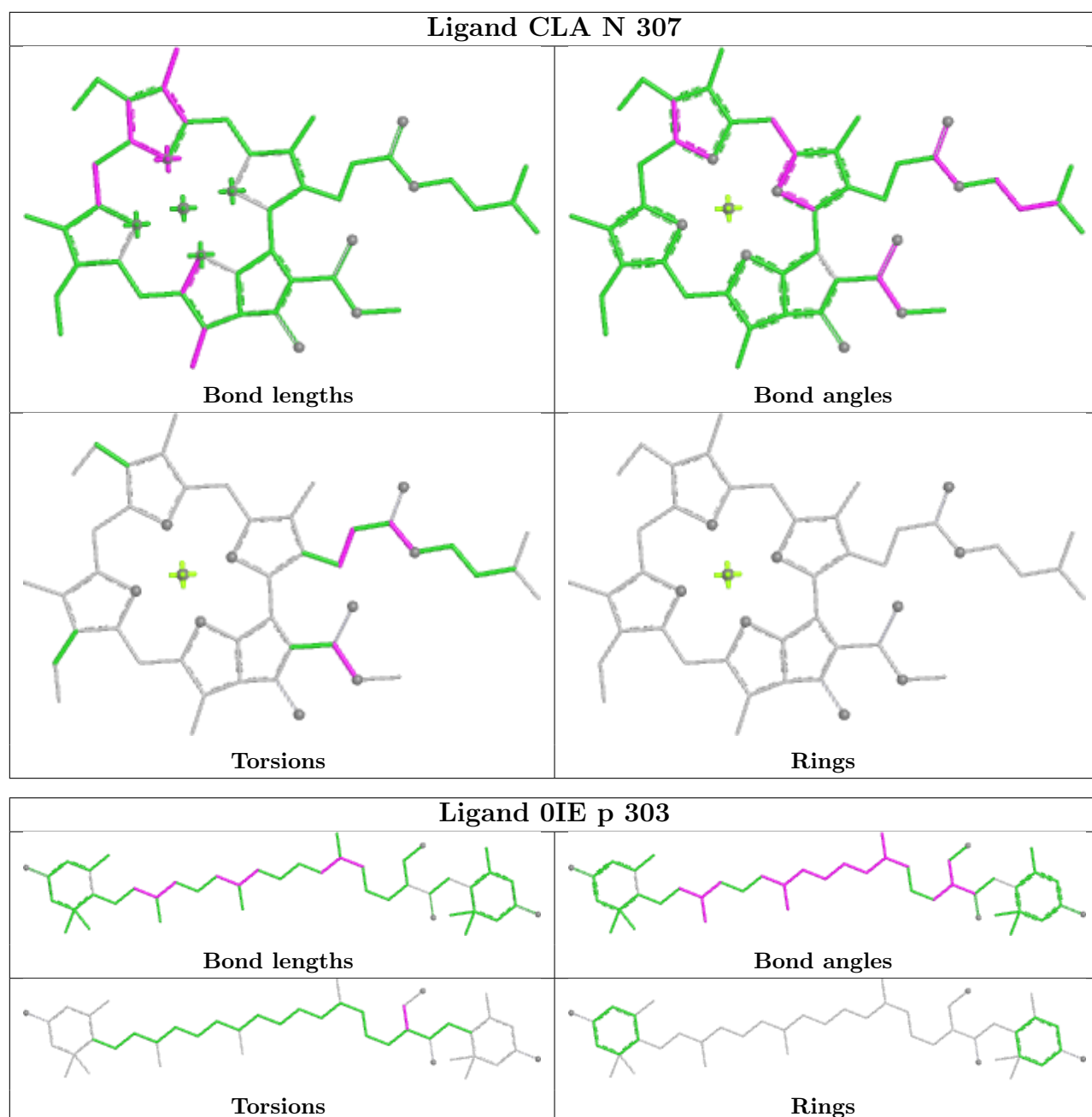


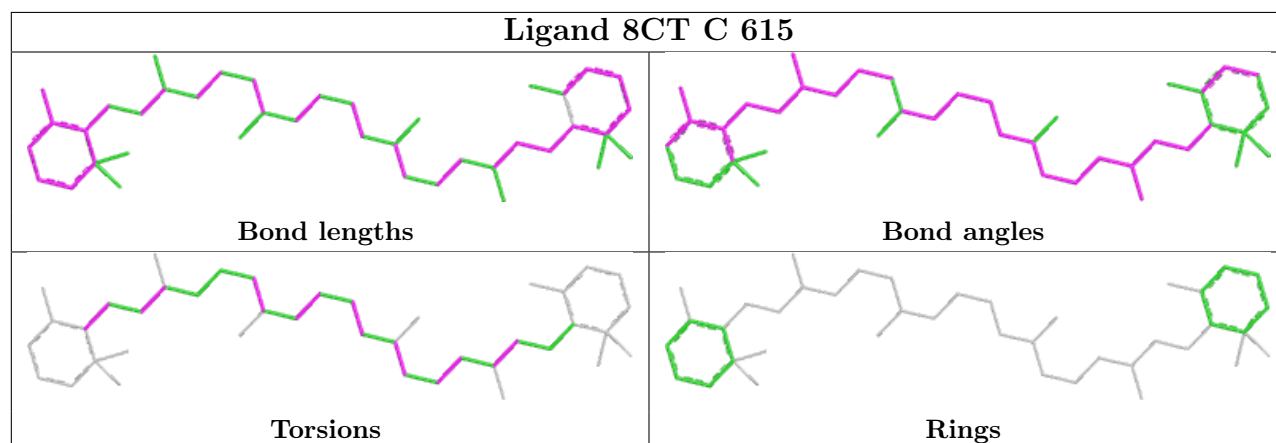
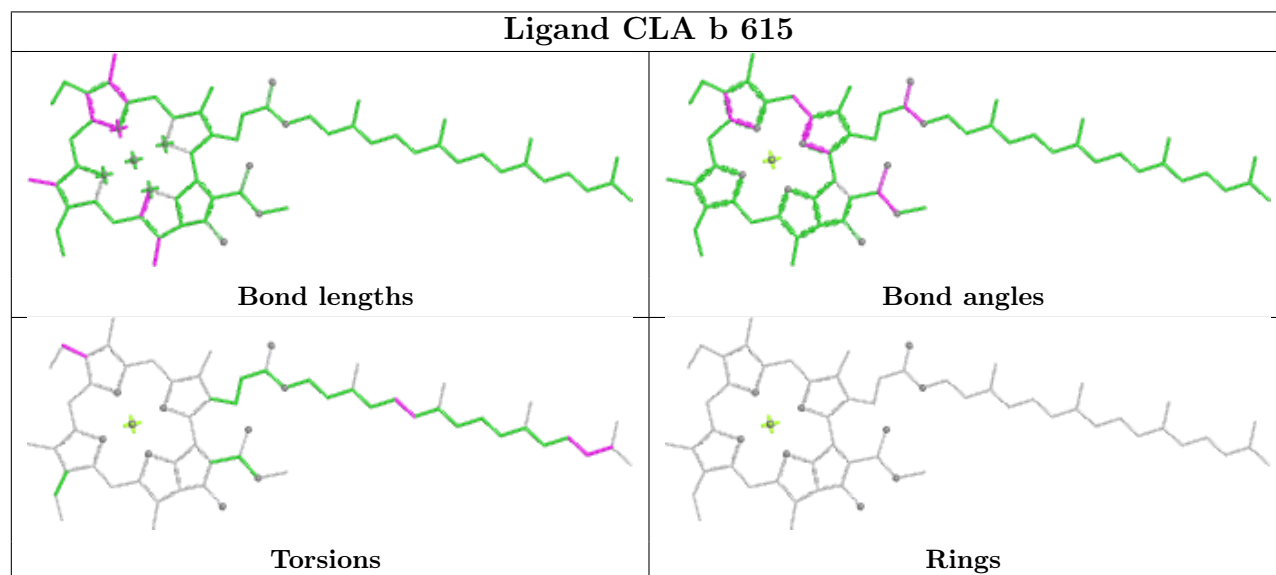
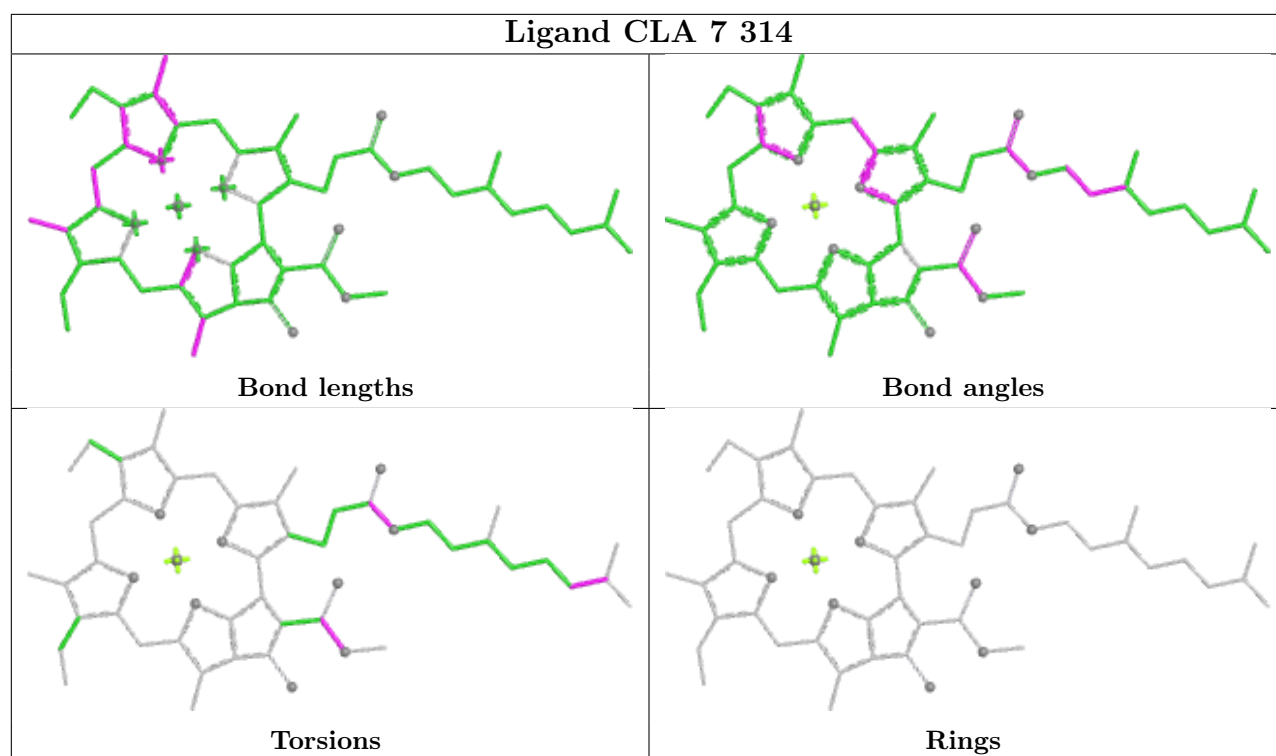
Torsions

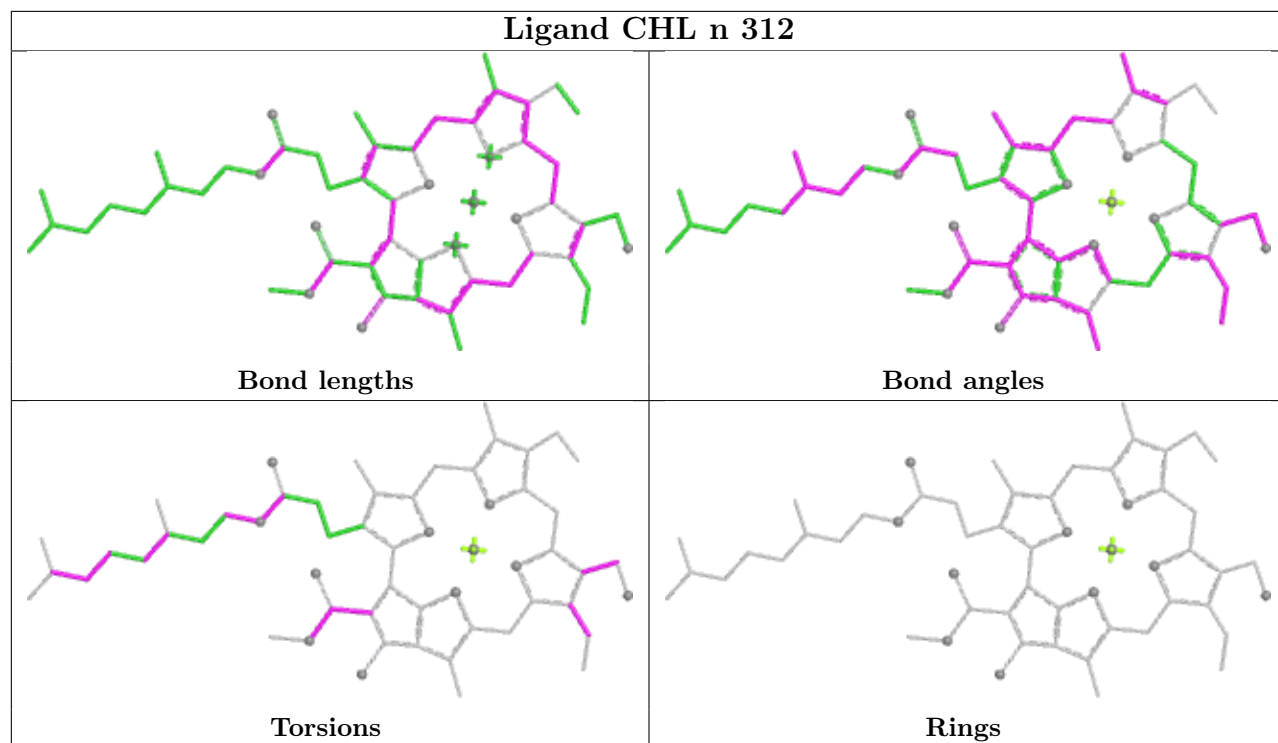


Rings

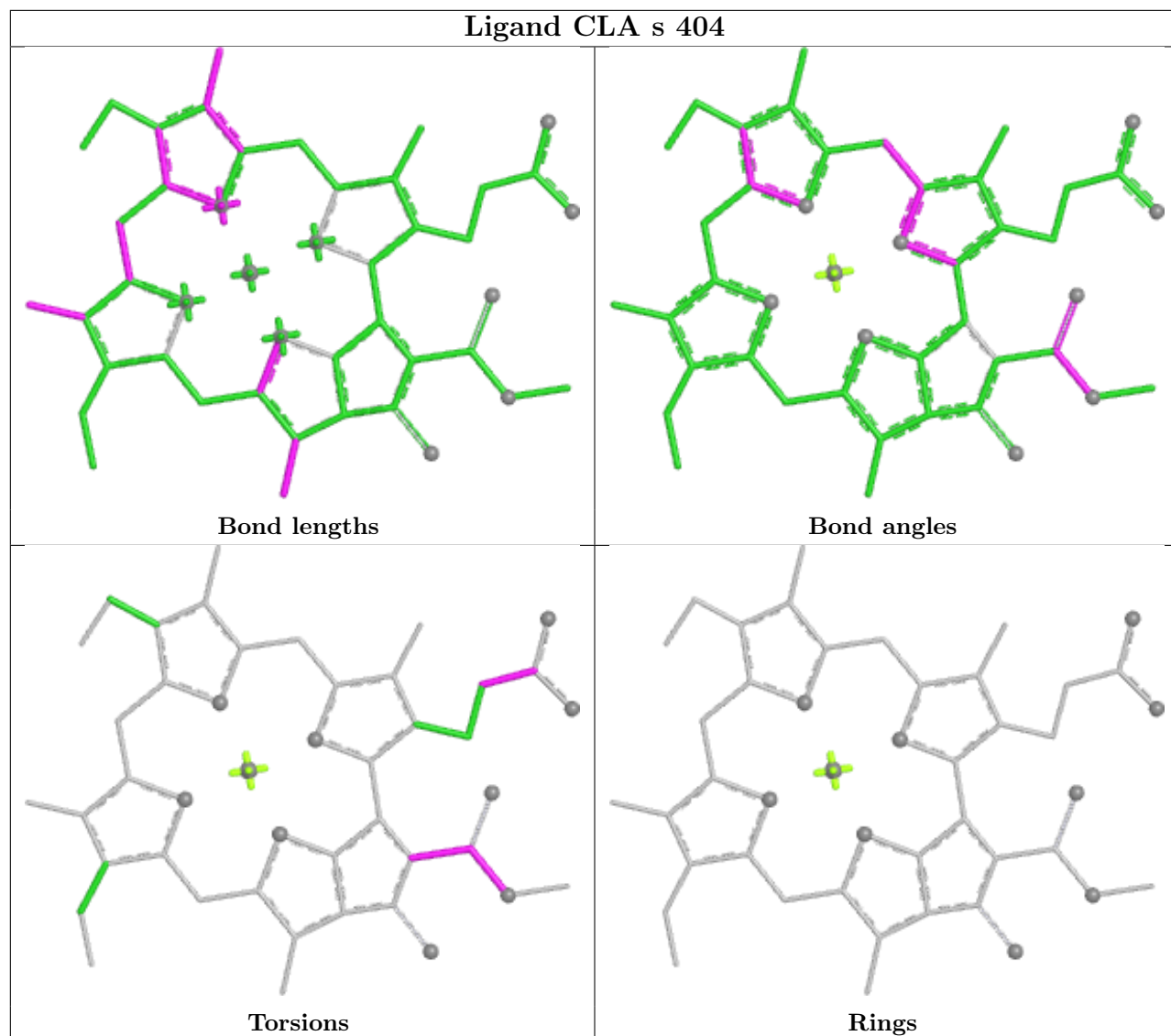




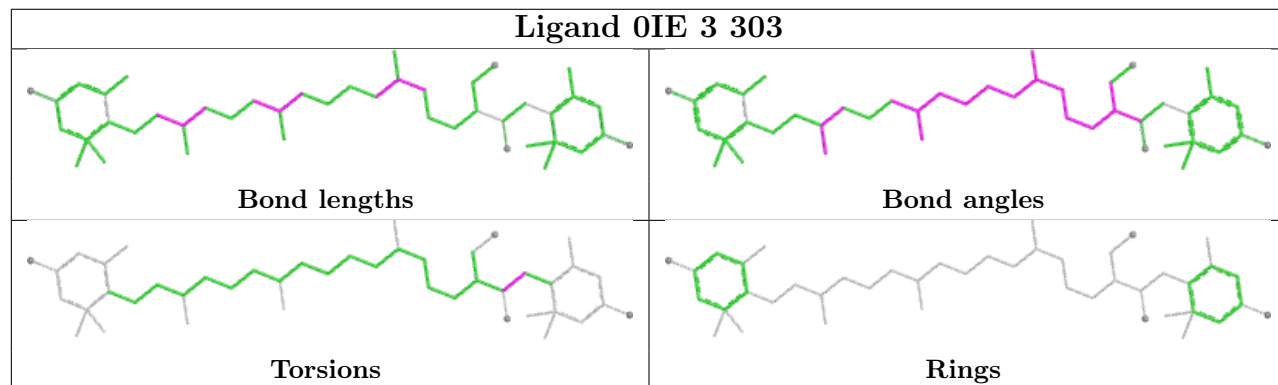


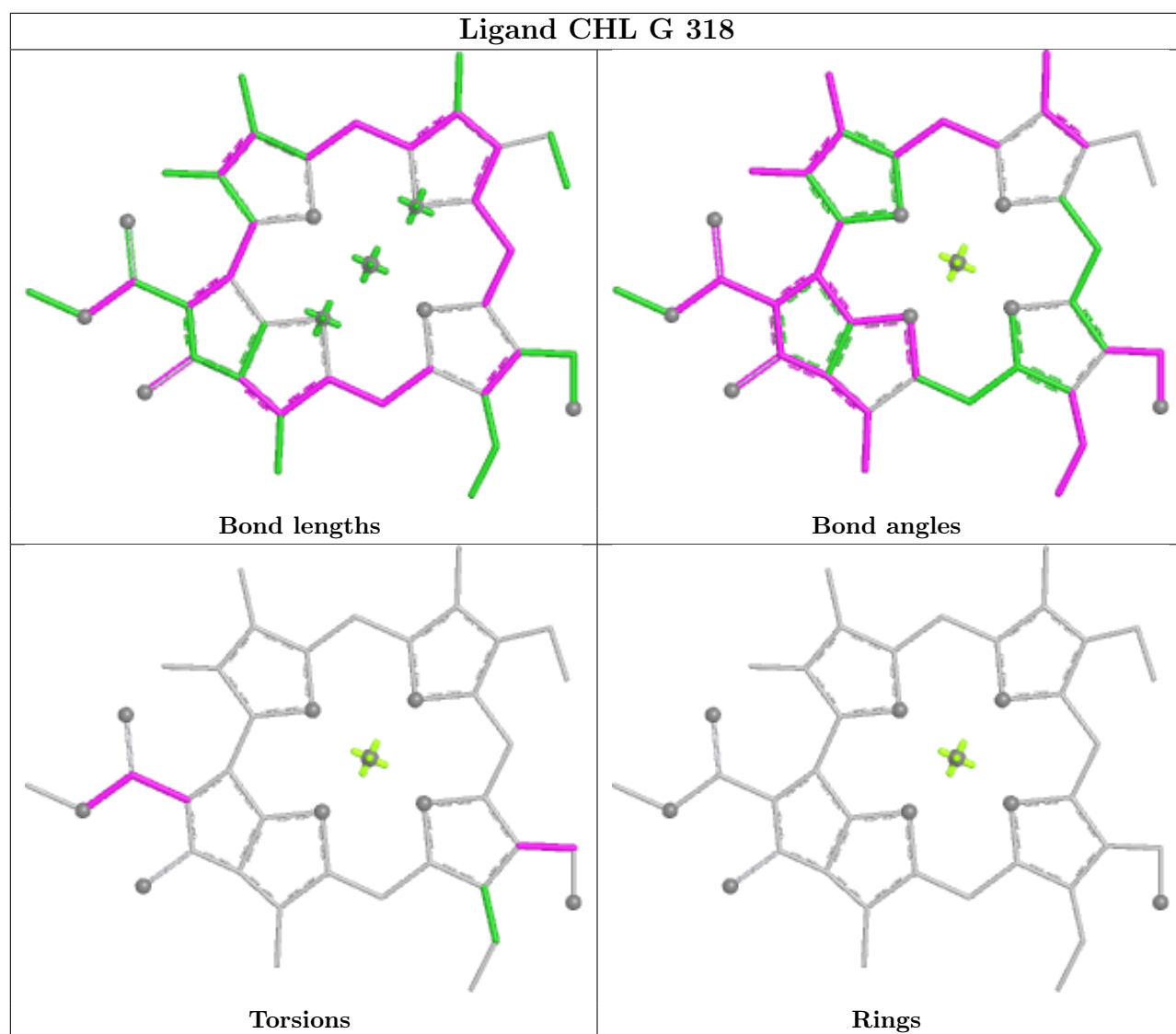


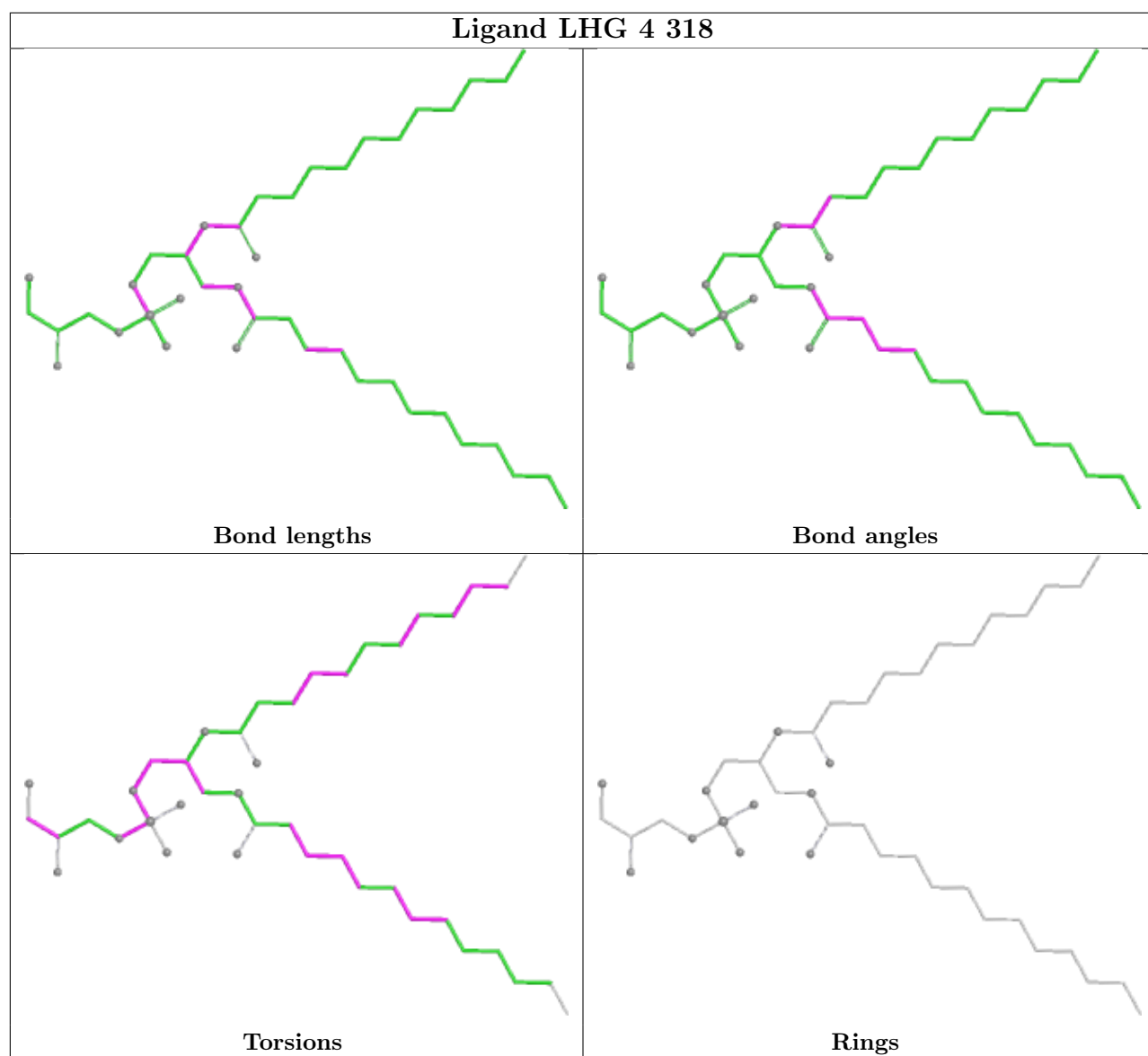
Ligand CLA s 404

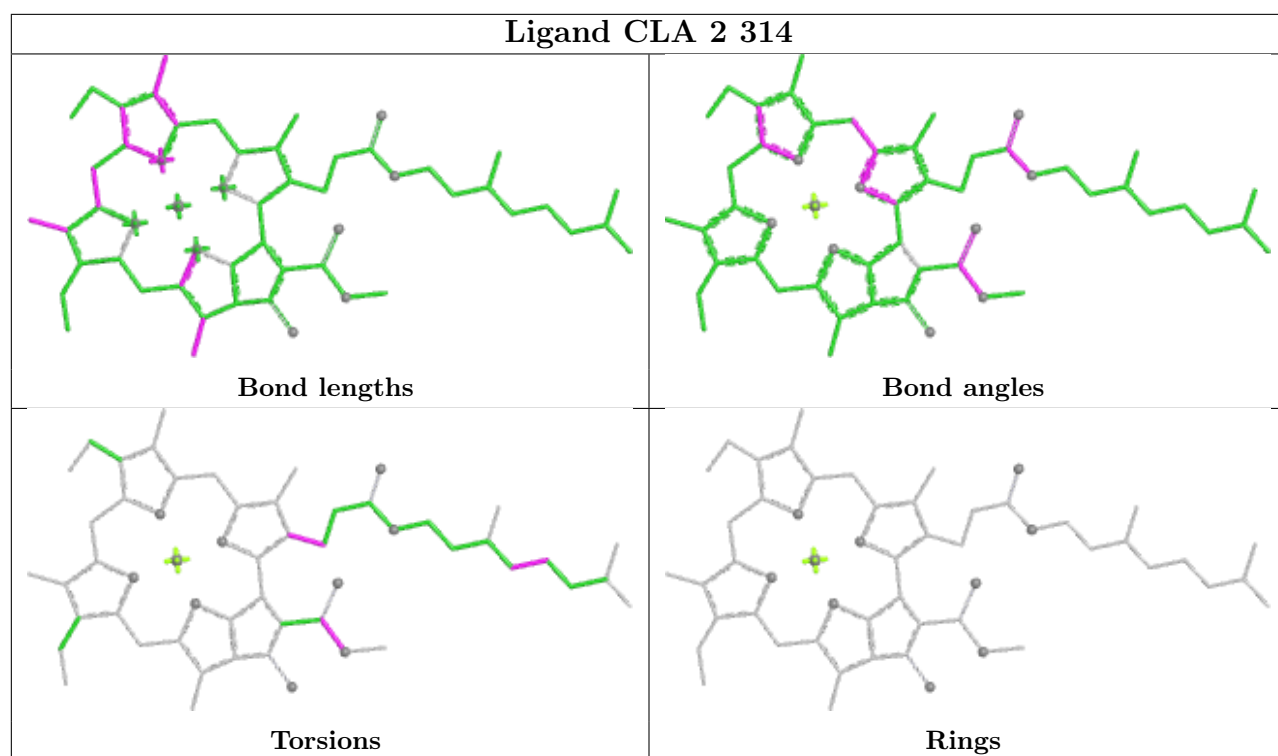


Ligand OIE 3 303

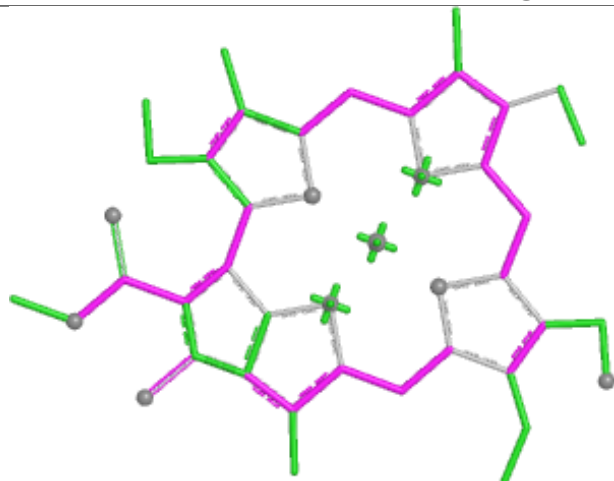




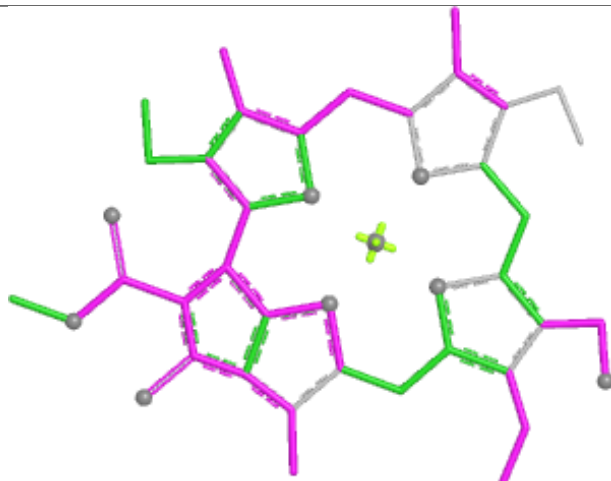




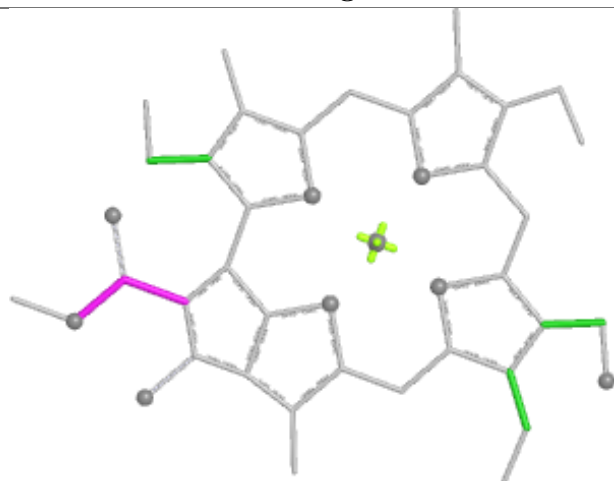
Ligand CHL 5 309



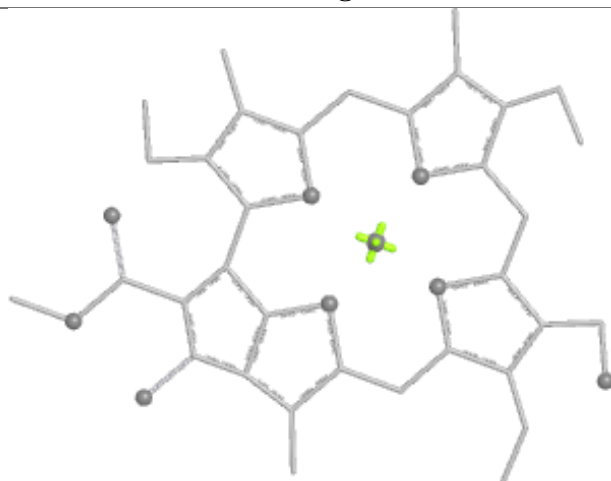
Bond lengths



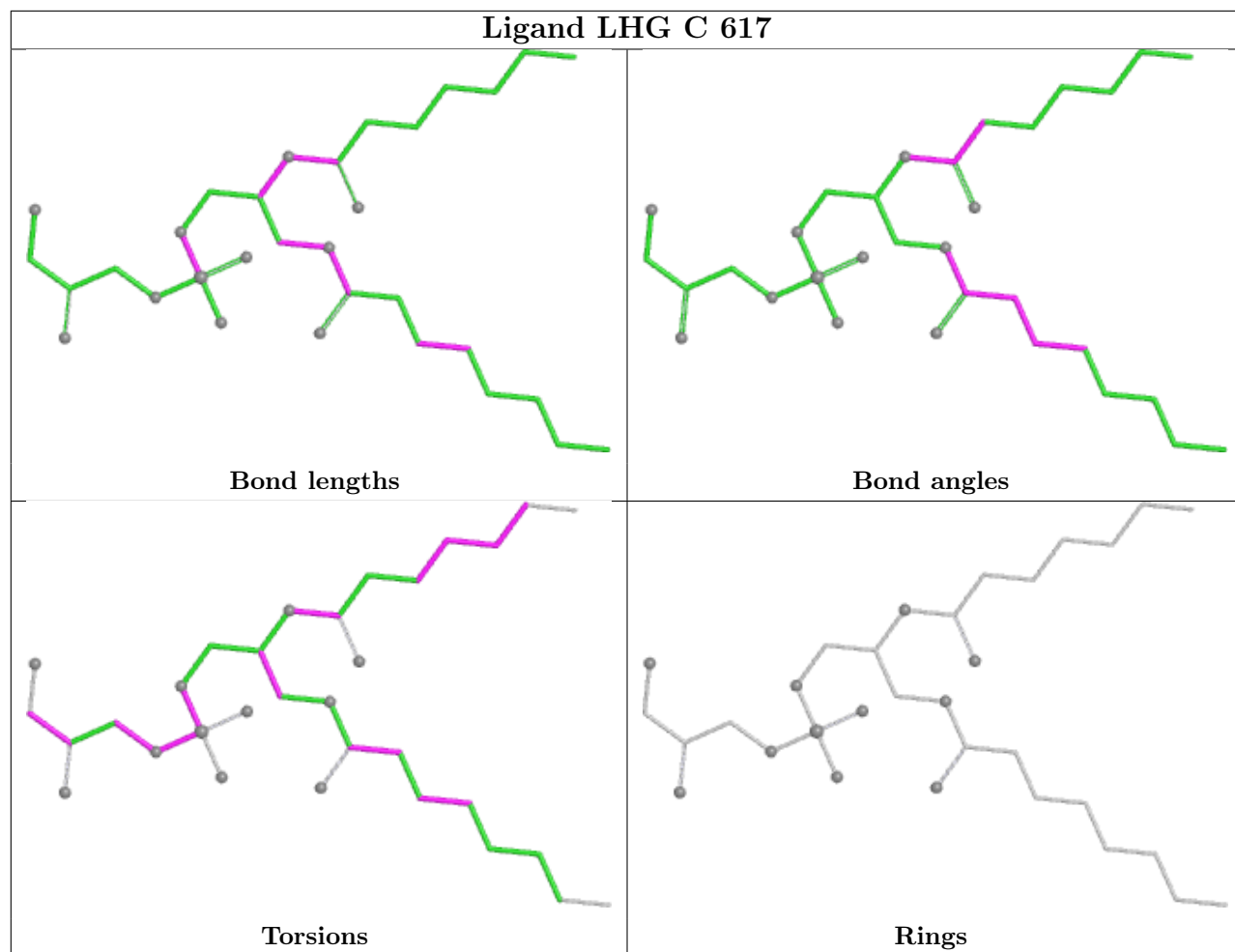
Bond angles



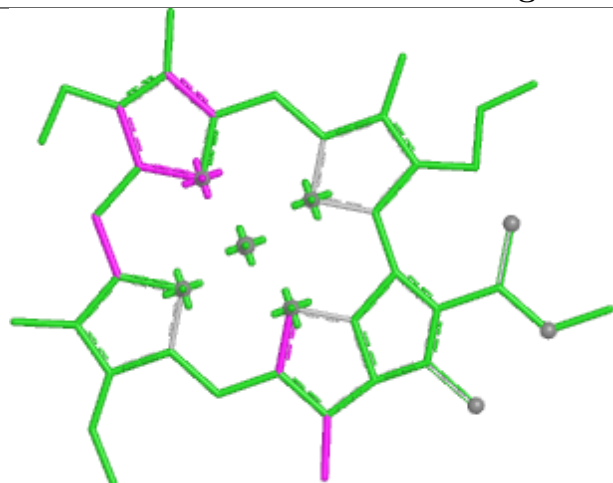
Torsions



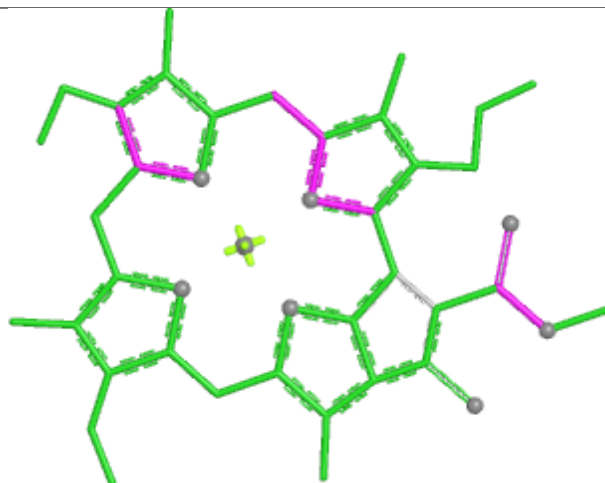
Rings



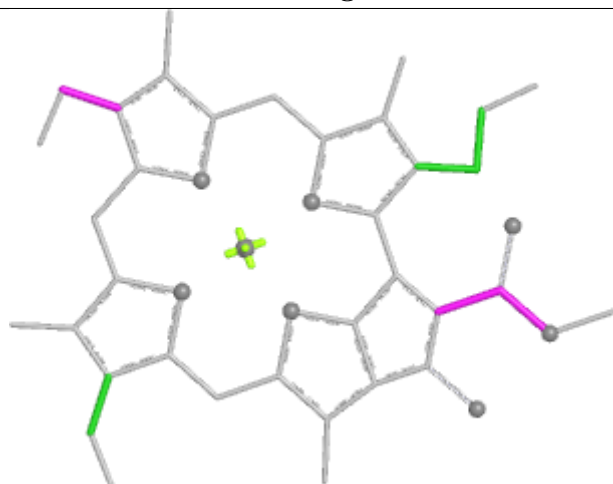
Ligand CLA 6 307



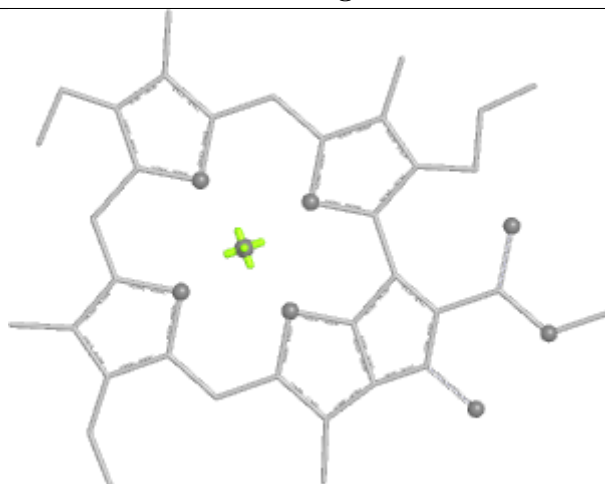
Bond lengths



Bond angles

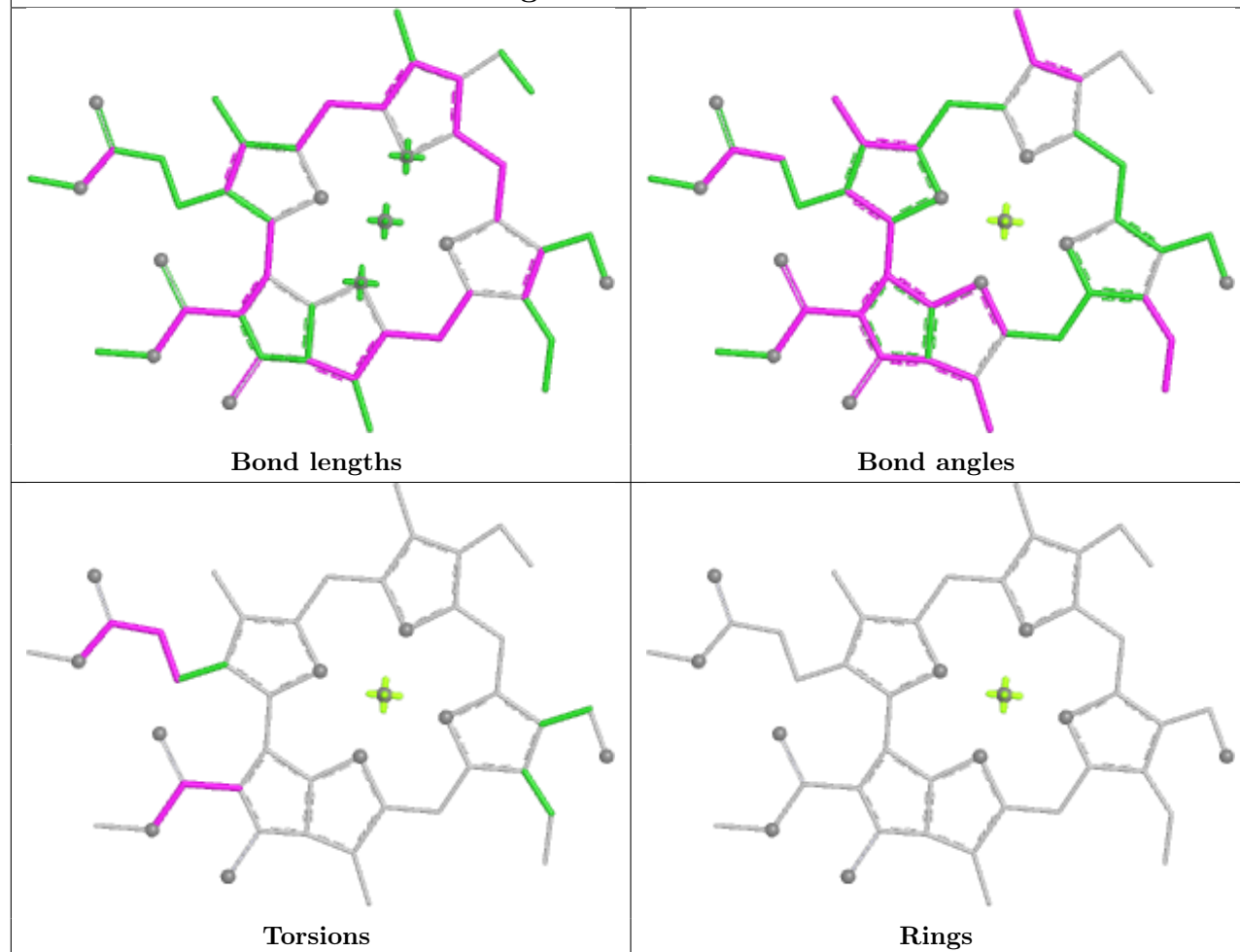


Torsions

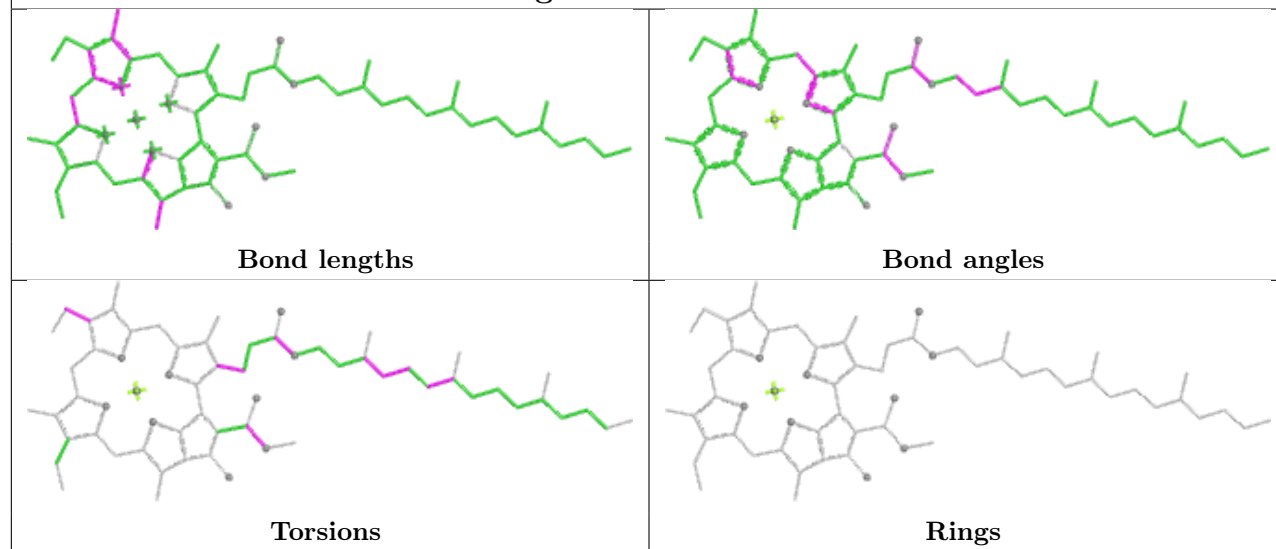


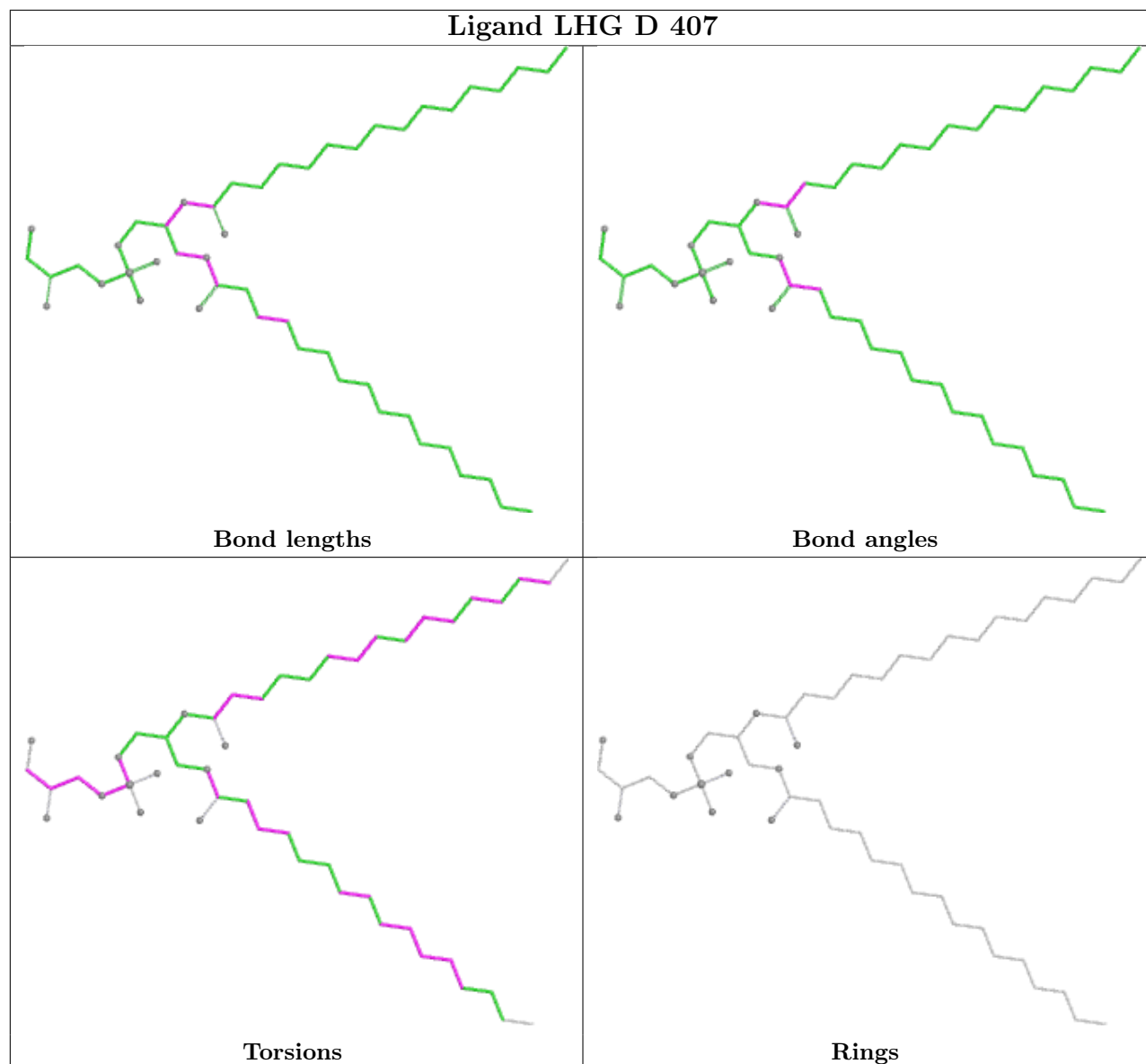
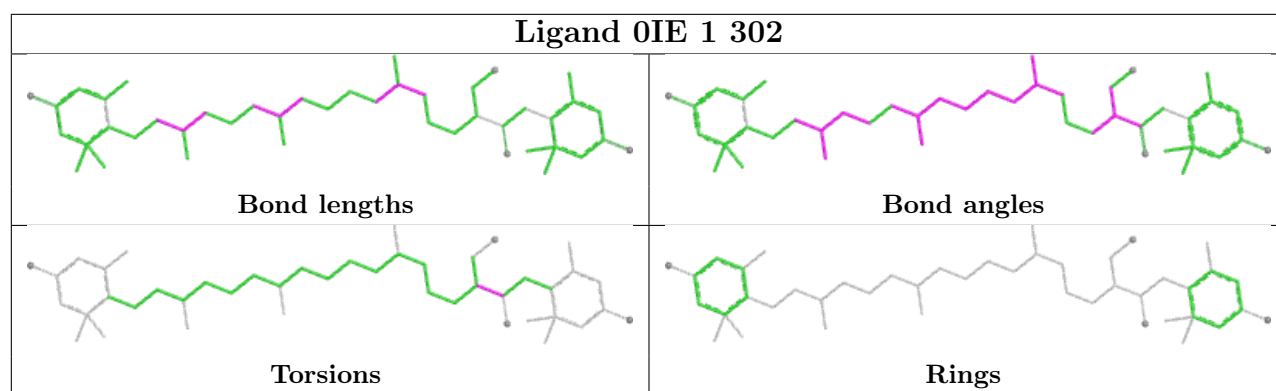
Rings

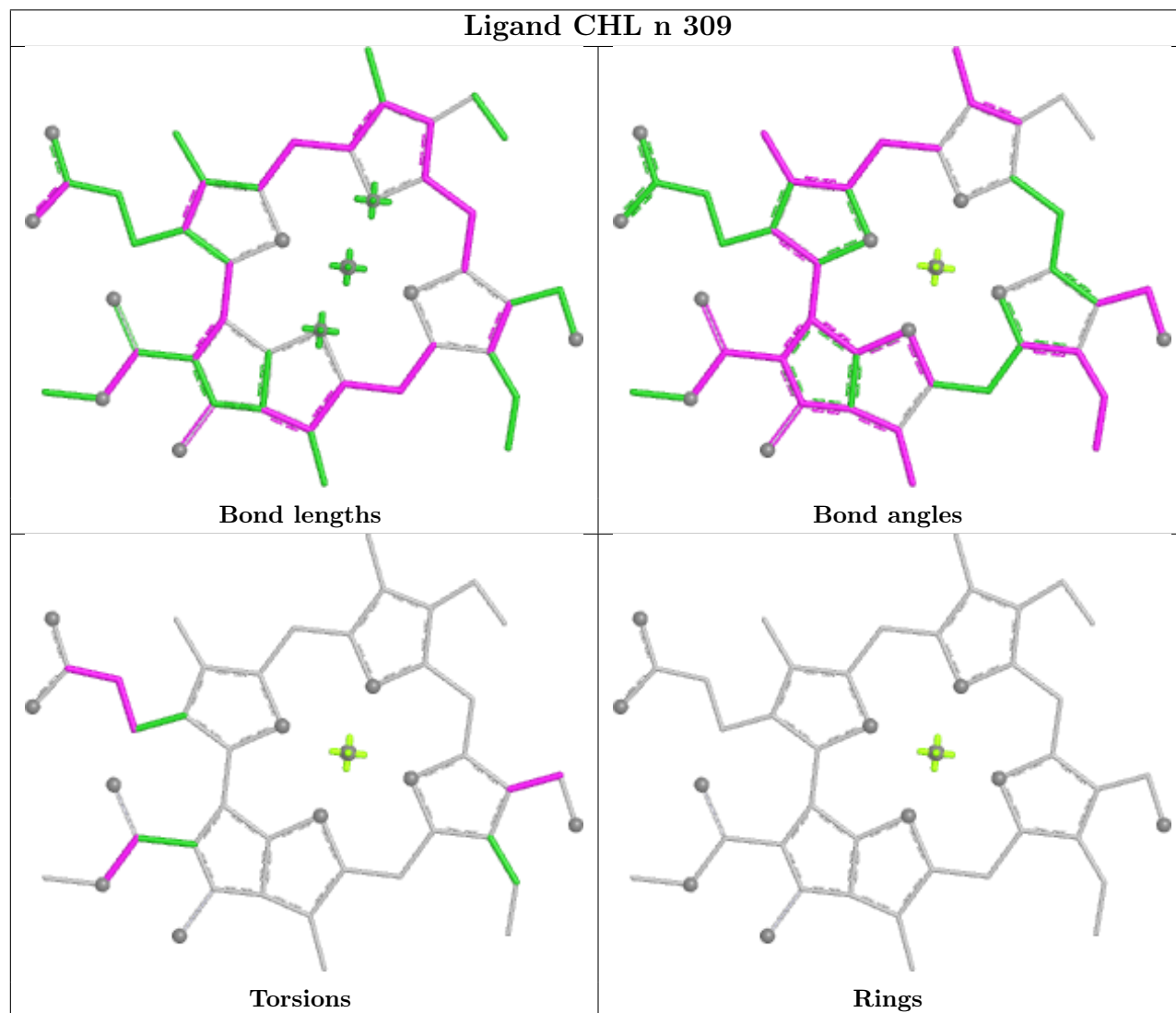
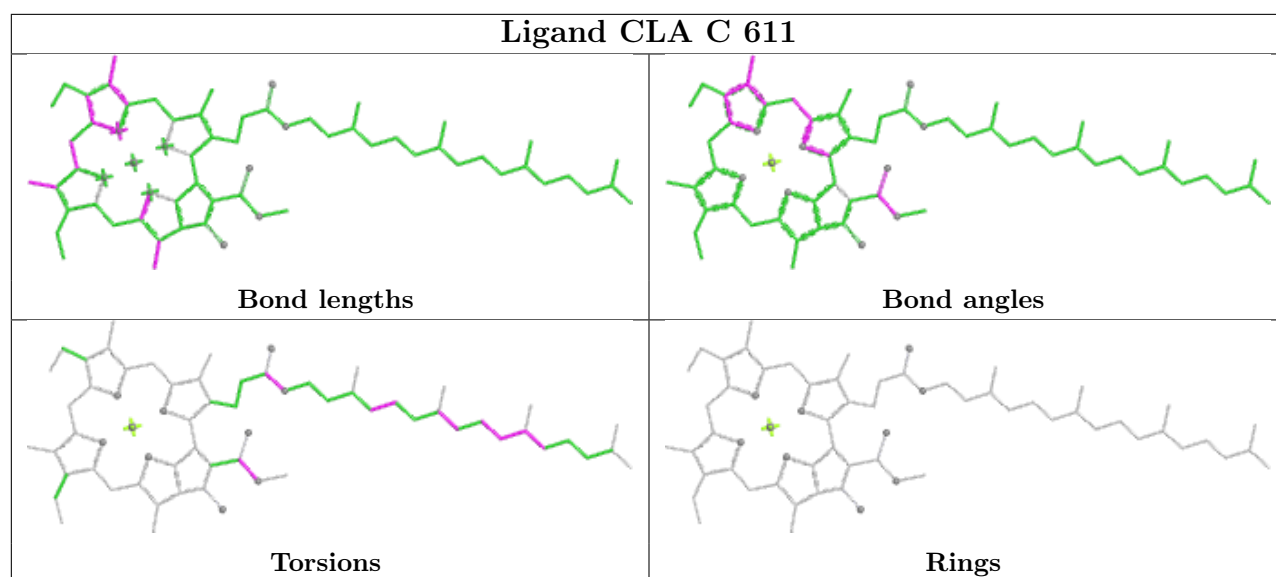
Ligand CHL 2 311



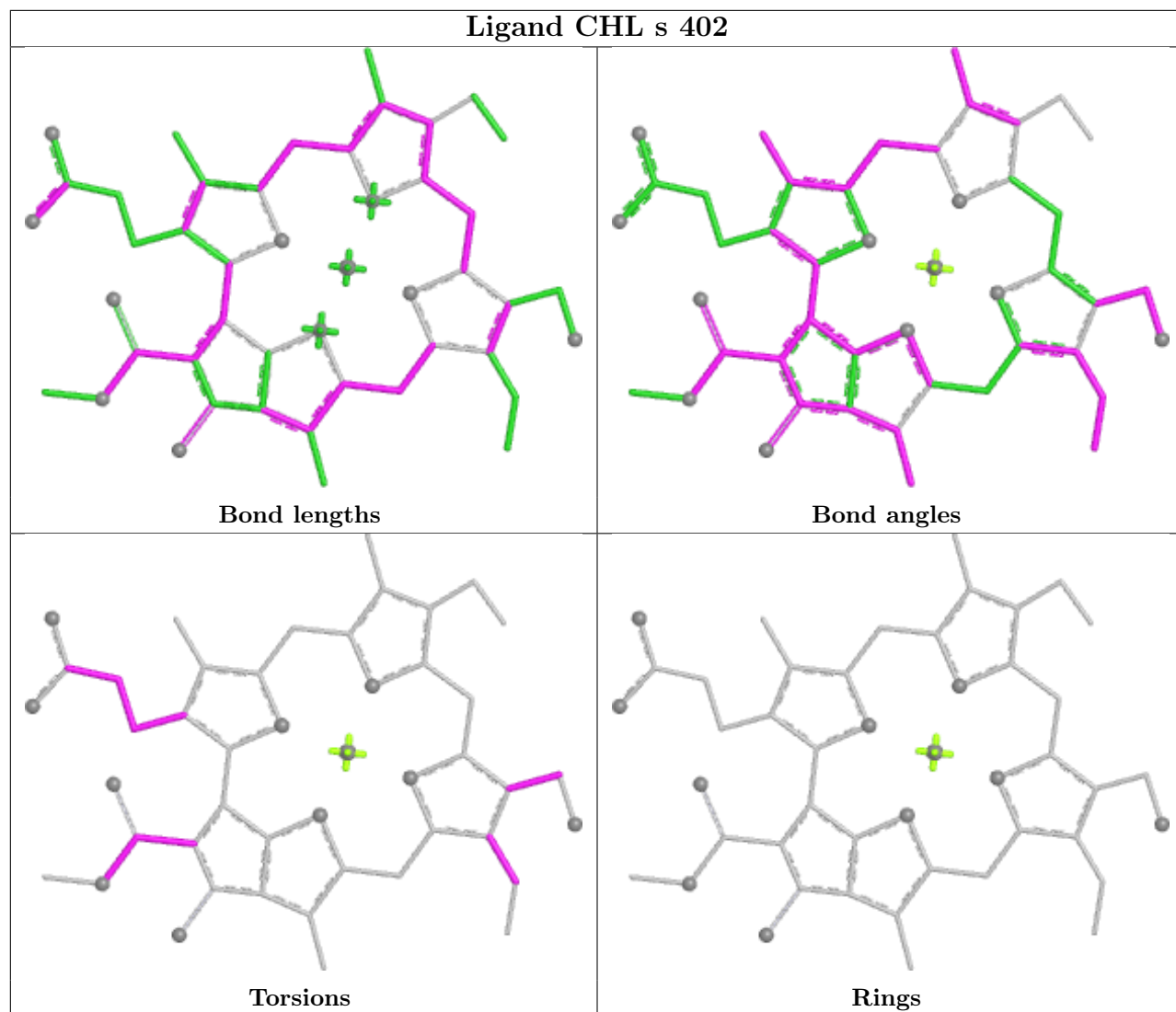
Ligand CLA u 315



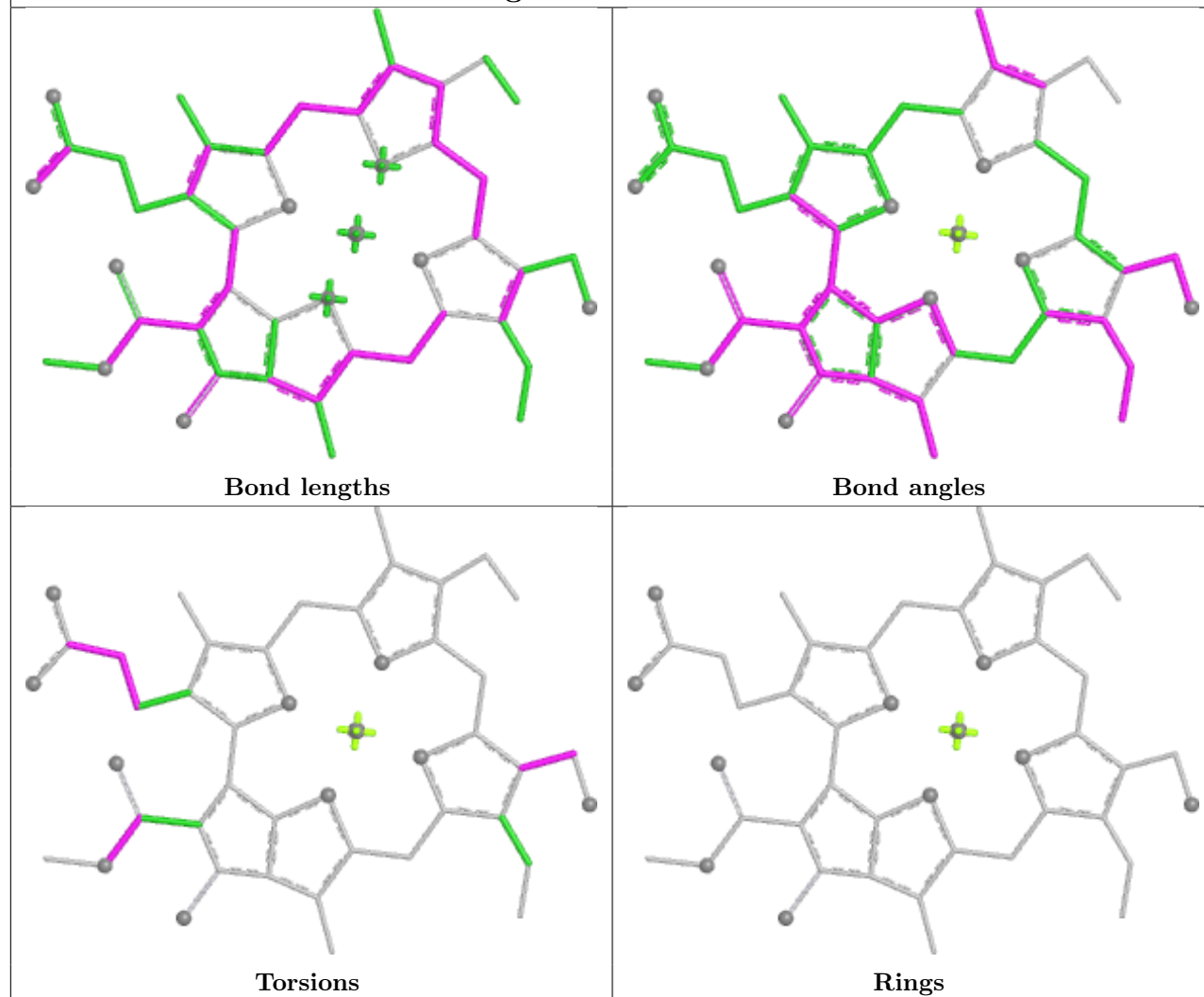




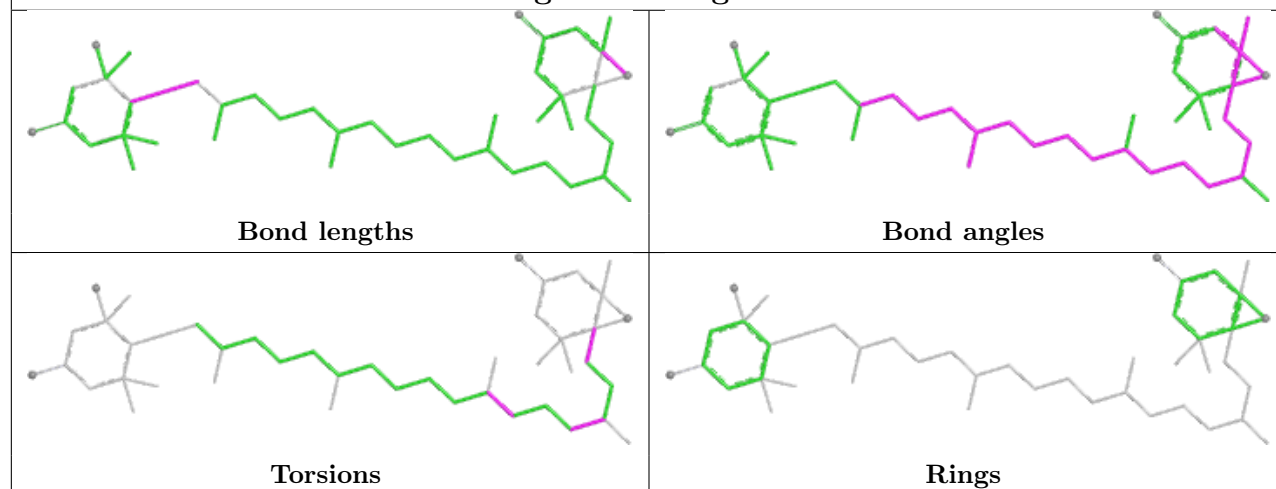
Ligand CHL s 402

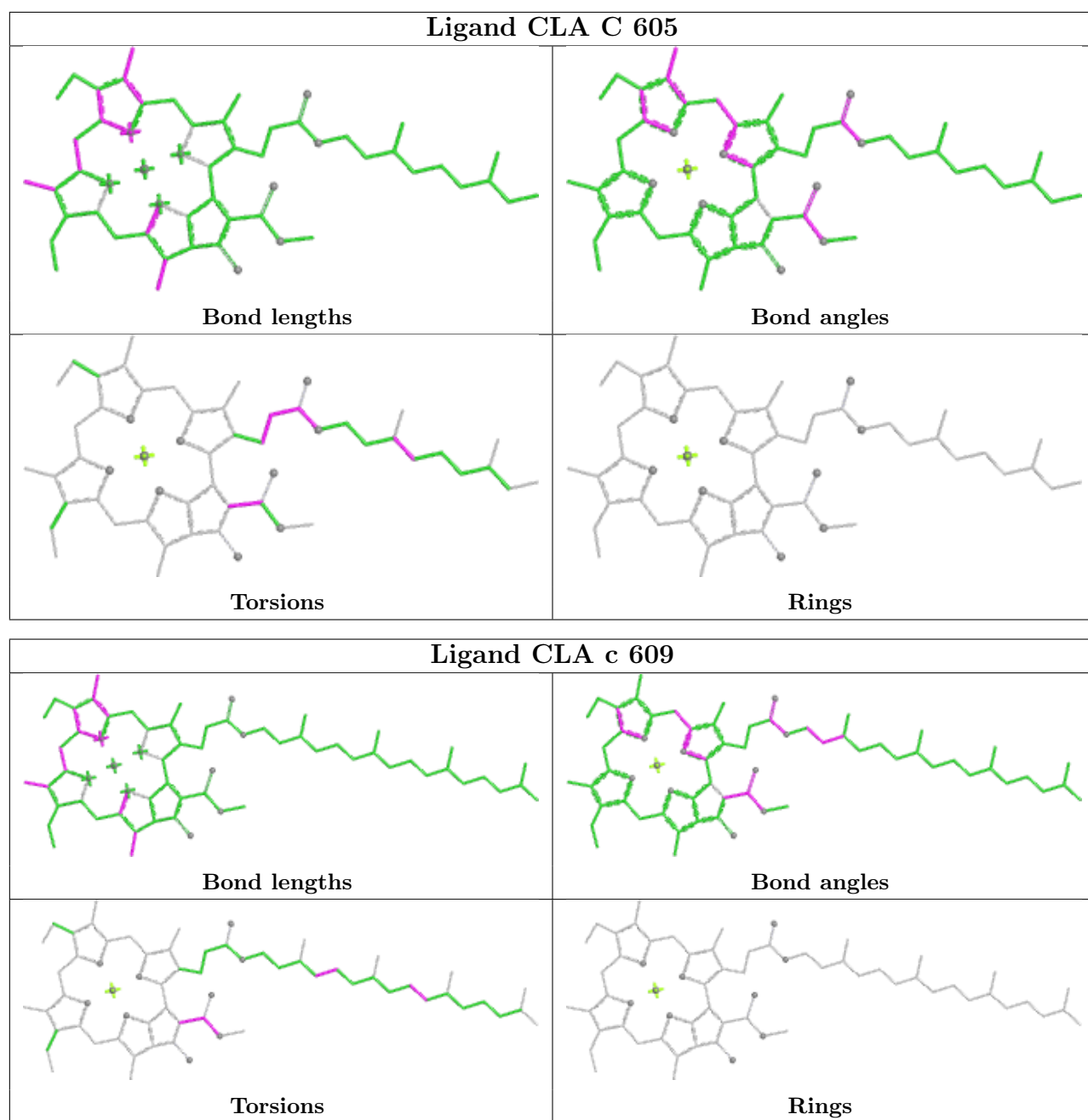


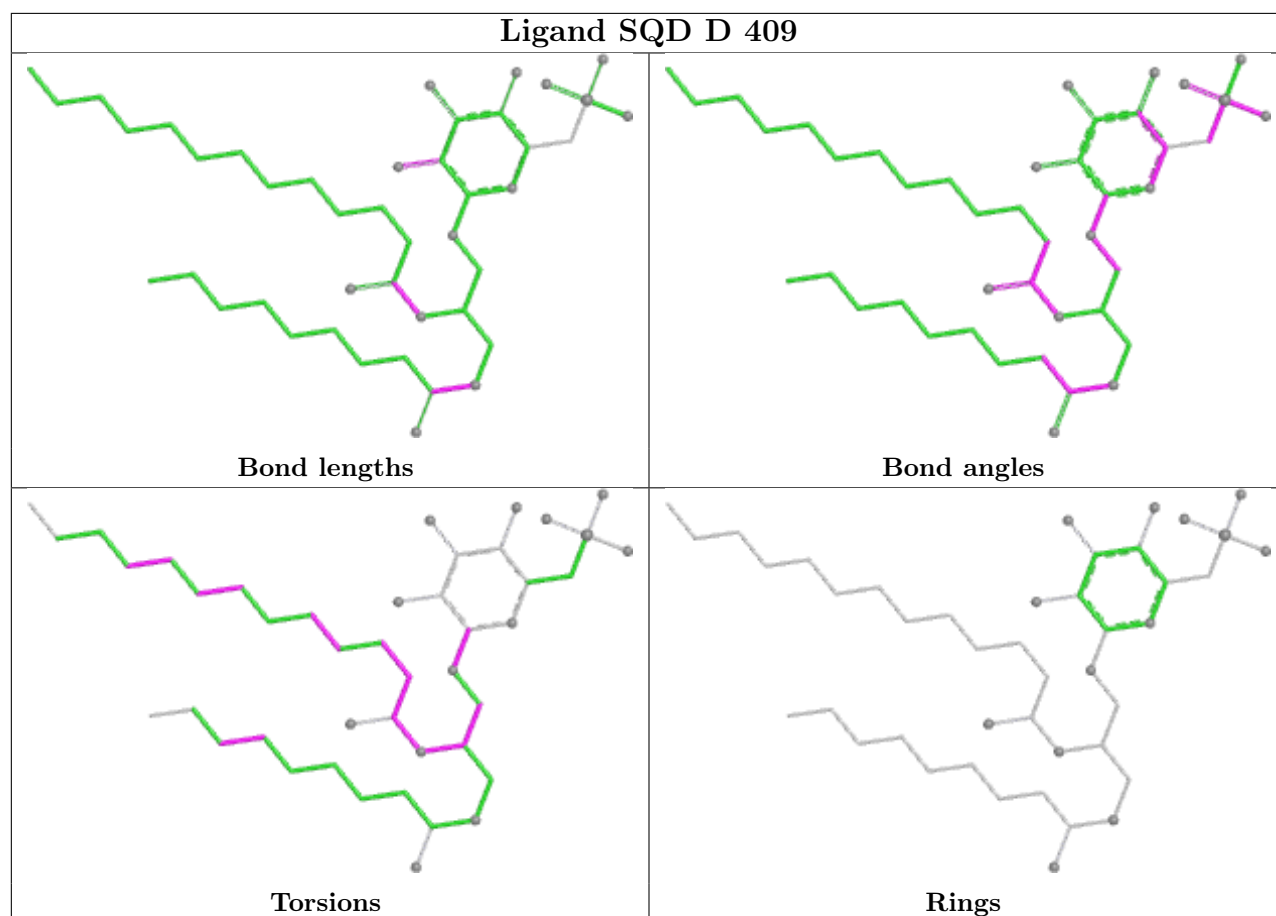
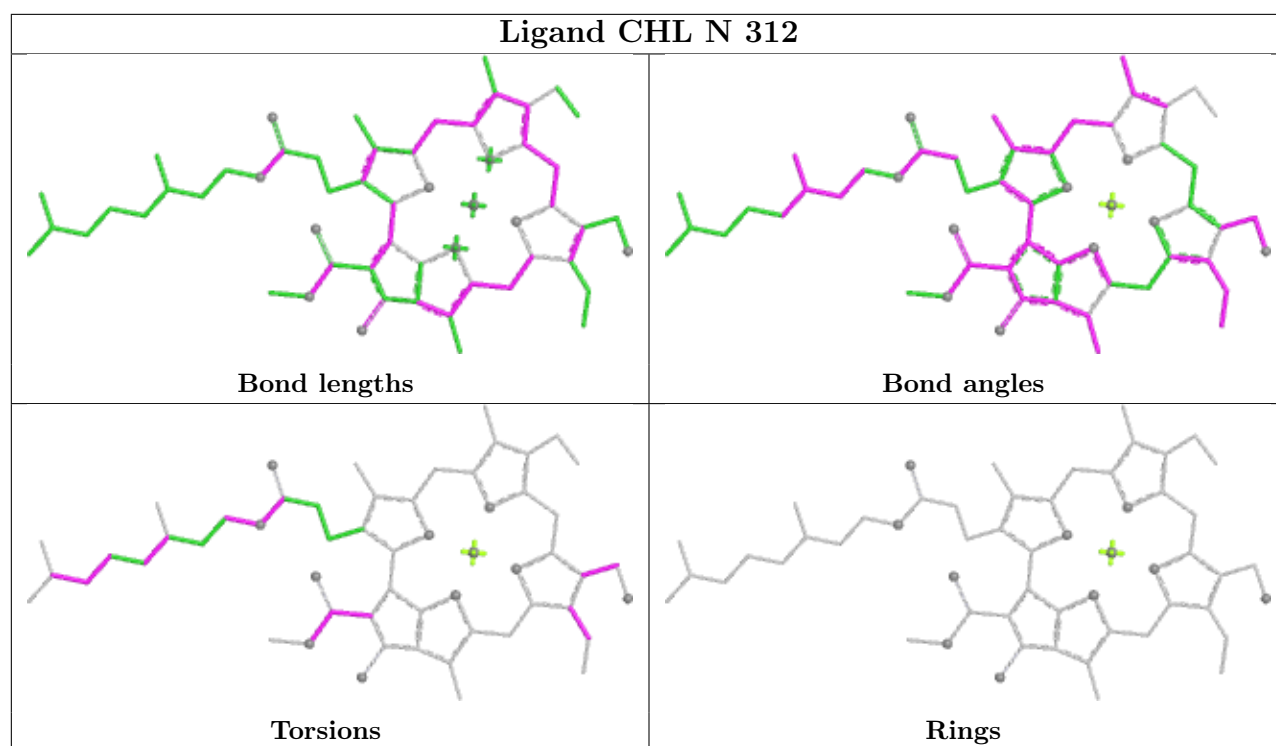
Ligand CHL 7 310



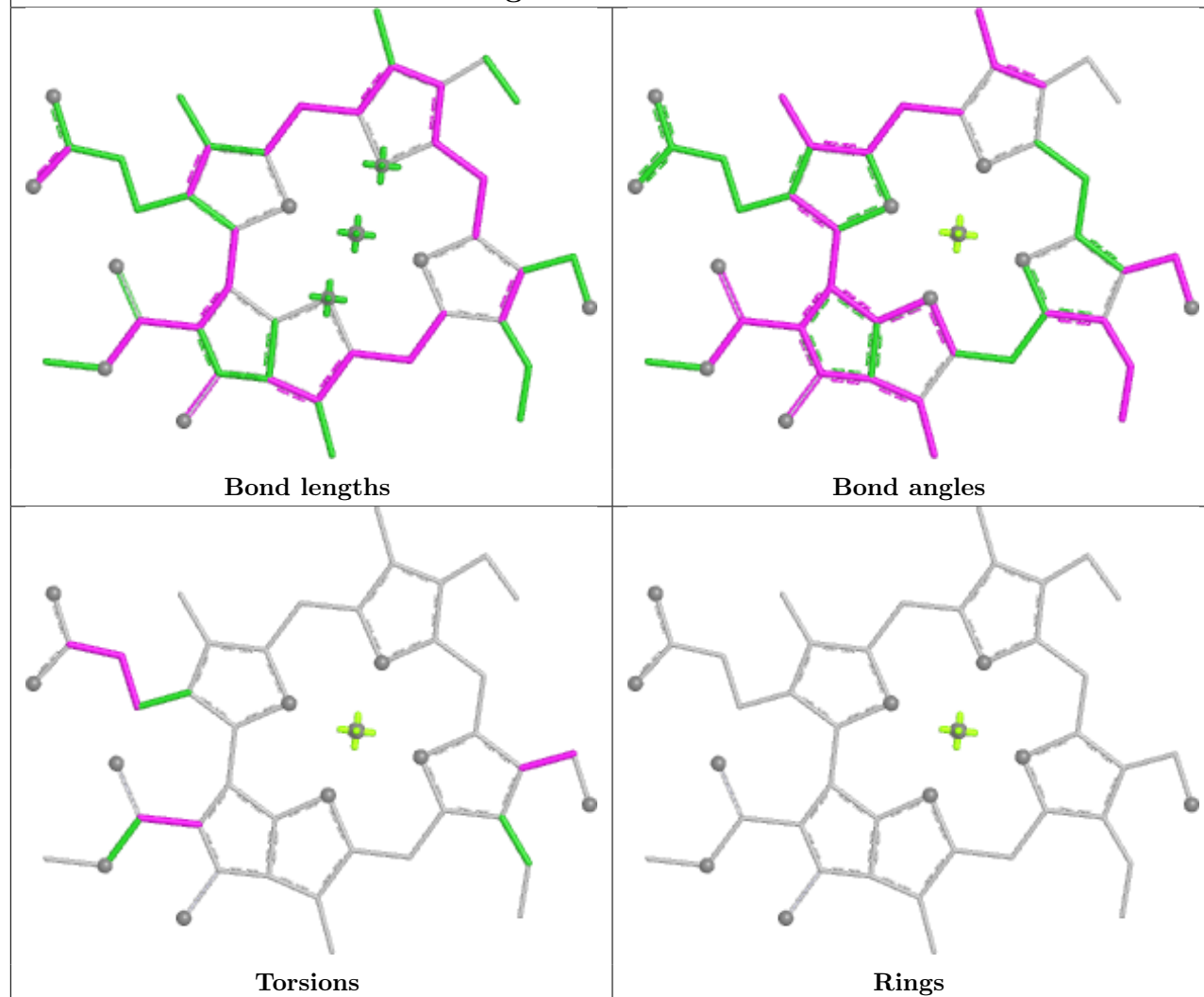
Ligand NEX g 304



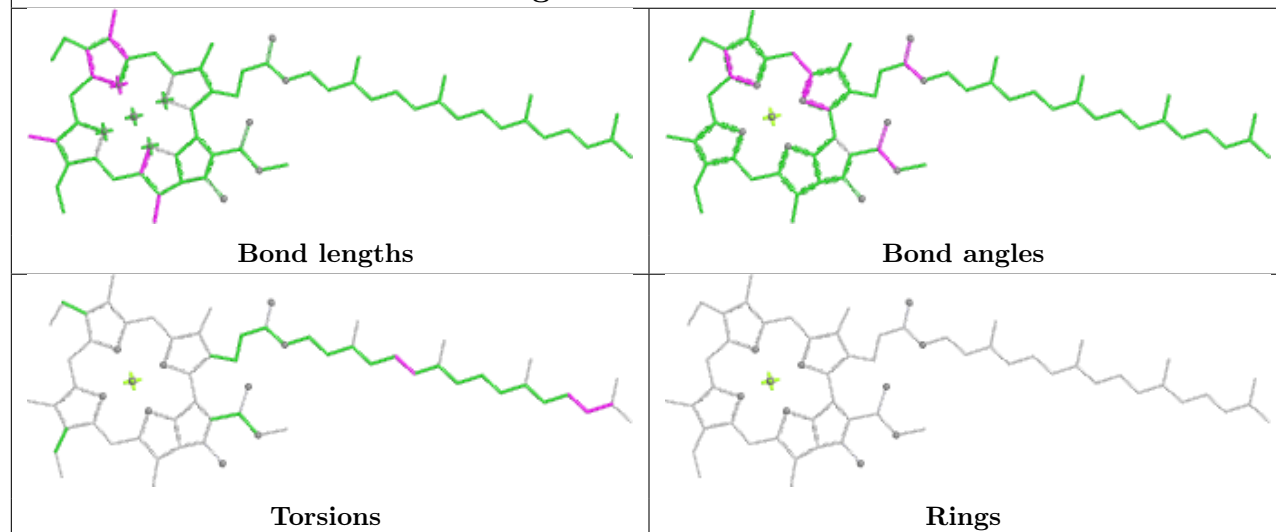




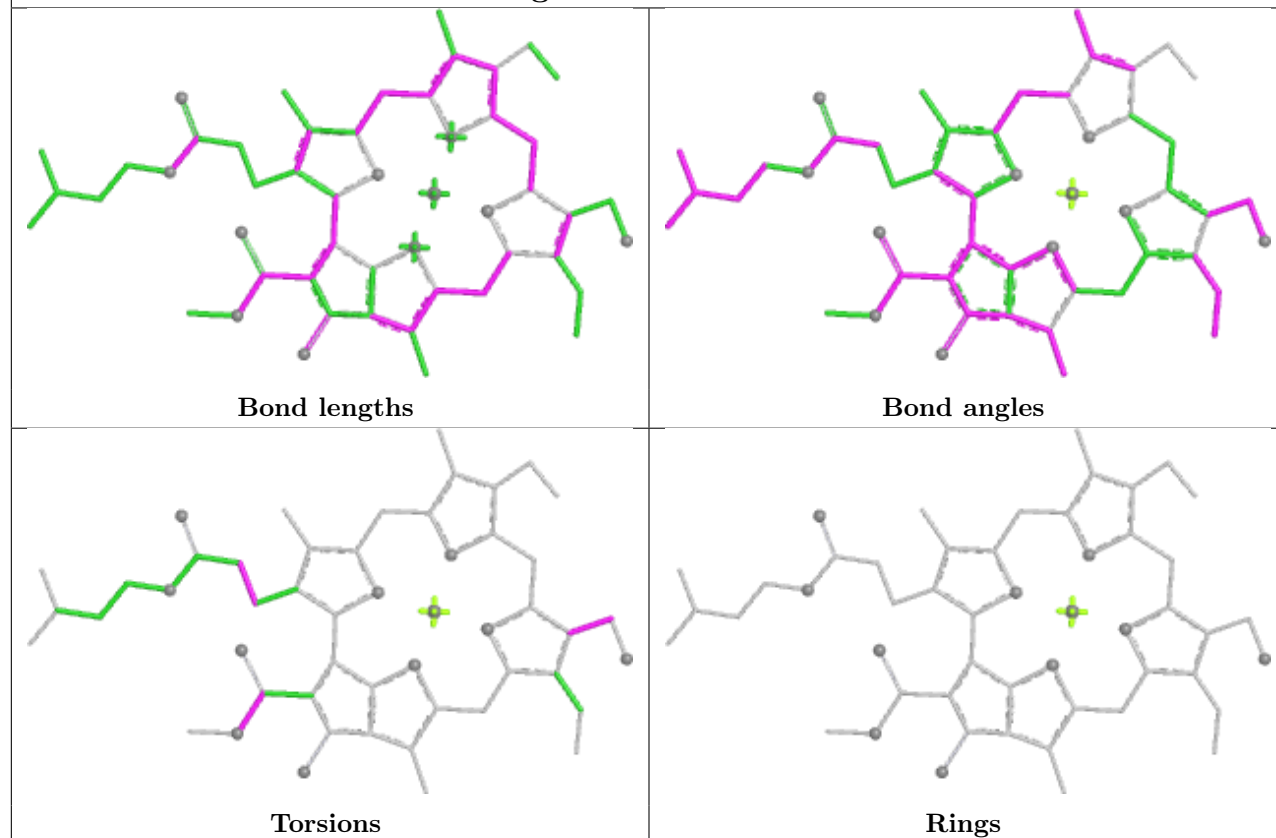
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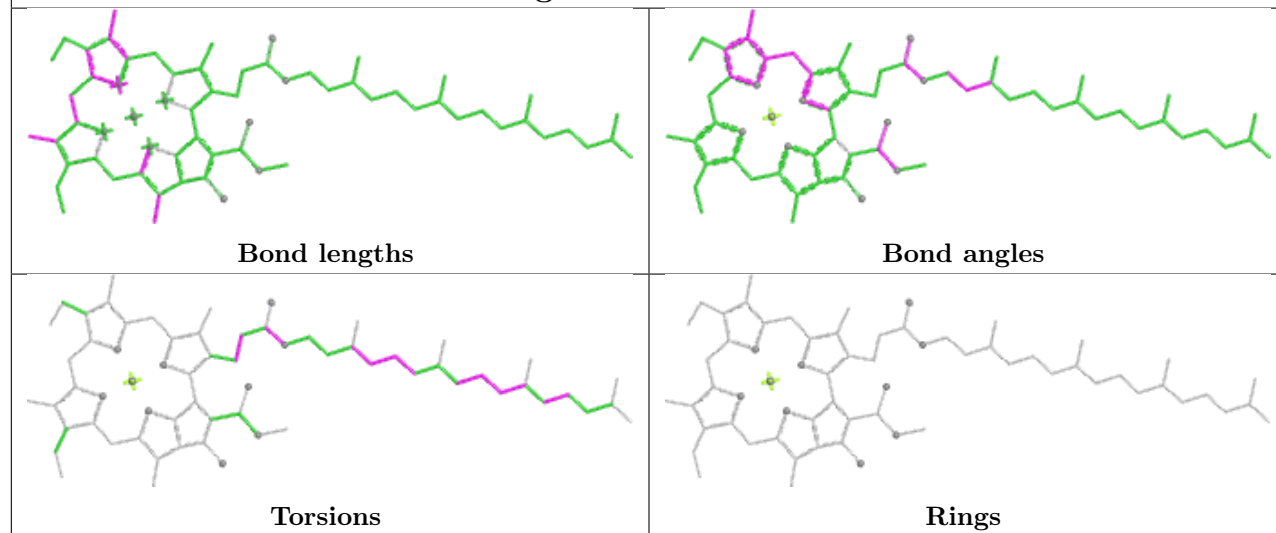
Ligand CLA B 615

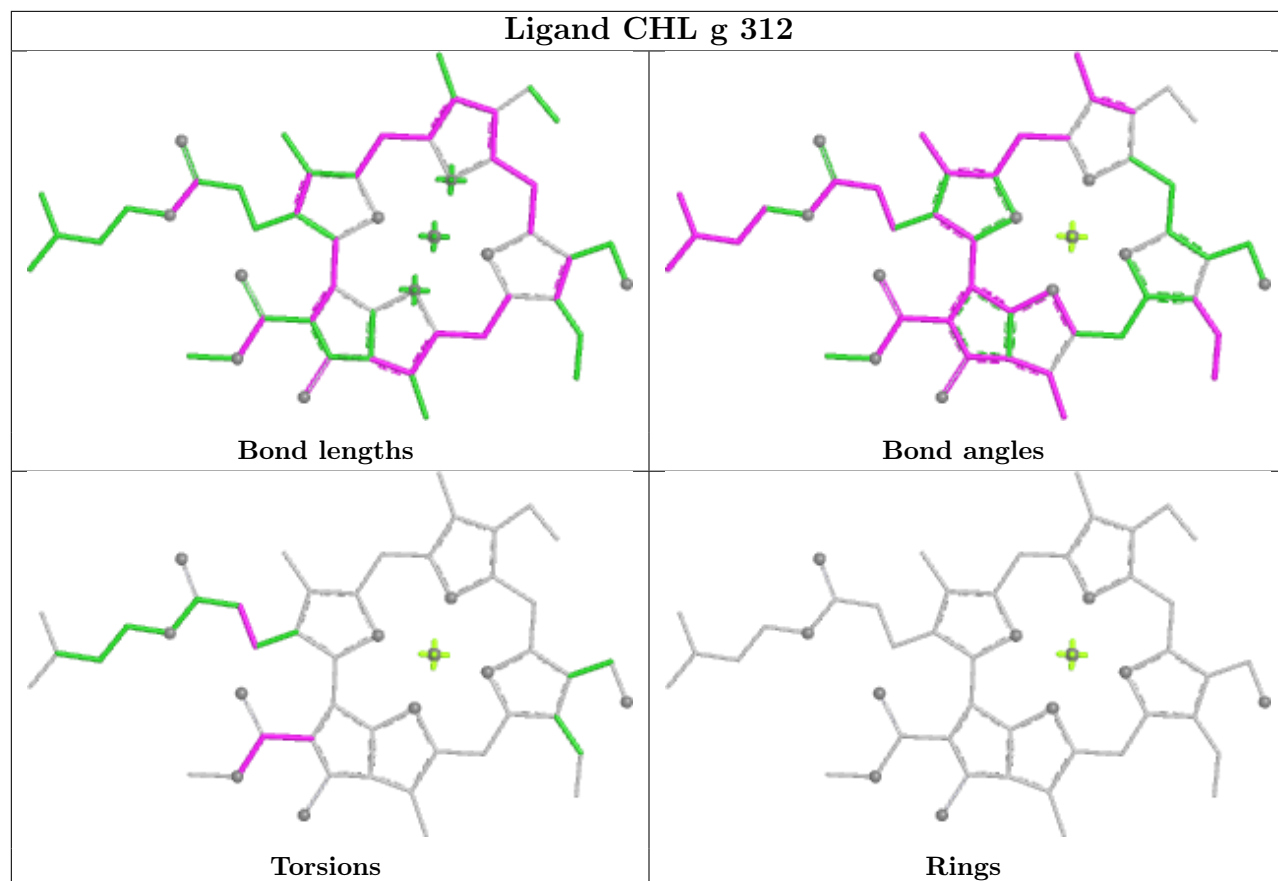


Ligand CHL Y 311

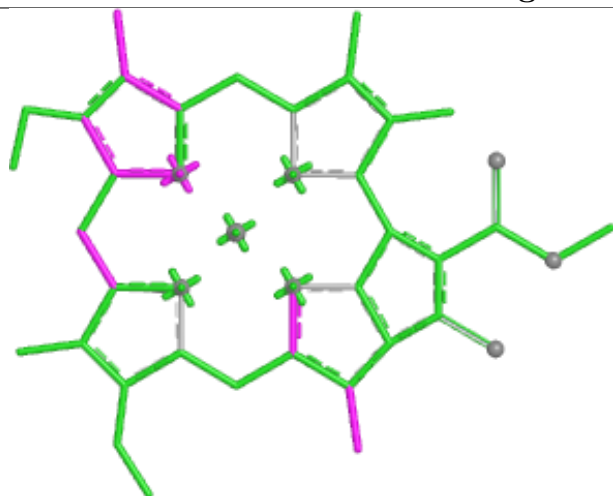


Ligand CLA b 612

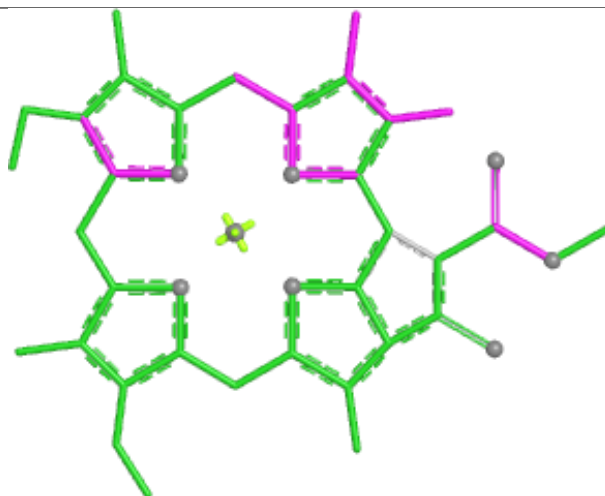




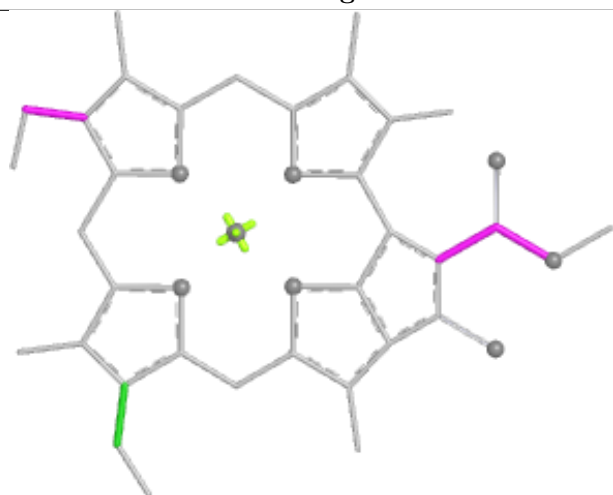
Ligand CLA 3 306



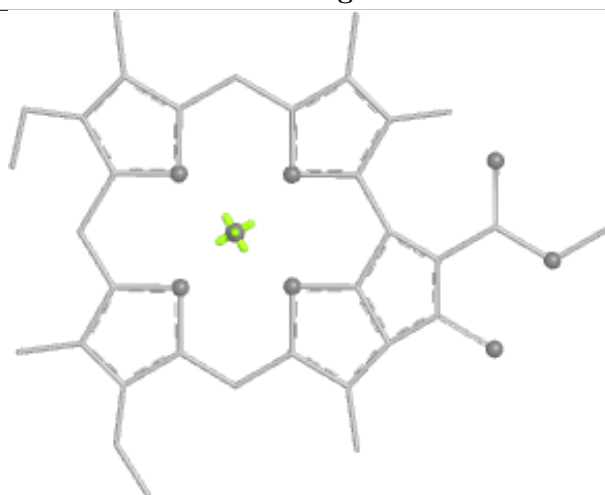
Bond lengths



Bond angles

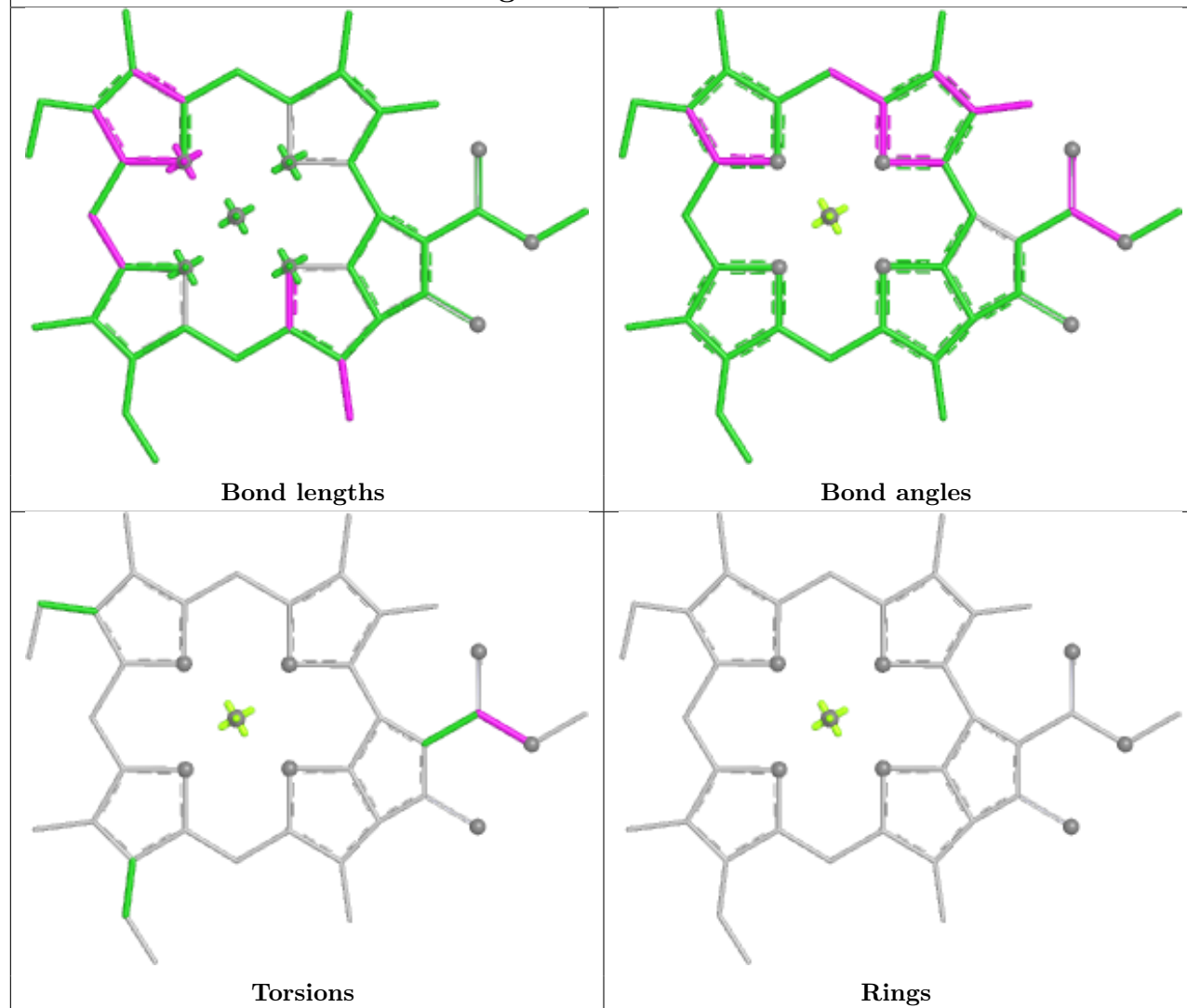


Torsions

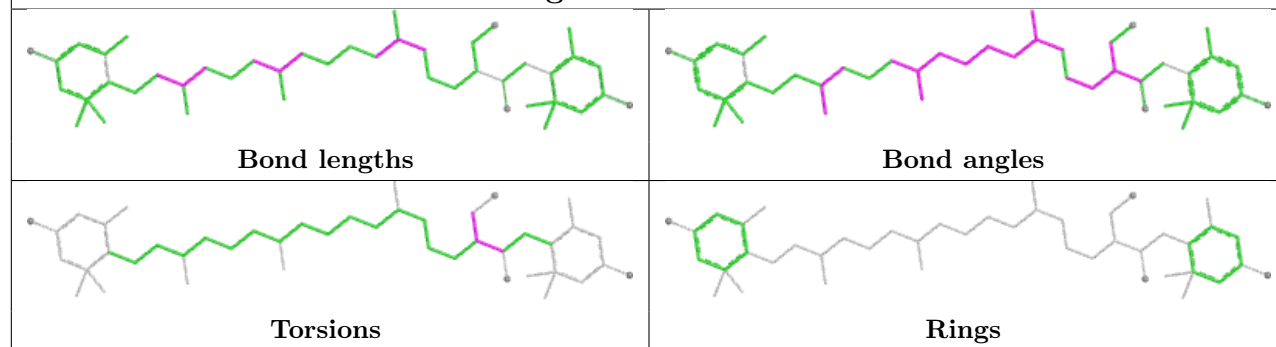


Rings

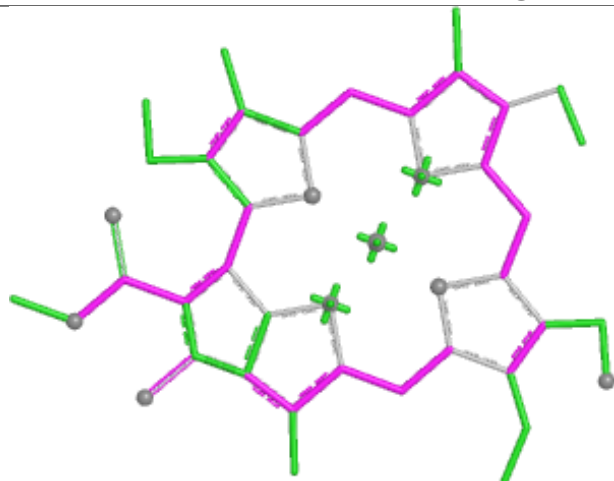
Ligand CLA 6 314



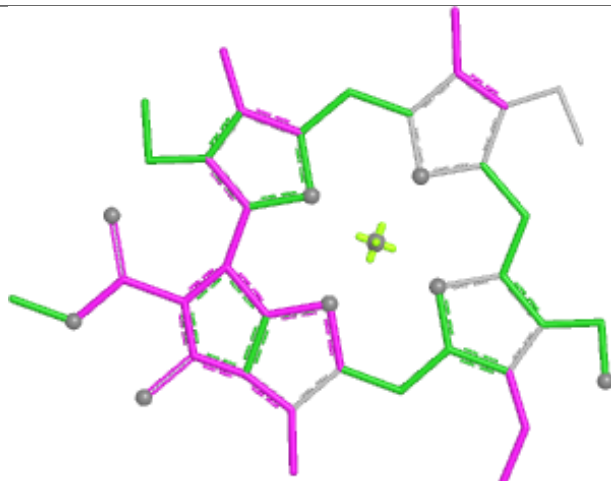
Ligand OIE 9 302



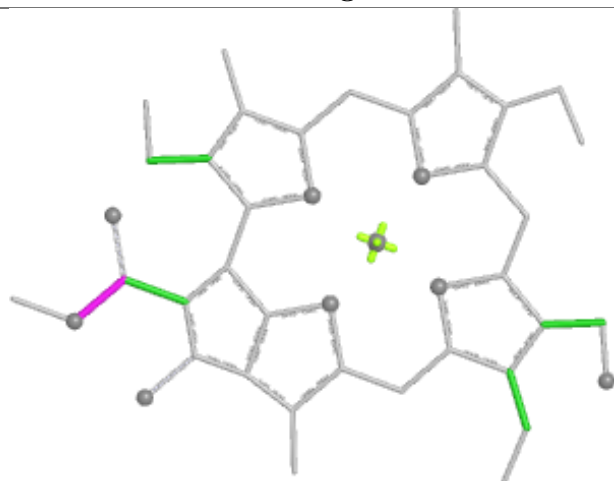
Ligand CHL N 308



Bond lengths



Bond angles

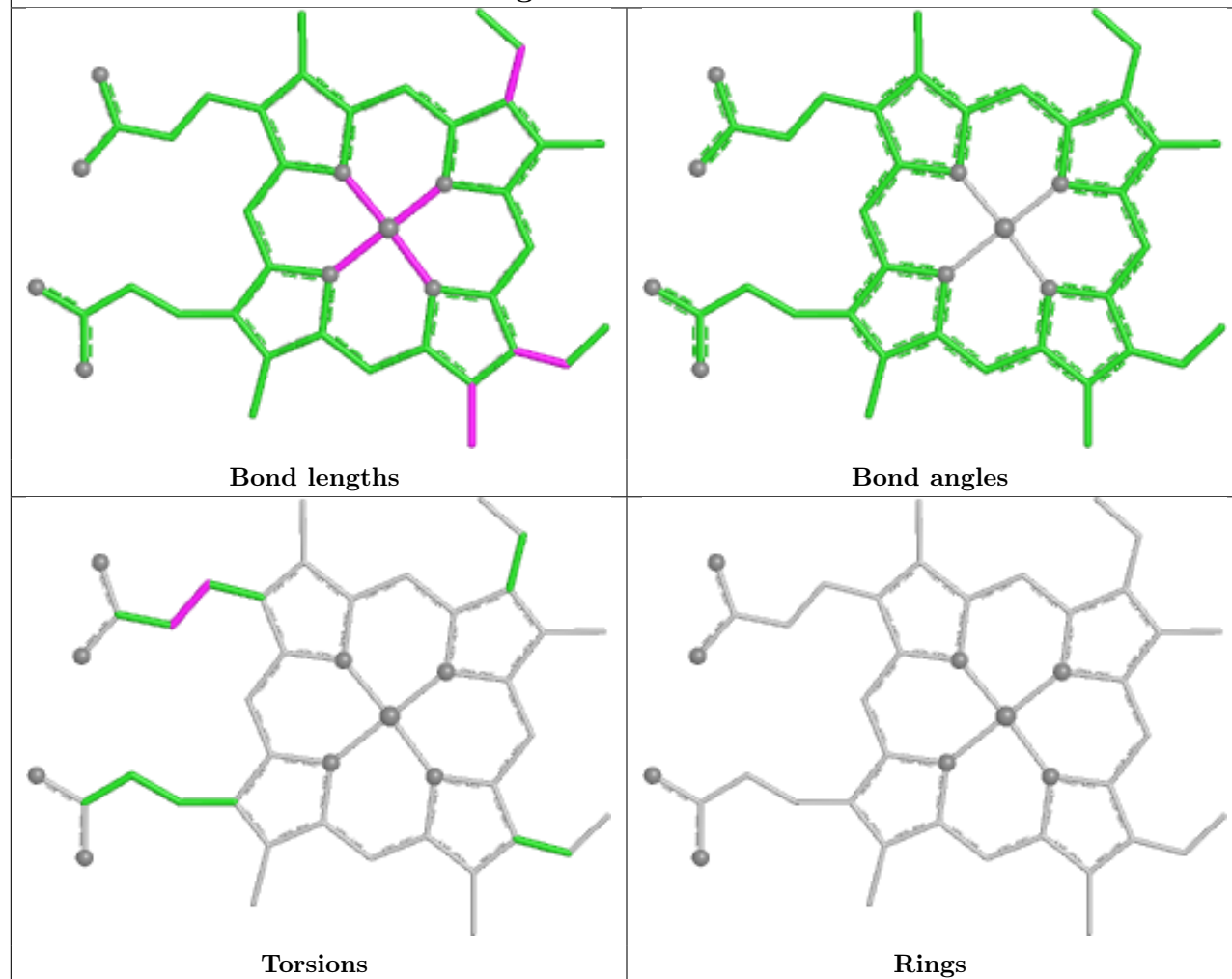


Torsions

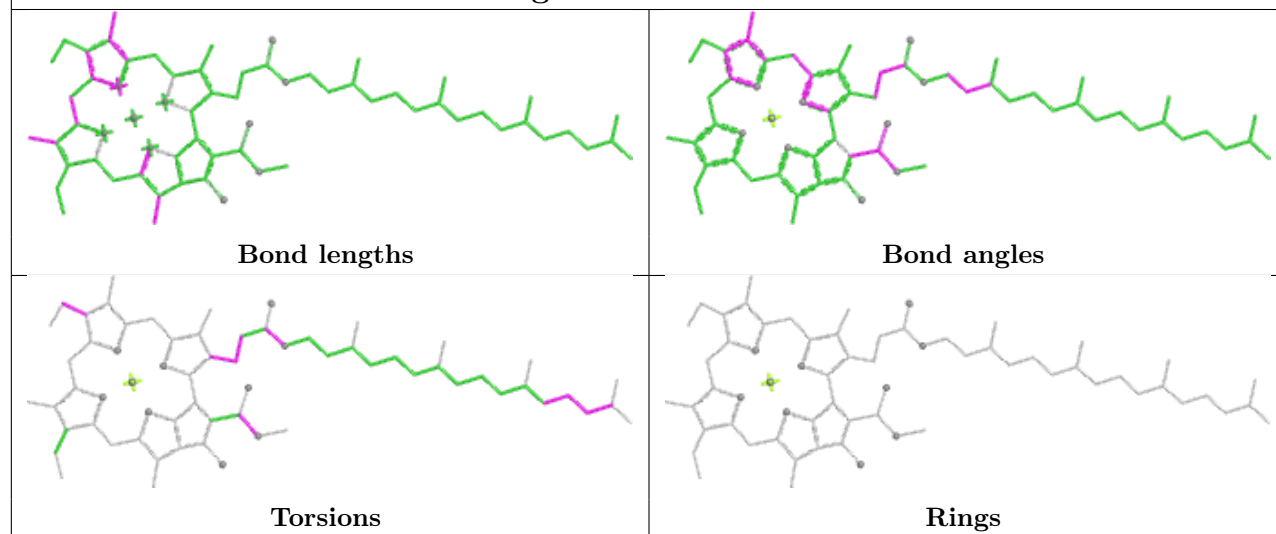


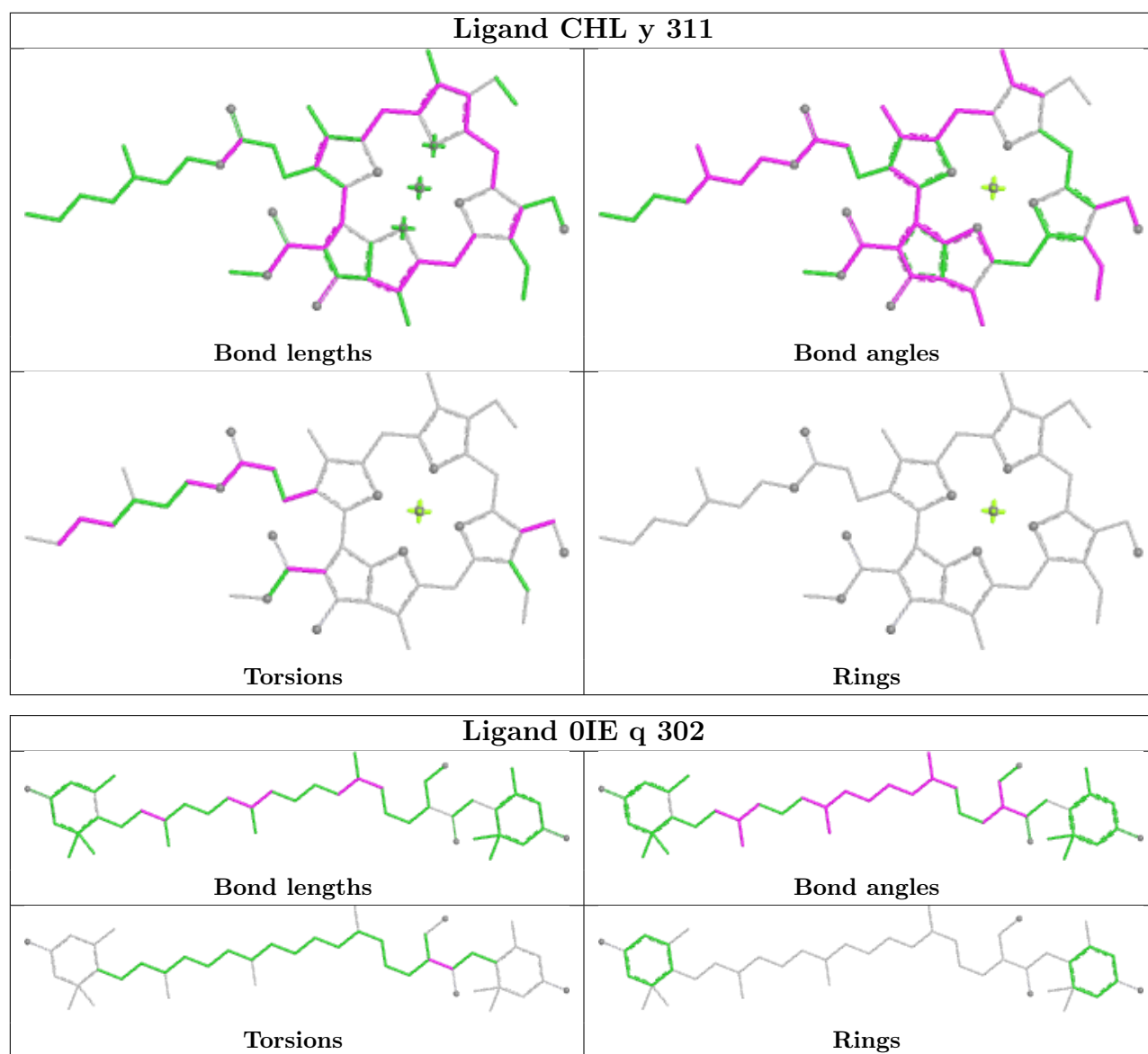
Rings

Ligand HEM f 201

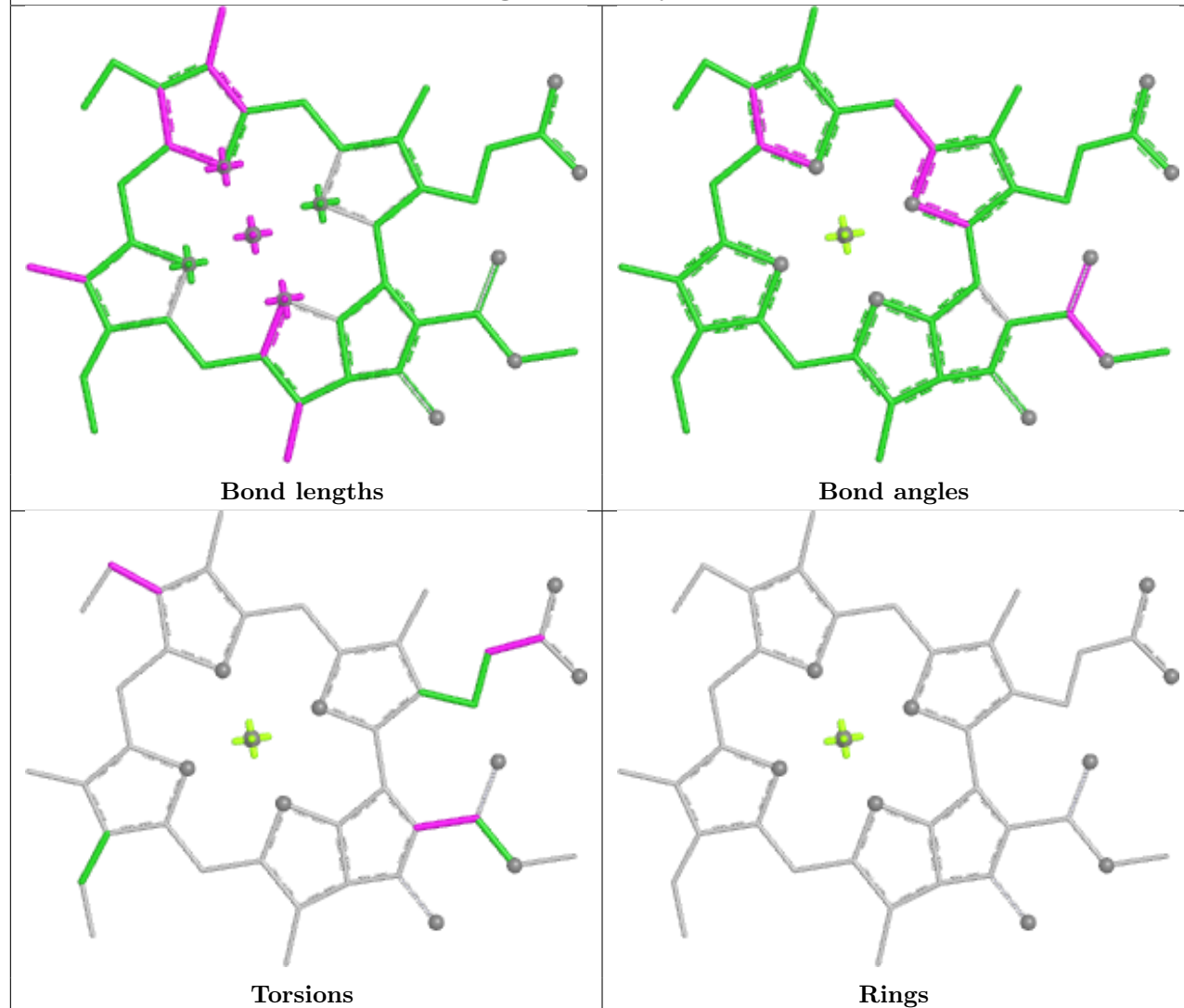


Ligand CLA A 603

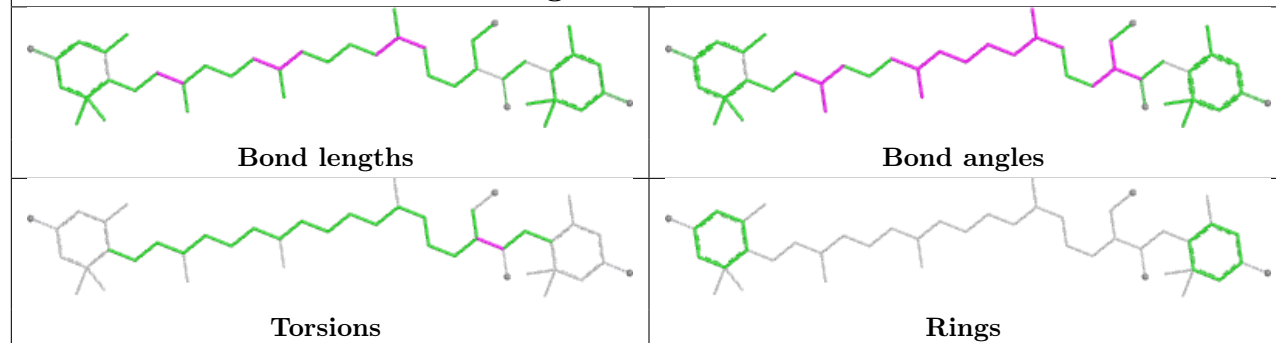


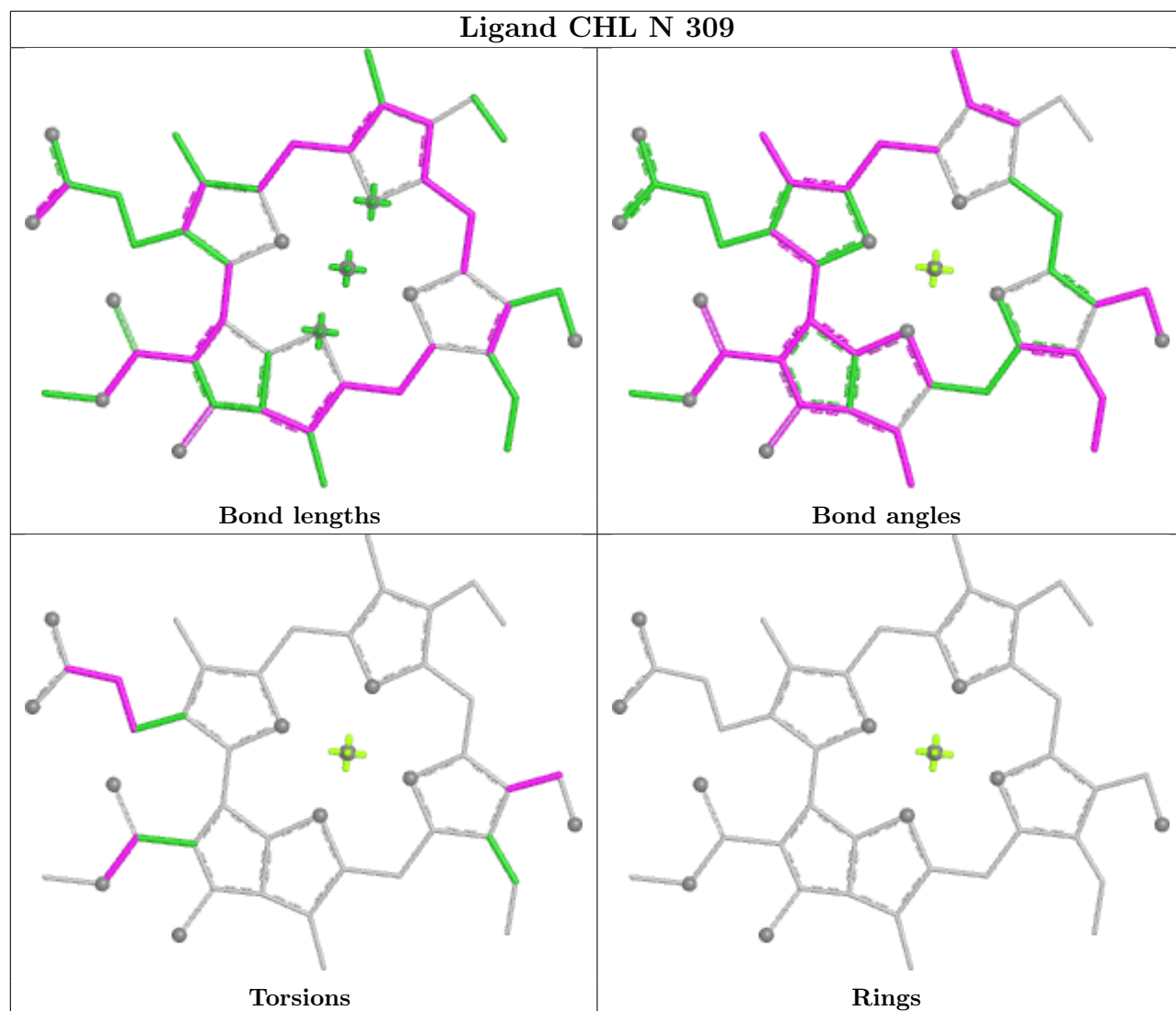
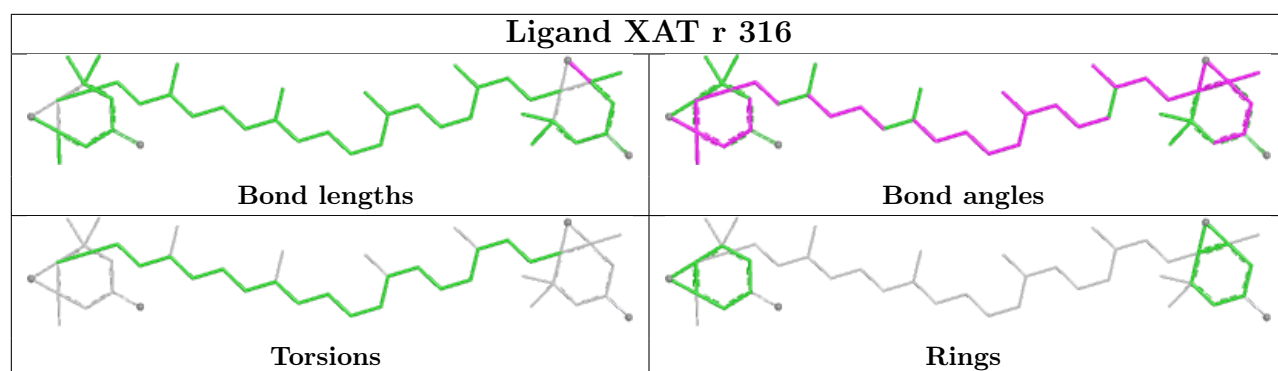


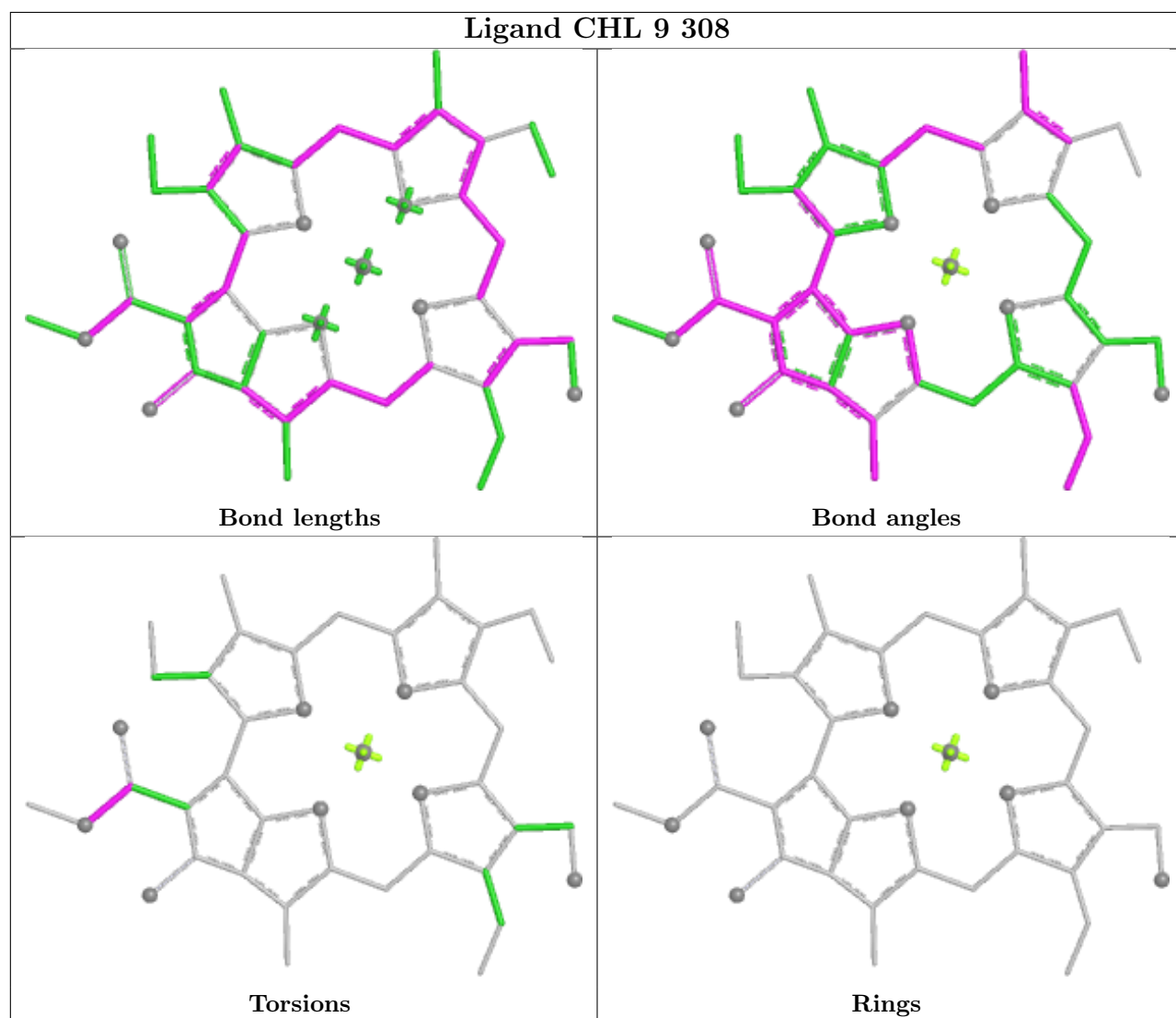
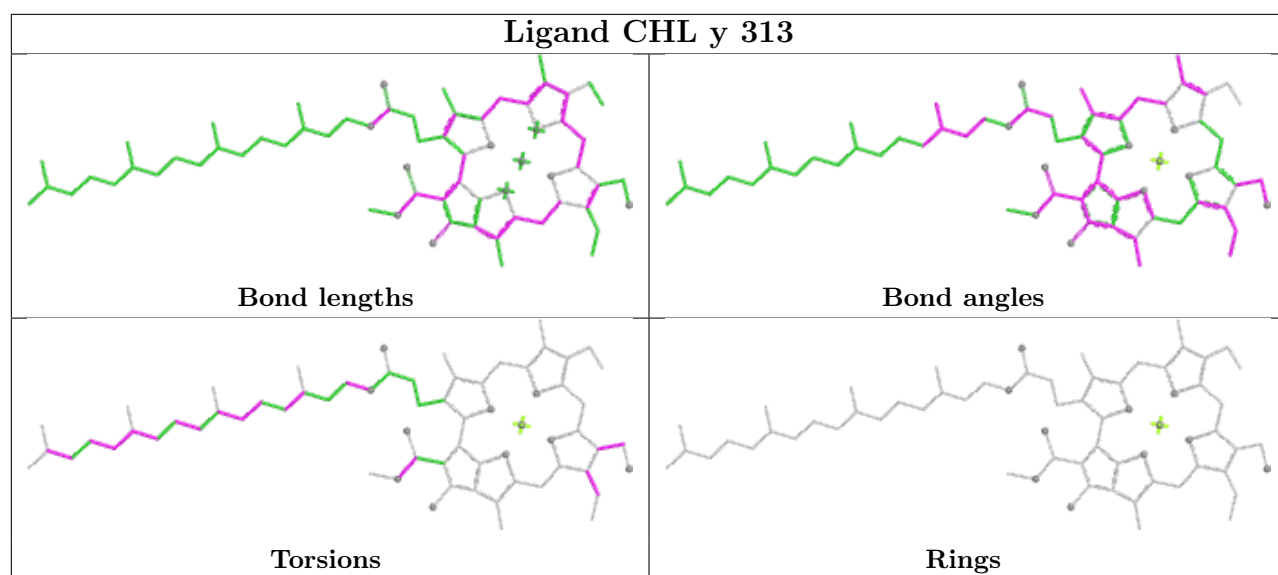
Ligand CLA y 316



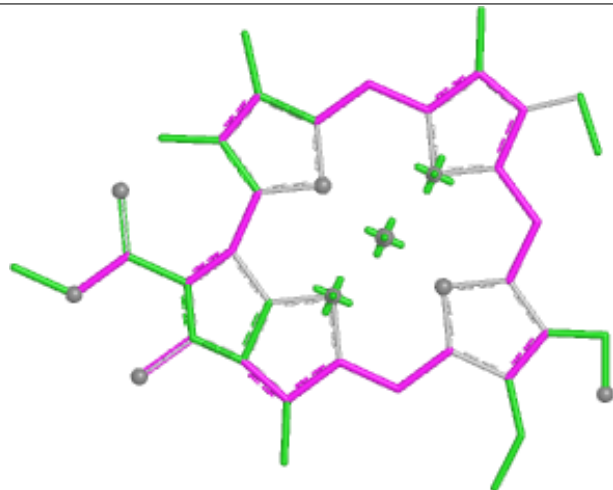
Ligand OIE 8 302



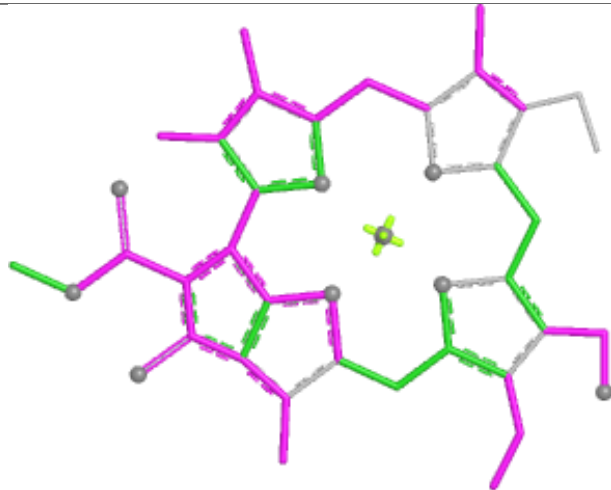




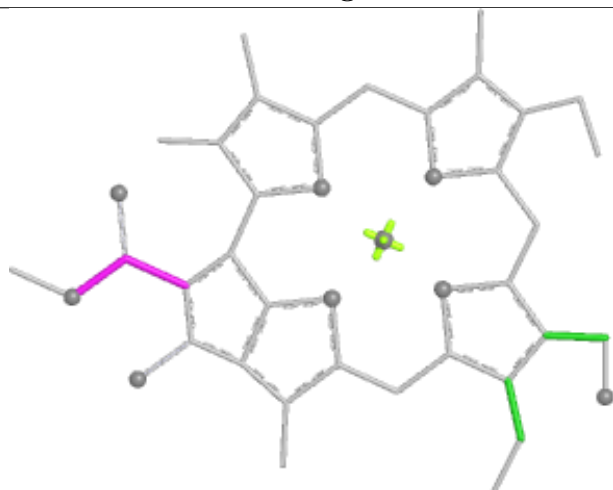
Ligand CHL 5 318



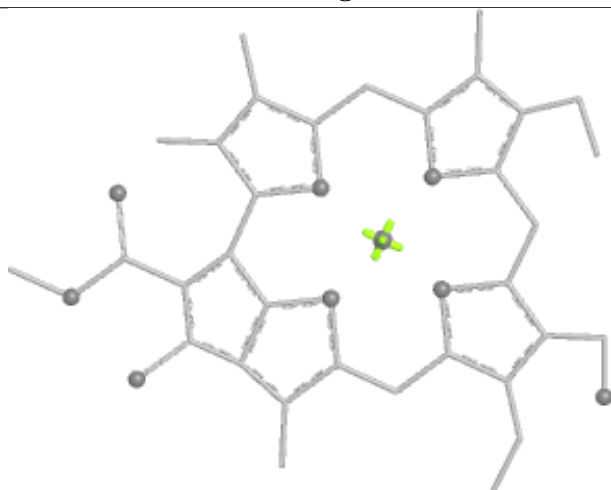
Bond lengths



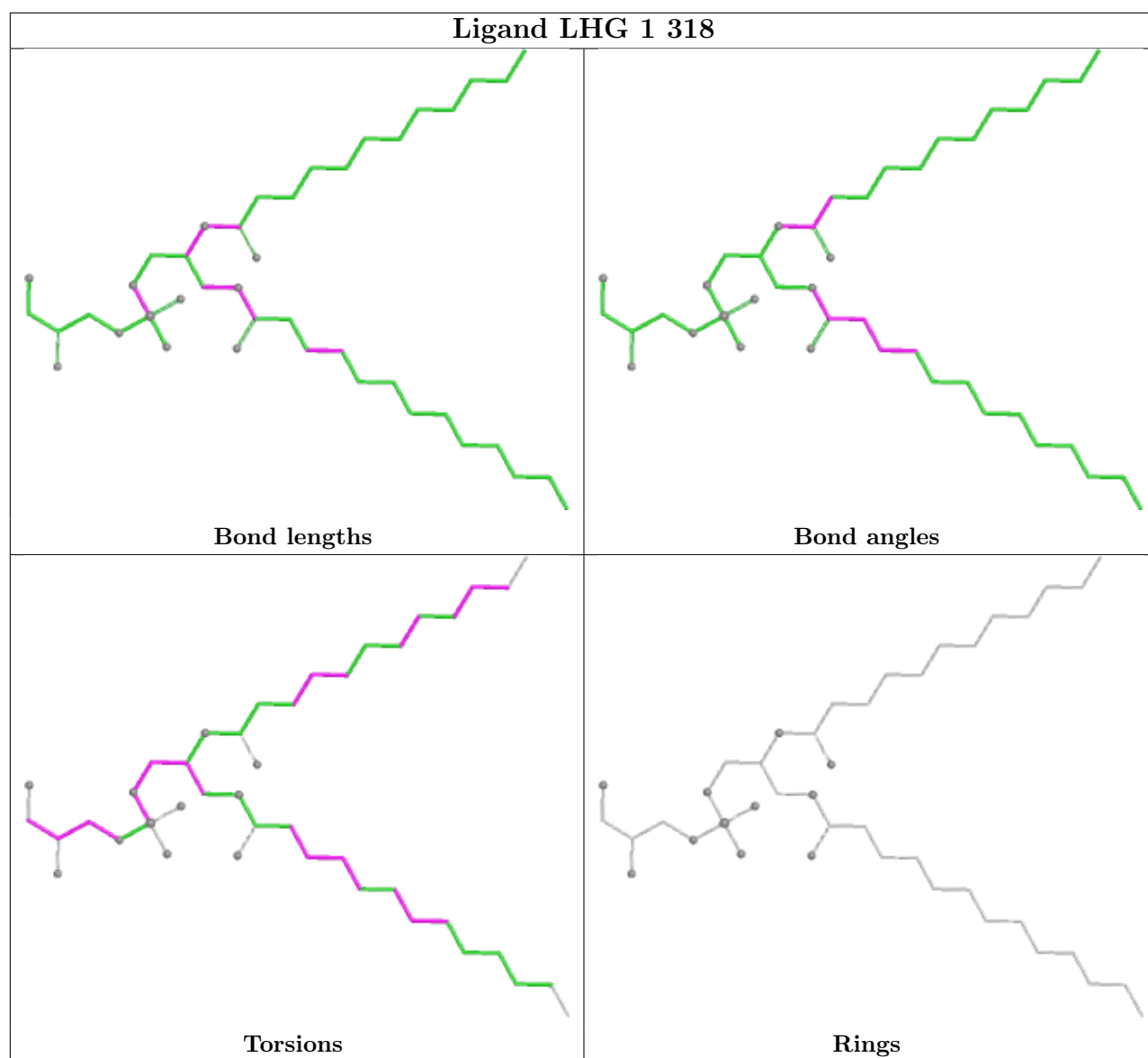
Bond angles

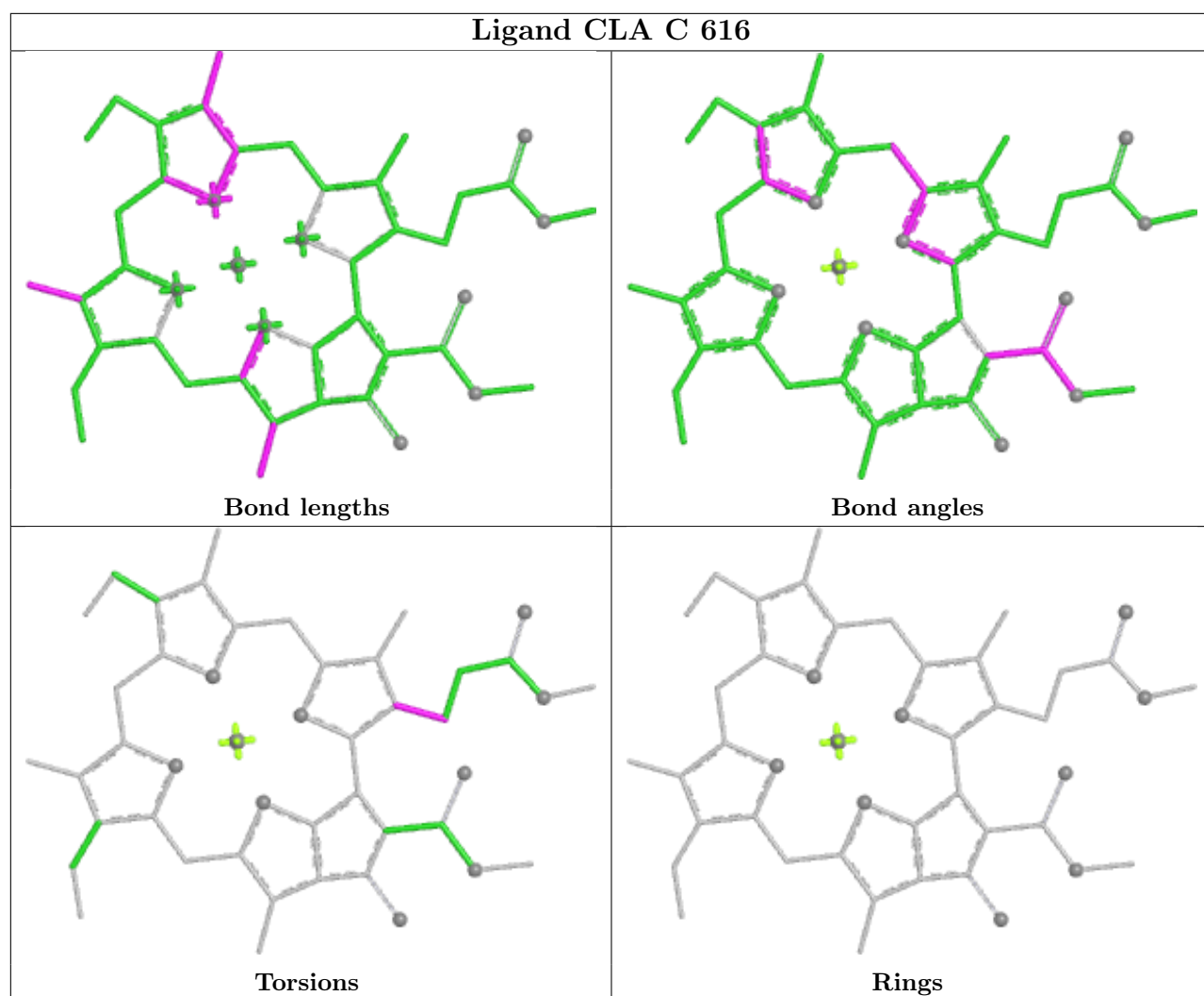


Torsions

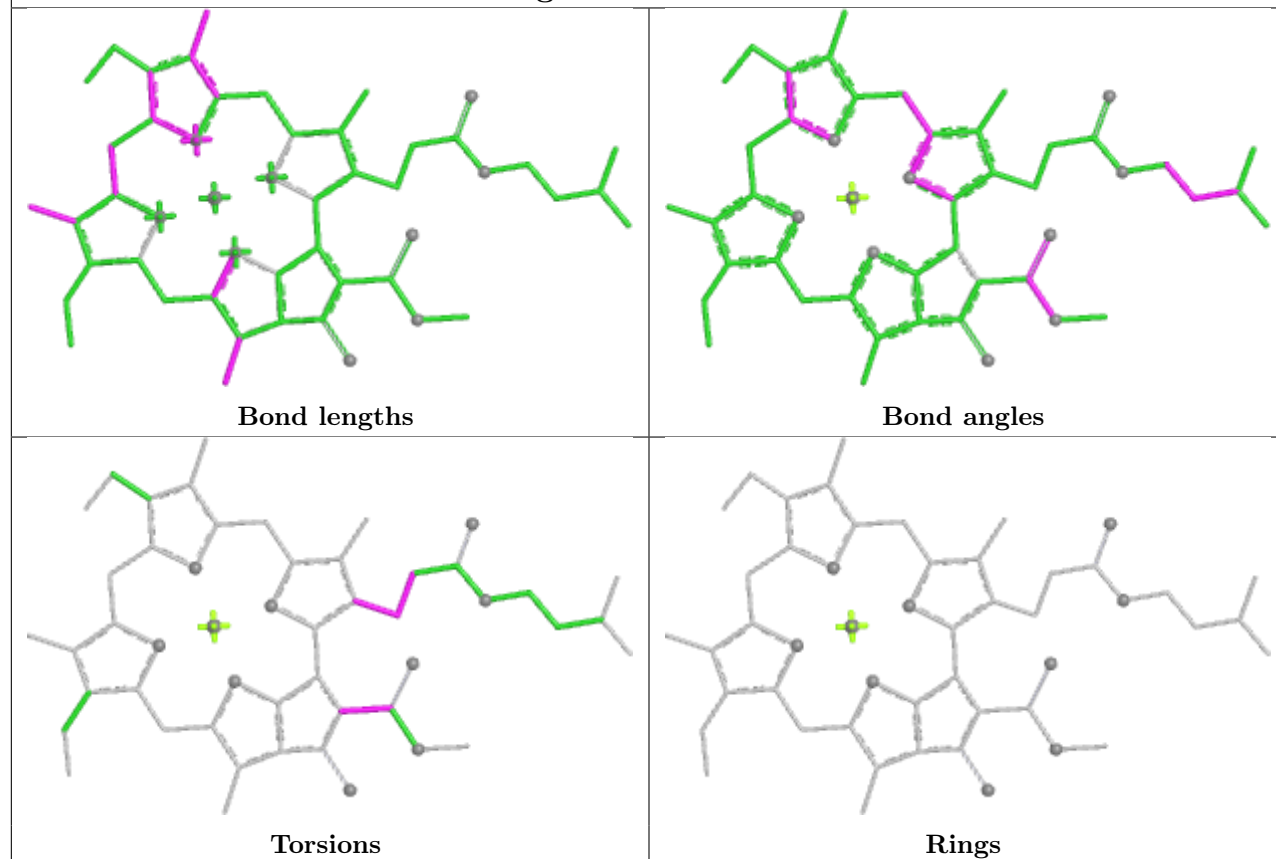


Rings

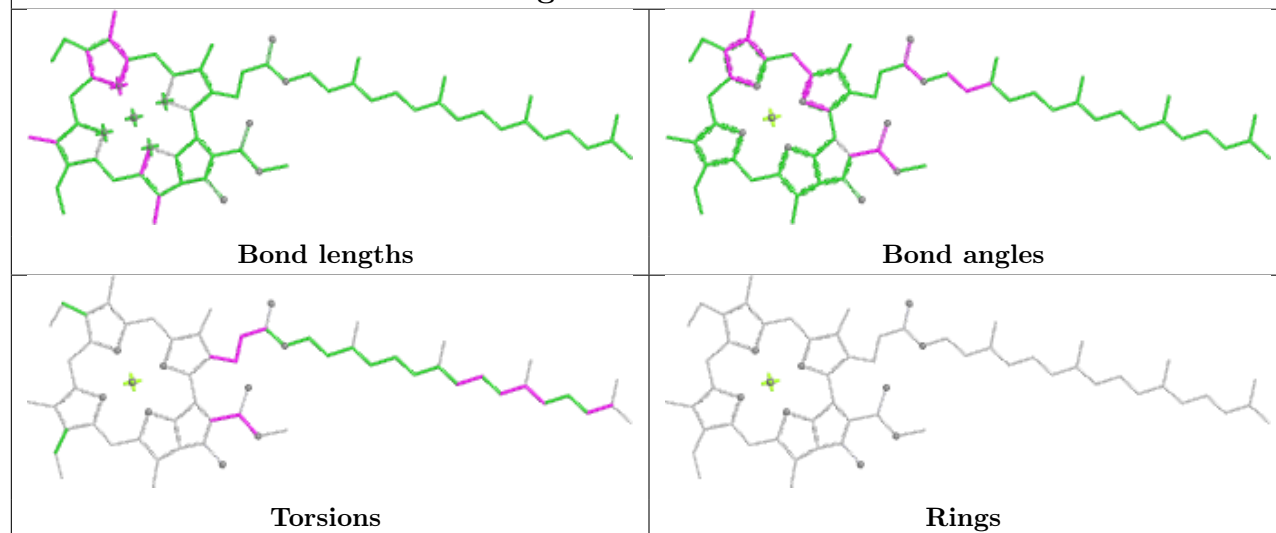




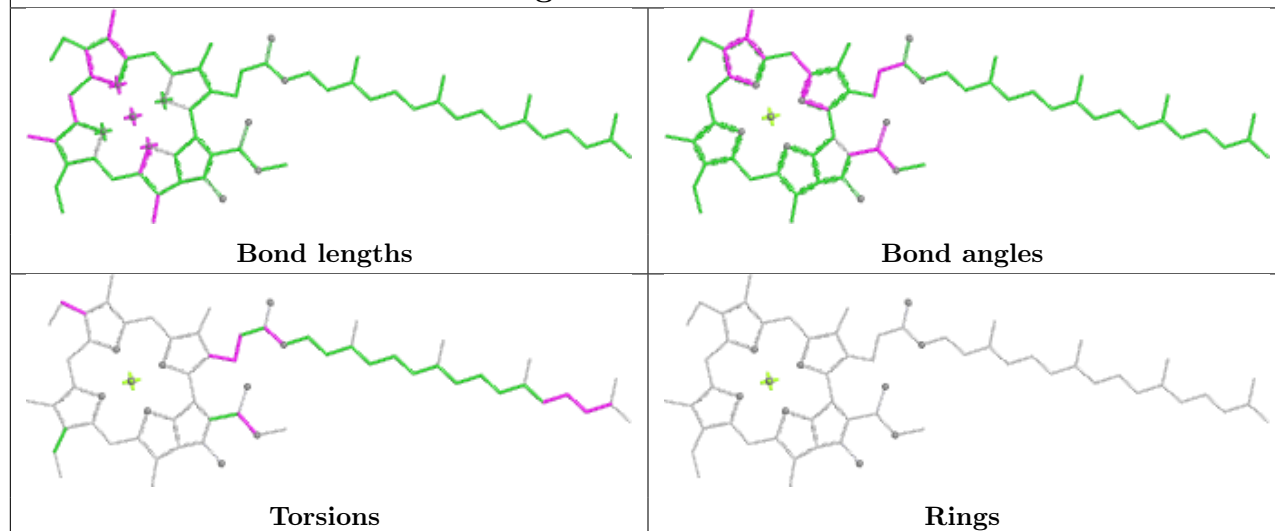
Ligand CLA 7 308



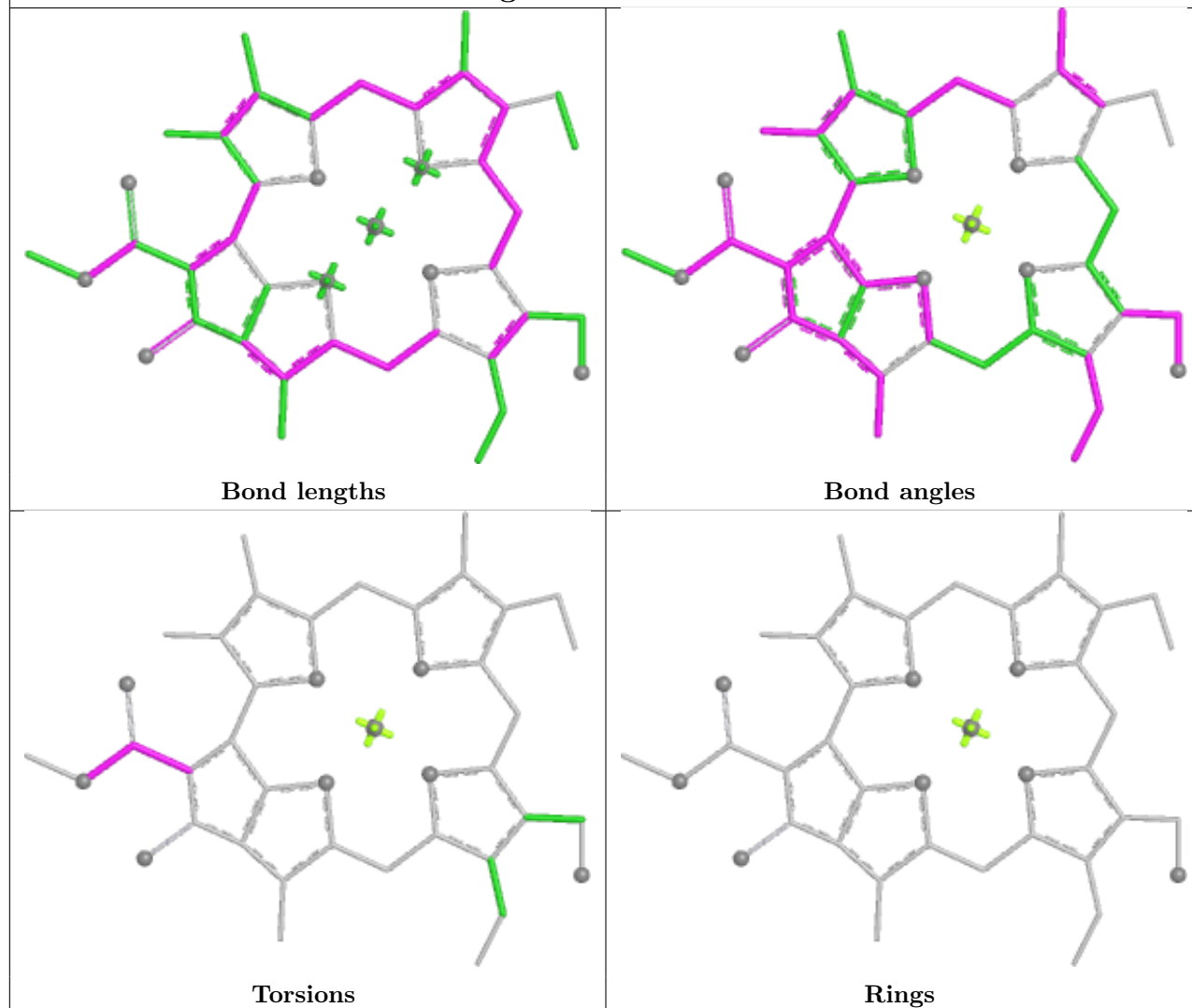
Ligand CLA c 601



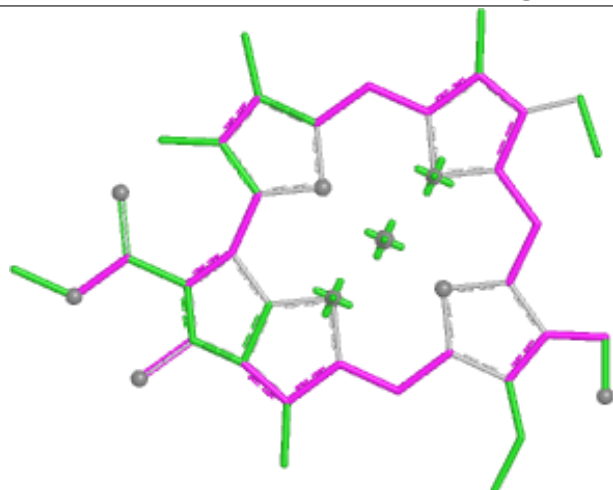
Ligand CLA a 603



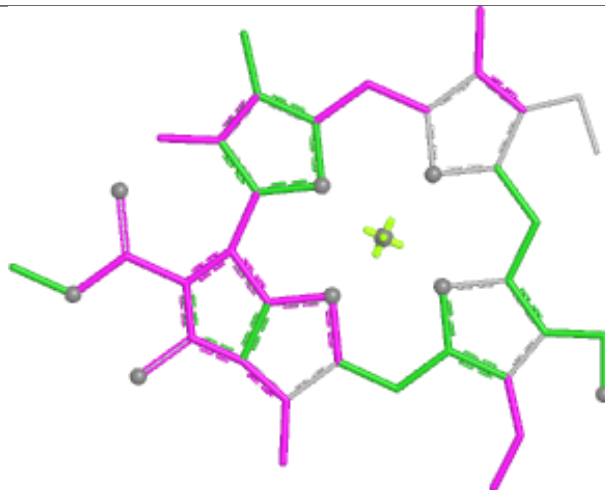
Ligand CHL 9 317



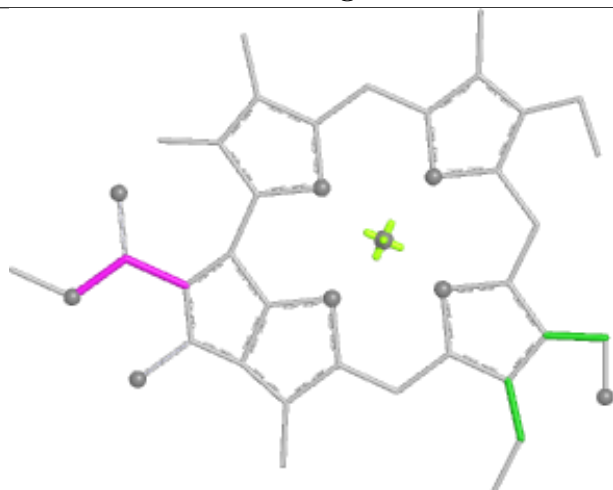
Ligand CHL 4 304



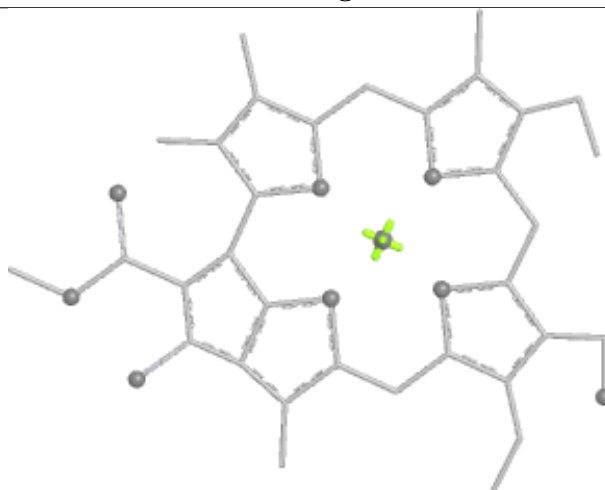
Bond lengths



Bond angles

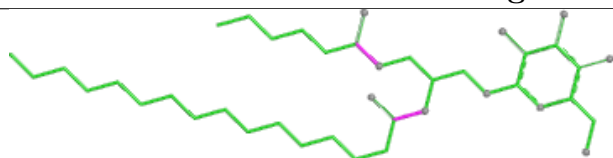


Torsions

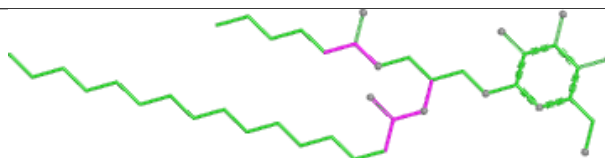


Rings

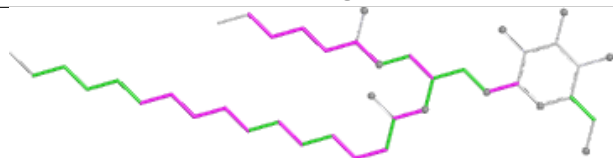
Ligand LMG m 101



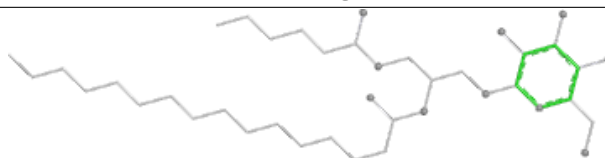
Bond lengths



Bond angles

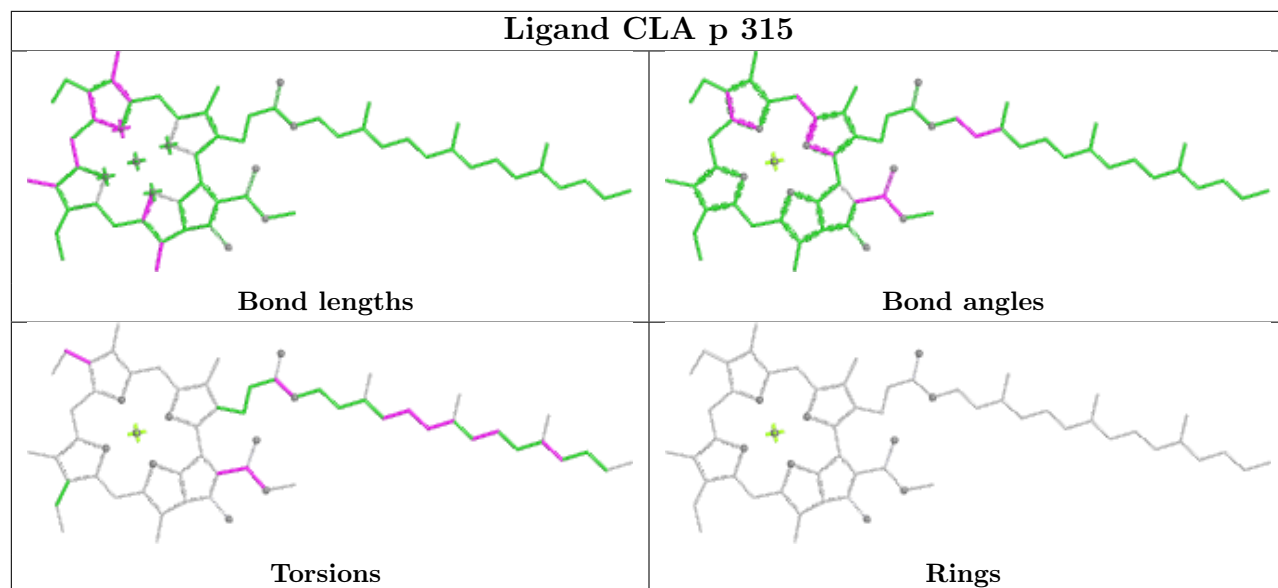


Torsions

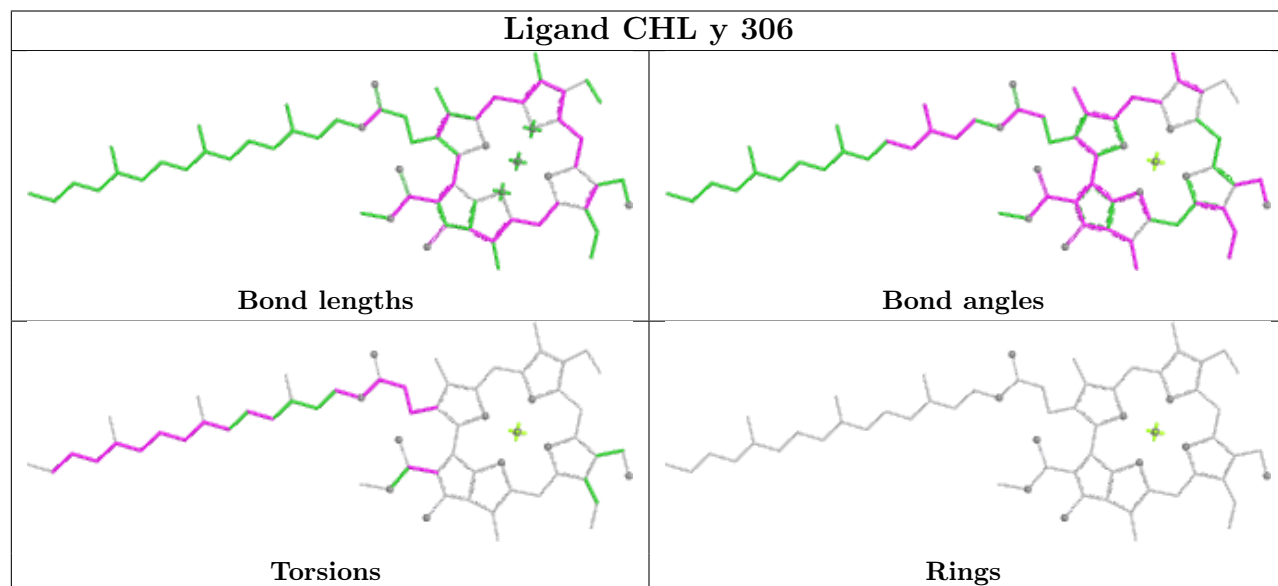


Rings

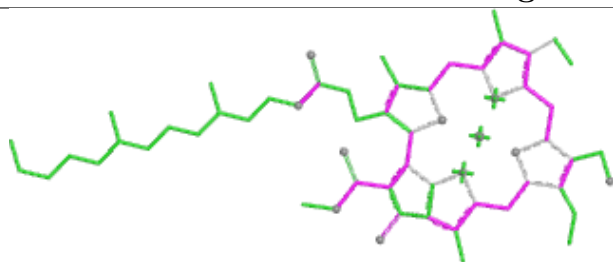
Ligand CLA p 315



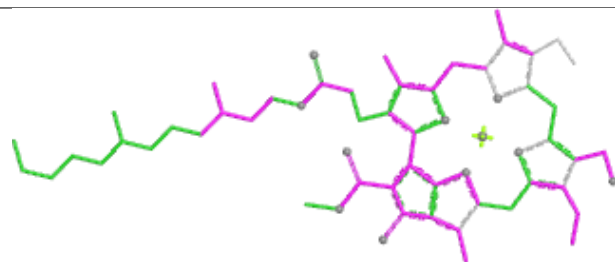
Ligand CHL y 306



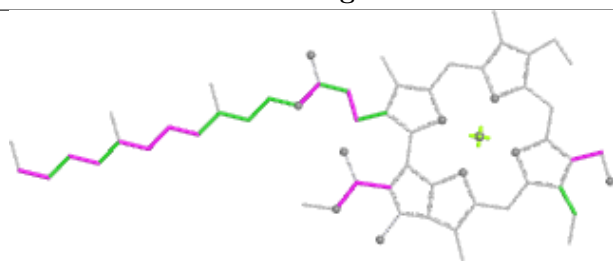
Ligand CHL 8 304



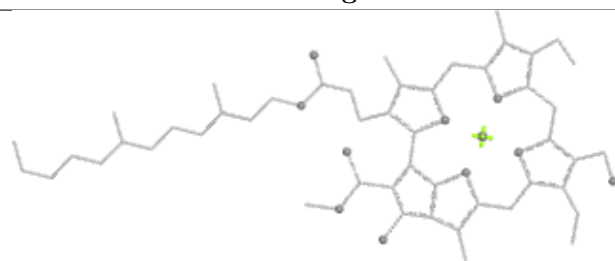
Bond lengths



Bond angles

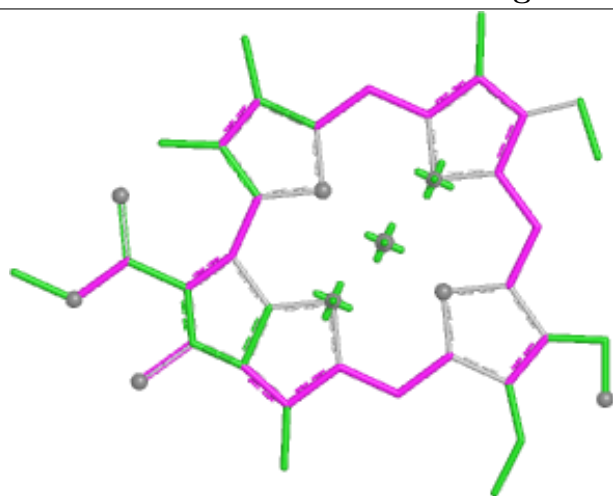


Torsions

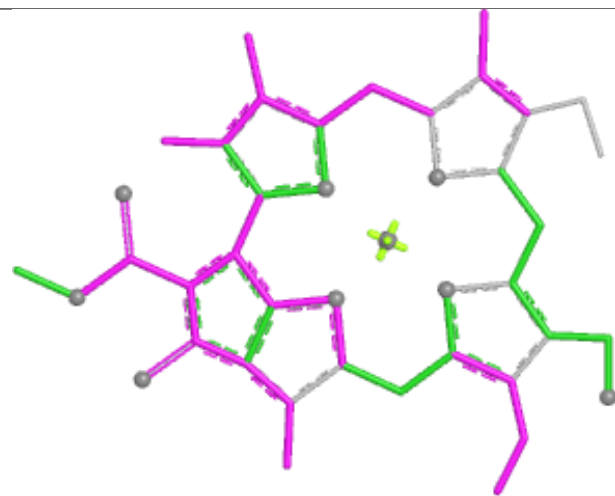


Rings

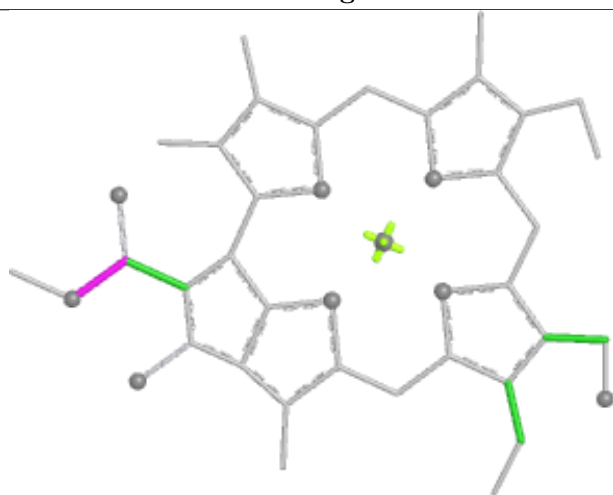
Ligand CHL R 605



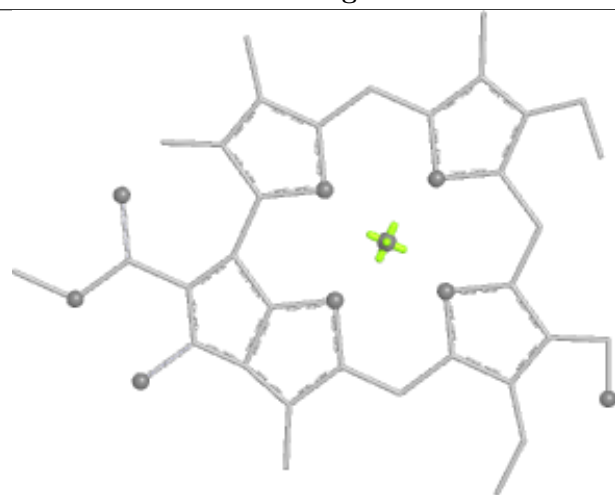
Bond lengths



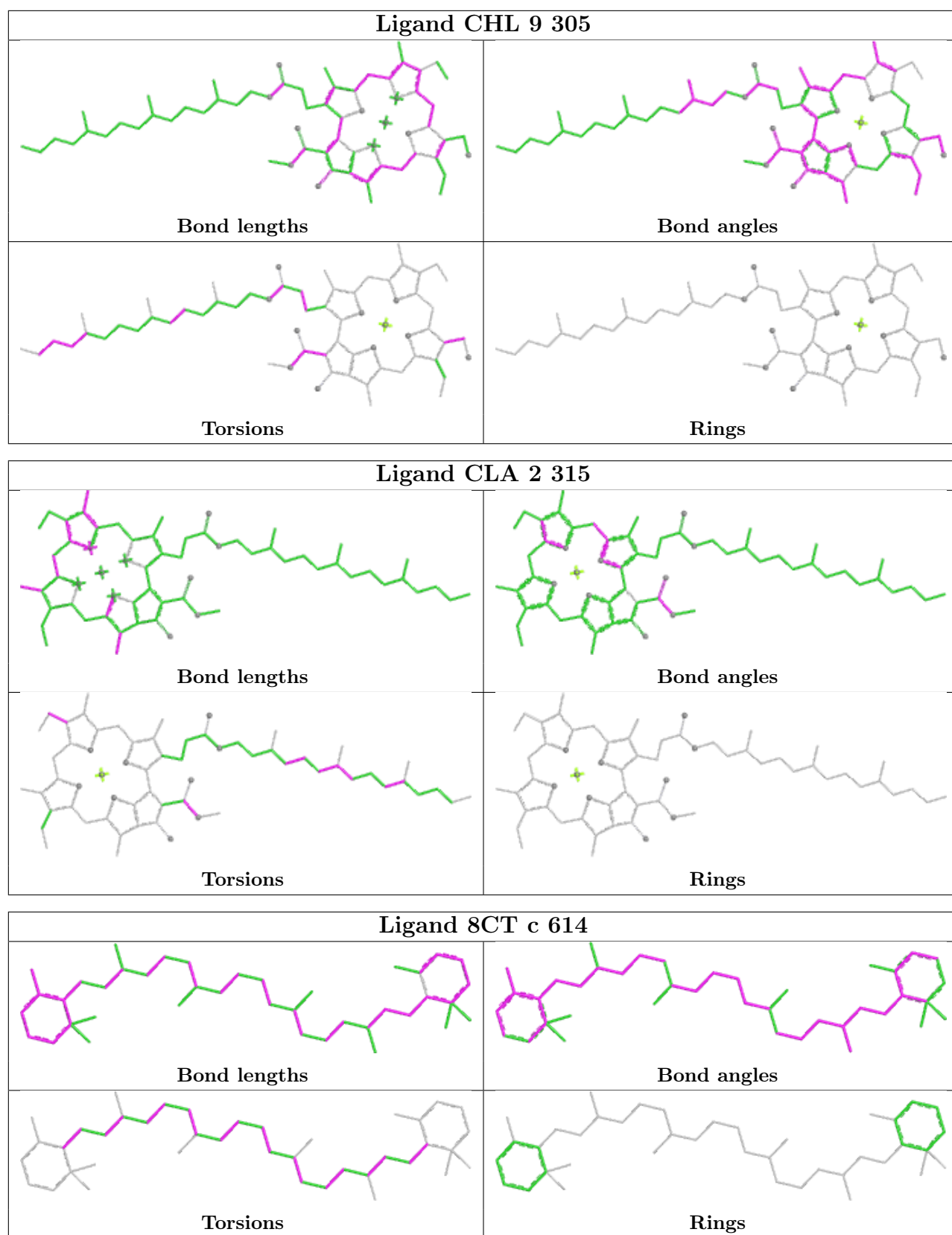
Bond angles



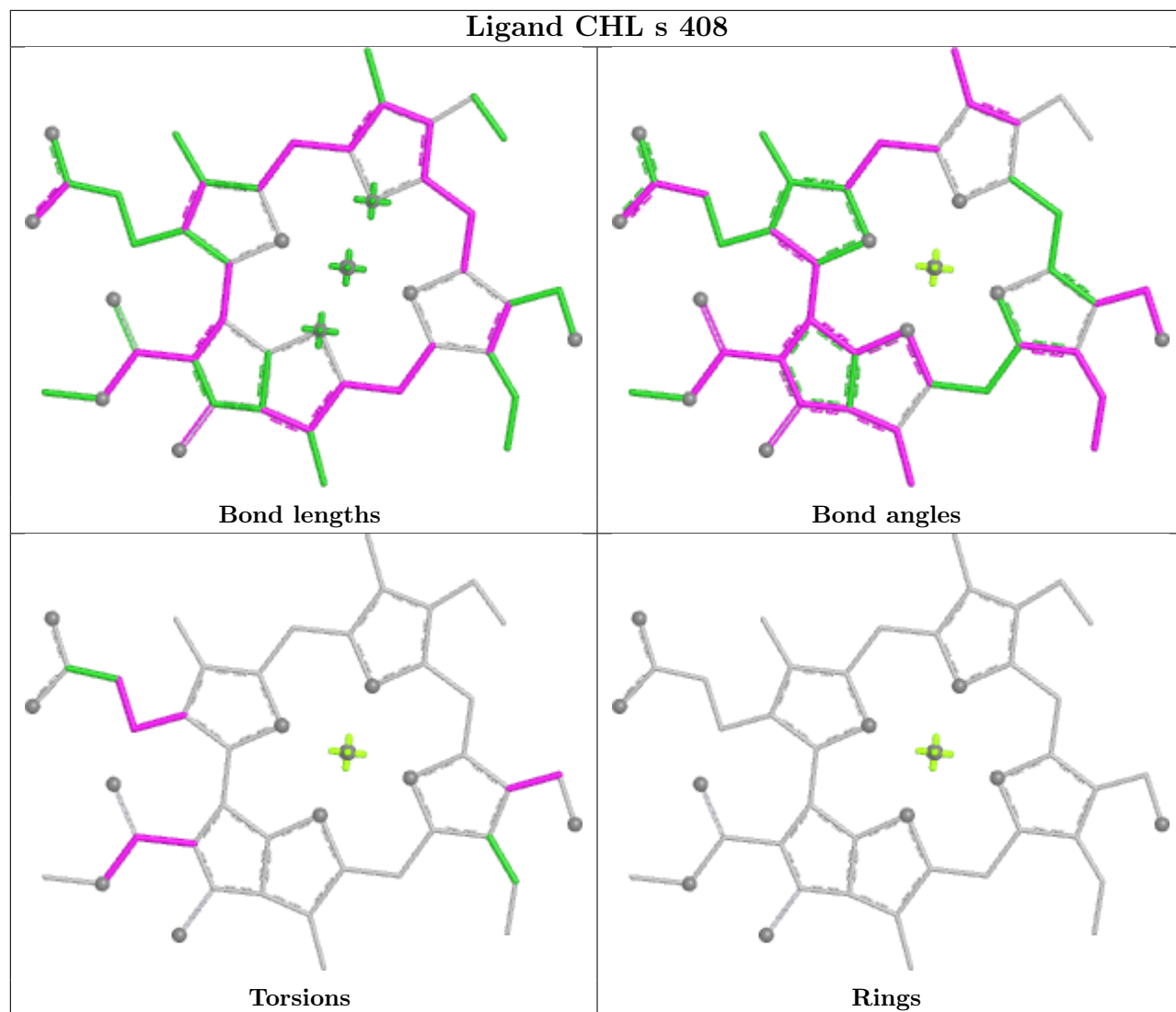
Torsions



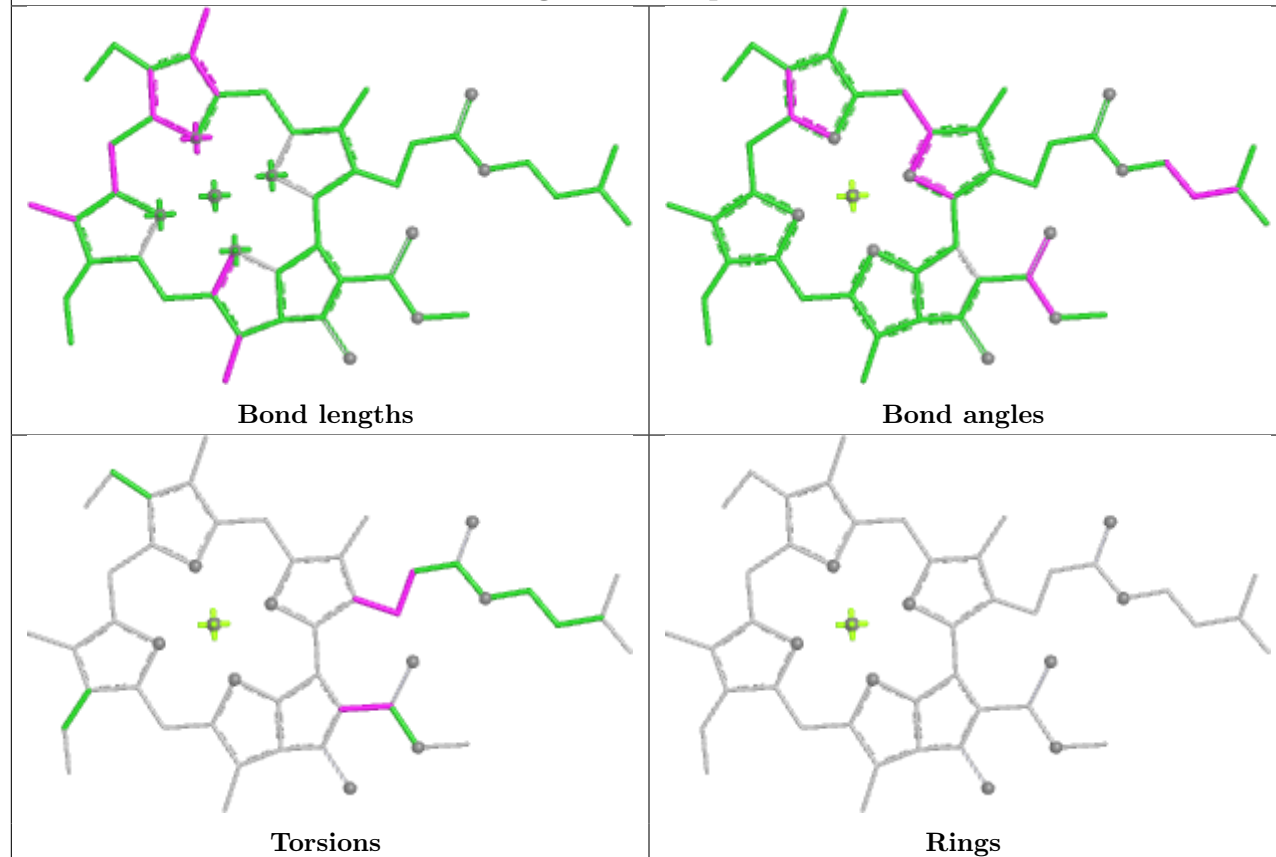
Rings



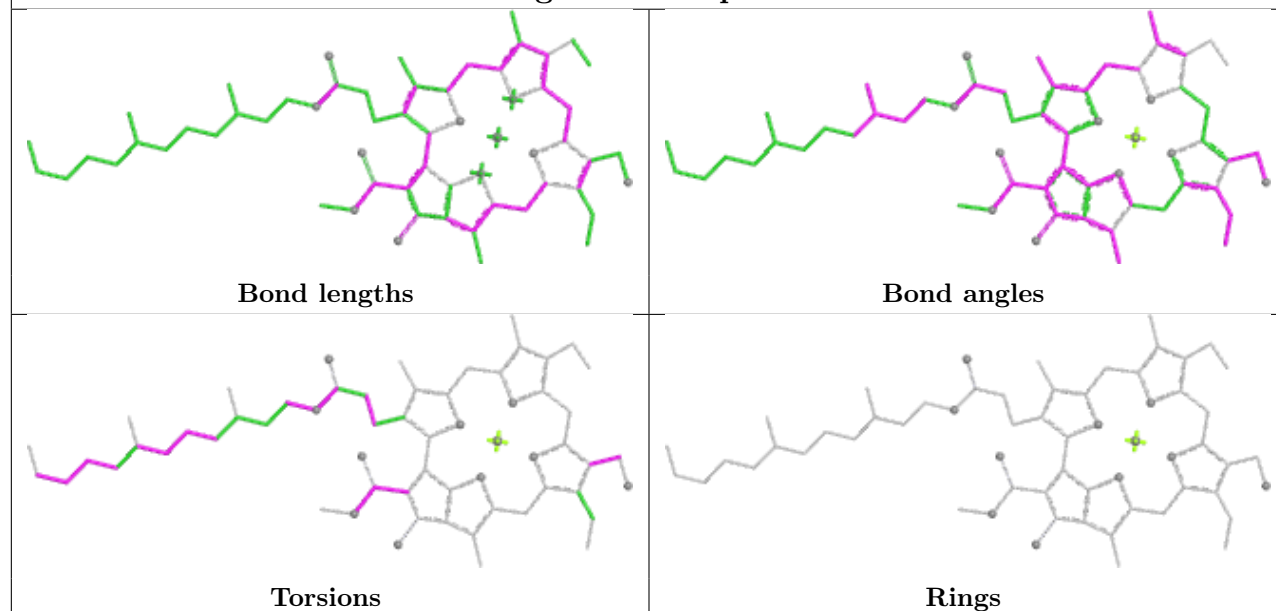
Ligand CHL s 408



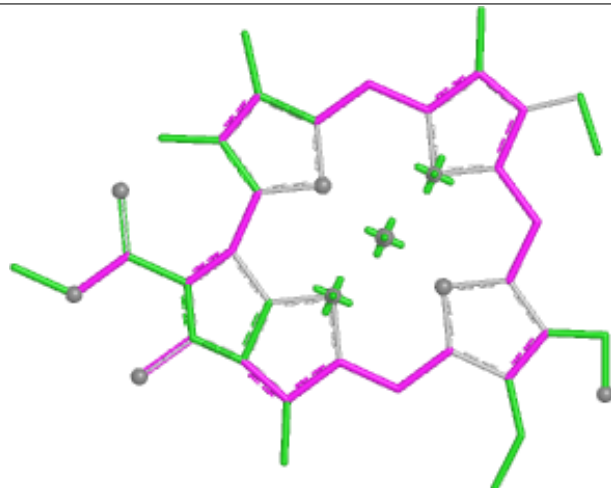
Ligand CLA p 308



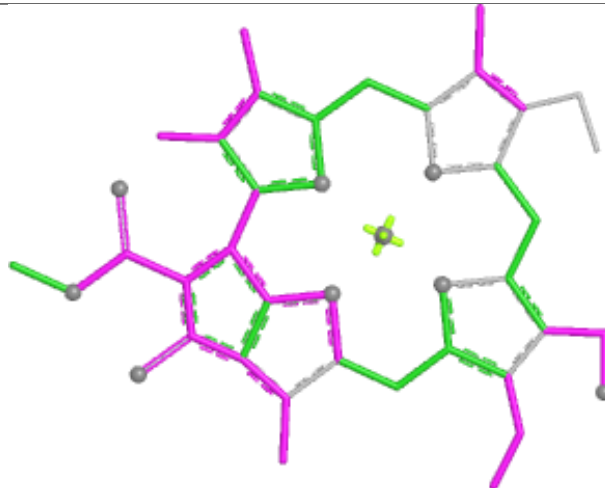
Ligand CHL q 304



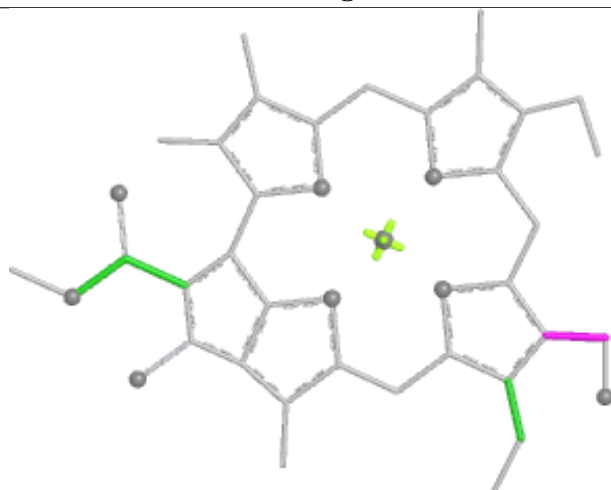
Ligand CHL 3 317



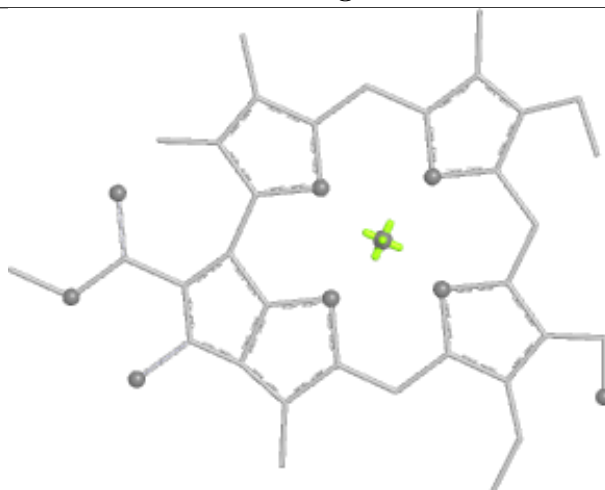
Bond lengths



Bond angles

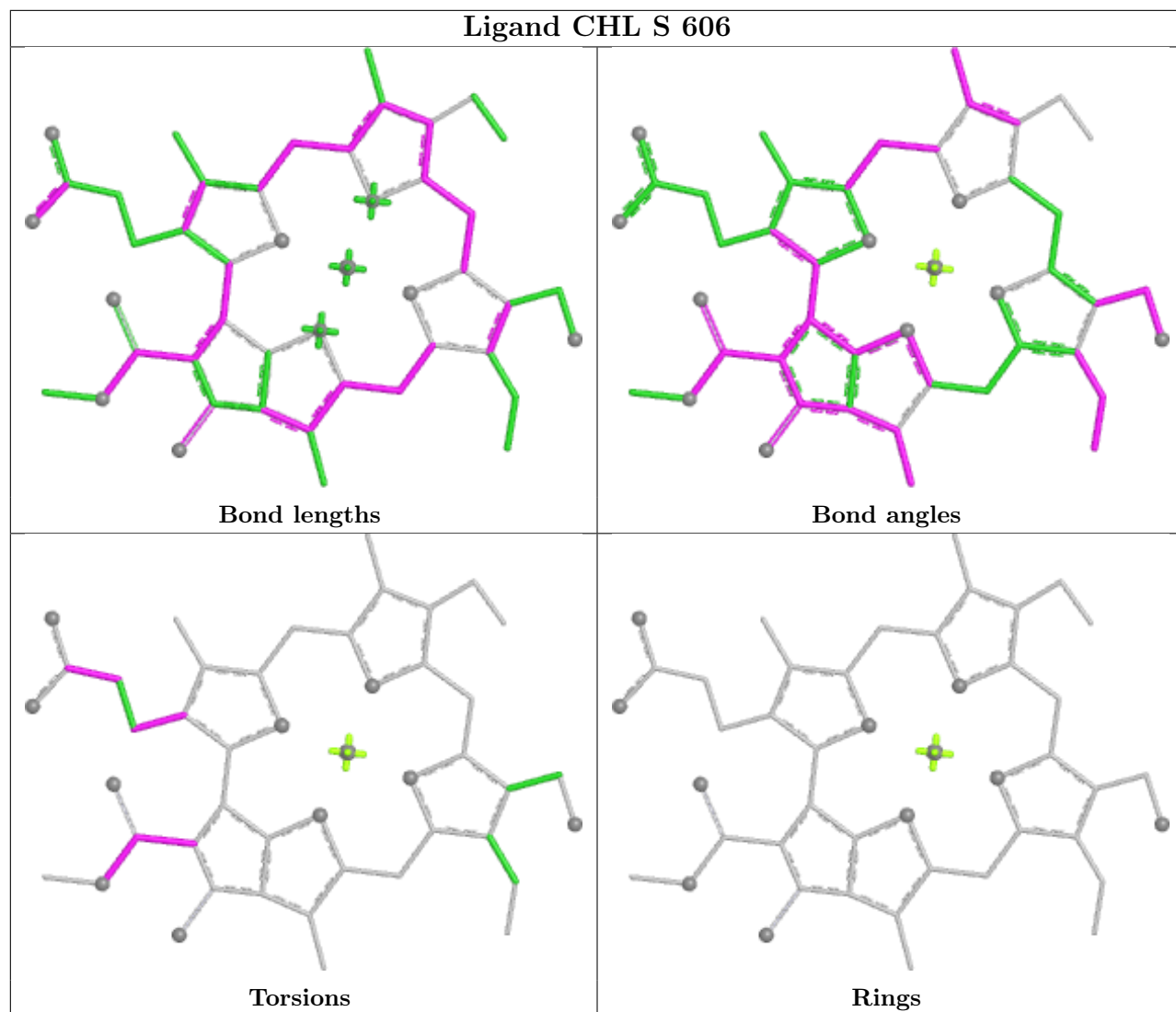


Torsions

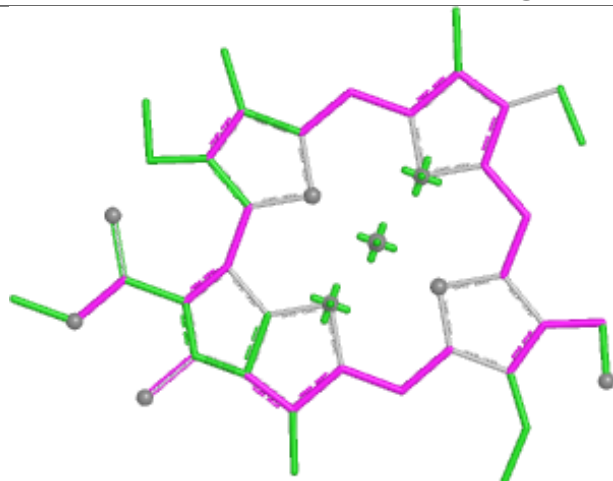


Rings

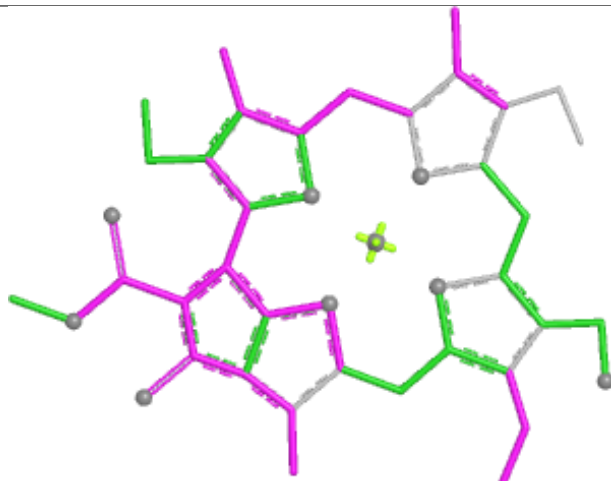
Ligand CHL S 606



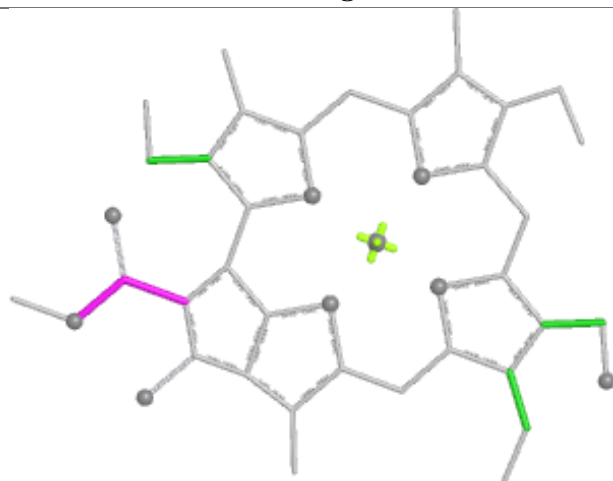
Ligand CHL 3 308



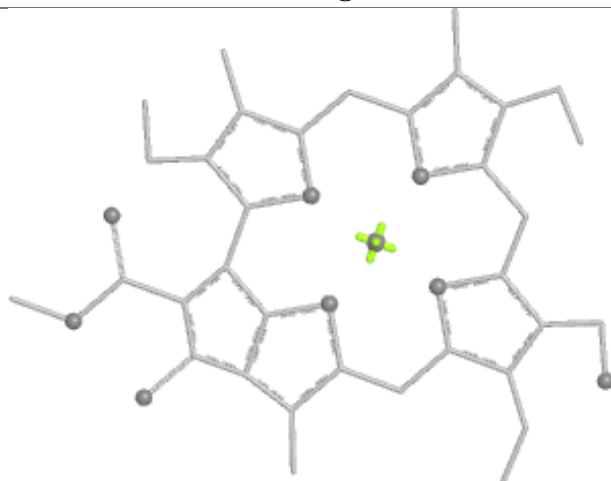
Bond lengths



Bond angles

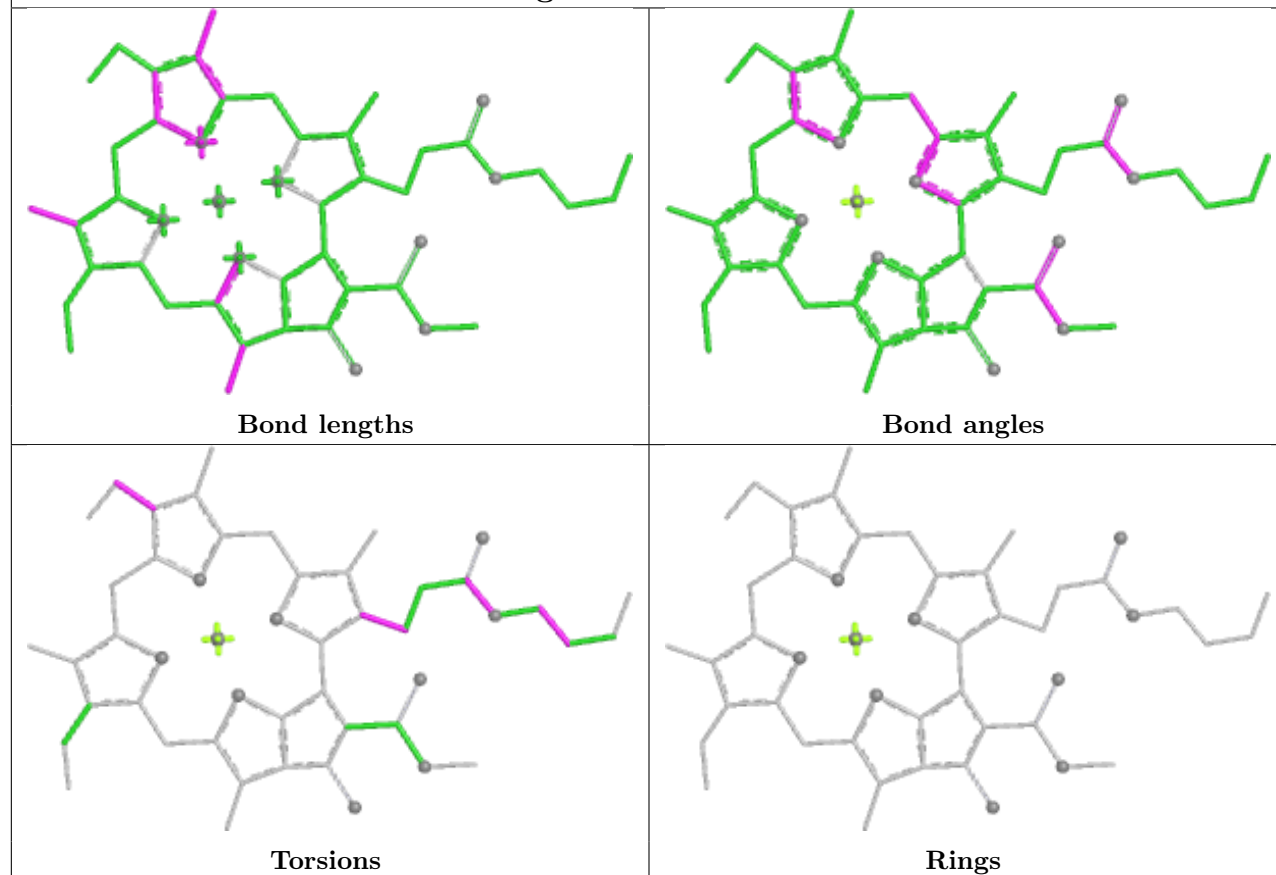


Torsions

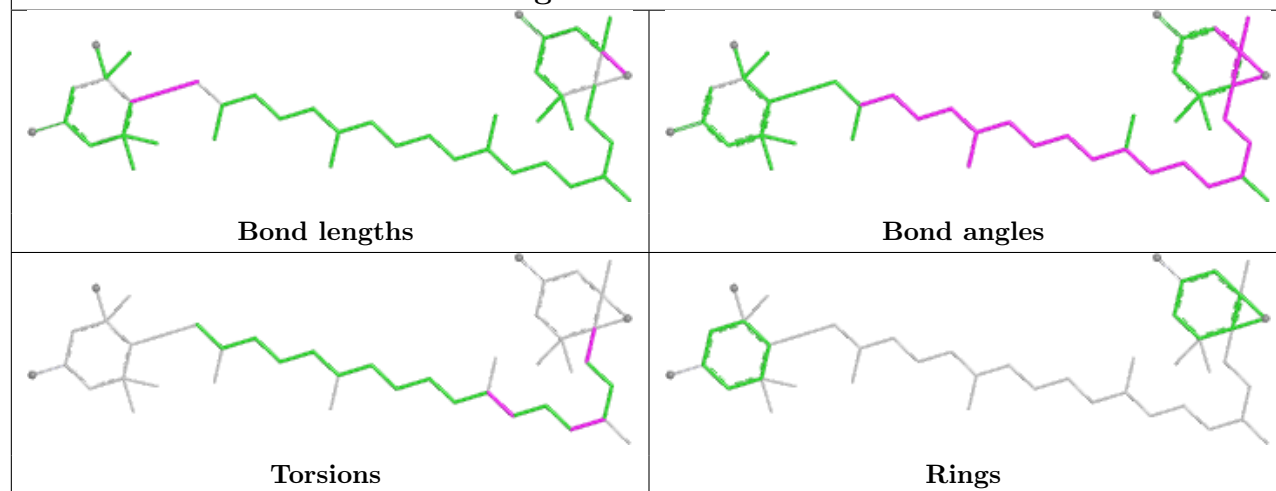


Rings

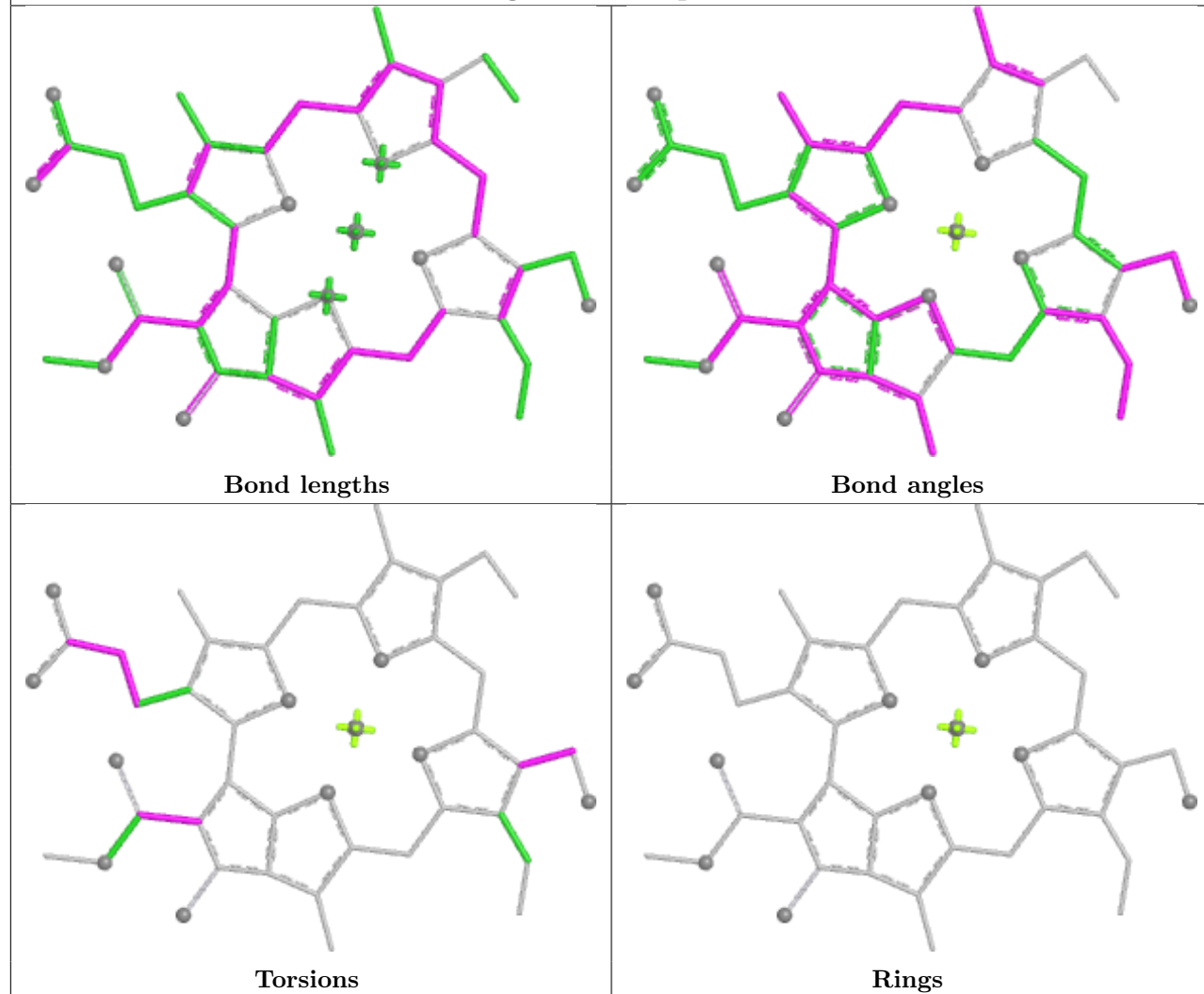
Ligand CLA a 605



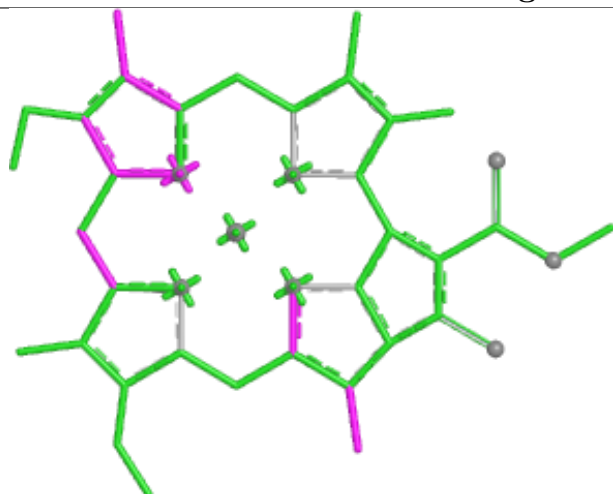
Ligand NEX 4 303



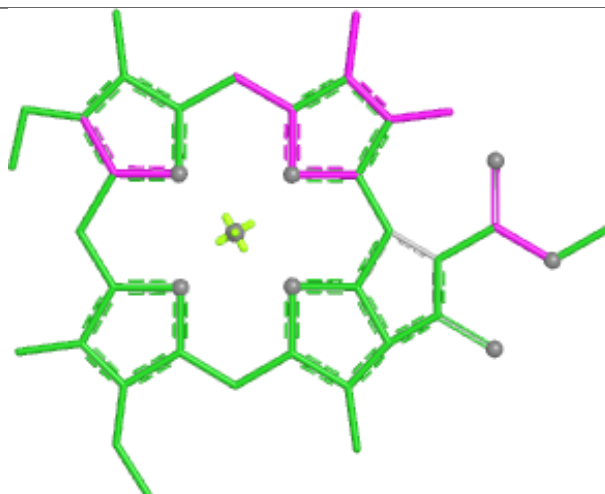
Ligand CHL q 308



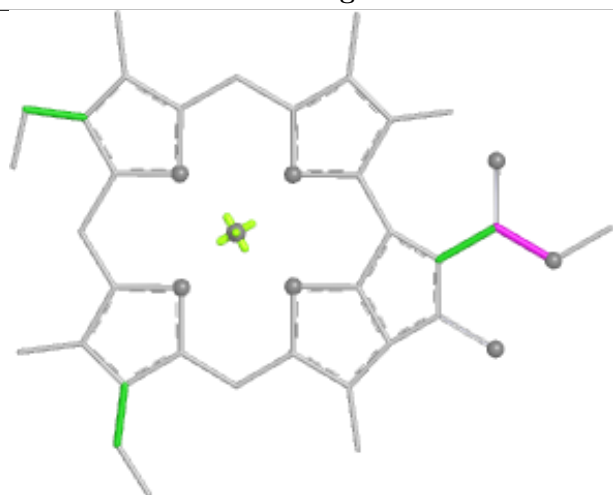
Ligand CLA 3 313



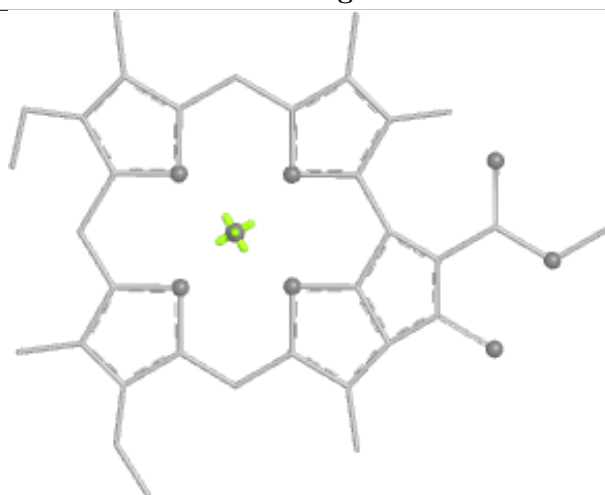
Bond lengths



Bond angles

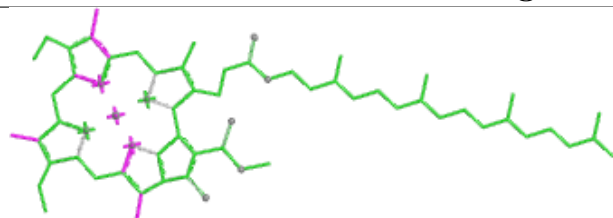


Torsions

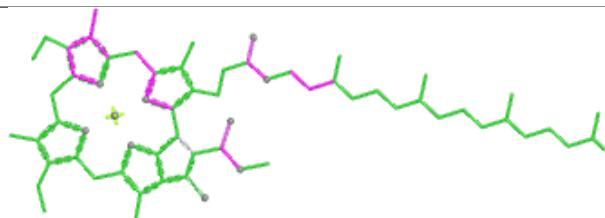


Rings

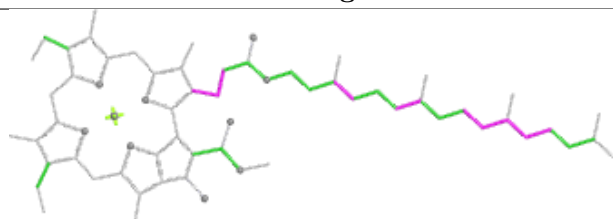
Ligand CLA b 603



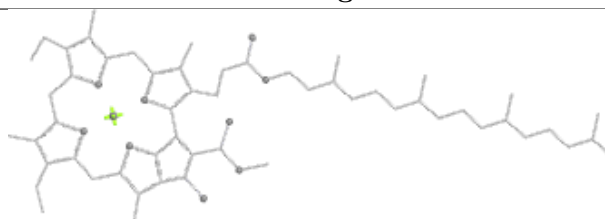
Bond lengths



Bond angles

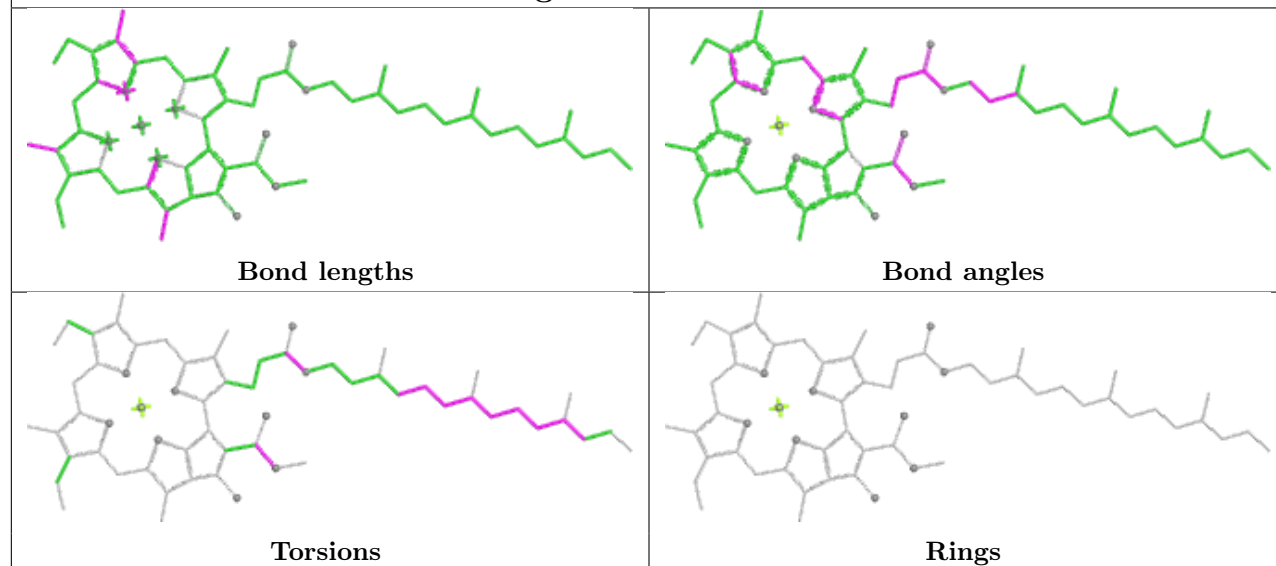


Torsions

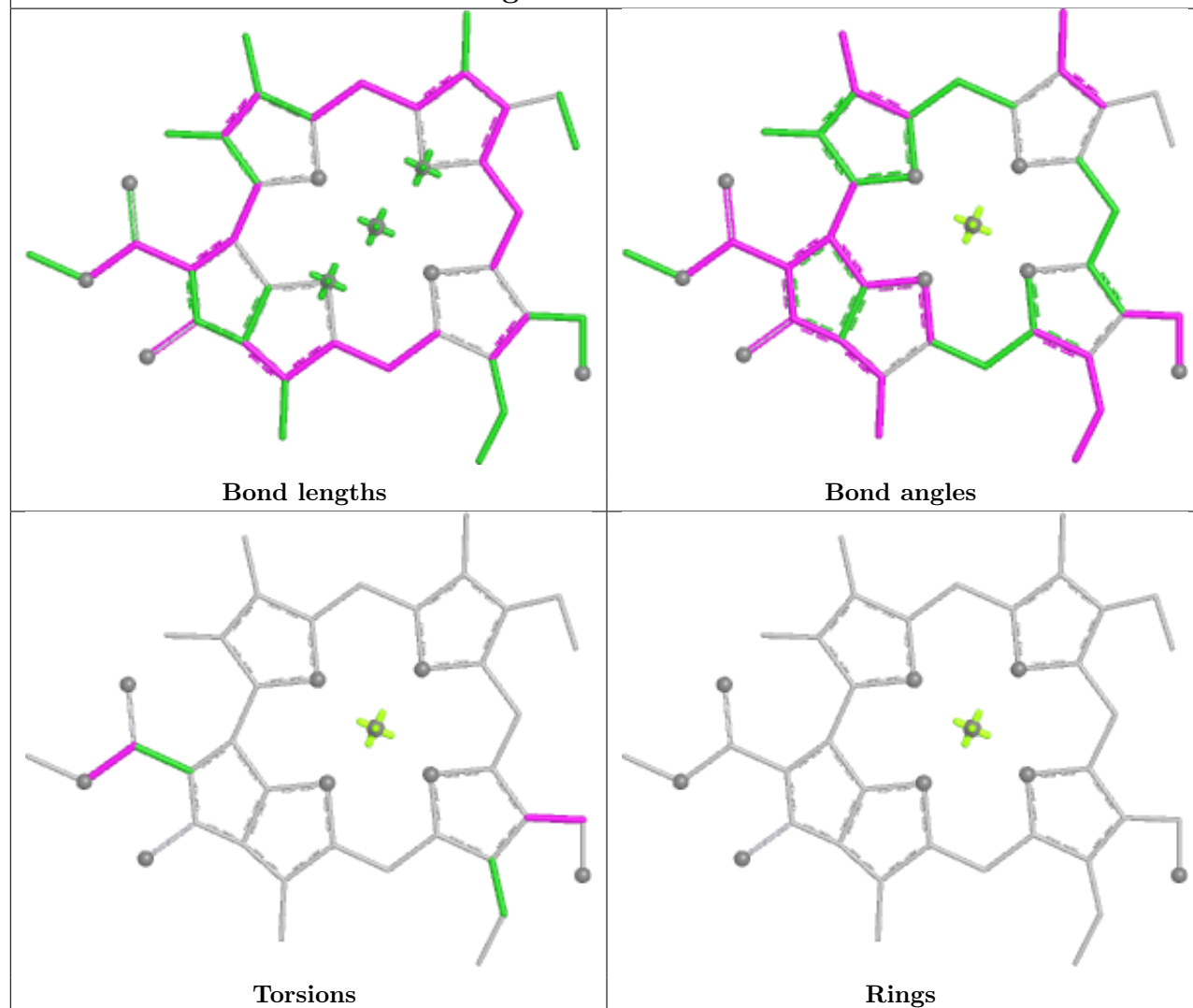


Rings

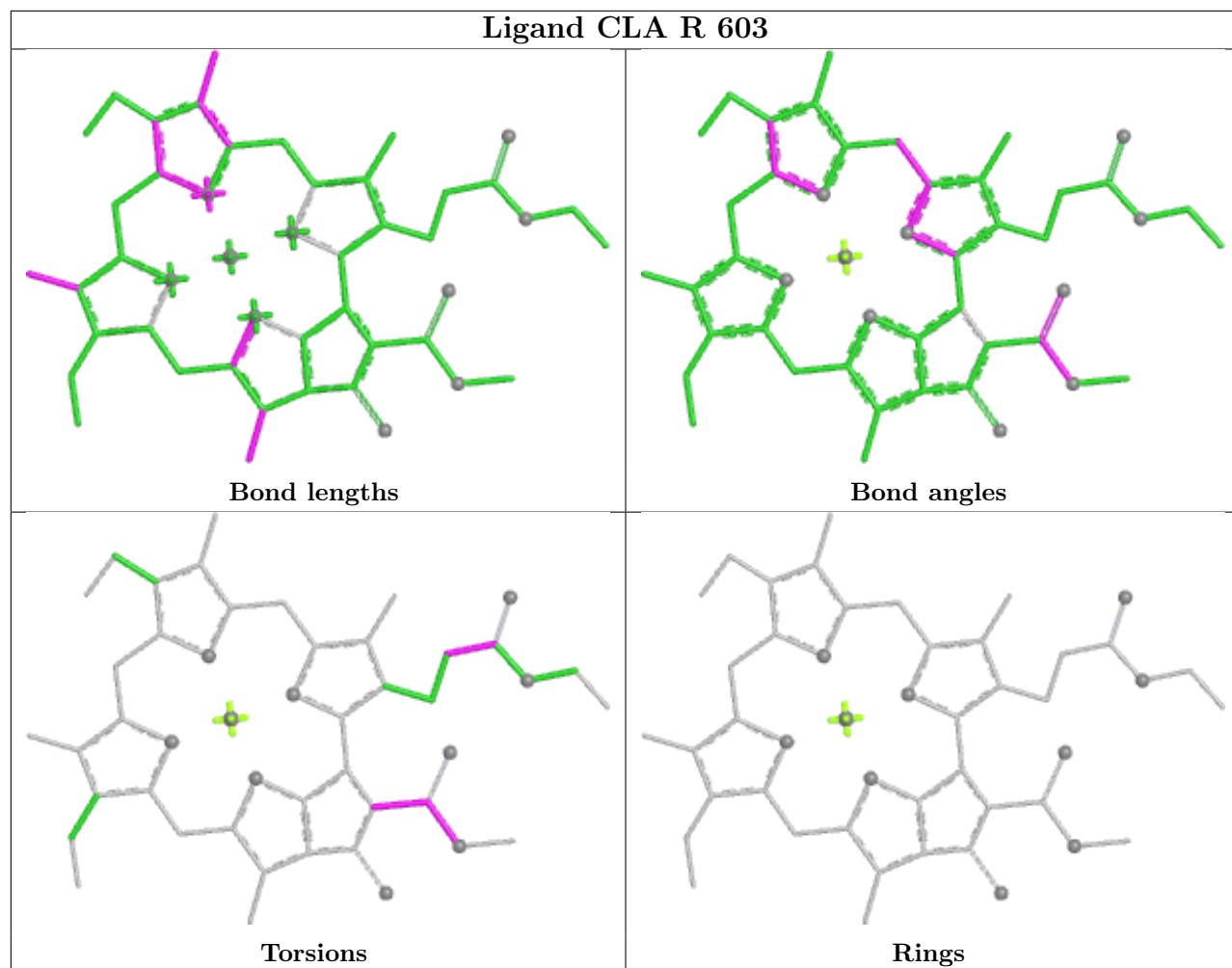
Ligand CLA b 604



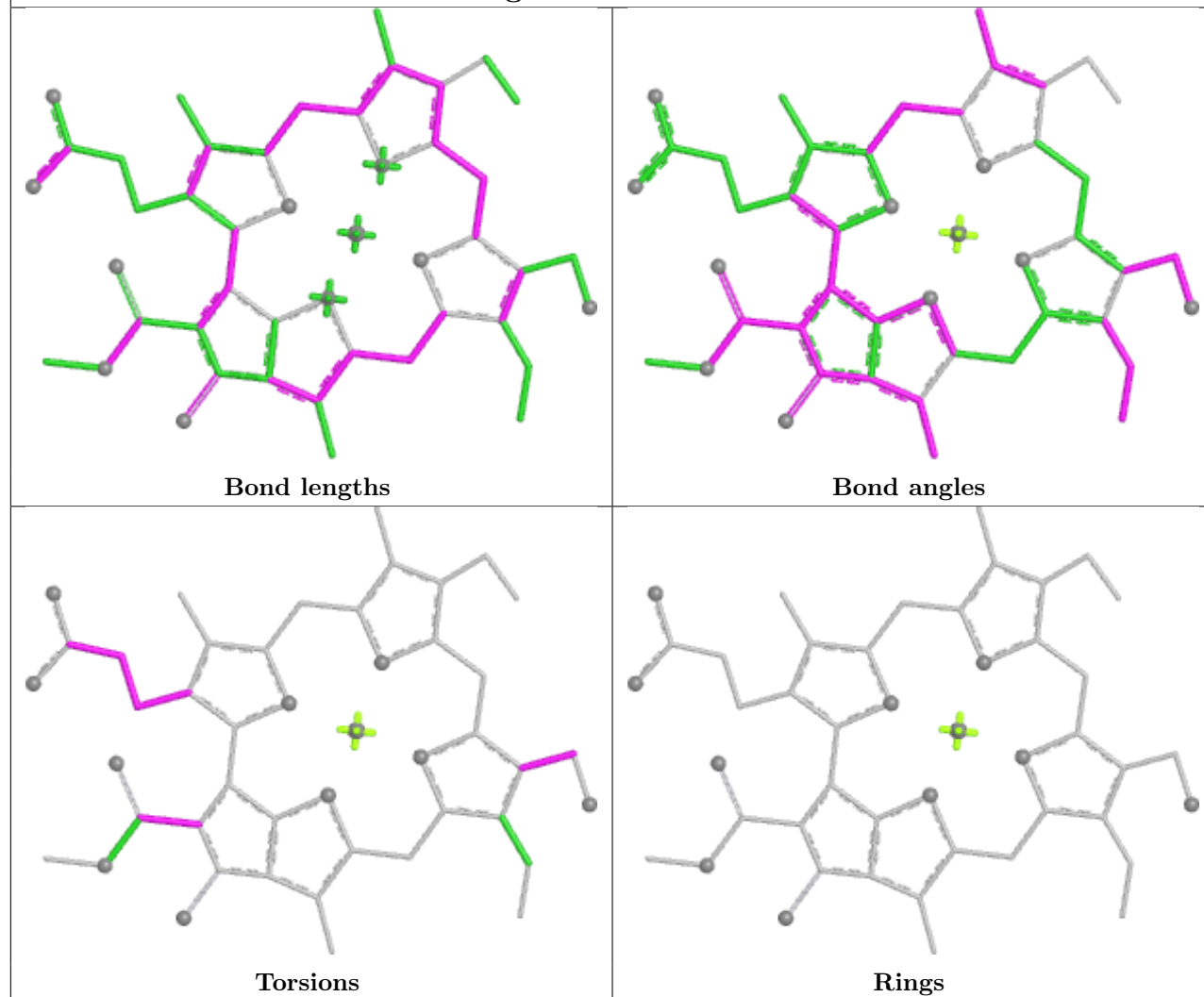
Ligand CHL r 306



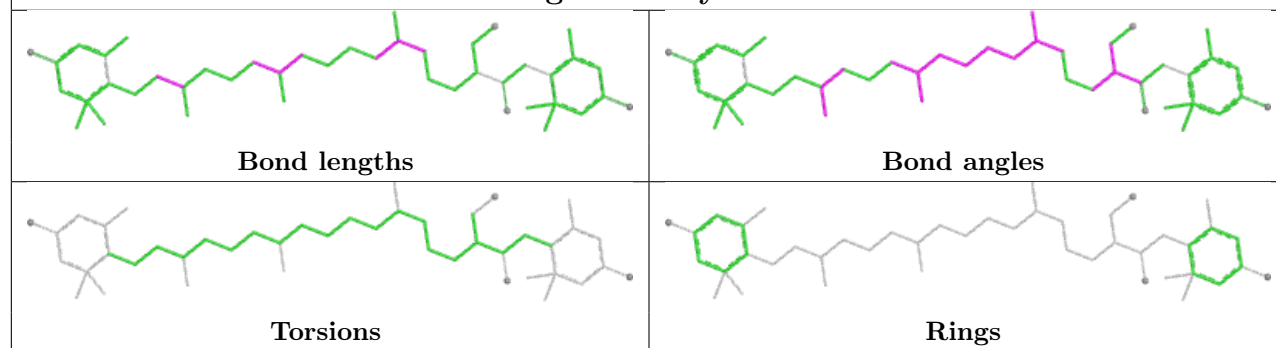
Ligand CLA R 603



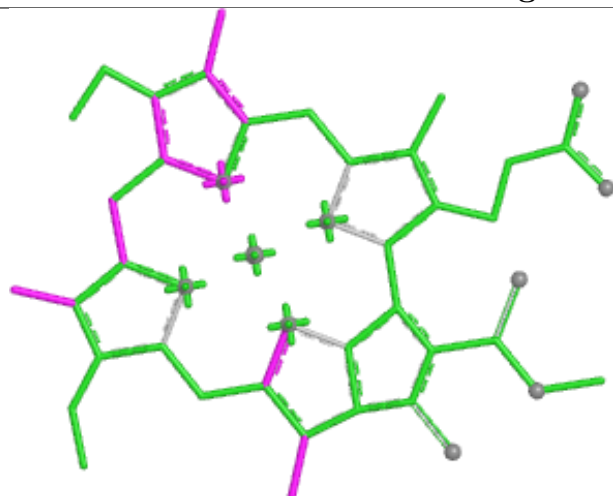
Ligand CHL 4 305



Ligand OIE y 303



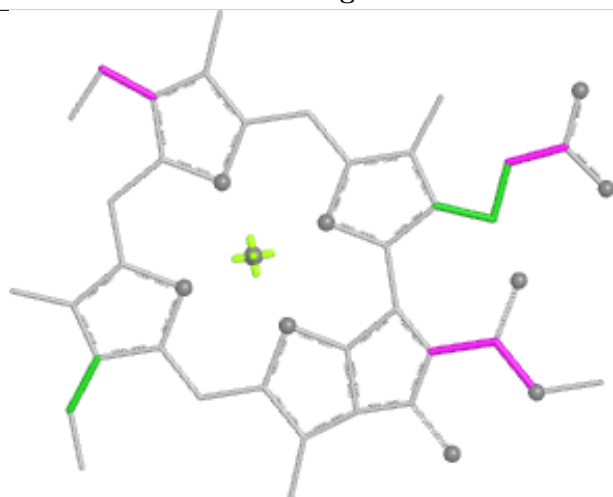
Ligand CLA 1 315



Bond lengths



Bond angles

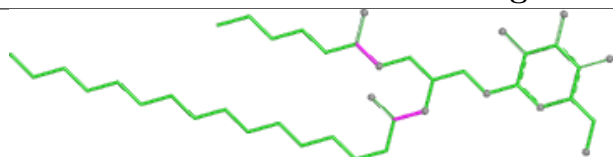


Torsions

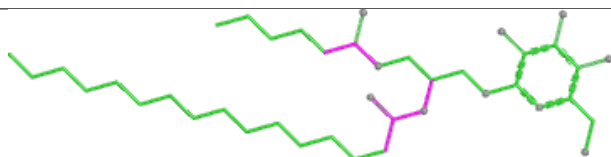


Rings

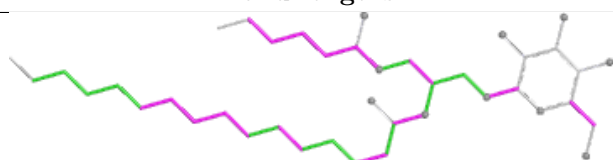
Ligand LMG B 619



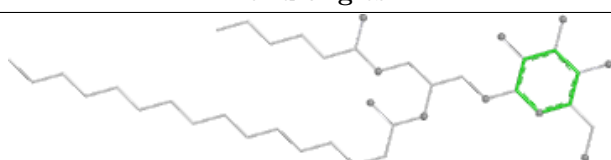
Bond lengths



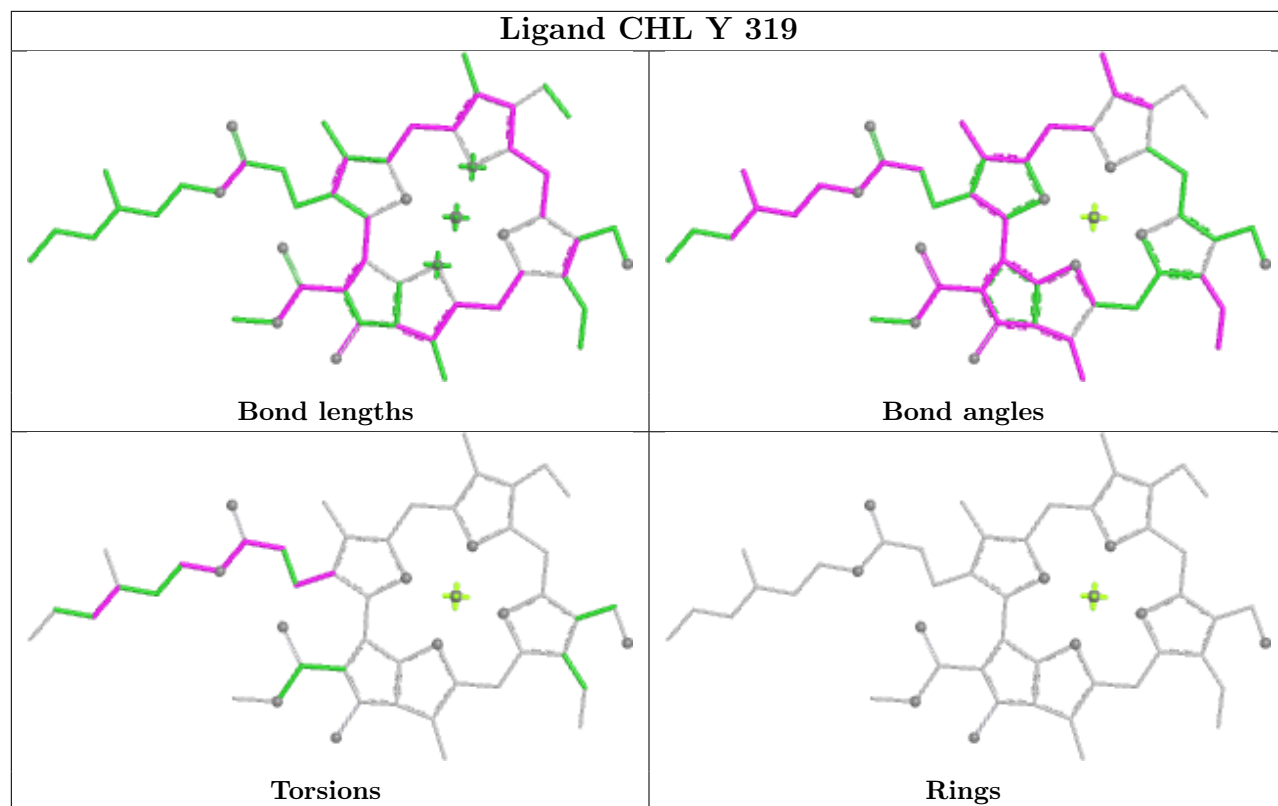
Bond angles



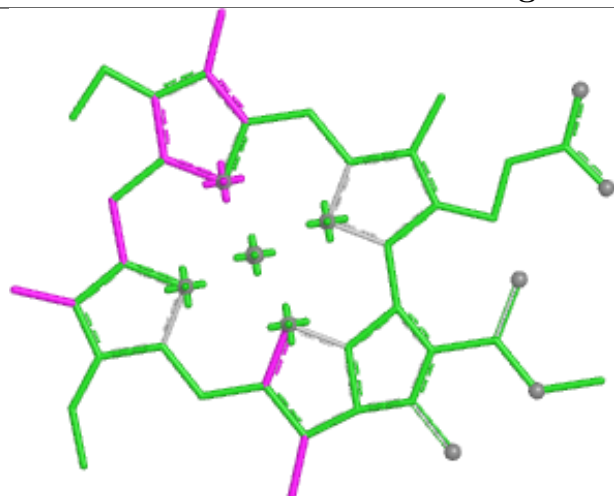
Torsions



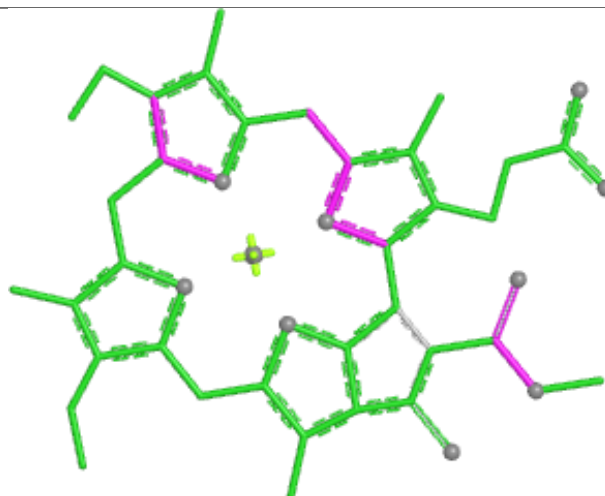
Rings



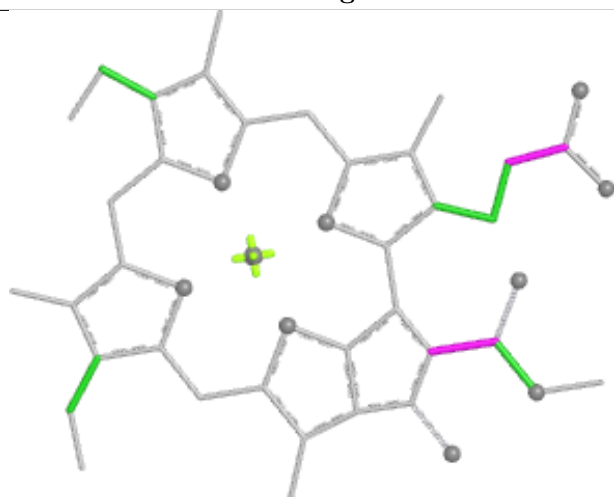
Ligand CLA 5 316



Bond lengths



Bond angles

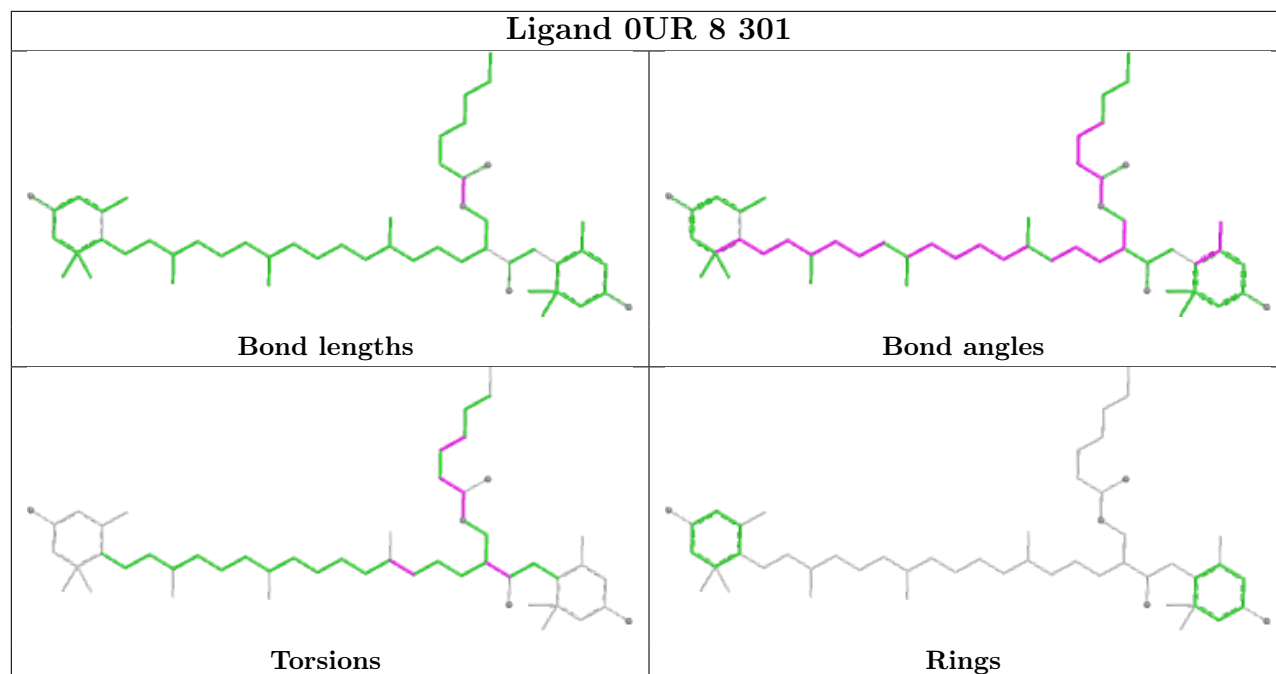


Torsions

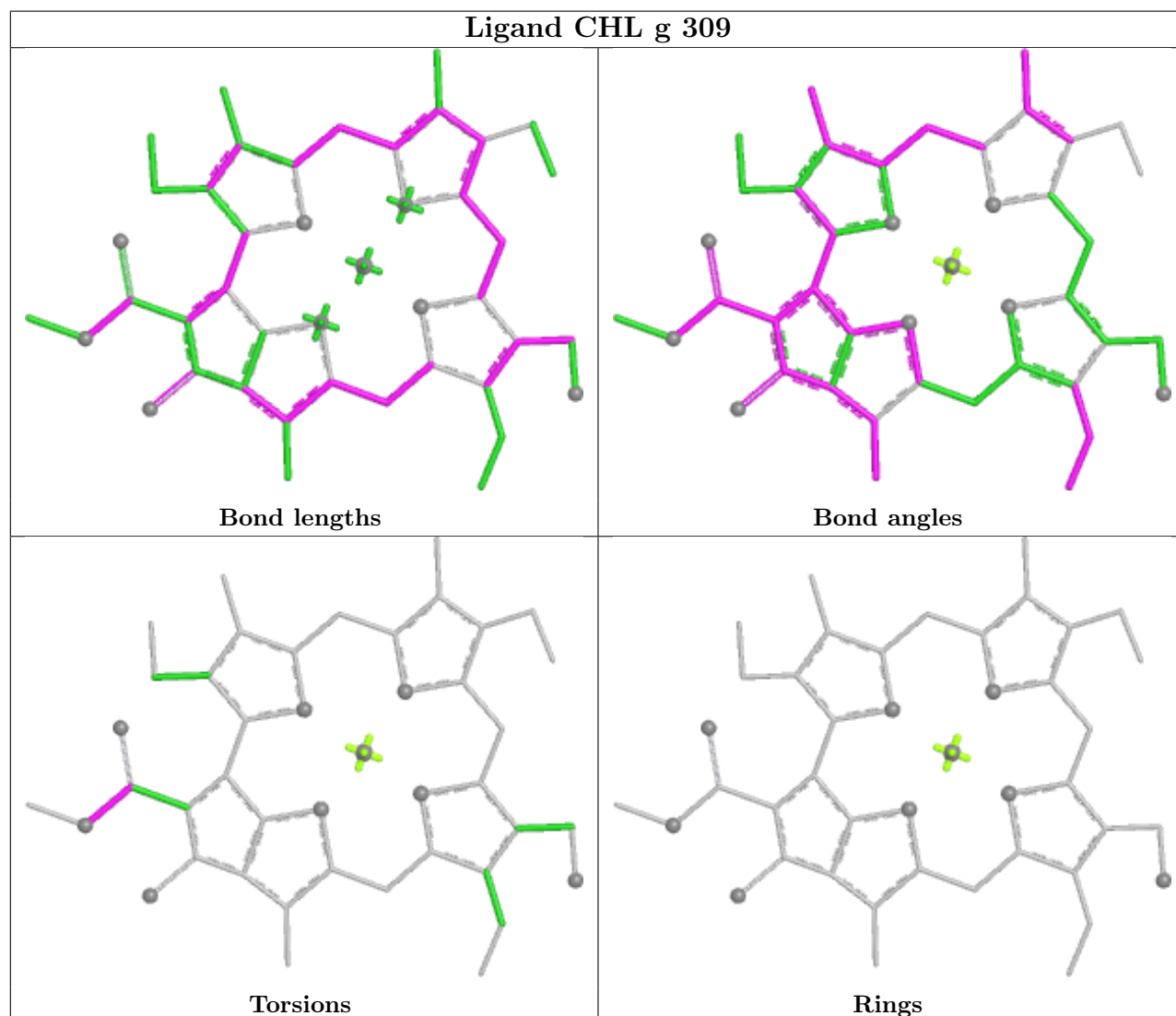


Rings

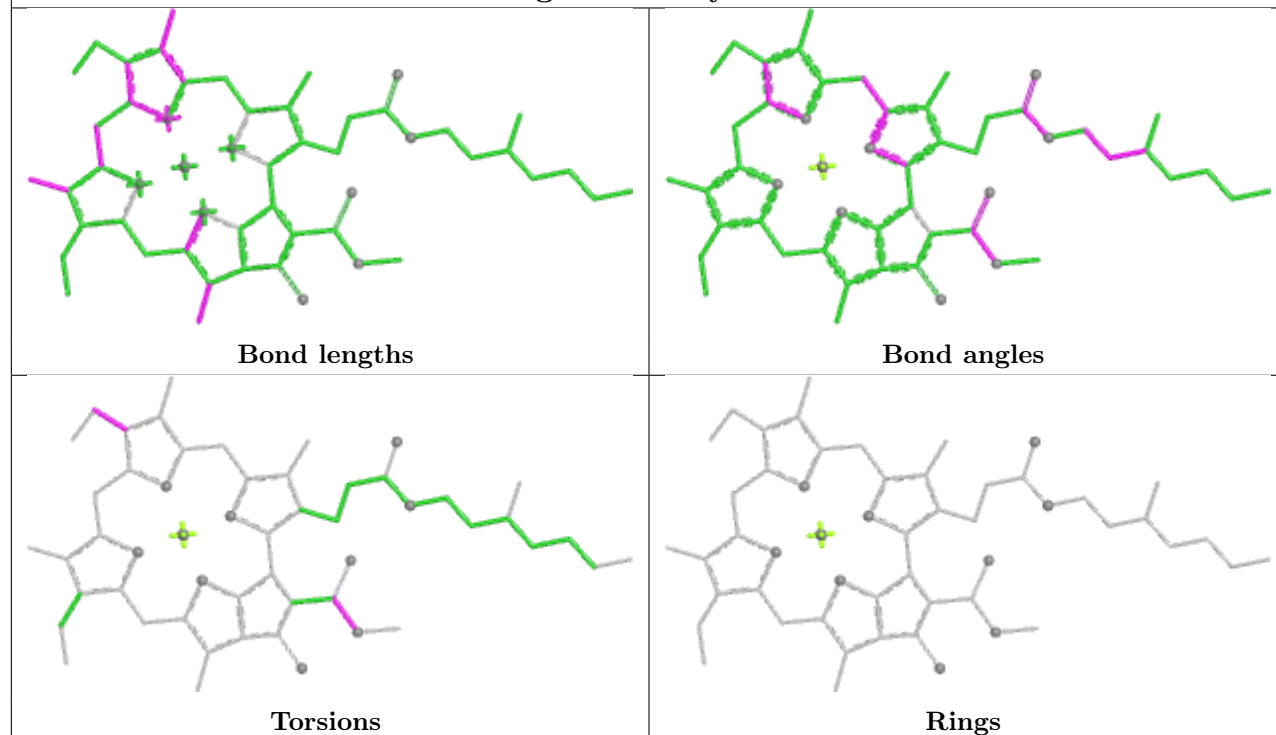
Ligand OUR 8 301



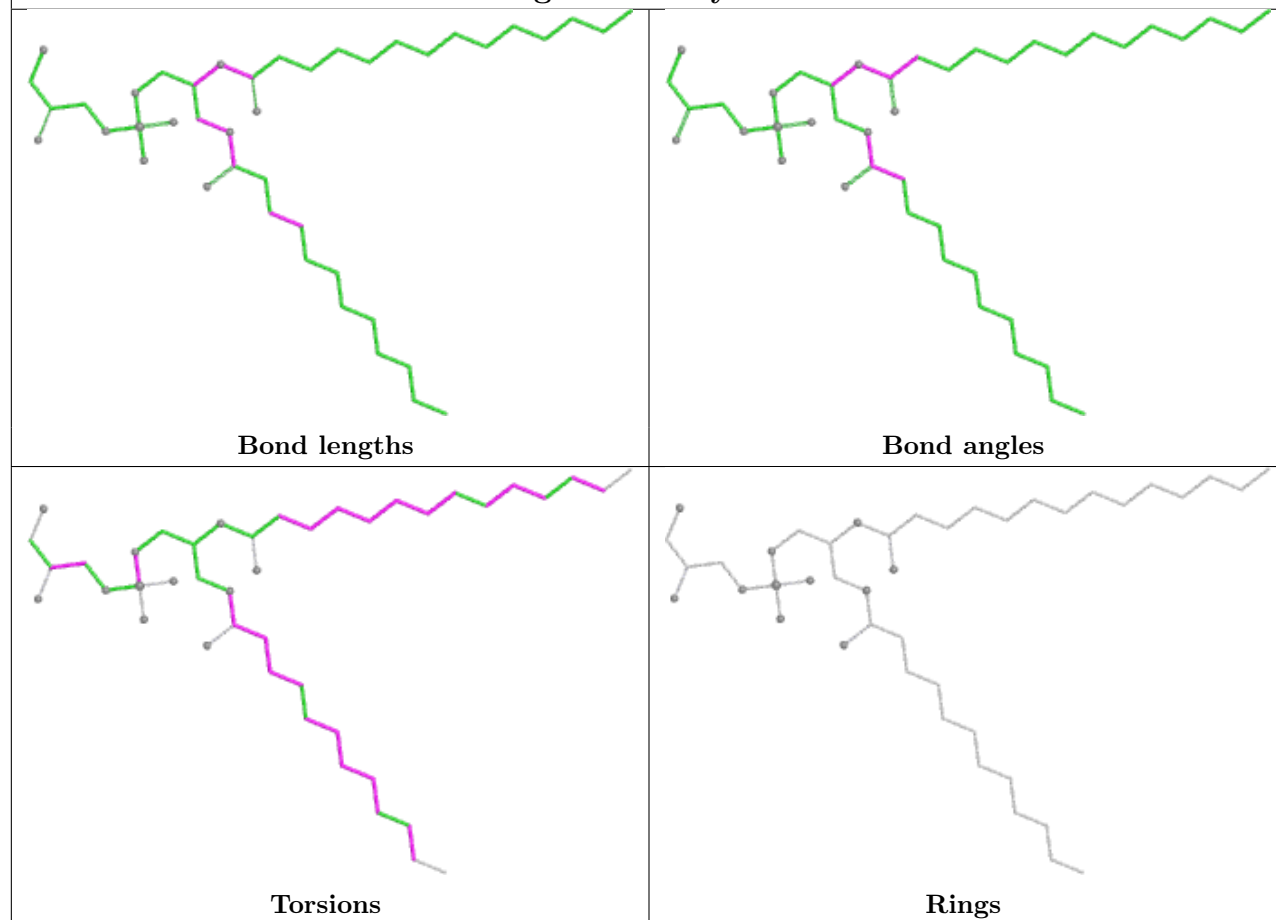
Ligand CHL g 309

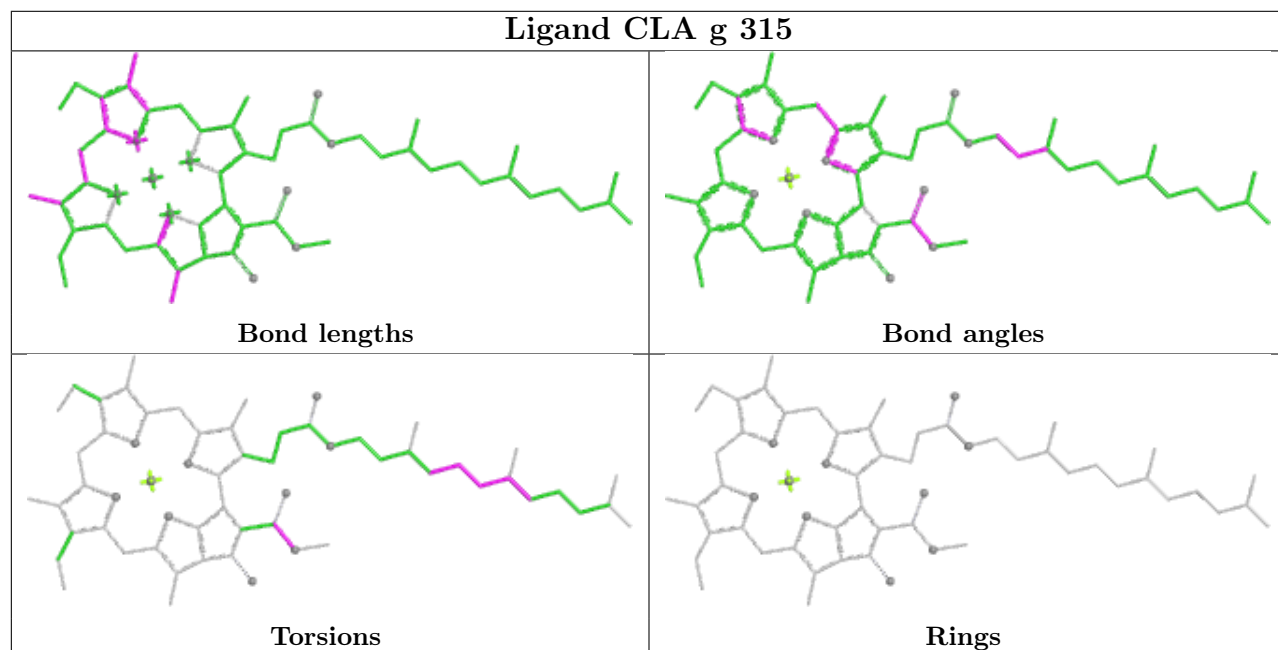
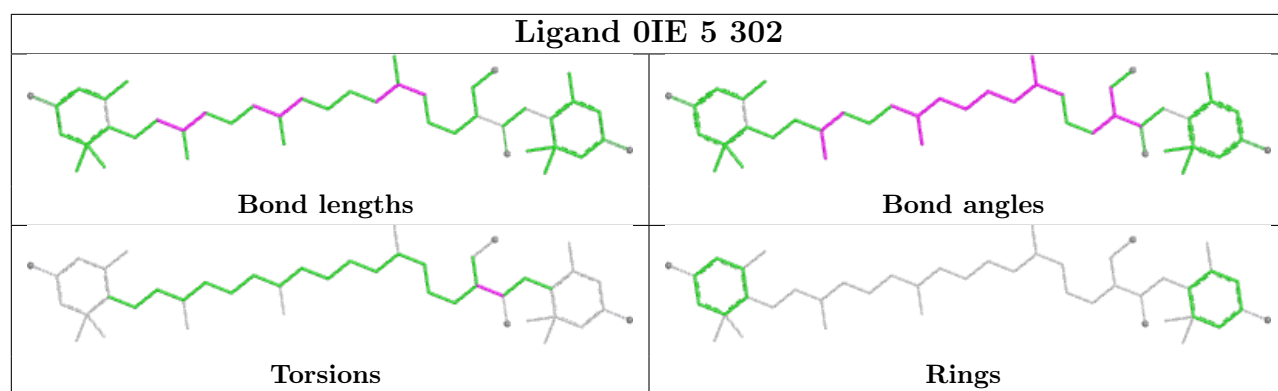


Ligand CLA y 307

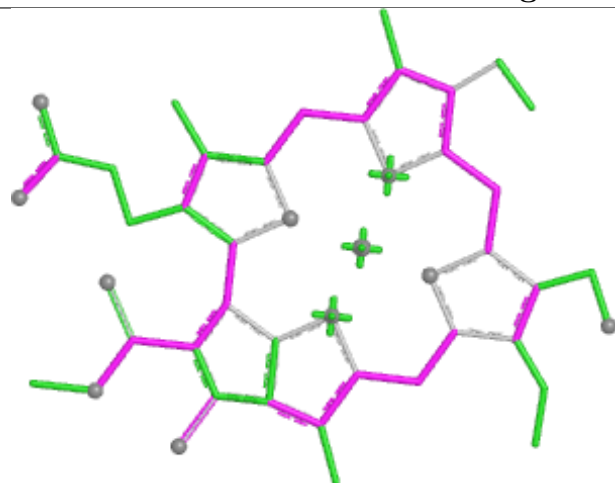


Ligand LHG y 319

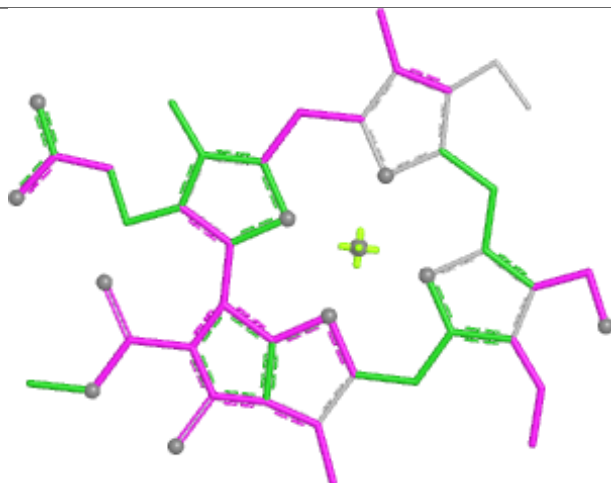




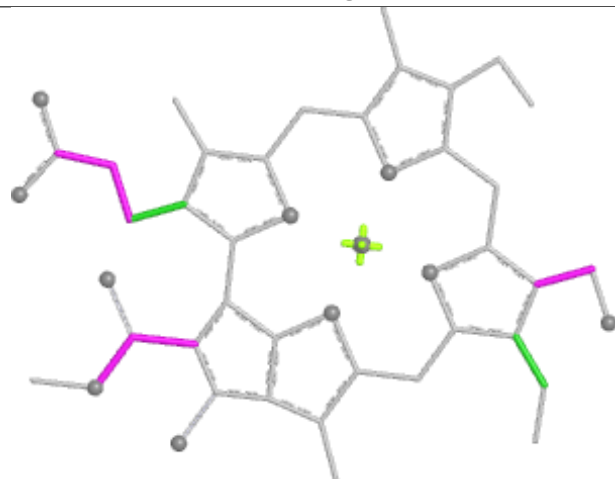
Ligand CHL 2 312



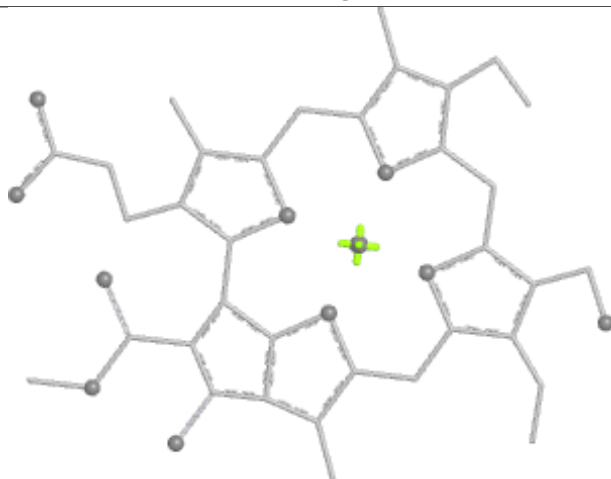
Bond lengths



Bond angles

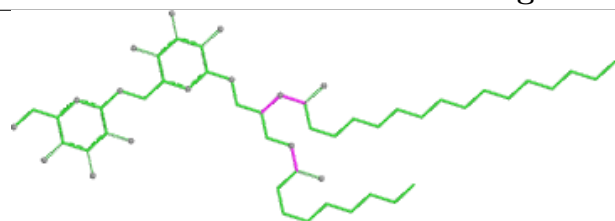


Torsions

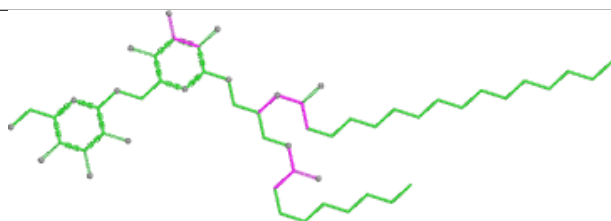


Rings

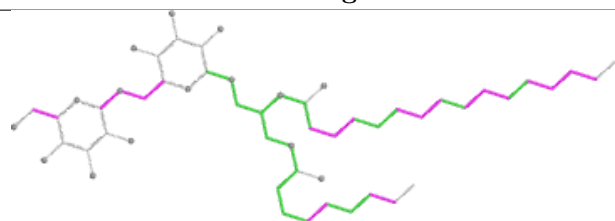
Ligand DGD c 619



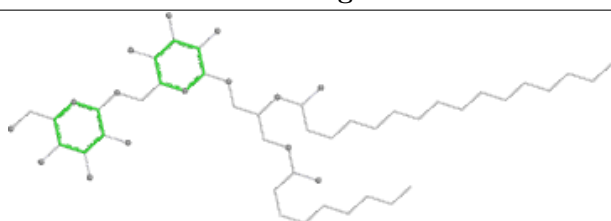
Bond lengths



Bond angles

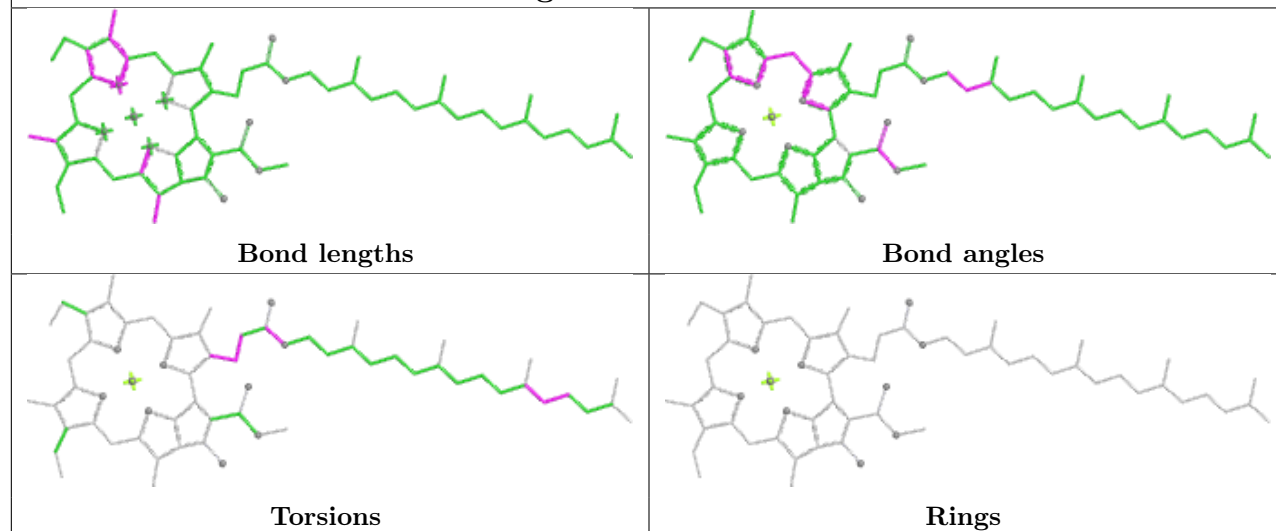


Torsions

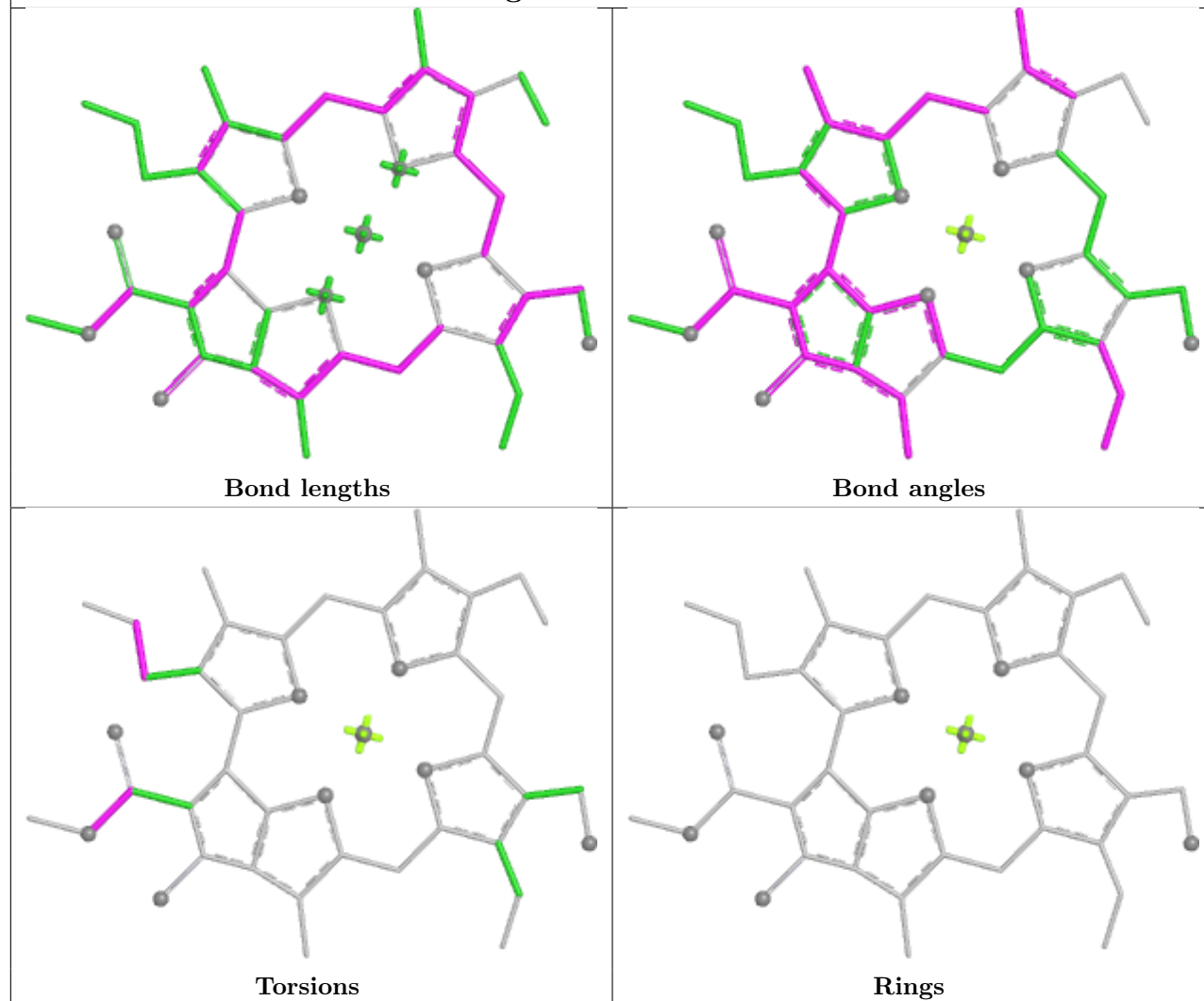


Rings

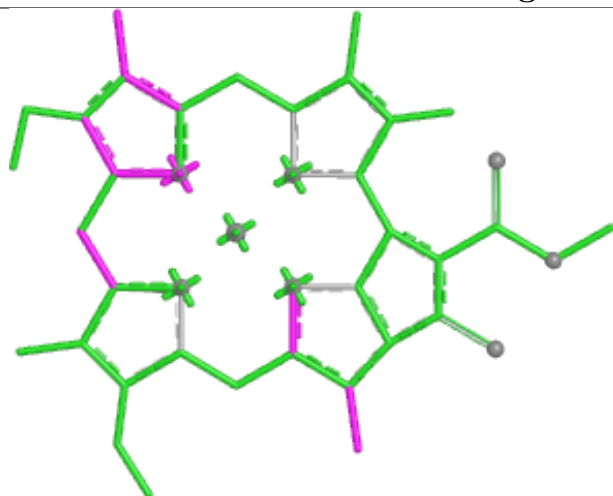
Ligand CLA a 604



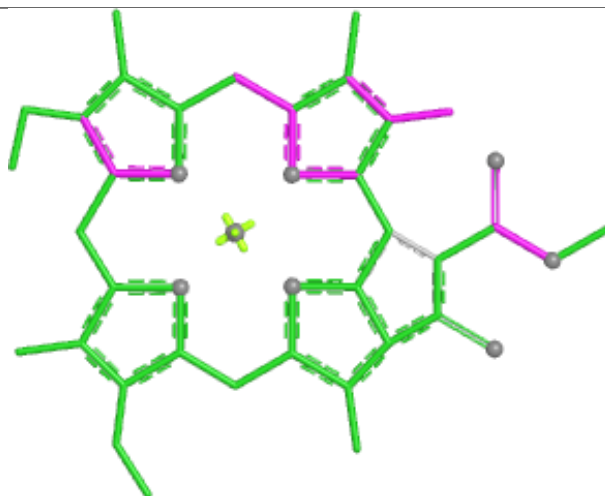
Ligand CHL 4 311



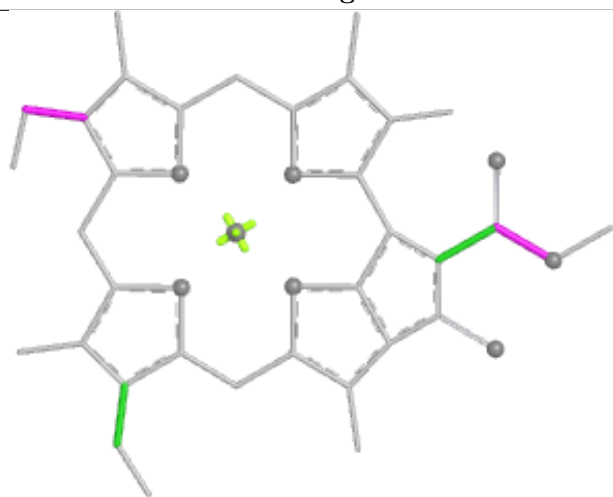
Ligand CLA 4 314



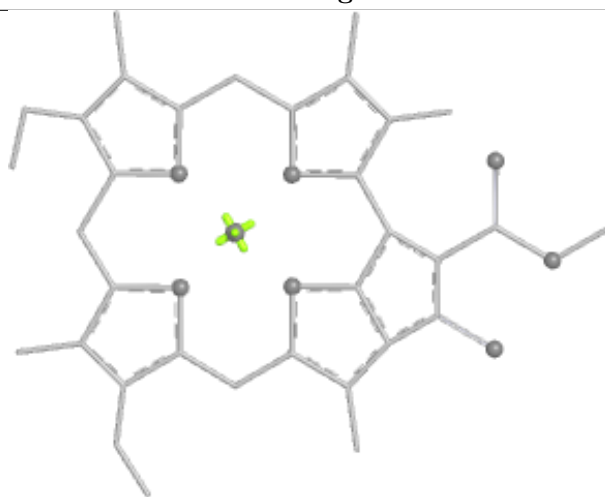
Bond lengths



Bond angles

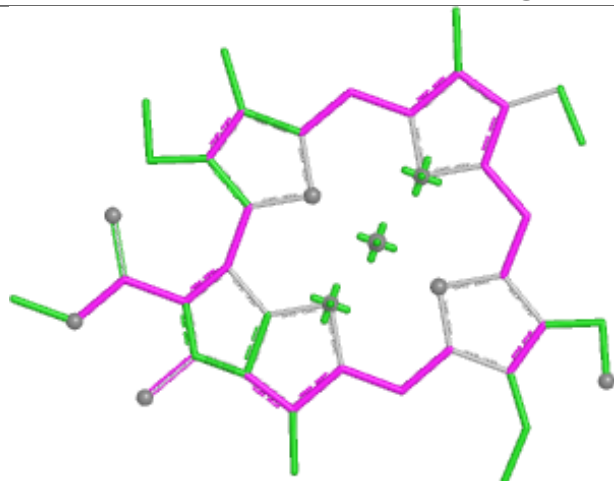


Torsions

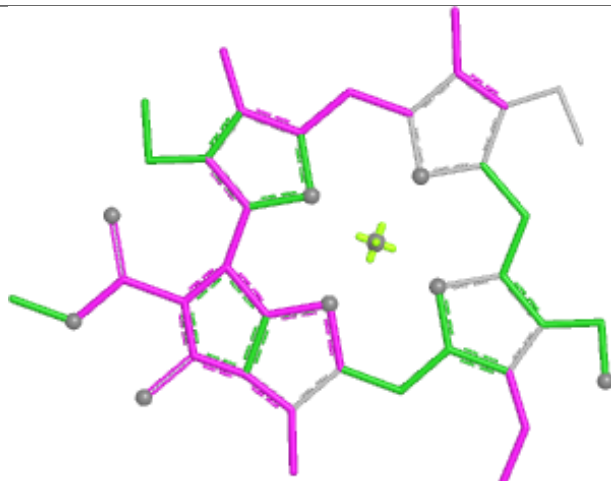


Rings

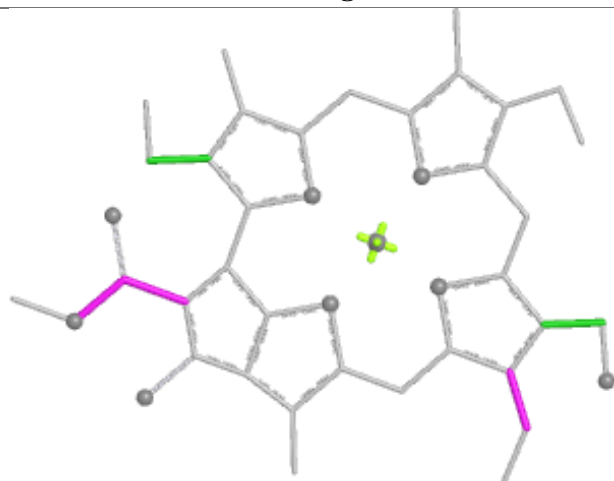
Ligand CHL 7 313



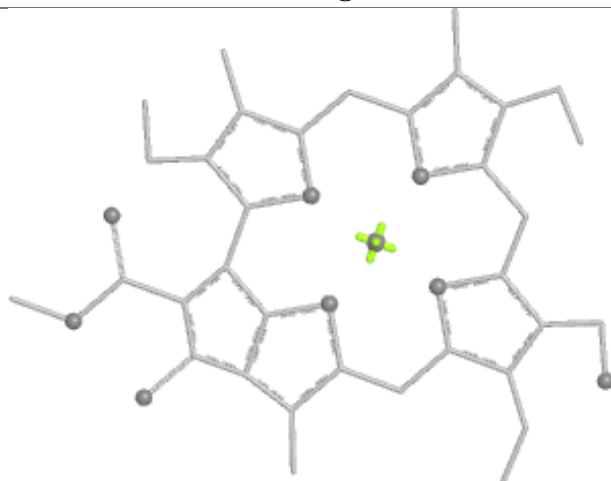
Bond lengths



Bond angles

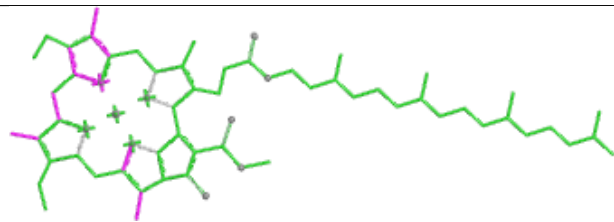


Torsions

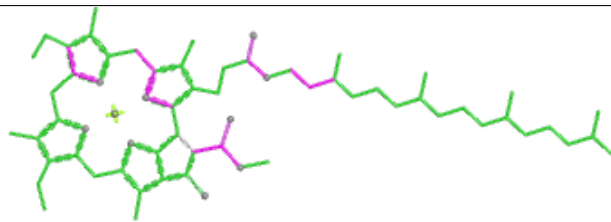


Rings

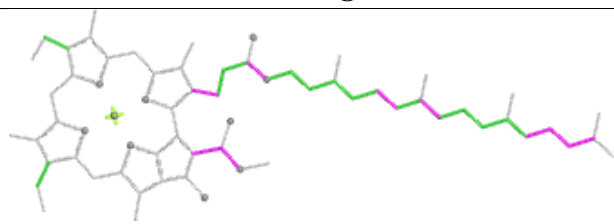
Ligand CLA d 405



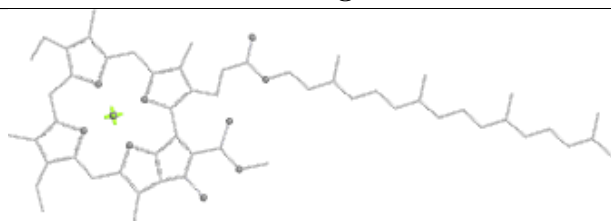
Bond lengths



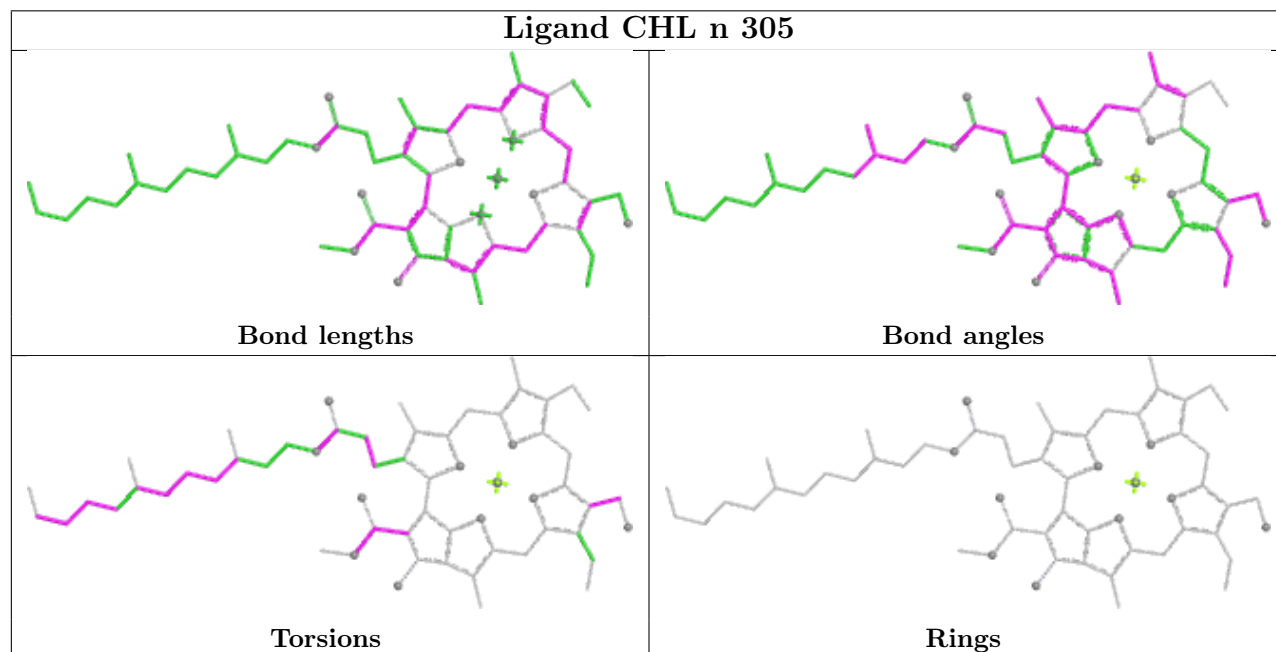
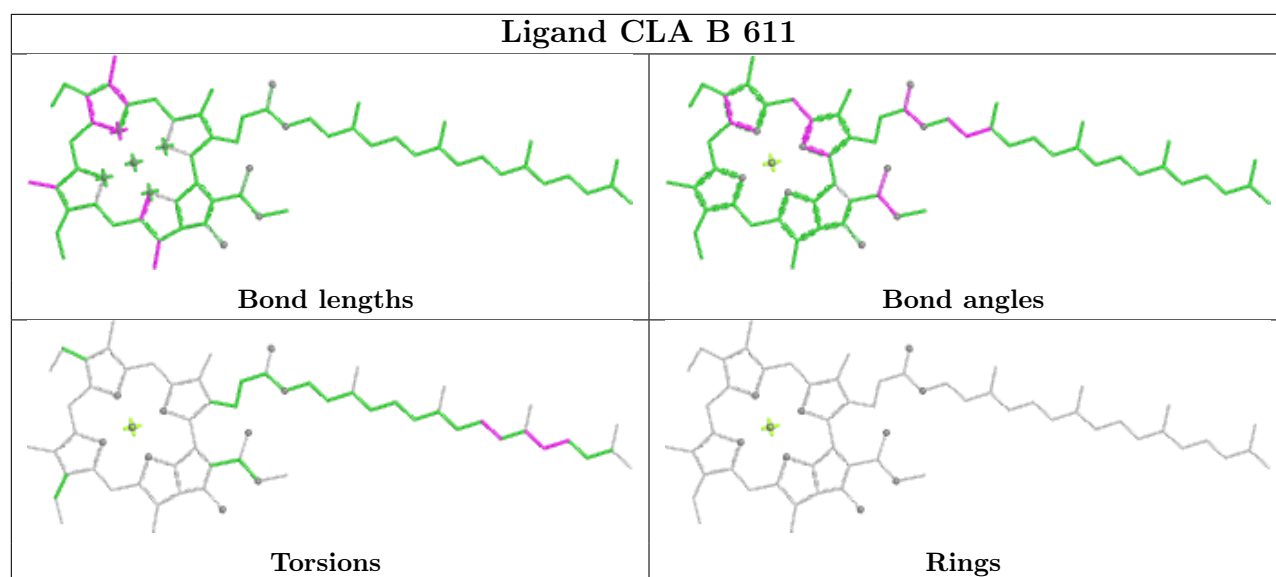
Bond angles



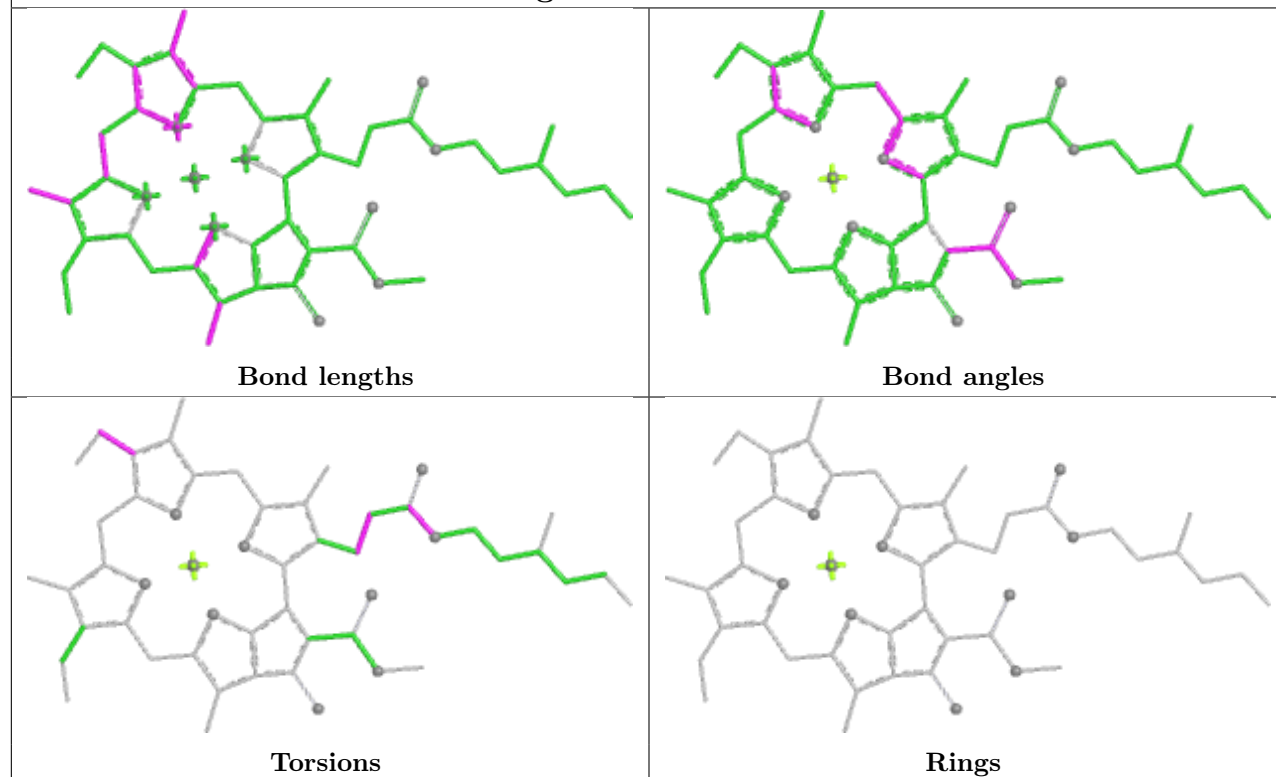
Torsions



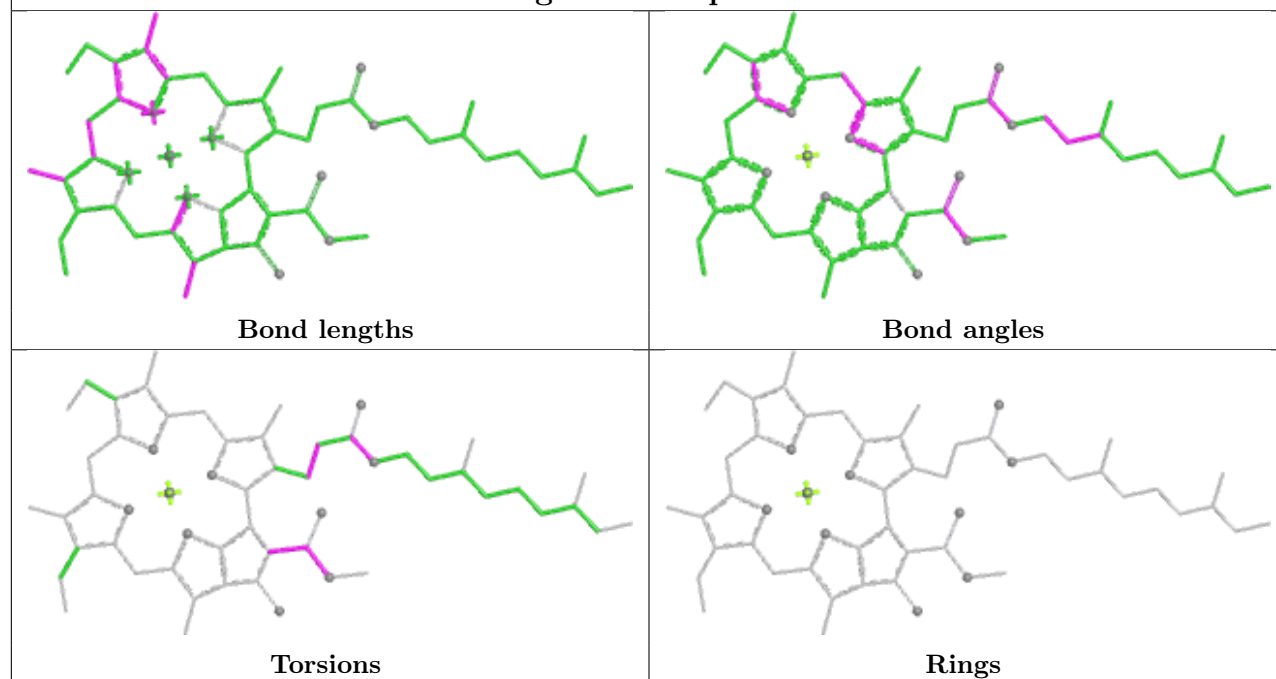
Rings



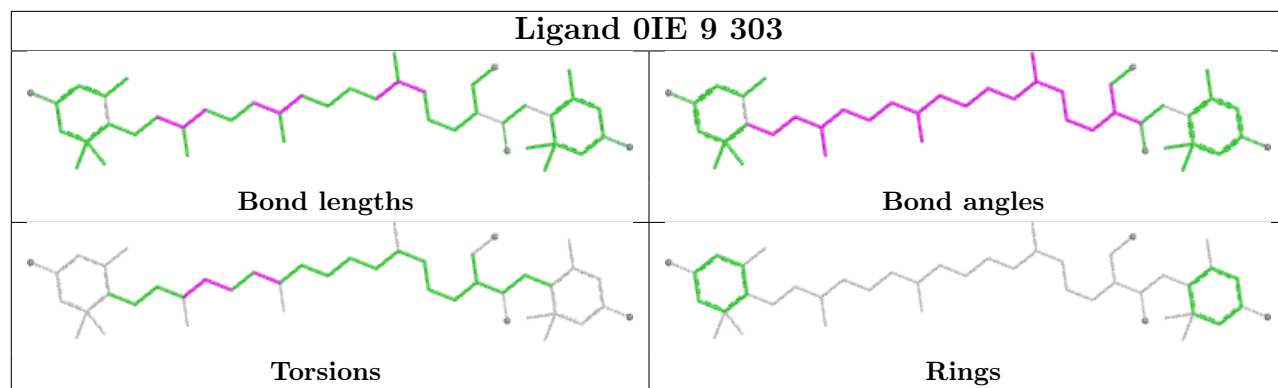
Ligand CLA 7 317



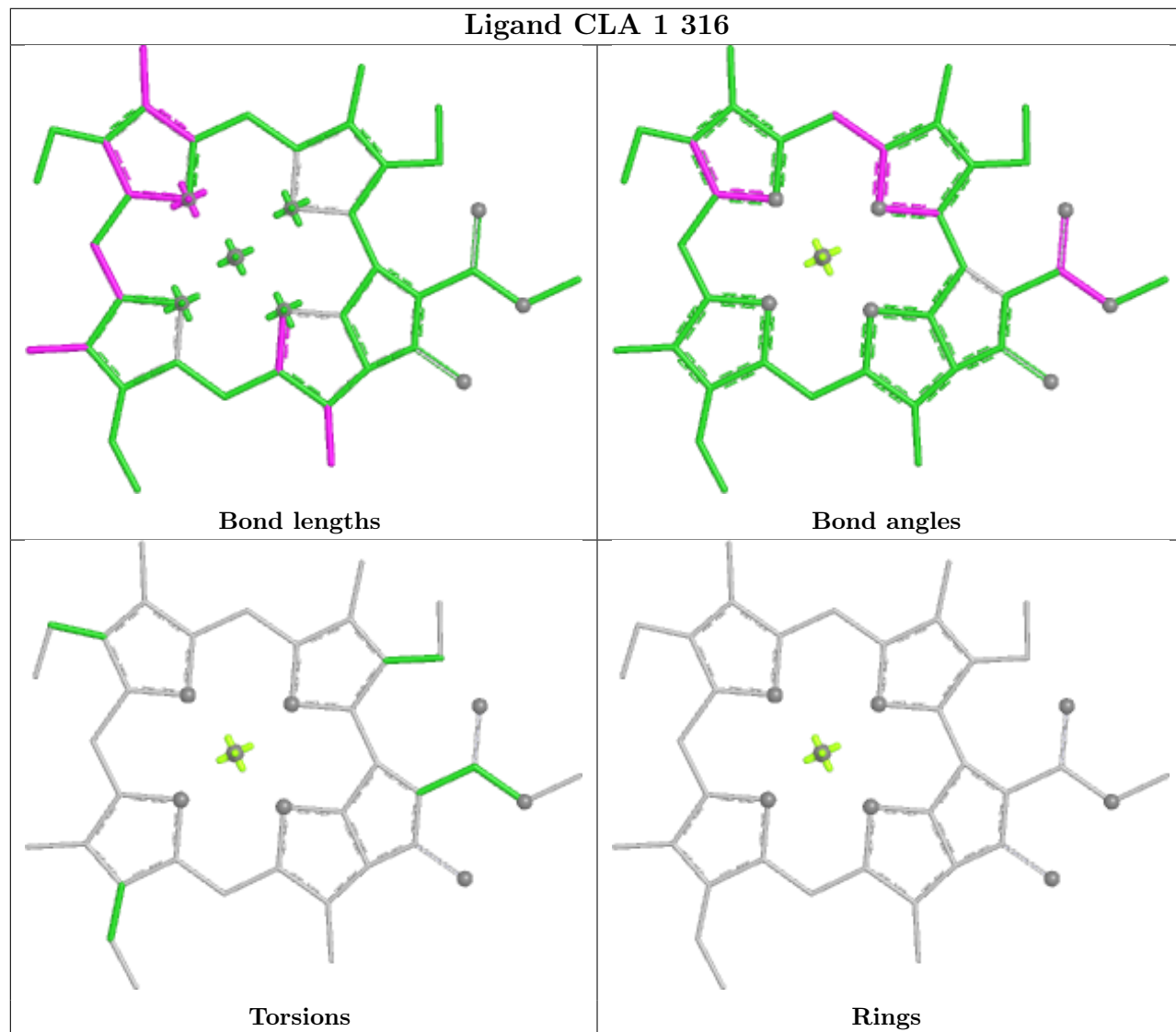
Ligand CLA p 307

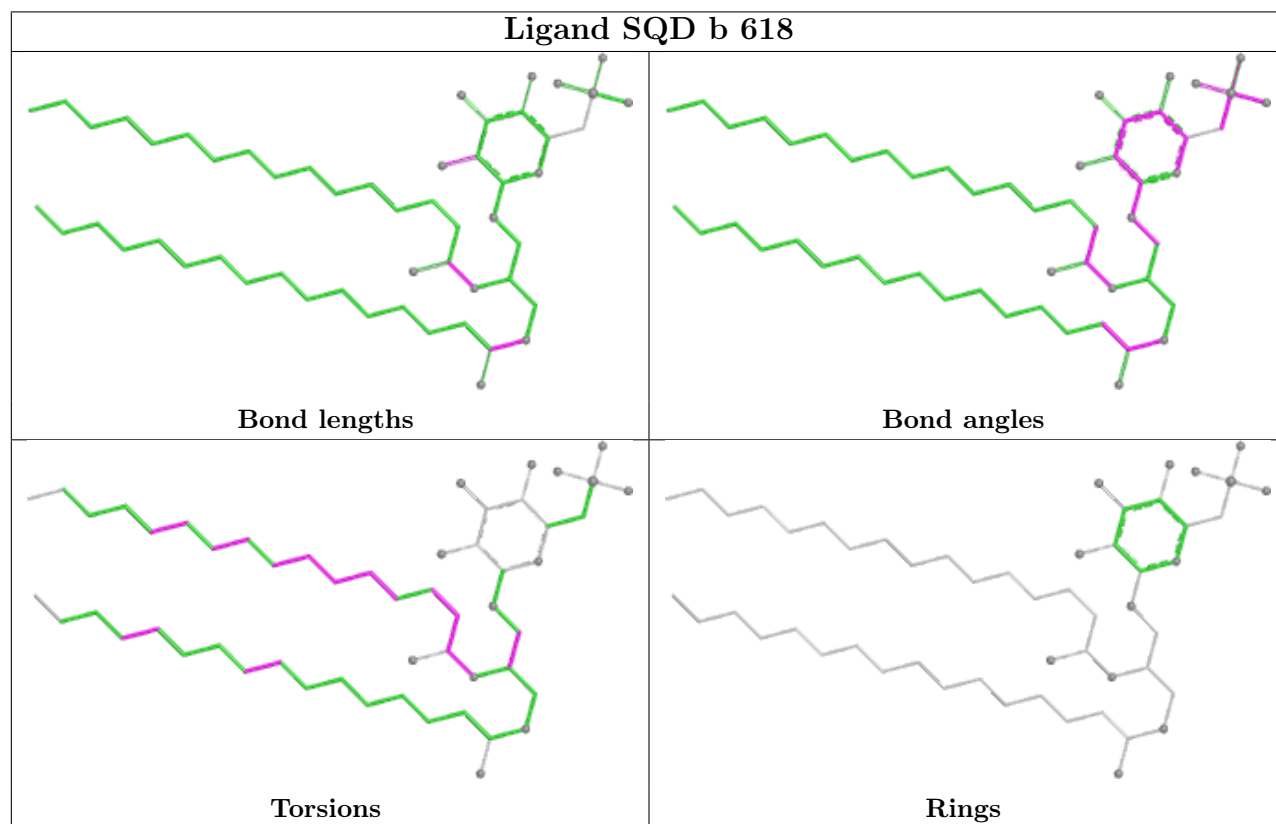
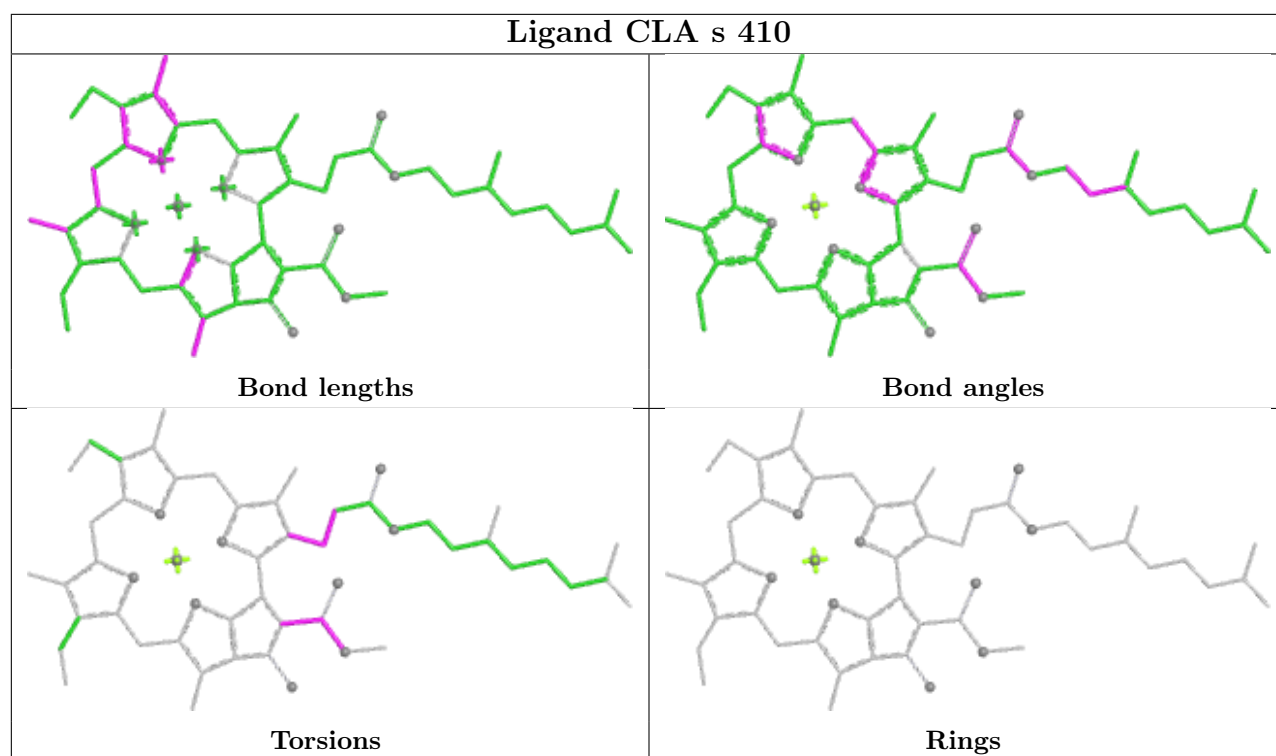


Ligand OIE 9 303

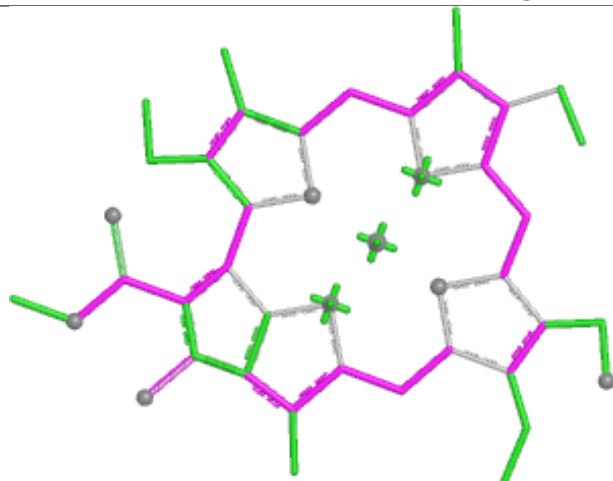


Ligand CLA 1 316

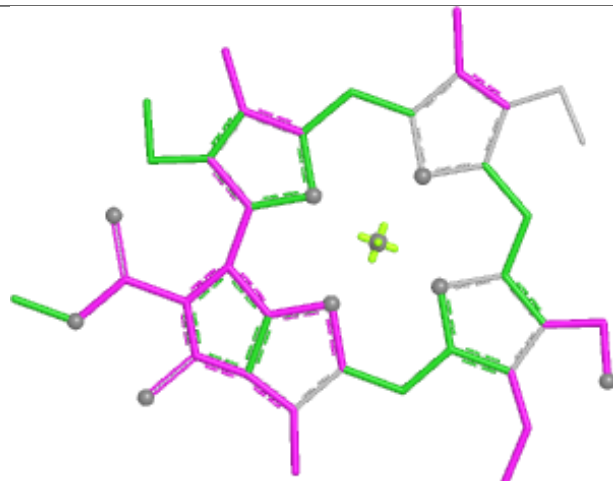




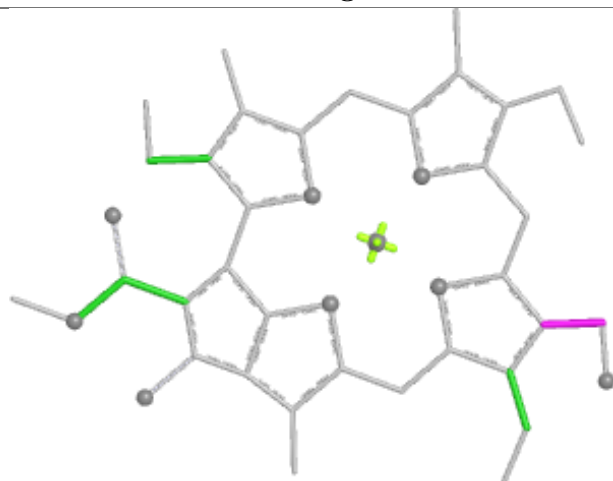
Ligand CHL 8 307



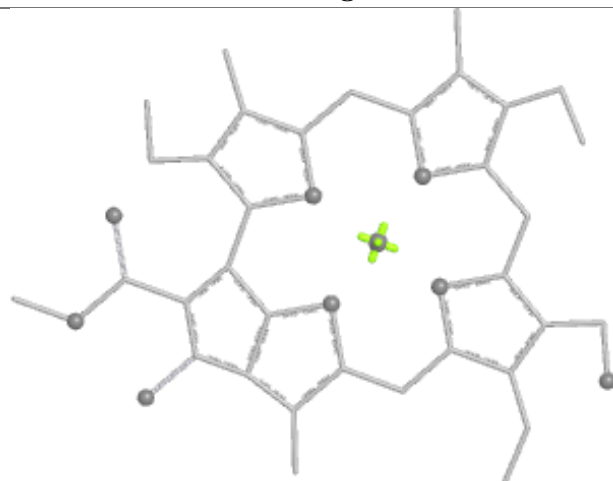
Bond lengths



Bond angles

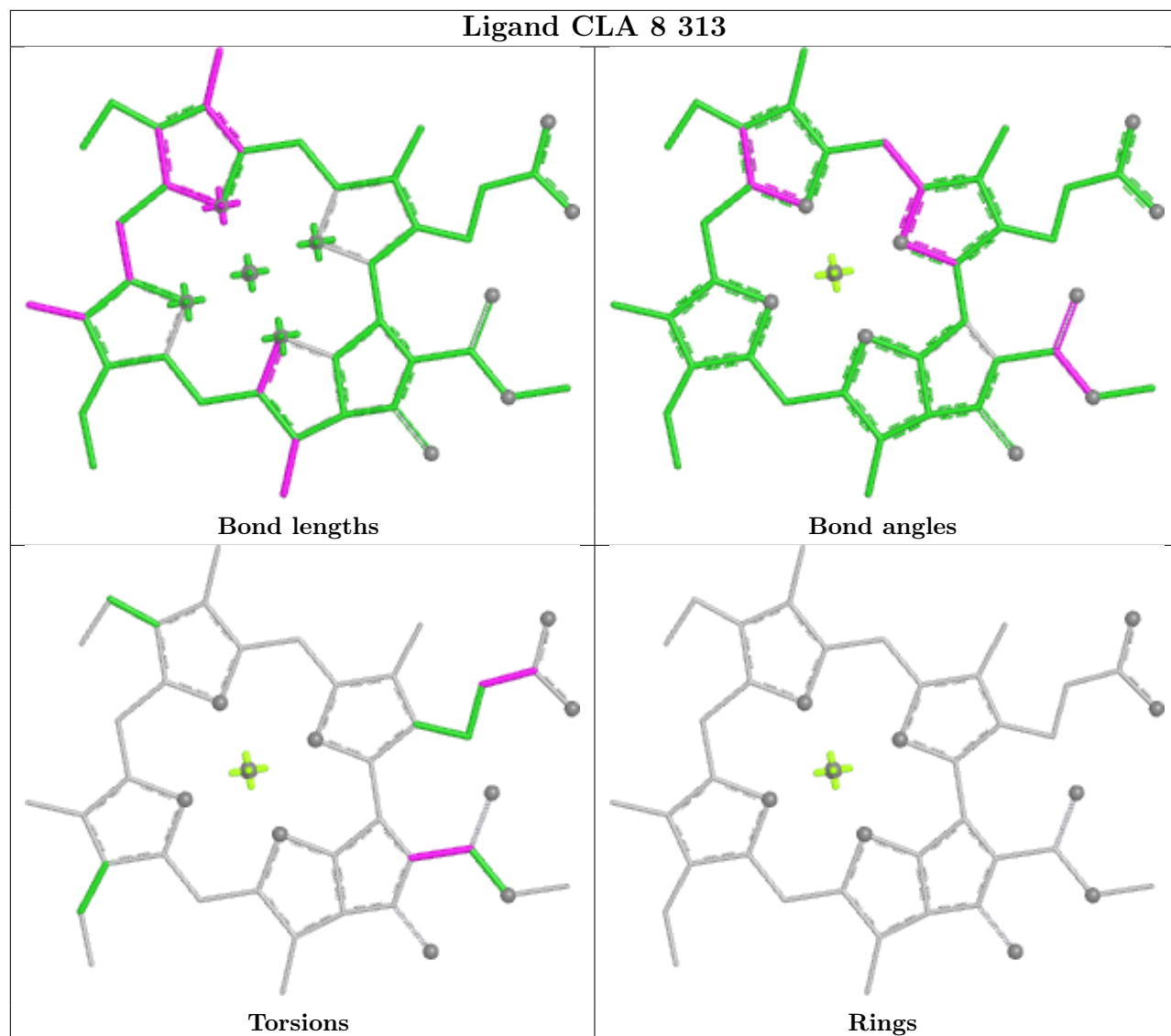


Torsions

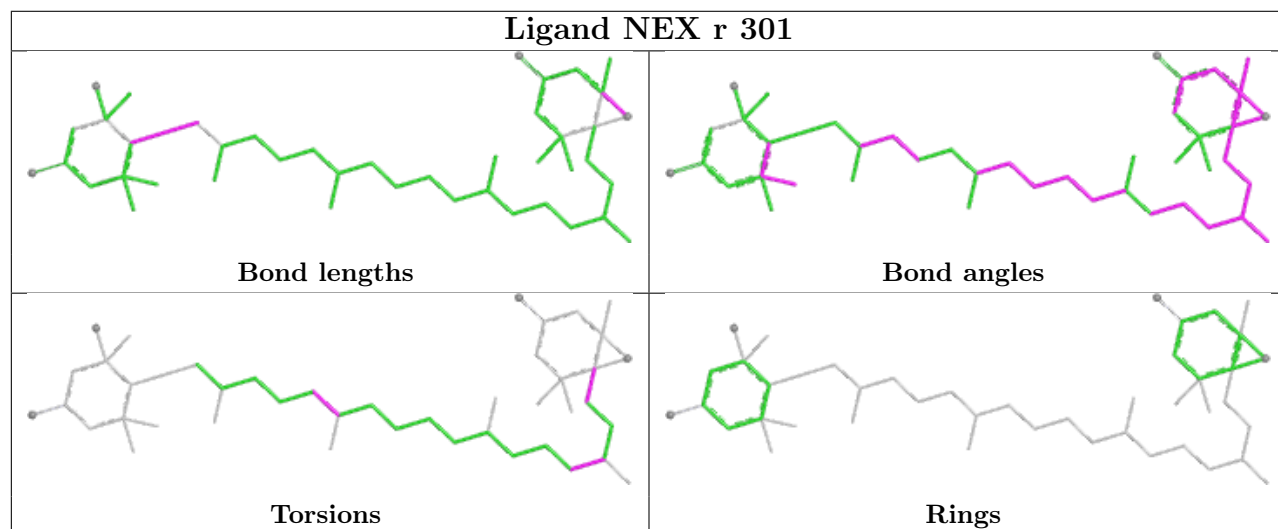


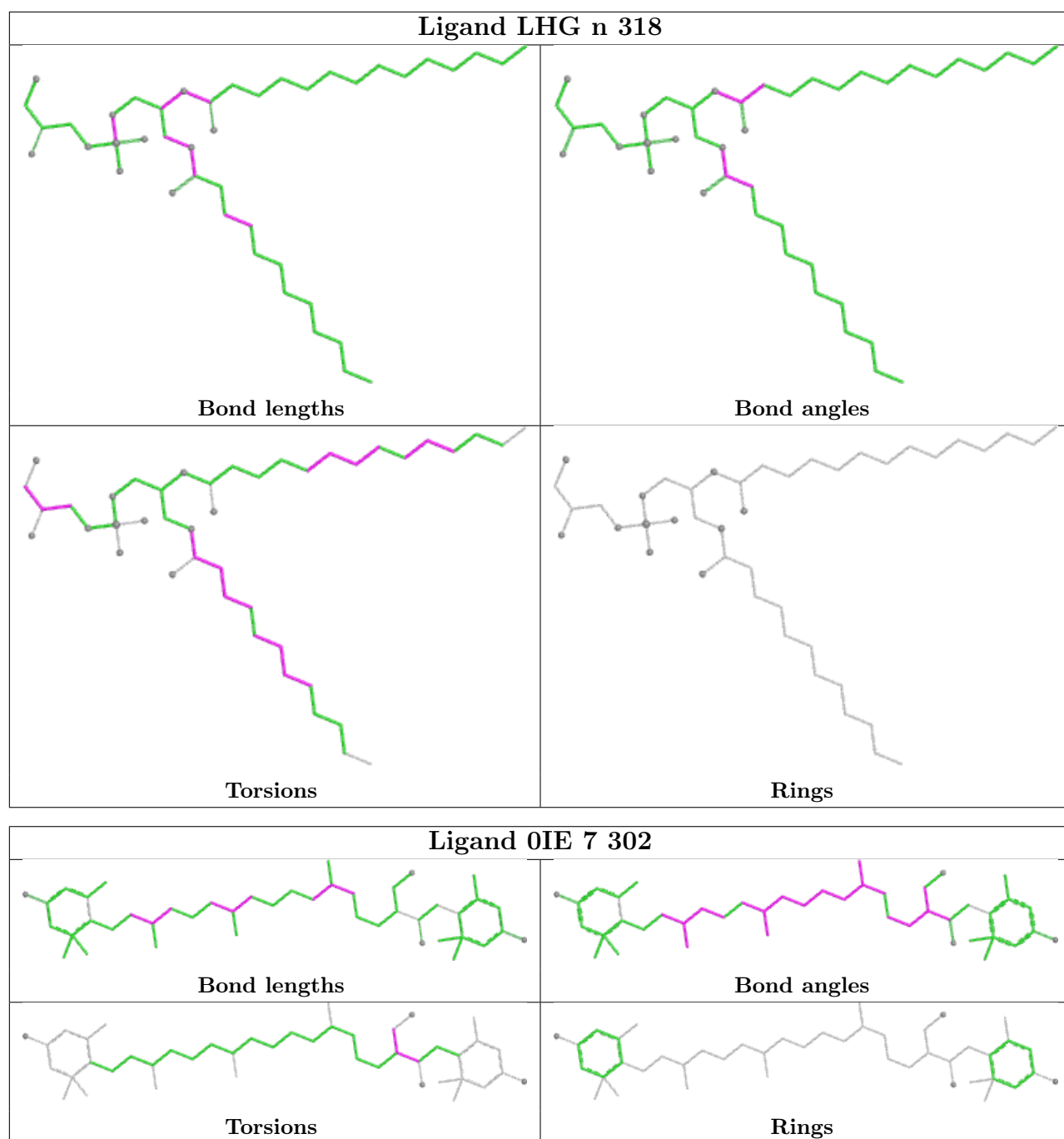
Rings

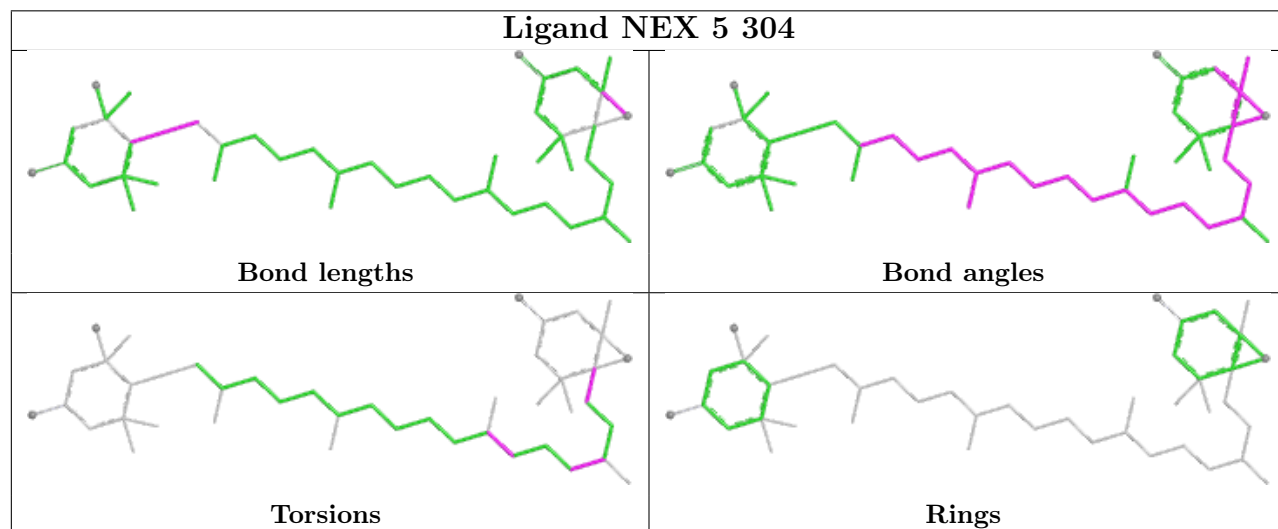
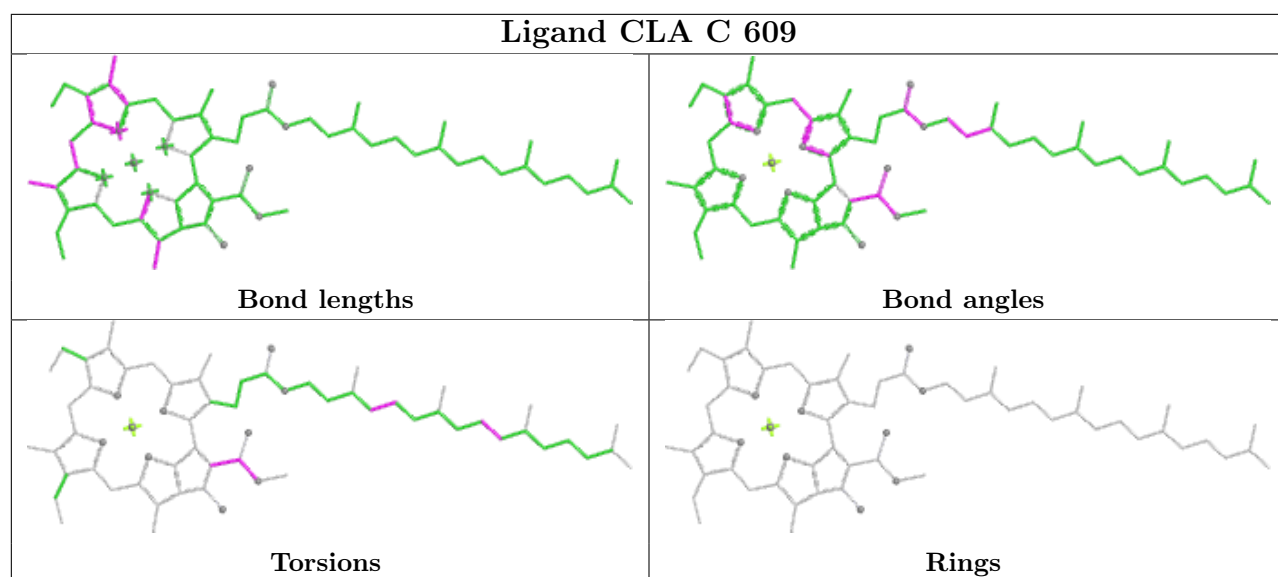
Ligand CLA 8 313



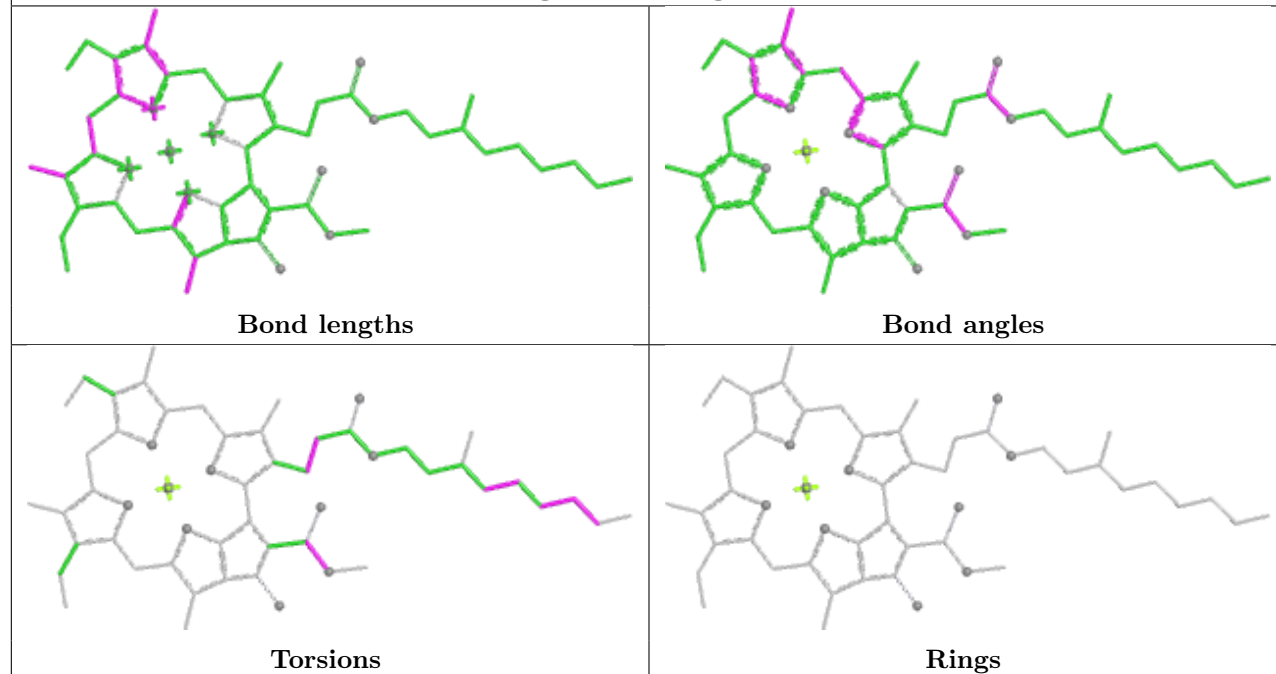
Ligand NEX r 301



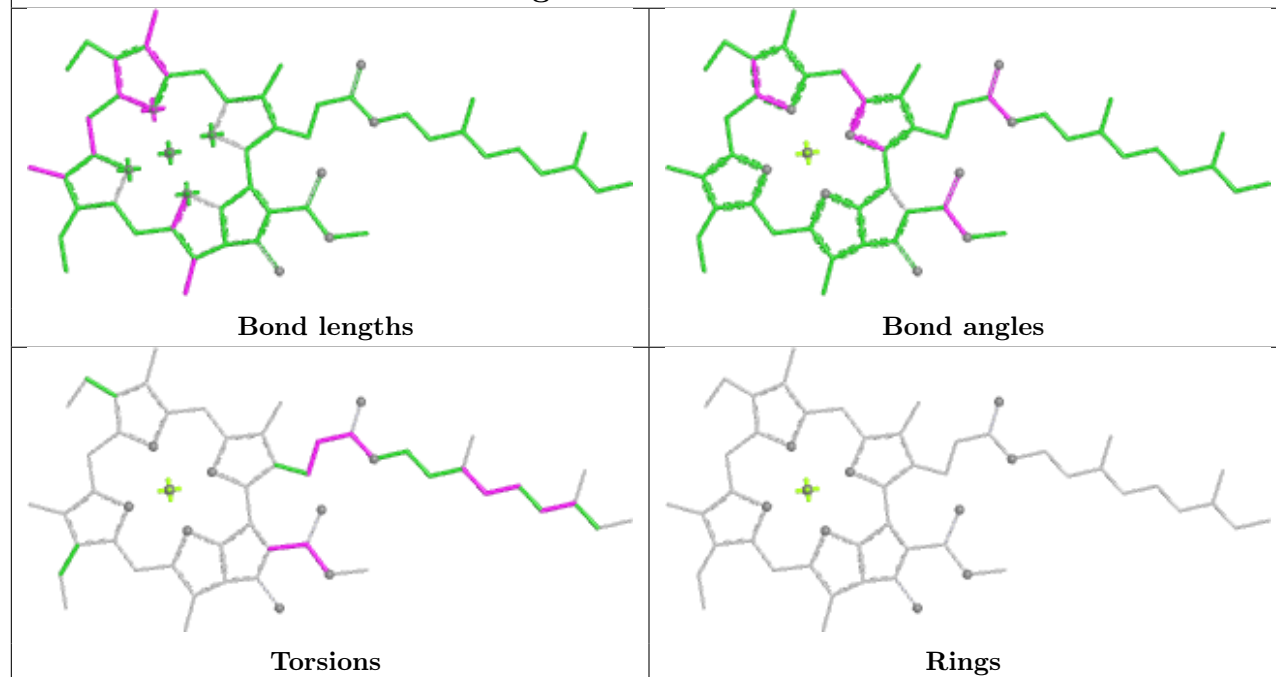




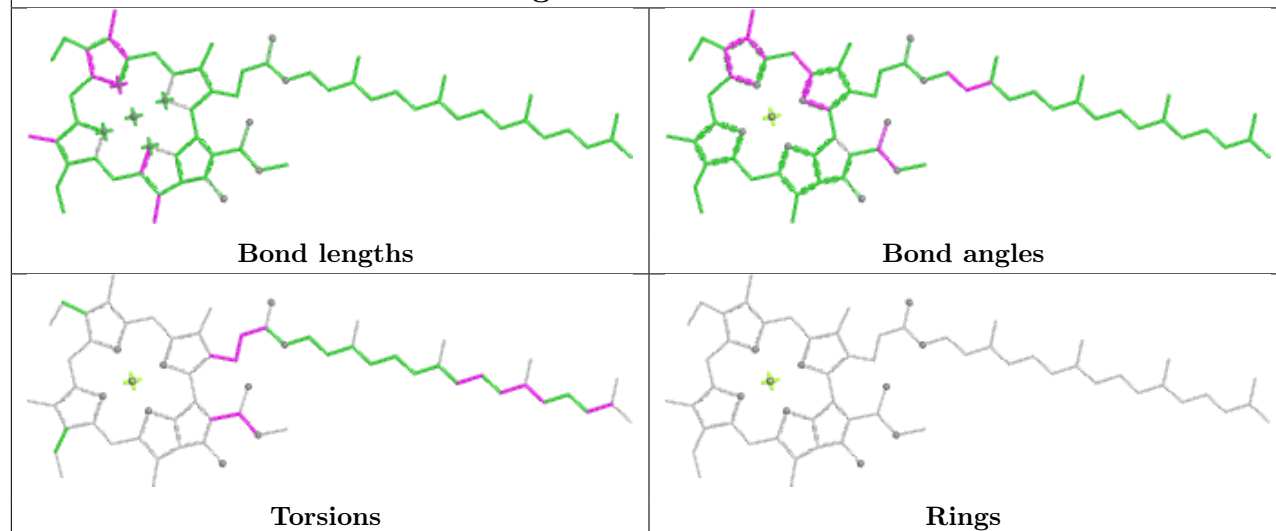
Ligand CLA g 317



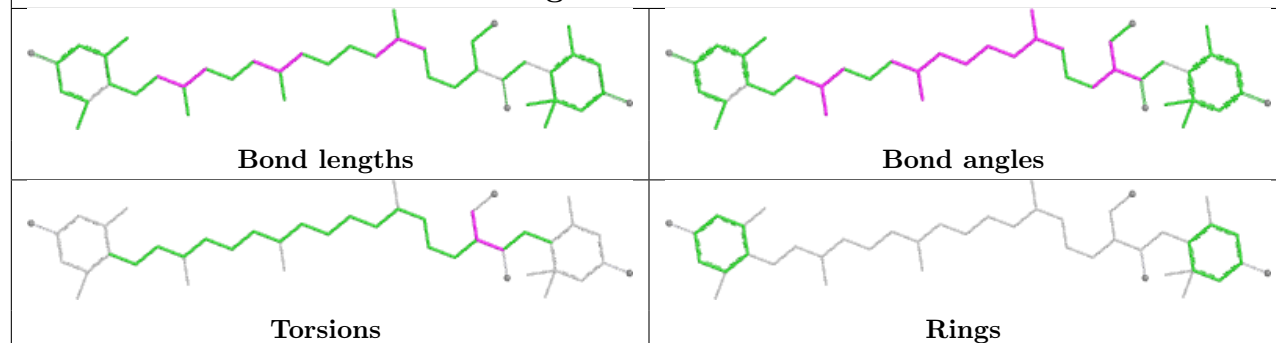
Ligand CLA B 614



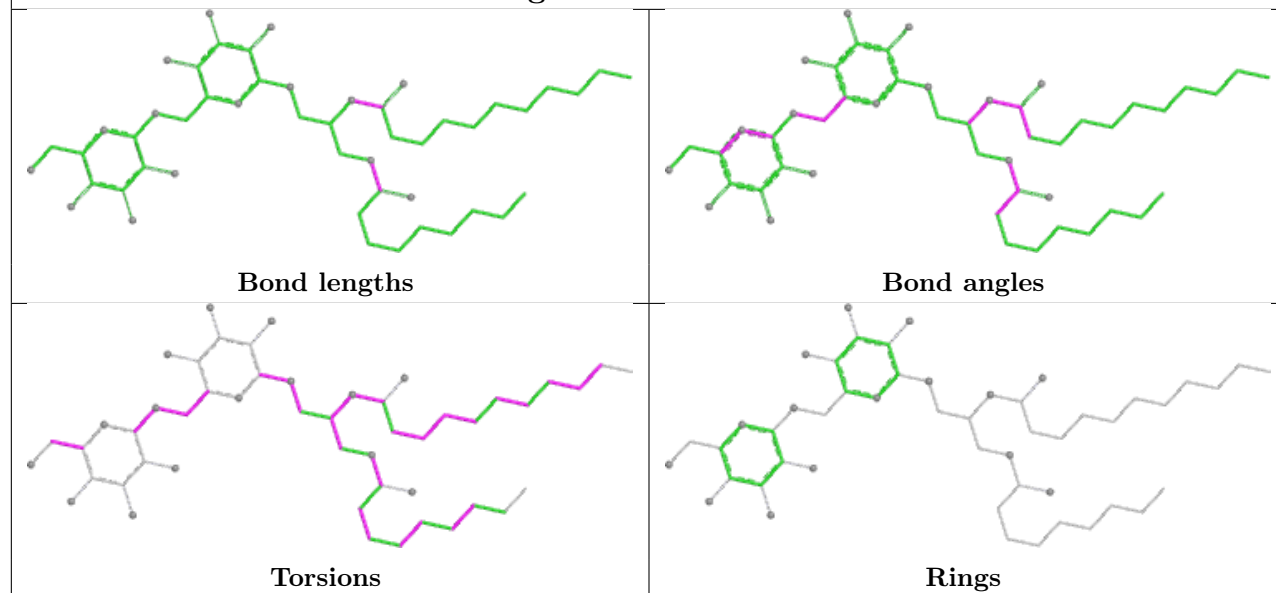
Ligand CLA C 601

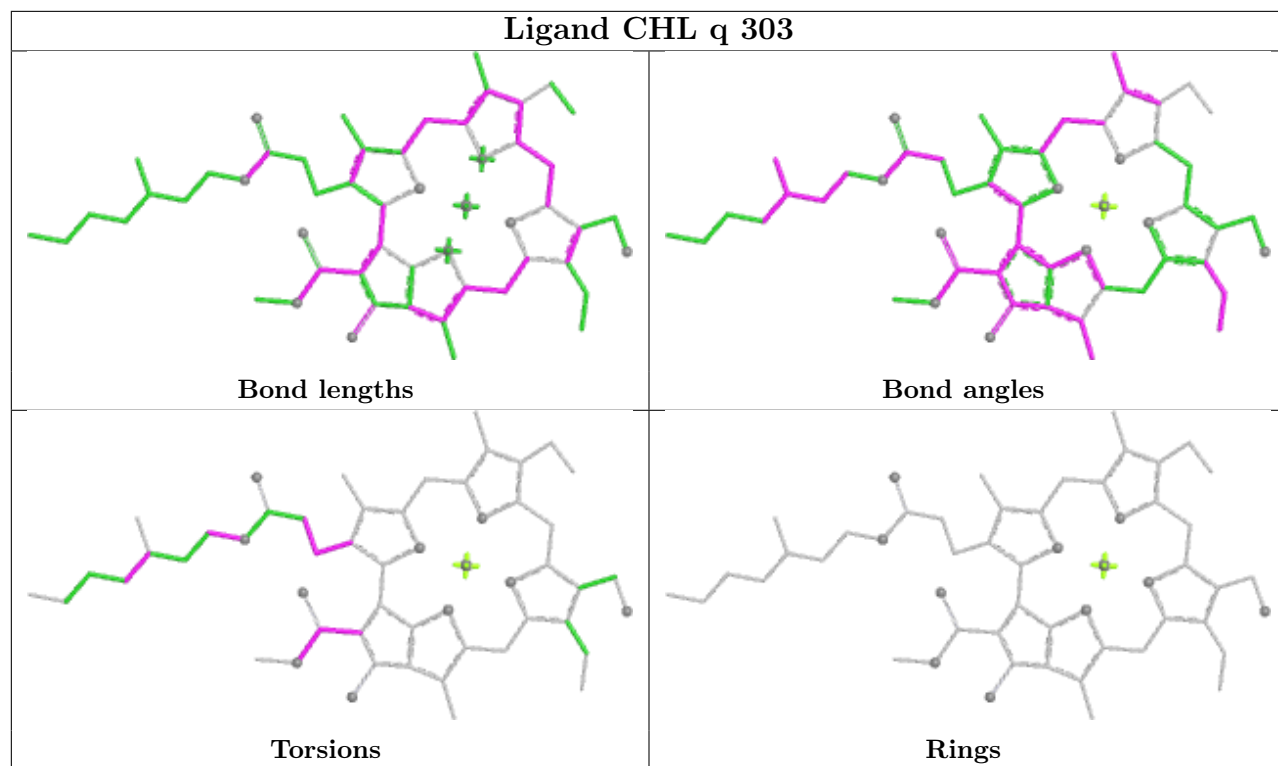


Ligand OIE 3 302

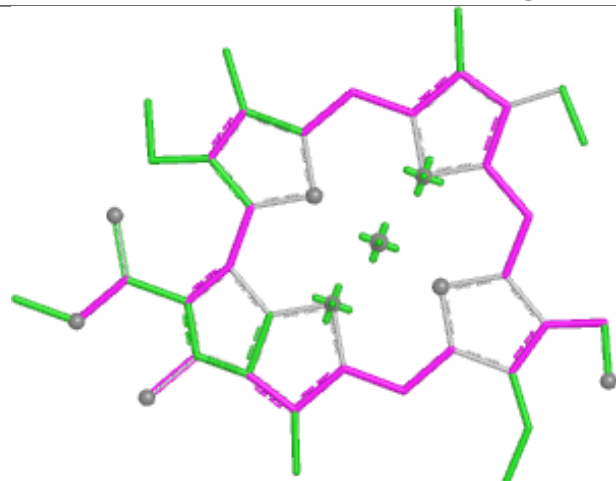


Ligand DGD C 619

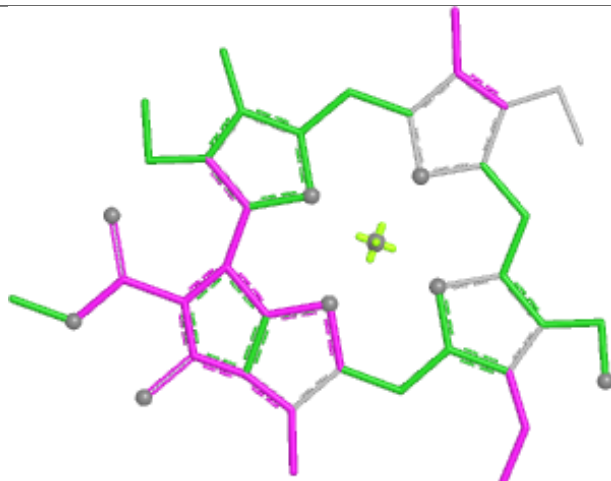




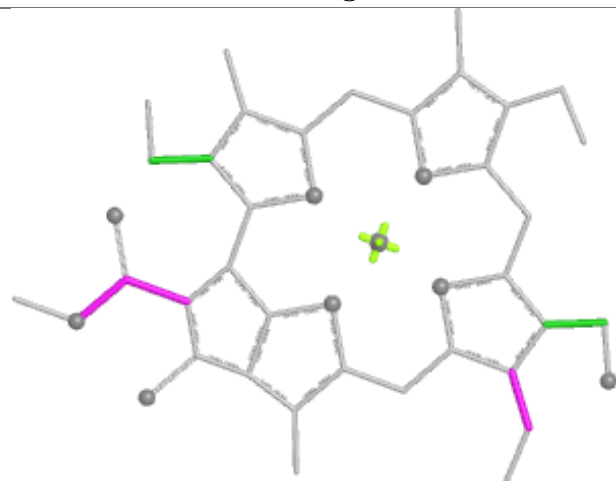
Ligand CHL 6 312



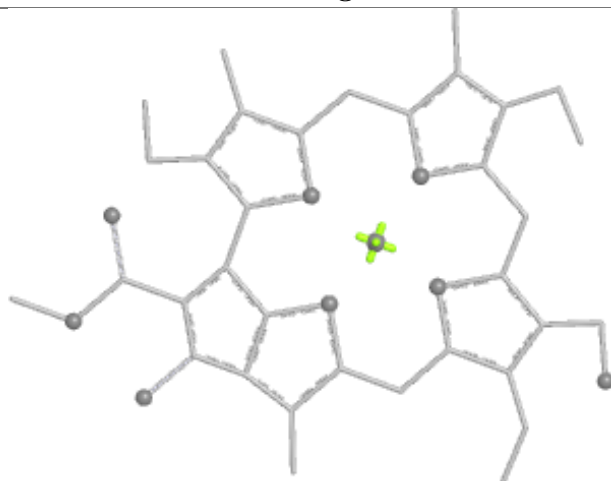
Bond lengths



Bond angles

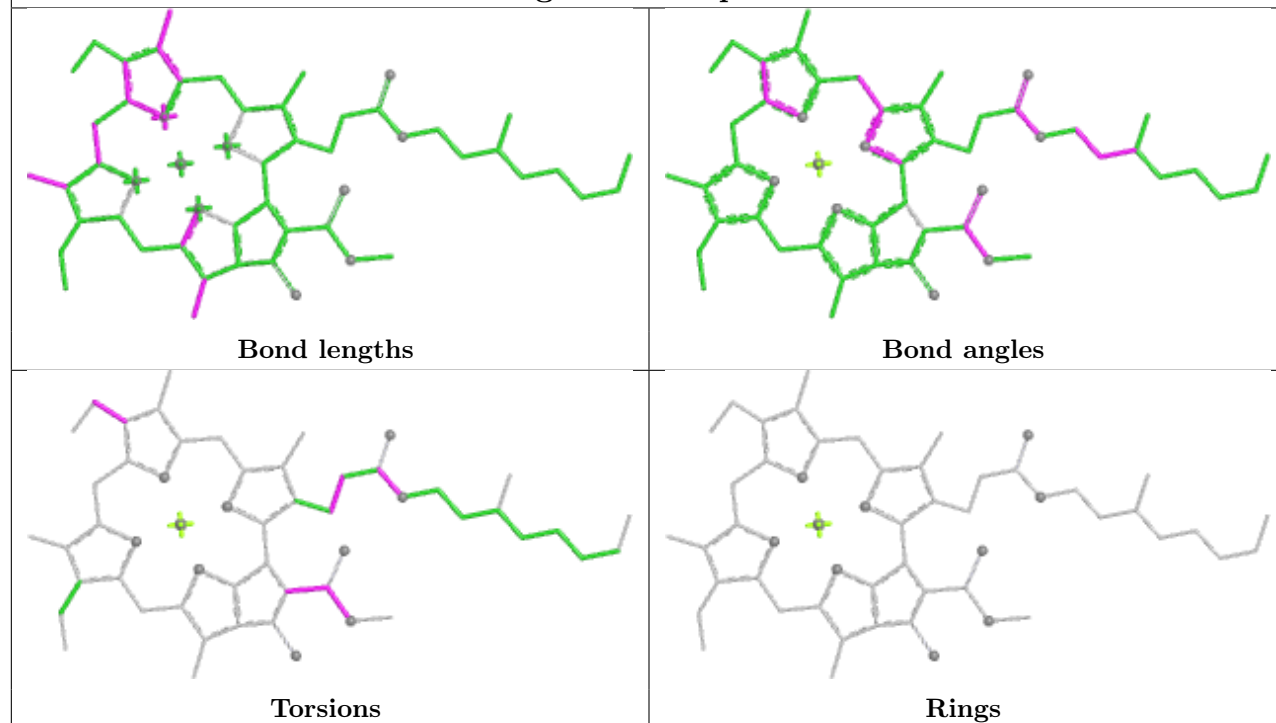


Torsions

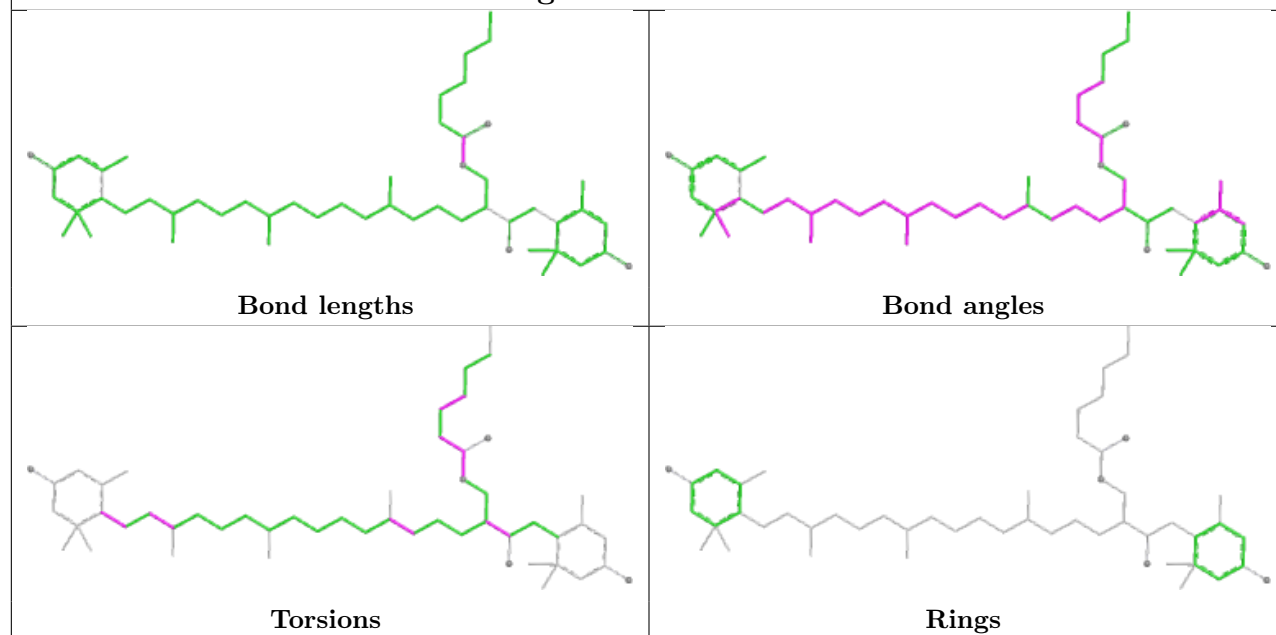


Rings

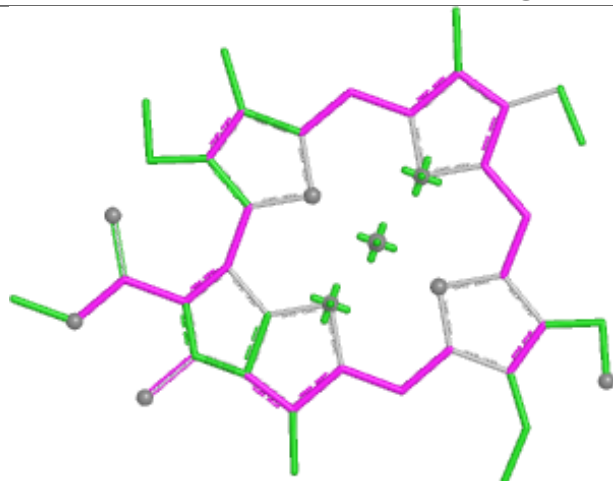
Ligand CLA q 305



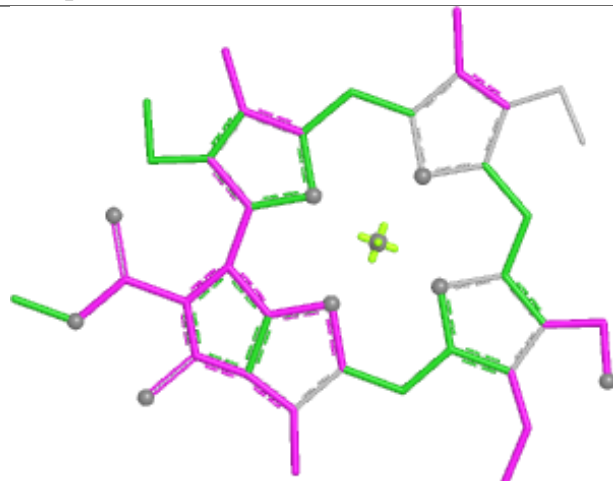
Ligand OUR 4 301



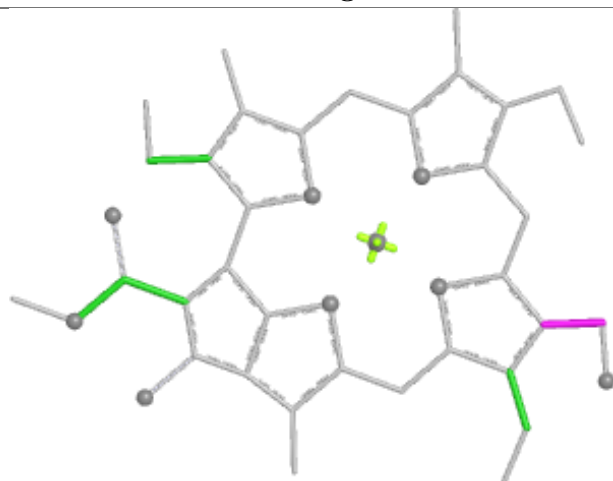
Ligand CHL q 307



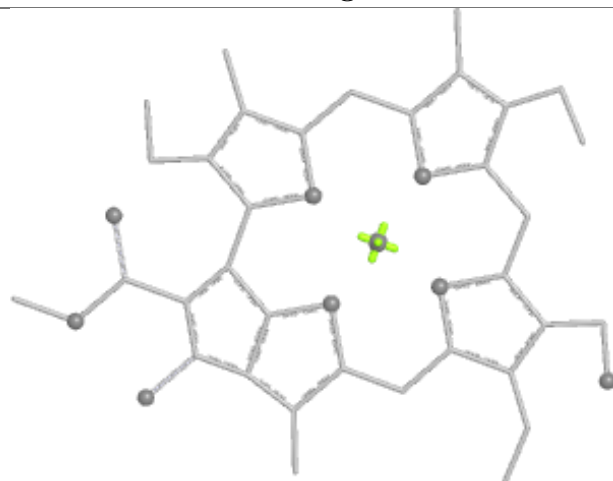
Bond lengths



Bond angles

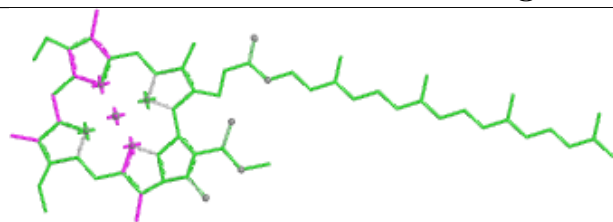


Torsions

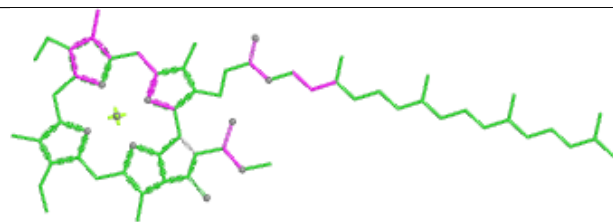


Rings

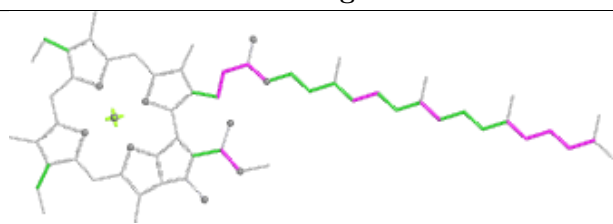
Ligand CLA b 606



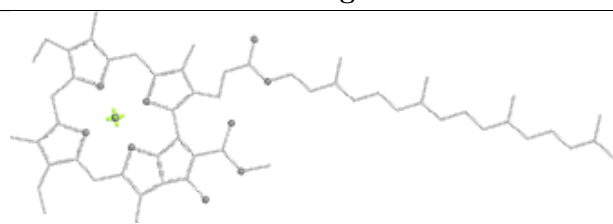
Bond lengths



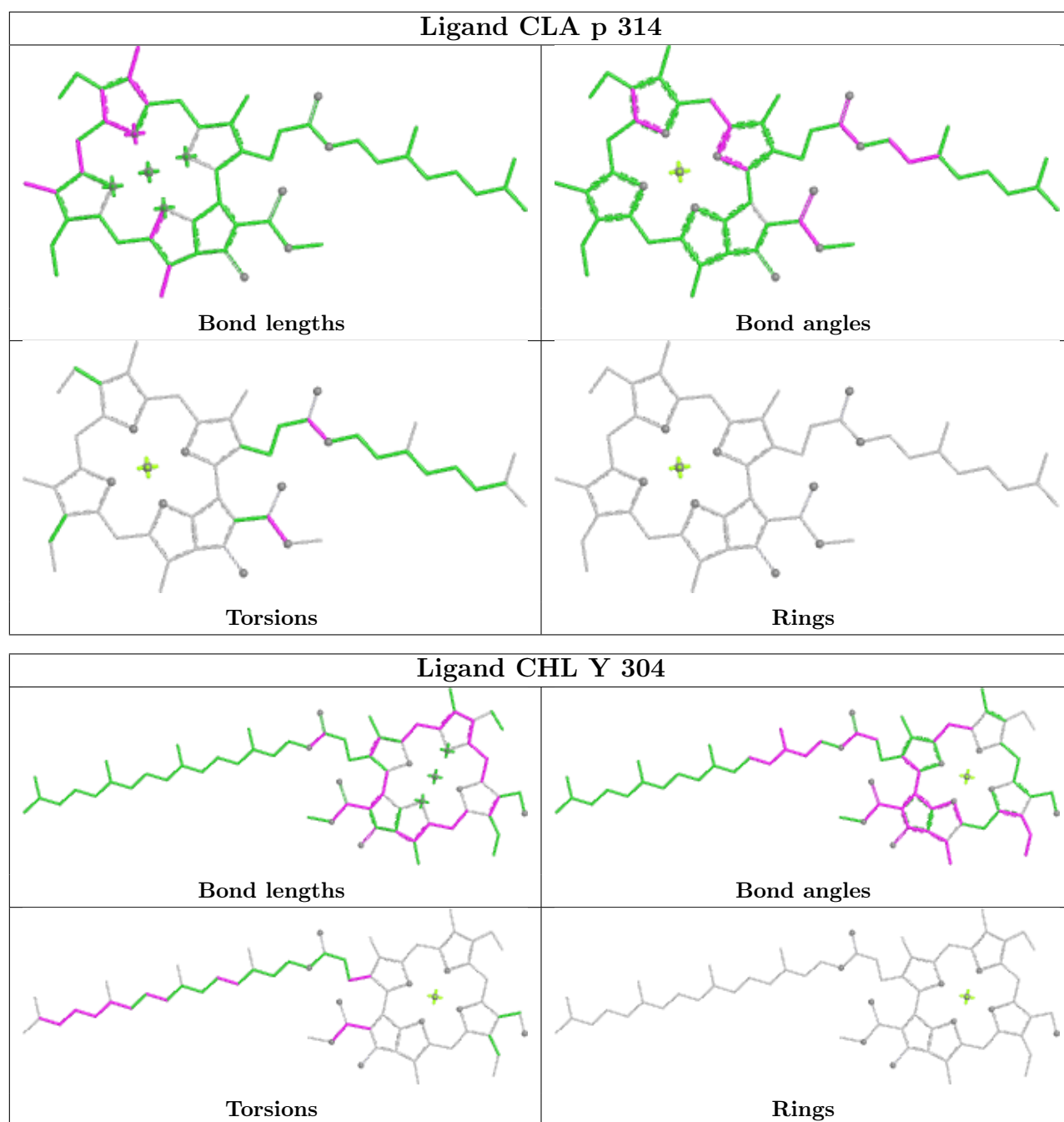
Bond angles

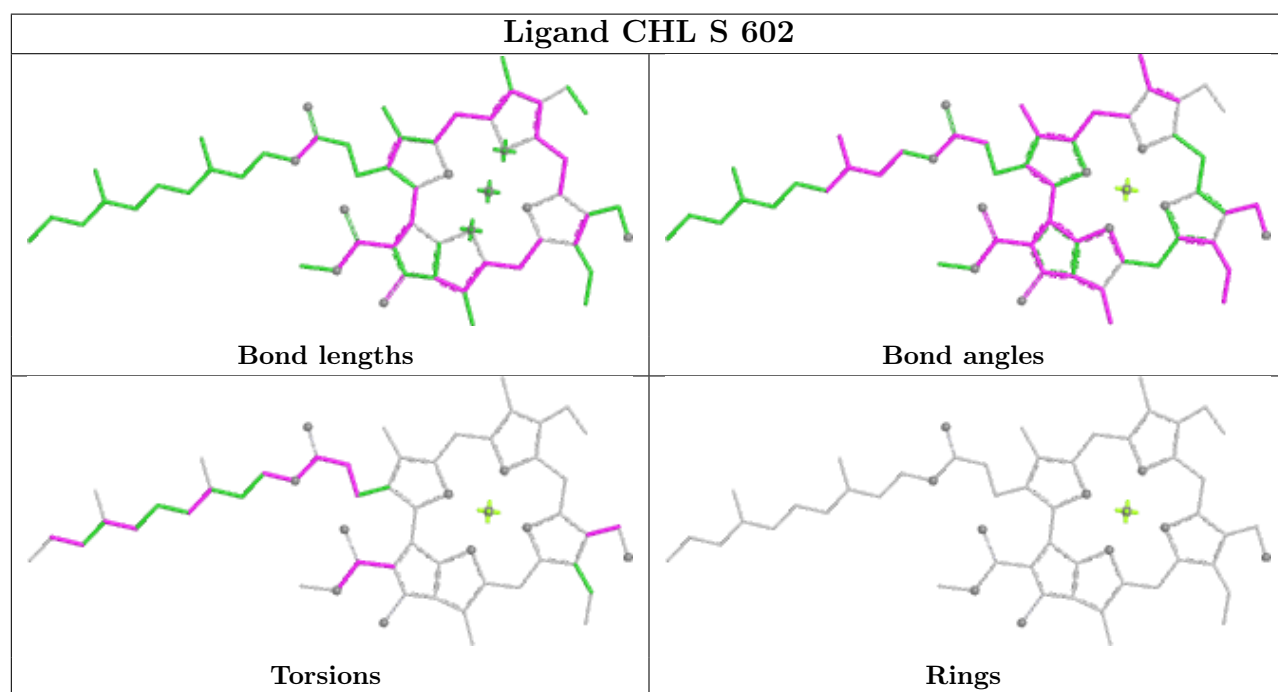
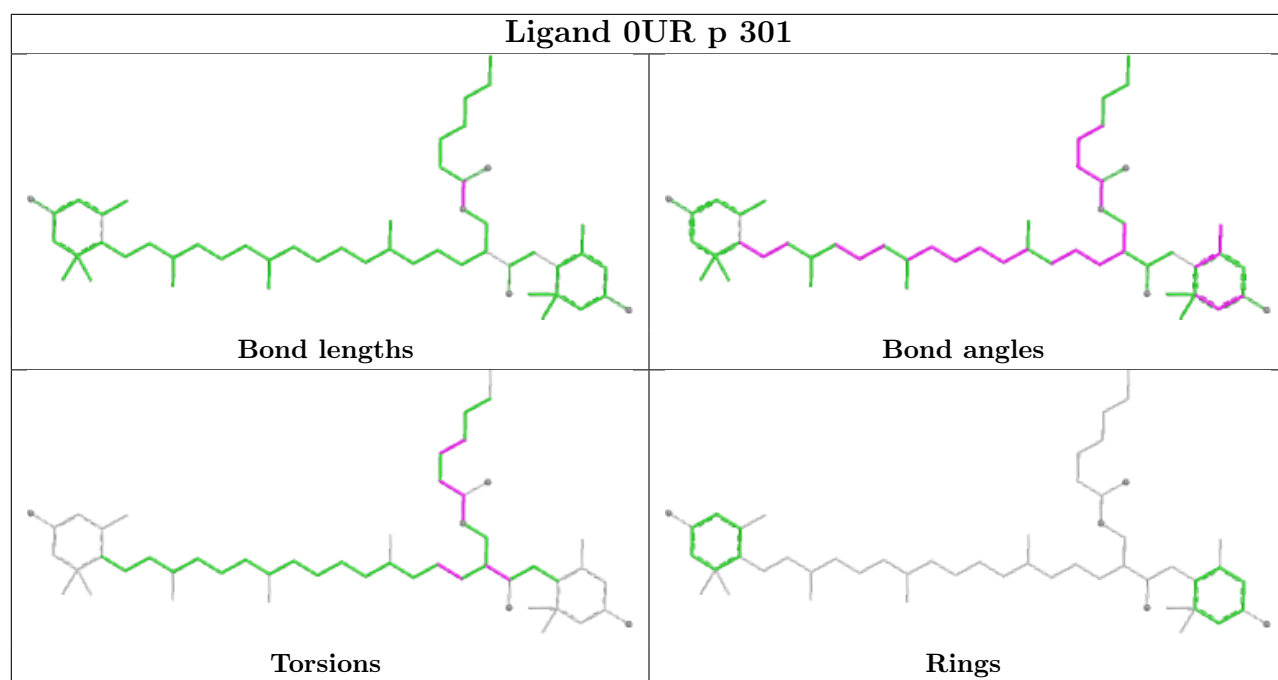


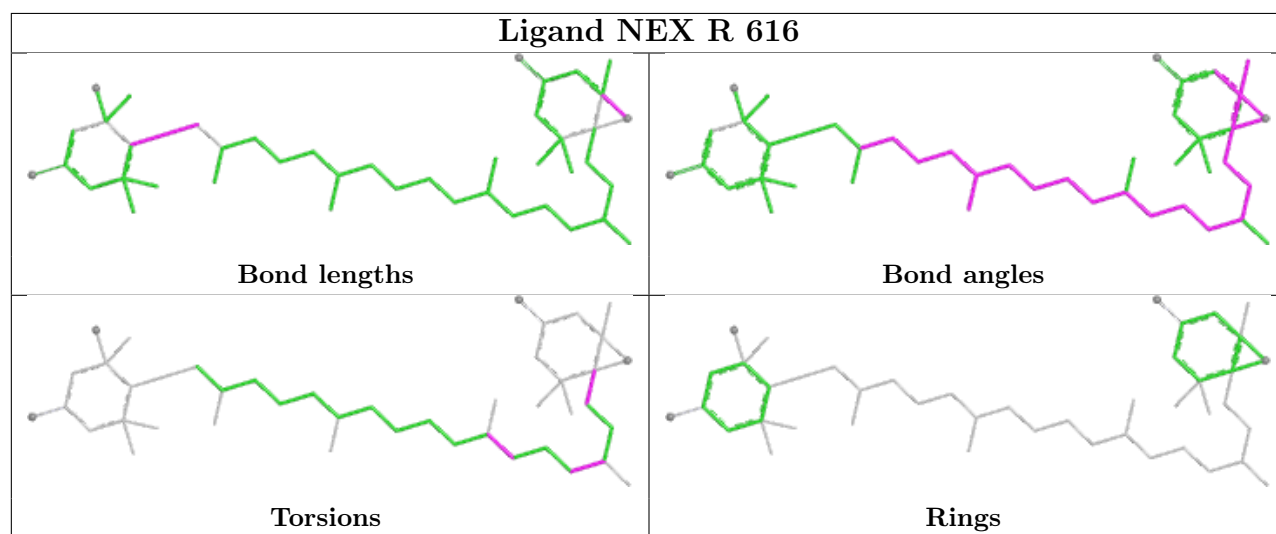
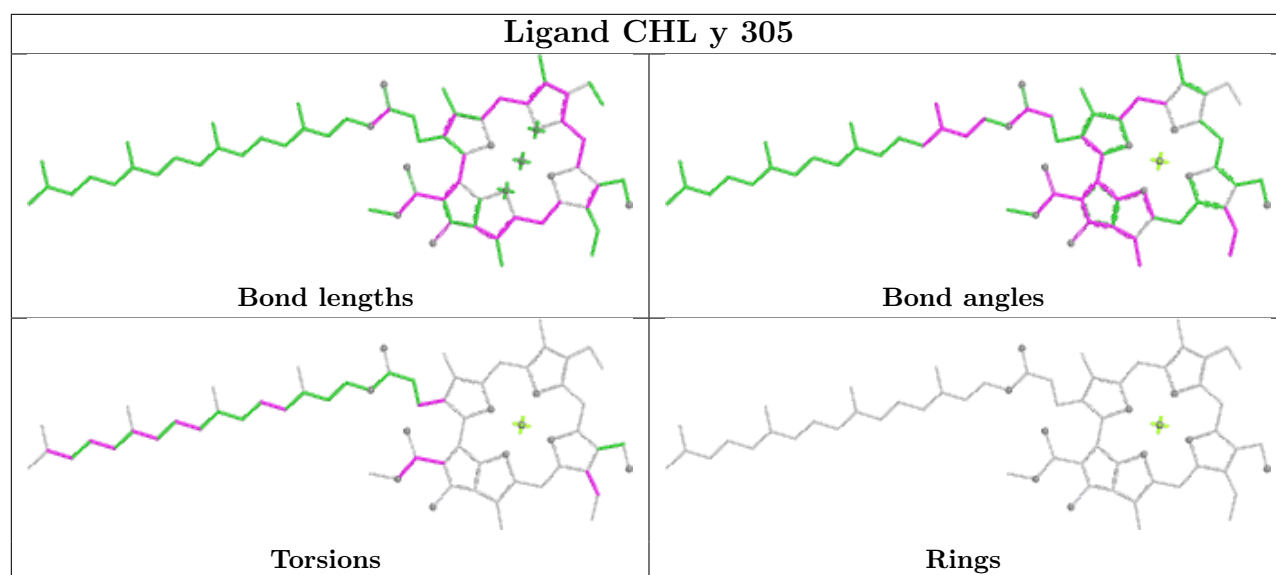
Torsions



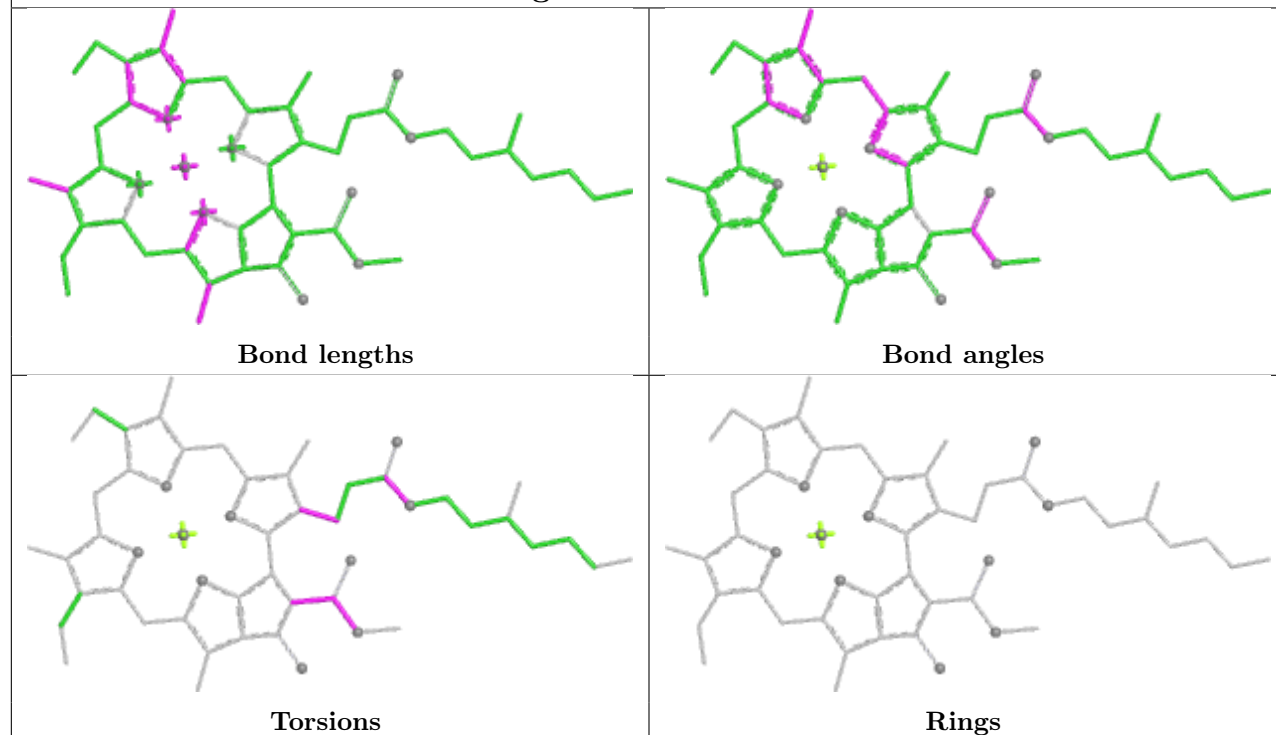
Rings



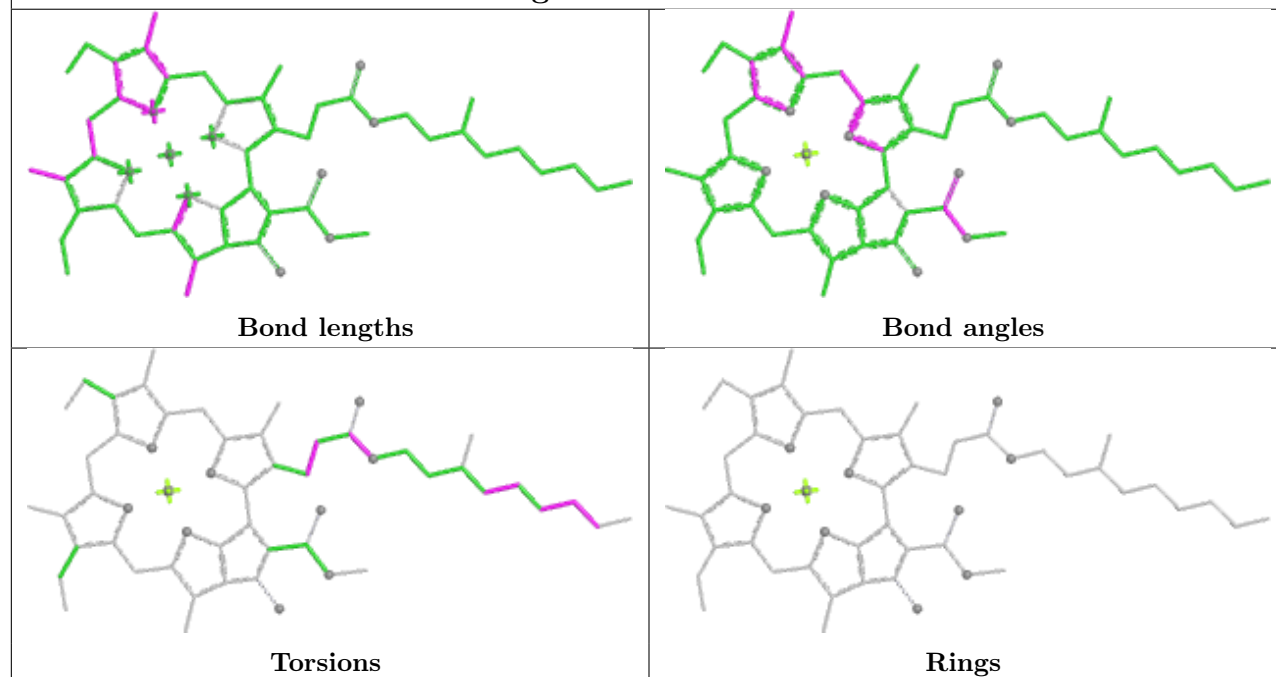




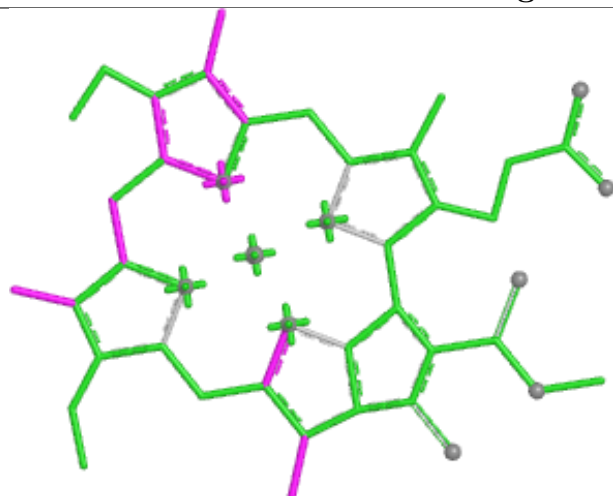
Ligand CLA C 606



Ligand CLA Y 316



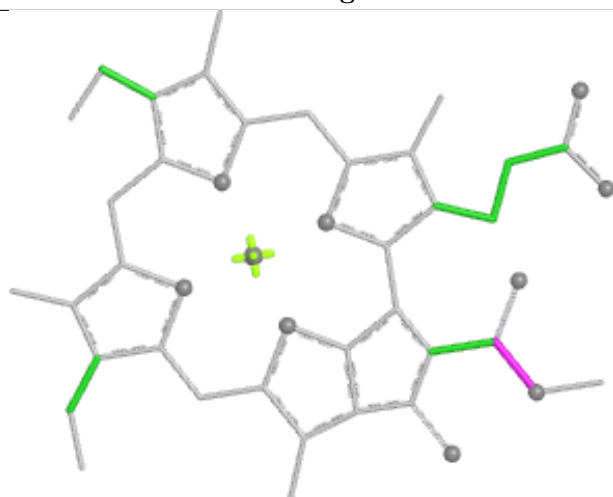
Ligand CLA S 610



Bond lengths



Bond angles

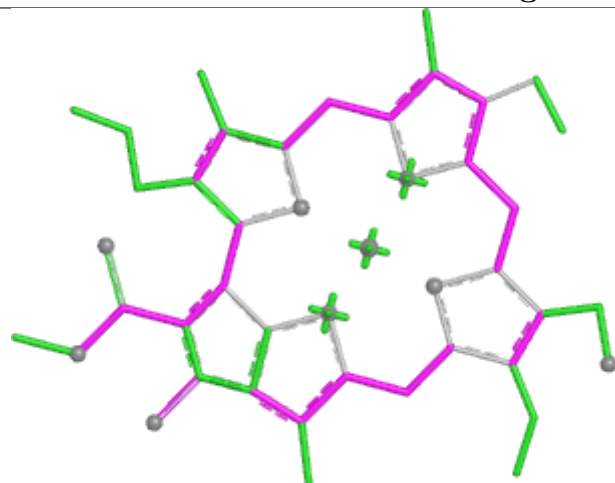


Torsions

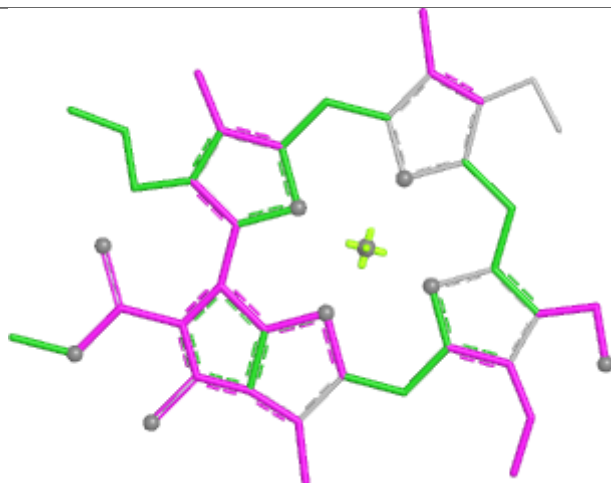


Rings

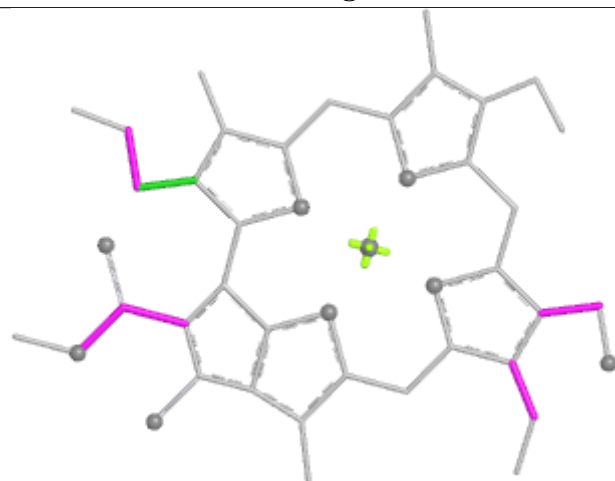
Ligand CHL 5 305



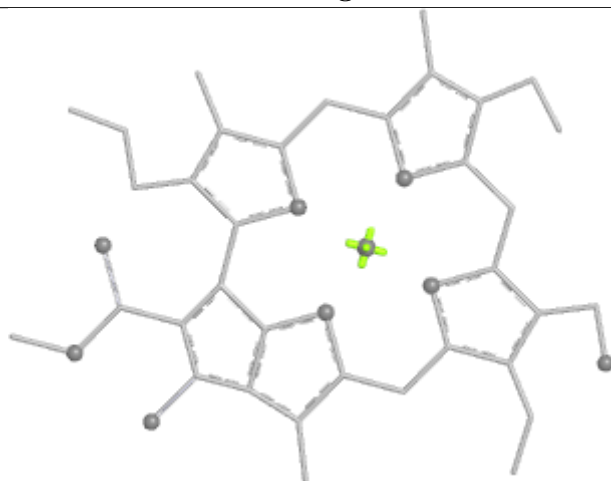
Bond lengths



Bond angles

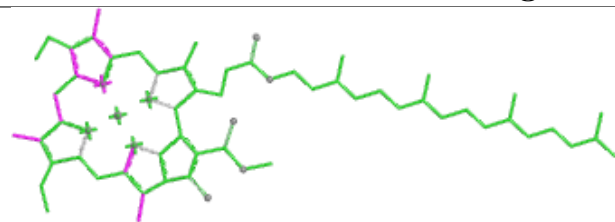


Torsions

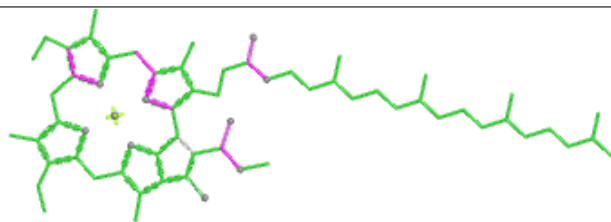


Rings

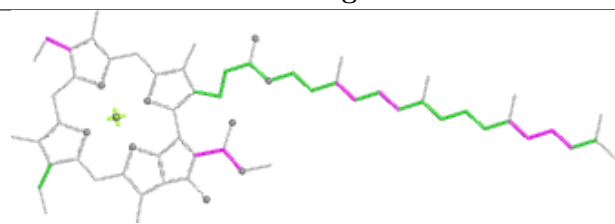
Ligand CLA b 605



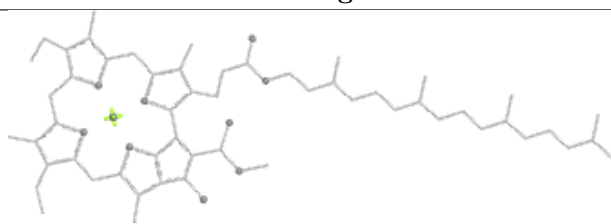
Bond lengths



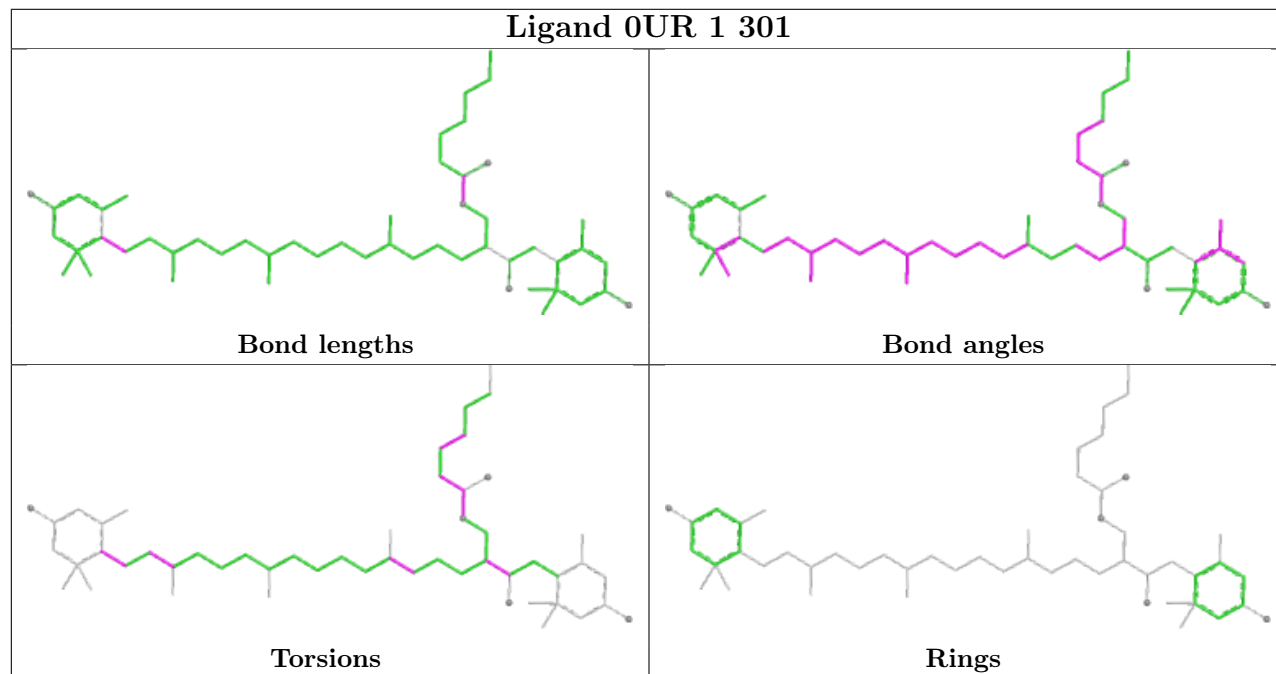
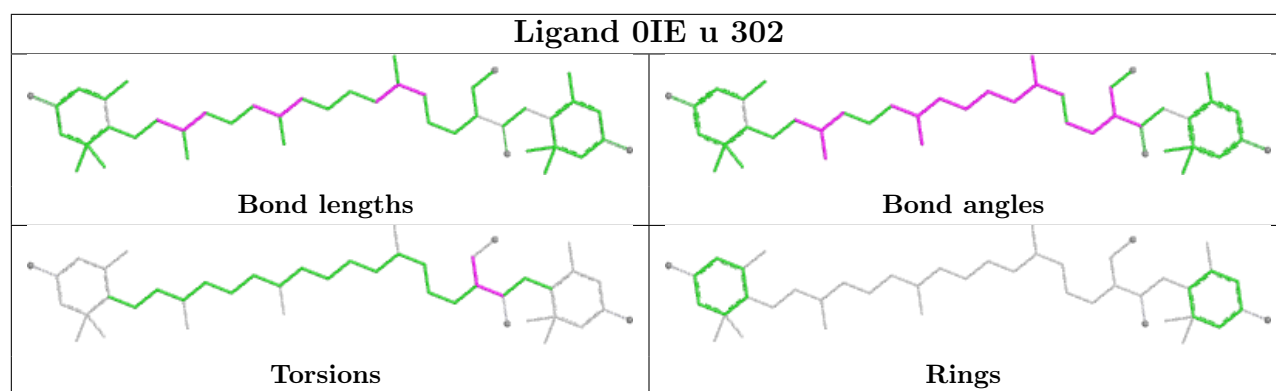
Bond angles



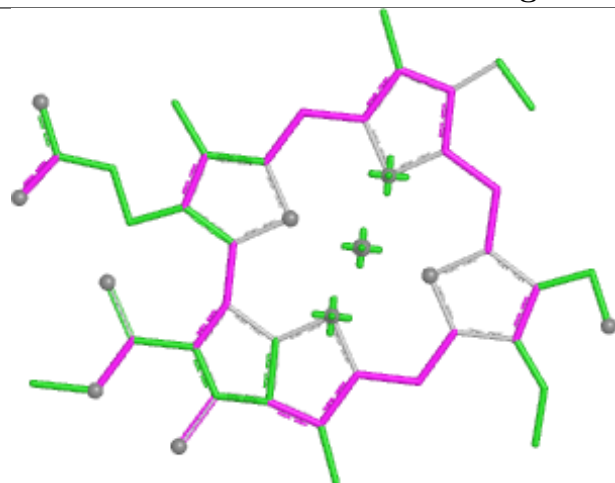
Torsions



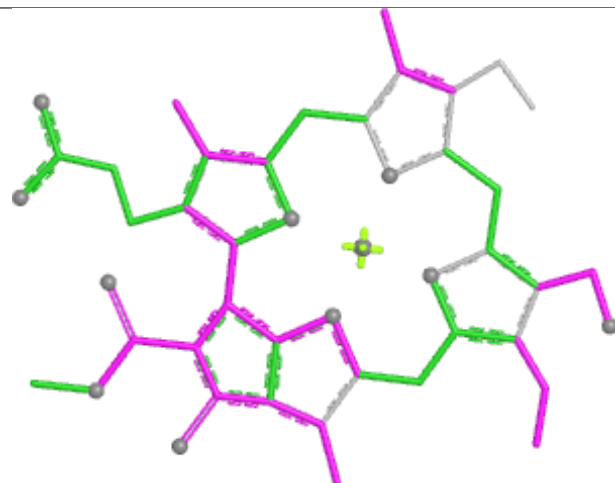
Rings



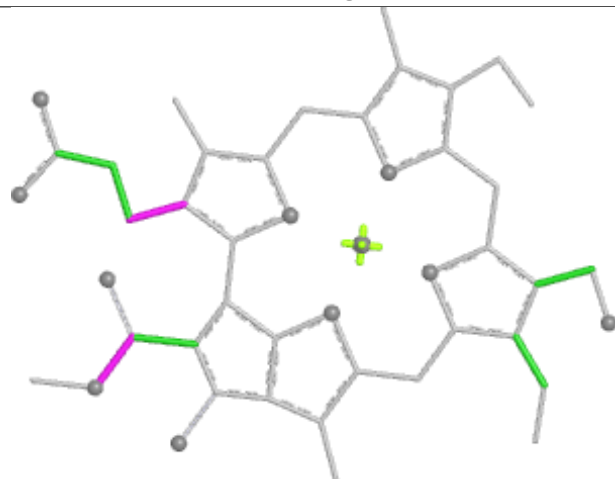
Ligand CHL 9 310



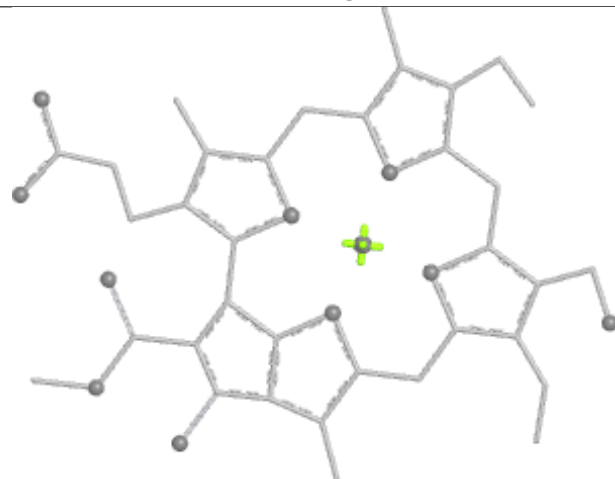
Bond lengths



Bond angles

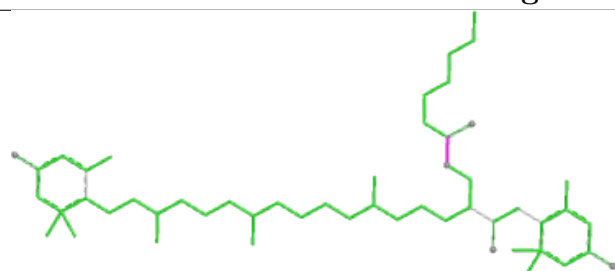


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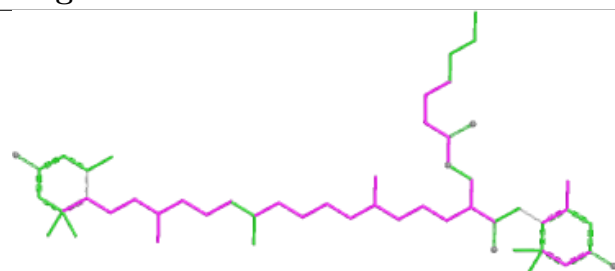


Rings

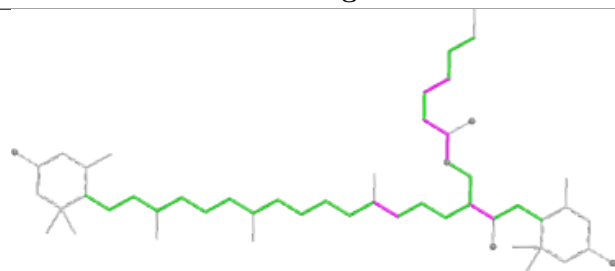
Ligand OUR g 301



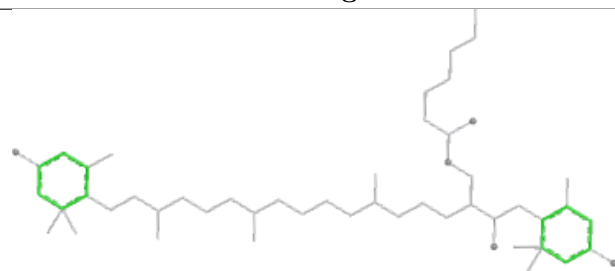
Bond lengths



Bond angles

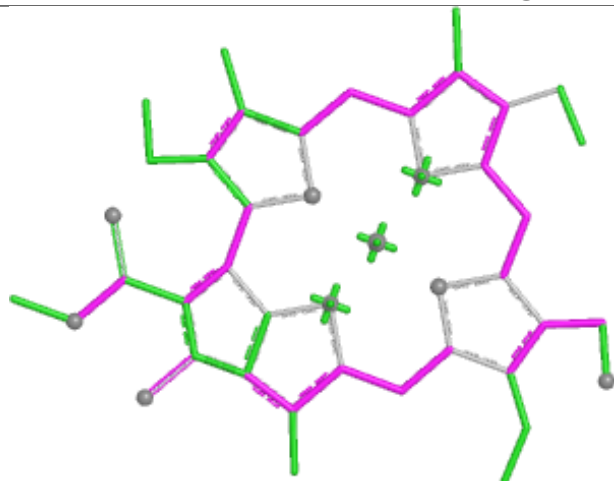


Torsions

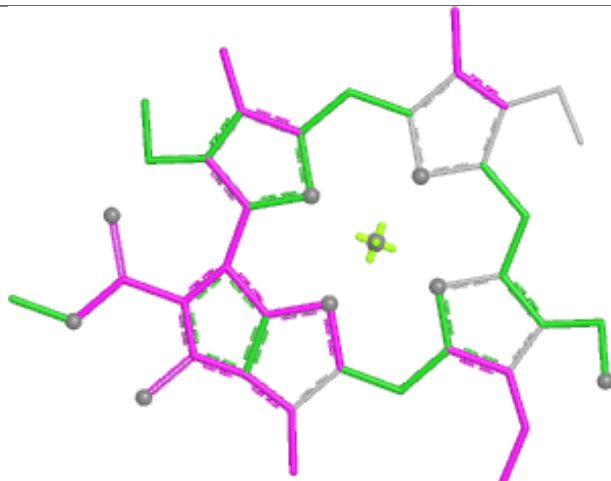


Rings

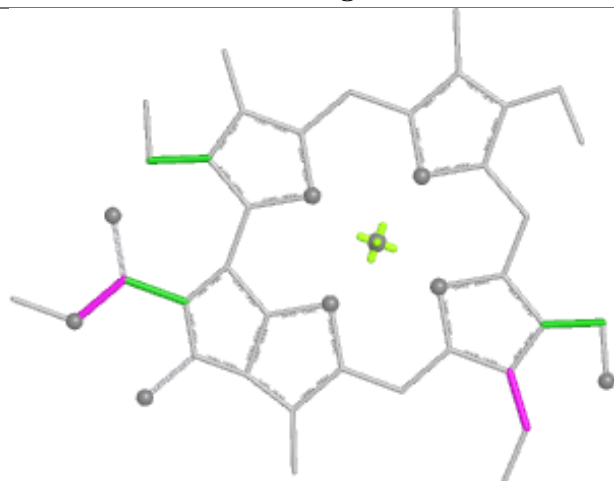
Ligand CHL 9 312



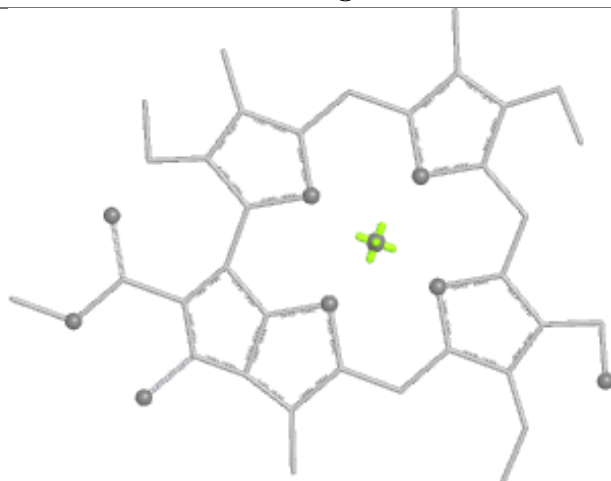
Bond lengths



Bond angles

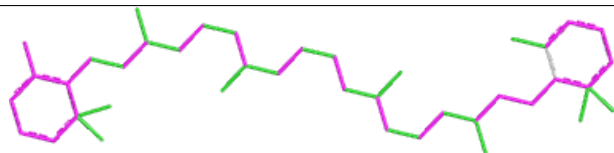


Torsions

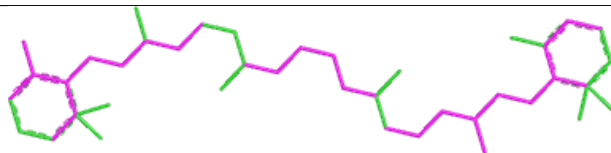


Rings

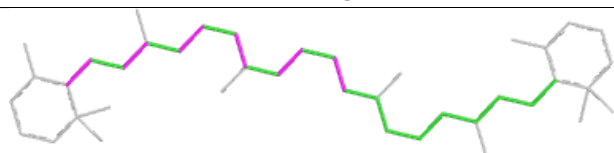
Ligand 8CT A 608



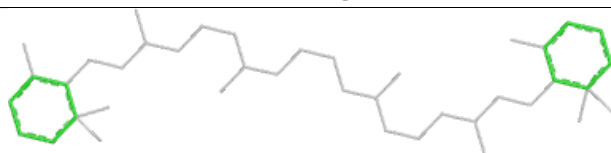
Bond lengths



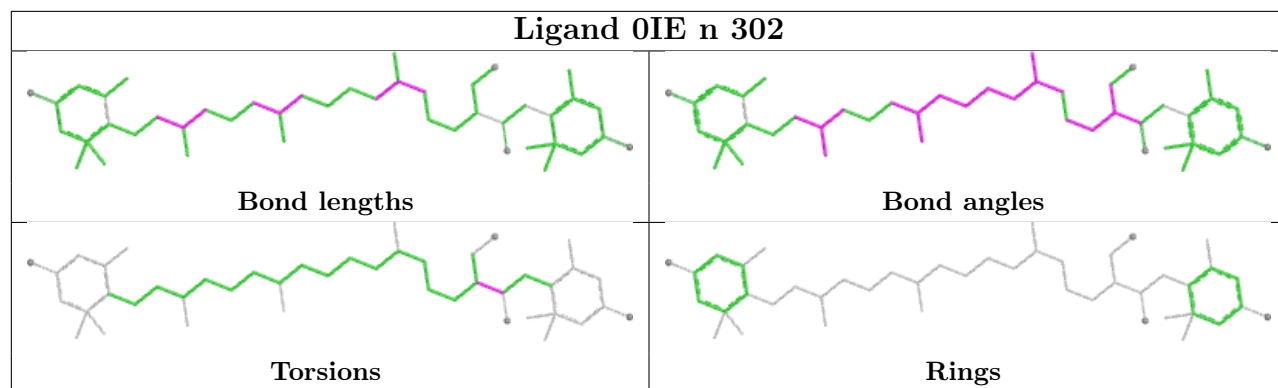
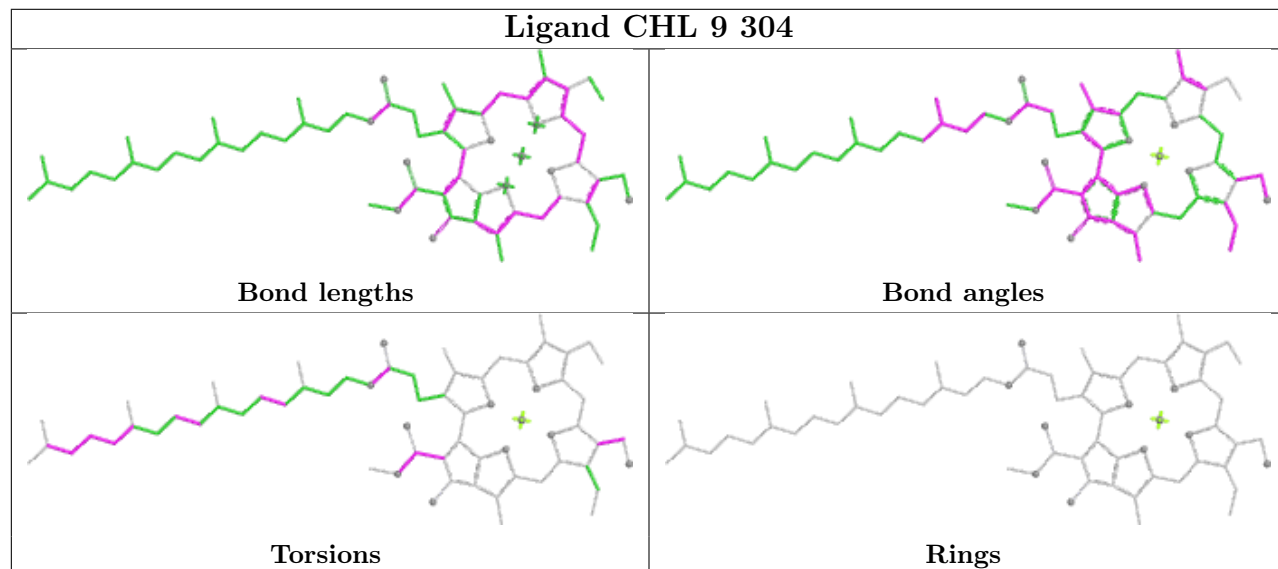
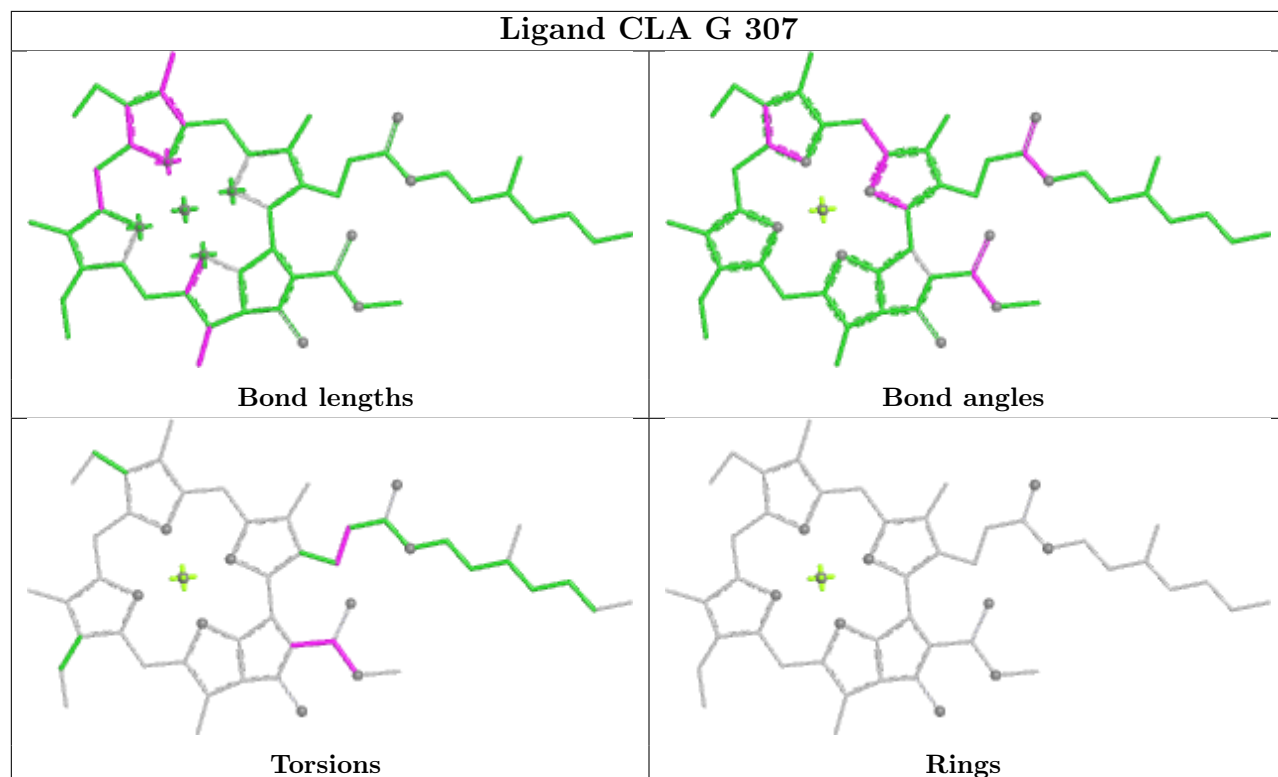
Bond angles



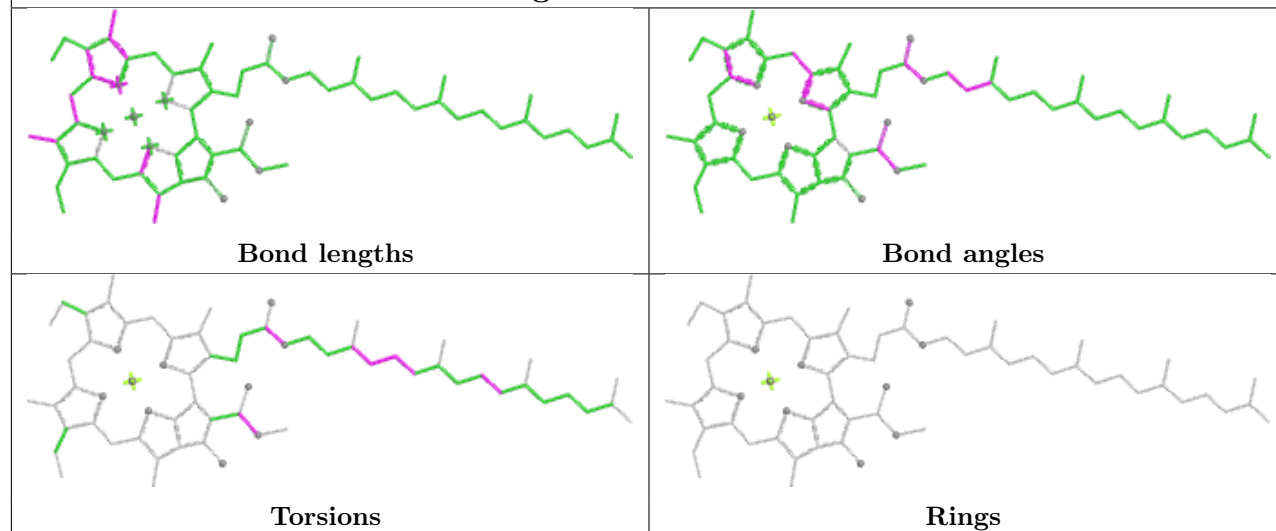
Torsions



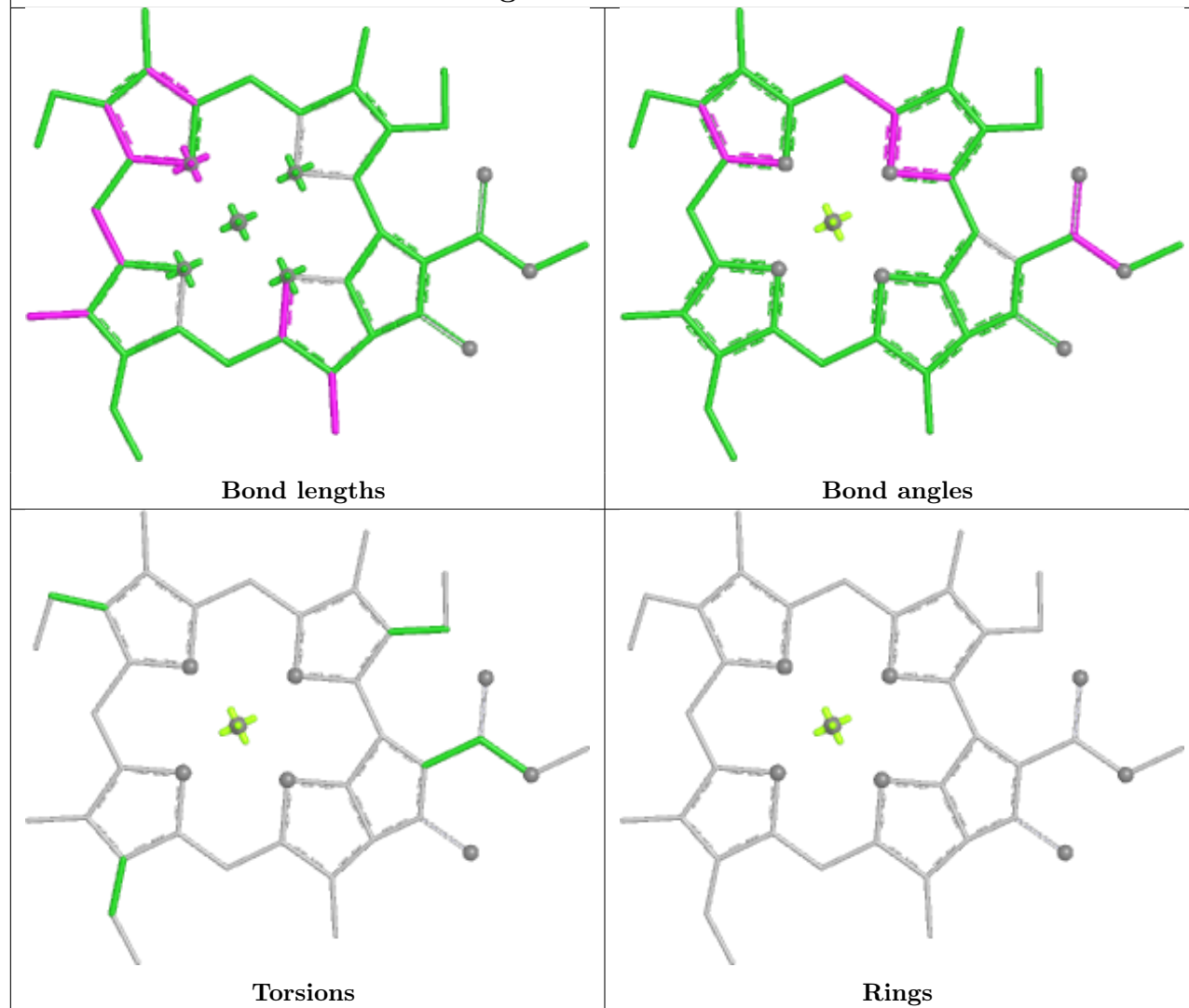
Rings

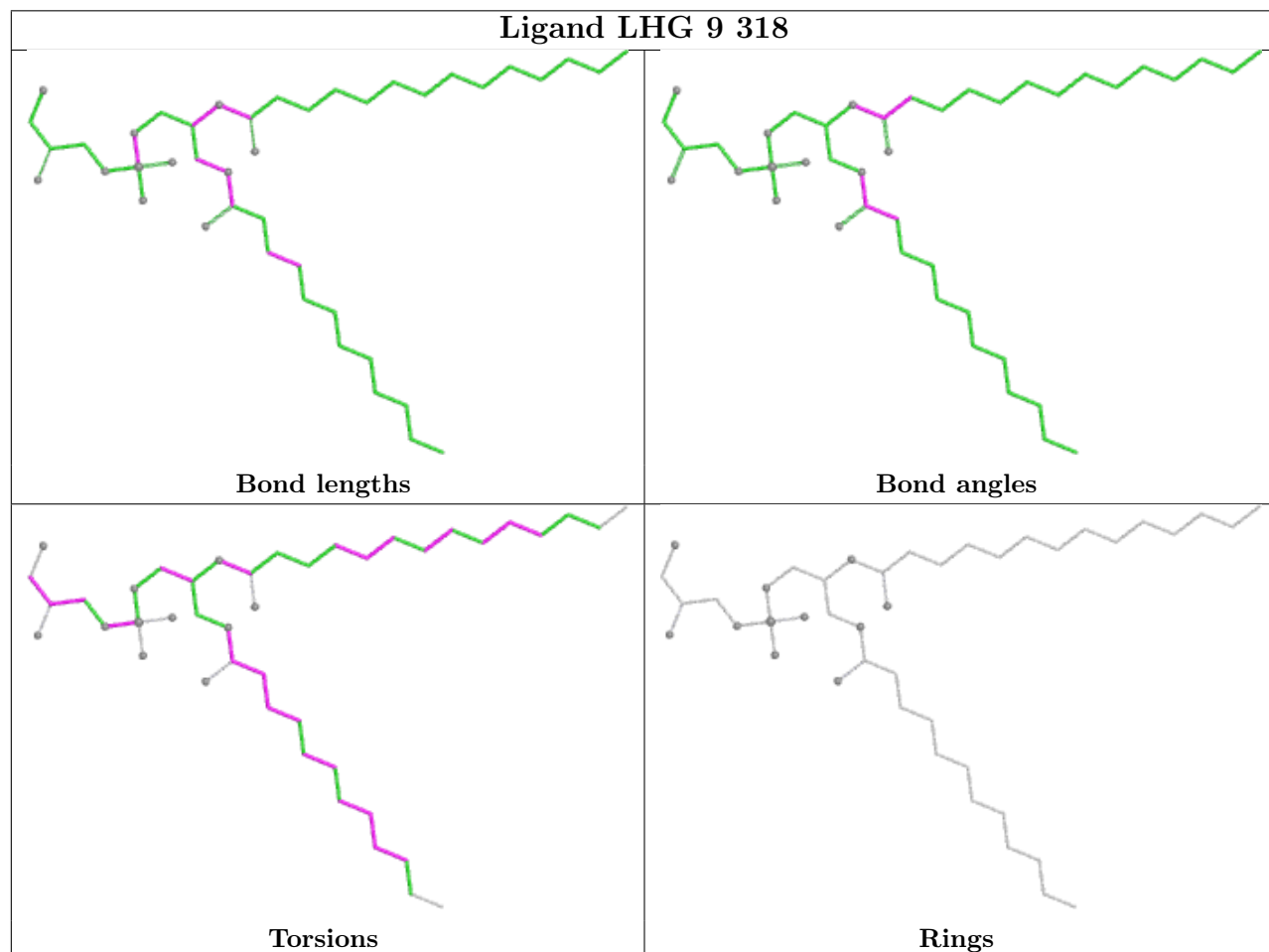
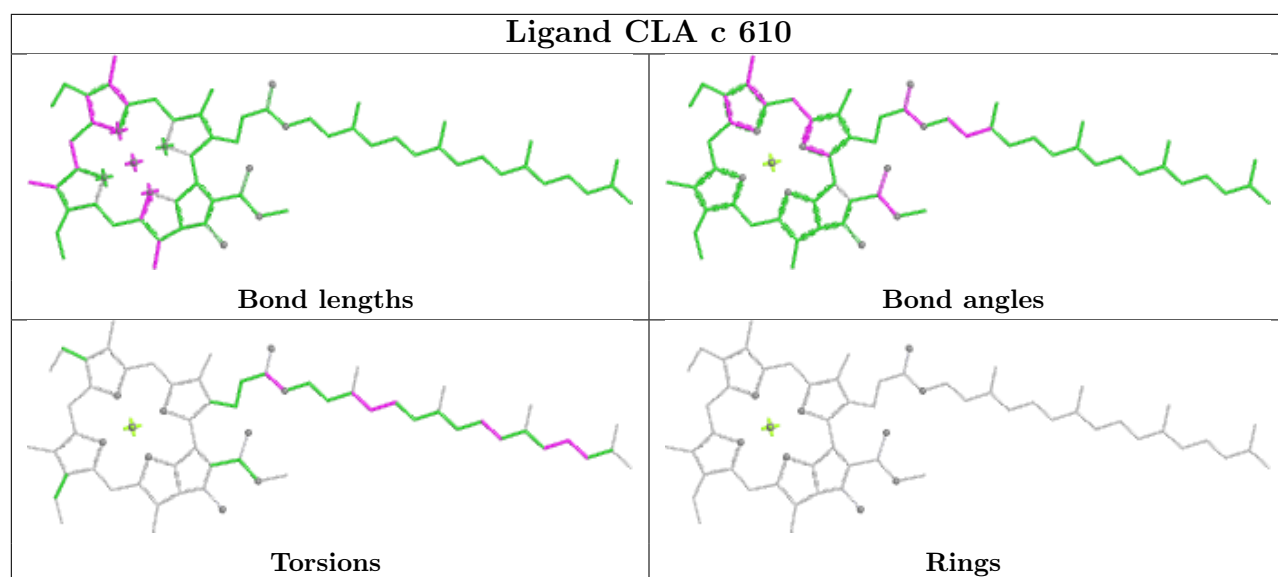
Ligand OIE n 302**Ligand CHL 9 304****Ligand CLA G 307**

Ligand CLA B 613

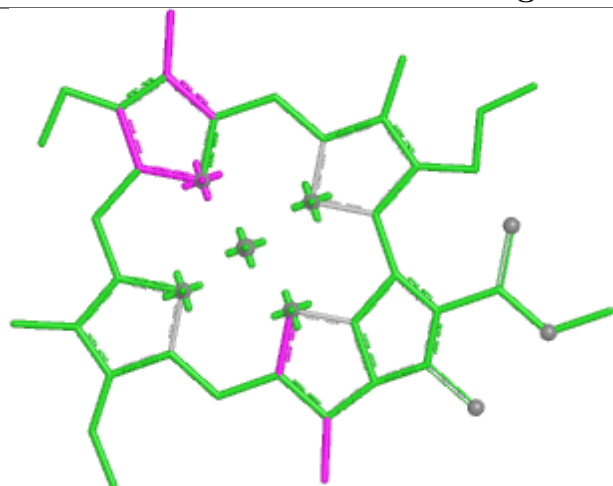


Ligand CLA 4 316

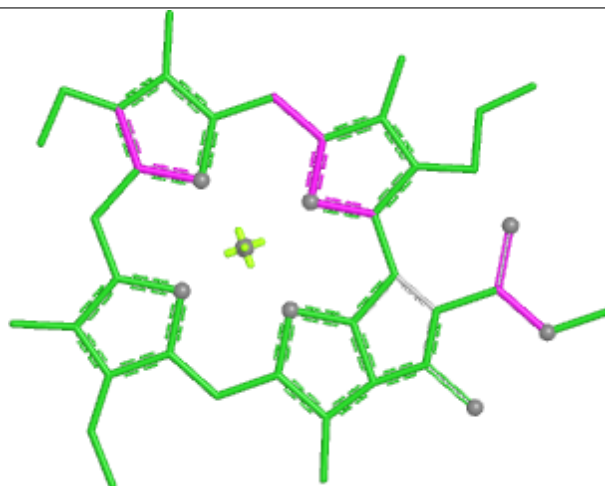




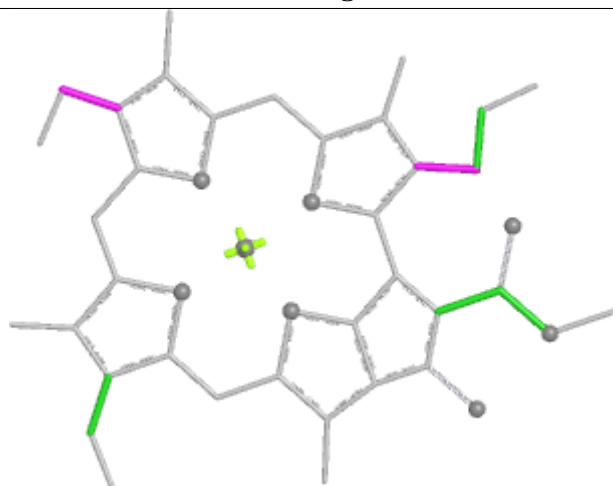
Ligand CLA S 604



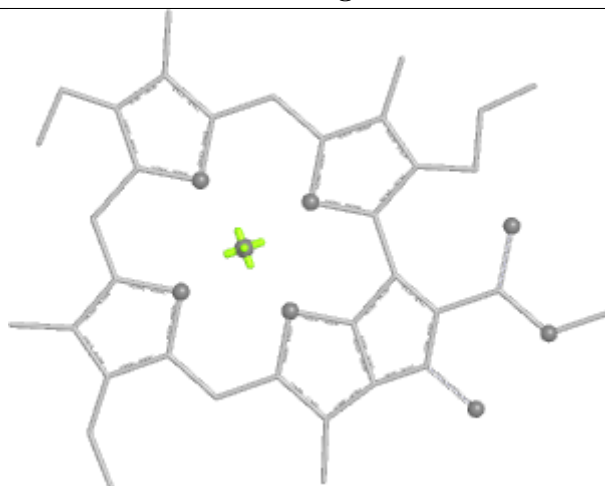
Bond lengths



Bond angles

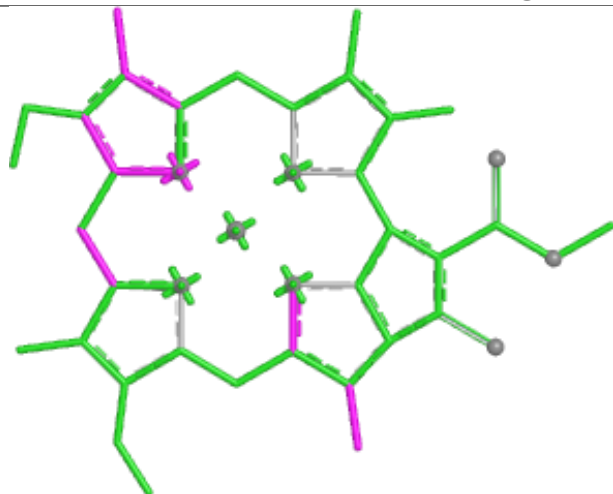


Torsions

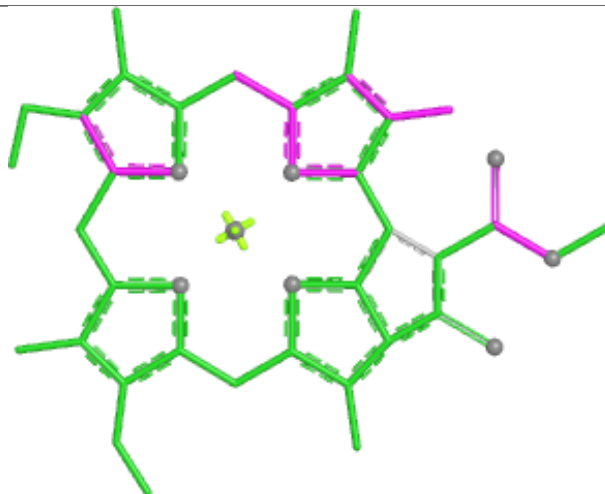


Rings

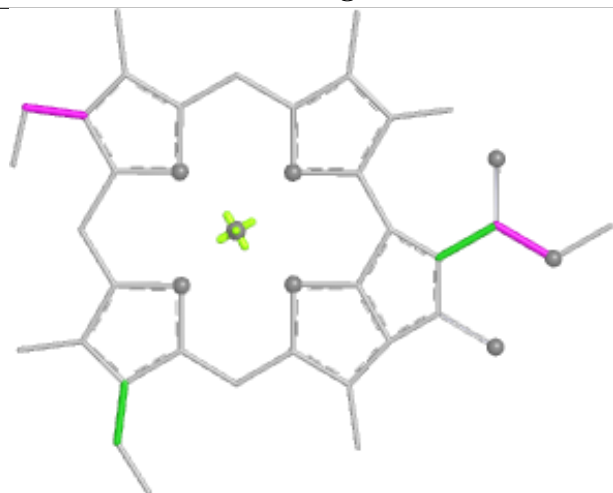
Ligand CLA 1 314



Bond lengths



Bond angles

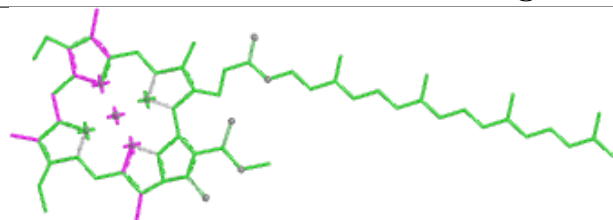


Torsions

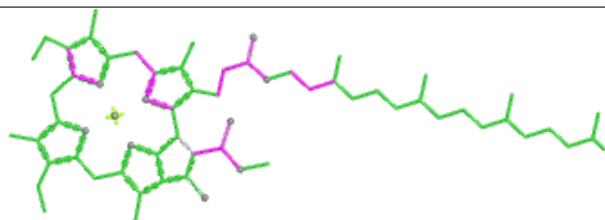


Rings

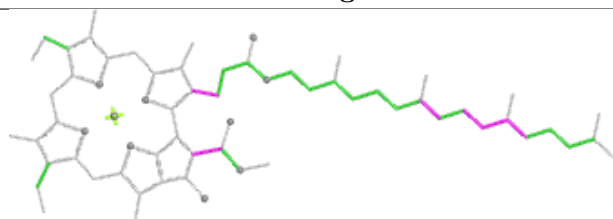
Ligand CLA d 404



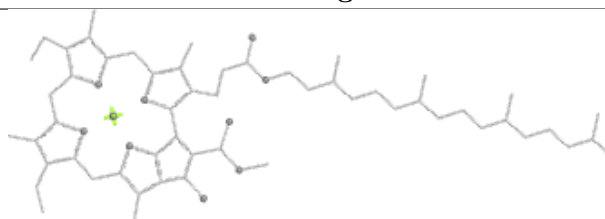
Bond lengths



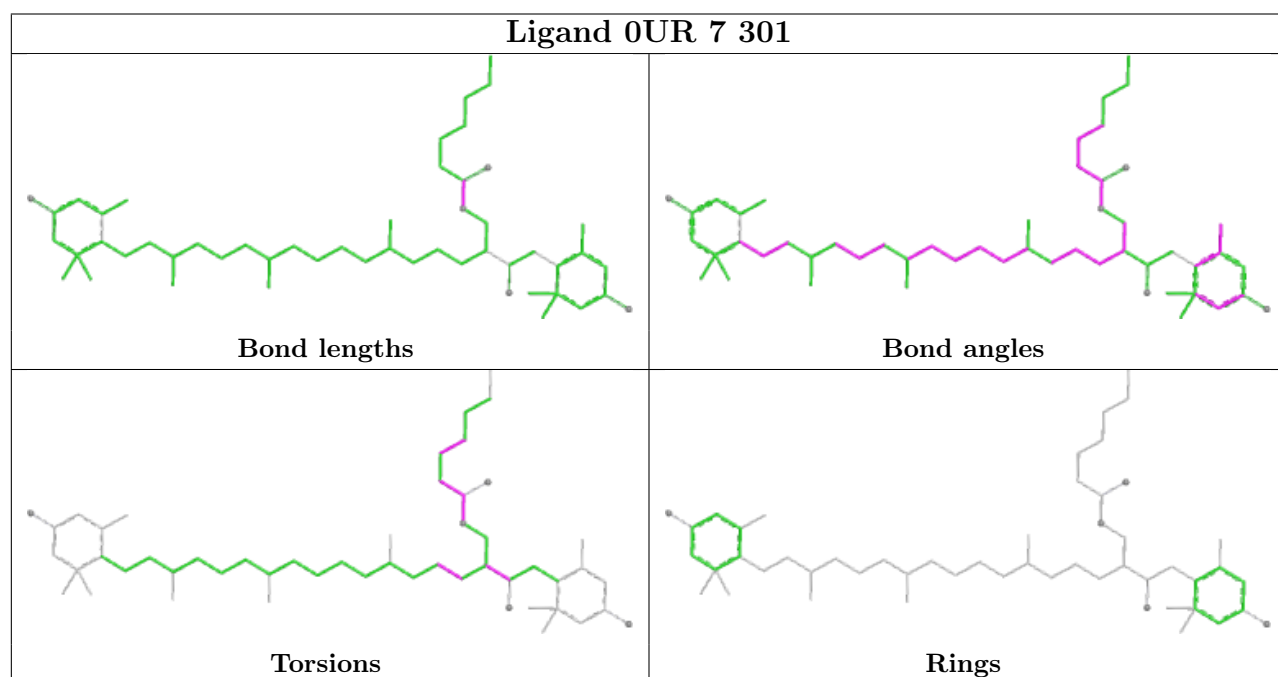
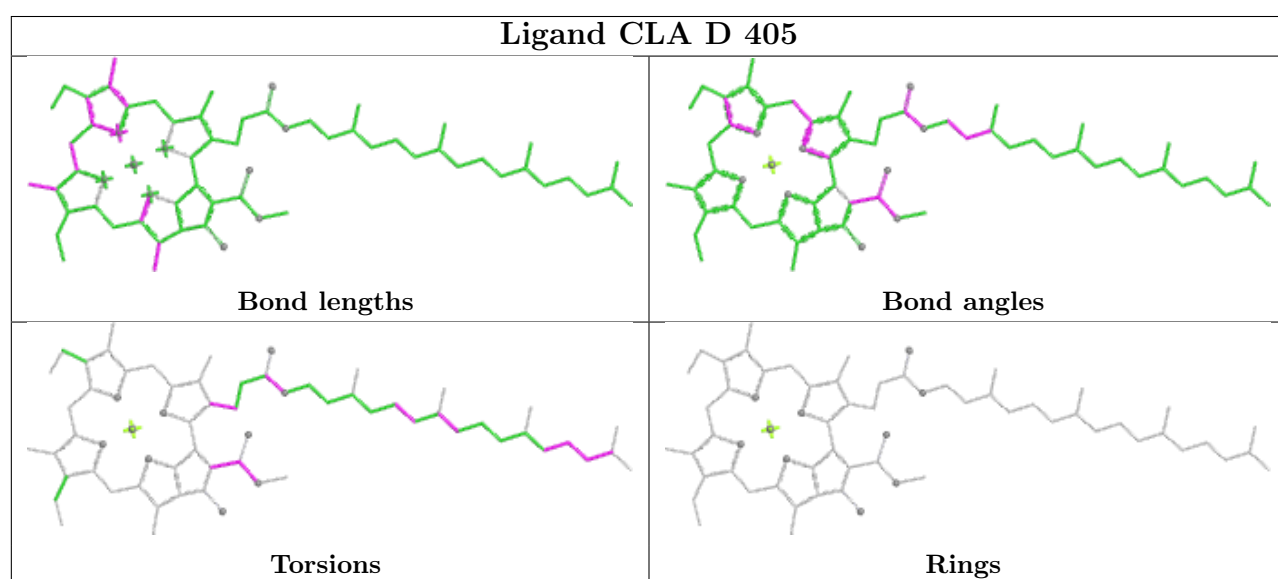
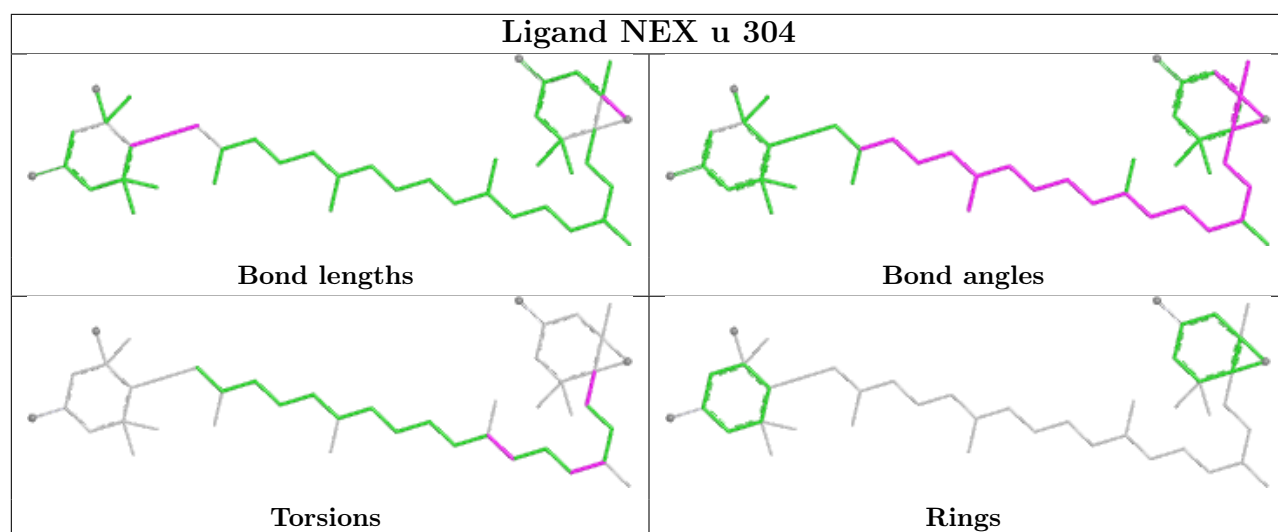
Bond angles



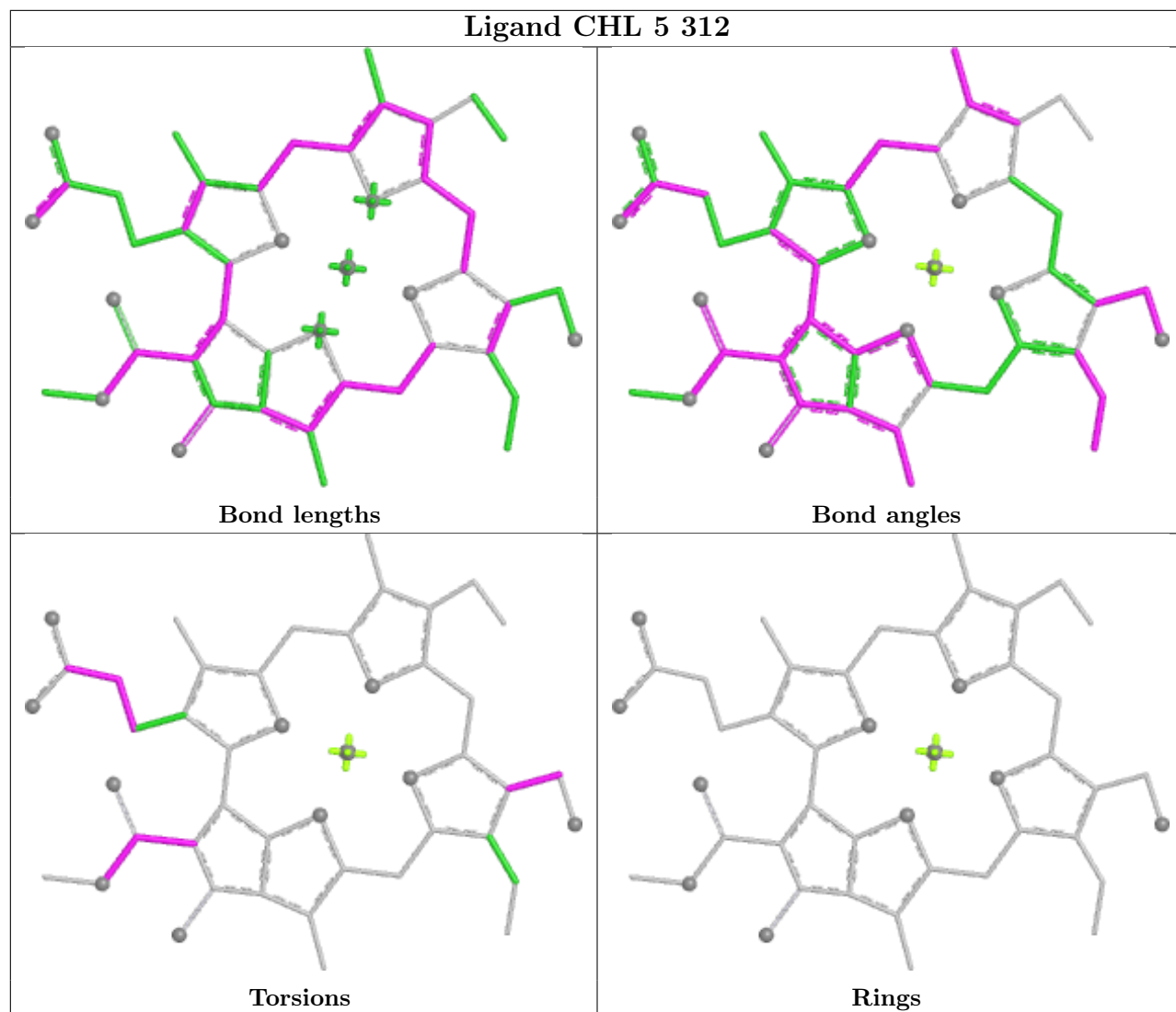
Torsions

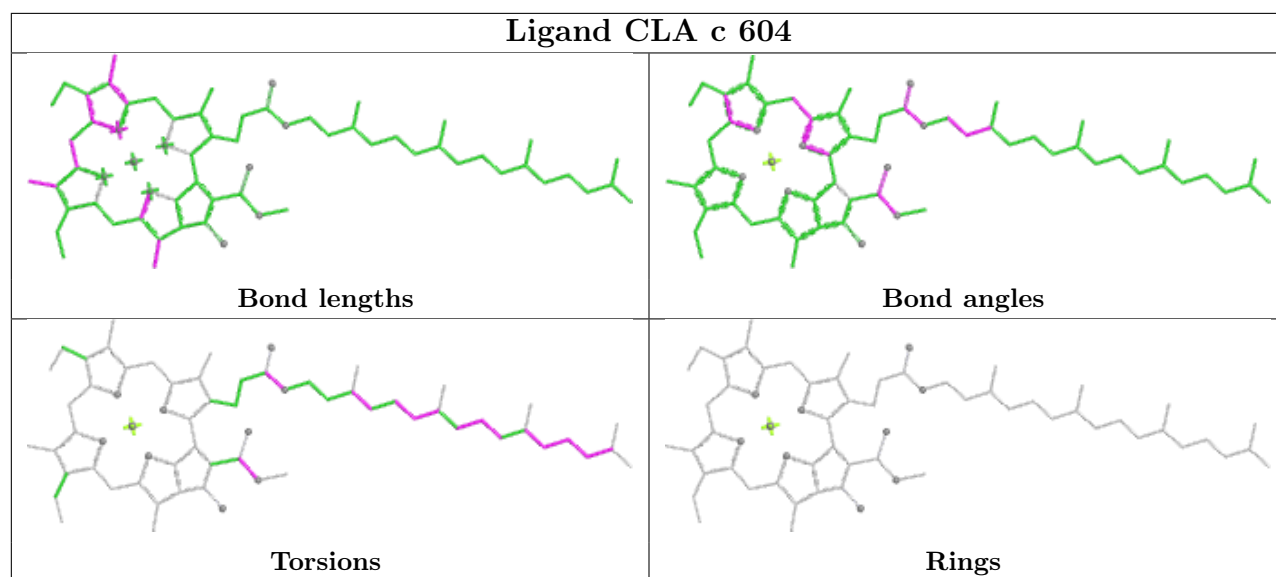
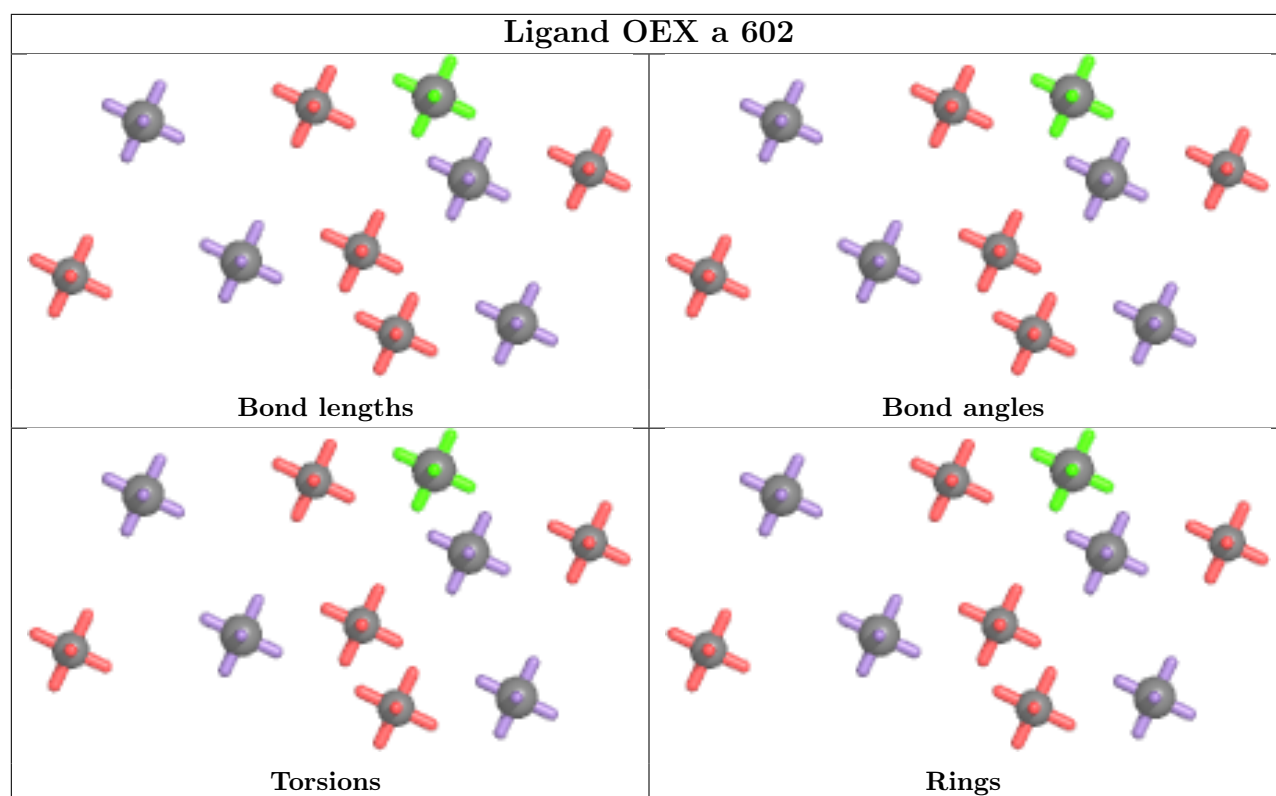


Rings

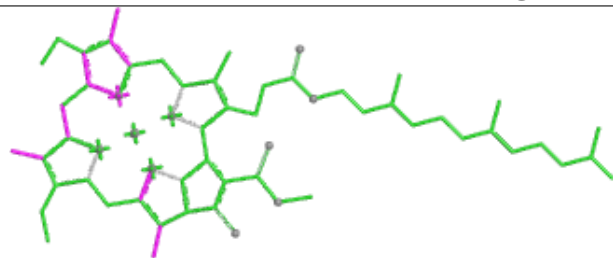


Ligand CHL 5 312

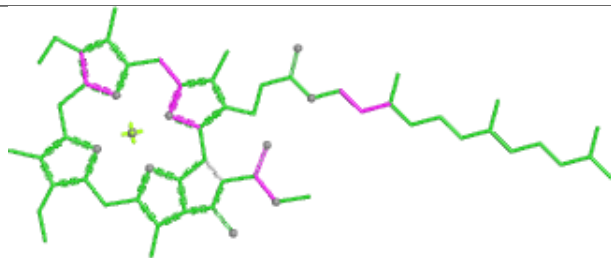




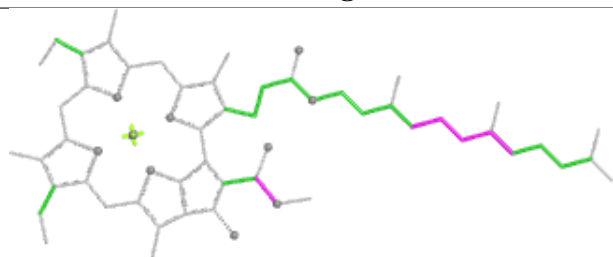
Ligand CLA G 315



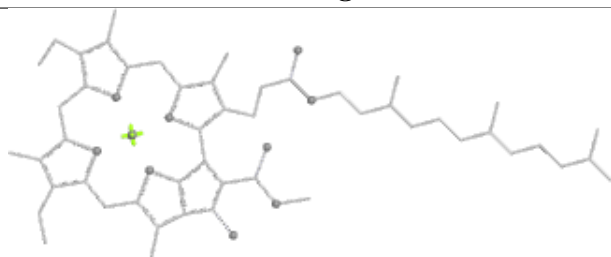
Bond lengths



Bond angles

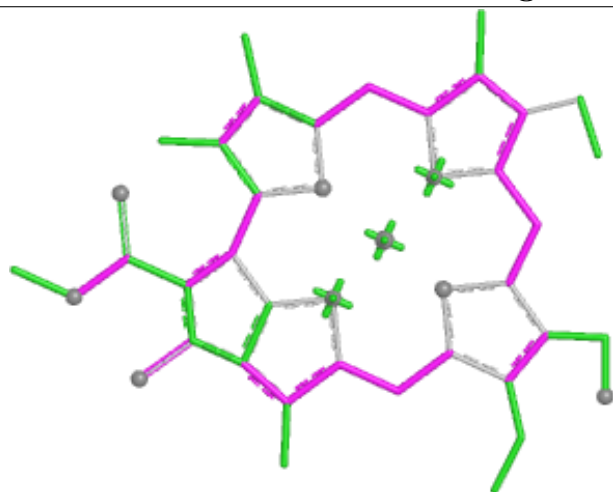


Torsions

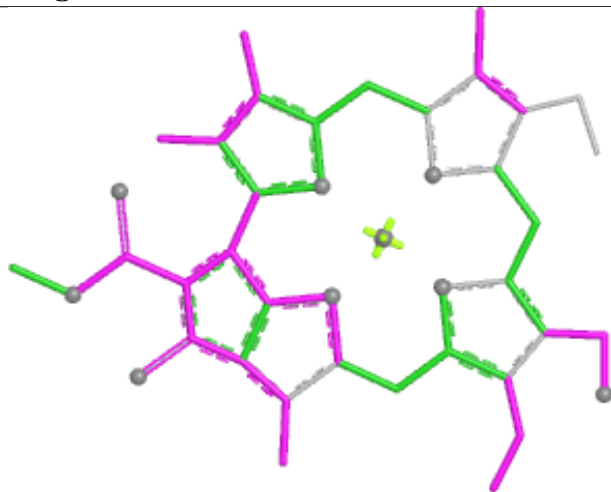


Rings

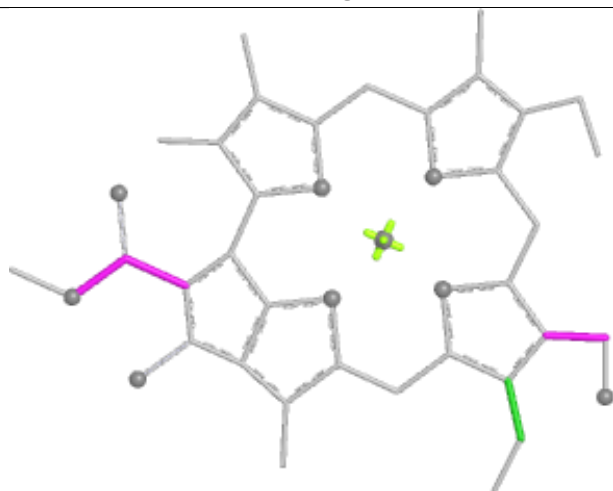
Ligand CHL g 318



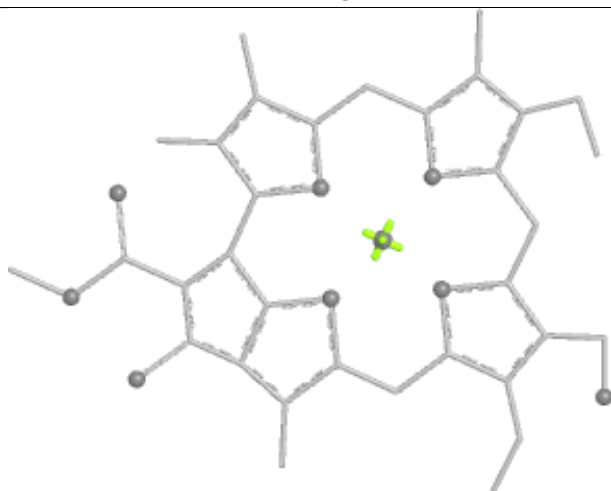
Bond lengths



Bond angles

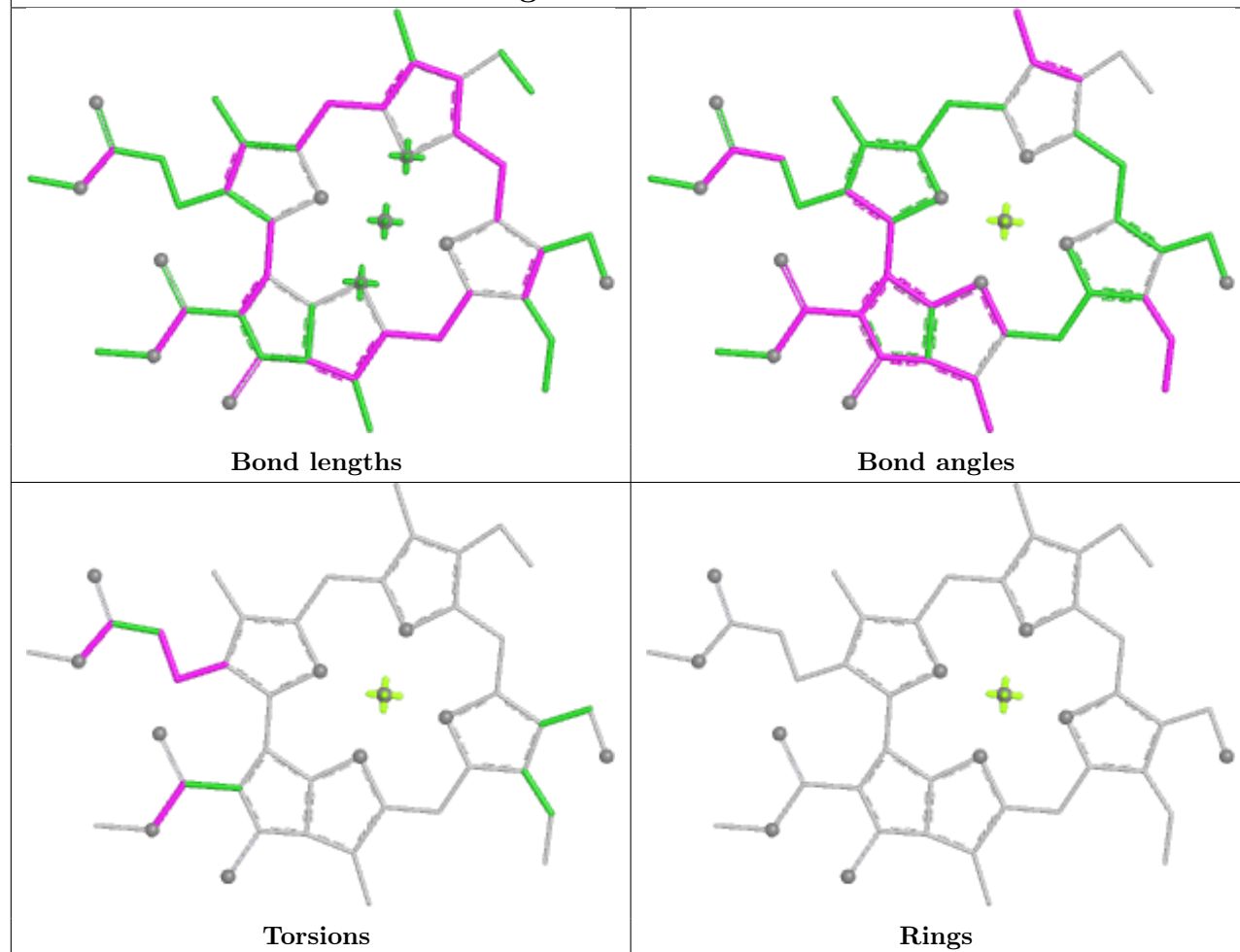


Torsions

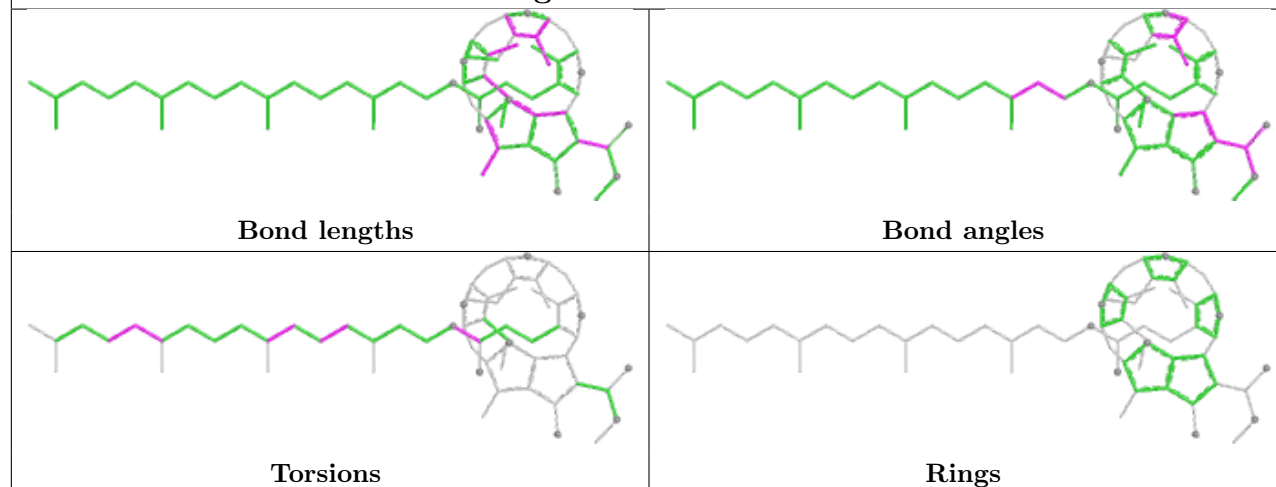


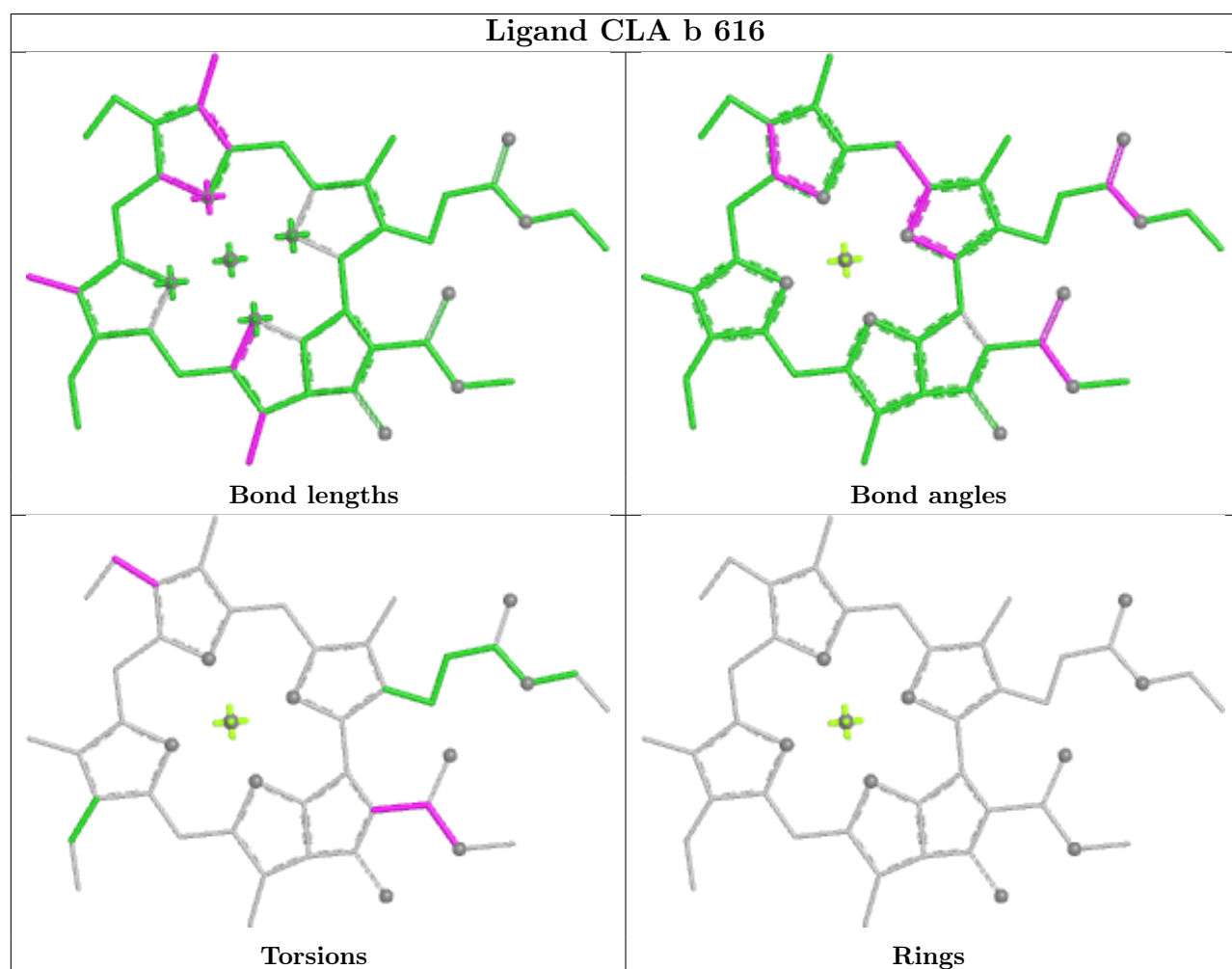
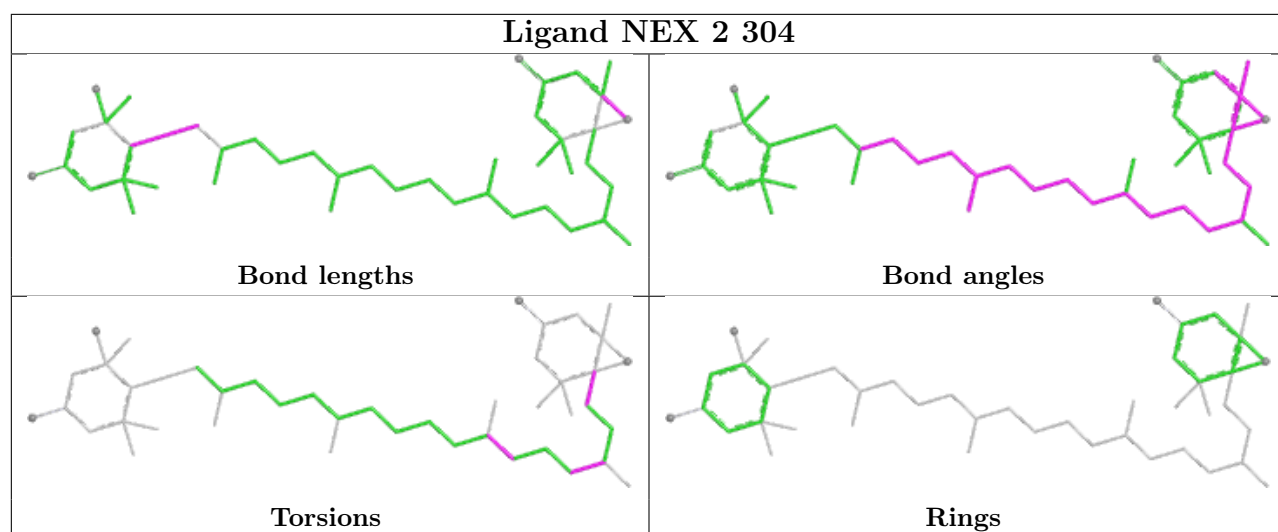
Rings

Ligand CHL u 312

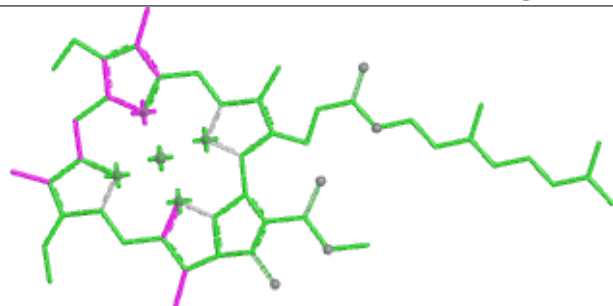


Ligand PHO a 606

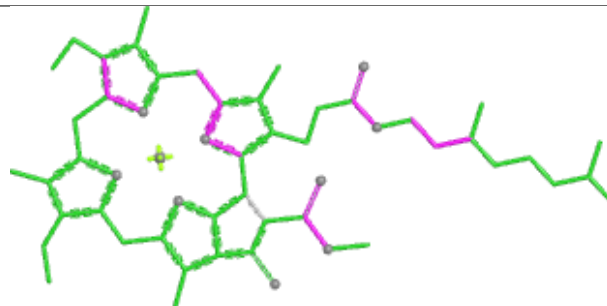




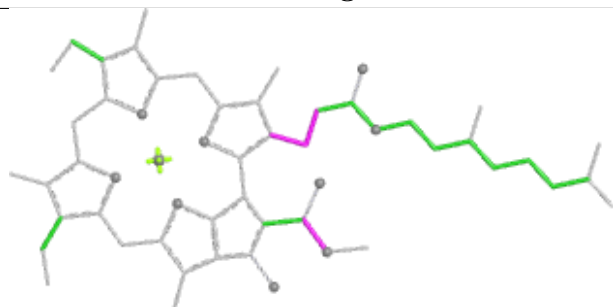
Ligand CLA S 609



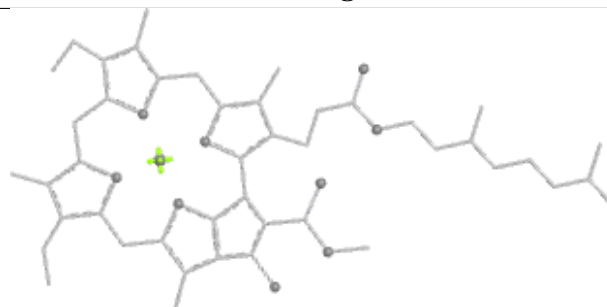
Bond lengths



Bond angles

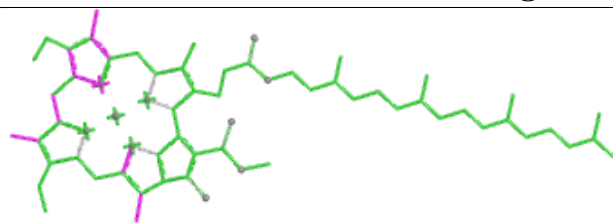


Torsions

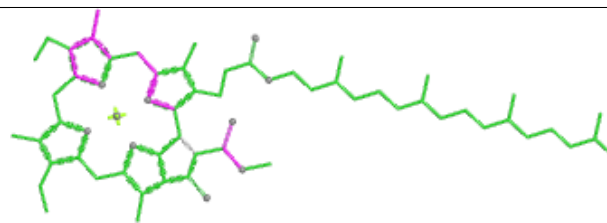


Rings

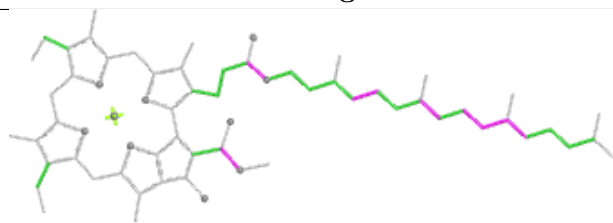
Ligand CLA c 611



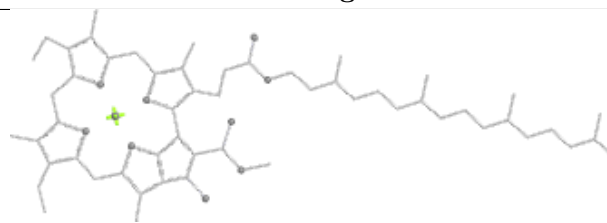
Bond lengths



Bond angles

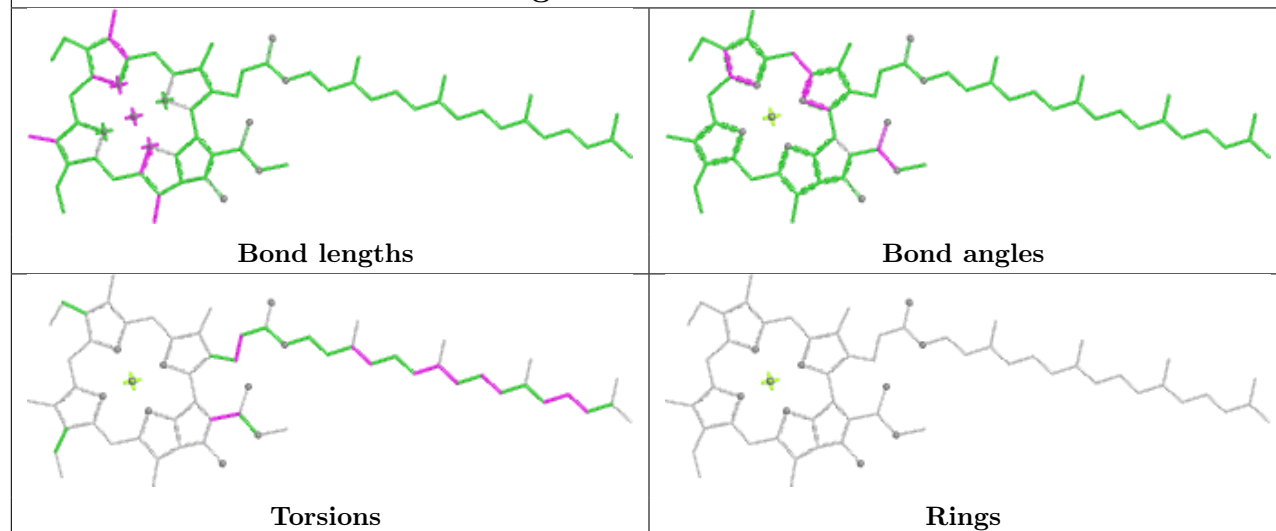


Torsions

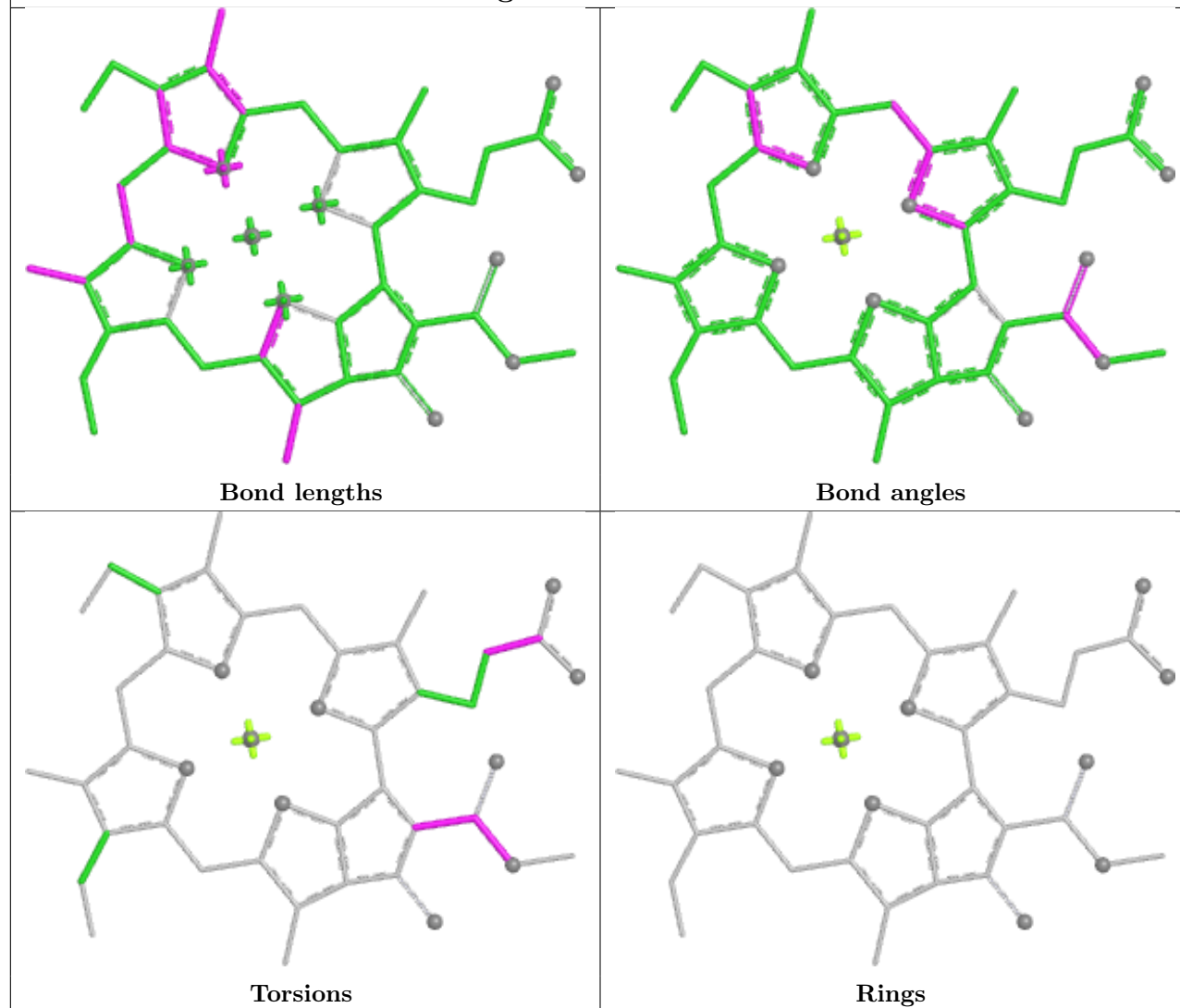


Rings

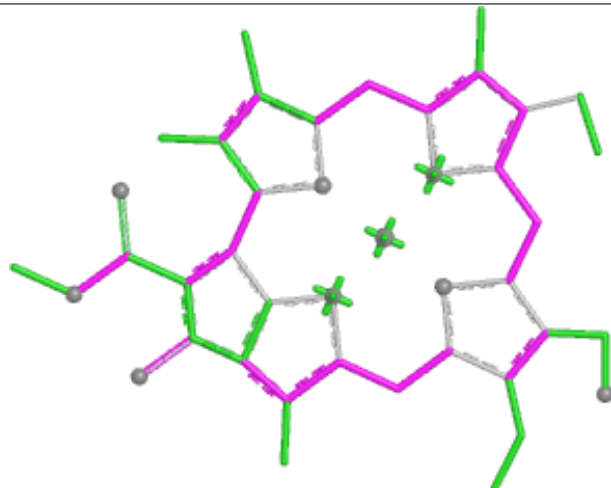
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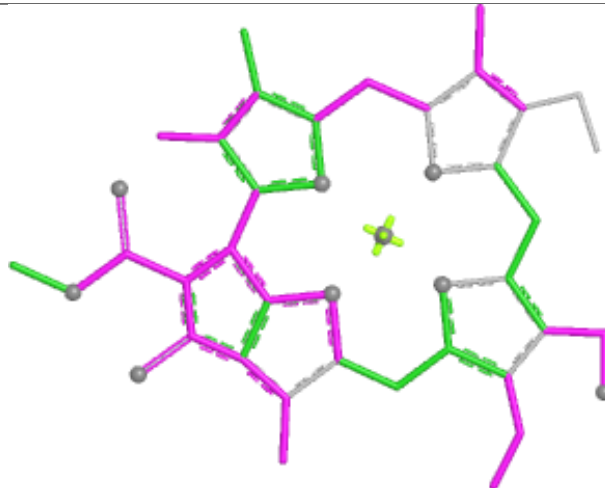
Ligand CLA s 412



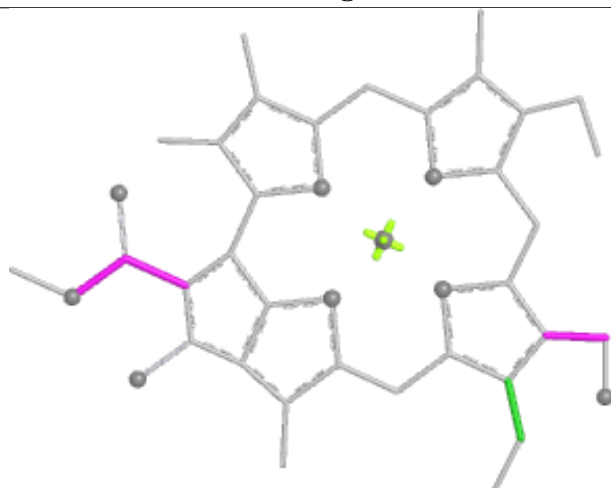
Ligand CHL 1 317



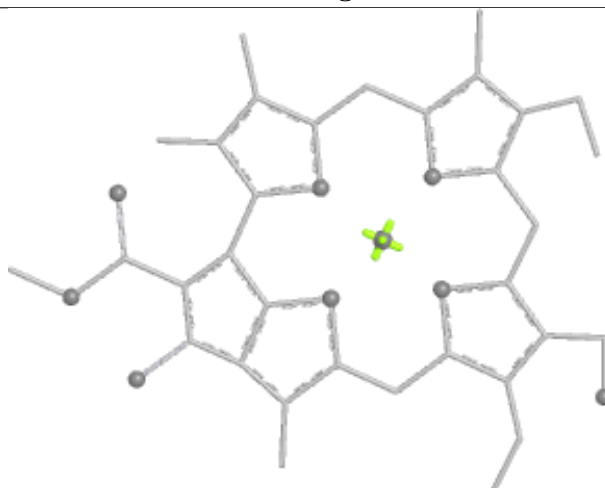
Bond lengths



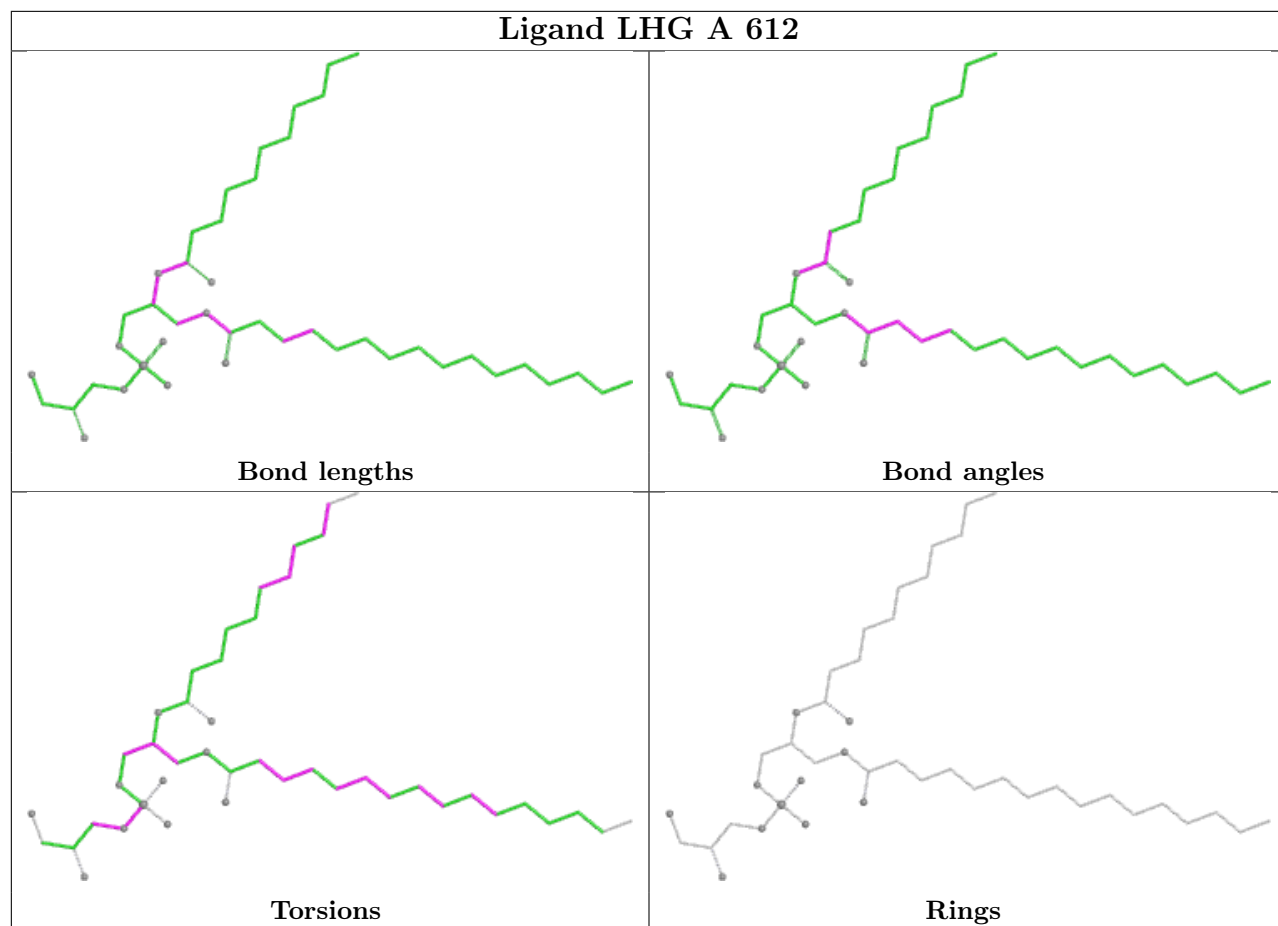
Bond angles



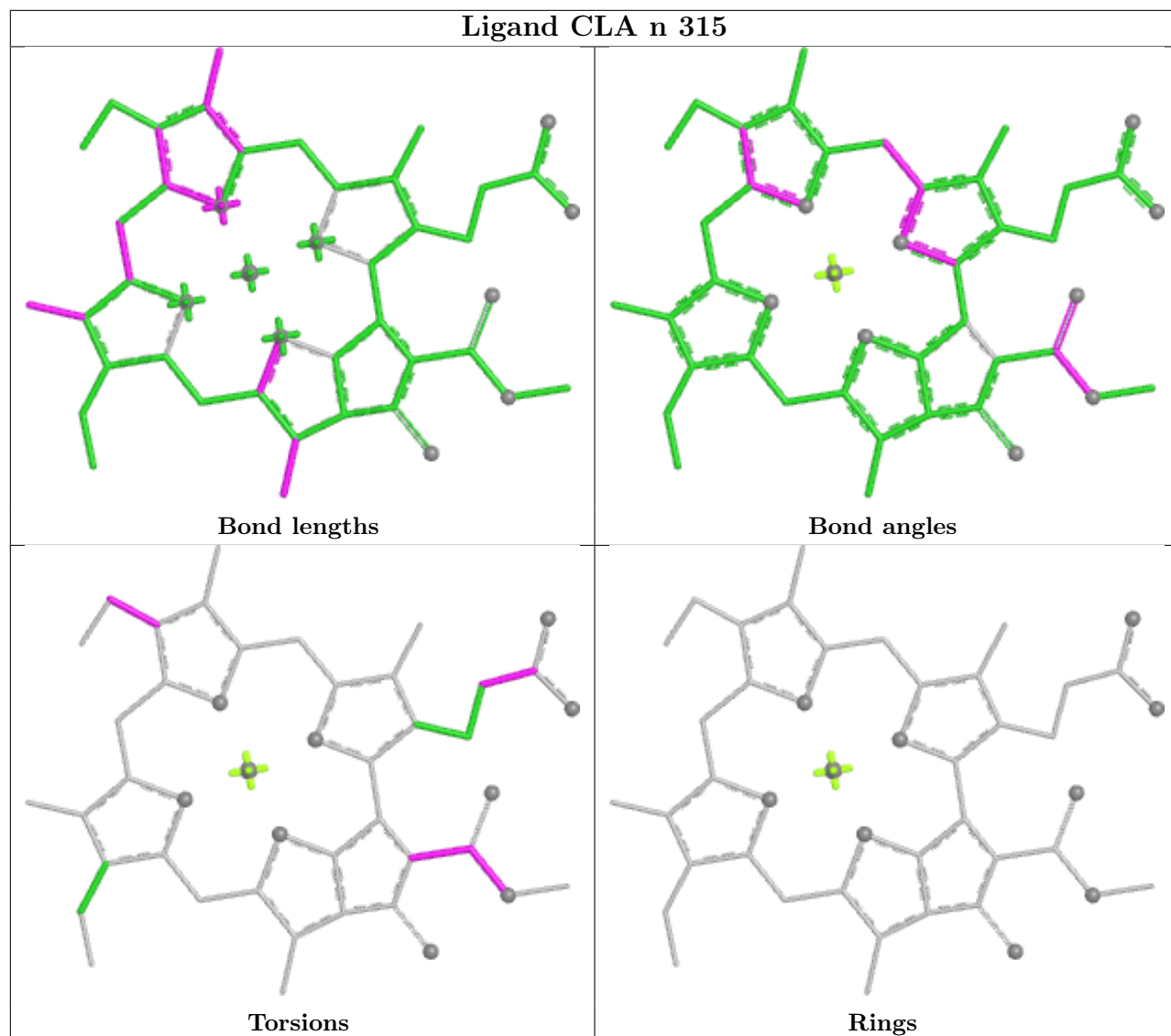
Torsions



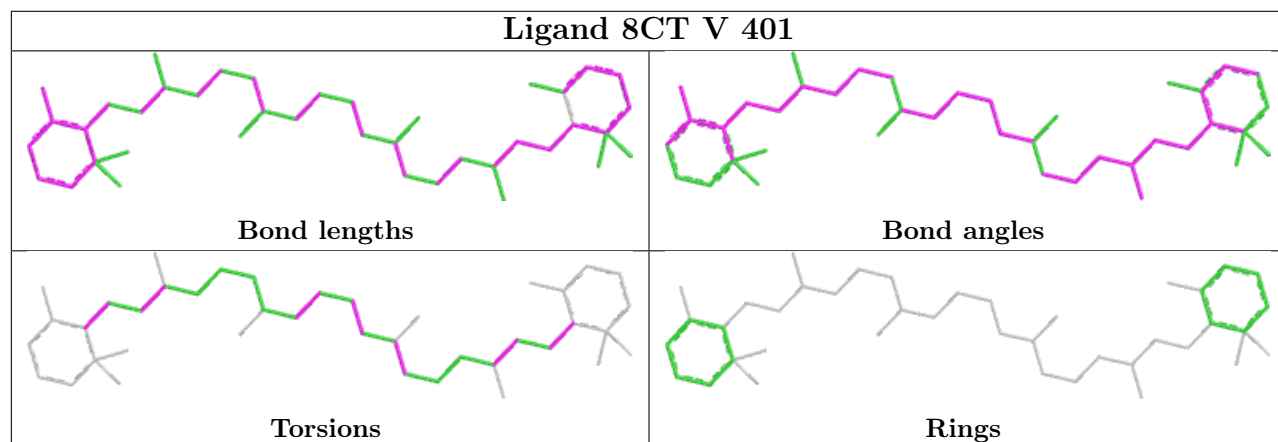
Rings

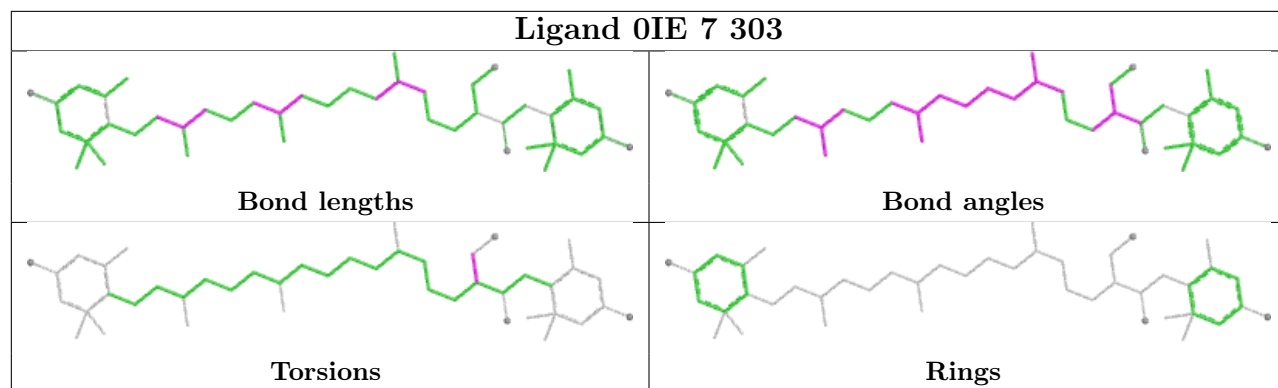
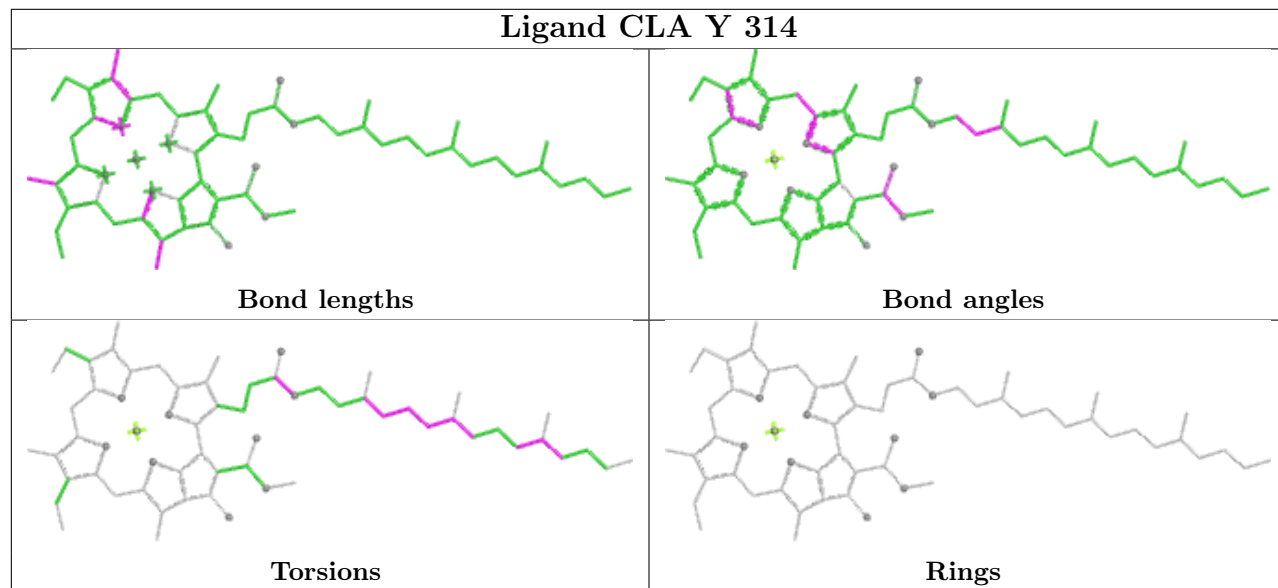


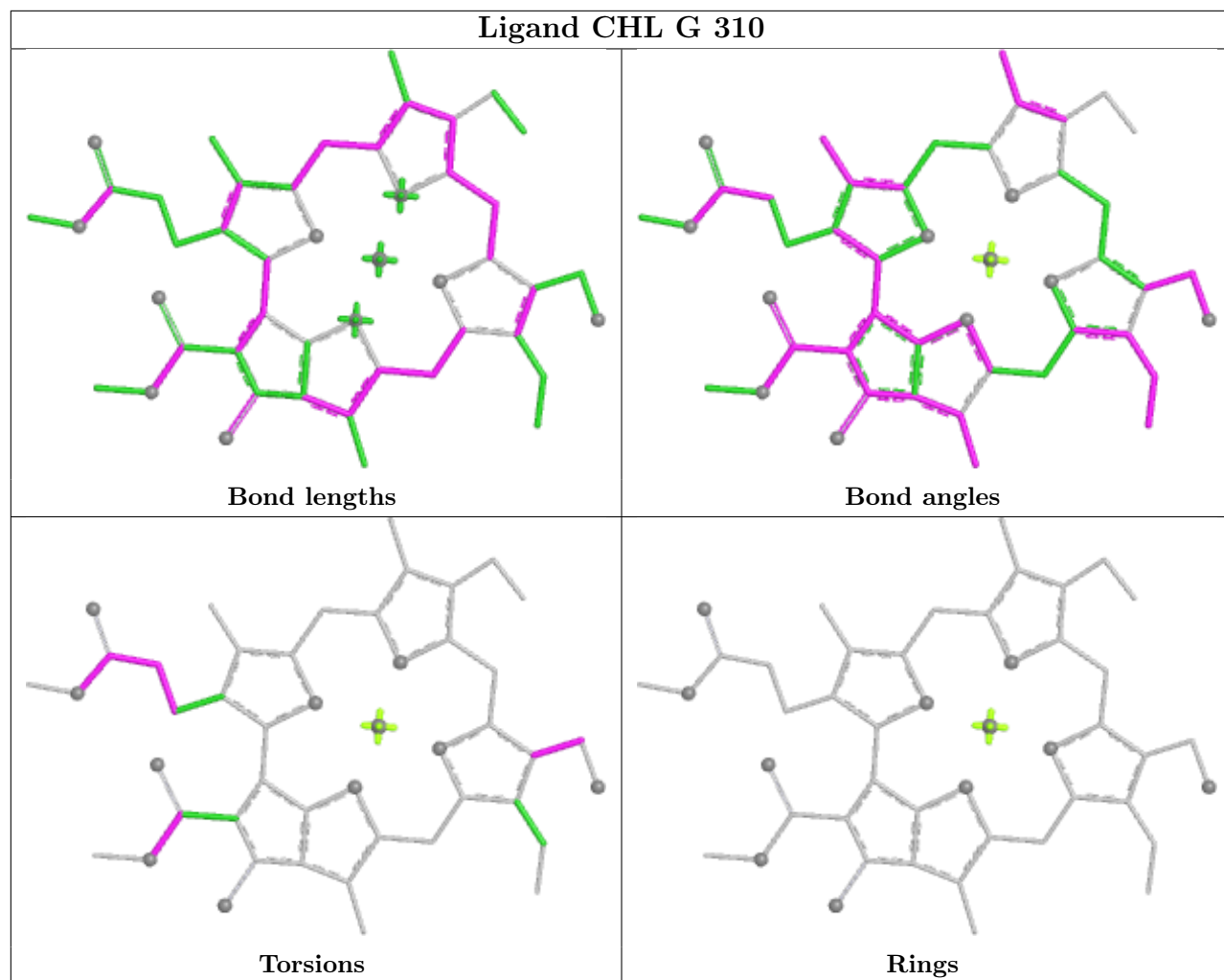
Ligand CLA n 315

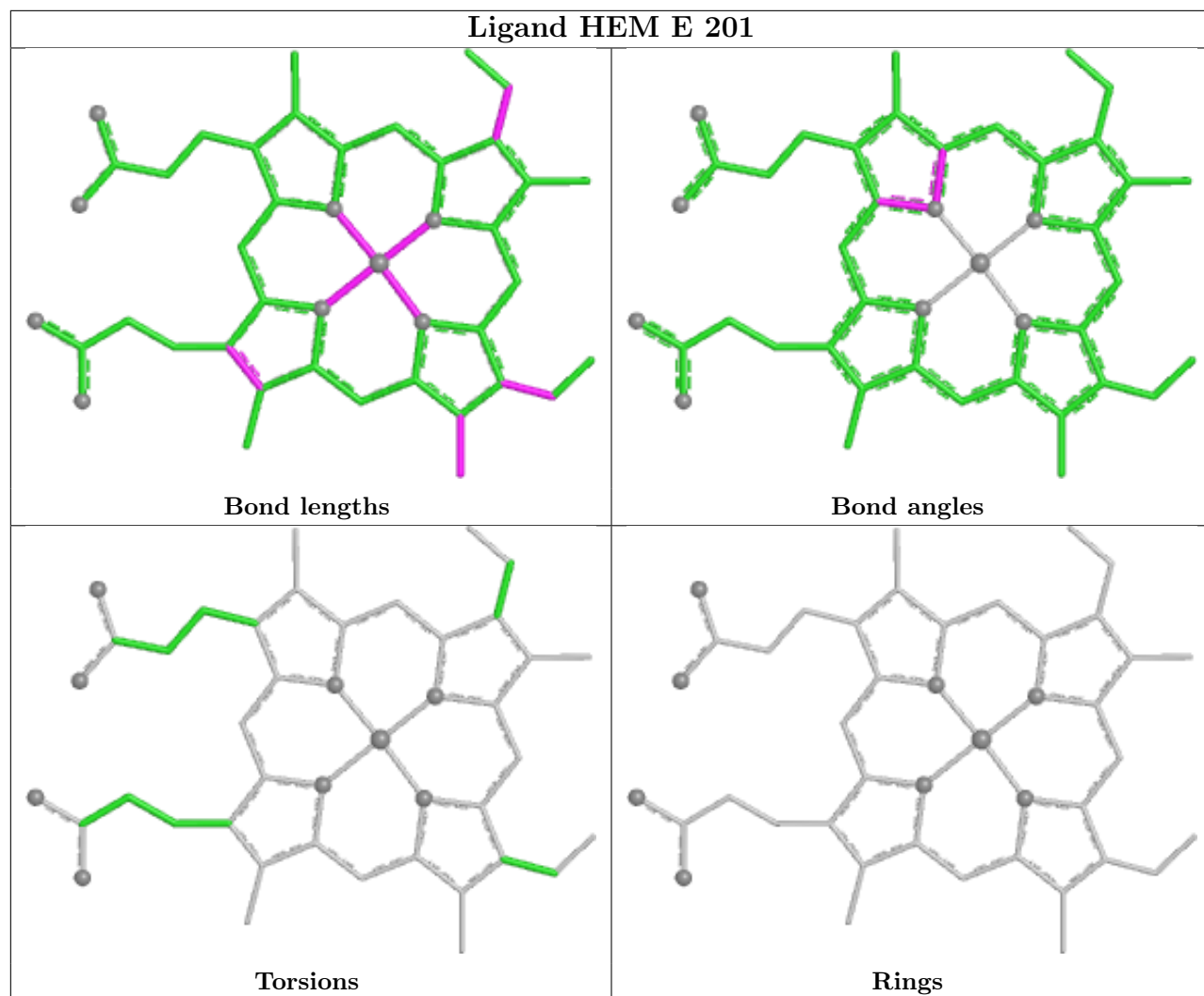


Ligand 8CT V 401

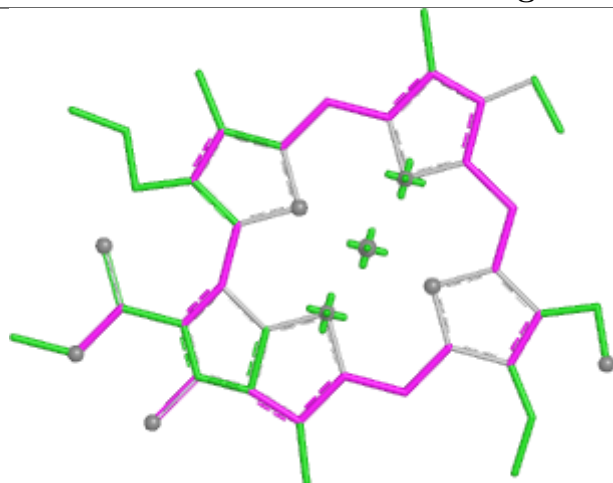


Ligand OIE 7 303**Ligand CLA Y 314**

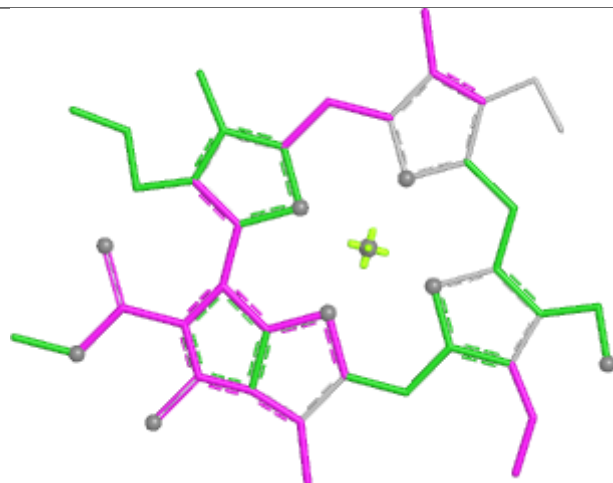




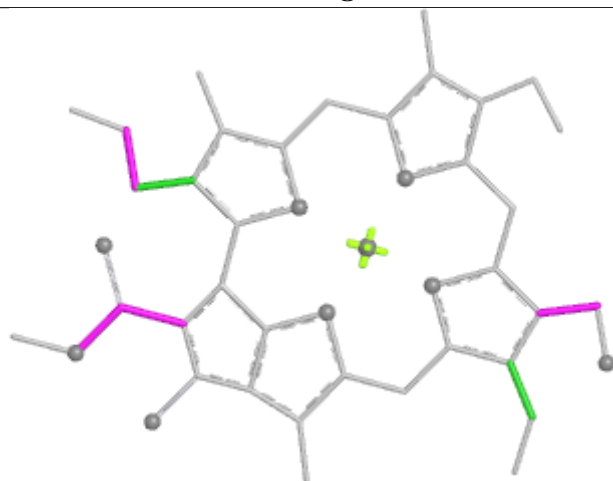
Ligand CHL 3 311



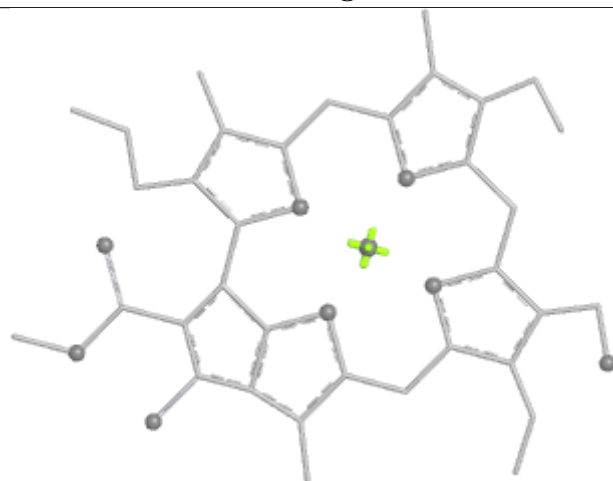
Bond lengths



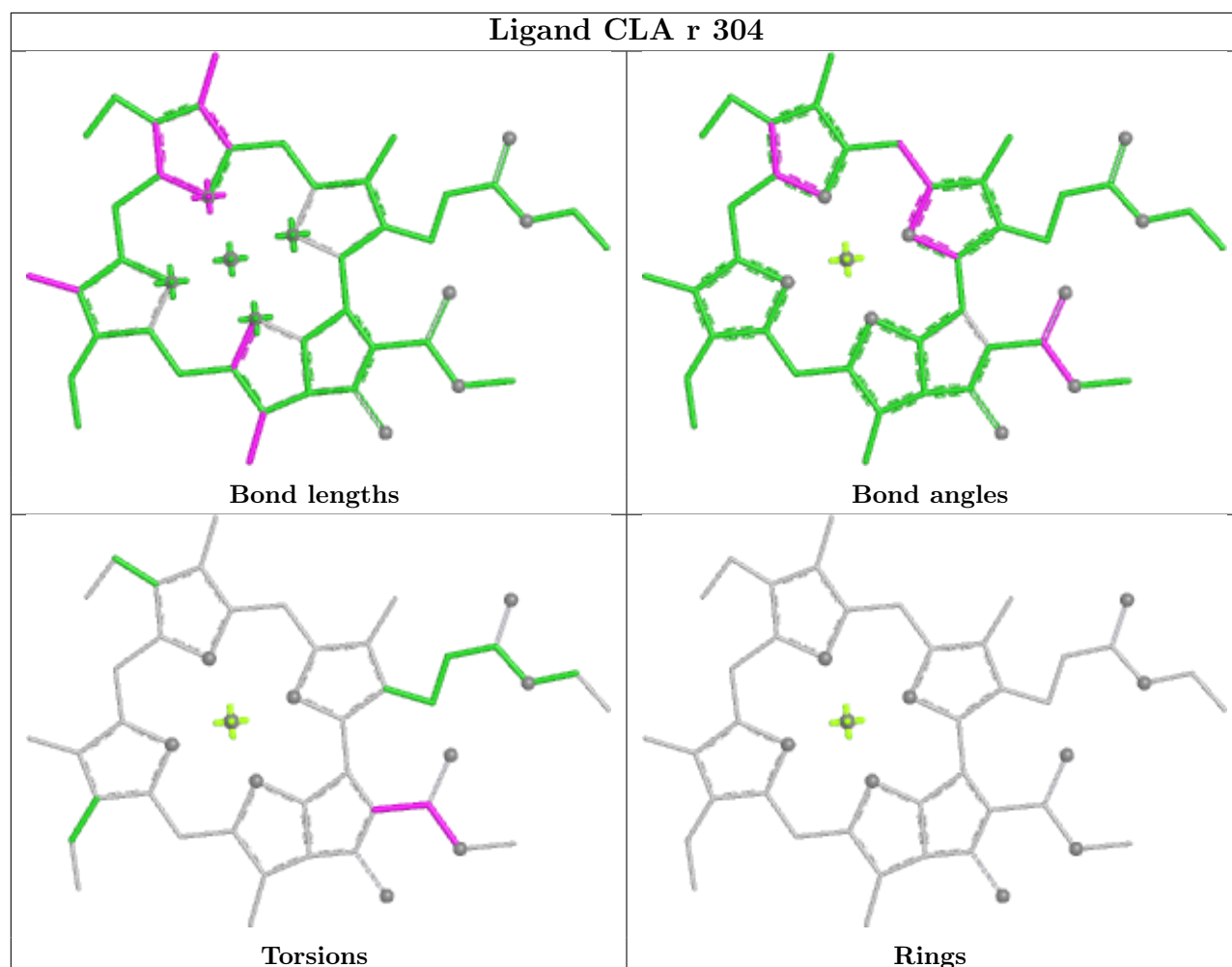
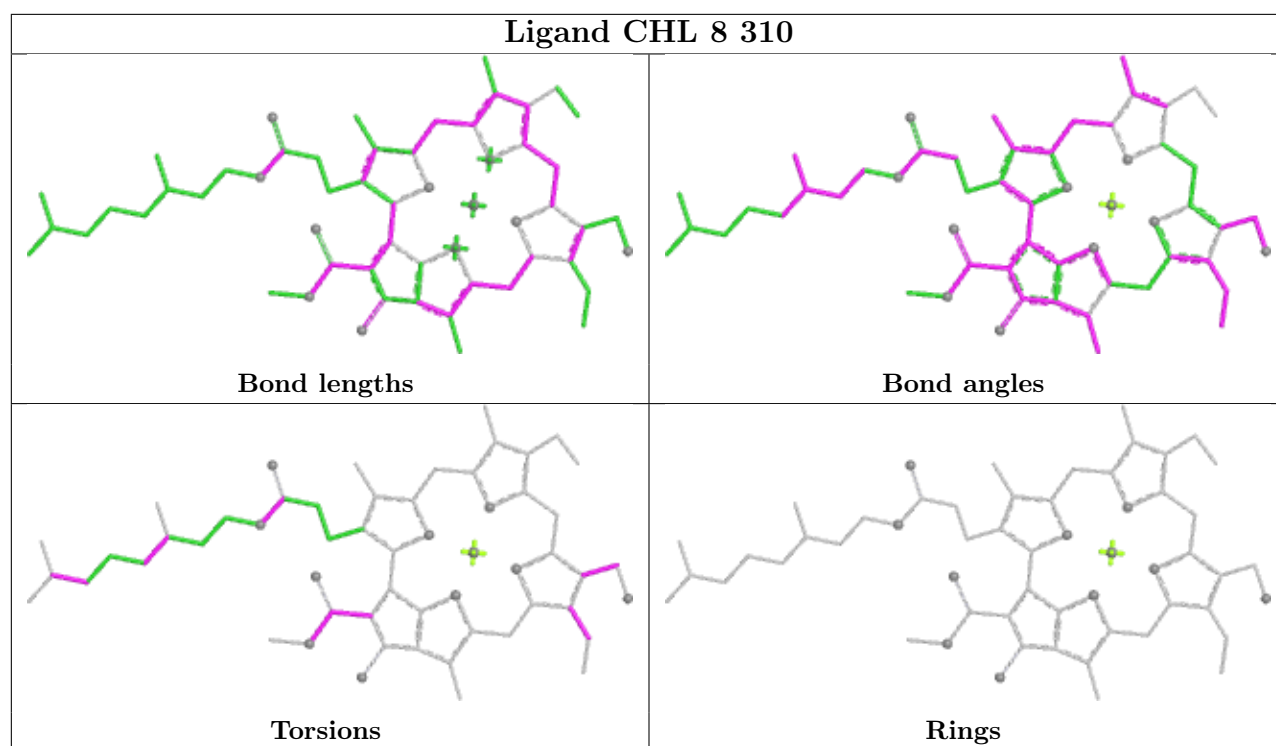
Bond angles

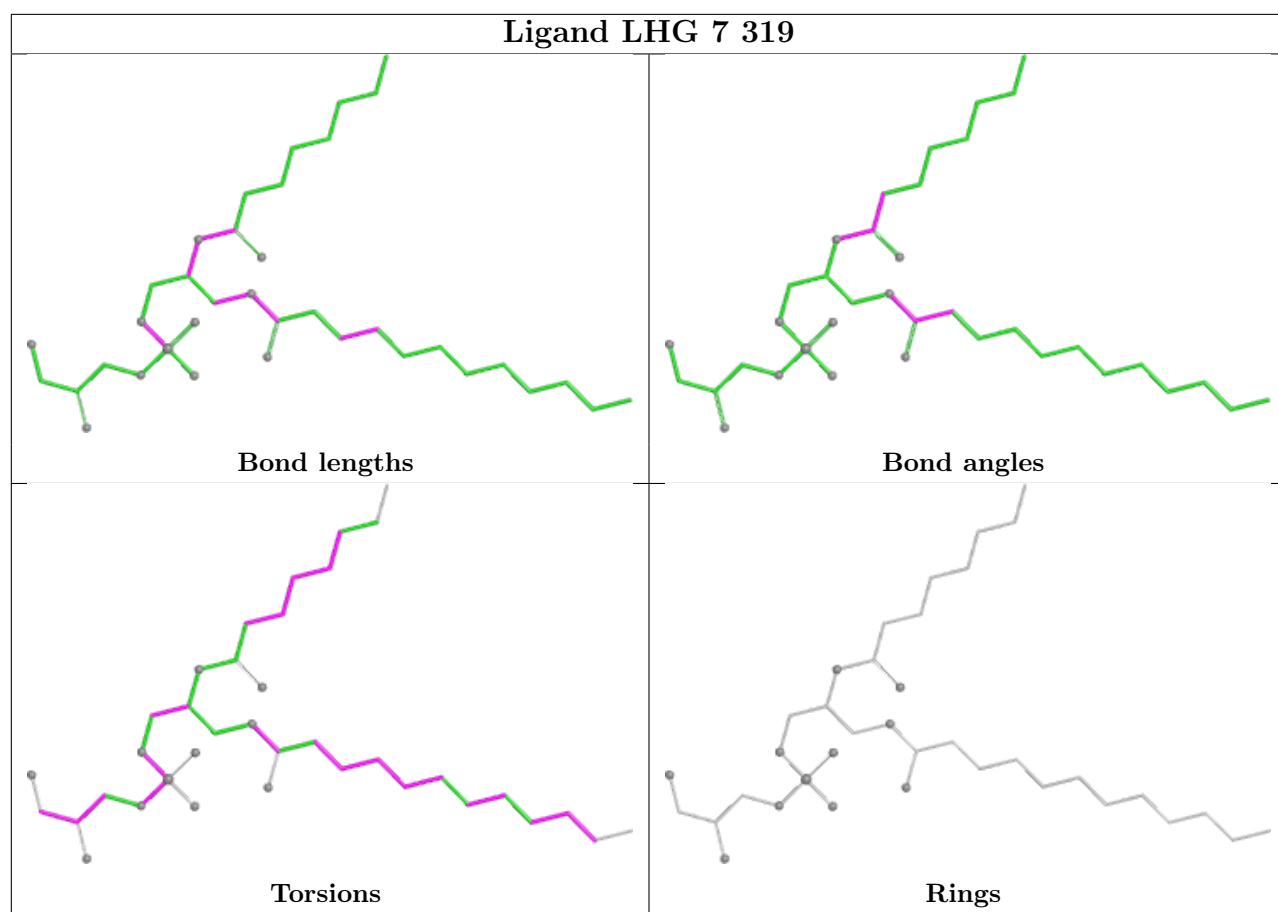


Torsions

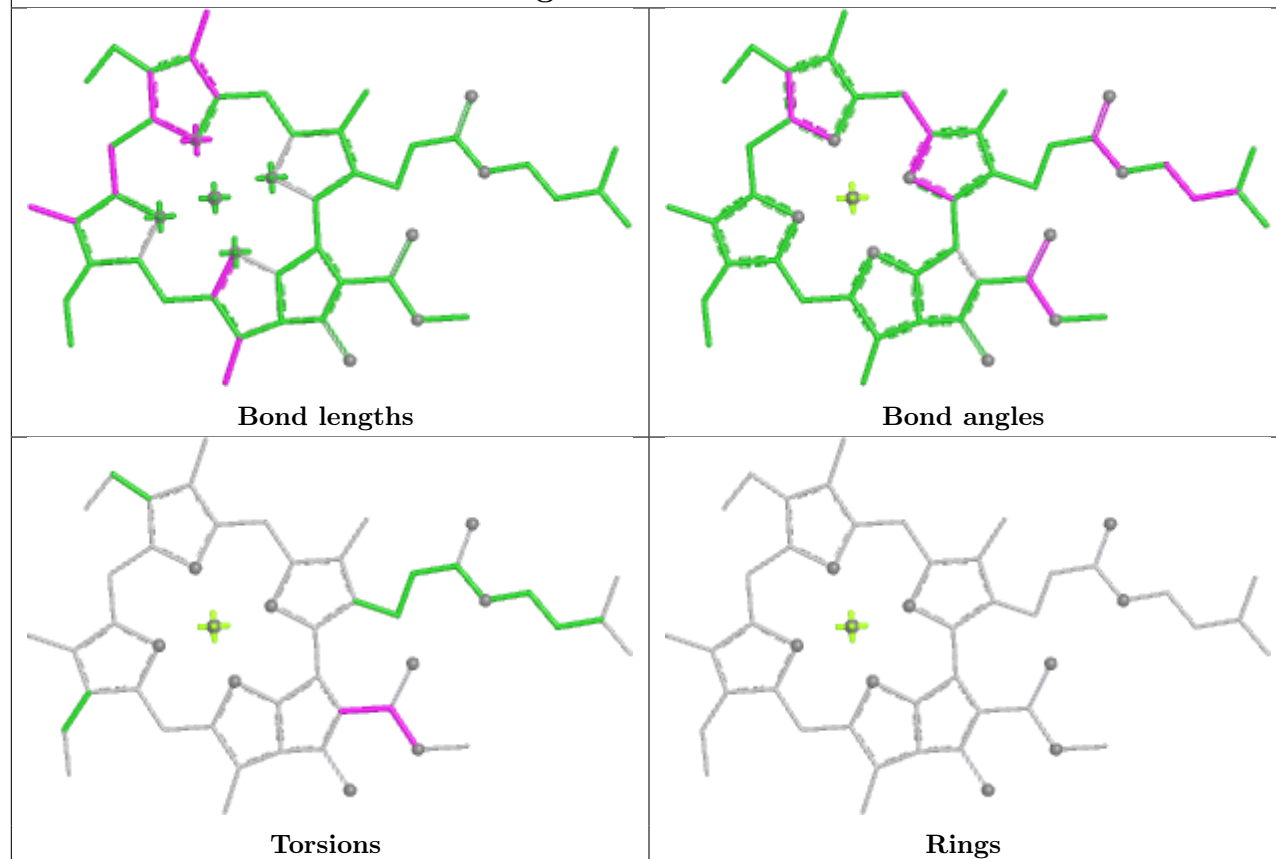


Rings

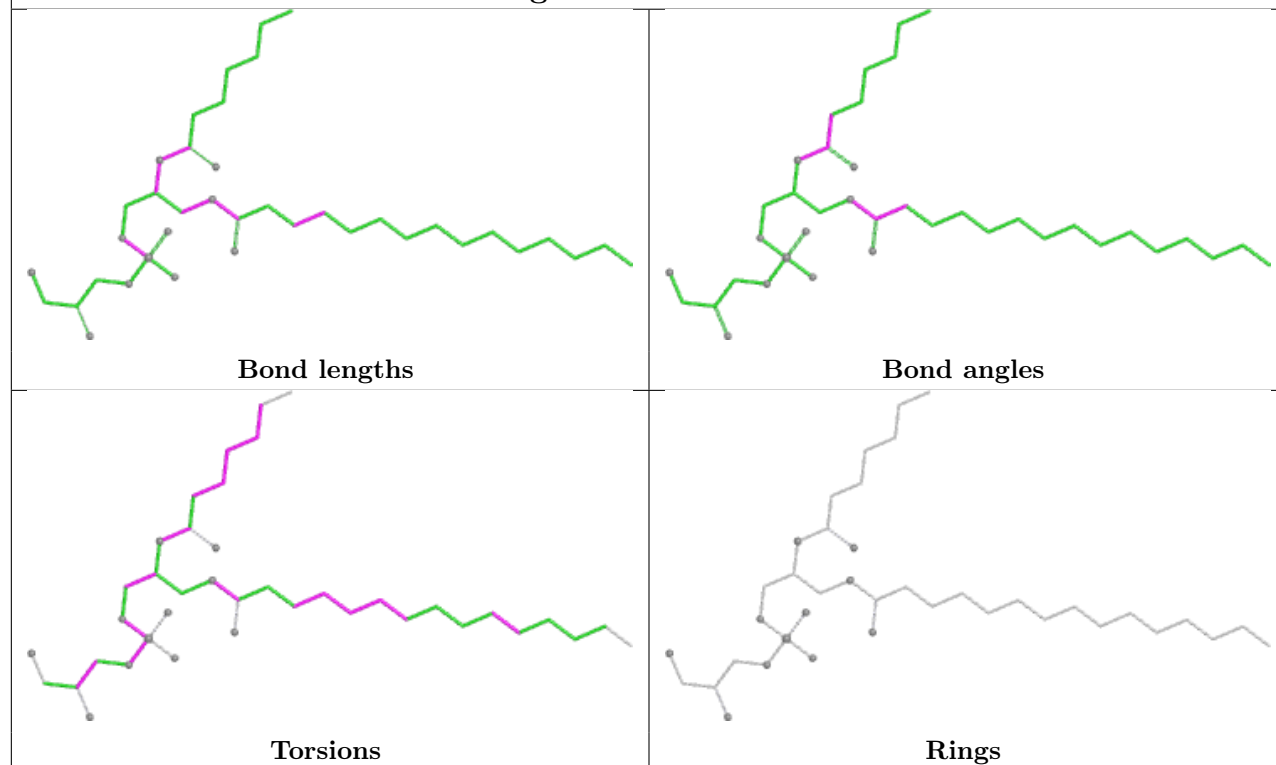


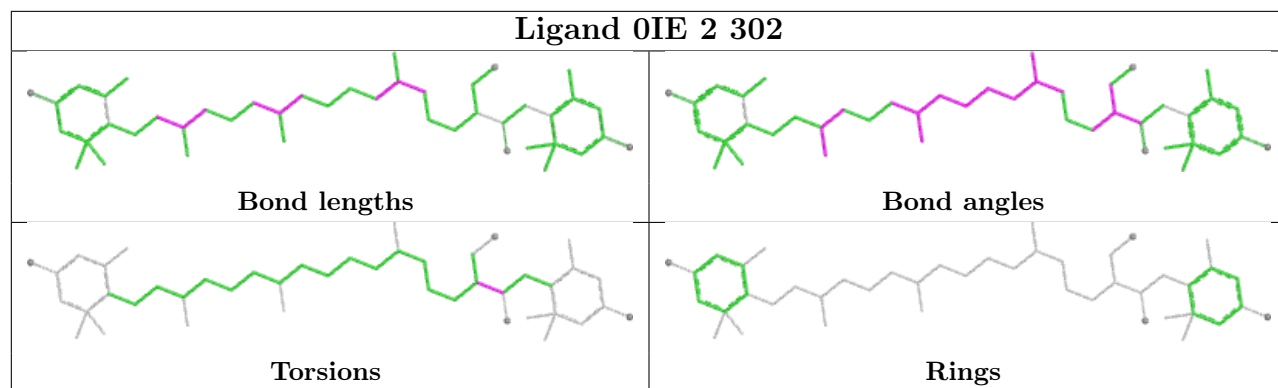
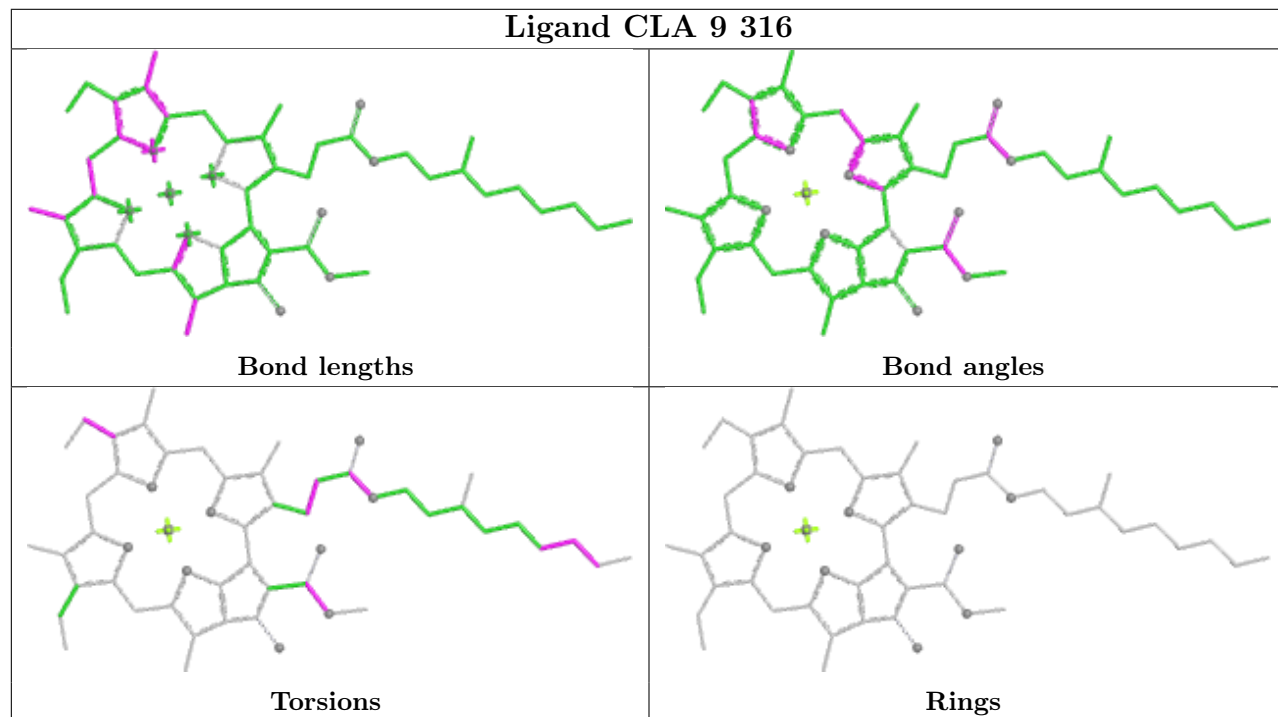


Ligand CLA 5 308

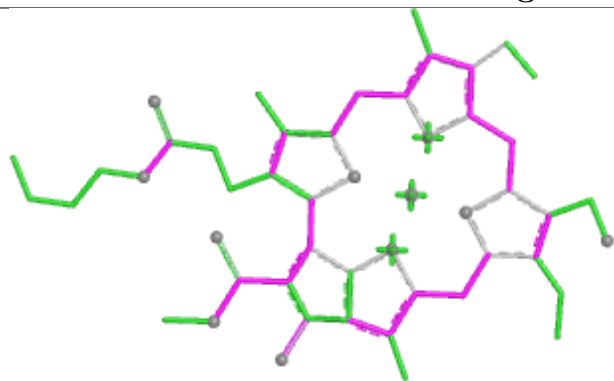


Ligand LHG D 408

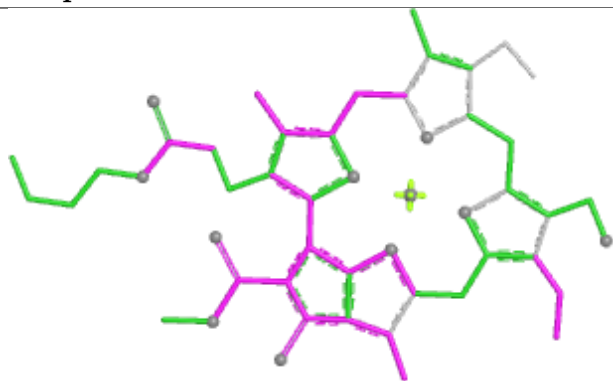


Ligand OIE 2 302**Ligand CLA 9 316**

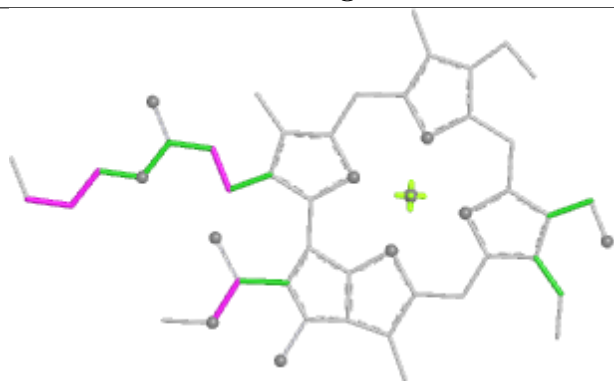
Ligand CHL q 310



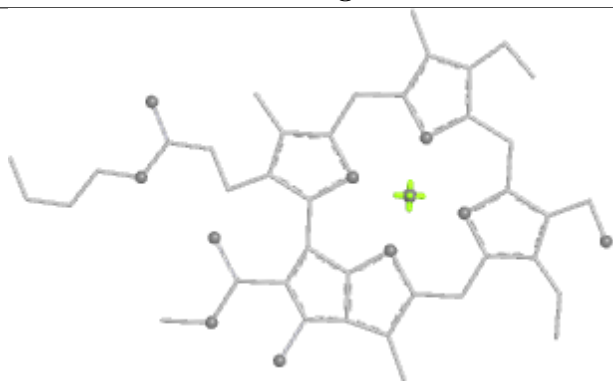
Bond lengths



Bond angles

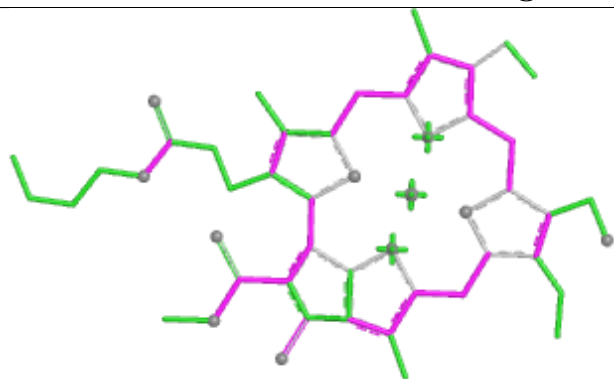


Torsions

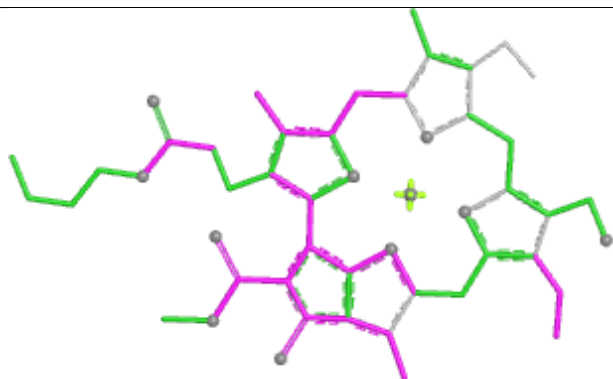


Rings

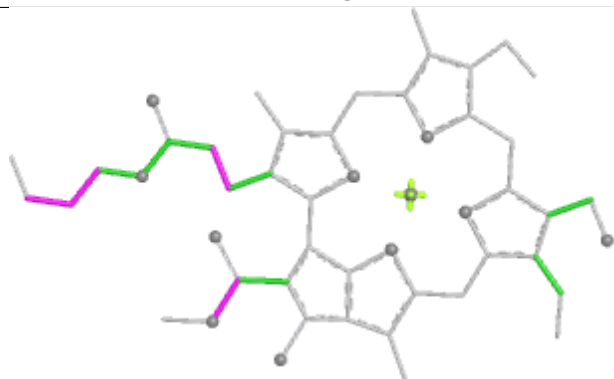
Ligand CHL 8 309



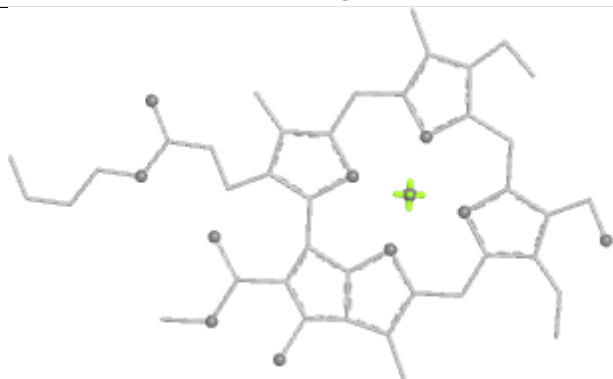
Bond lengths



Bond angles

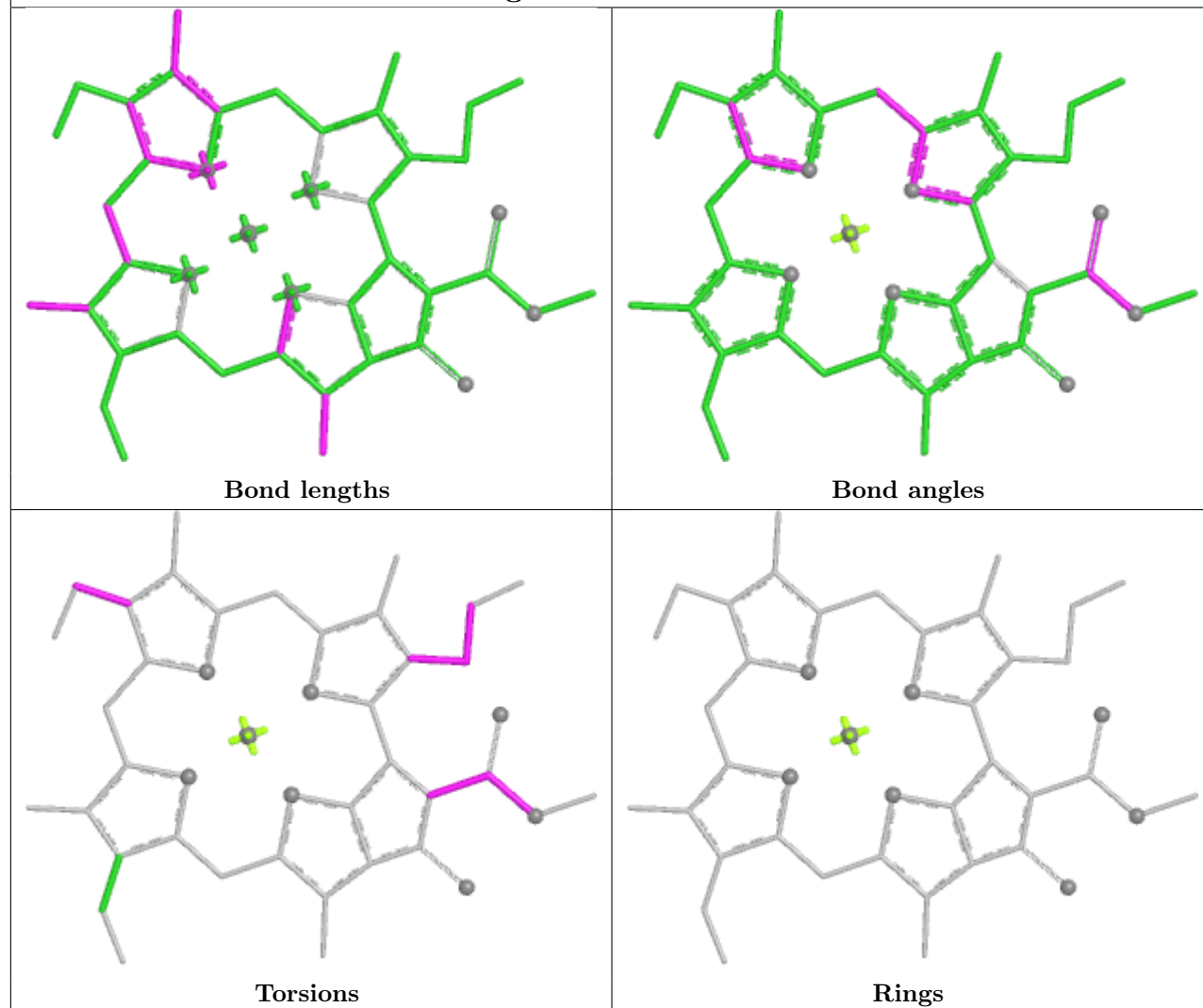


Torsions

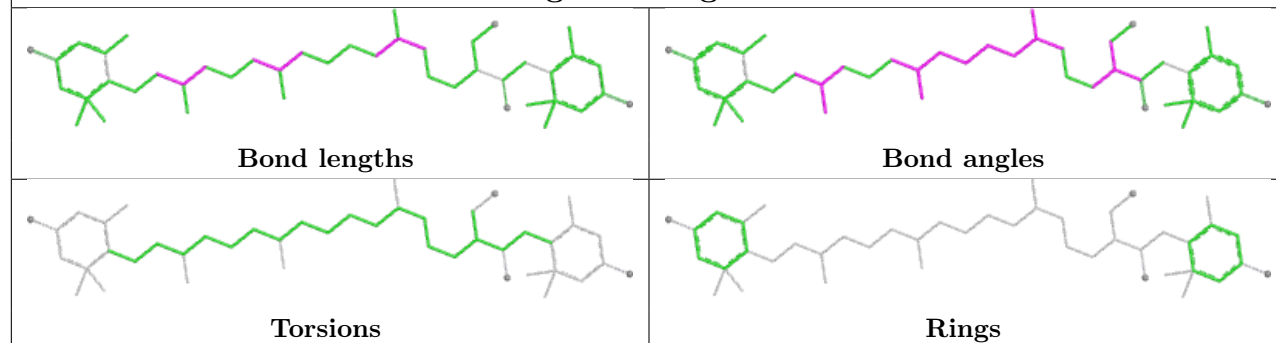


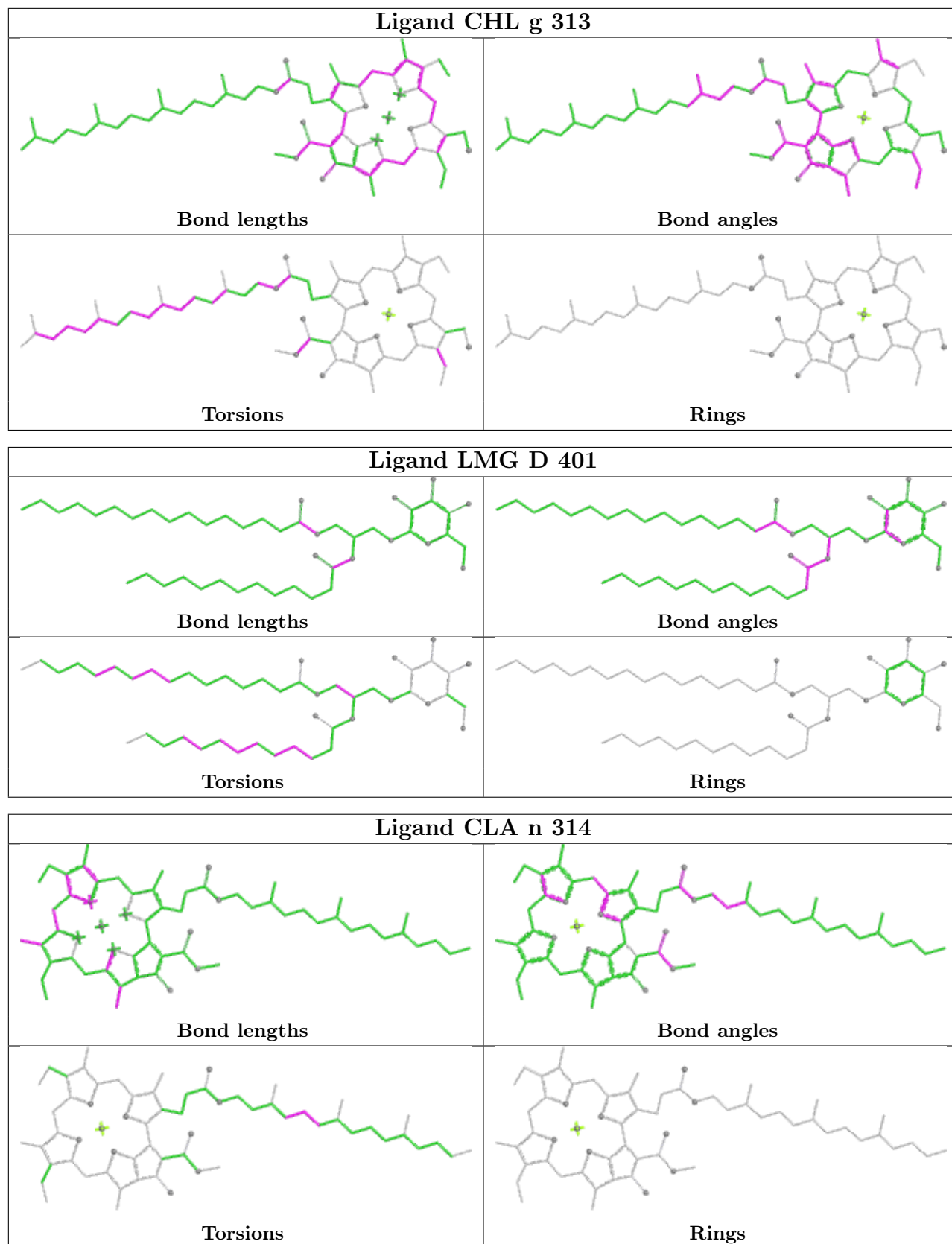
Rings

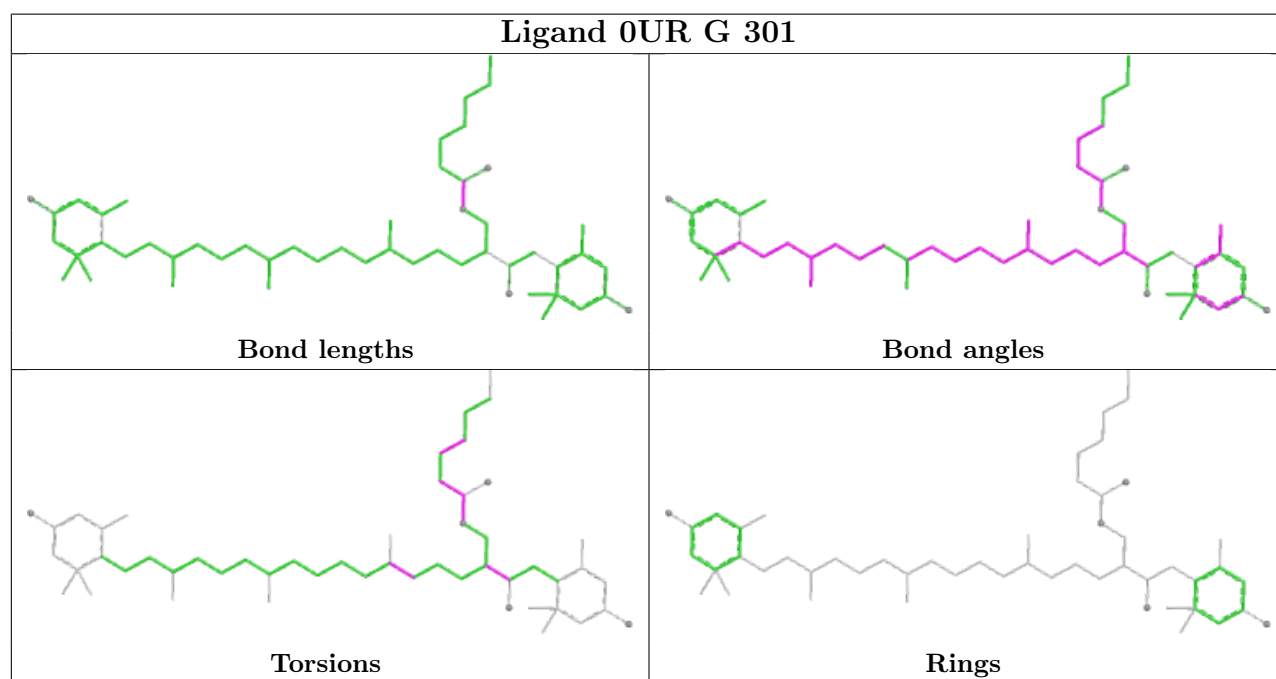
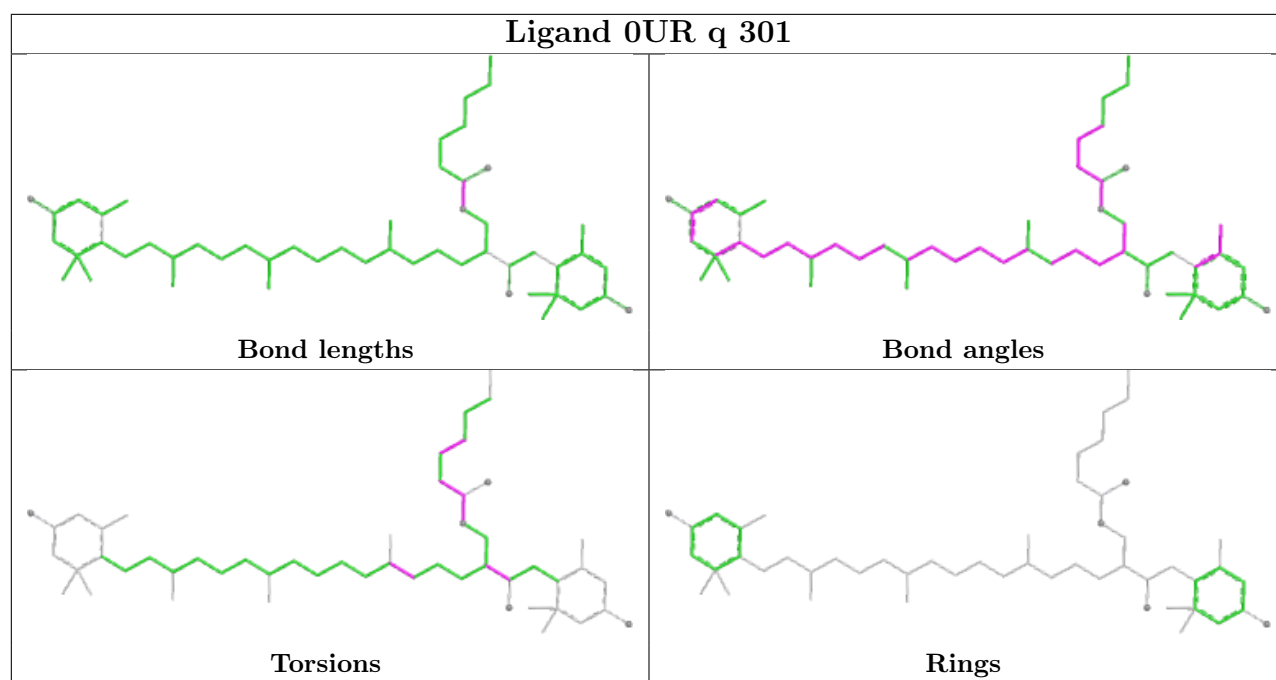
Ligand CLA 5 307

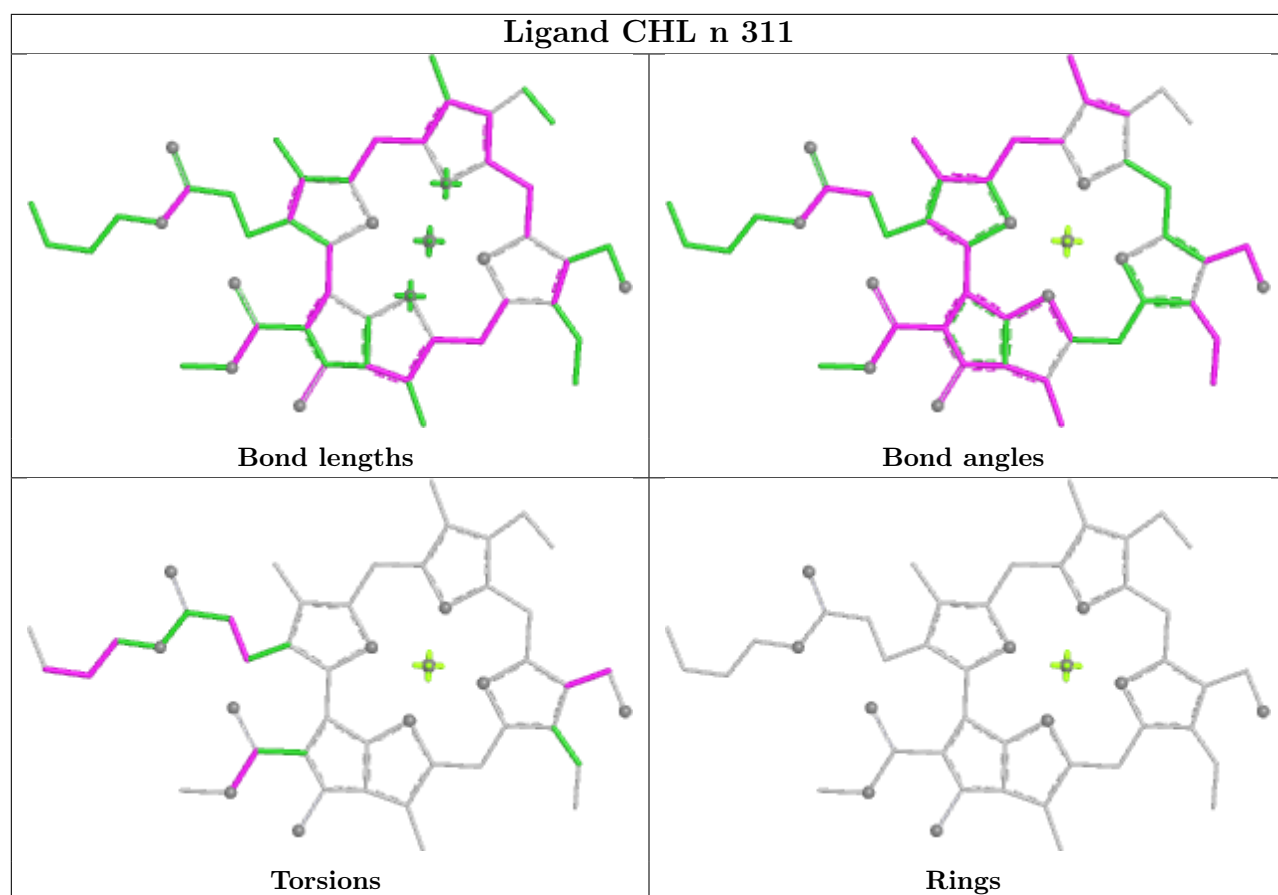


Ligand OIE g 303

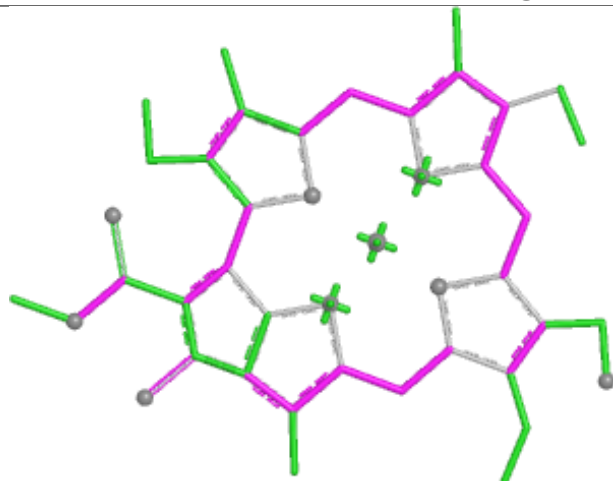




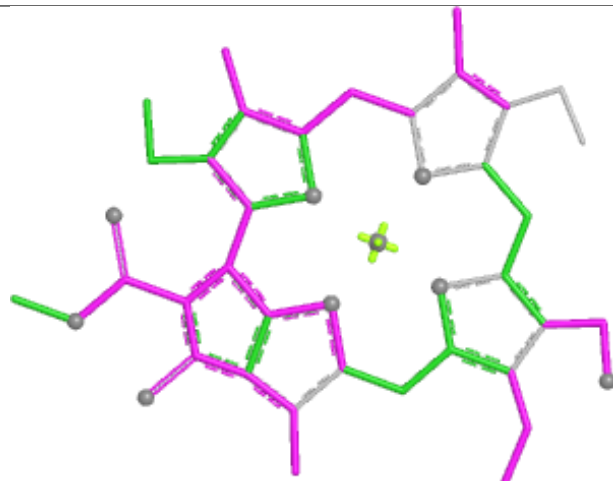




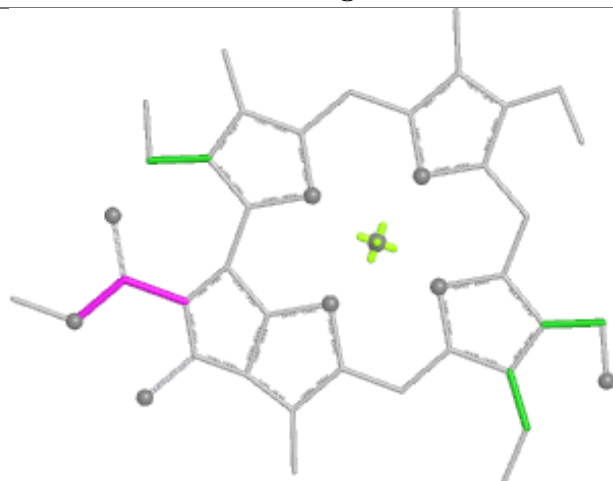
Ligand CHL 4 308



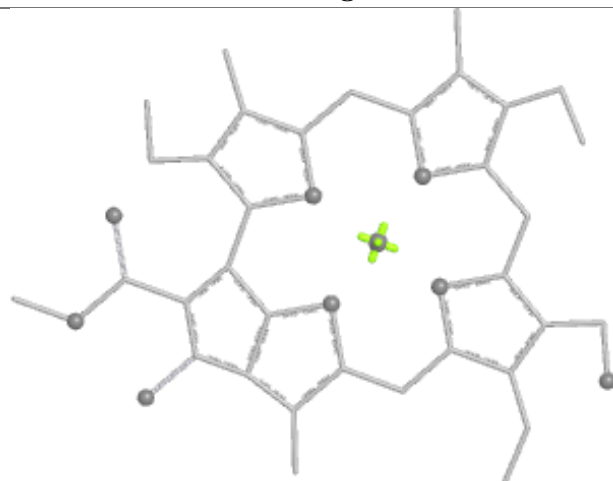
Bond lengths



Bond angles

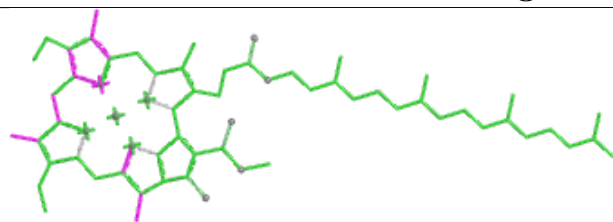


Torsions

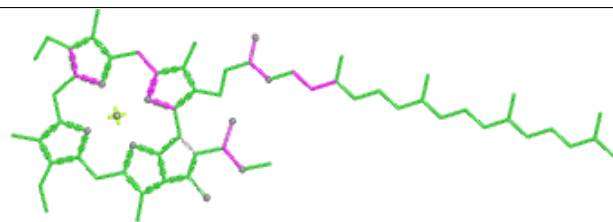


Rings

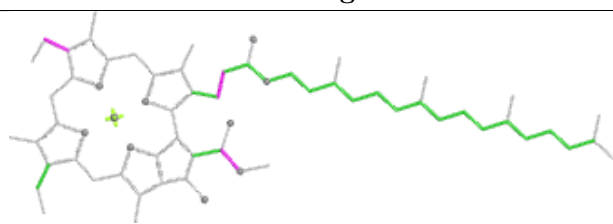
Ligand CLA b 610



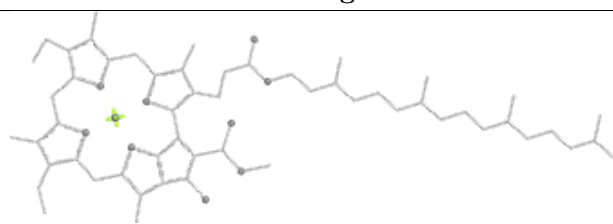
Bond lengths



Bond angles

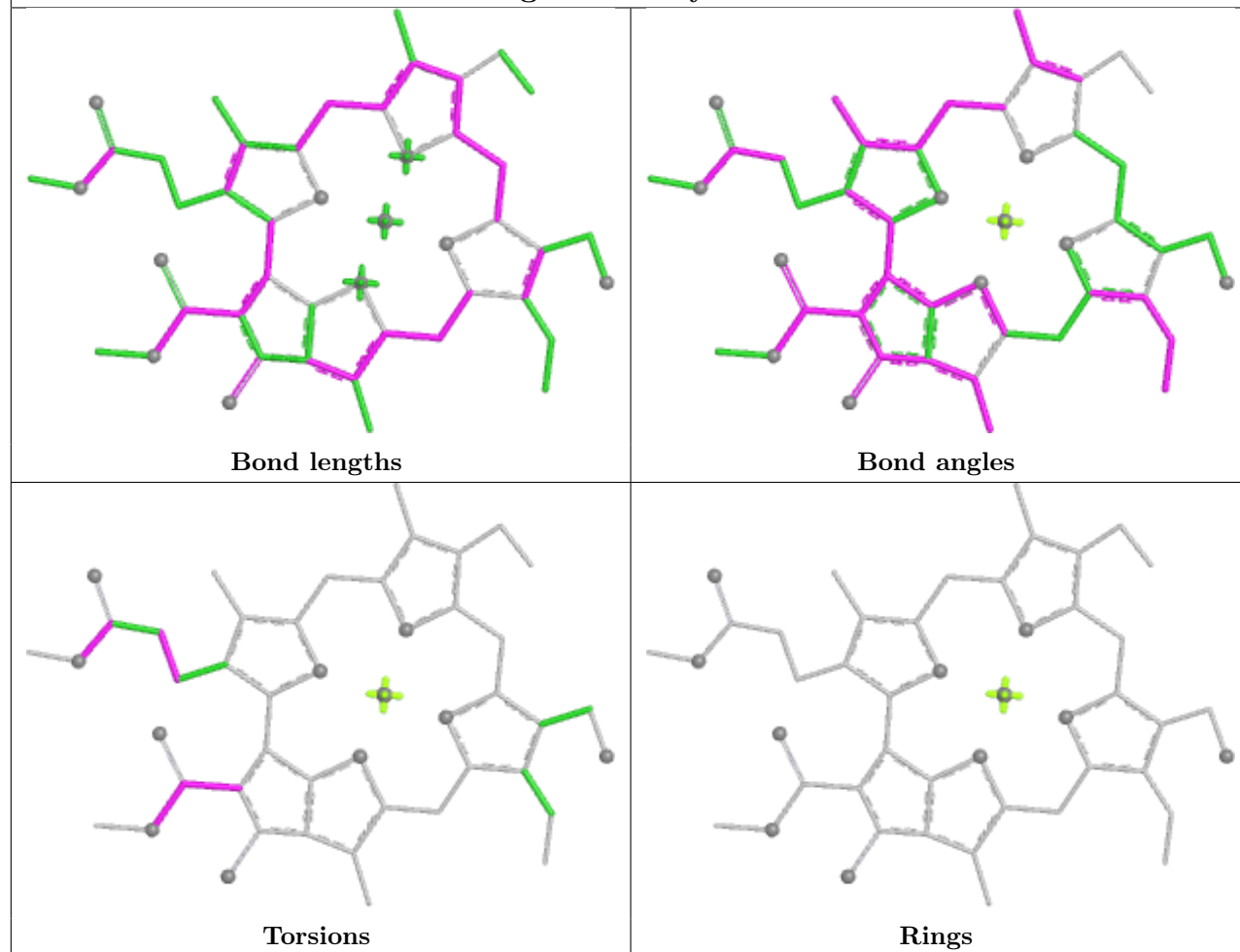


Torsions

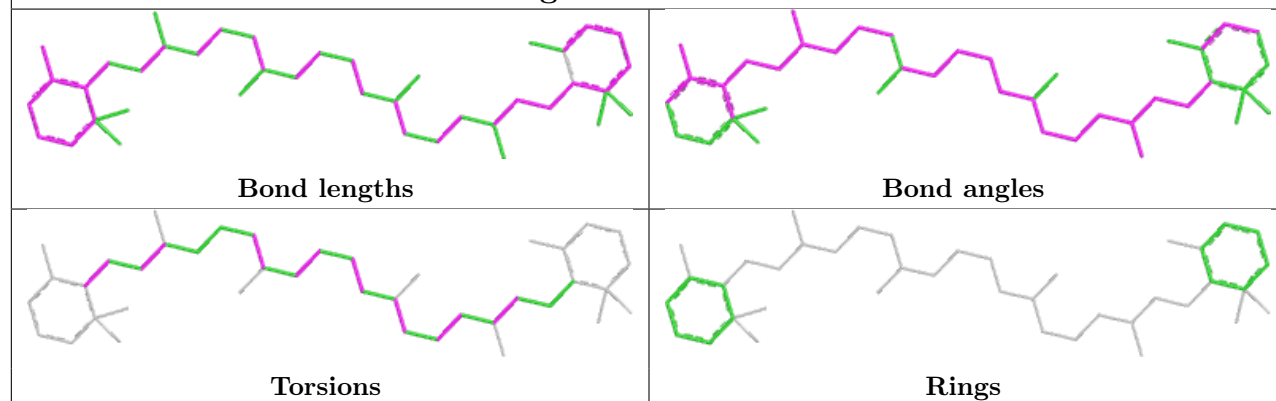


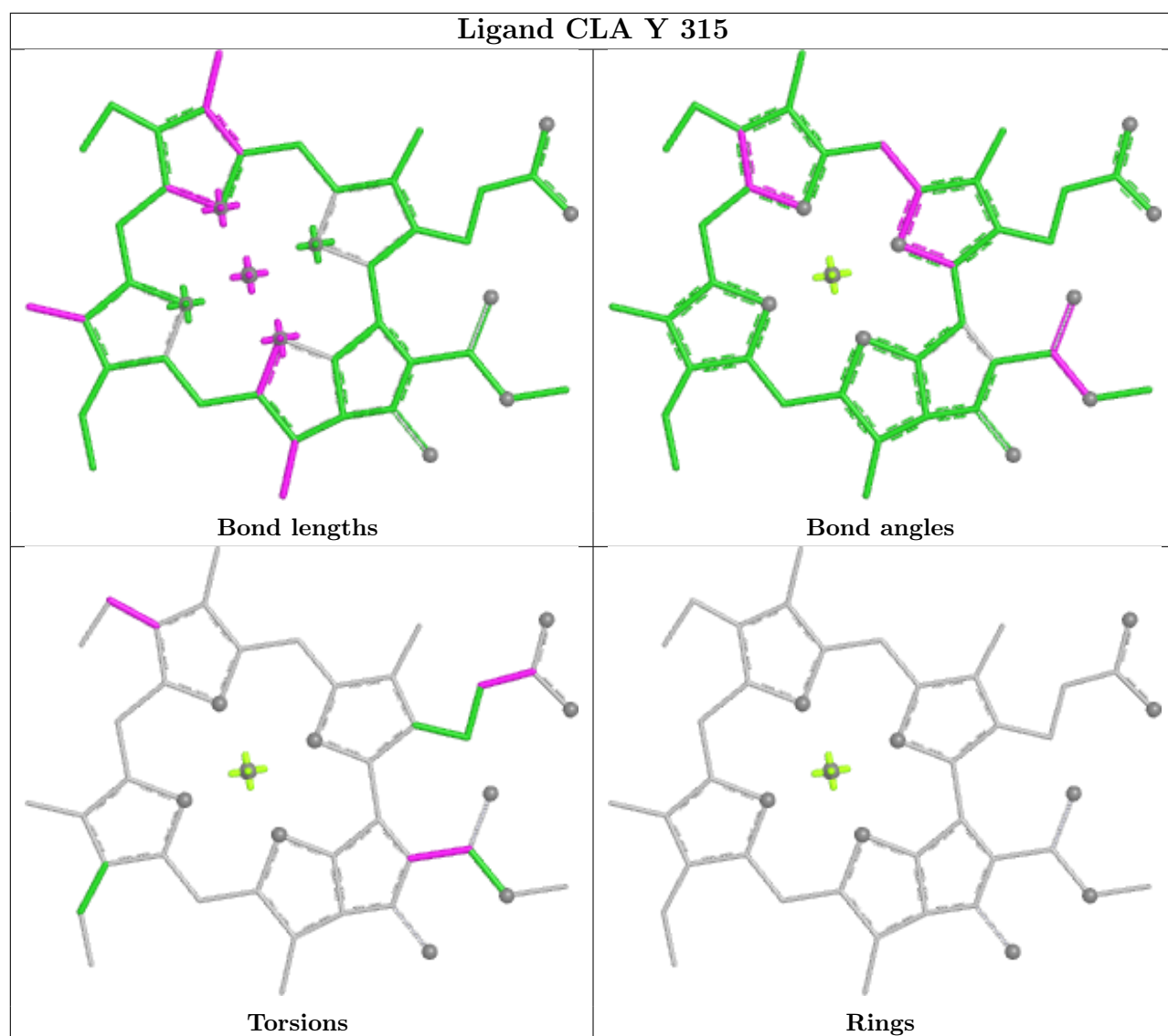
Rings

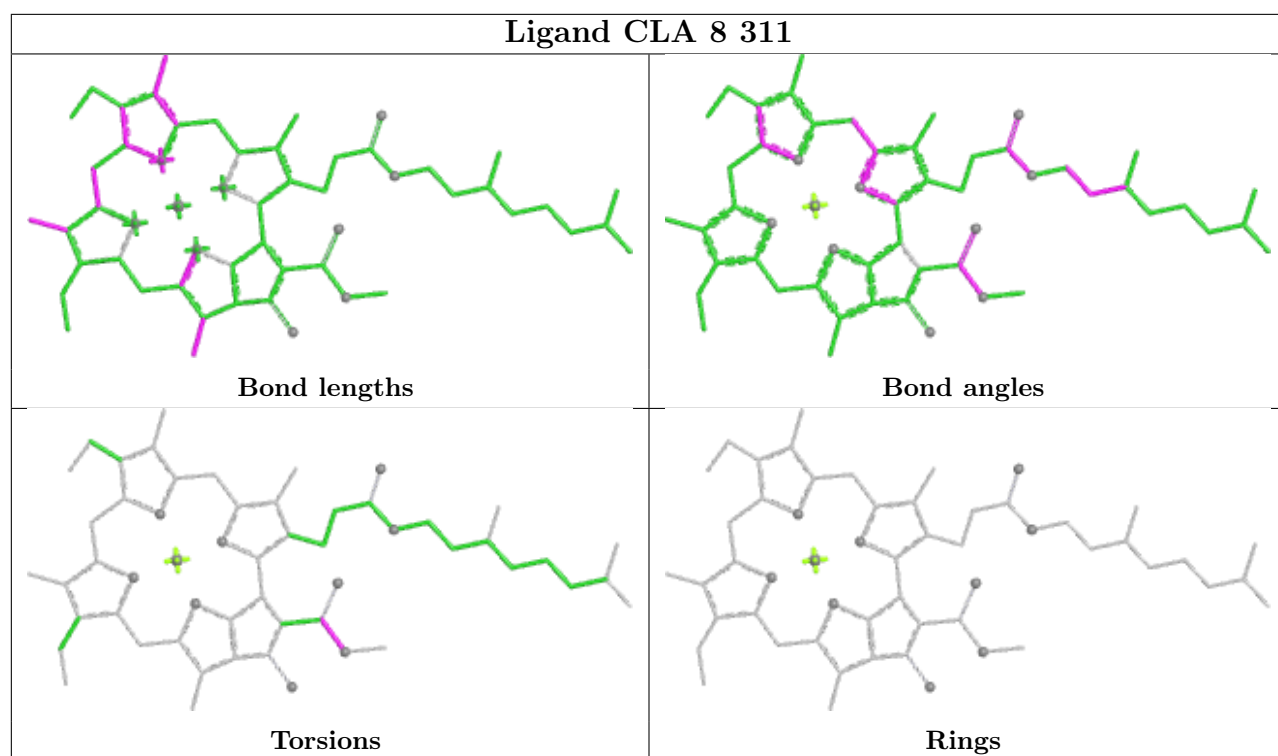
Ligand CHL y 310

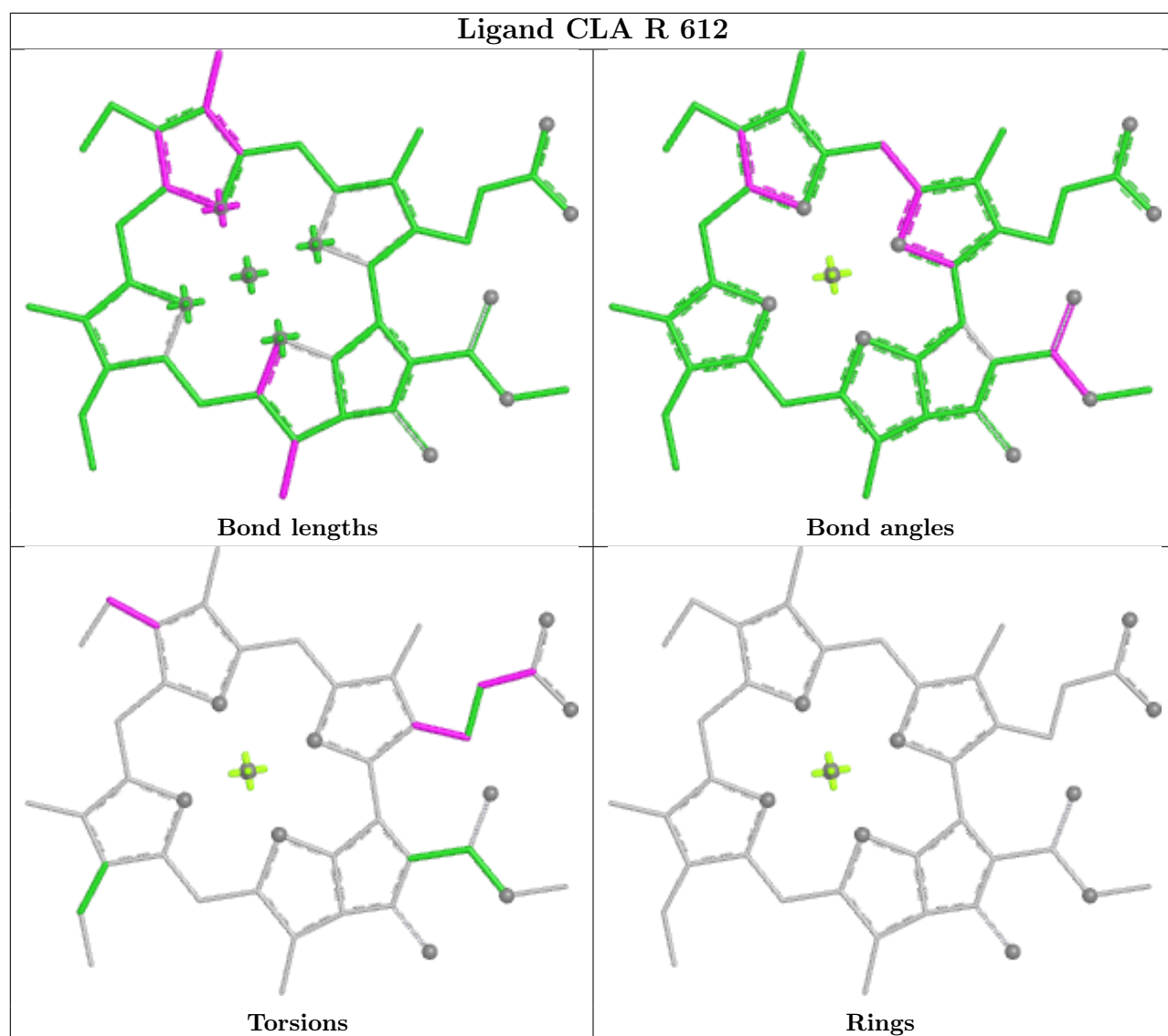


Ligand 8CT c 615

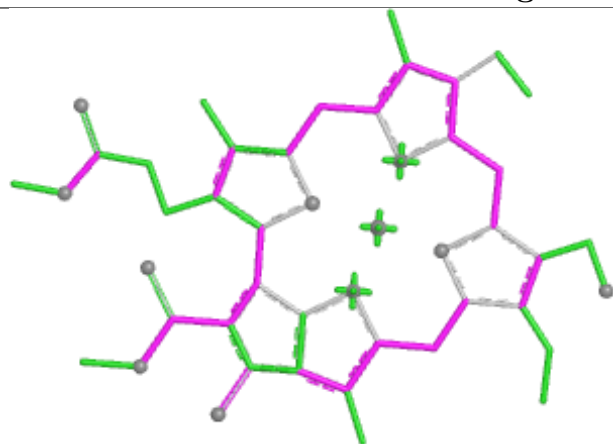




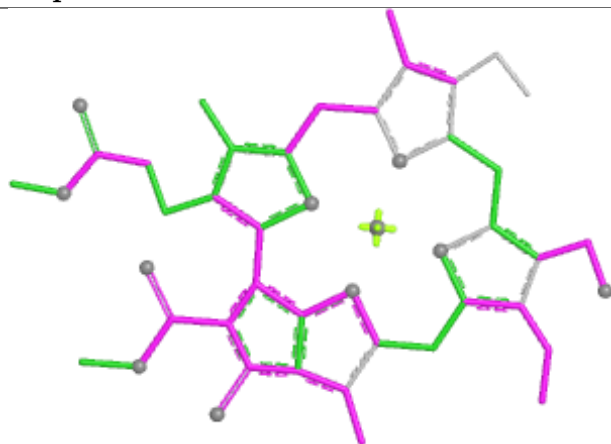




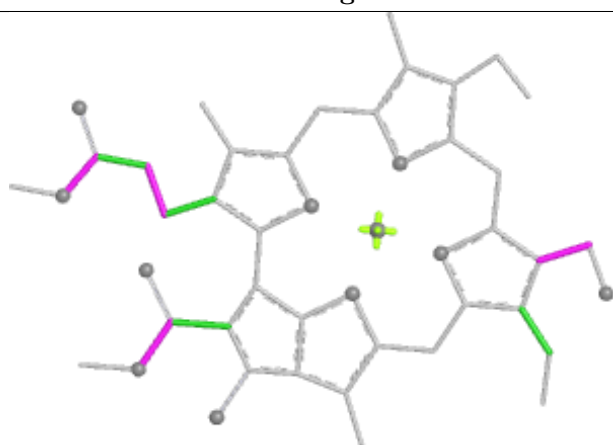
Ligand CHL p 312



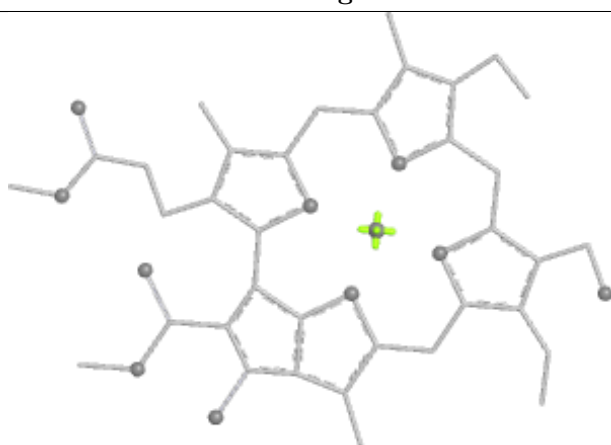
Bond lengths



Bond angles

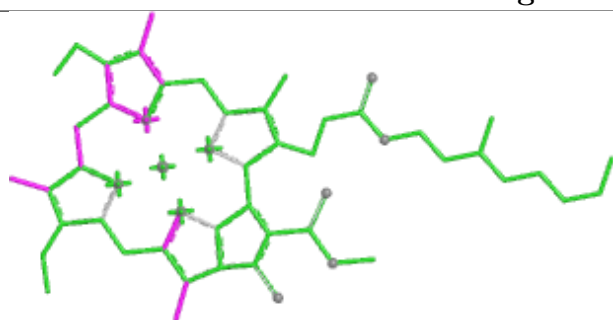


Torsions

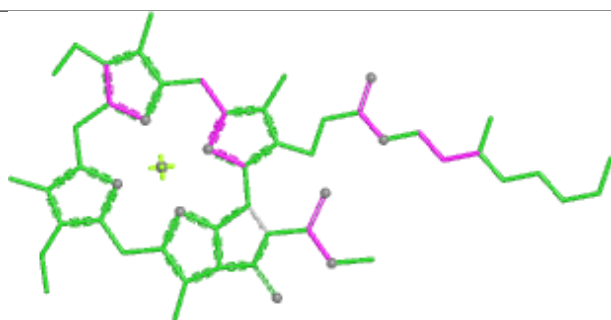


Rings

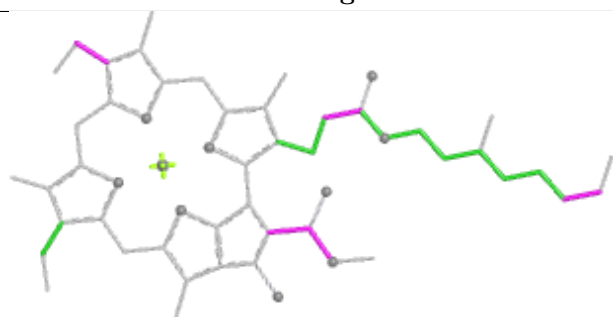
Ligand CLA n 306



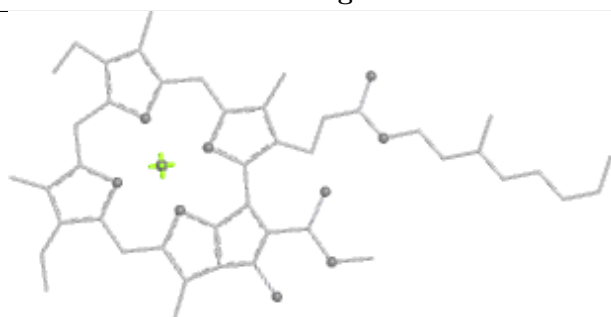
Bond lengths



Bond angles

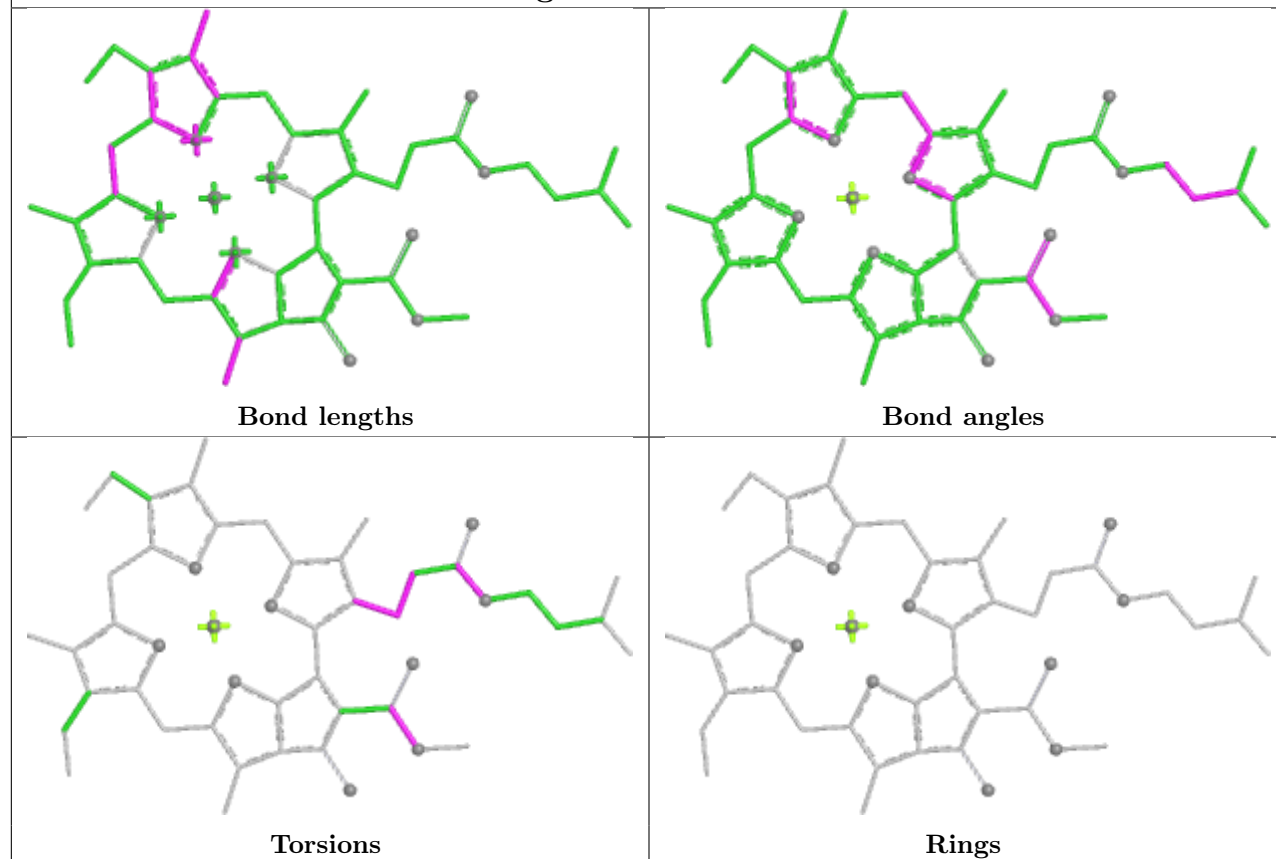


Torsions

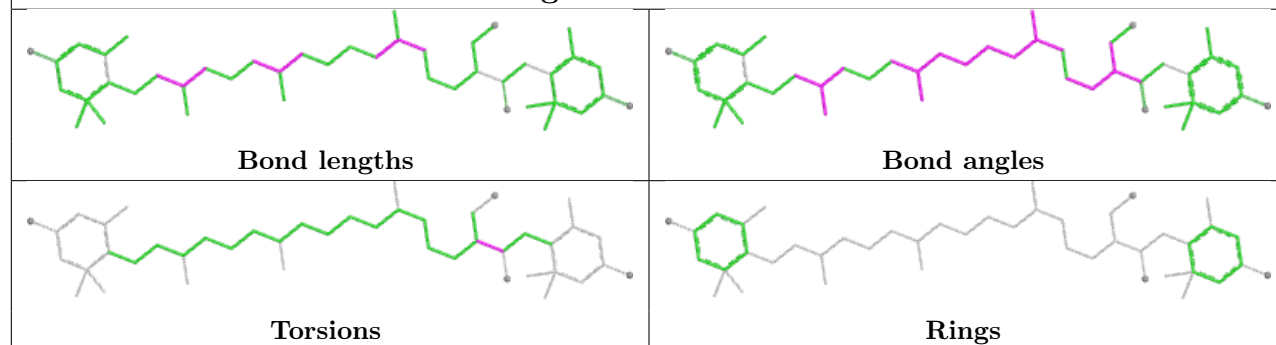


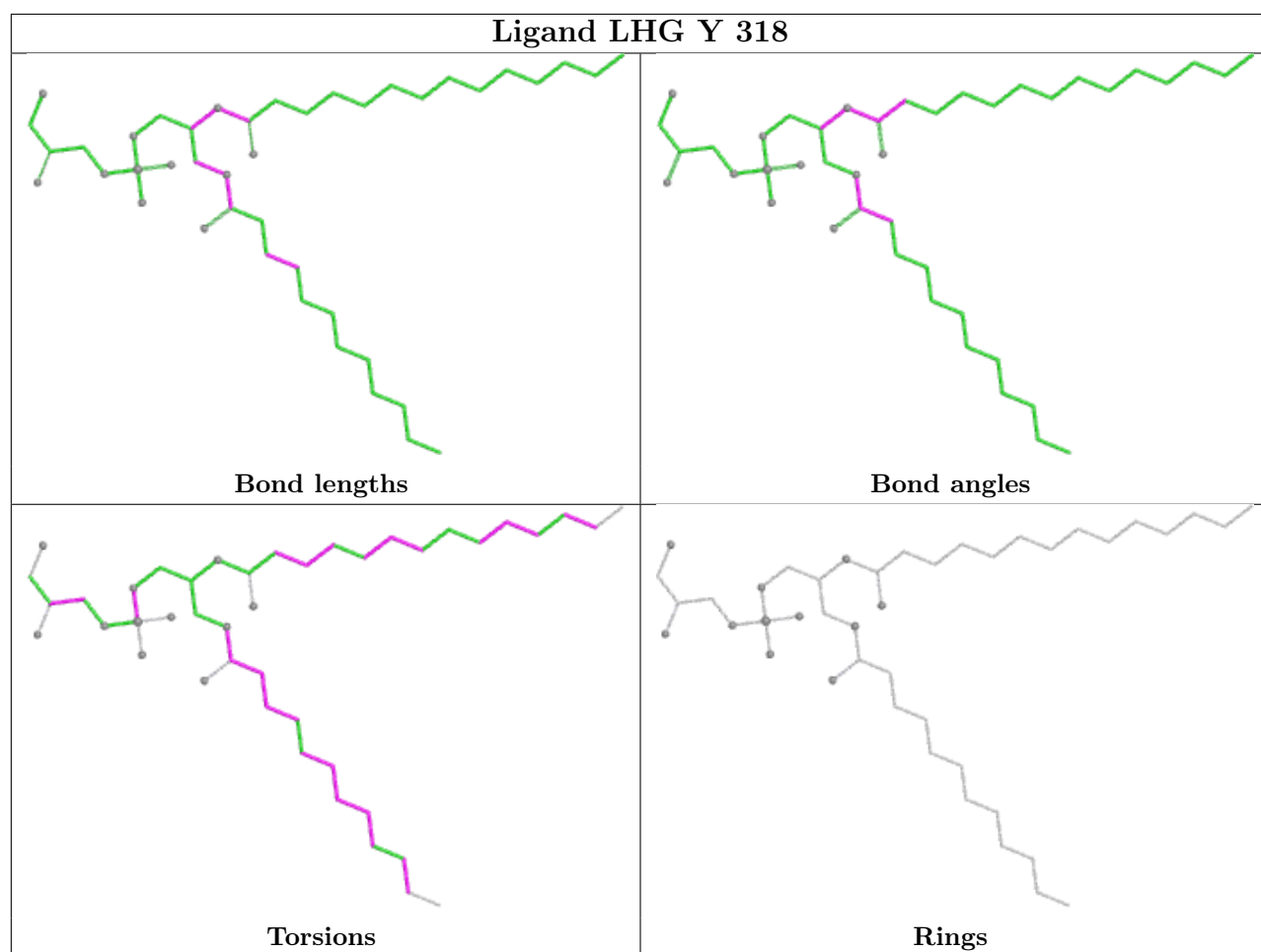
Rings

Ligand CLA 9 307

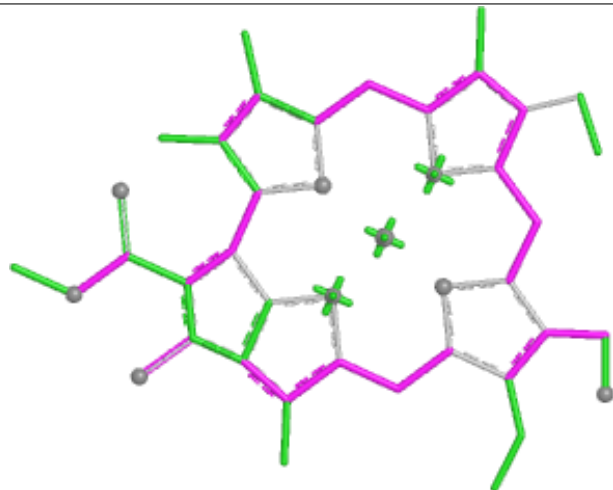


Ligand OIE N 302

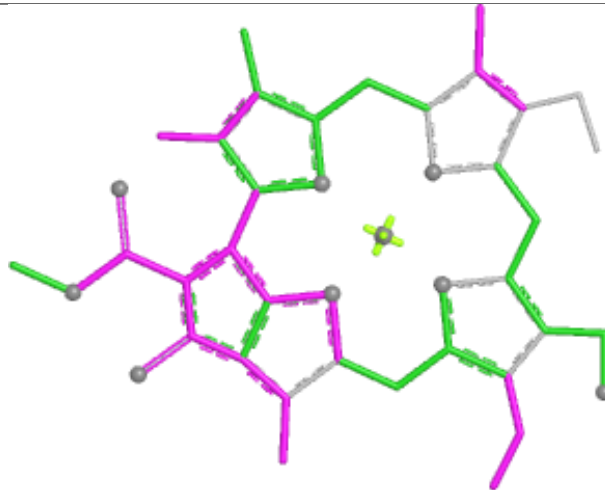




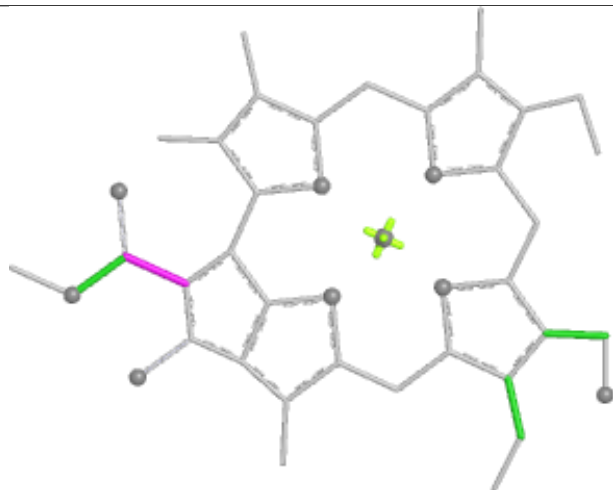
Ligand CHL q 316



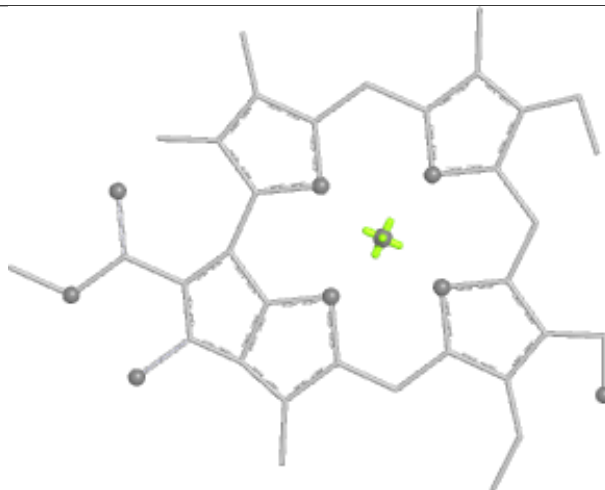
Bond lengths



Bond angles

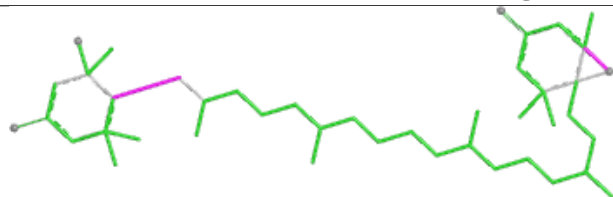


Torsions

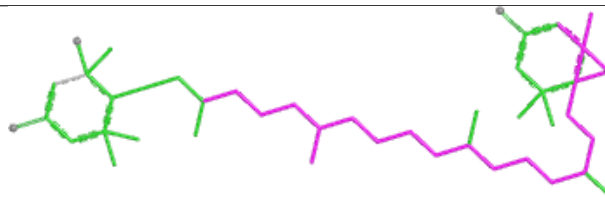


Rings

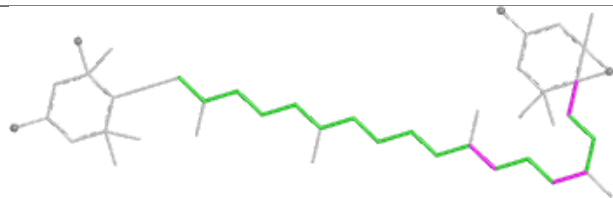
Ligand NEX r 317



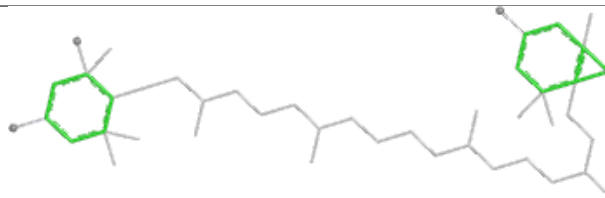
Bond lengths



Bond angles

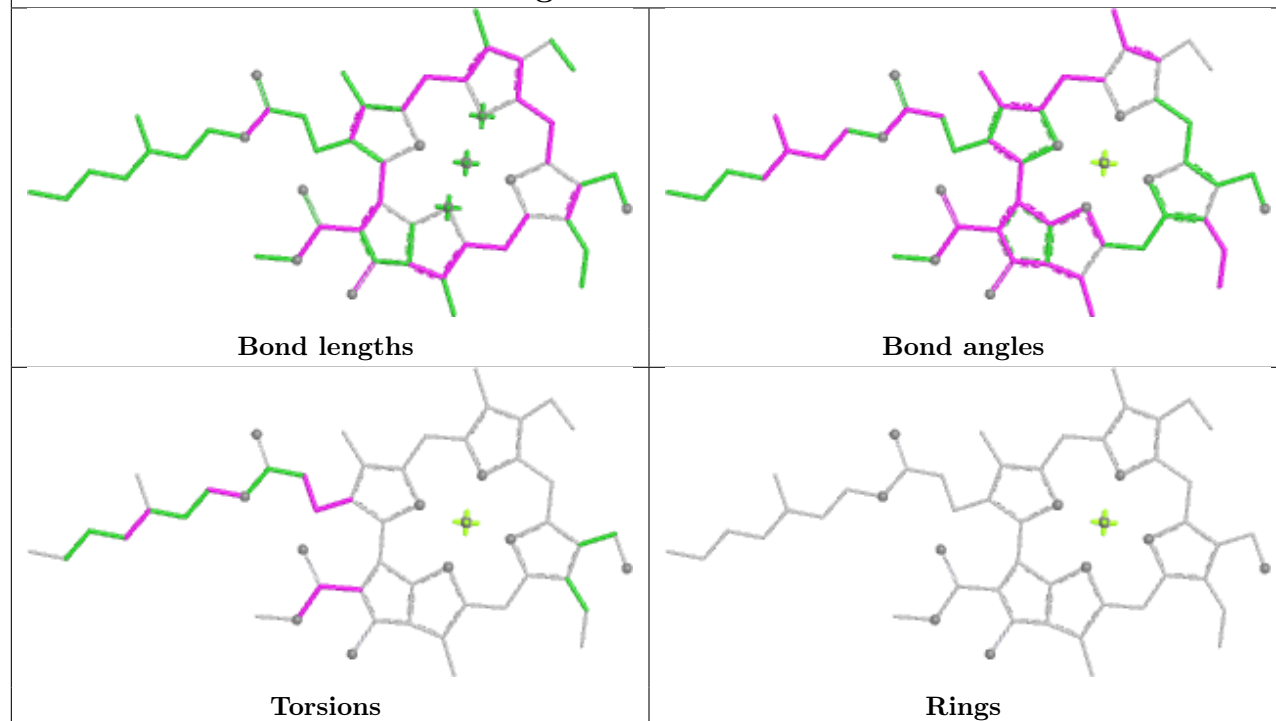


Torsions

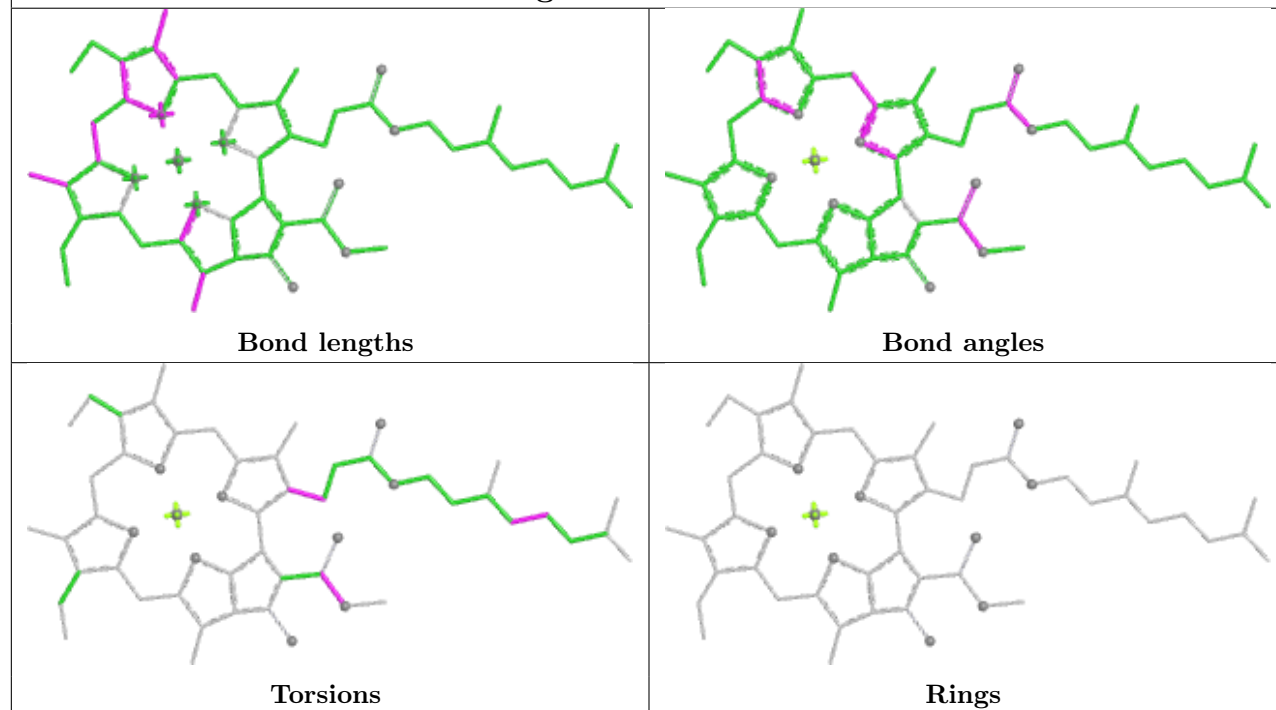


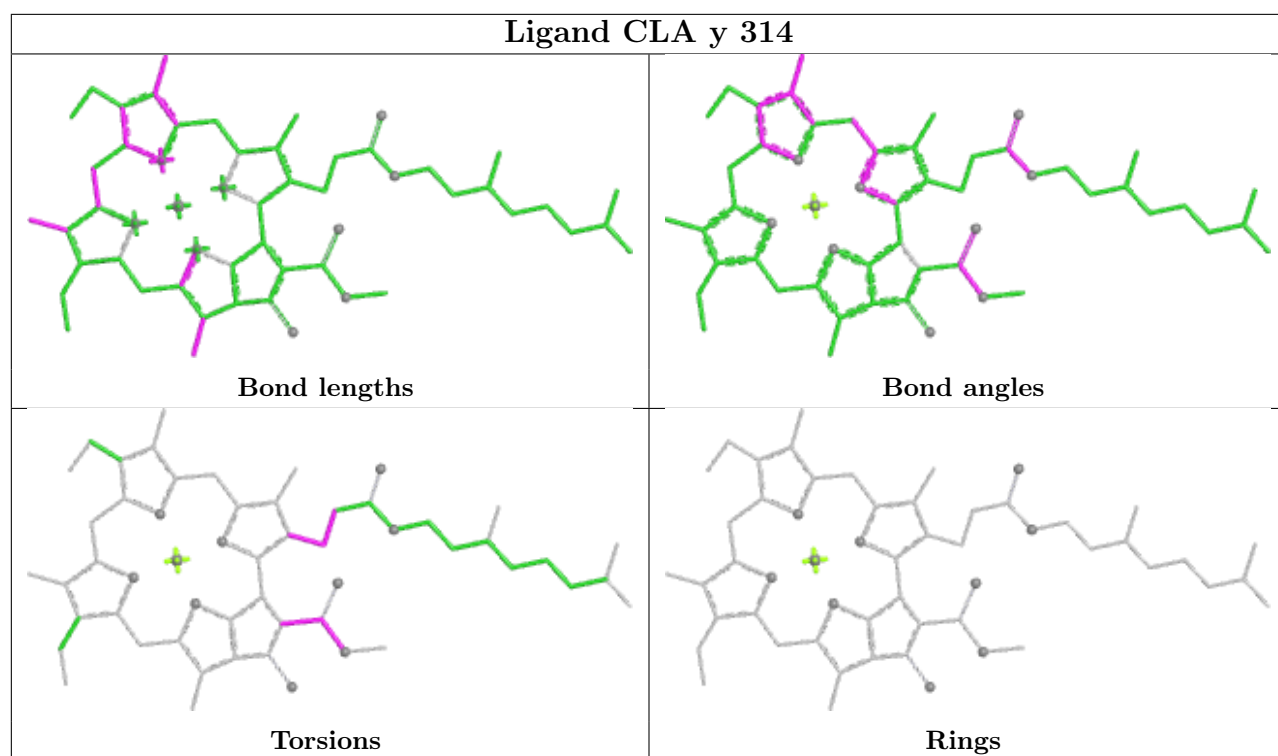
Rings

Ligand CHL 8 303

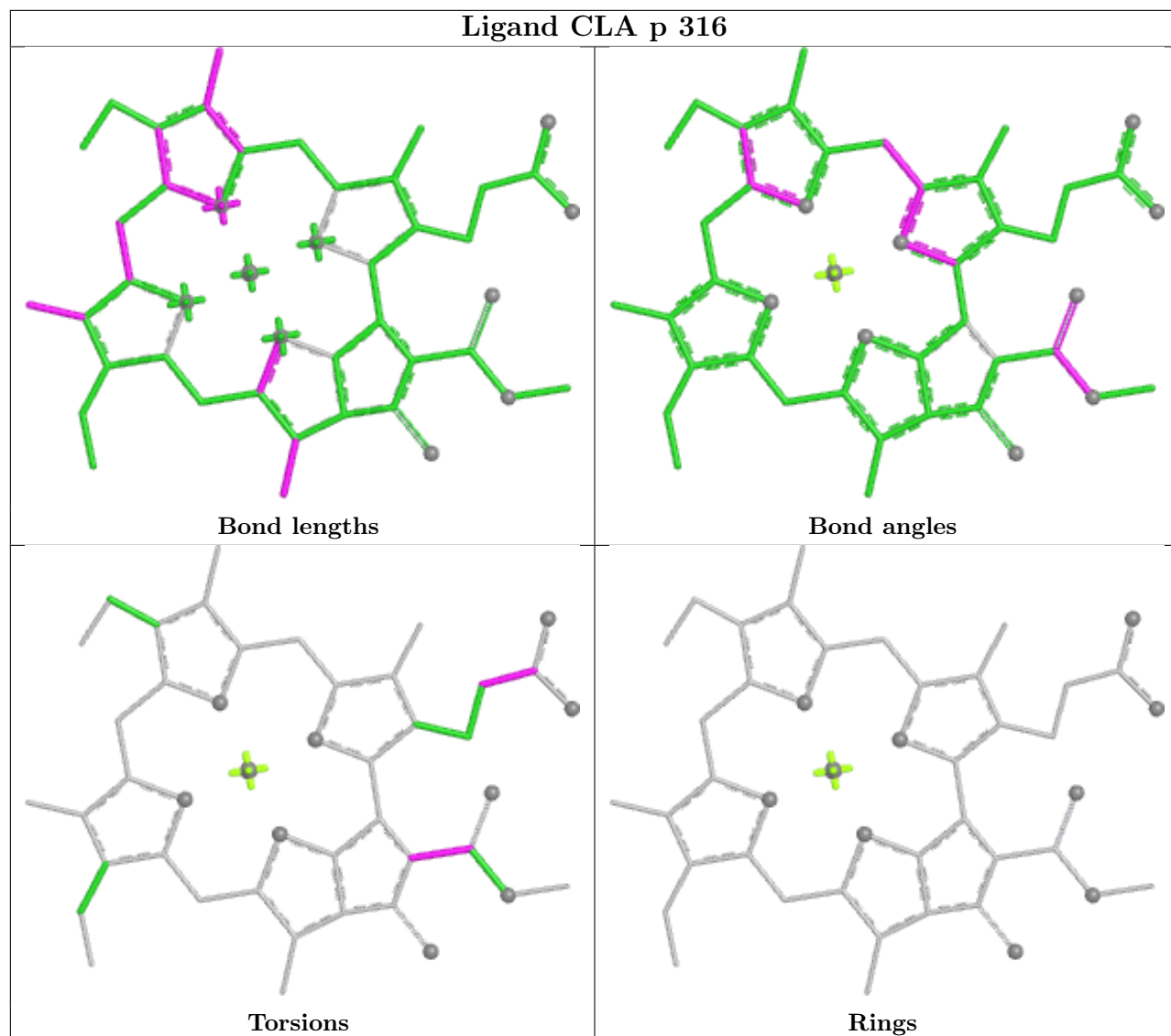


Ligand CLA 5 314

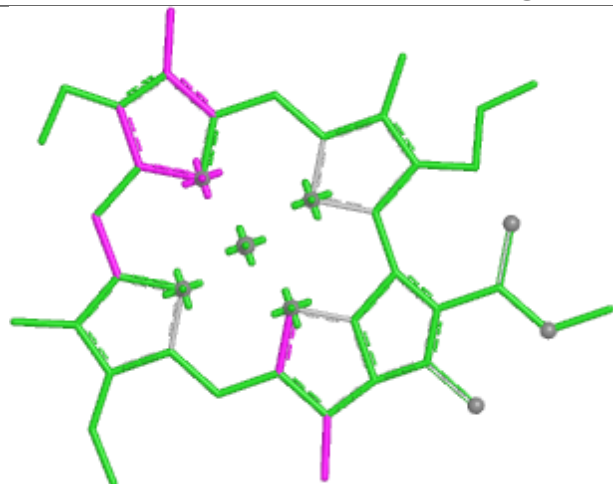




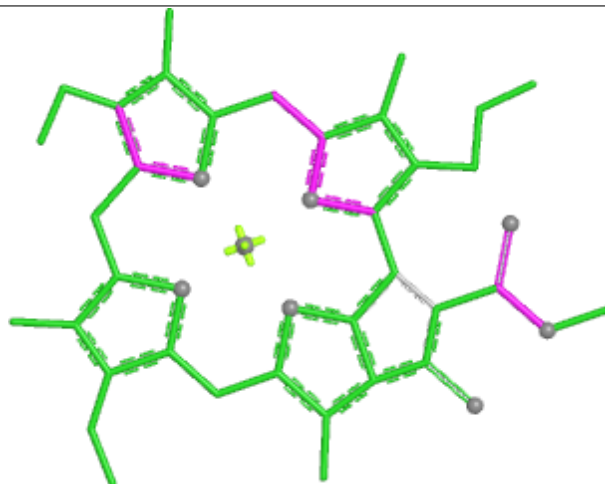
Ligand CLA p 316



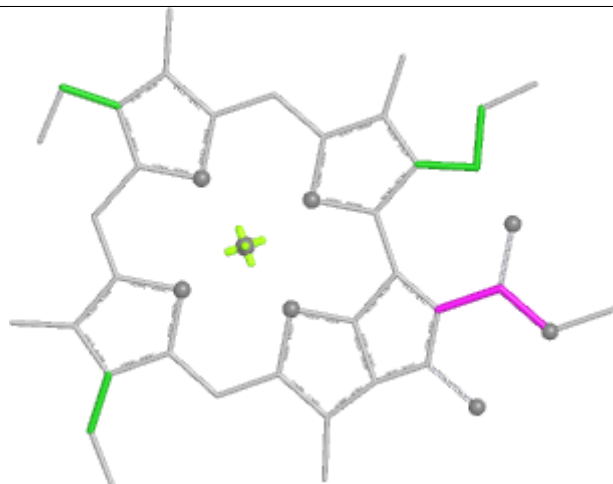
Ligand CLA 3 307



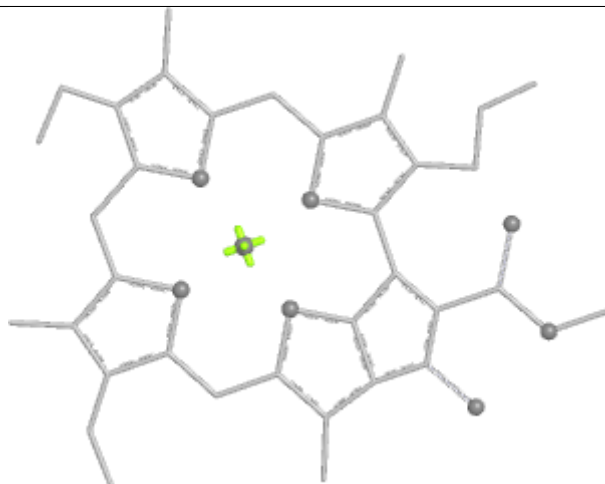
Bond lengths



Bond angles

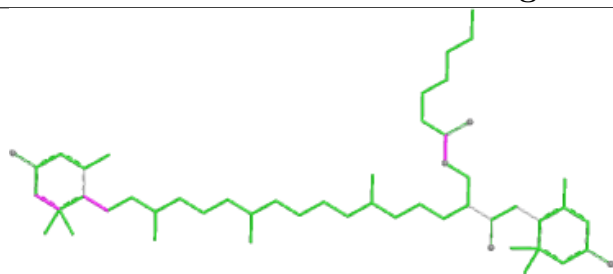


Torsions

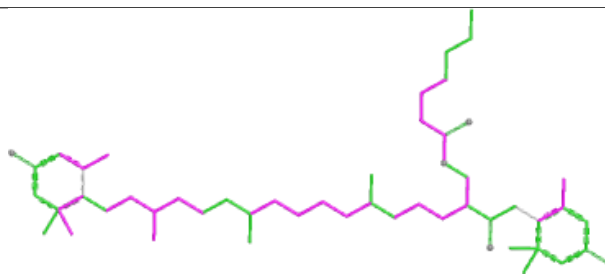


Rings

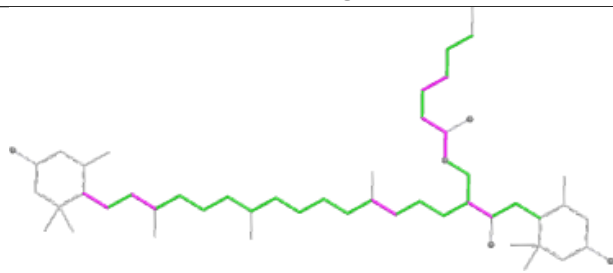
Ligand OUR 5 301



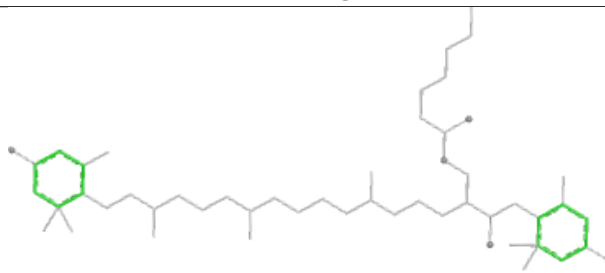
Bond lengths



Bond angles

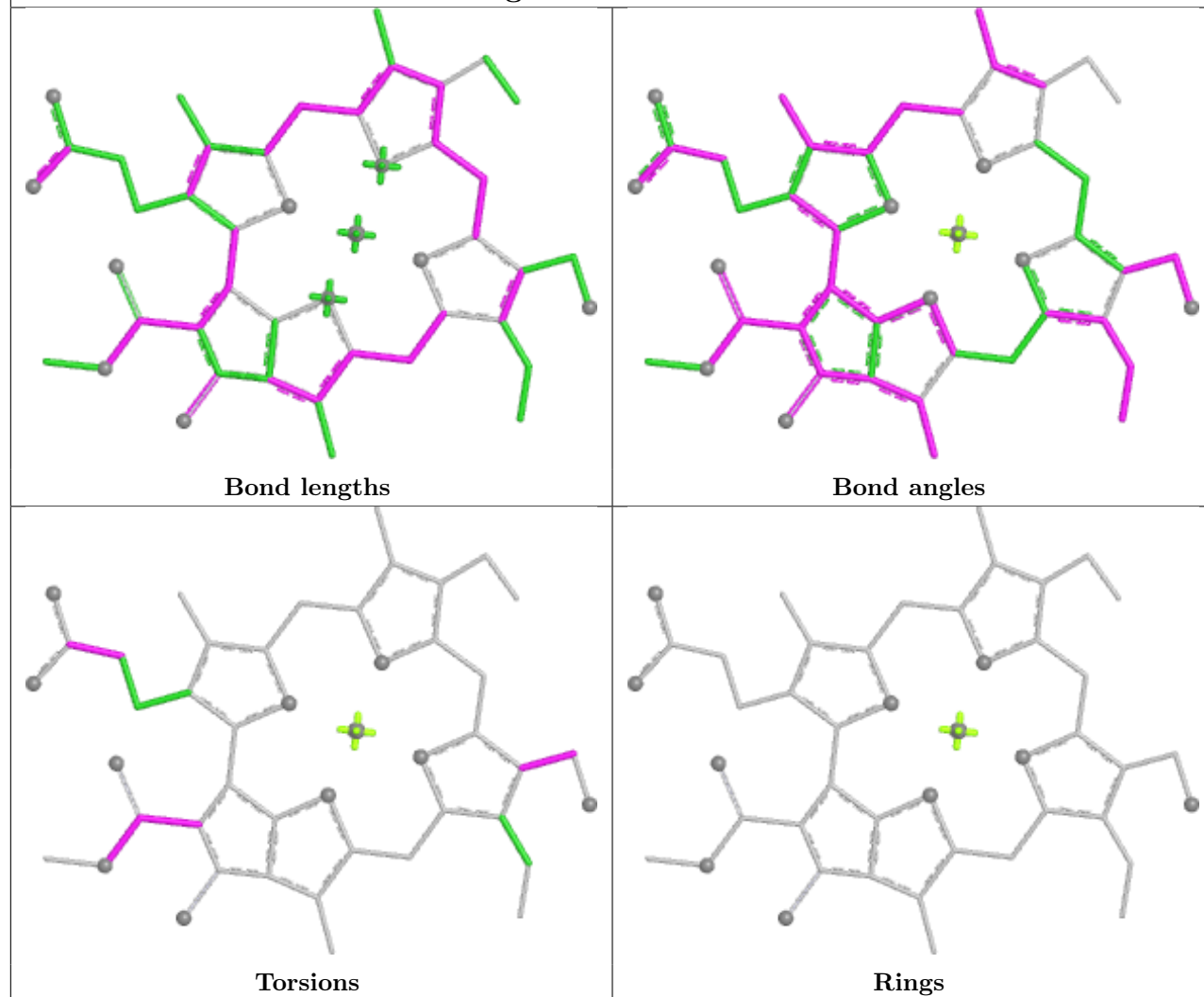


Torsions

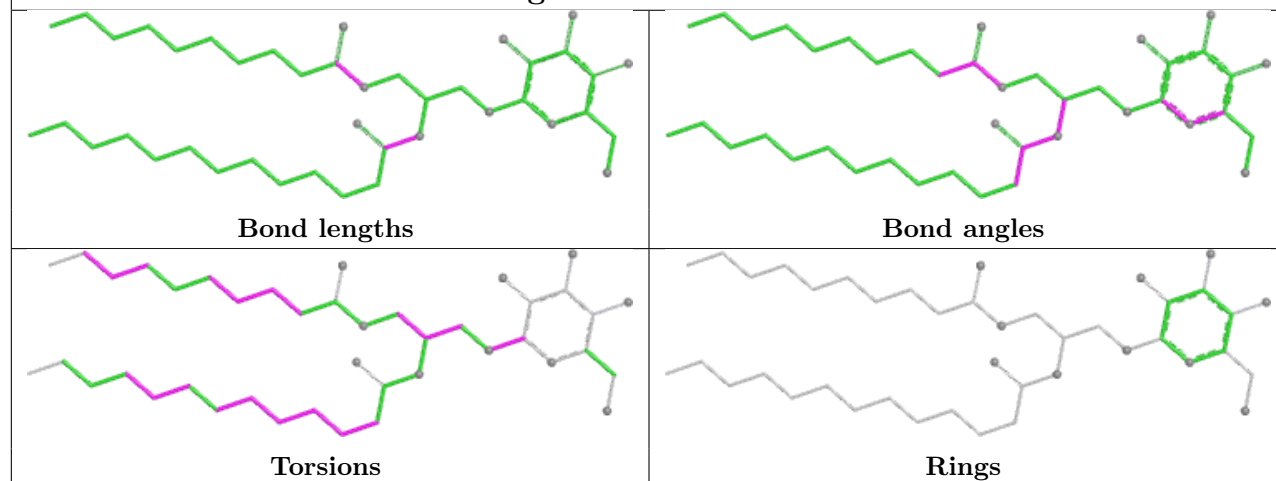


Rings

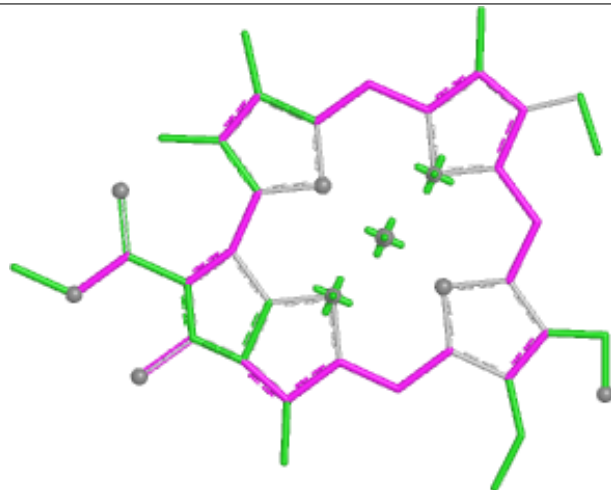
Ligand CHL 1 312



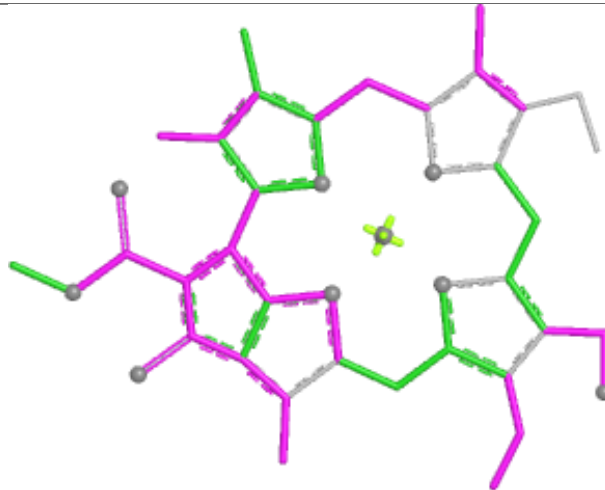
Ligand LMG C 618



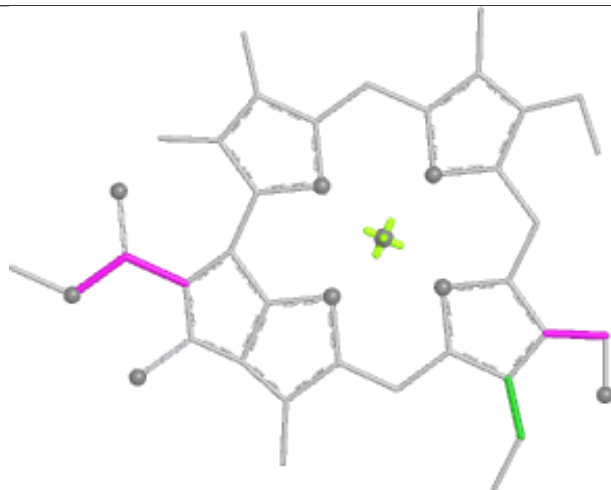
Ligand CHL 4 317



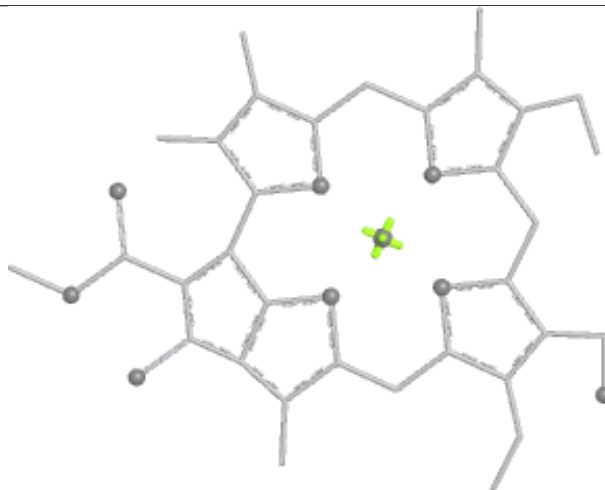
Bond lengths



Bond angles

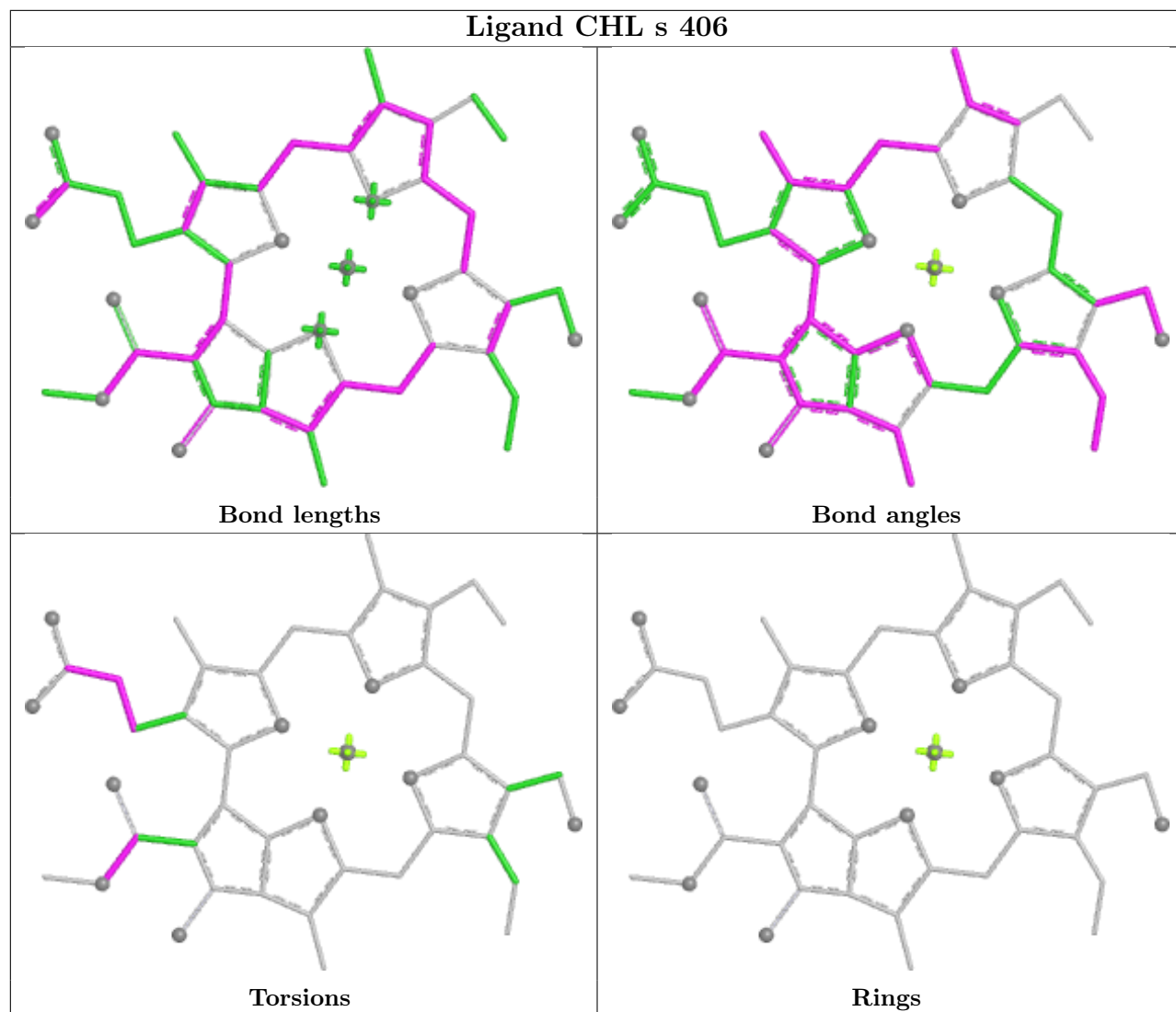


Torsions

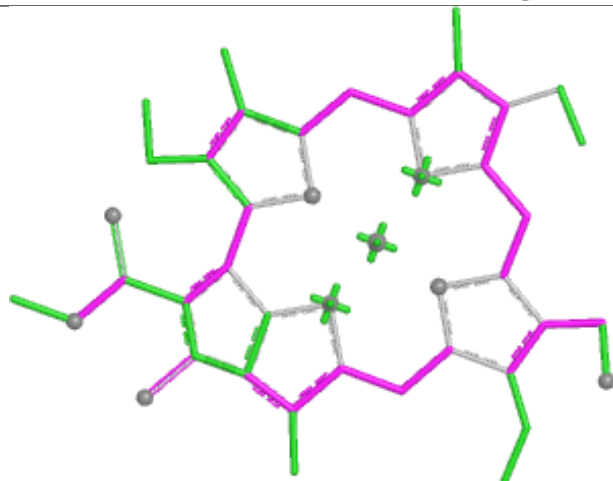


Rings

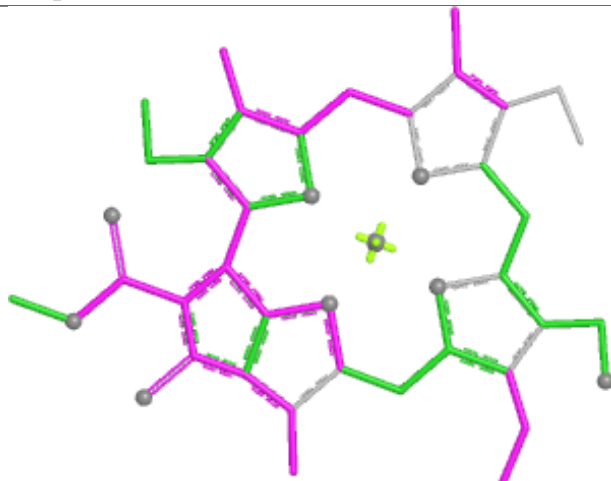
Ligand CHL s 406



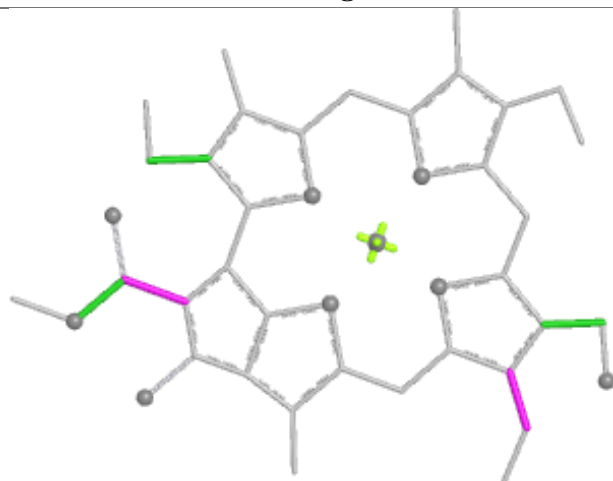
Ligand CHL p 309



Bond lengths



Bond angles

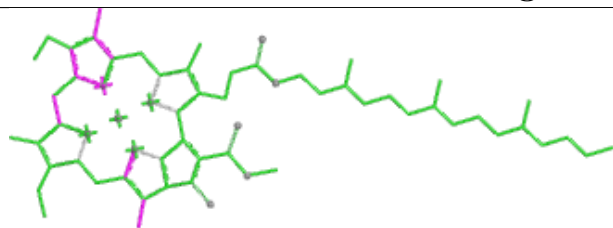


Torsions

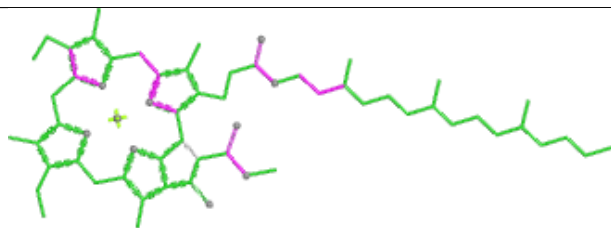


Rings

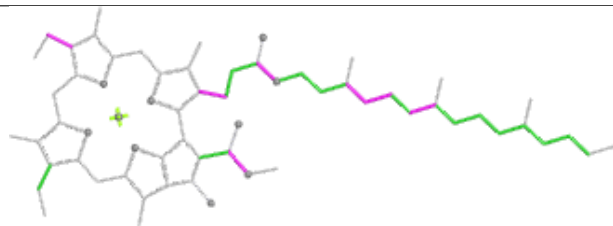
Ligand CLA 9 314



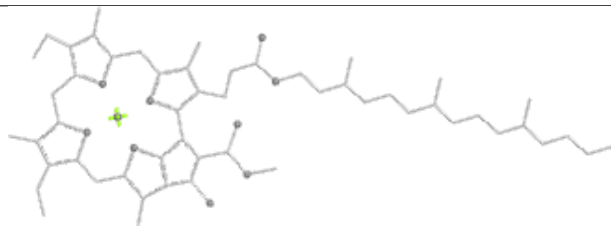
Bond lengths



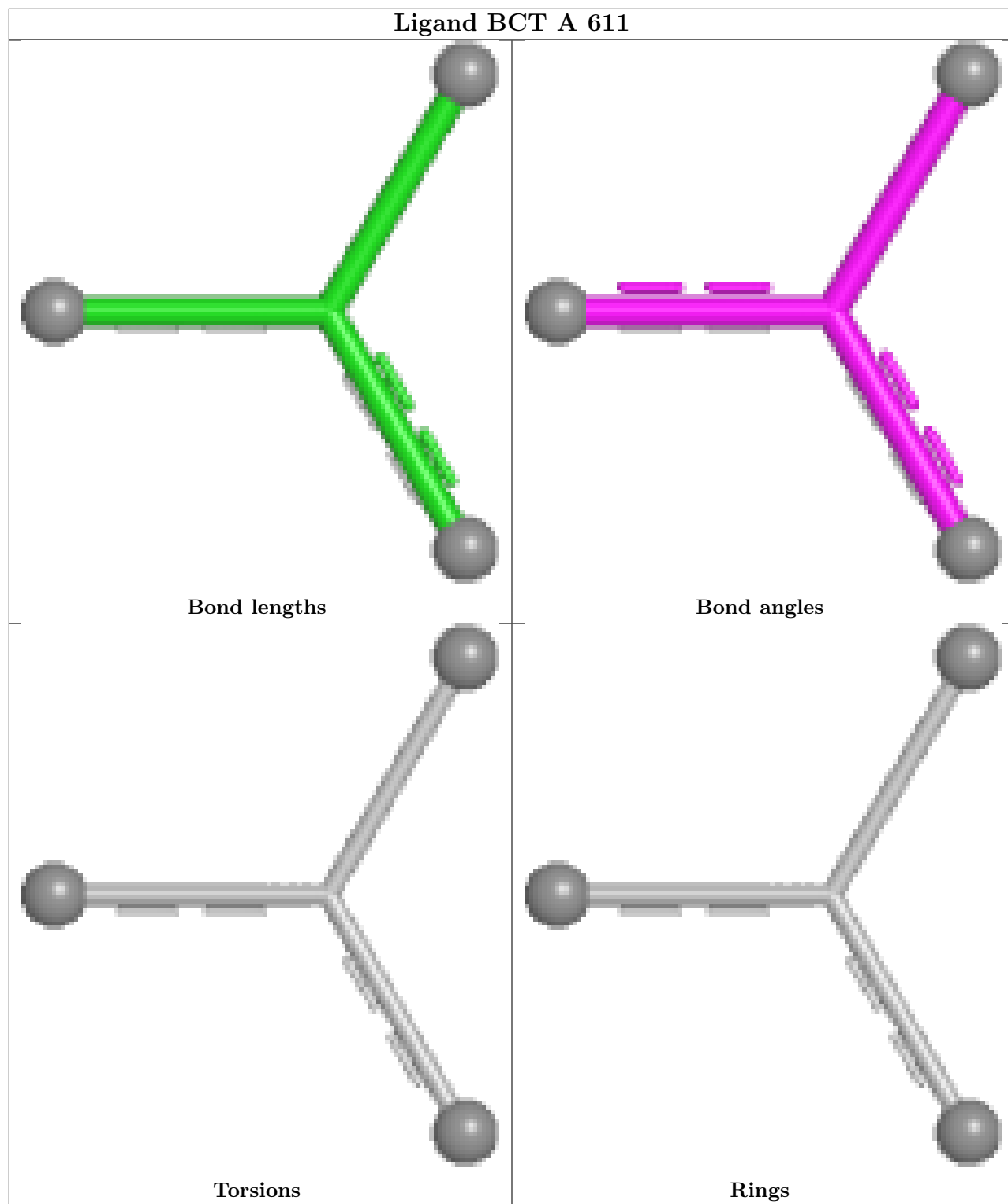
Bond angles



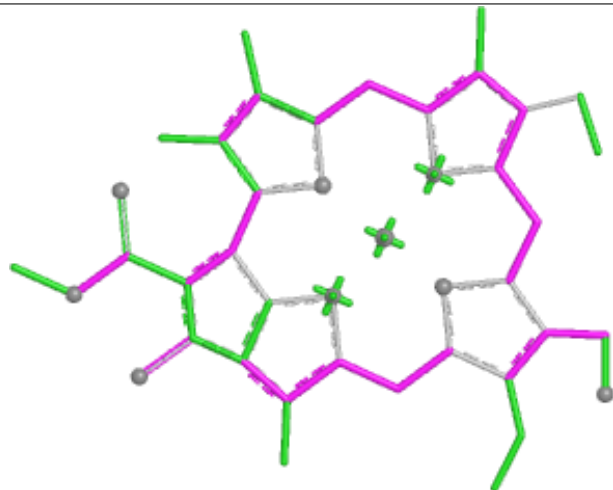
Torsions



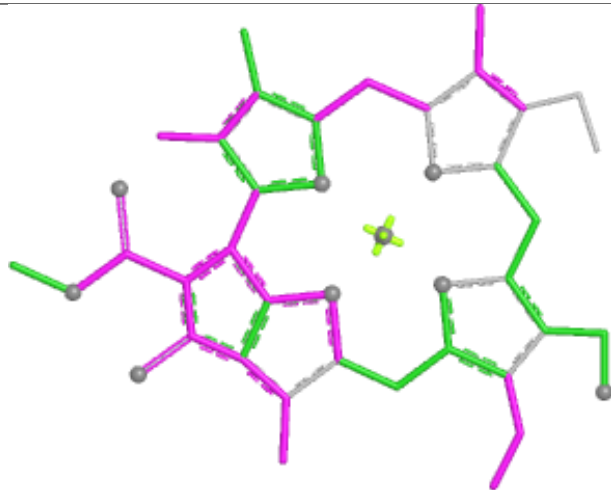
Rings



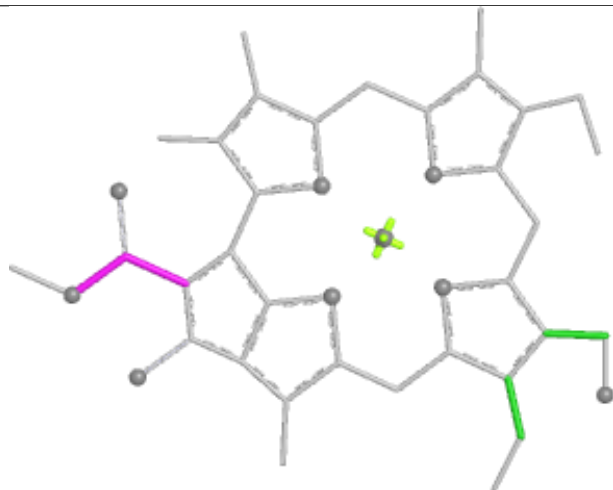
Ligand CHL 1 304



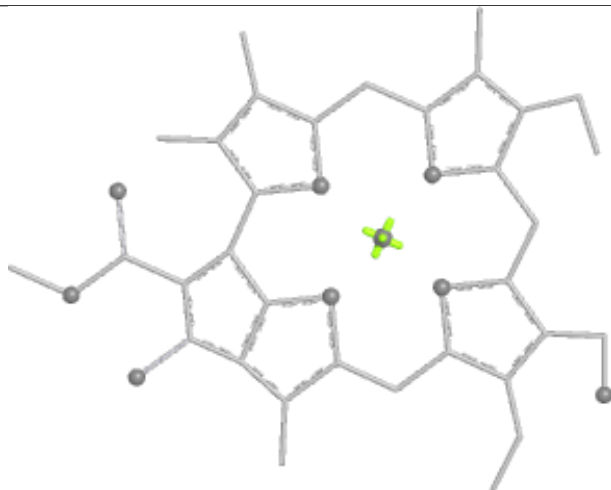
Bond lengths



Bond angles

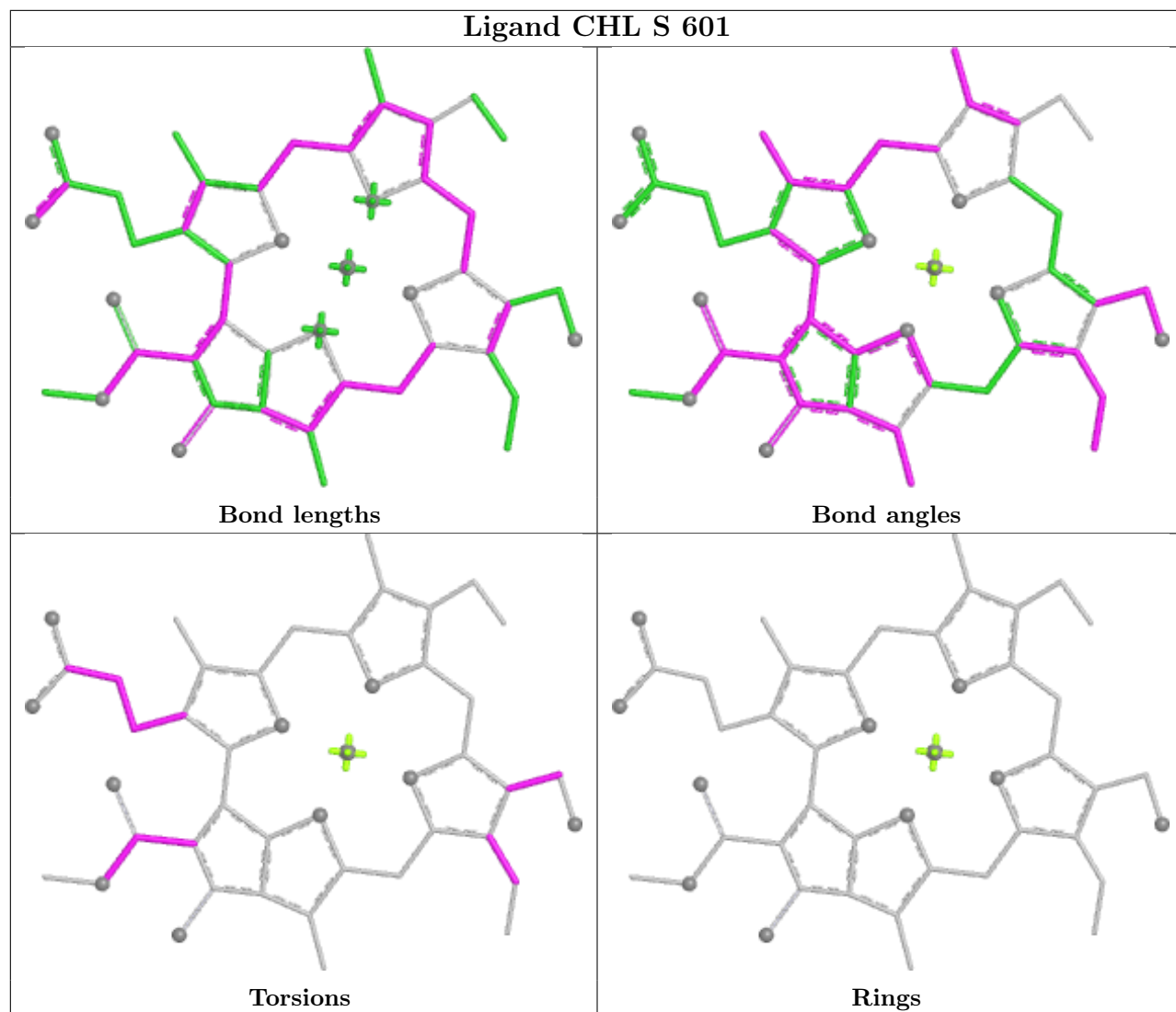


Torsions

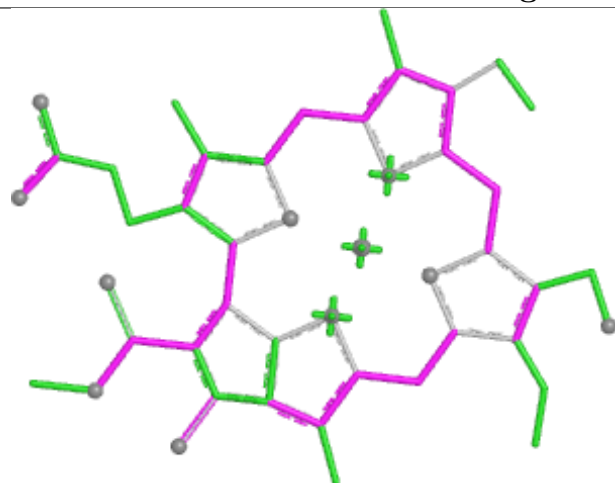


Rings

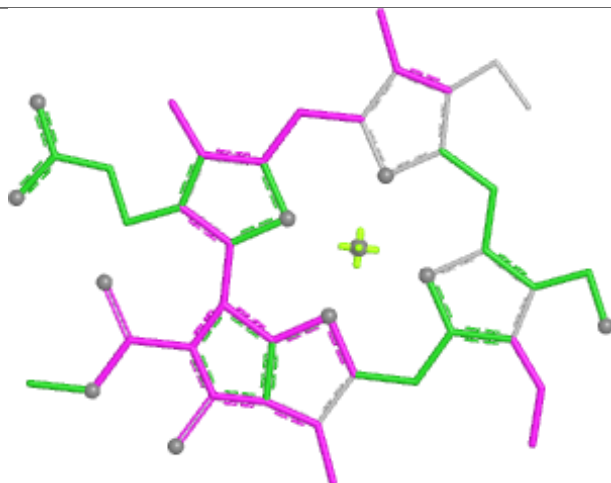
Ligand CHL S 601



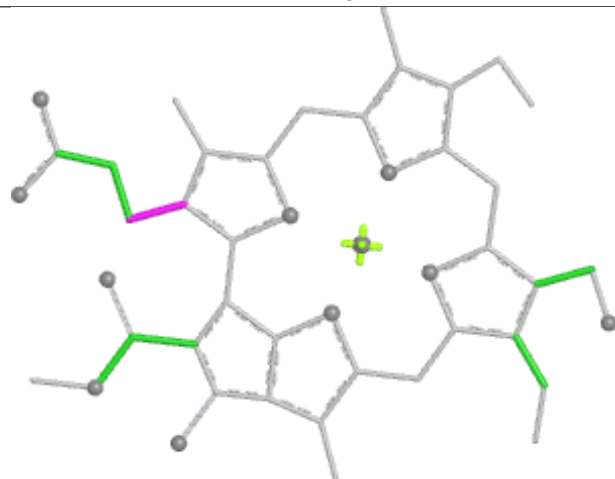
Ligand CHL 7 311



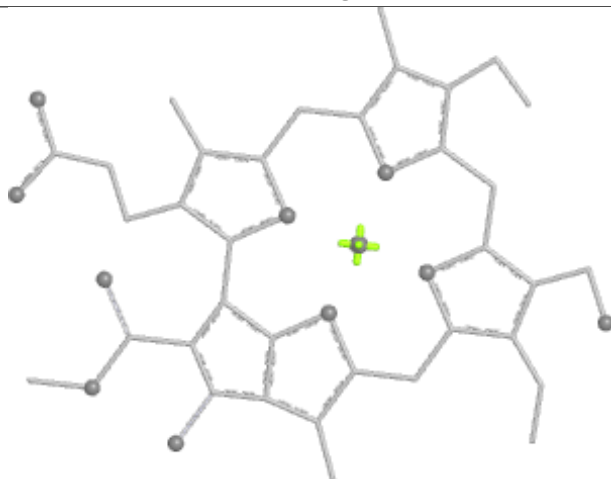
Bond lengths



Bond angles

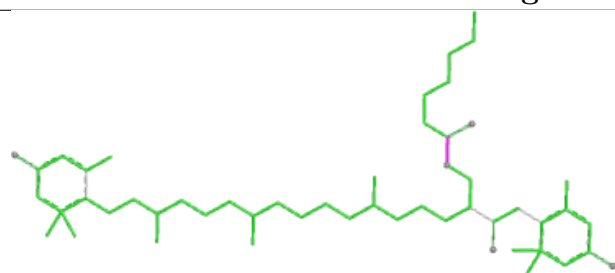


Torsions

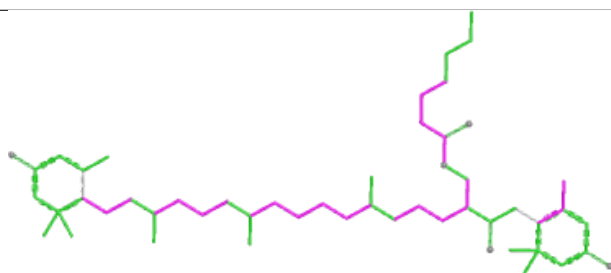


Rings

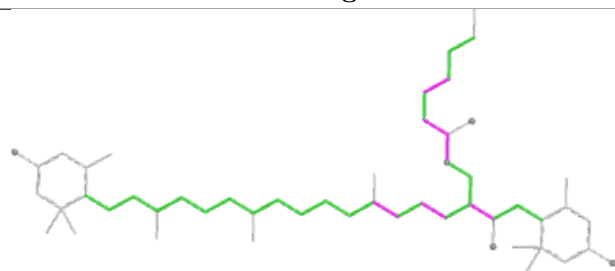
Ligand OUR 3 301



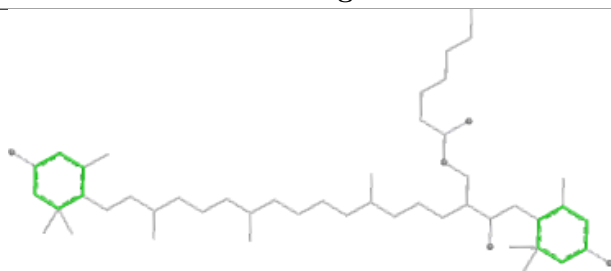
Bond lengths



Bond angles

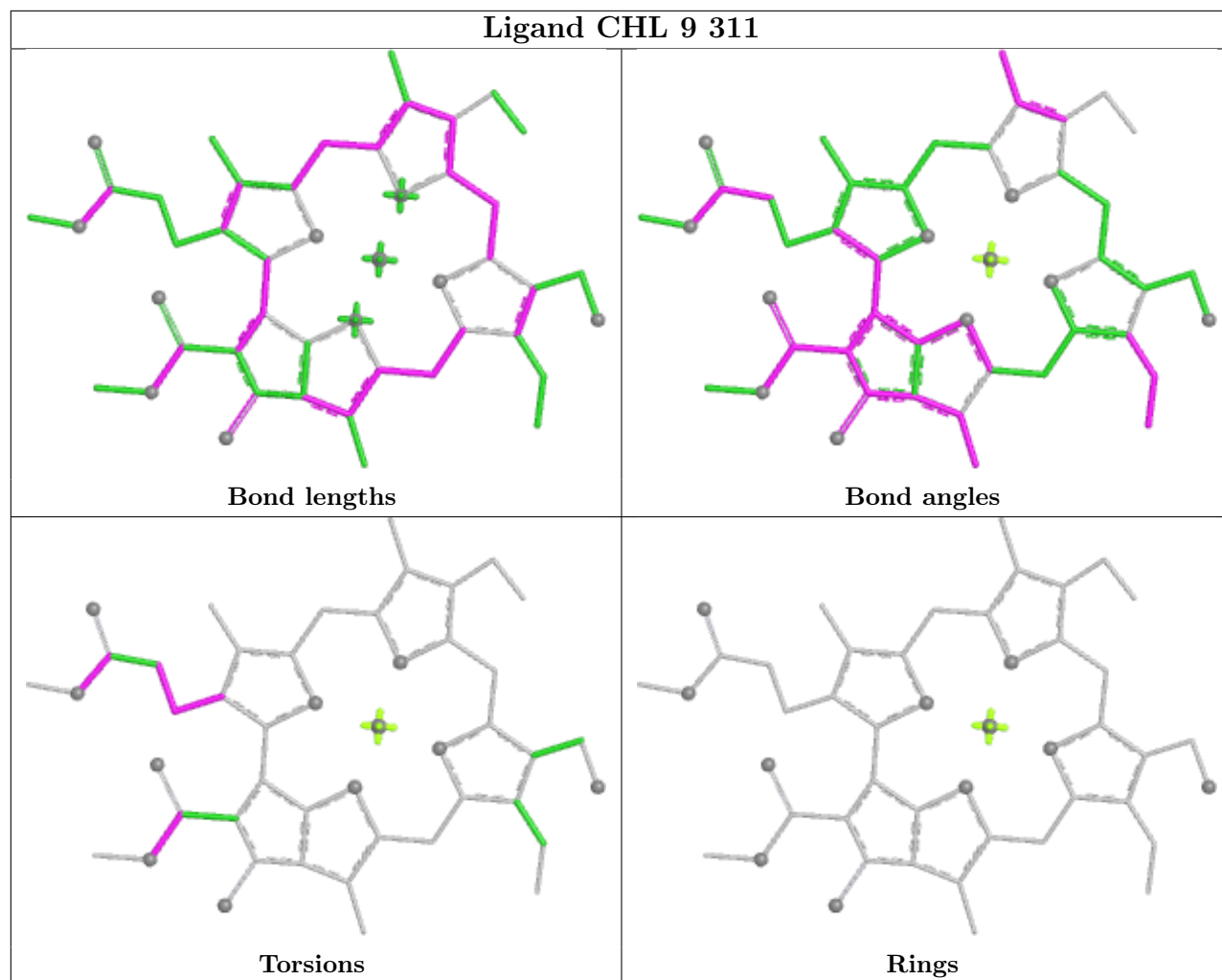


Torsions

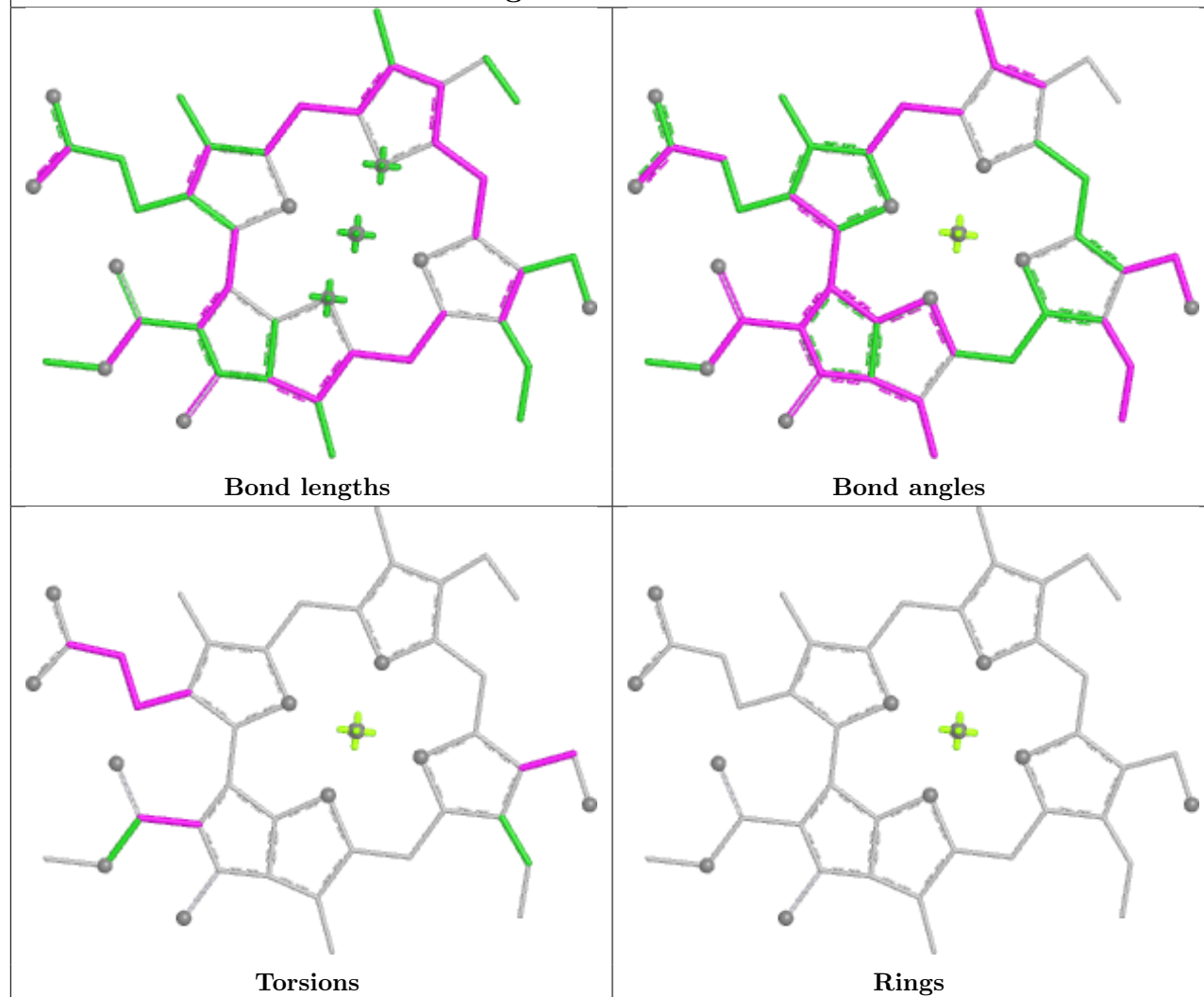


Rings

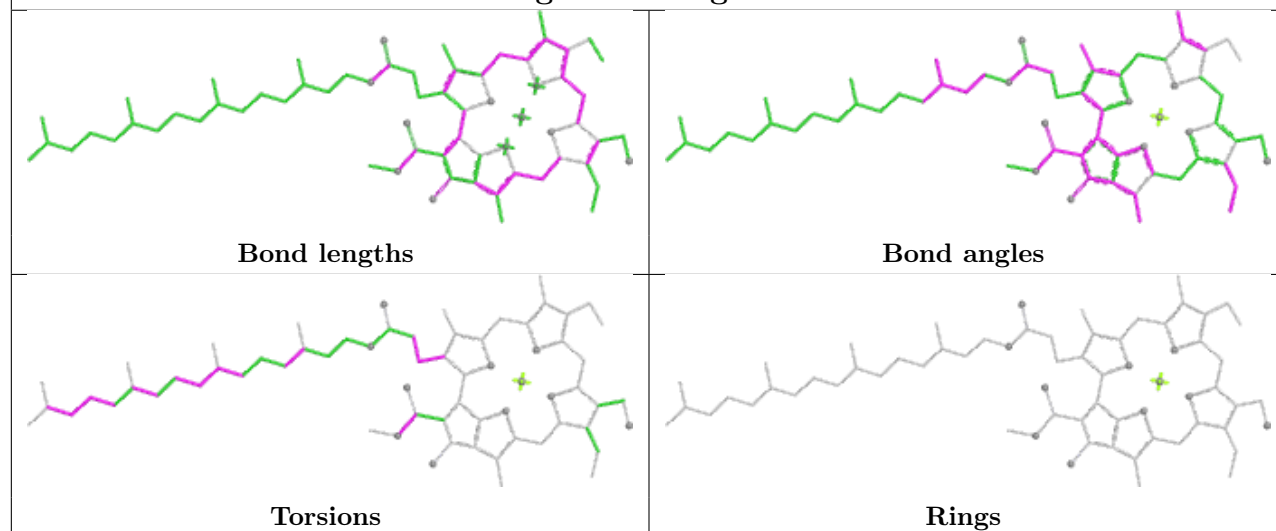
Ligand CHL 9 311



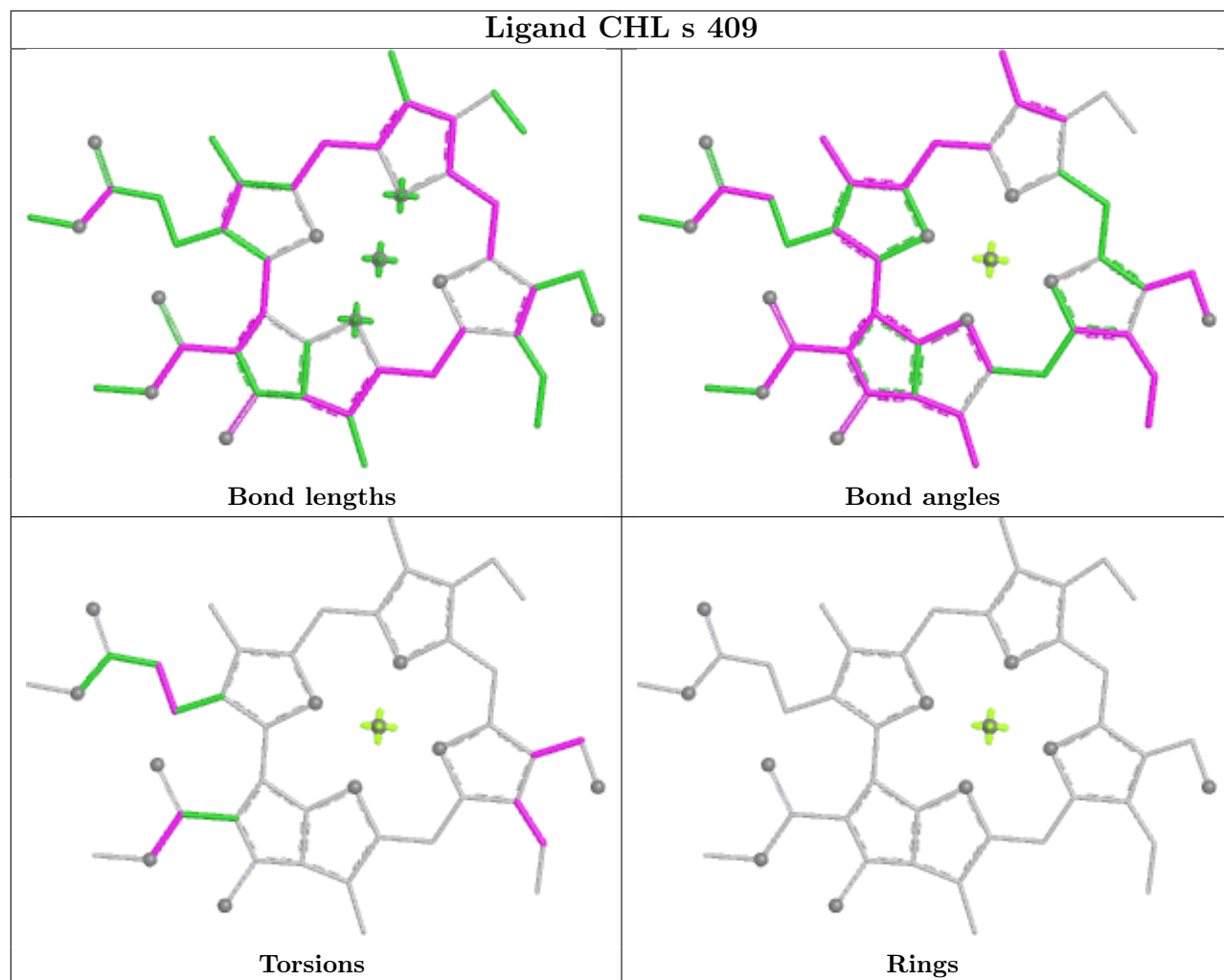
Ligand CHL 1 305



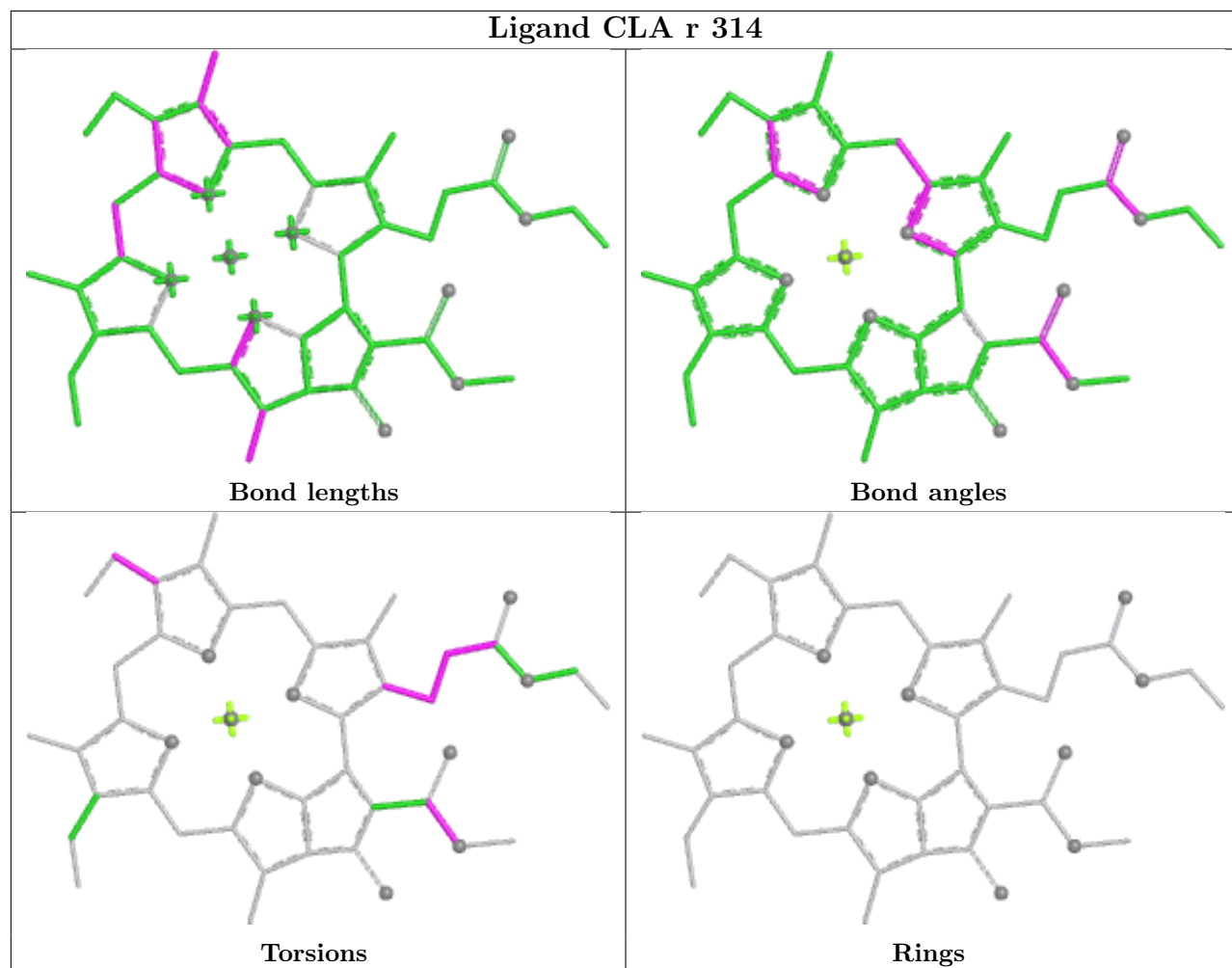
Ligand CHL g 305

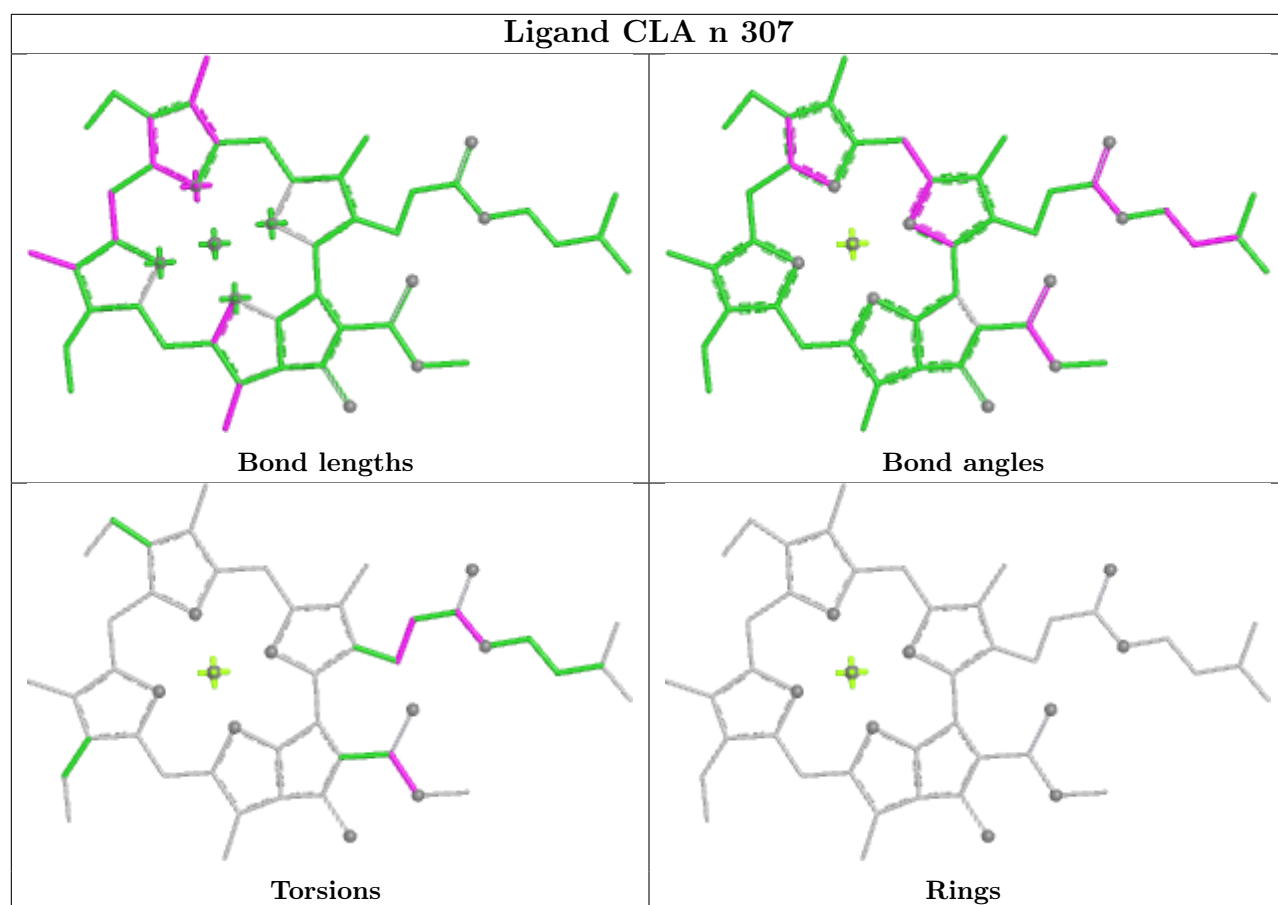


Ligand CHL s 409

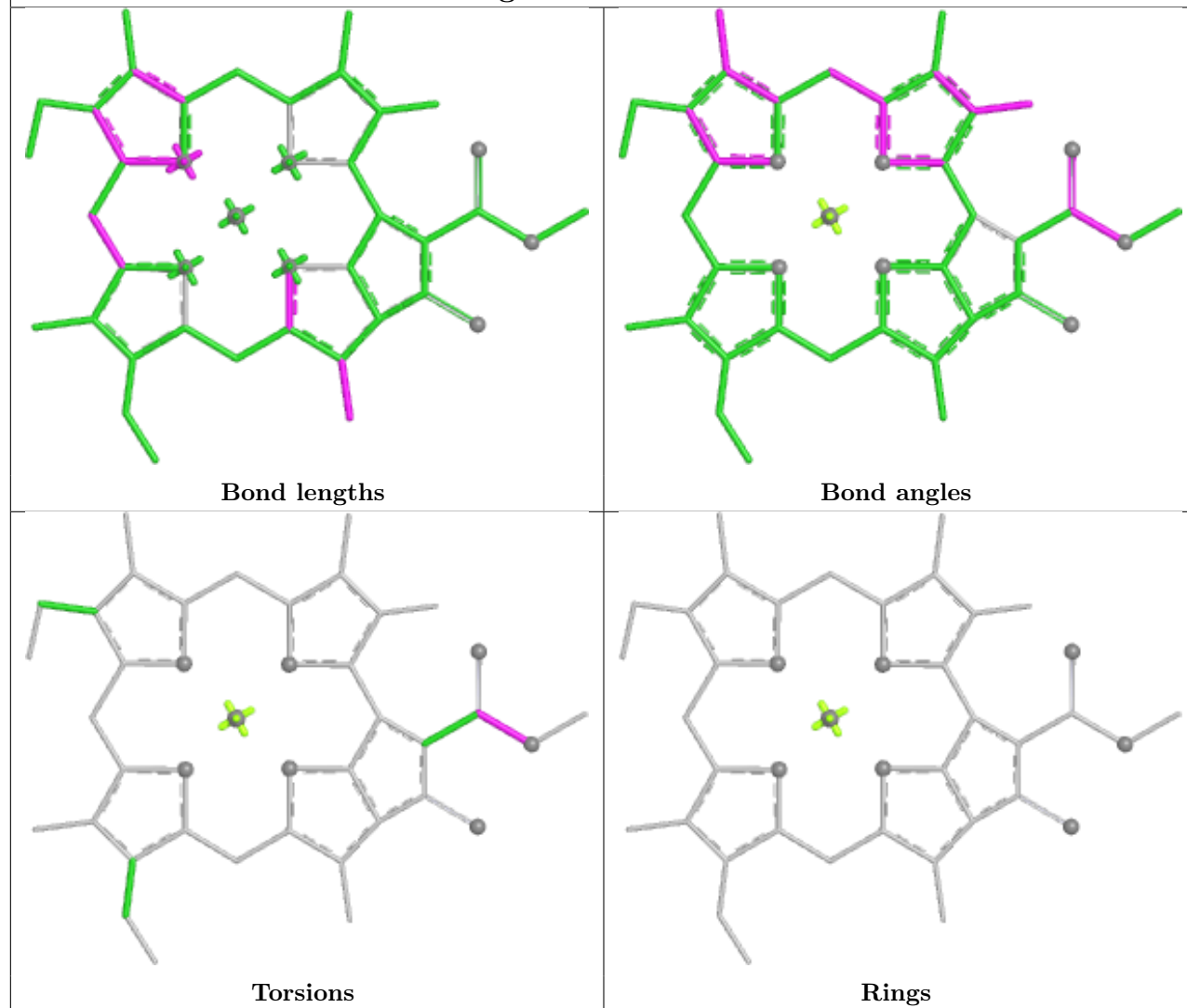


Ligand CLA r 314

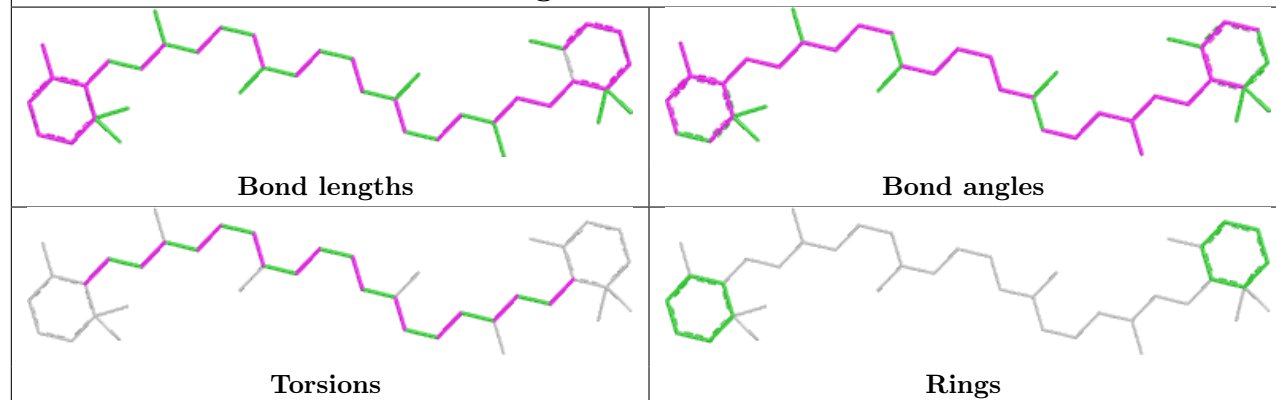




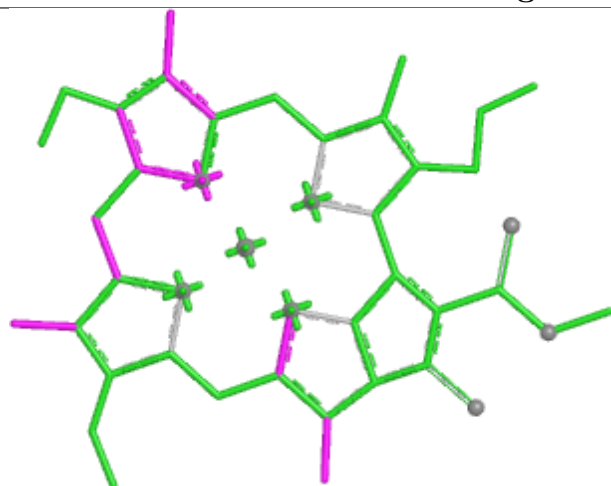
Ligand CLA 3 314



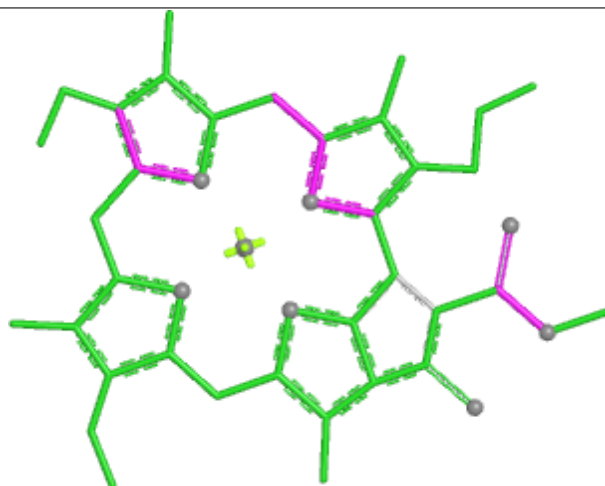
Ligand 8CT C 614



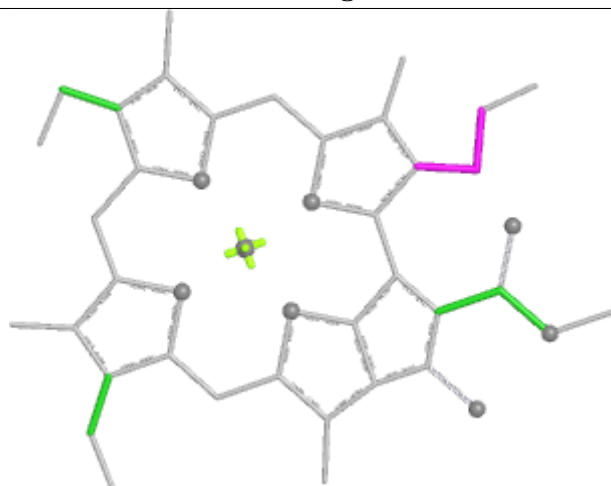
Ligand CLA n 316



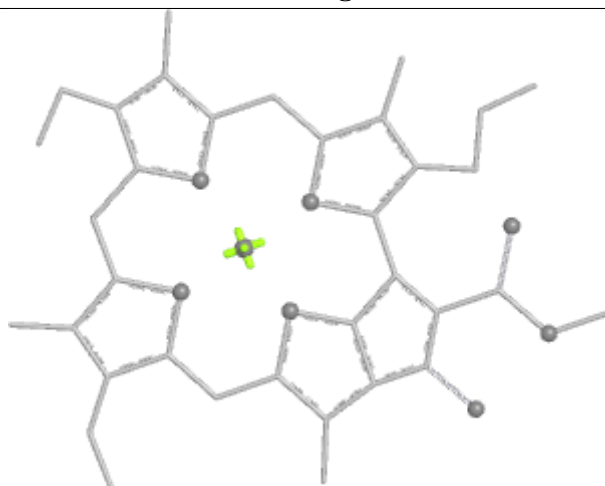
Bond lengths



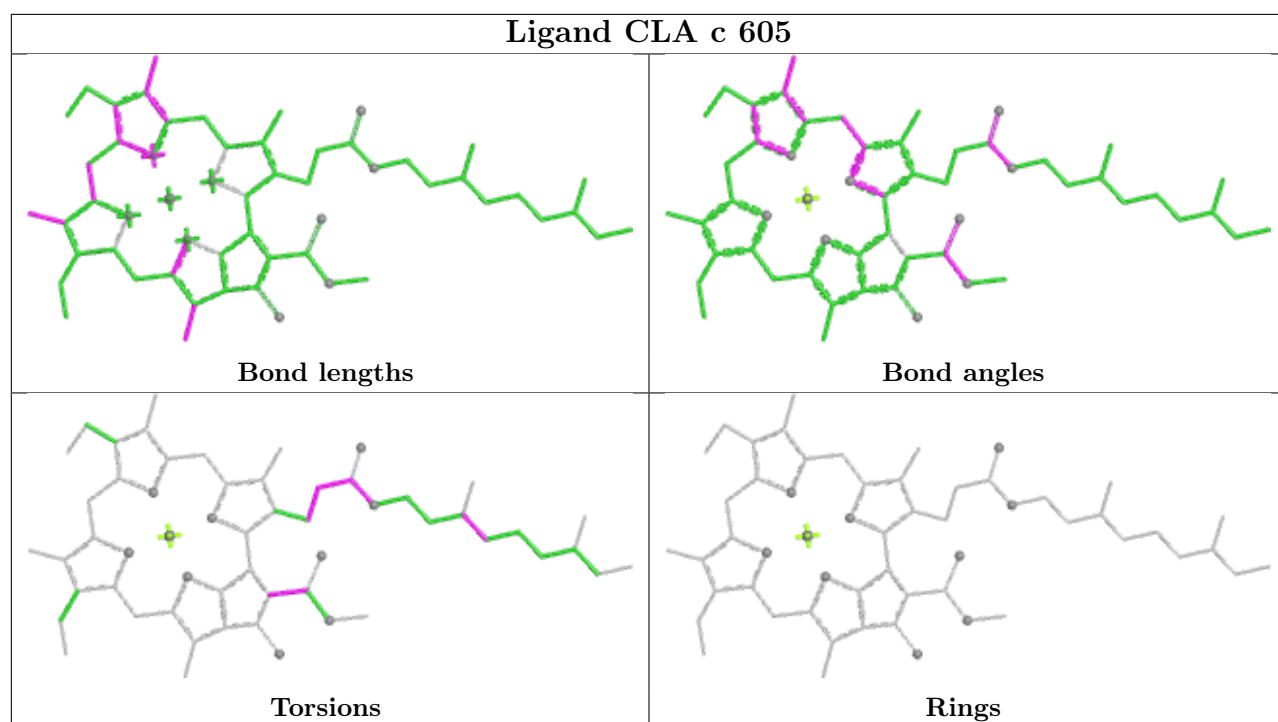
Bond angles

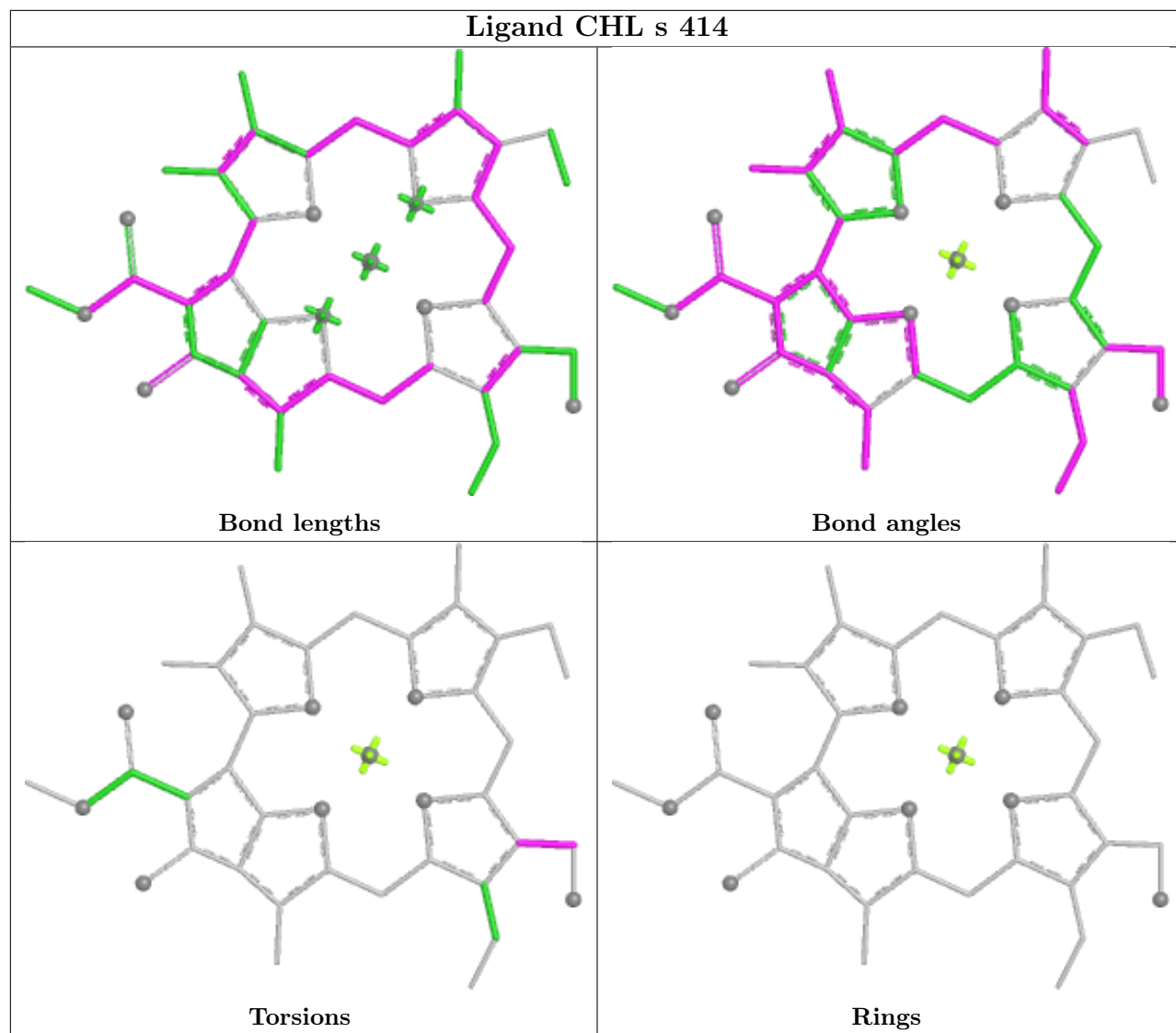


Torsions

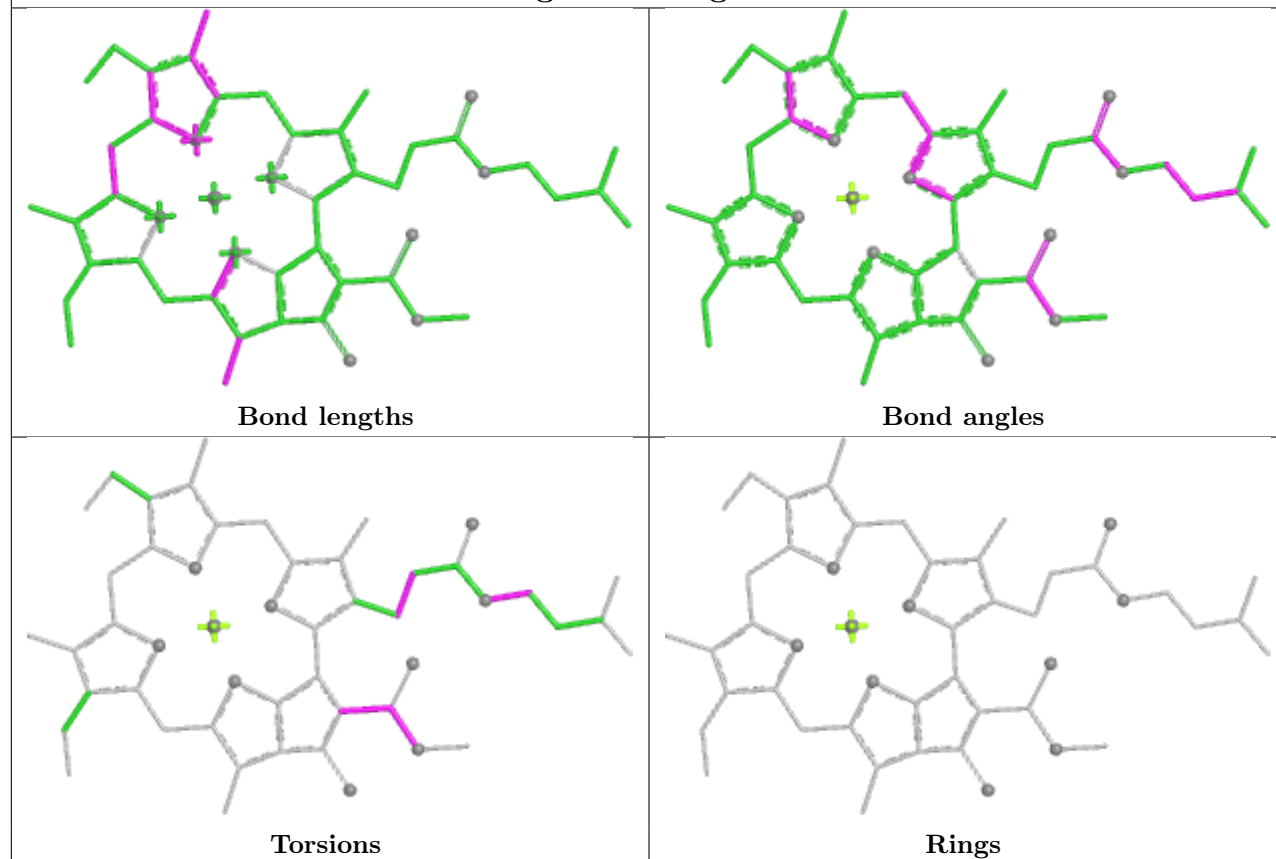


Rings

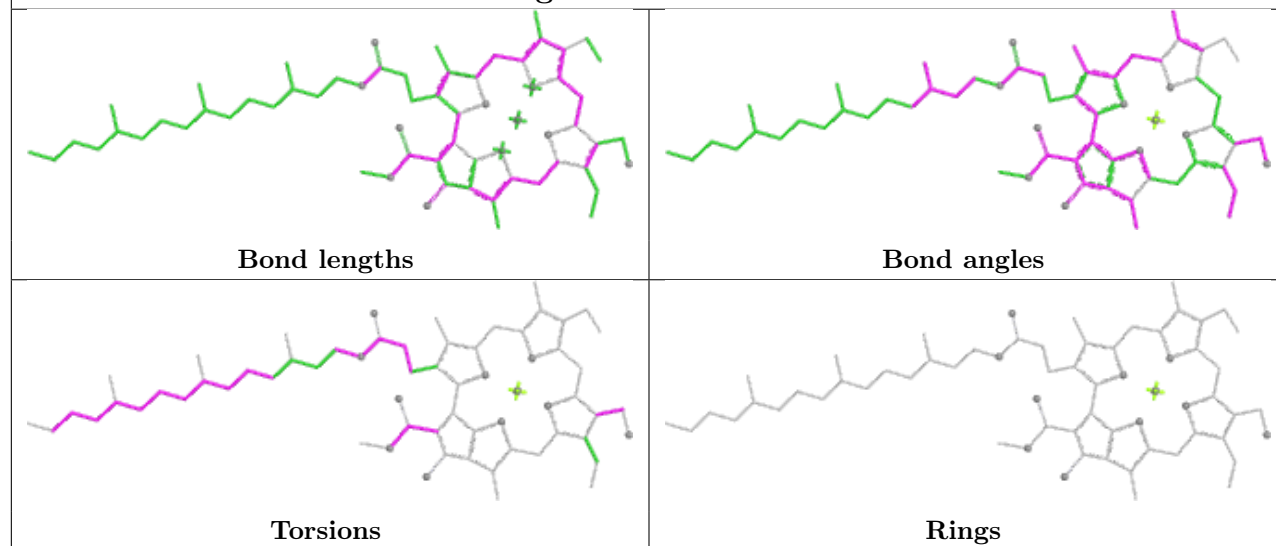


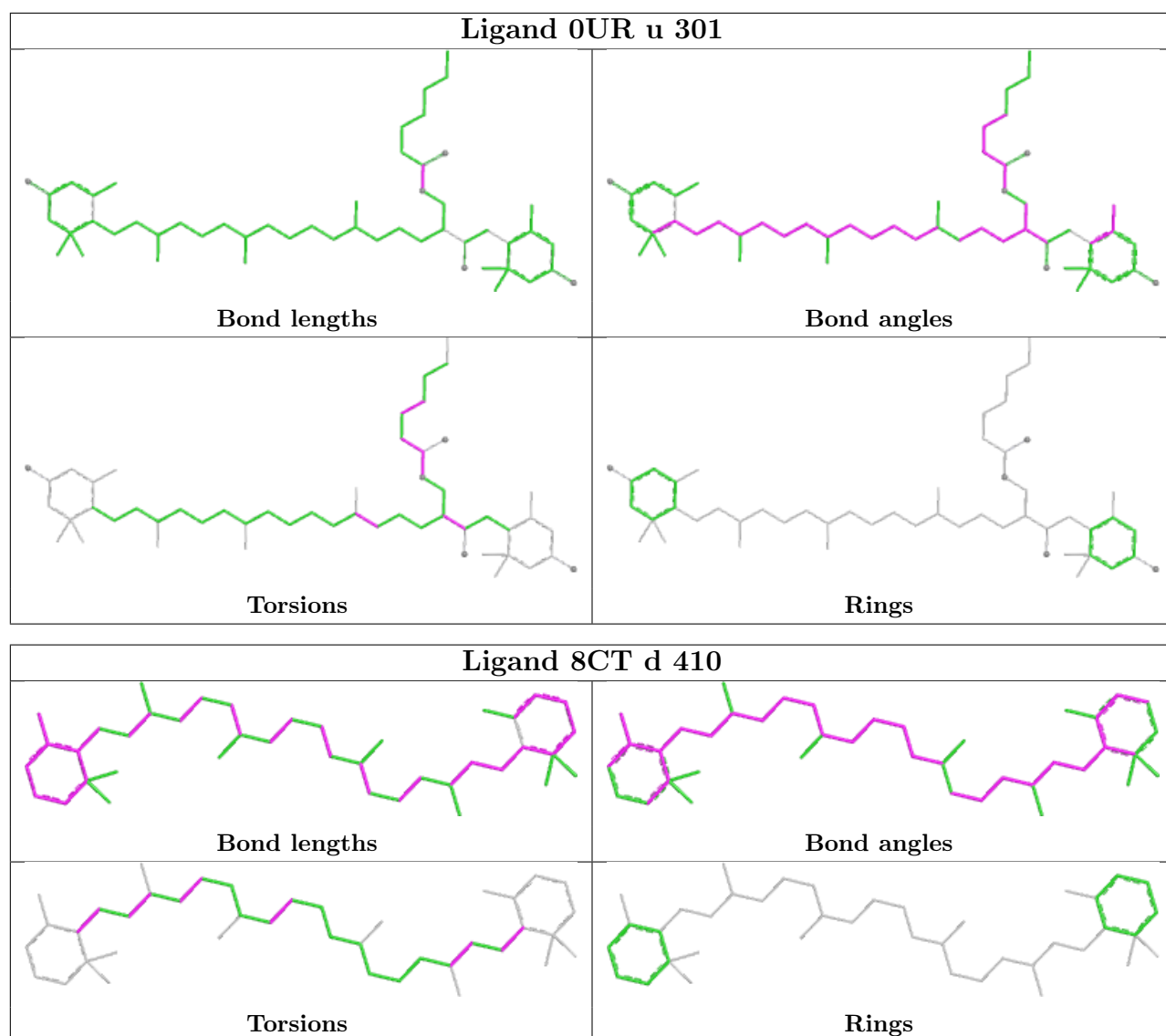


Ligand CLA g 308

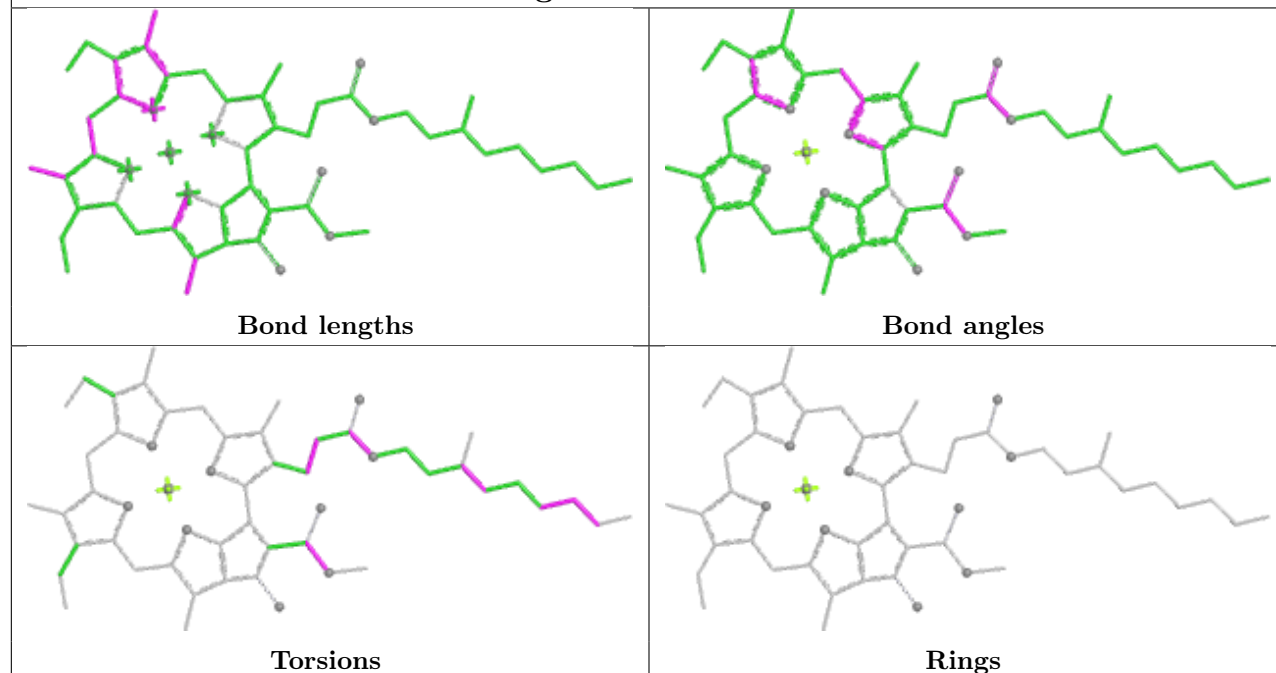


Ligand CHL 7 306

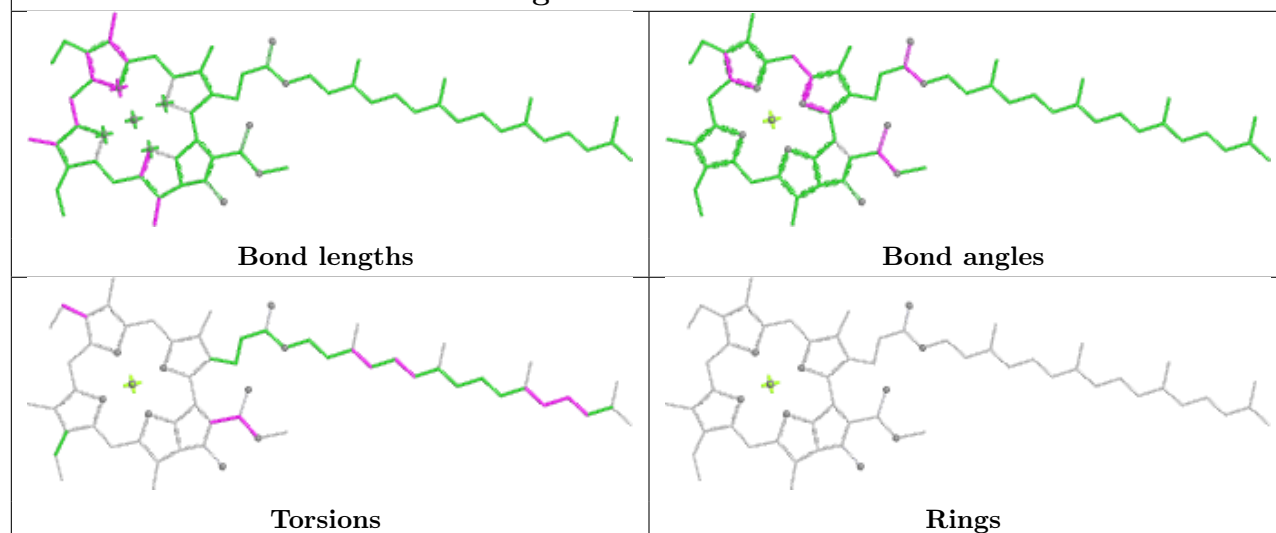




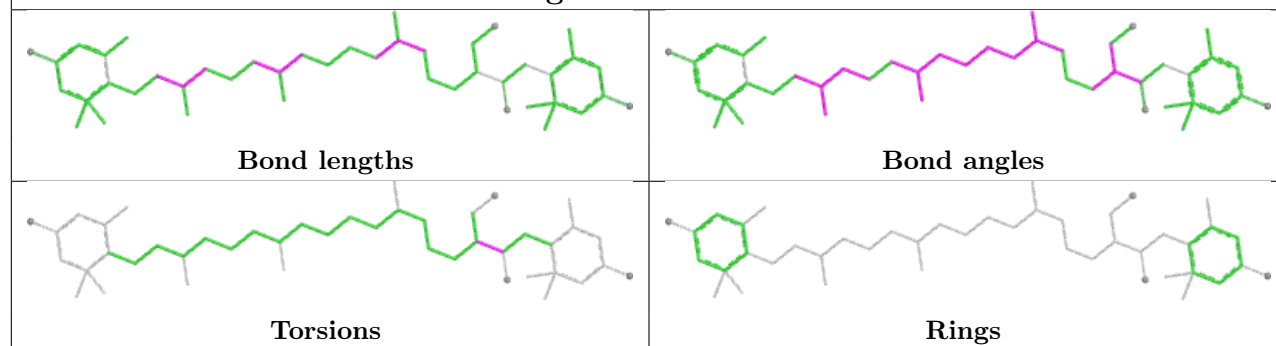
Ligand CLA S 612

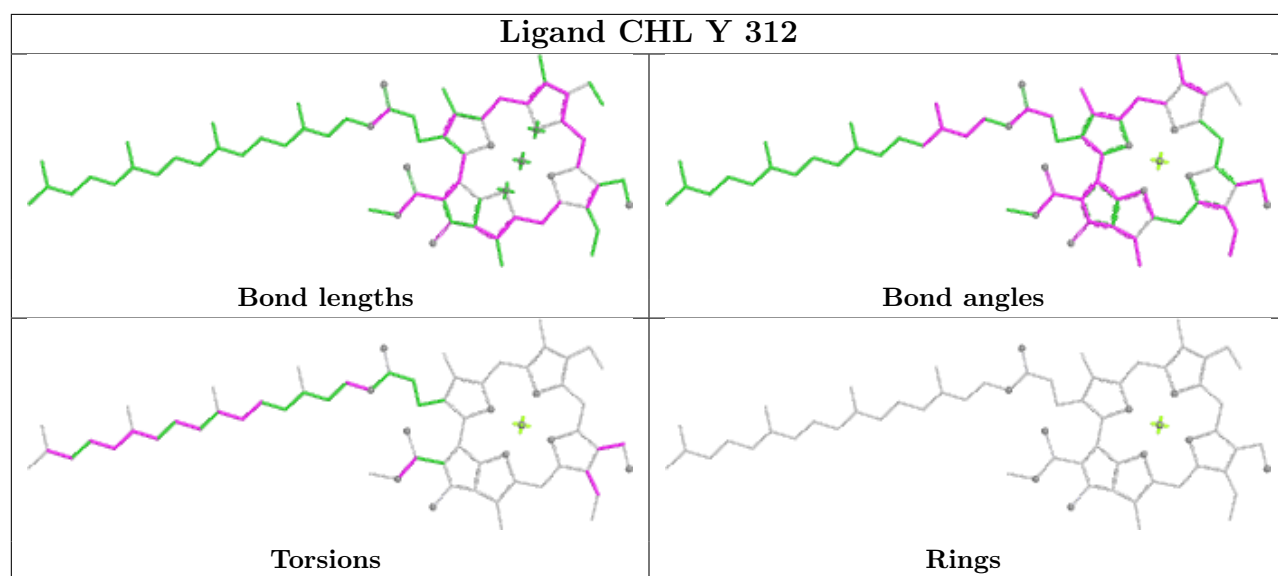
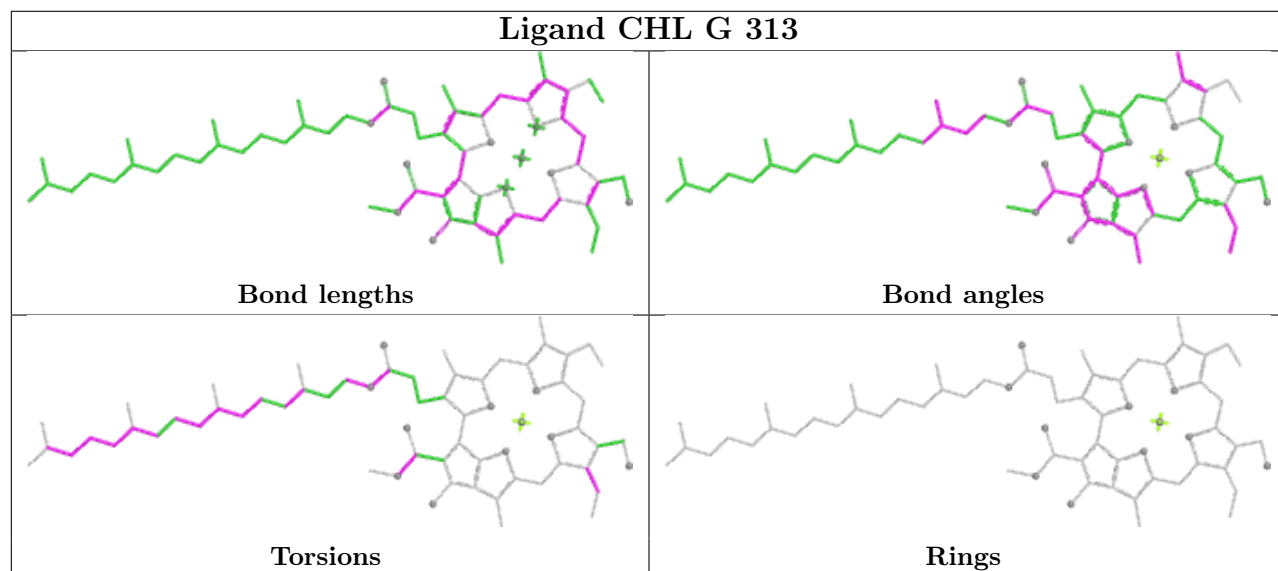
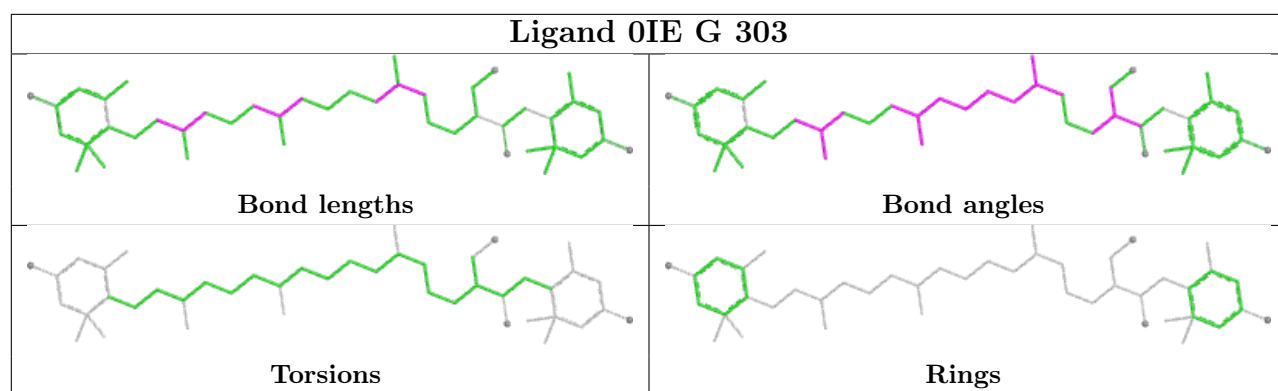


Ligand CLA B 605

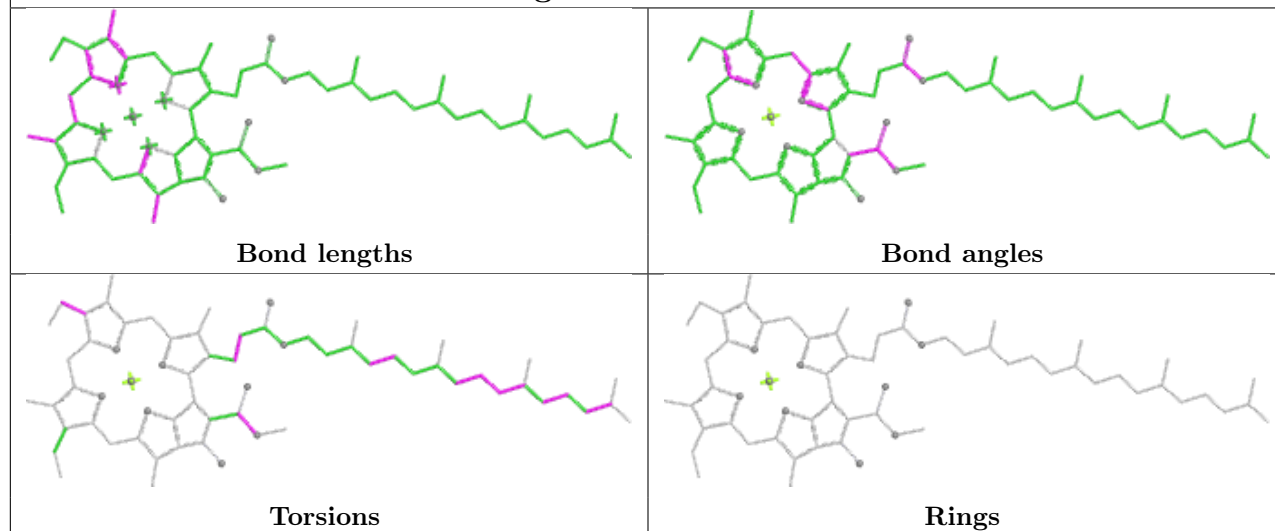


Ligand OIE 4 302

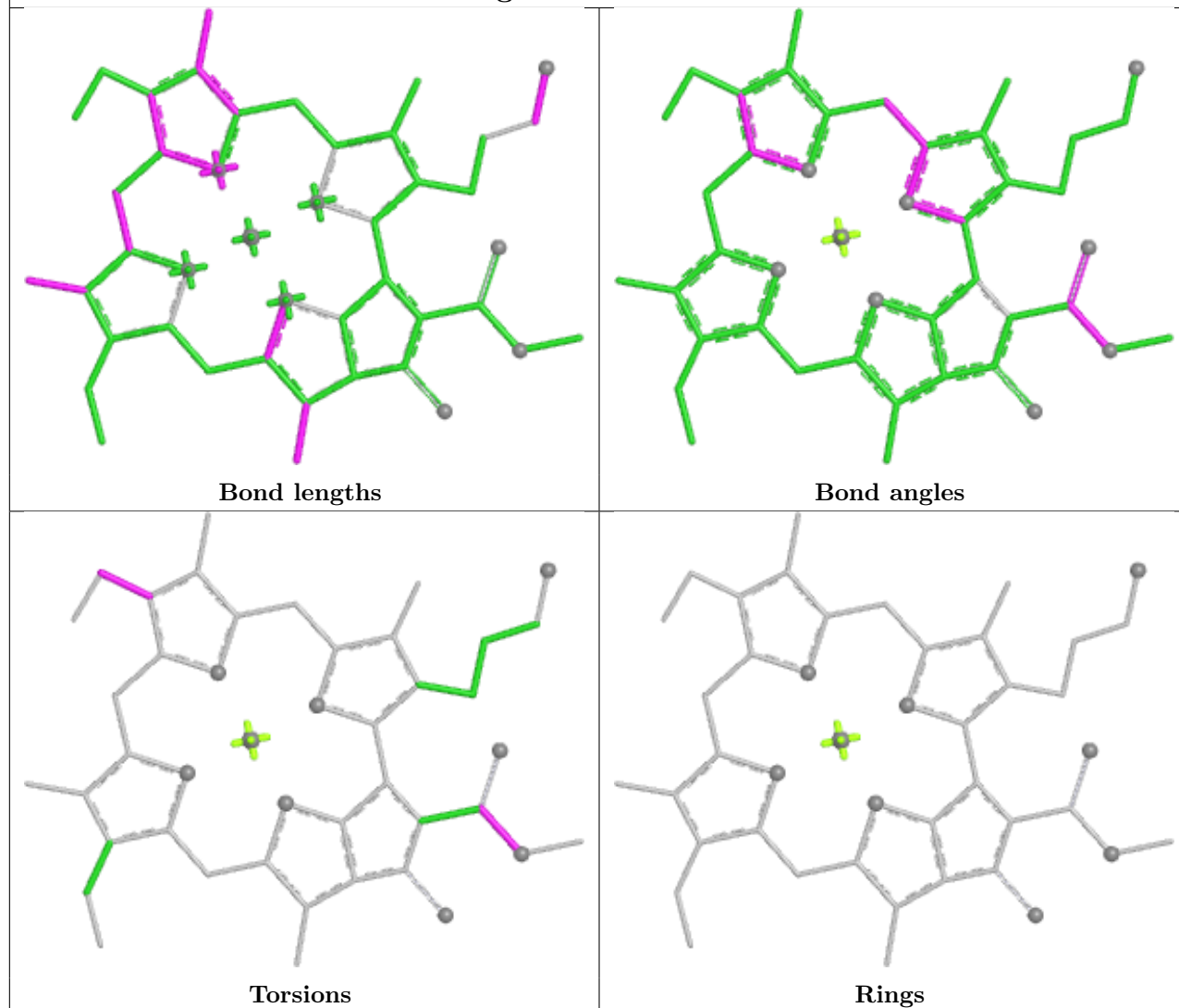


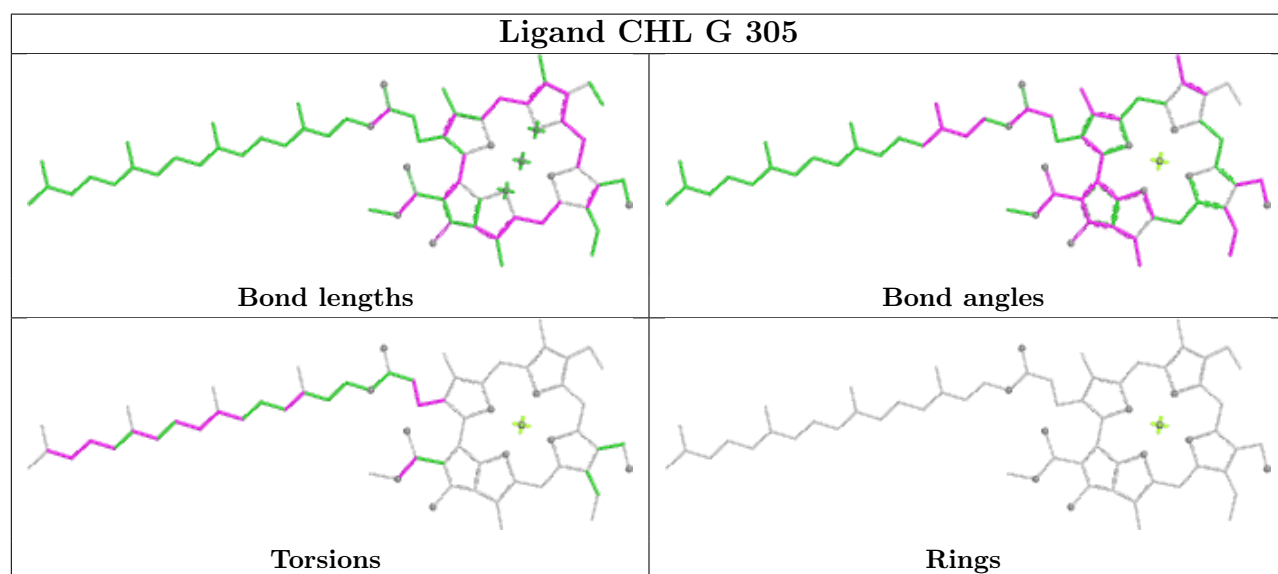
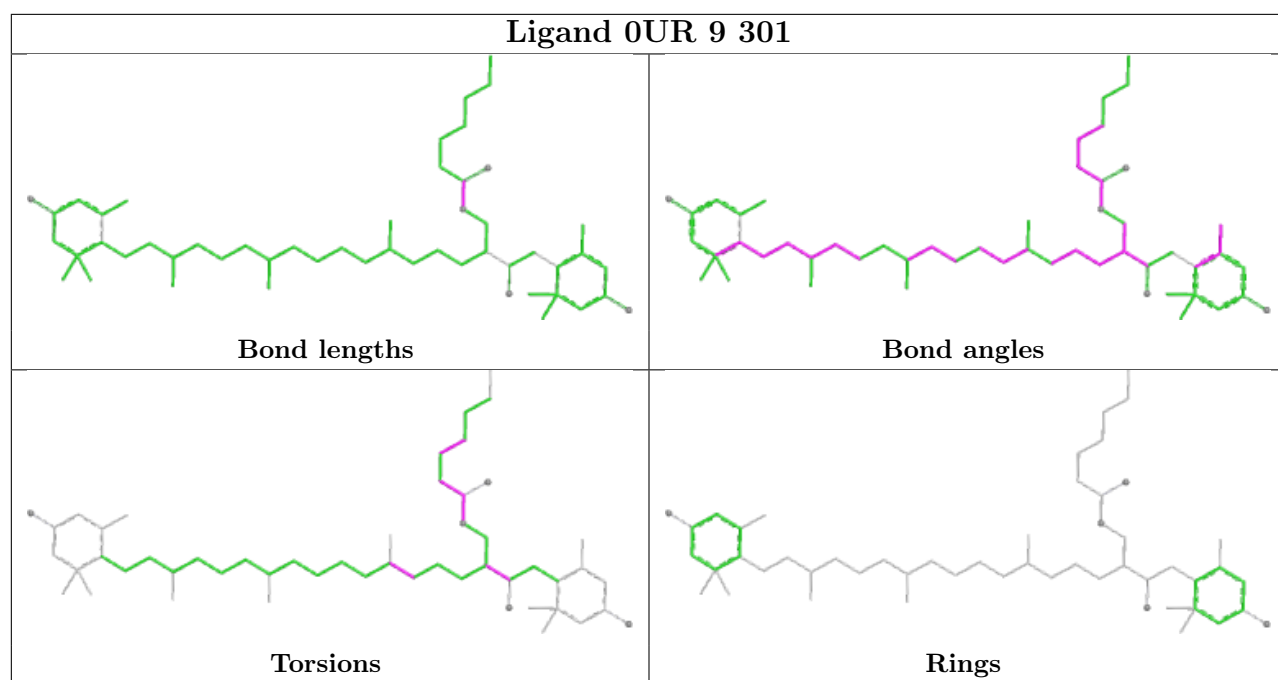


Ligand CLA b 607

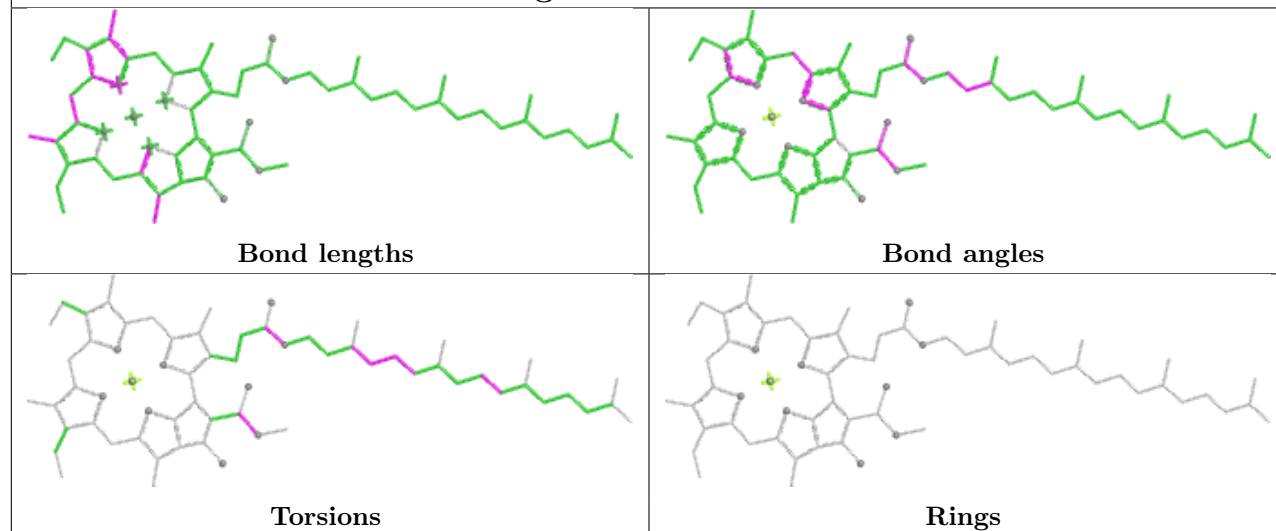


Ligand CLA s 411

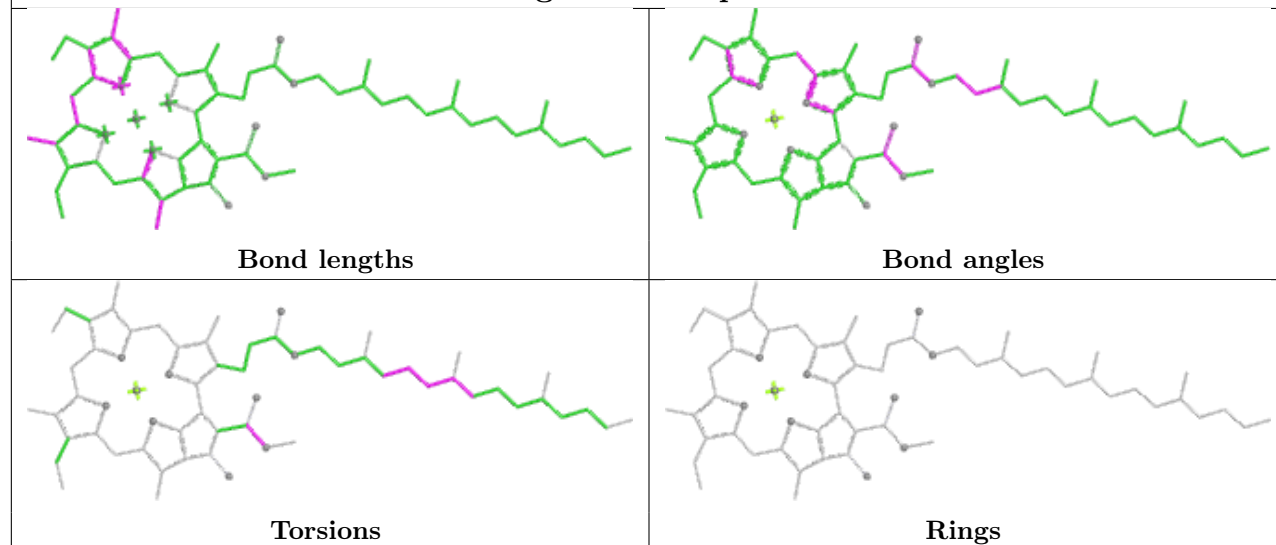




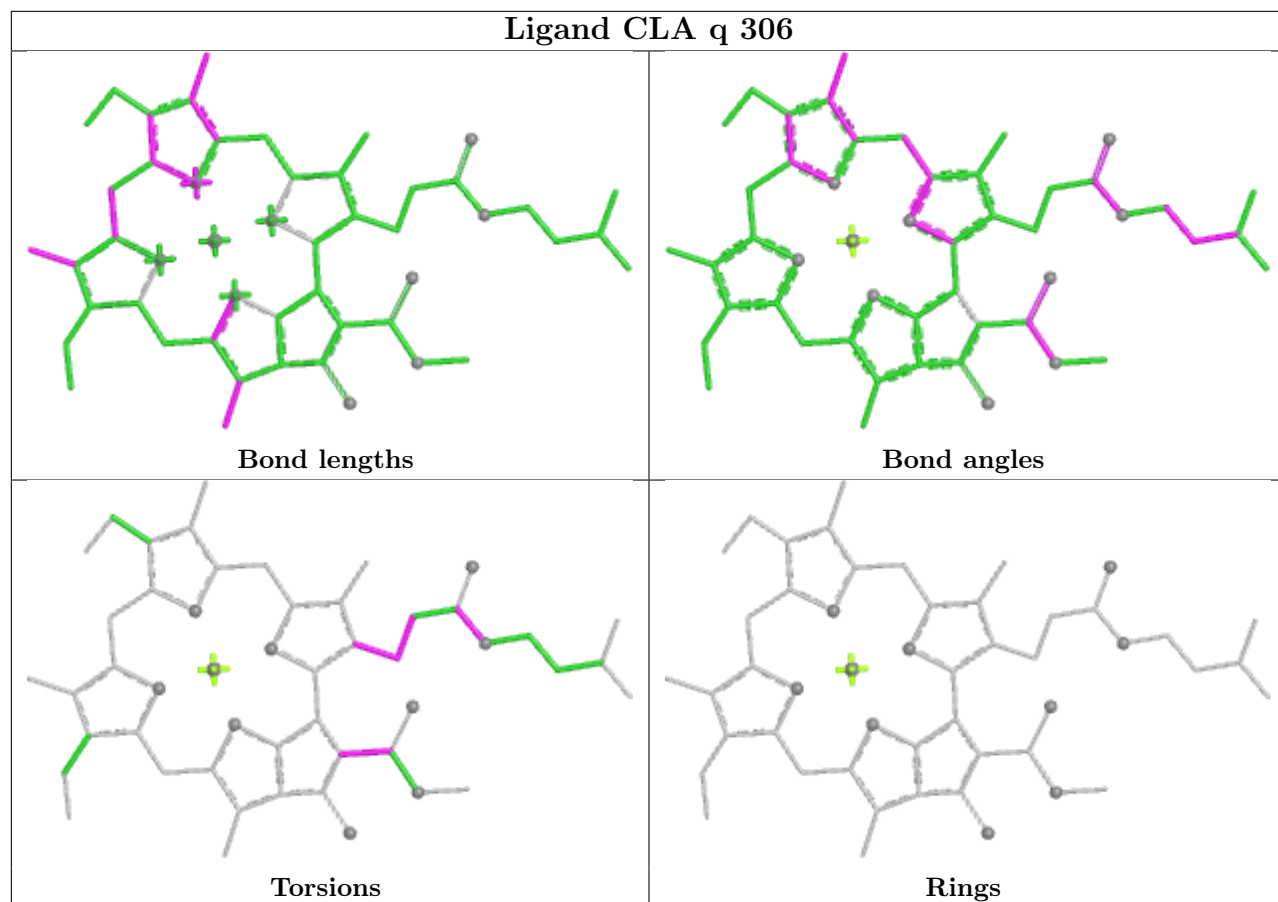
Ligand CLA b 613



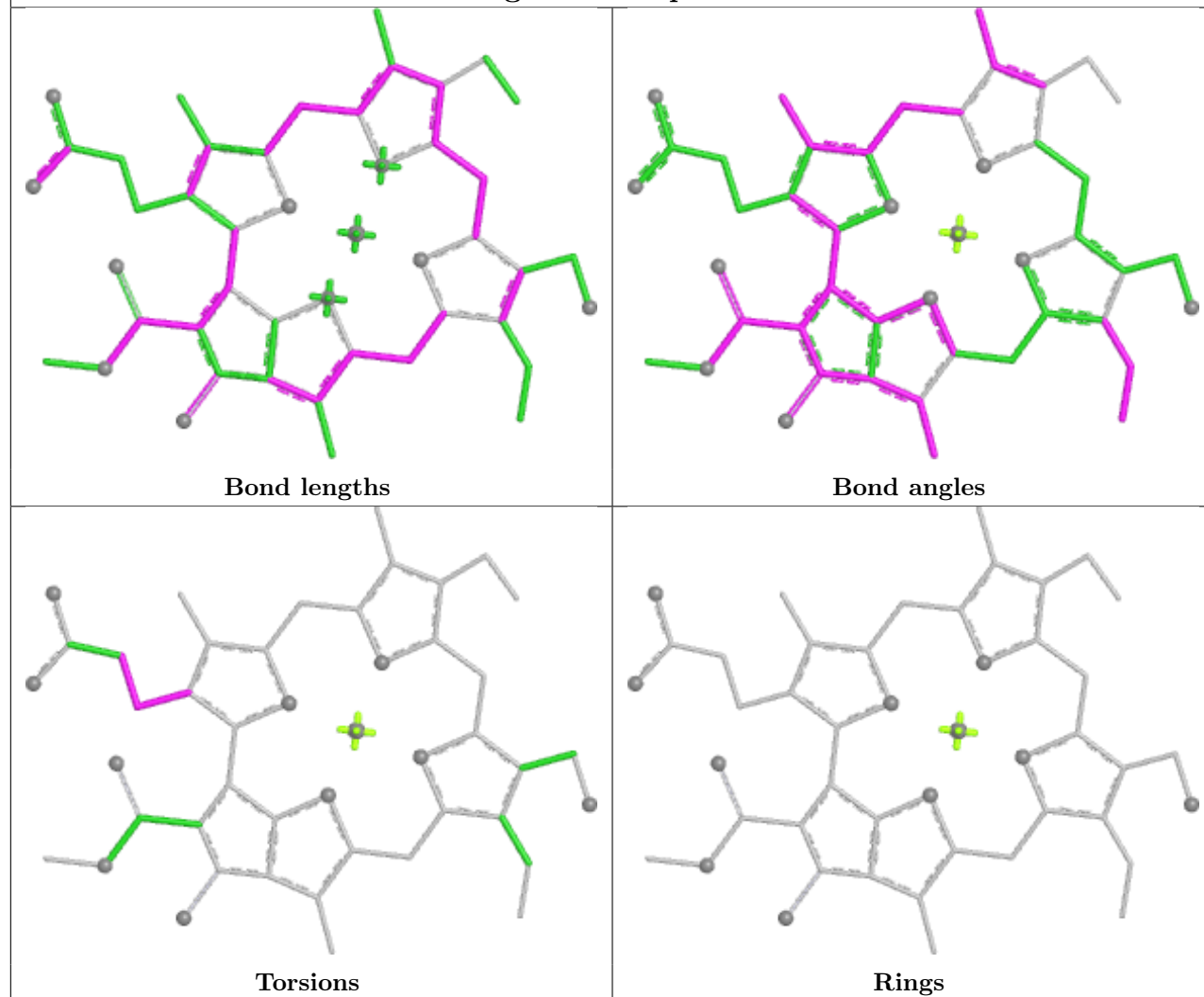
Ligand CLA q 313



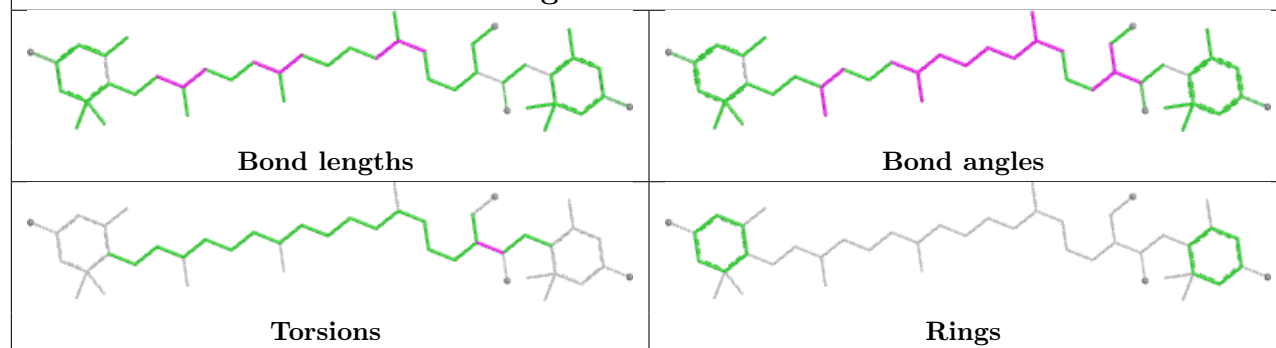
Ligand CLA q 306



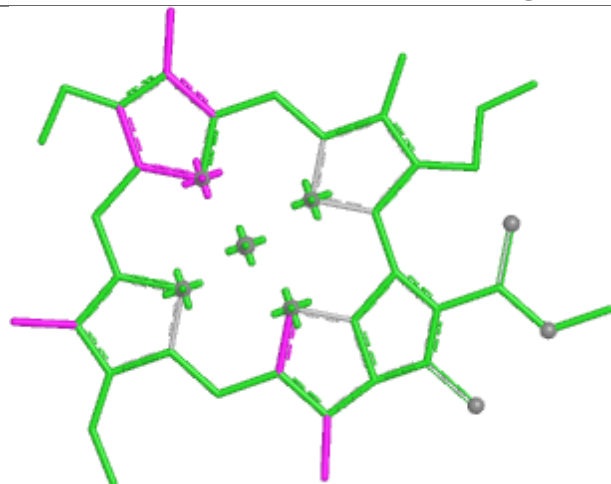
Ligand CHL p 311



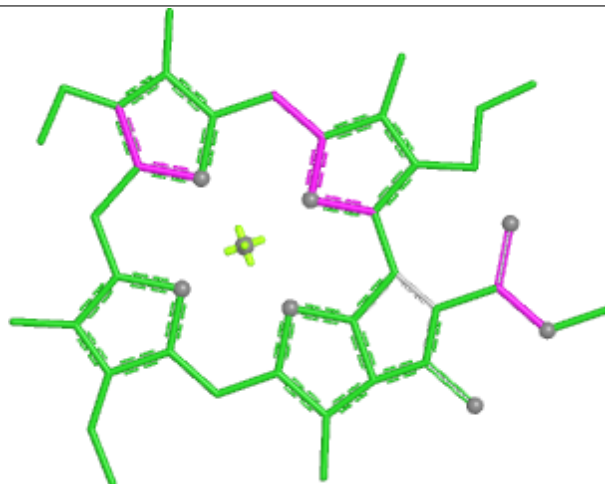
Ligand OIE G 302



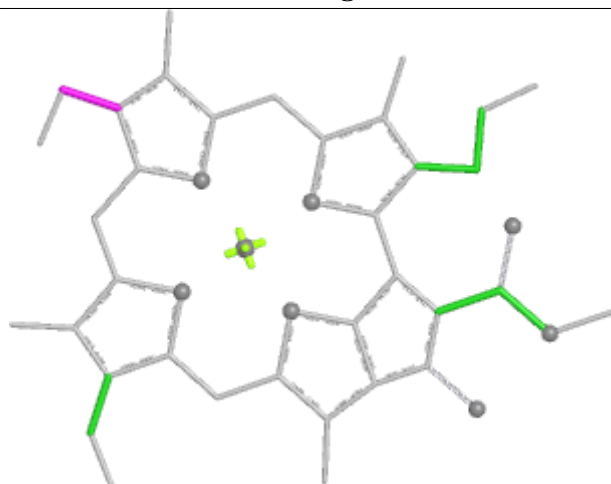
Ligand CLA s 405



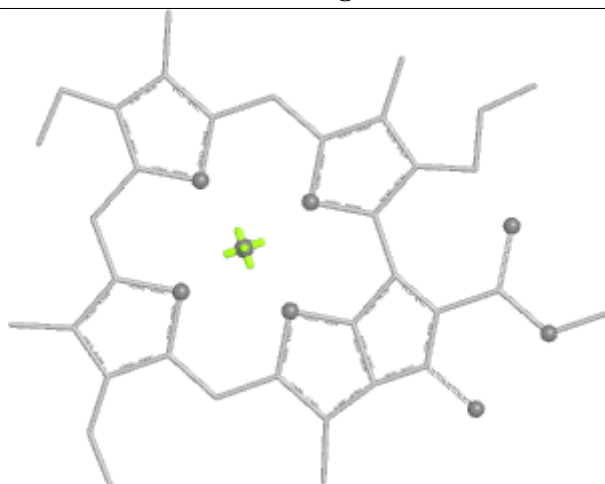
Bond lengths



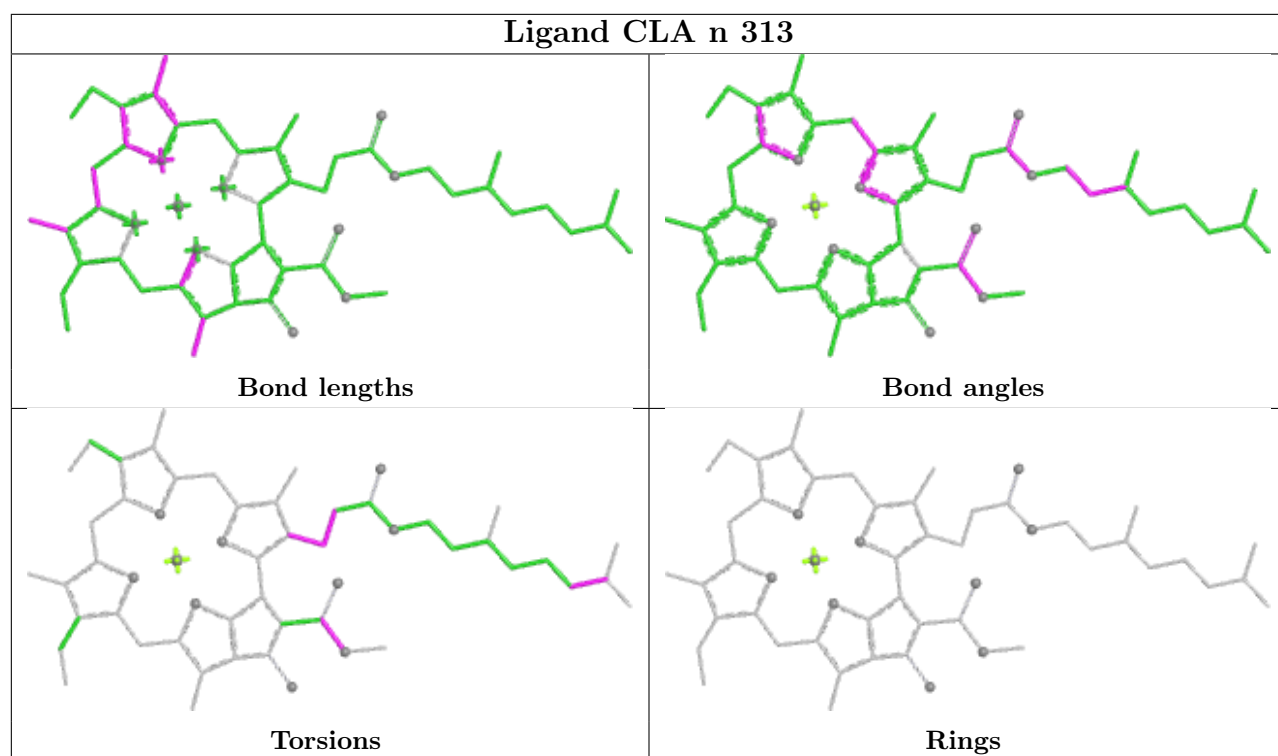
Bond angles



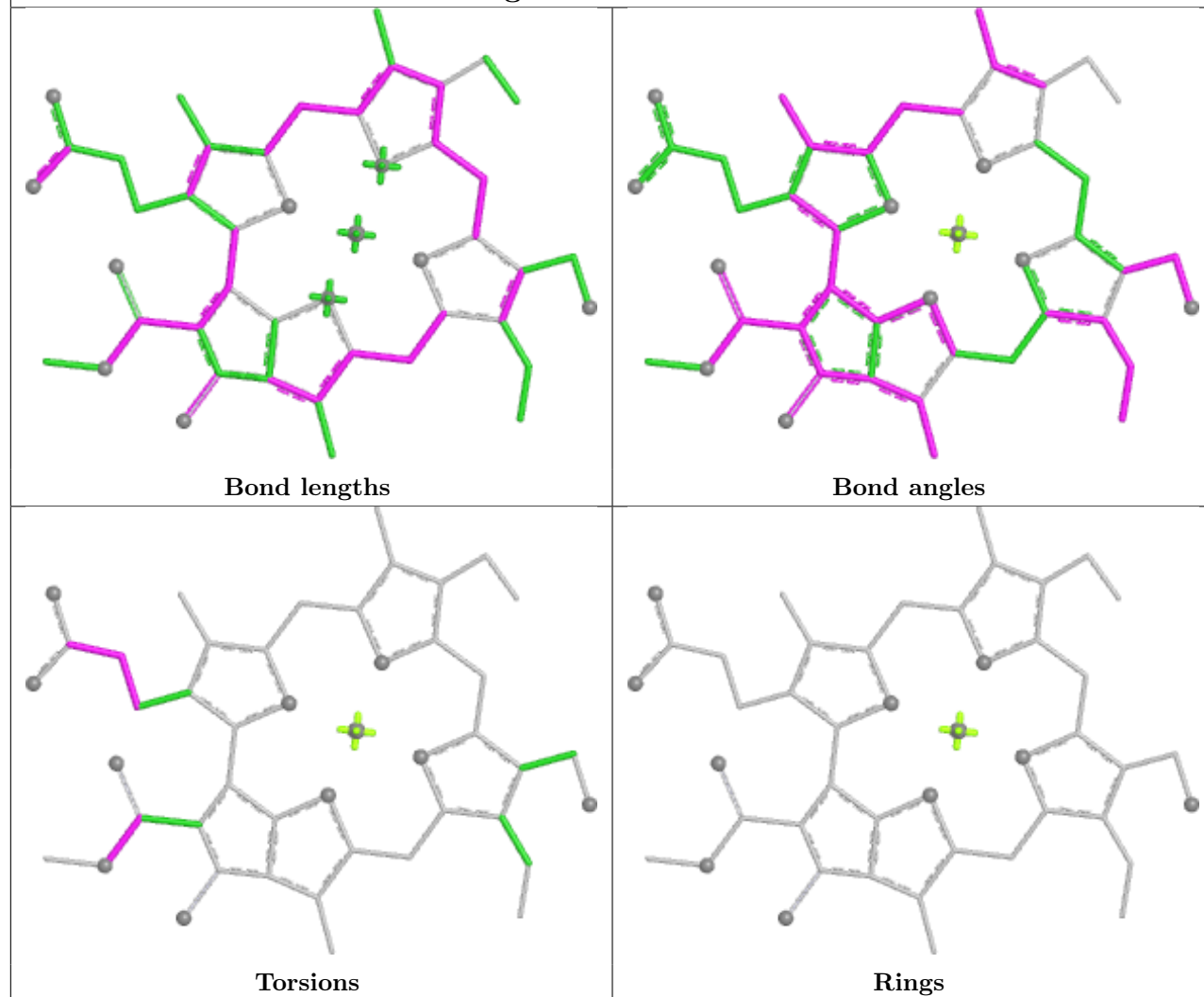
Torsions



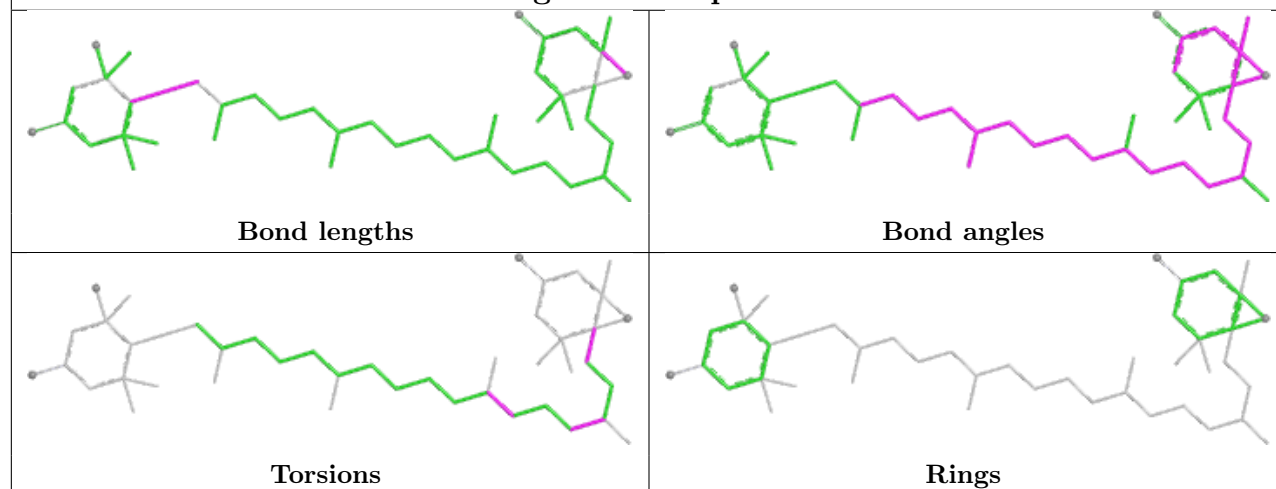
Rings



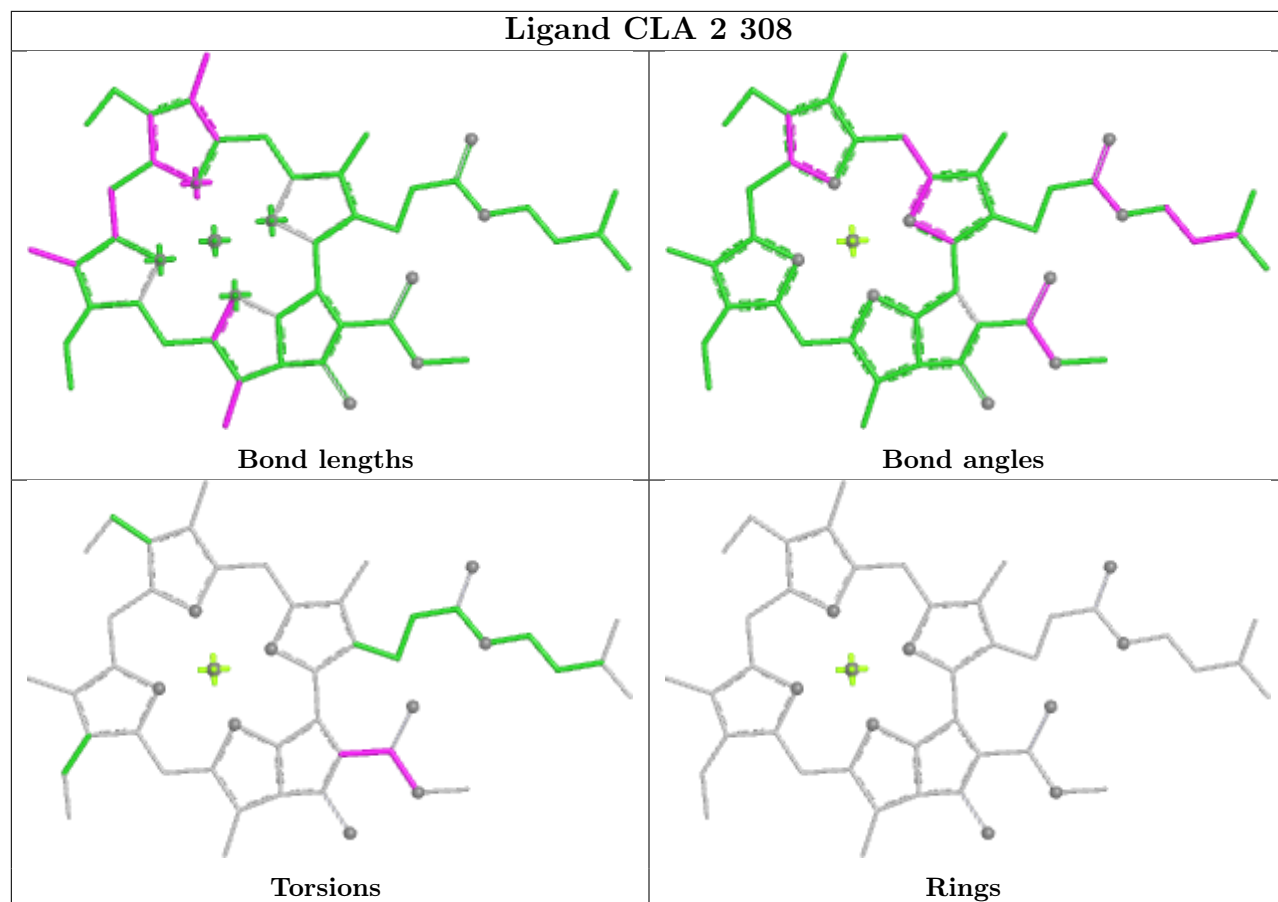
Ligand CHL S 605



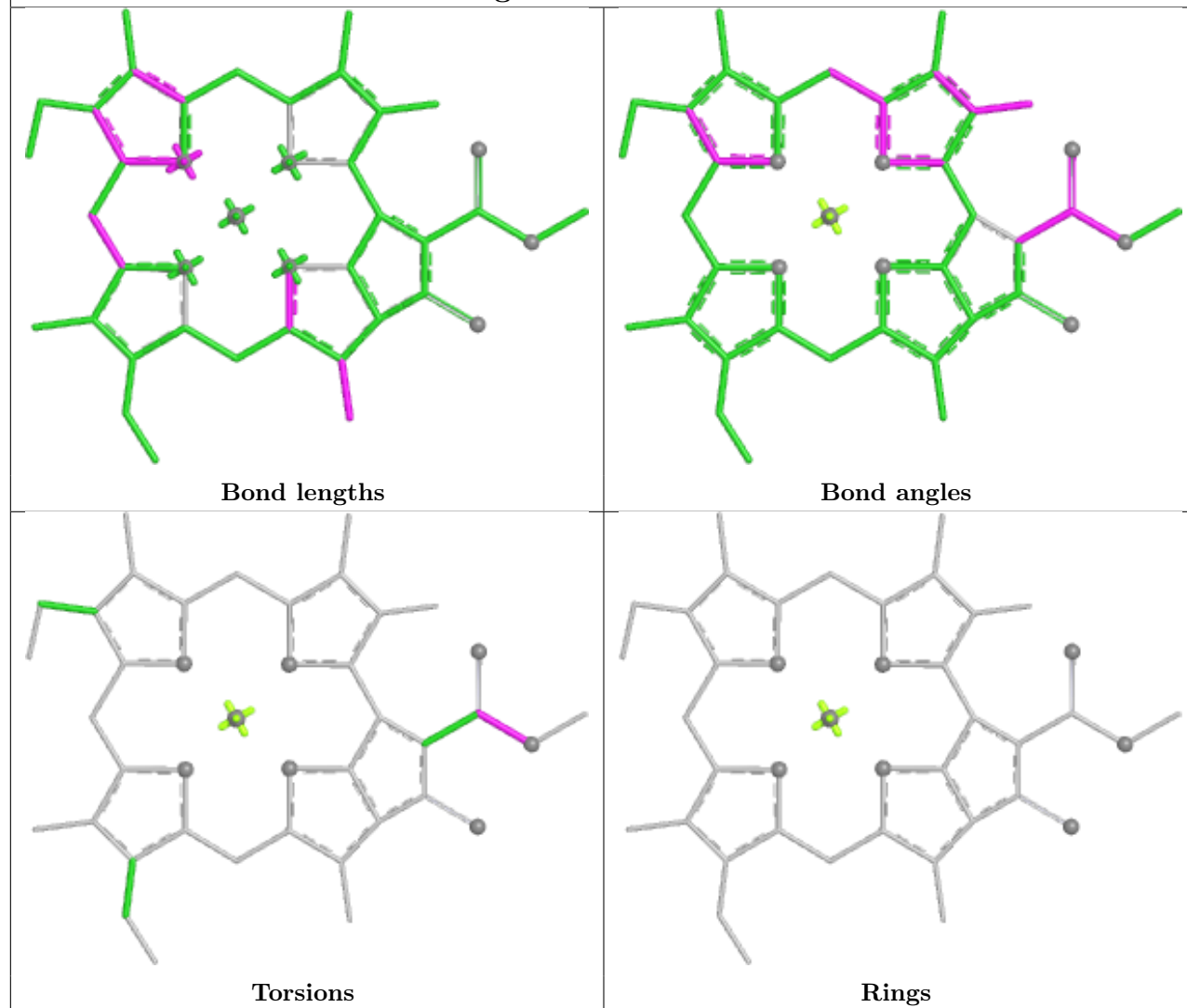
Ligand NEX p 304



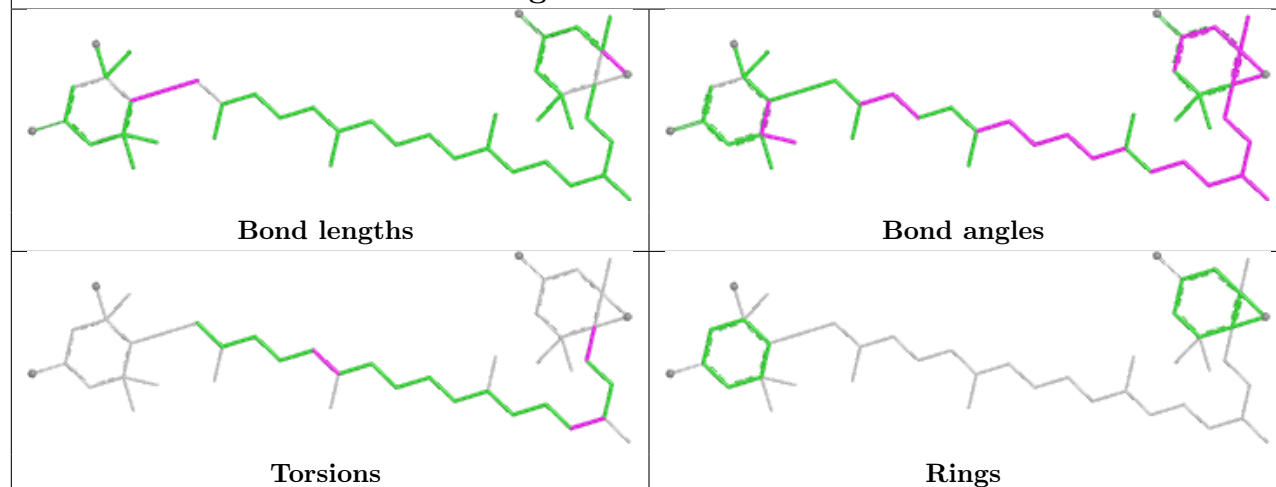
Ligand CLA 2 308



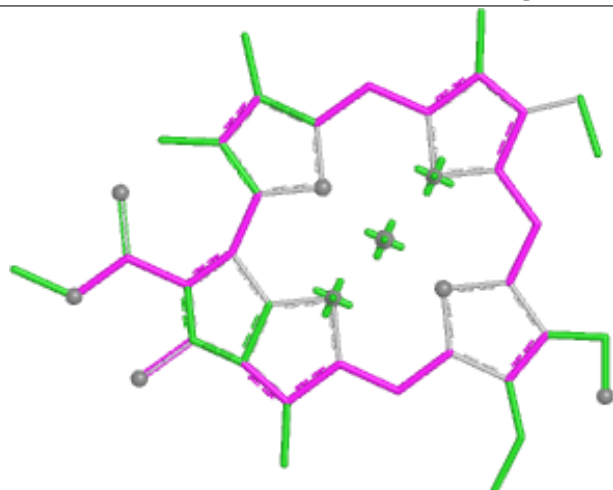
Ligand CLA A 610



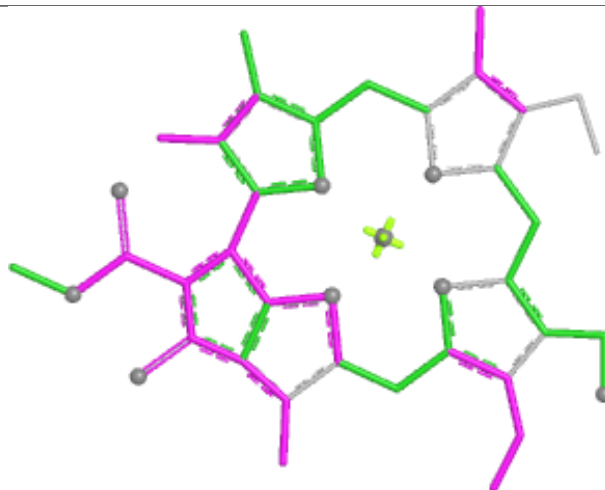
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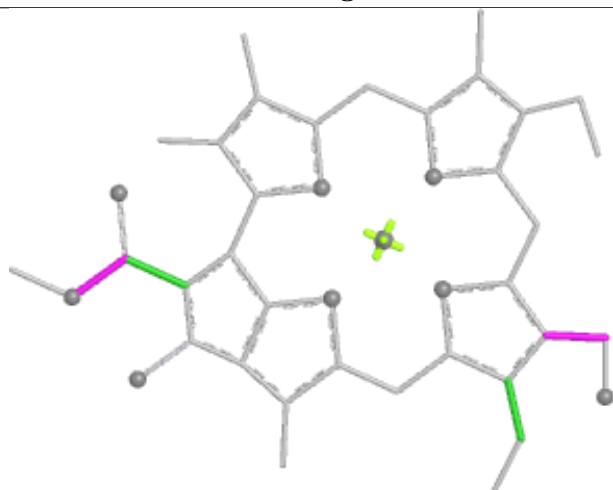
Ligand CHL 2 313



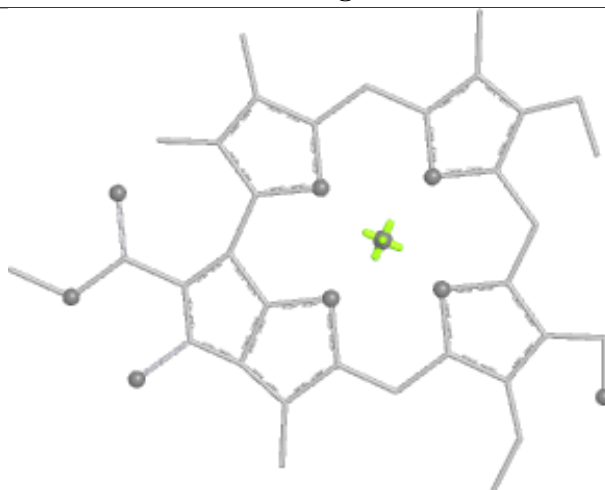
Bond lengths



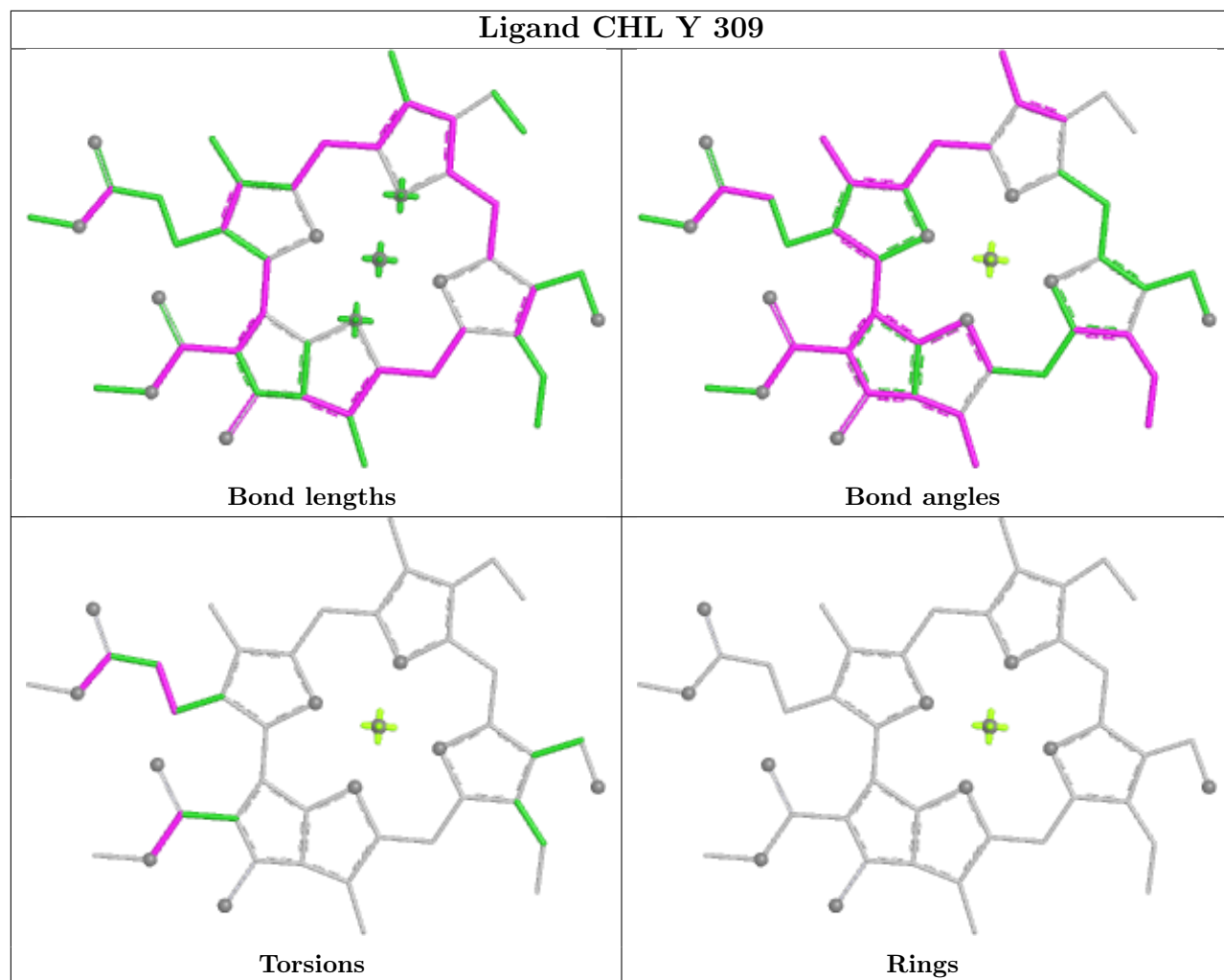
Bond angles



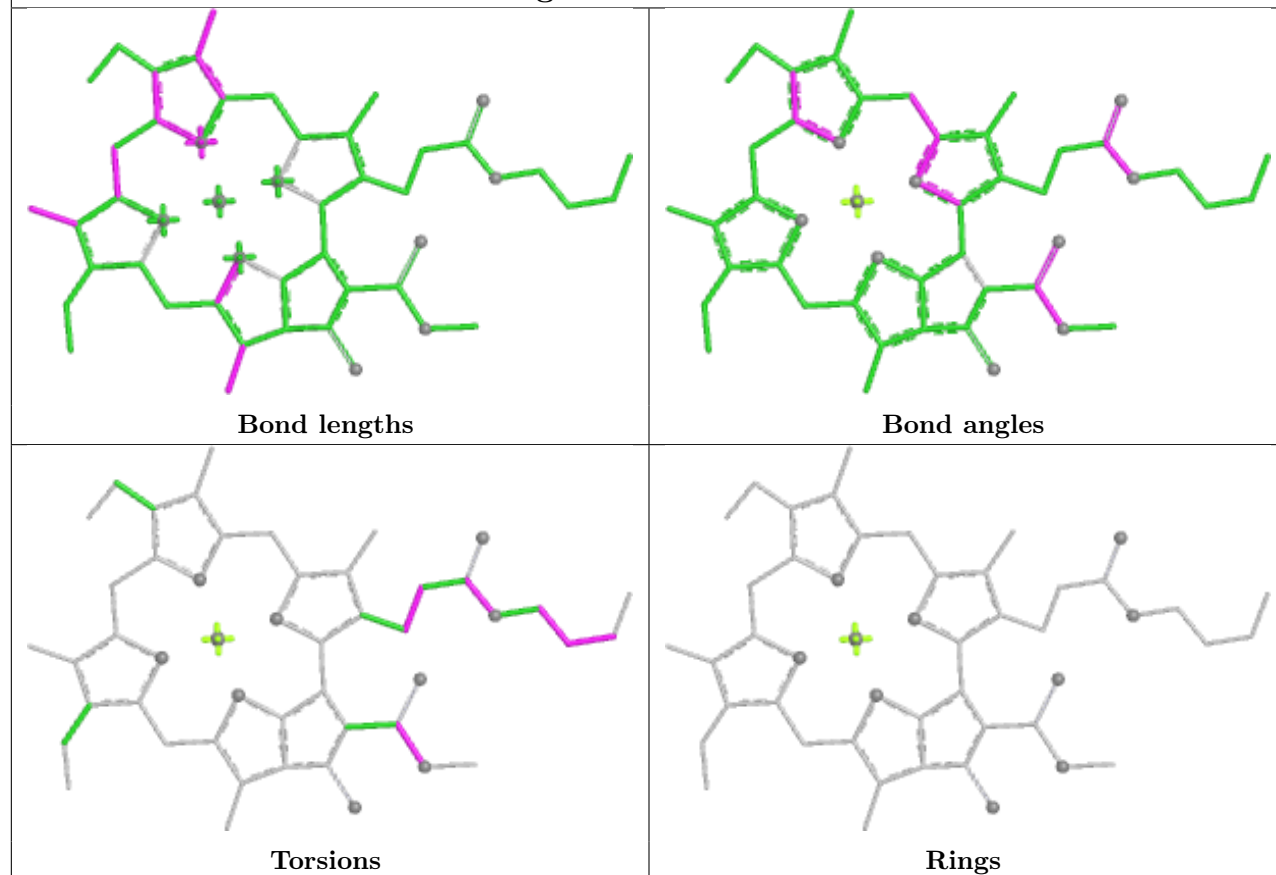
Torsions



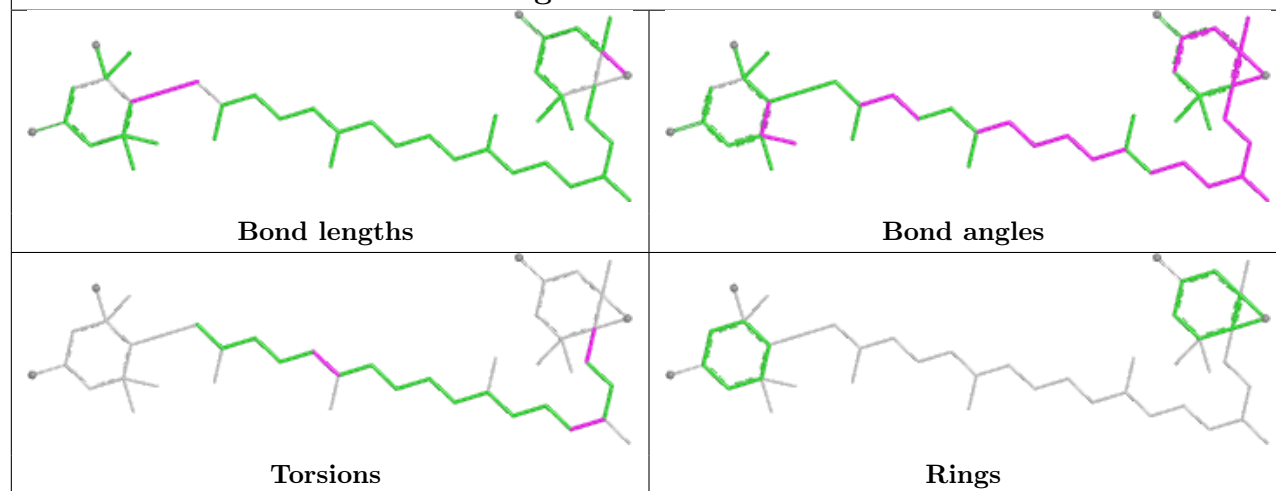
Rings



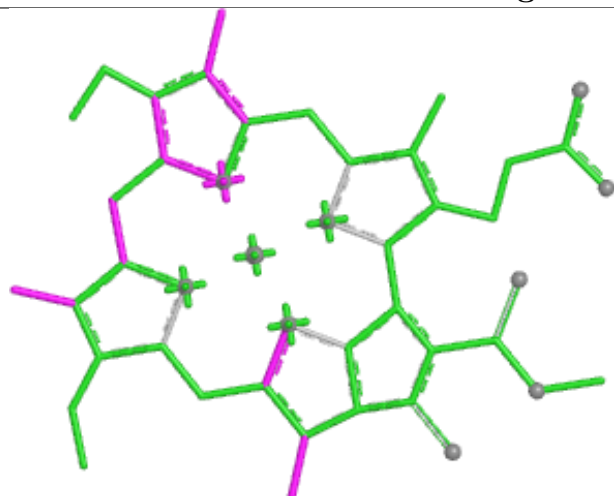
Ligand CLA 2 317



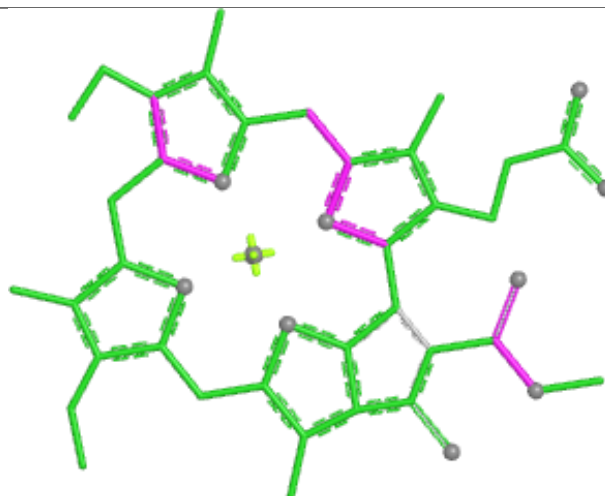
Ligand NEX 3 318



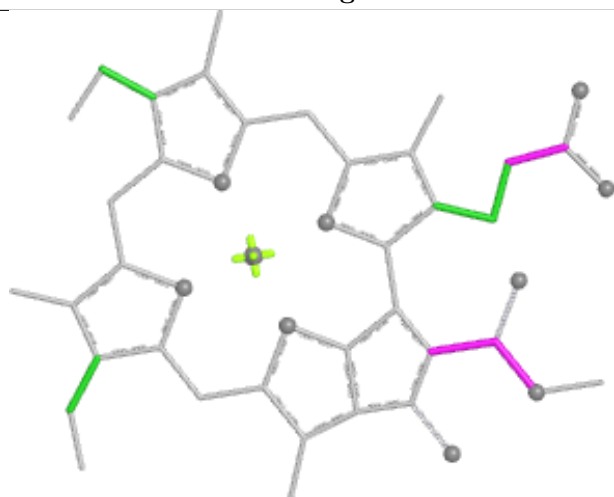
Ligand CLA S 603



Bond lengths



Bond angles

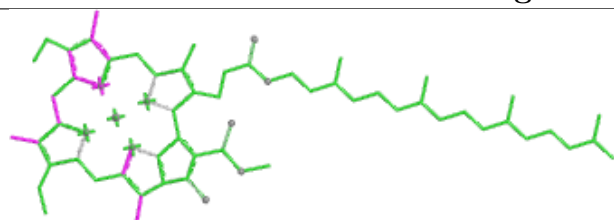


Torsions

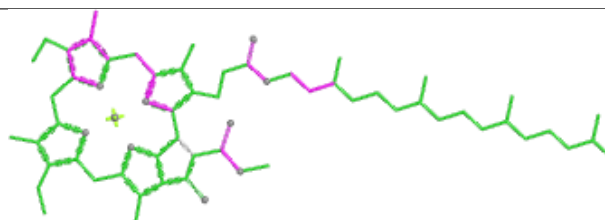


Rings

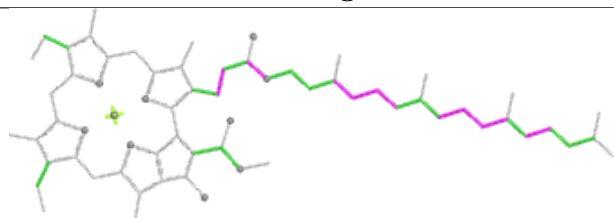
Ligand CLA B 612



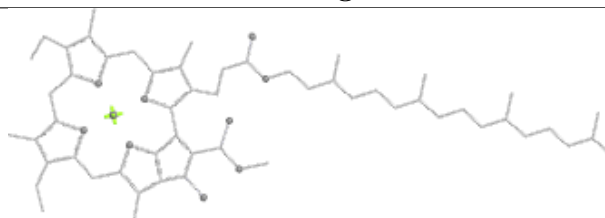
Bond lengths



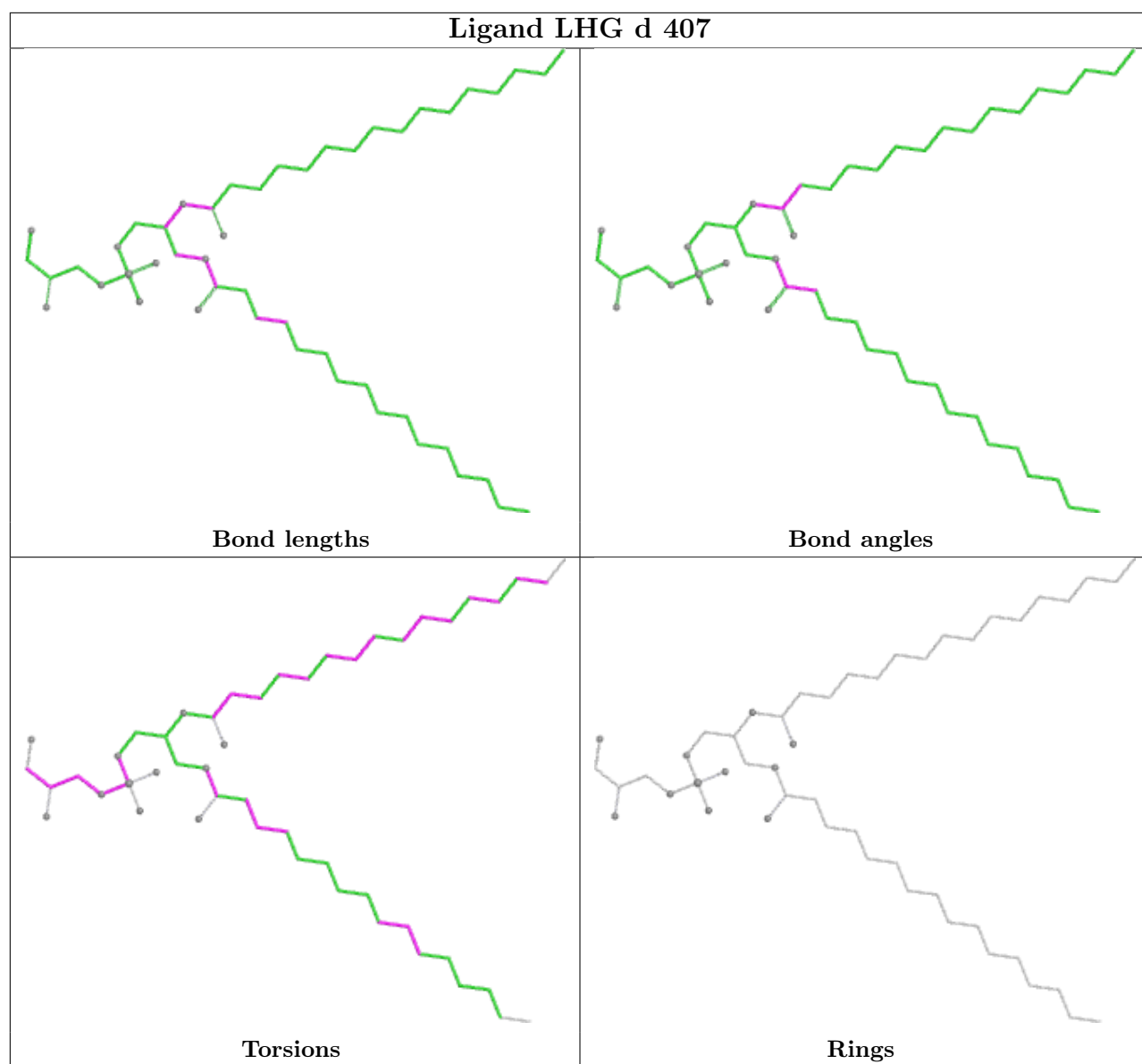
Bond angles



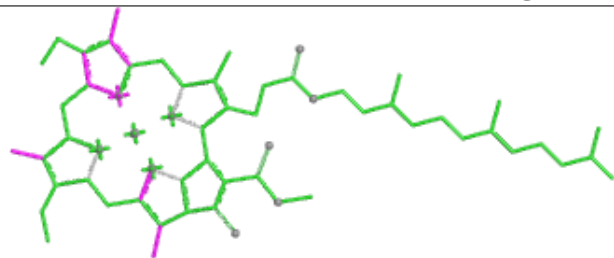
Torsions



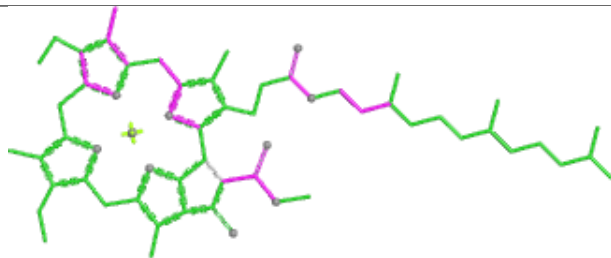
Rings



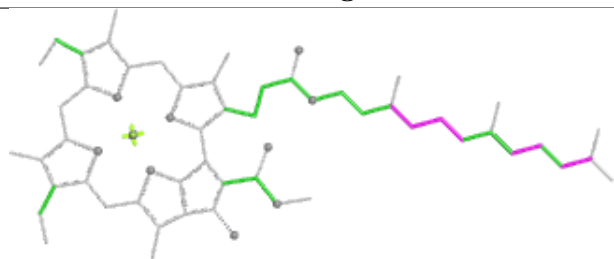
Ligand CLA a 607



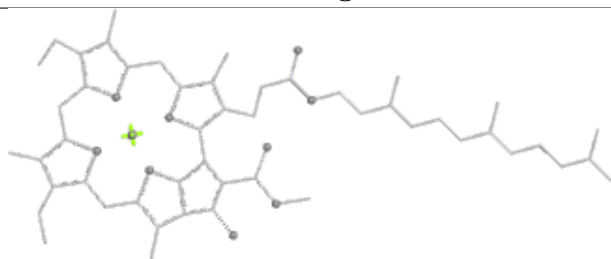
Bond lengths



Bond angles

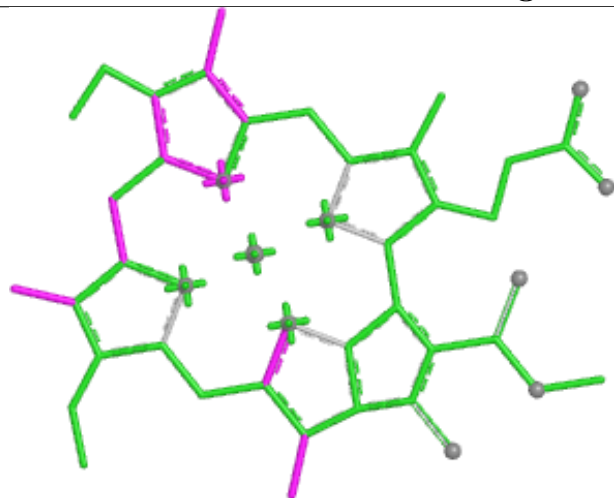


Torsions

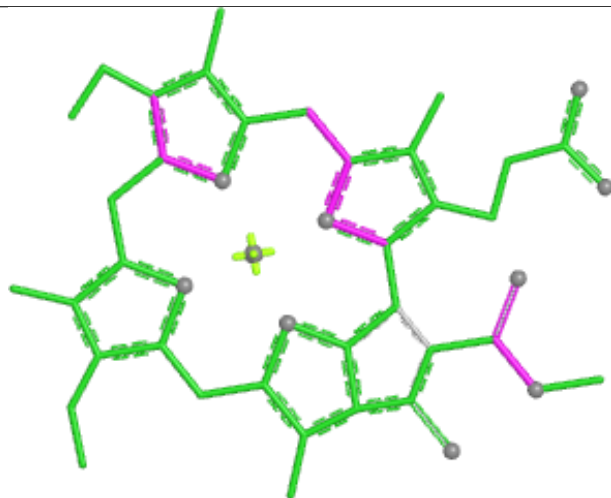


Rings

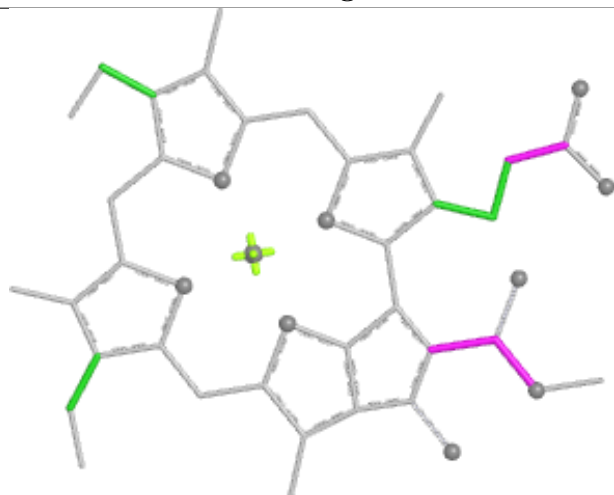
Ligand CLA S 611



Bond lengths



Bond angles

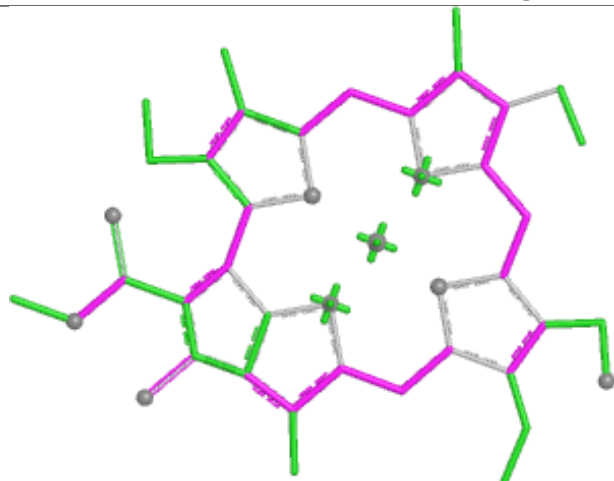


Torsions

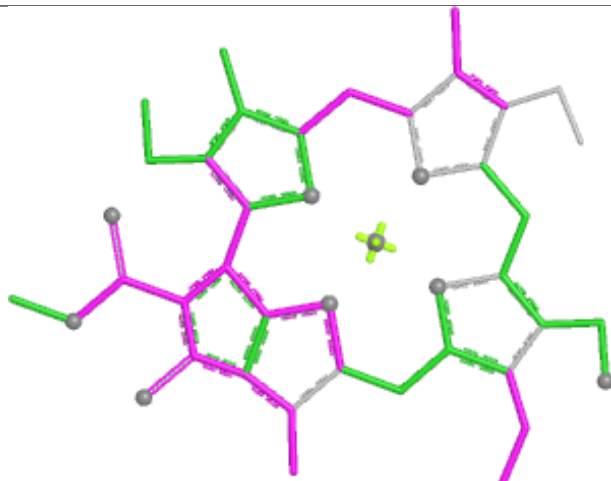


Rings

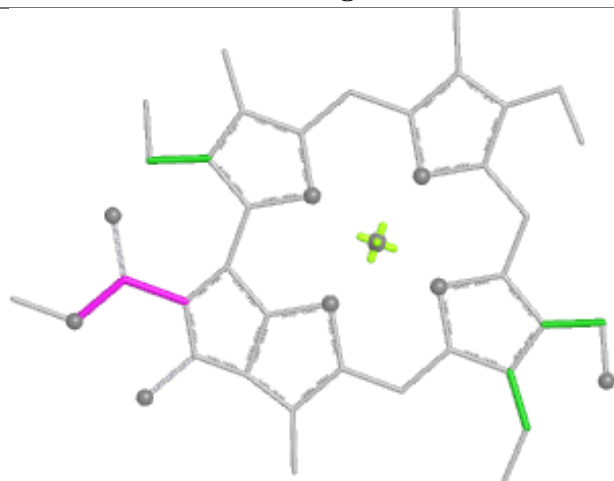
Ligand CHL 4 310



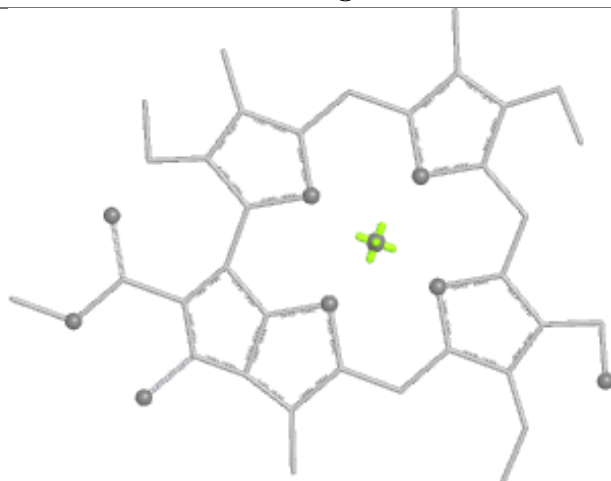
Bond lengths



Bond angles

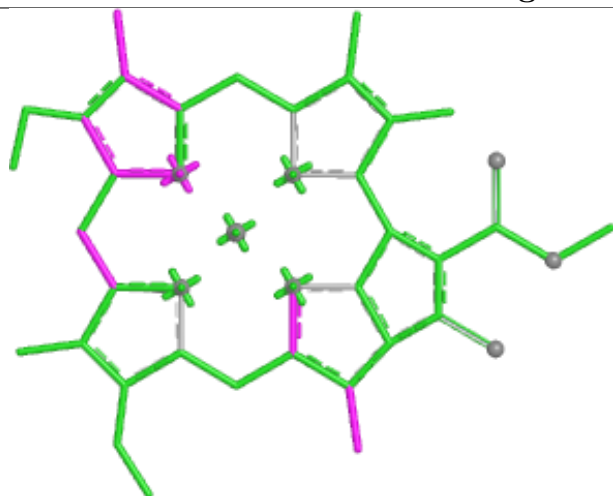


Torsions

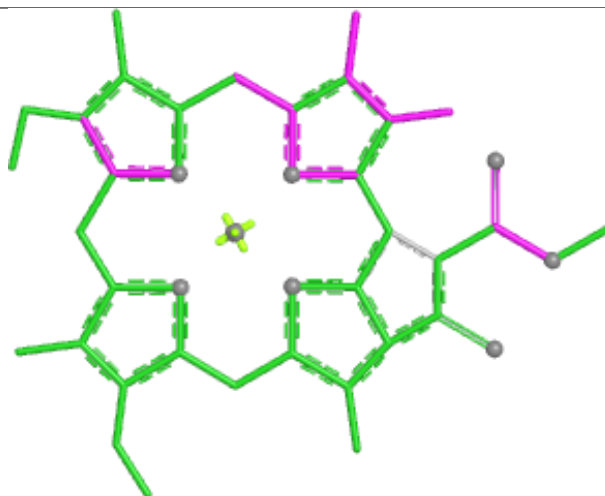


Rings

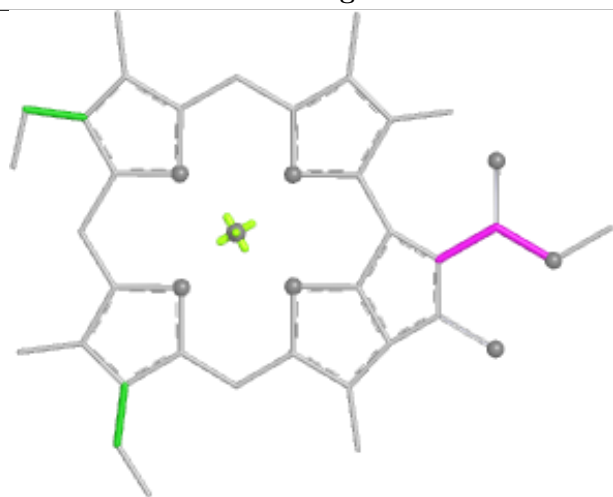
Ligand CLA 1 307



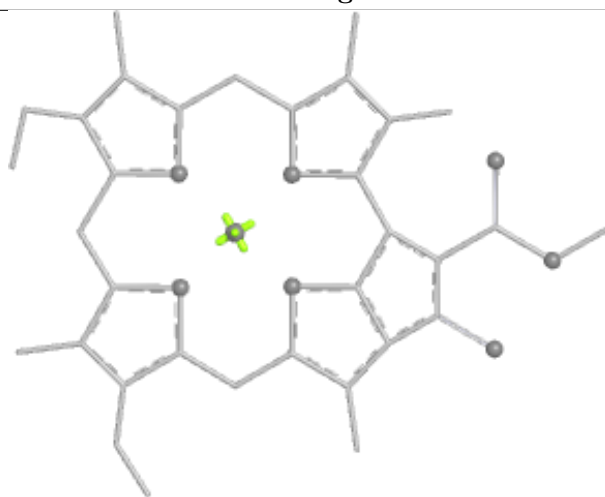
Bond lengths



Bond angles

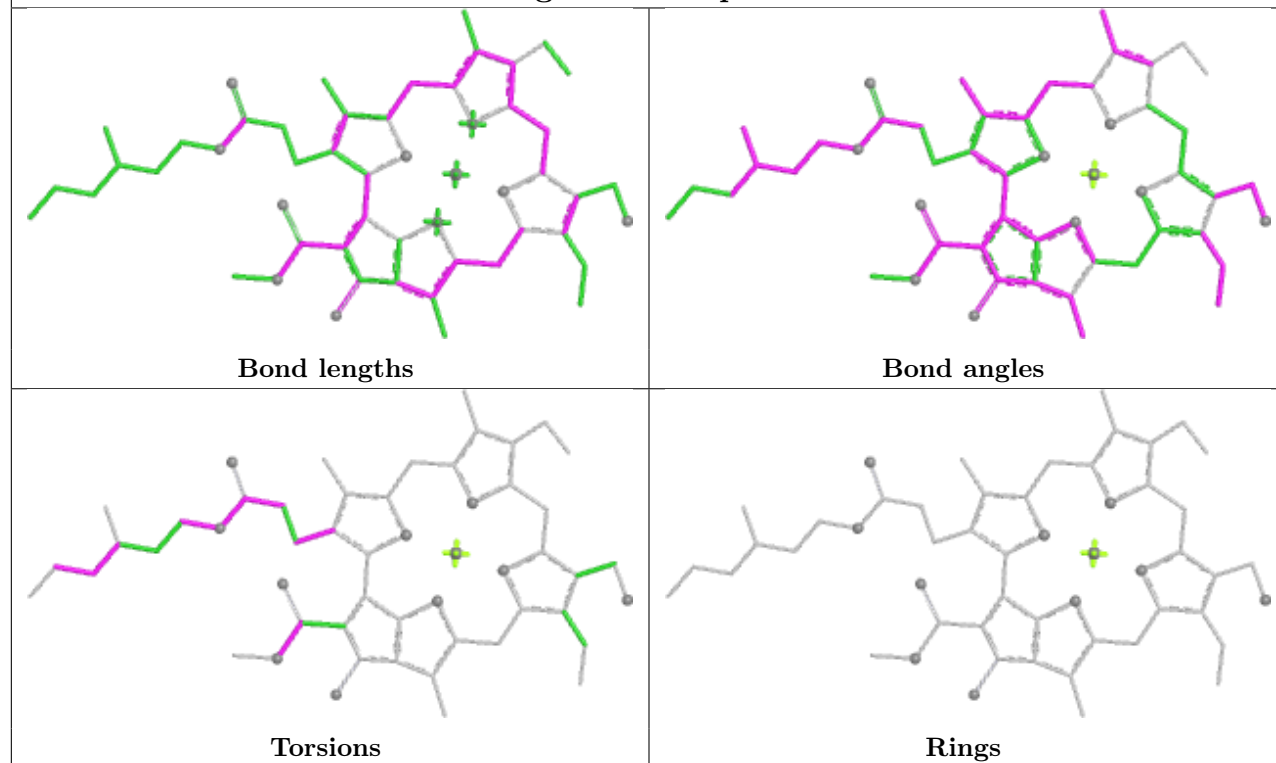


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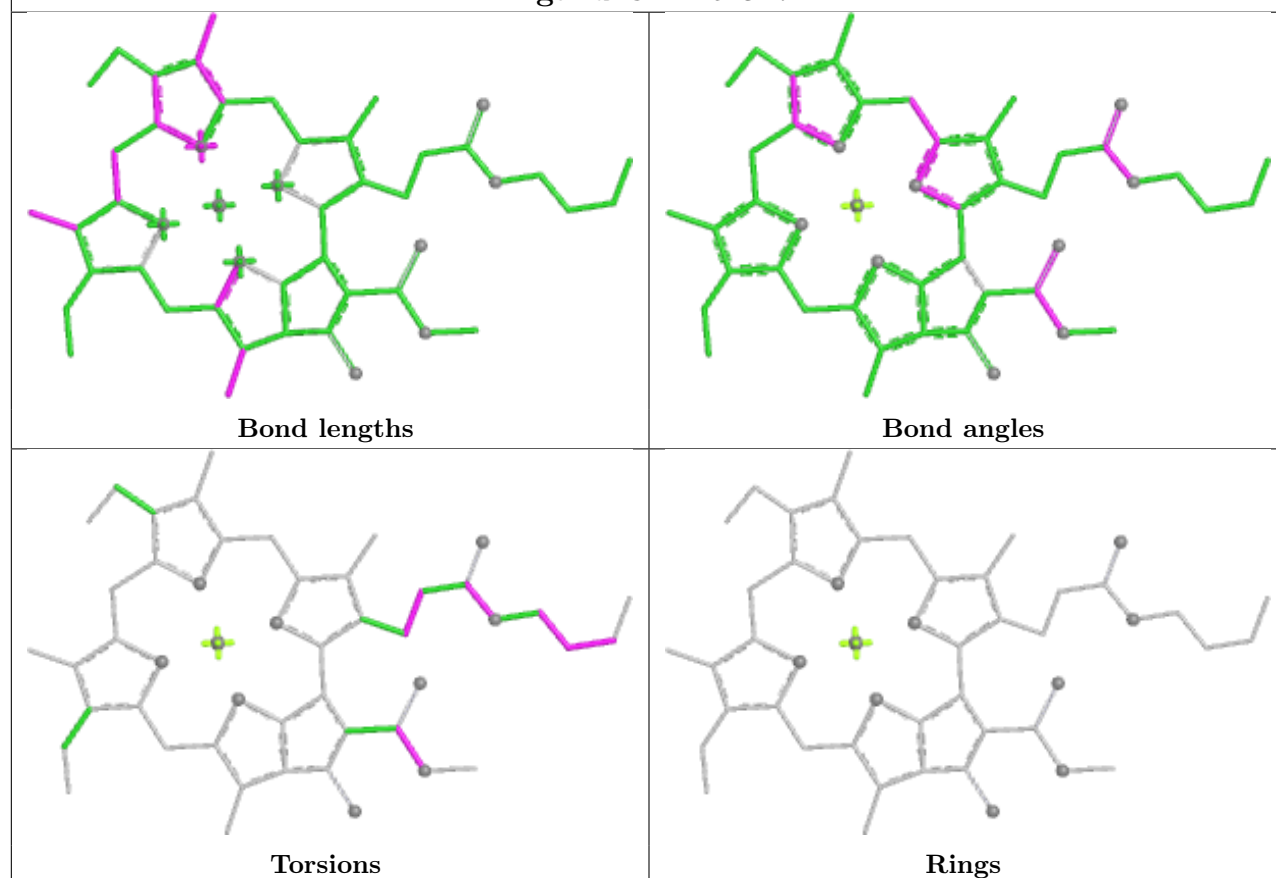


Rings

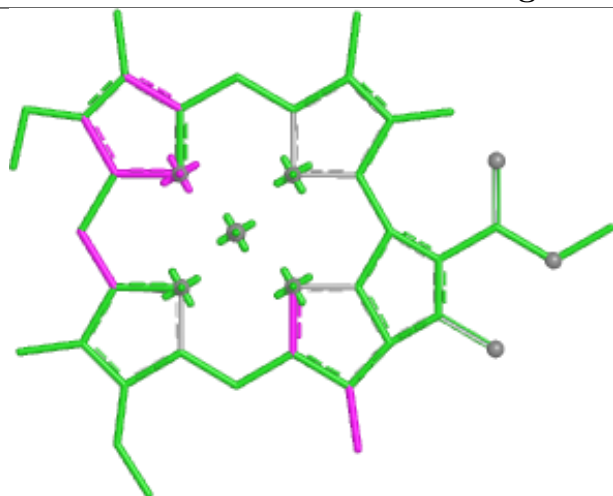
Ligand CHL q 309



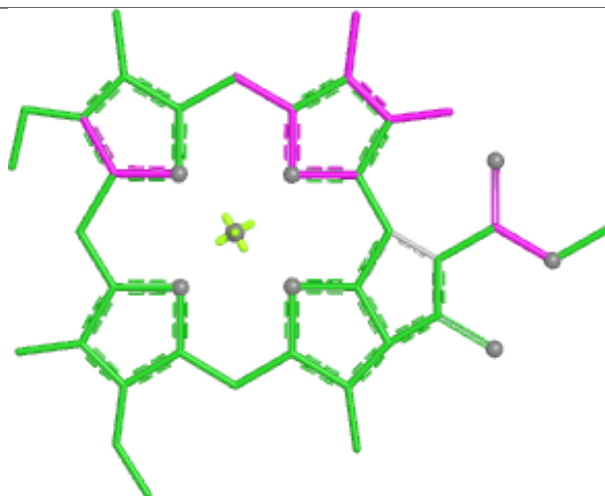
Ligand CLA 5 317



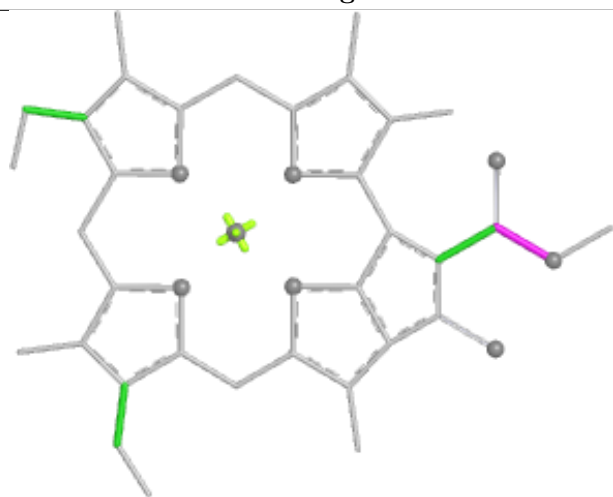
Ligand CLA 6 313



Bond lengths



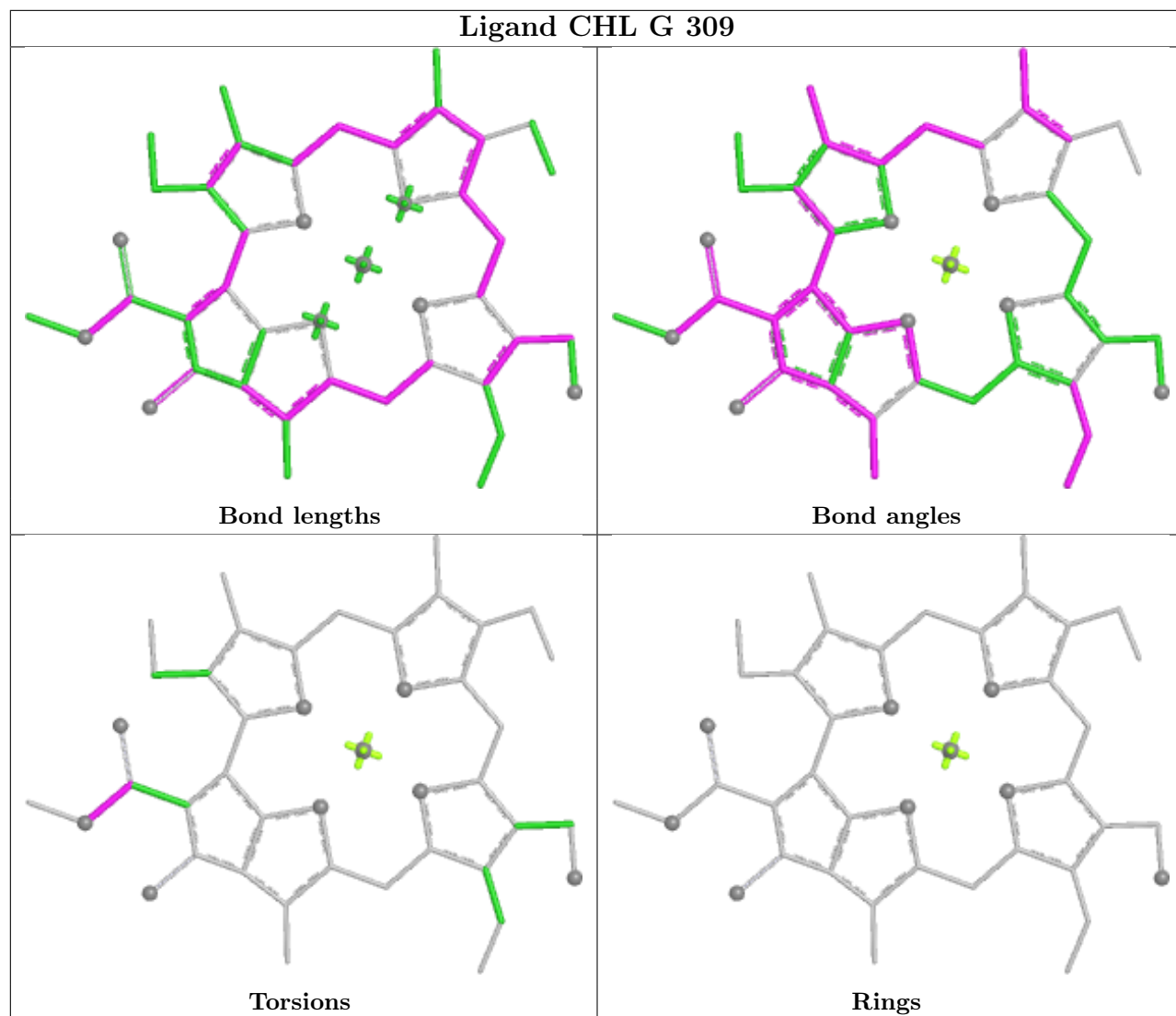
Bond angles



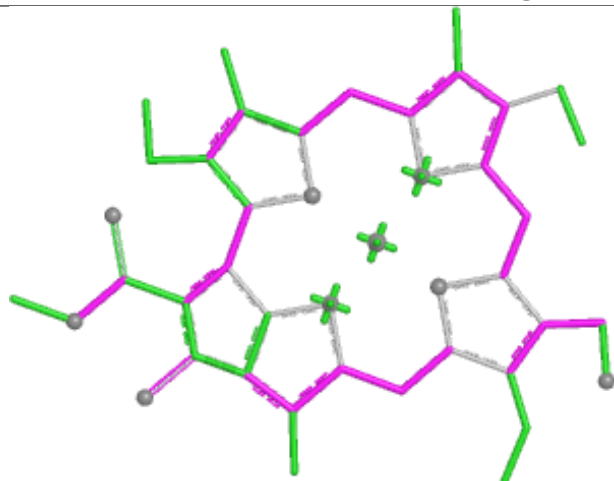
Torsions



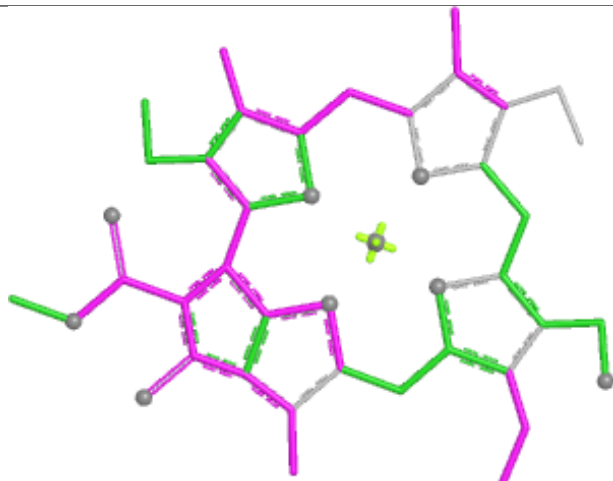
Rings



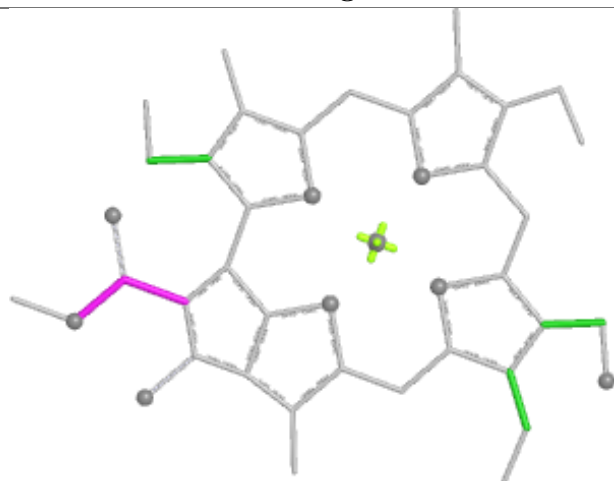
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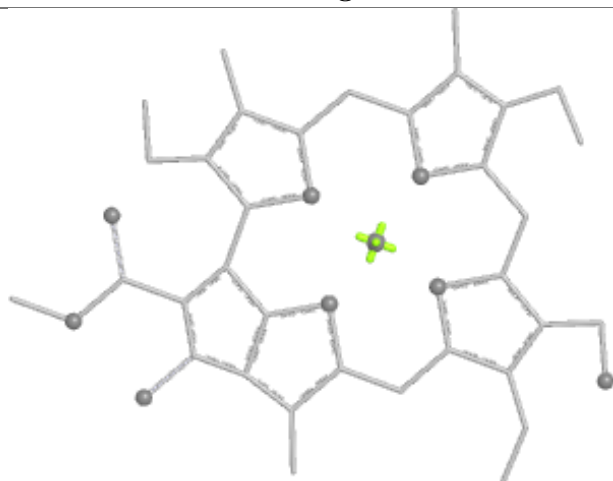
Bond lengths



Bond angles

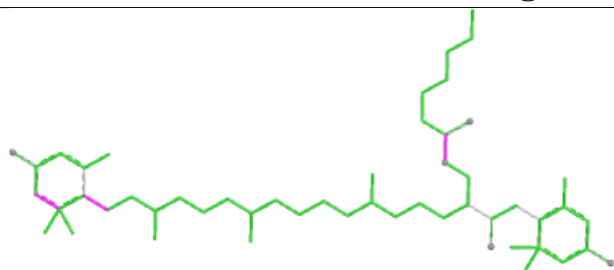


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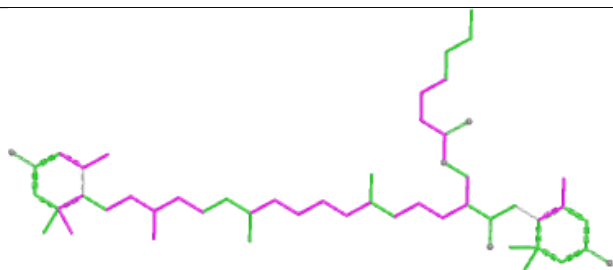


Rings

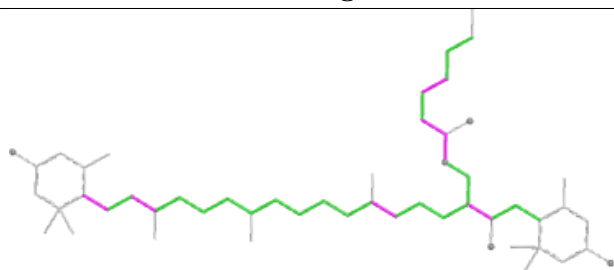
Ligand OUR 2 301



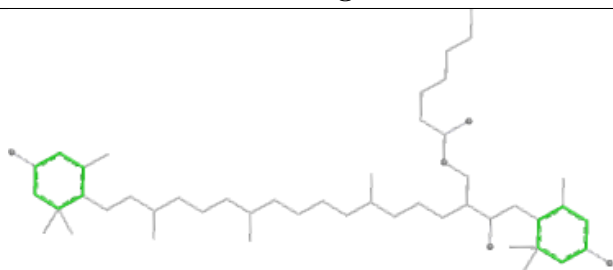
Bond lengths



Bond angles

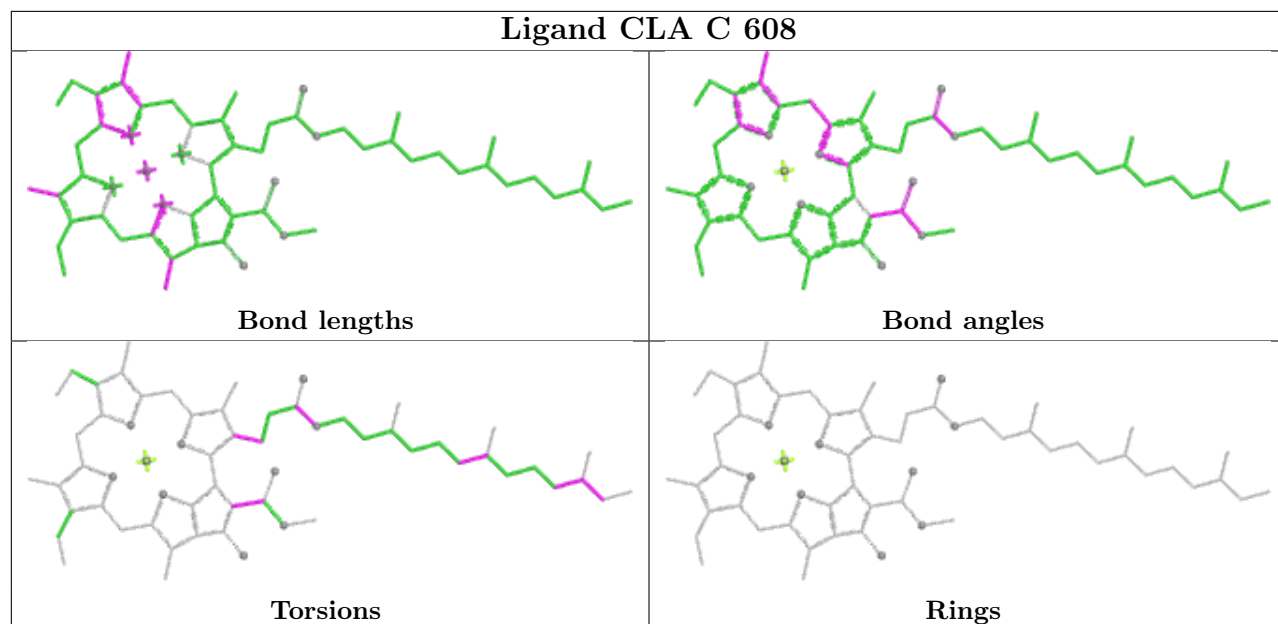


Torsions

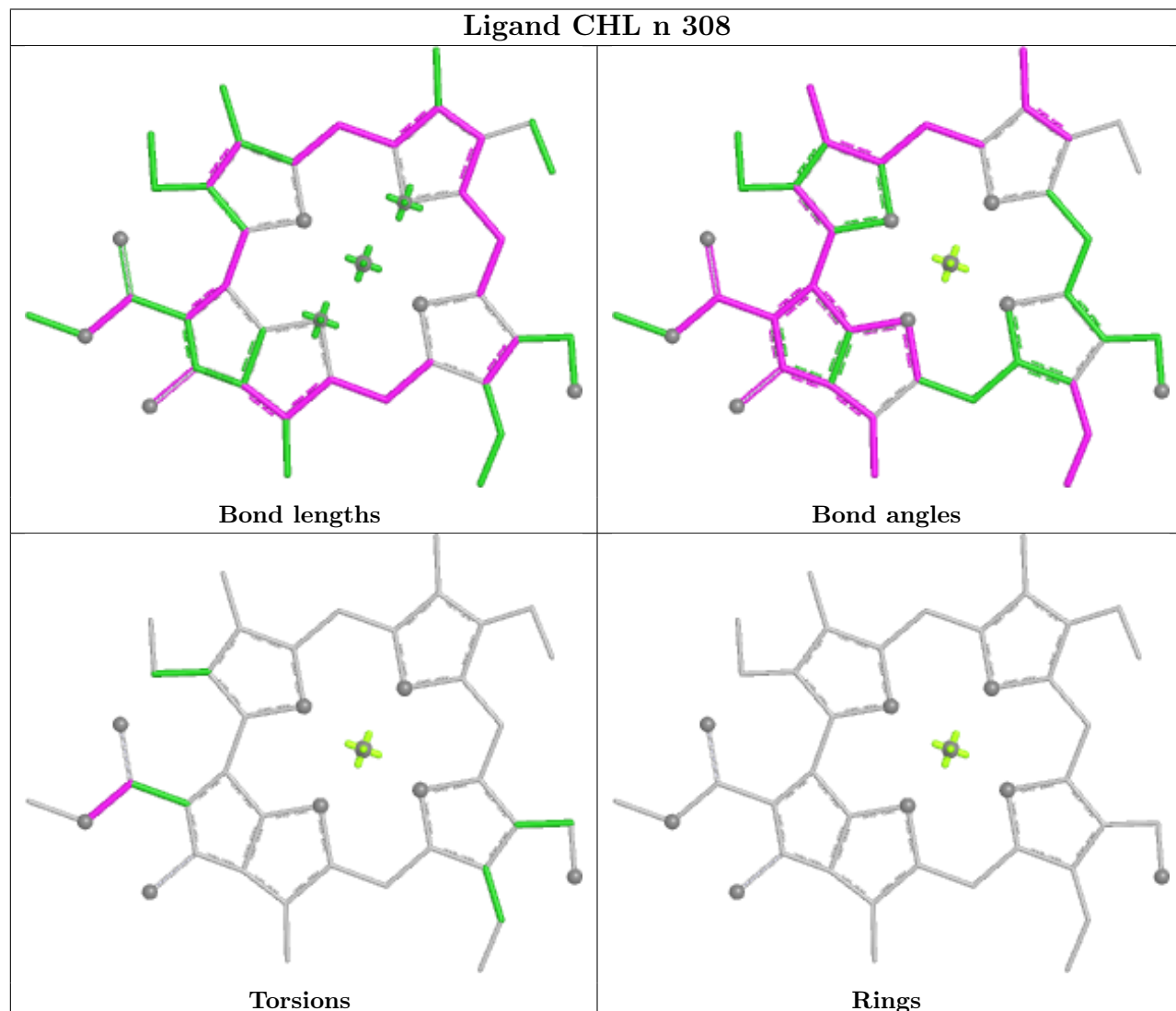


Rings

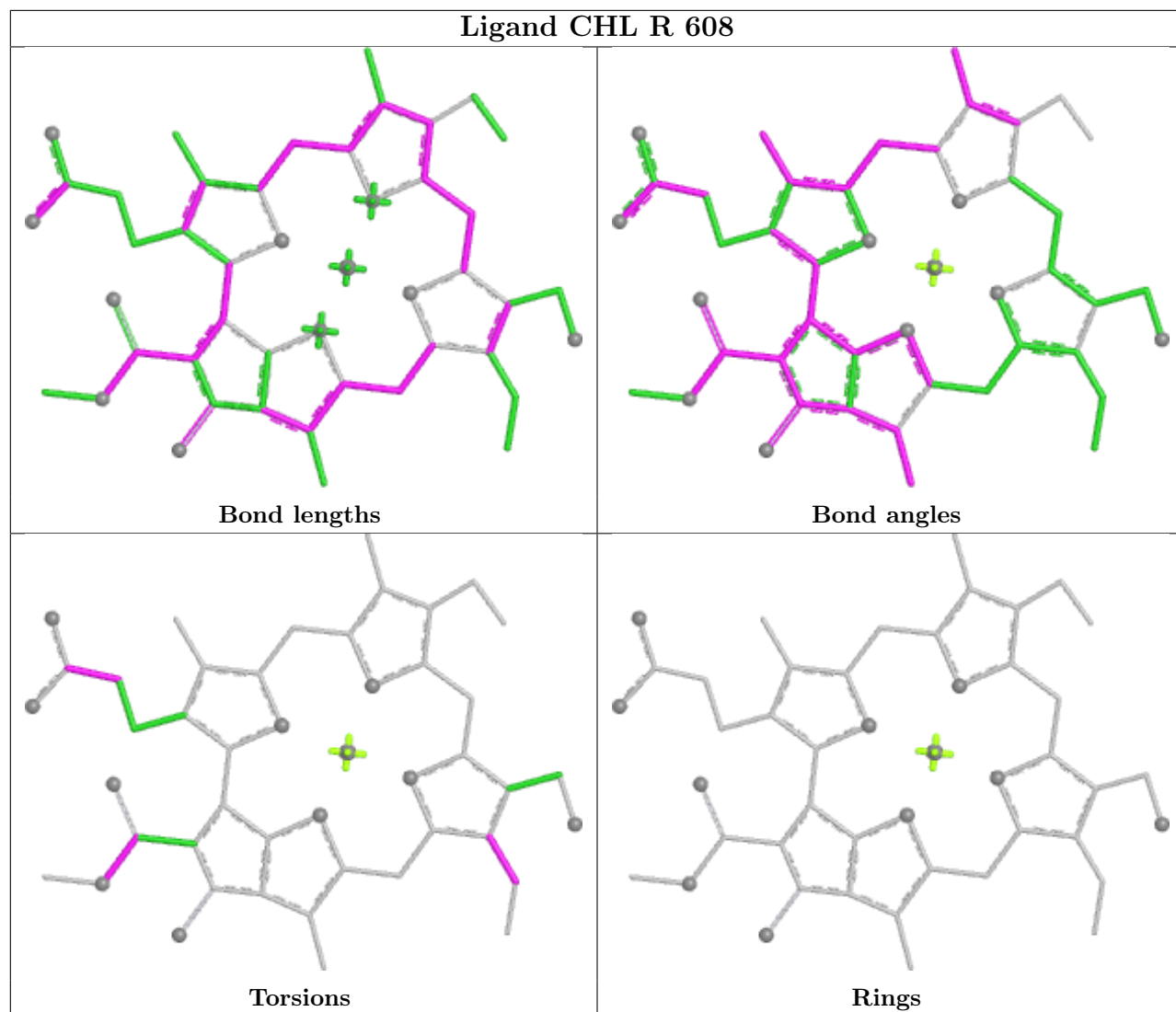
Ligand CLA C 608

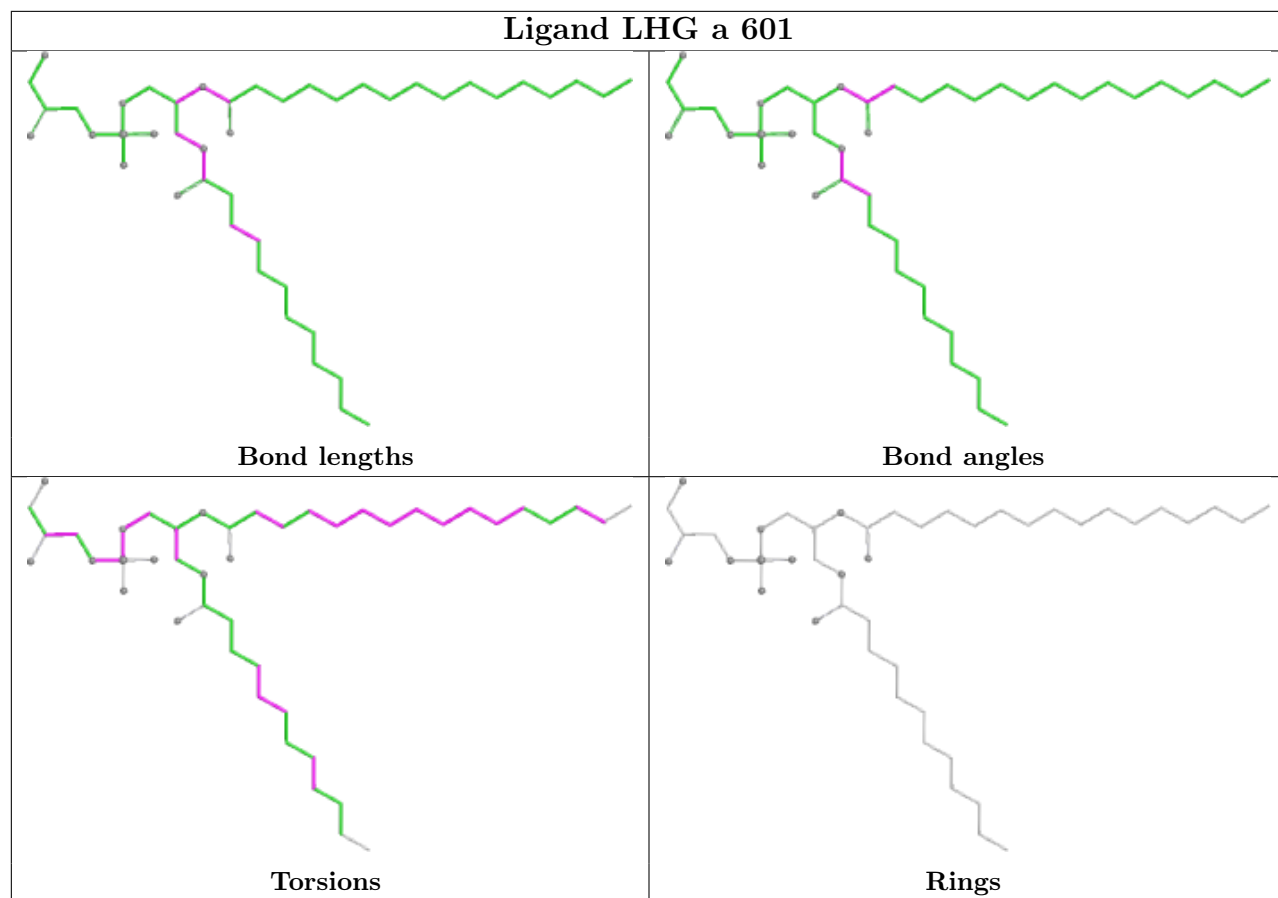


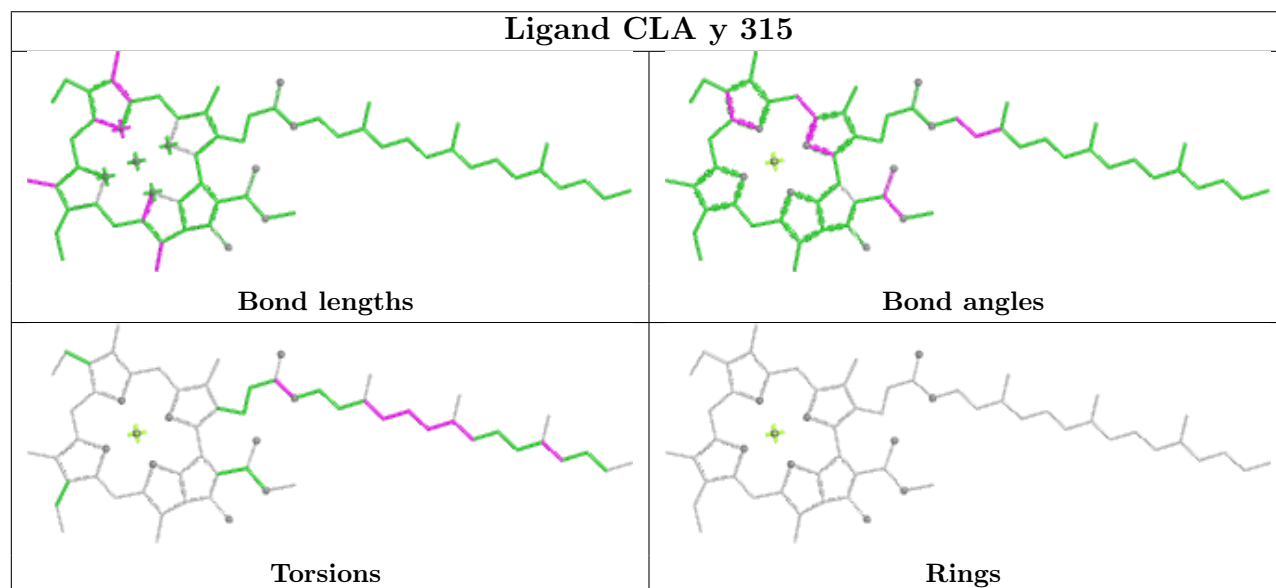
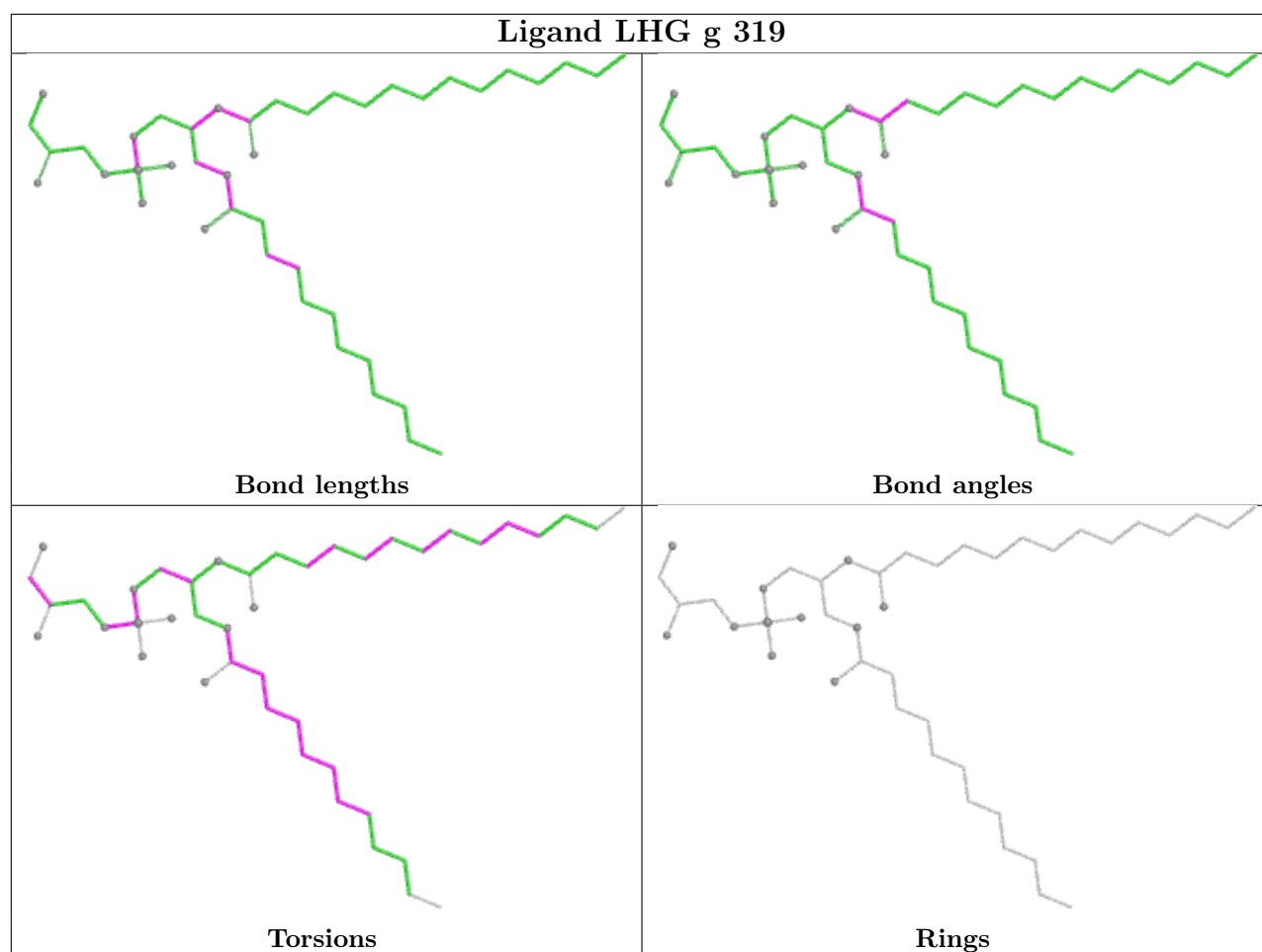
Ligand CHL n 308

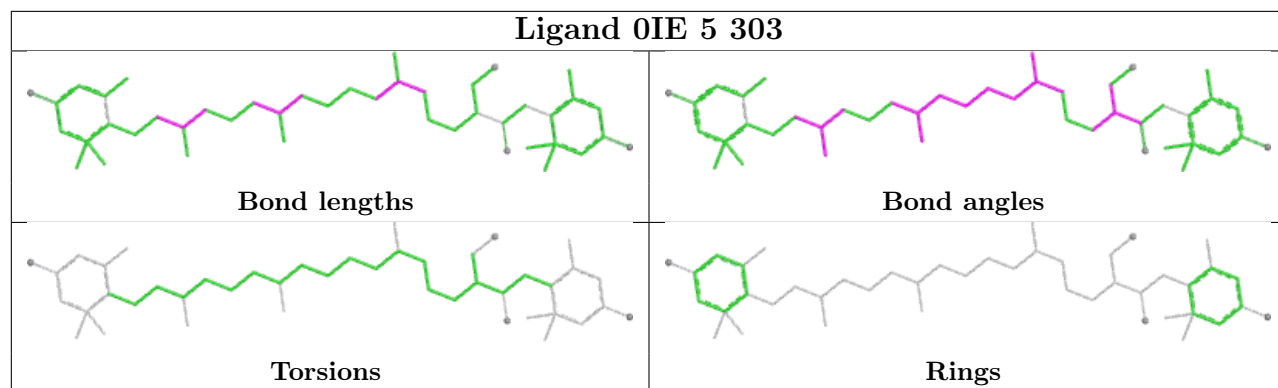
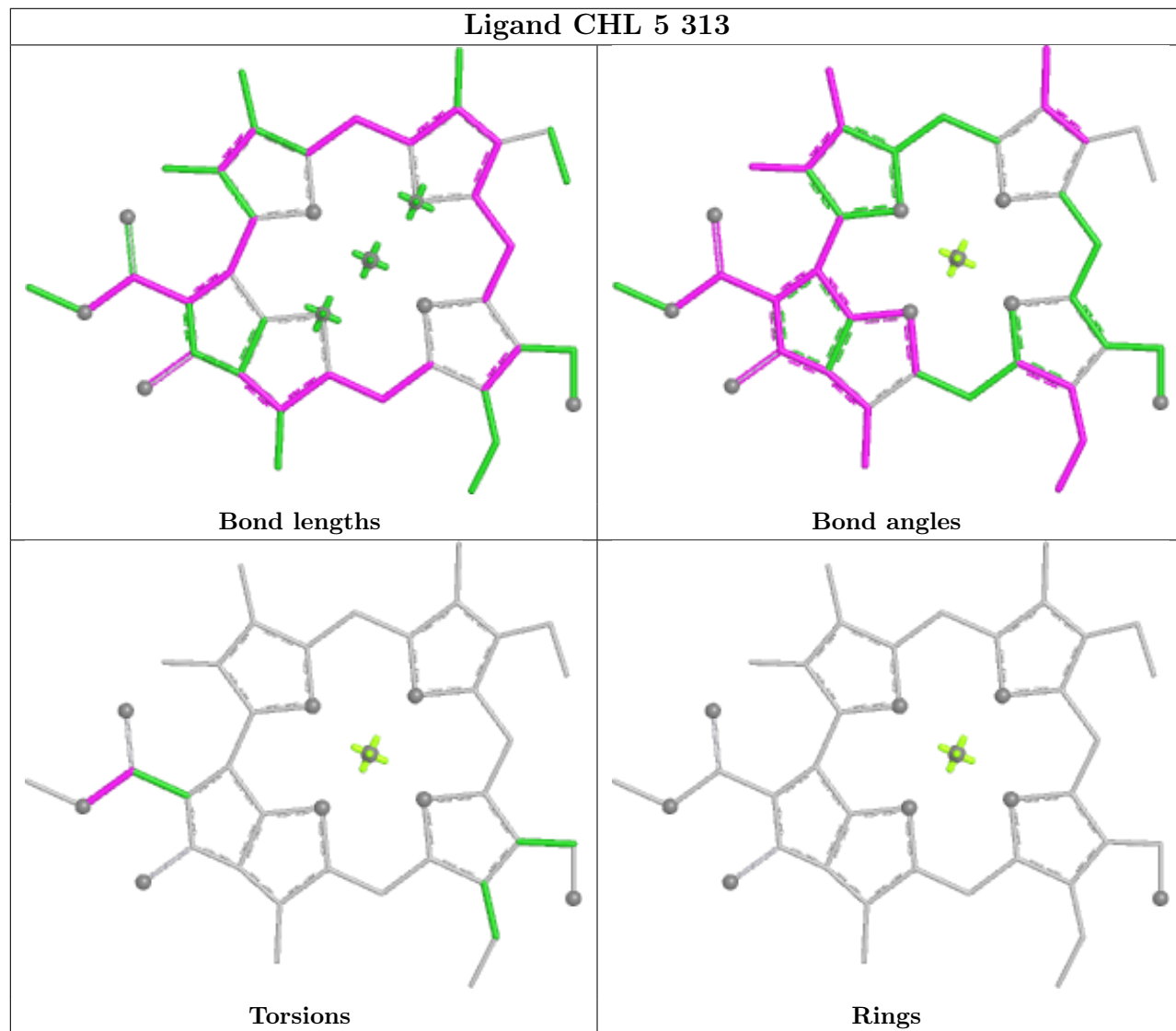


Ligand CHL R 608

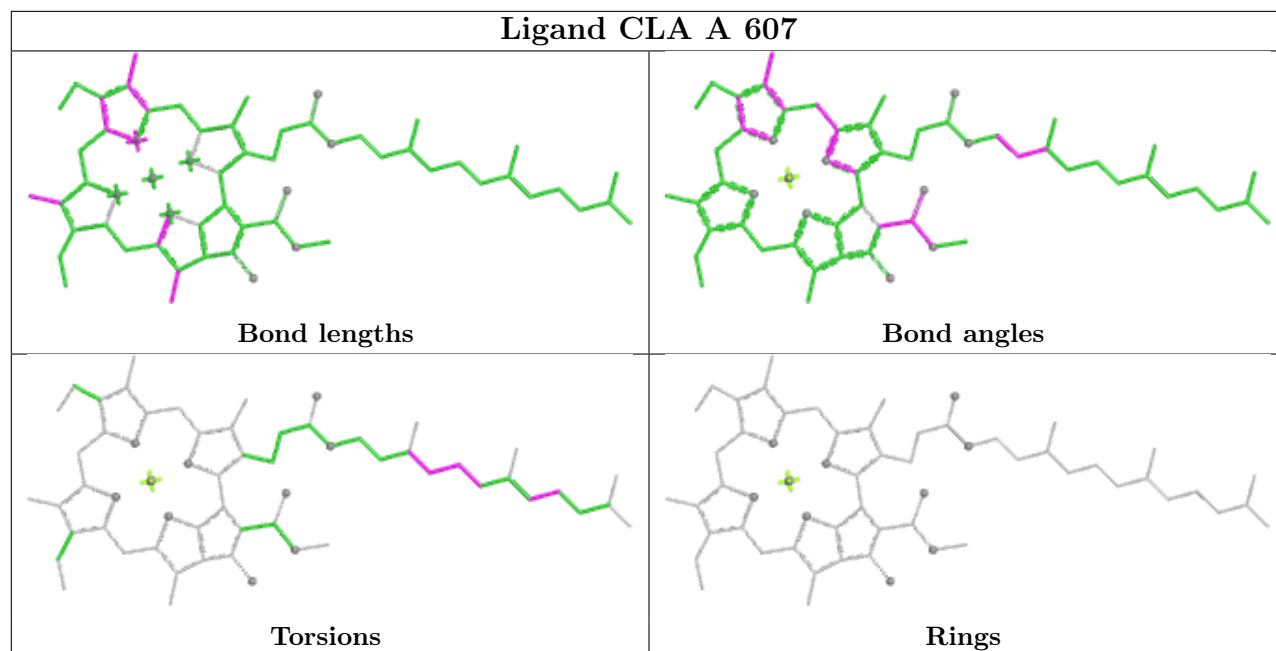




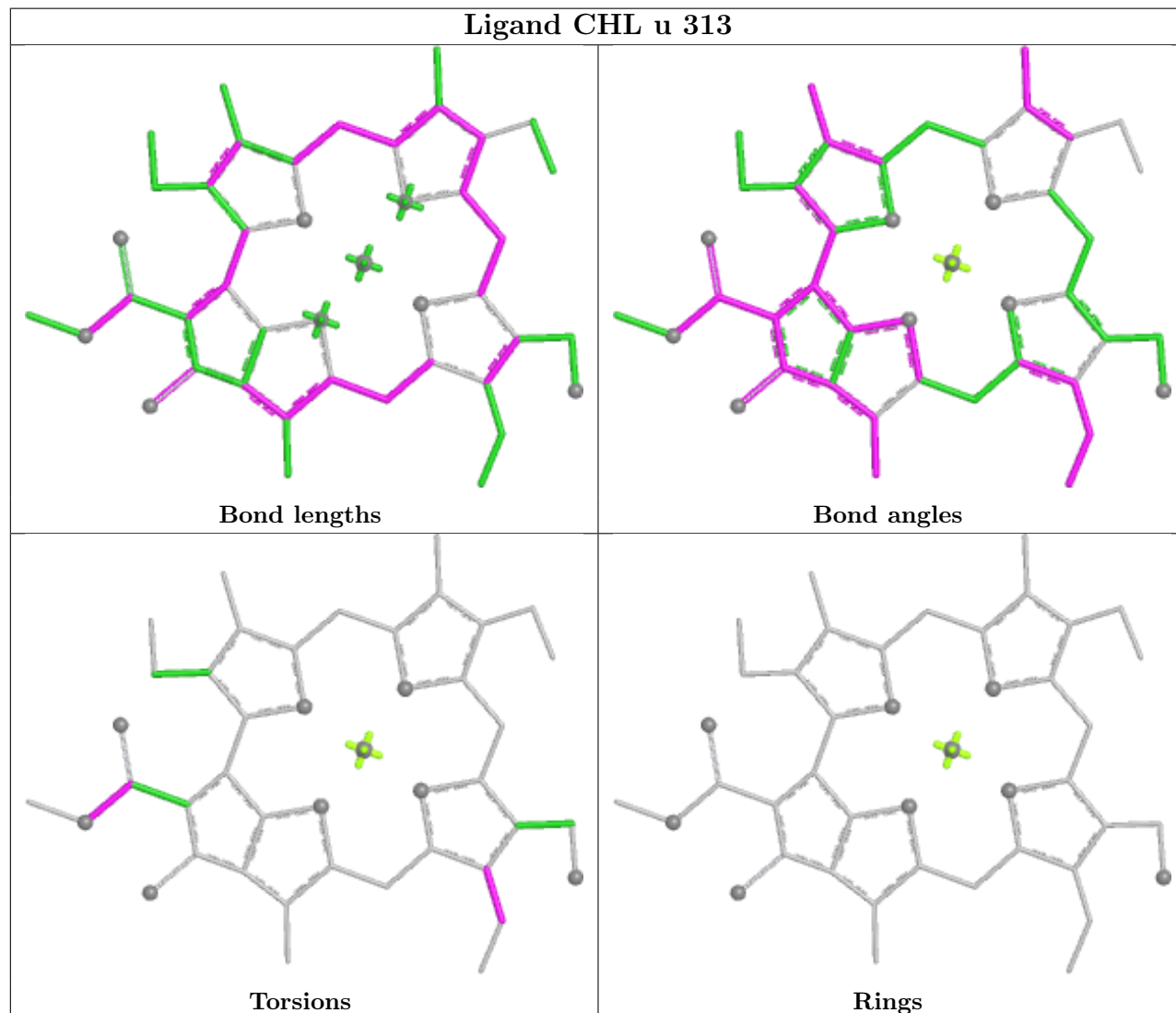


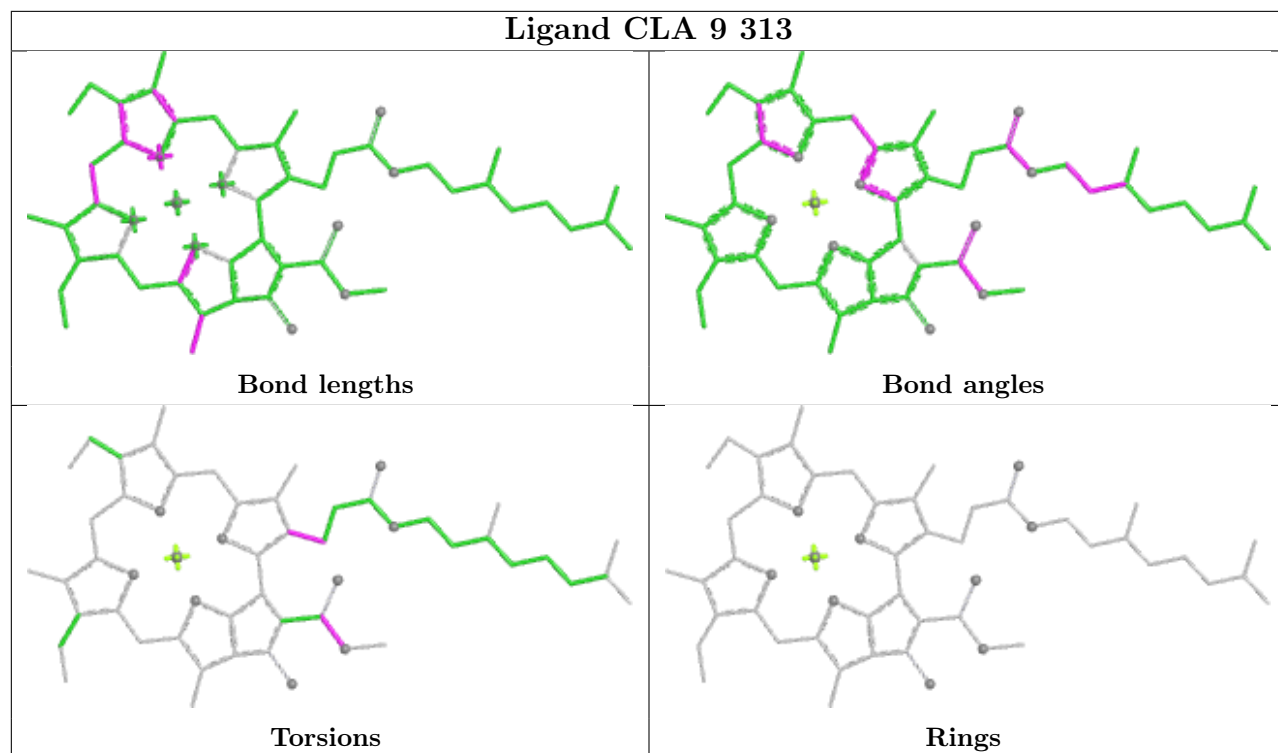
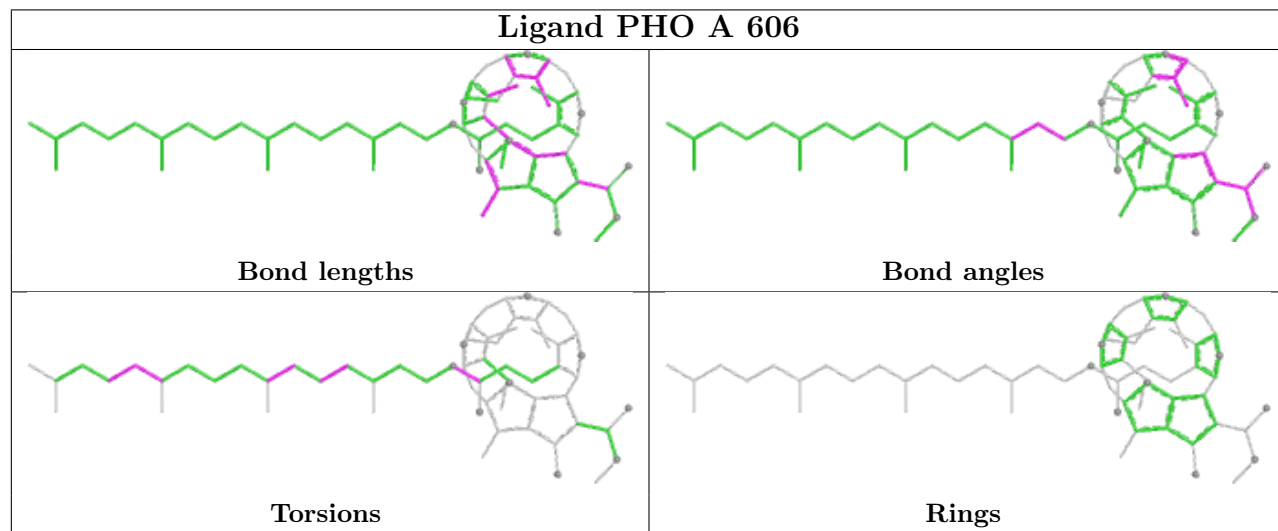
Ligand OIE 5 303**Ligand CHL 5 313**

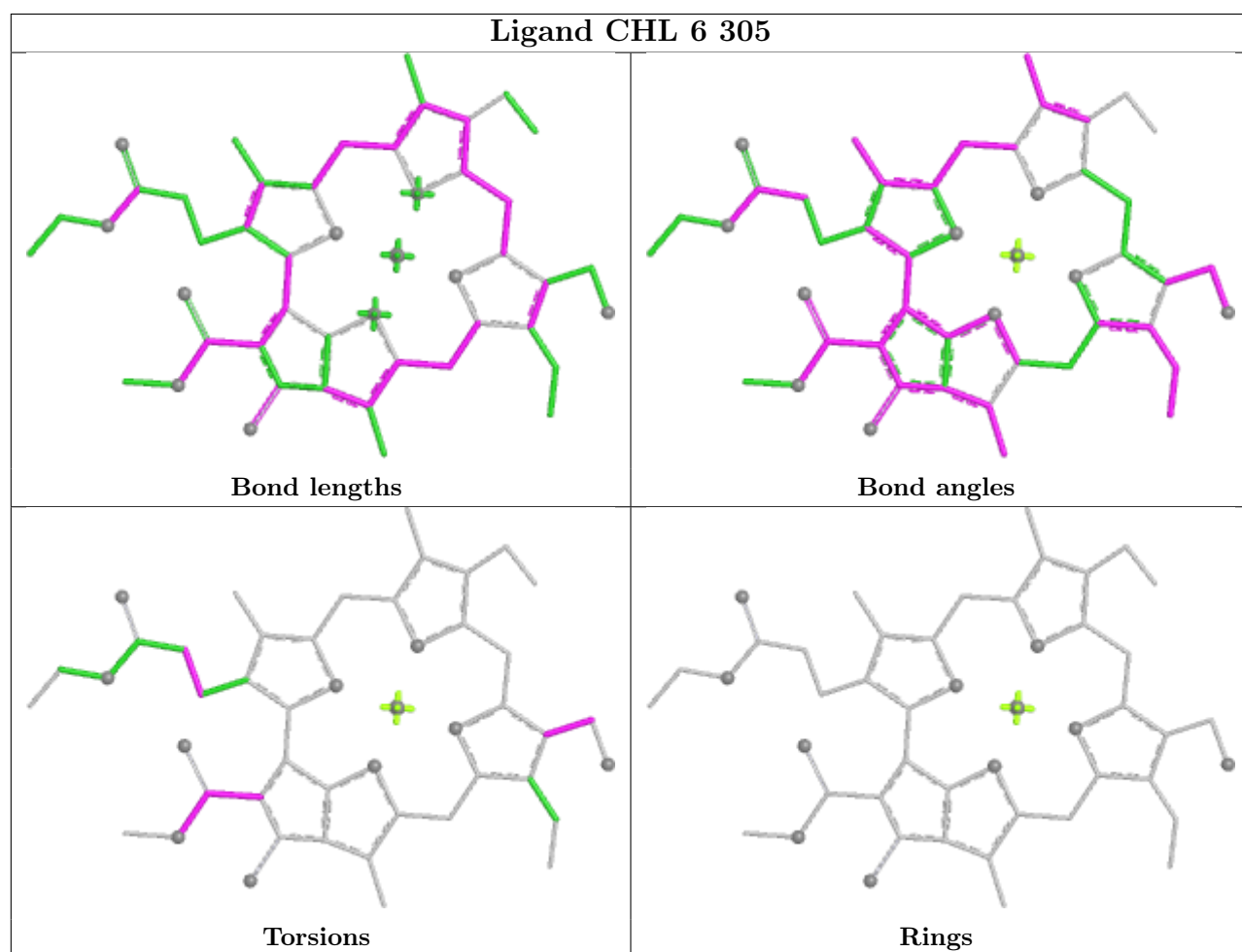
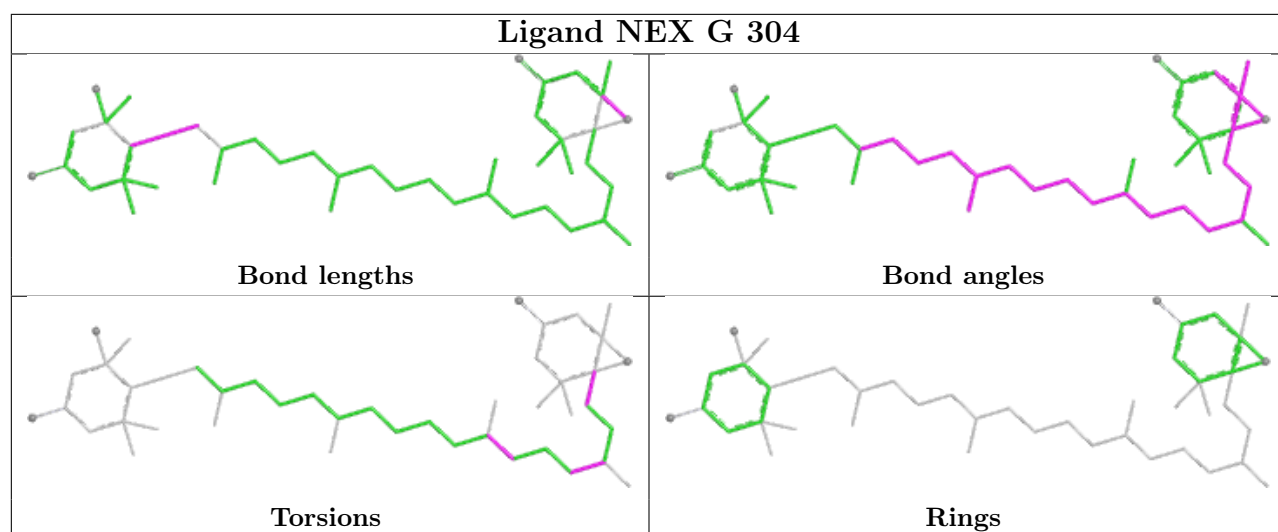
Ligand CLA A 607



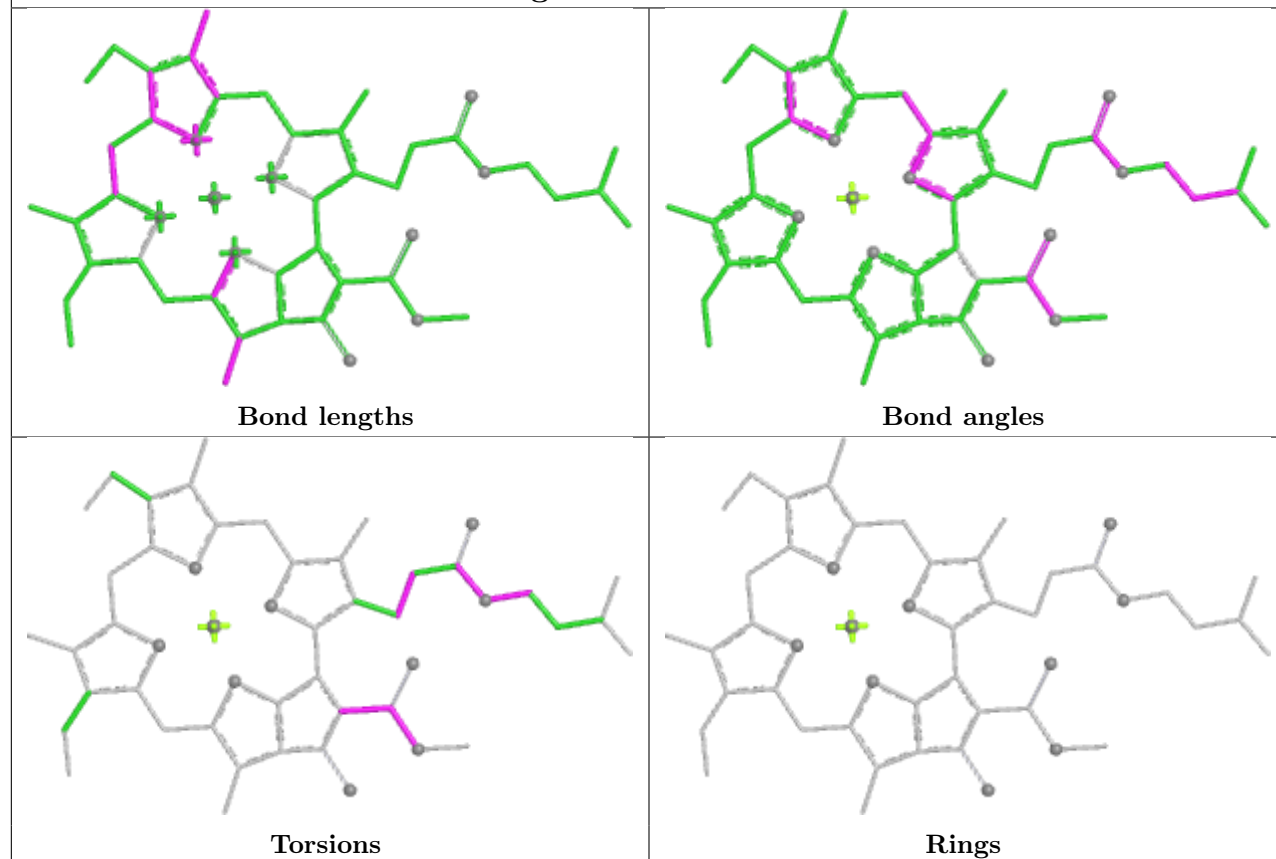
Ligand CHL u 313



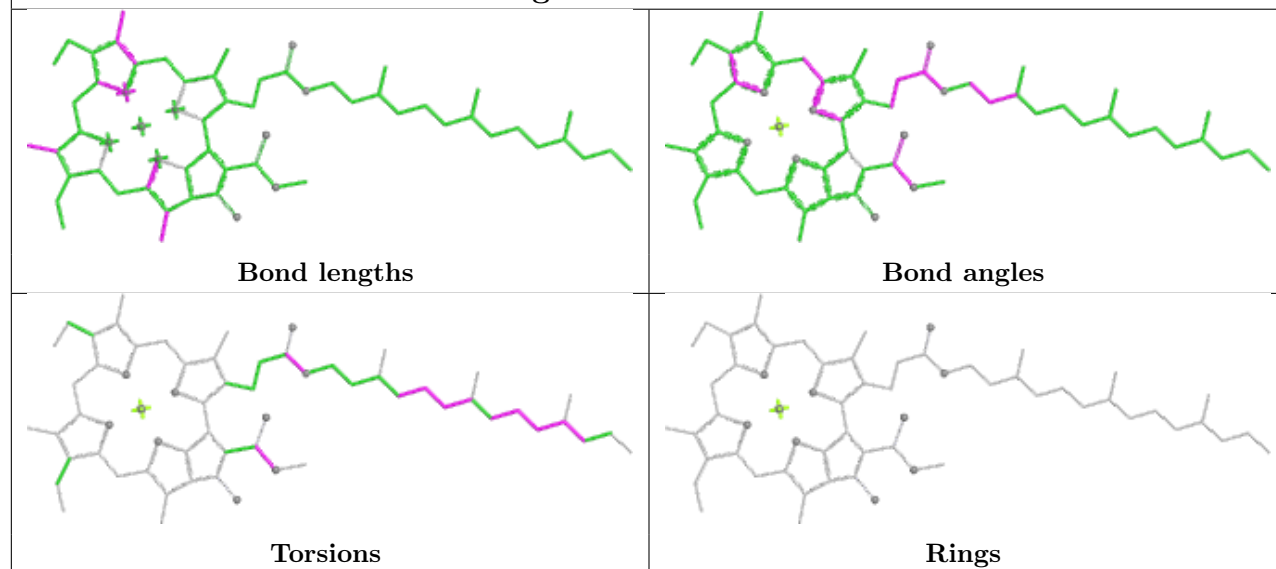
Ligand CLA 9 313**Ligand PHO A 606**

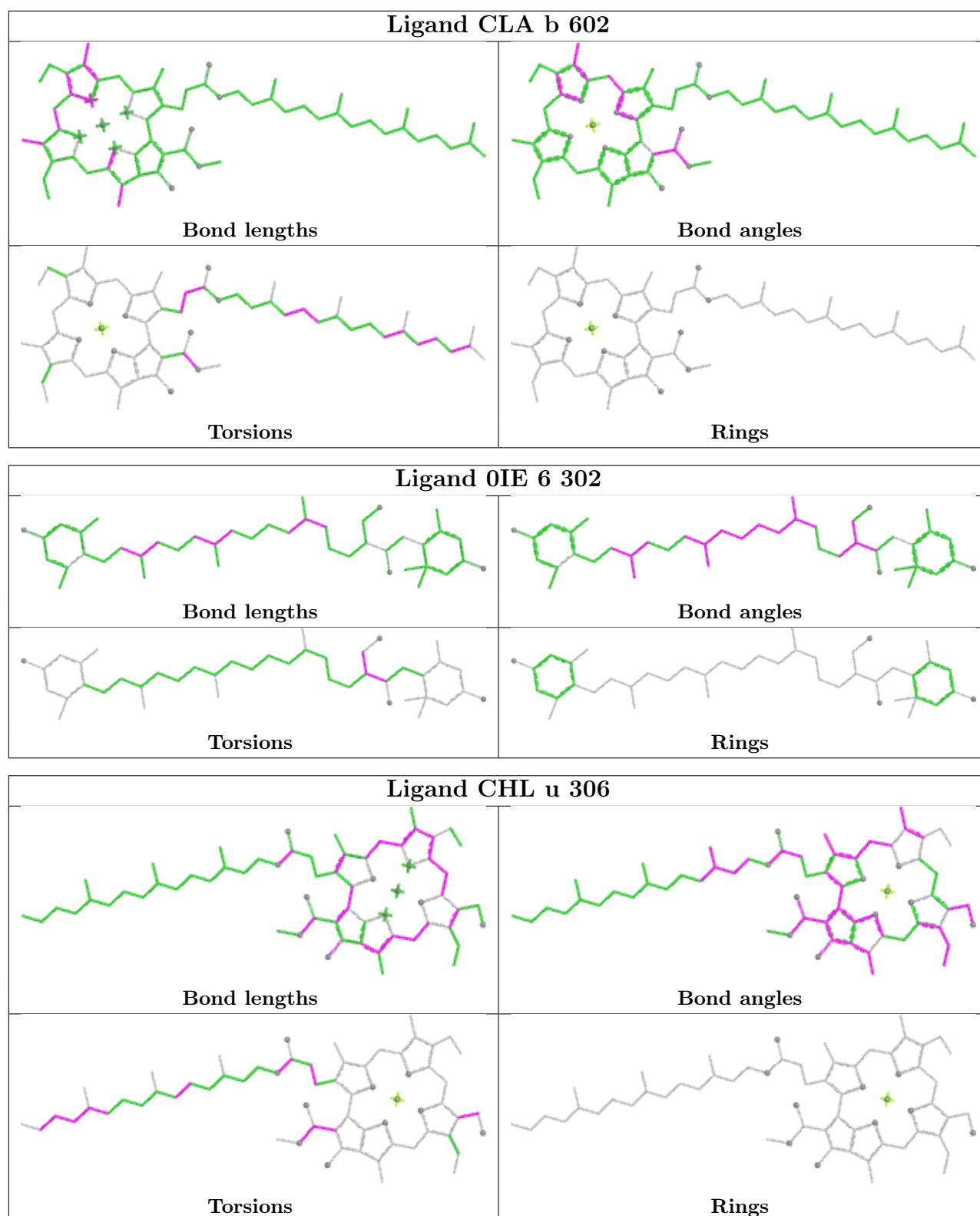


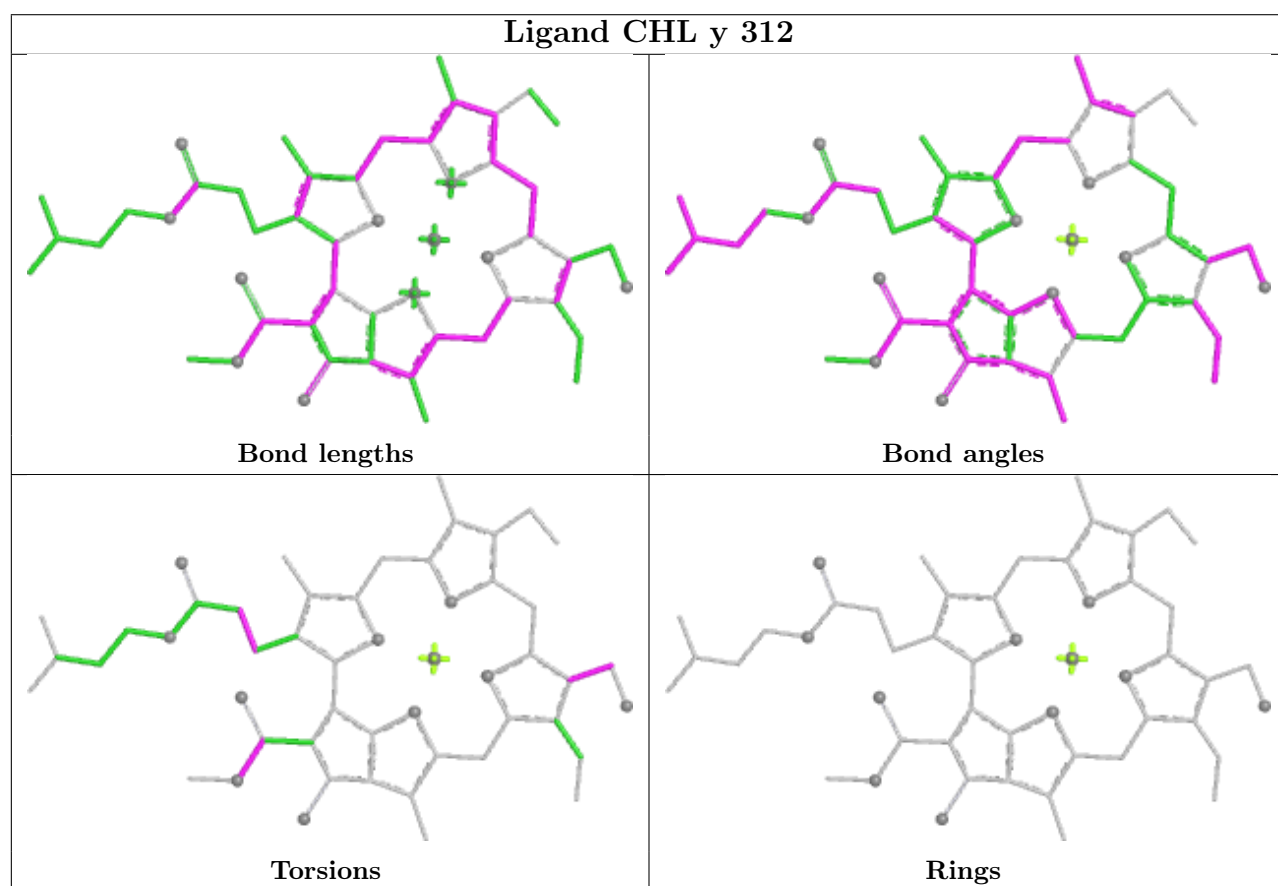
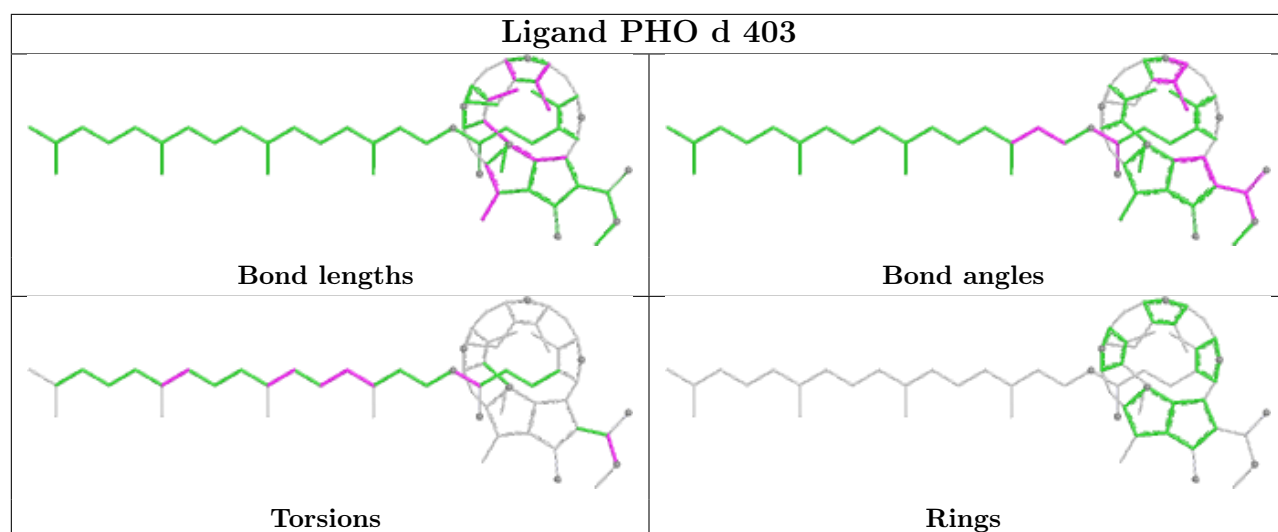
Ligand CLA G 308



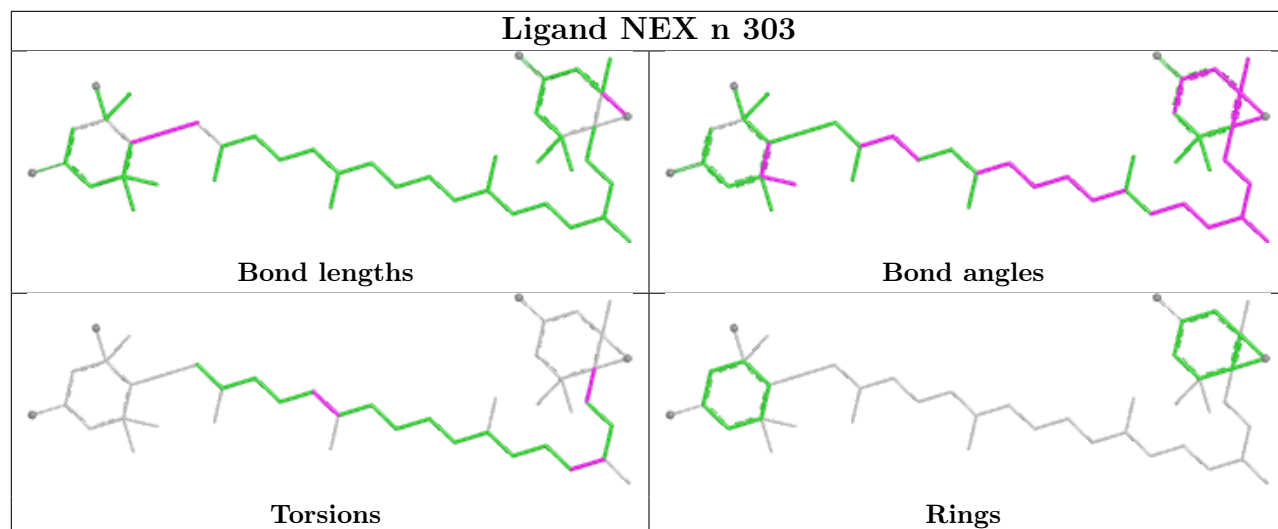
Ligand CLA B 604



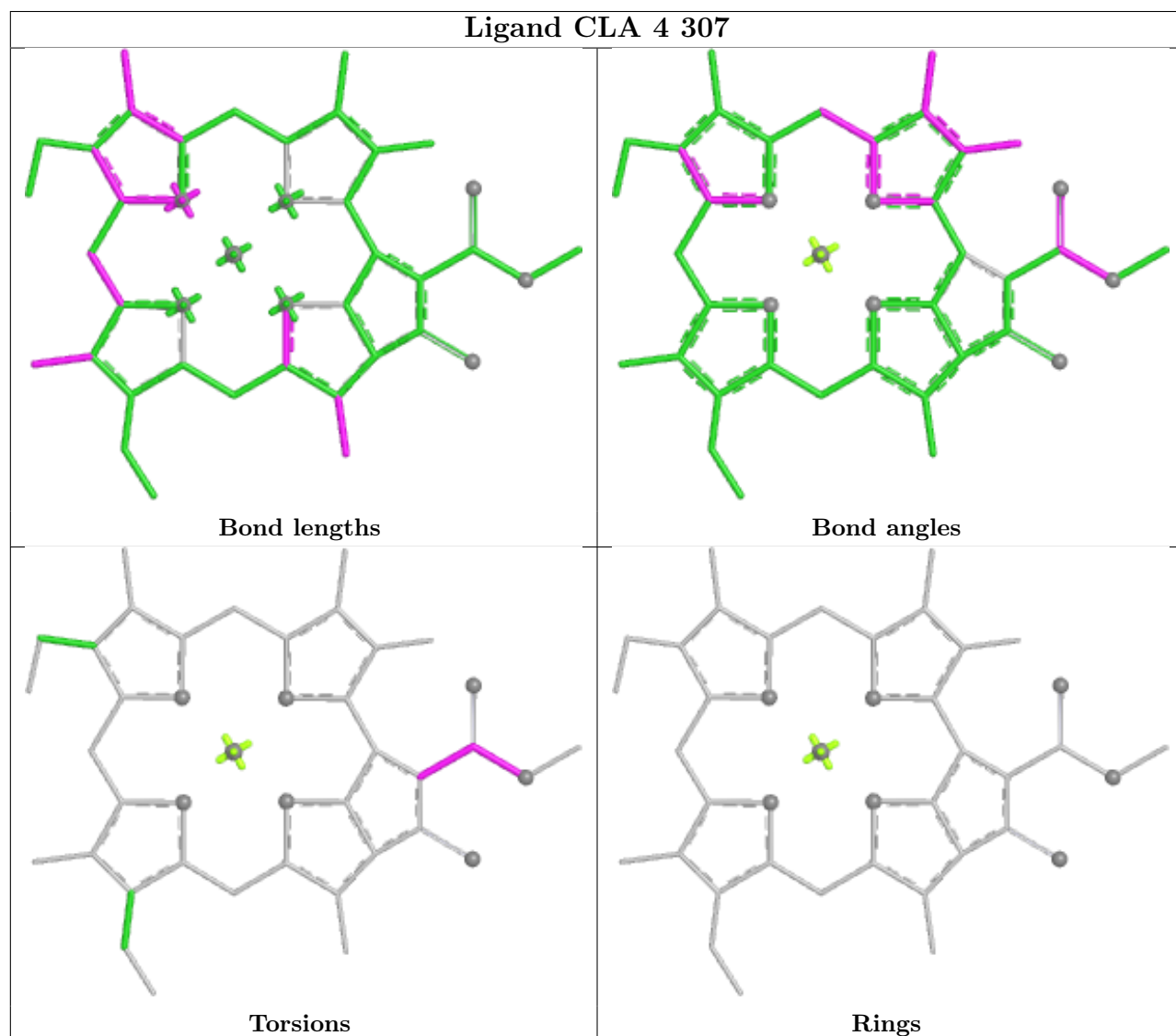




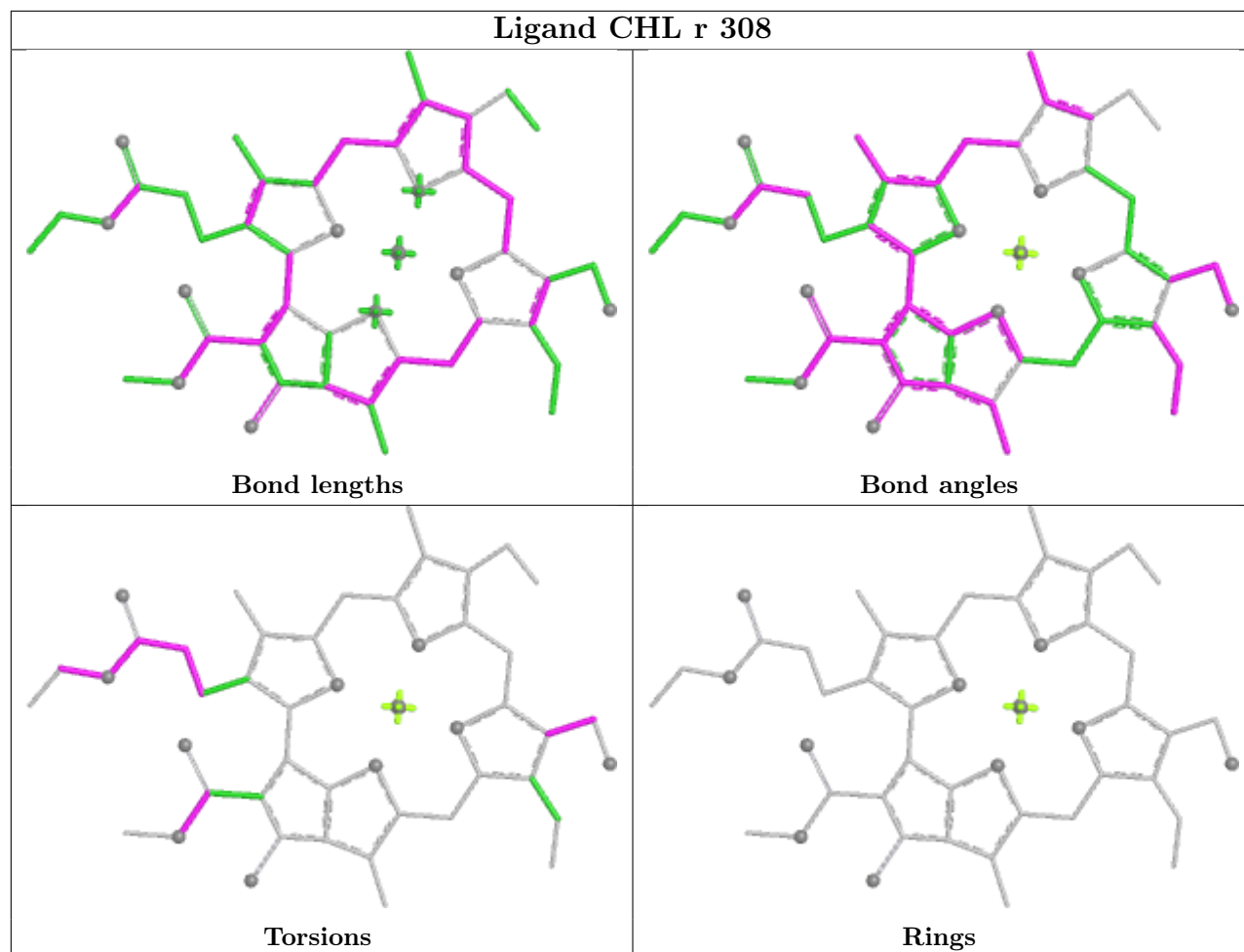
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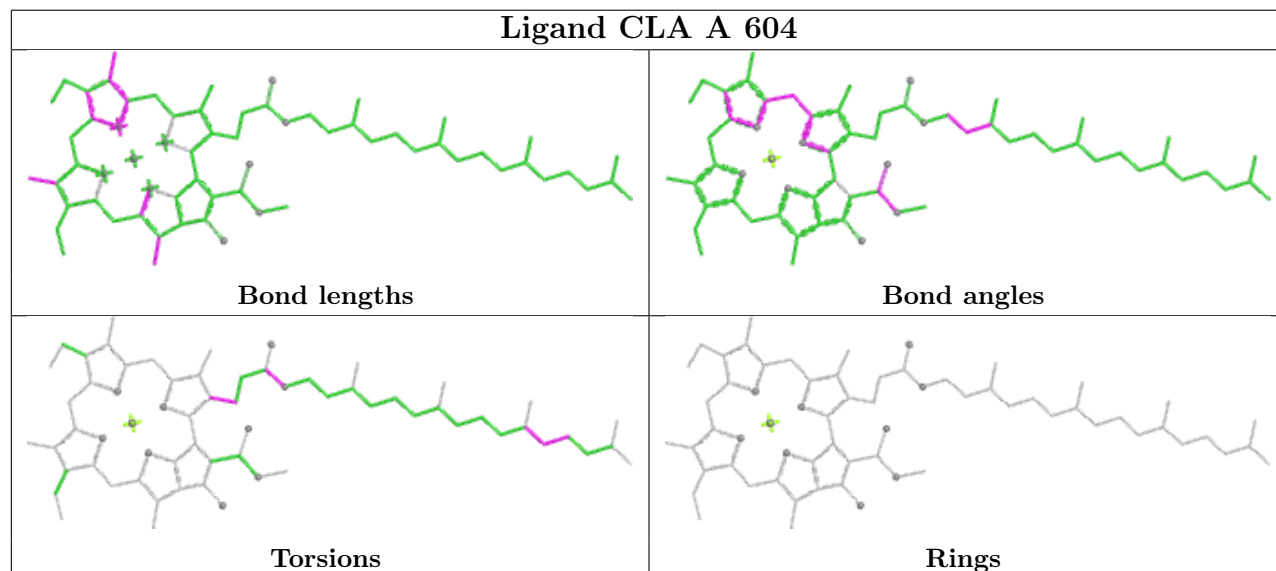
Ligand CLA 4 307

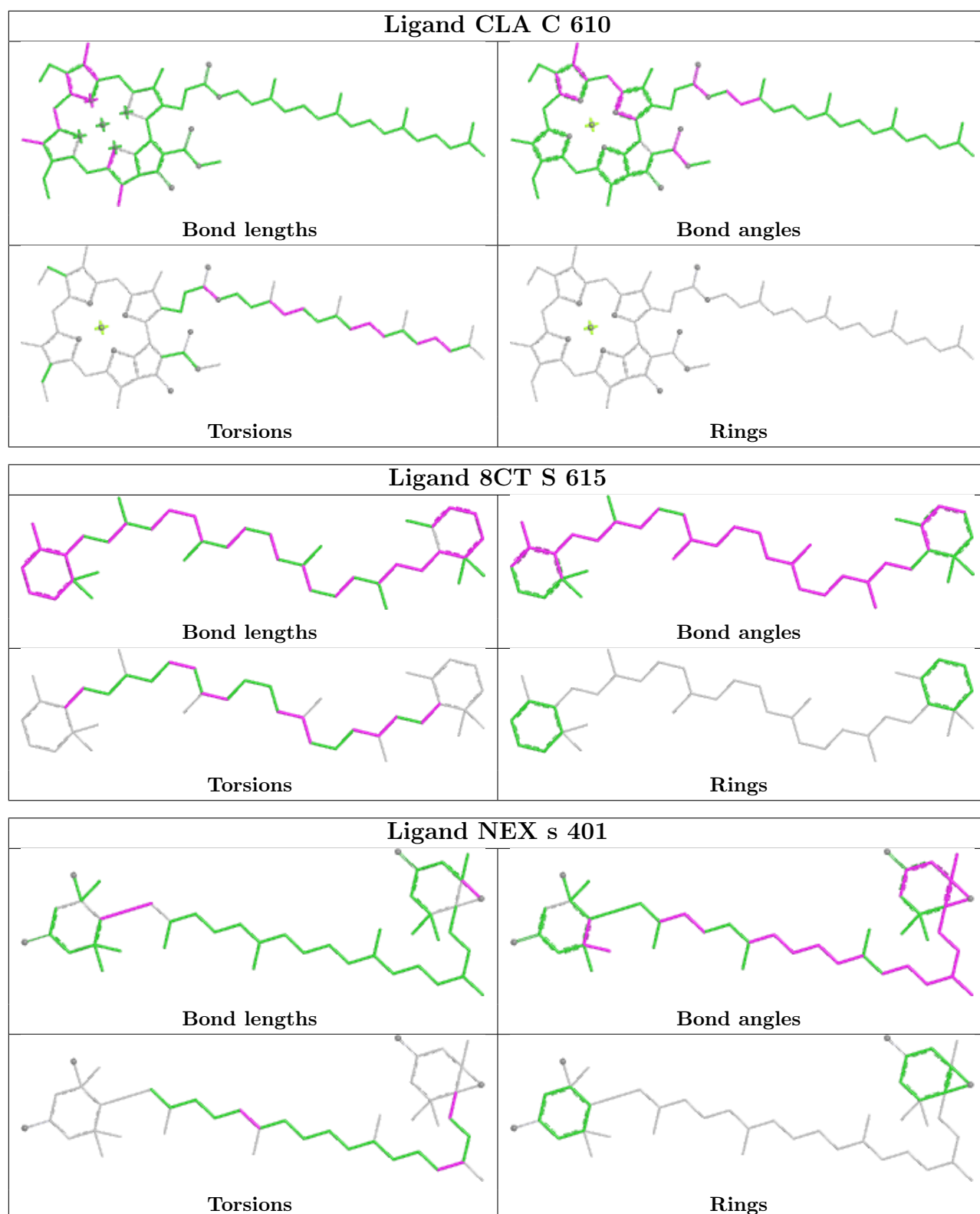


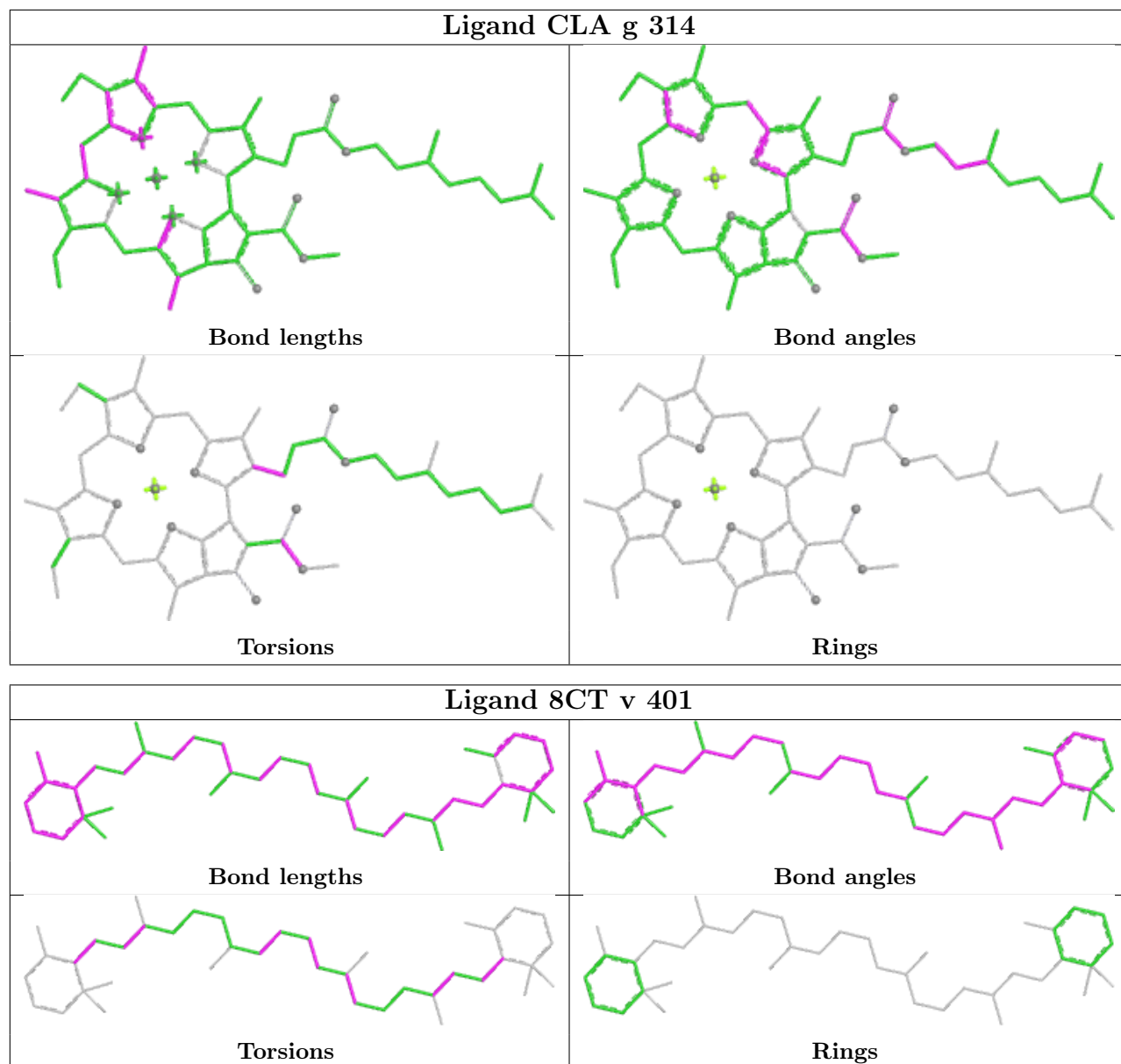
Ligand CHL r 308



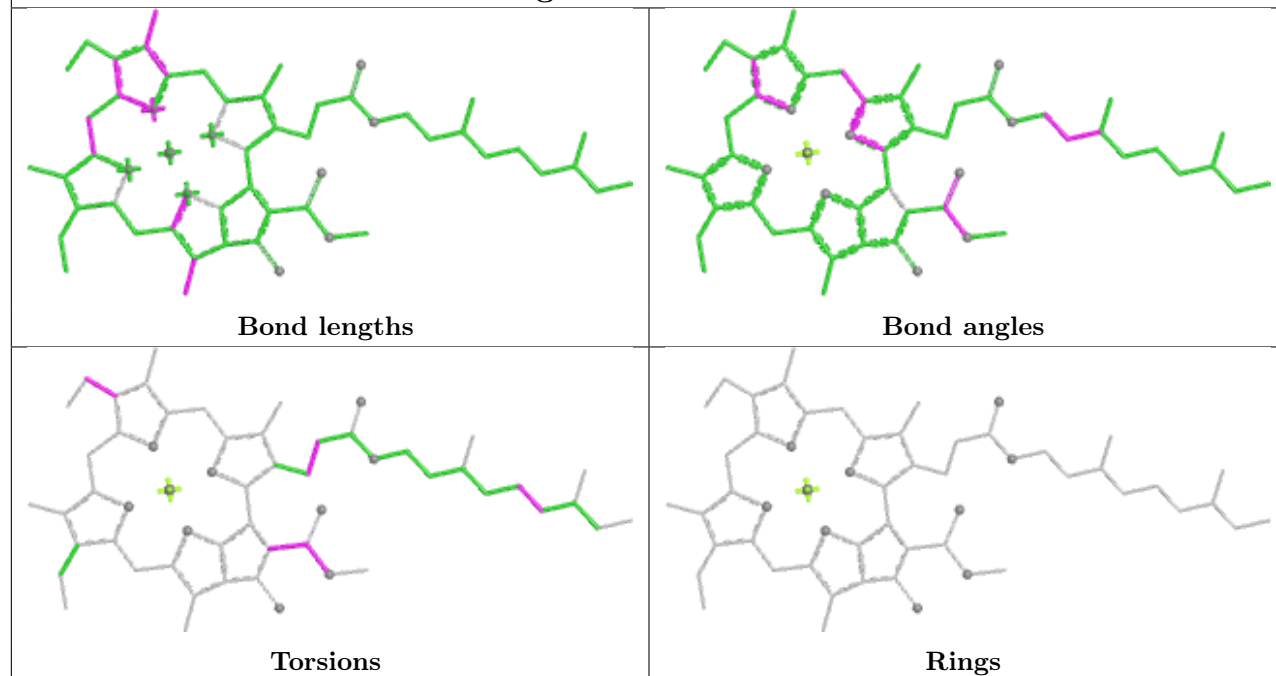
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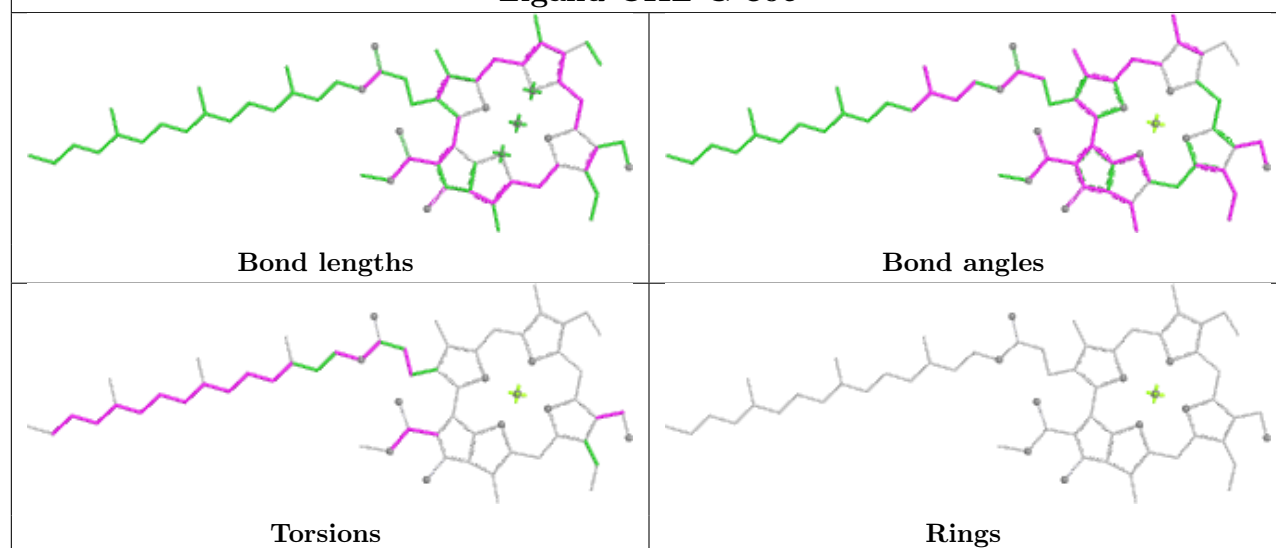




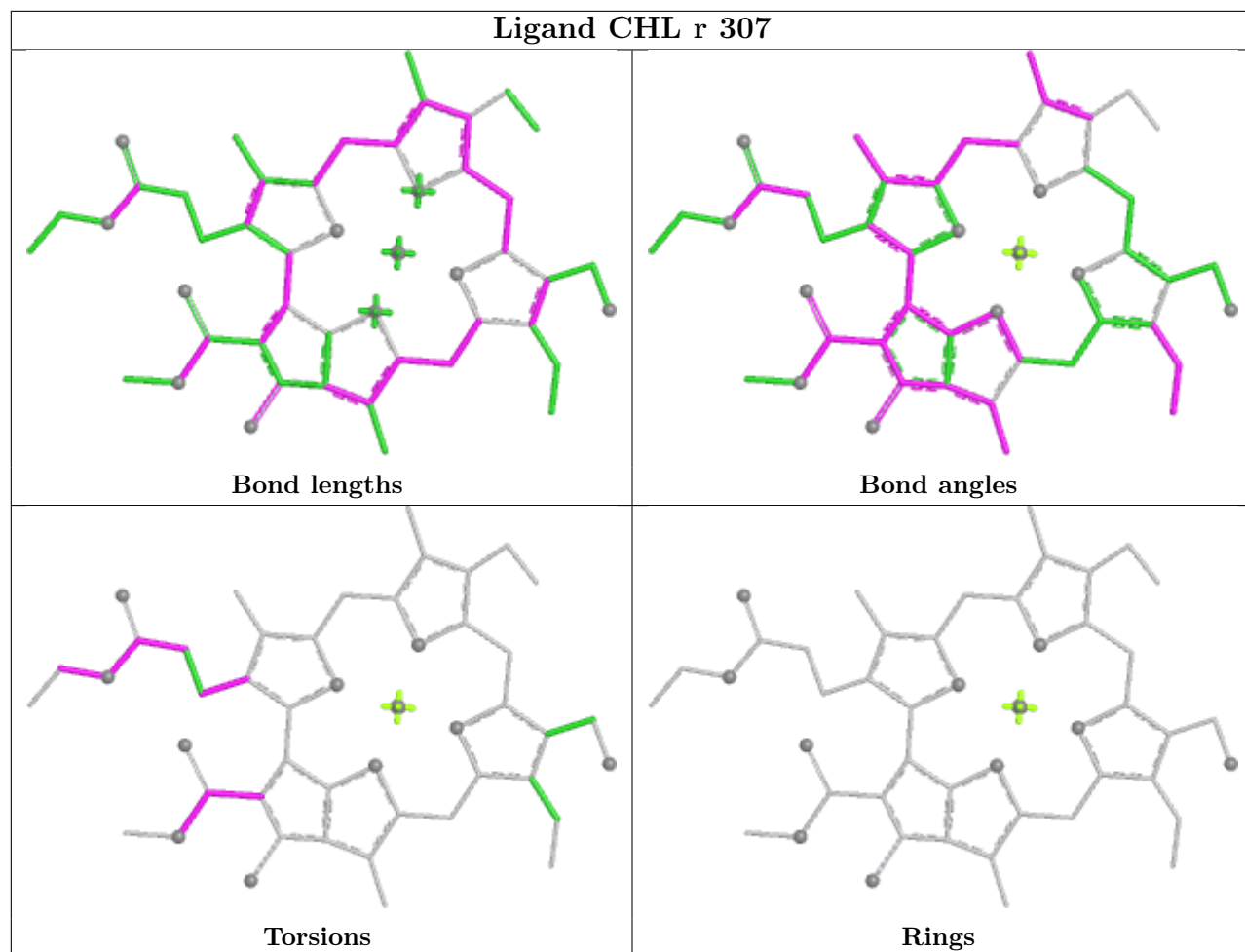
Ligand CLA 9 306



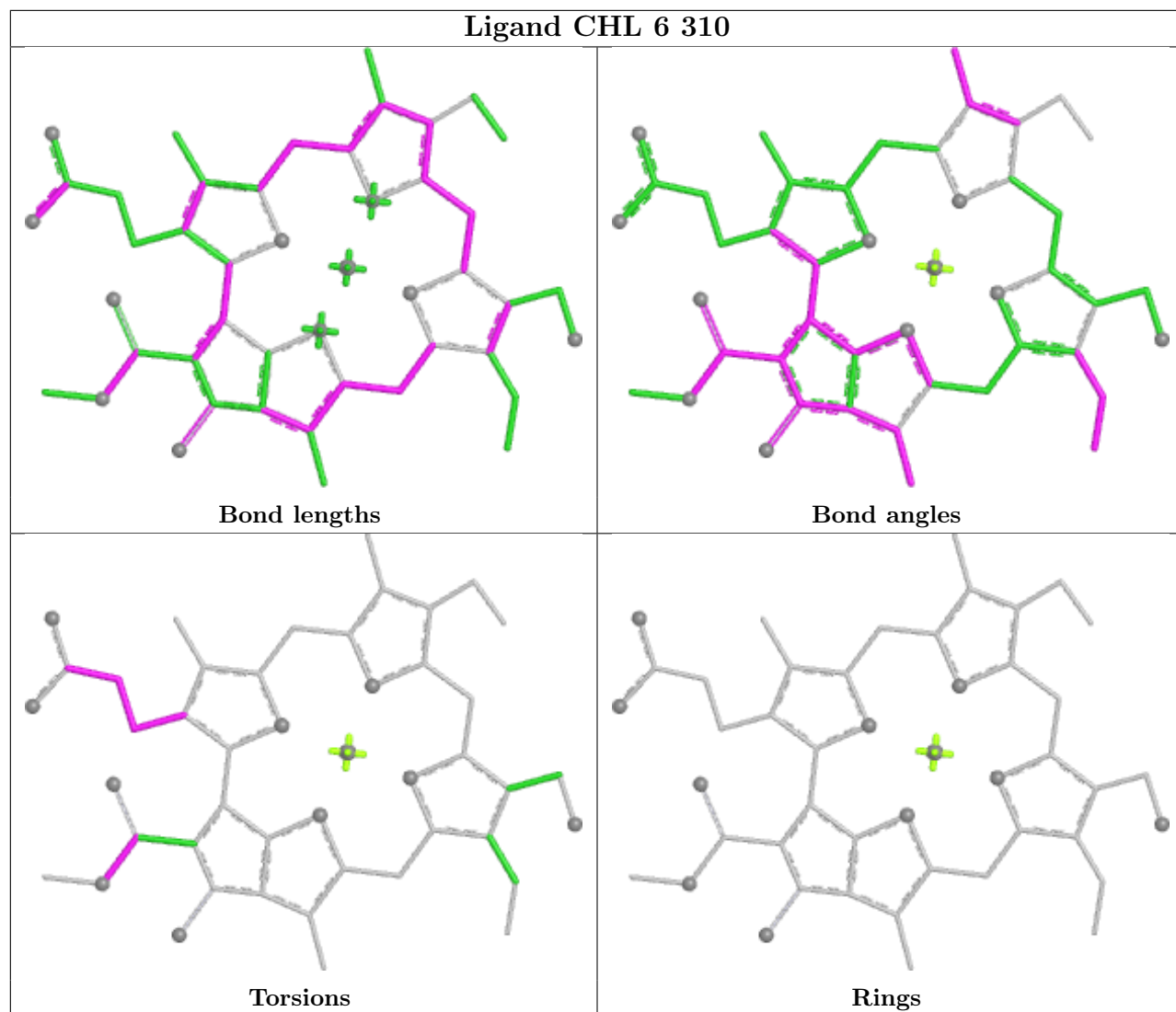
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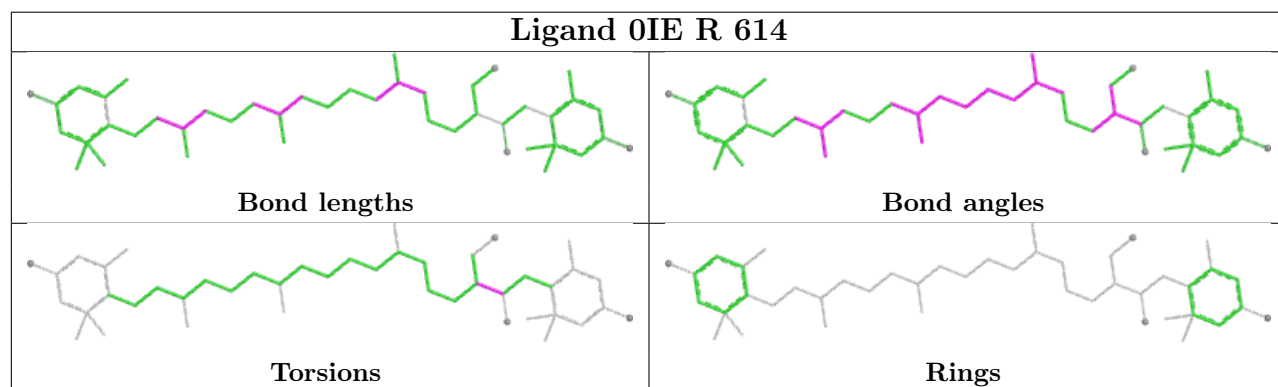
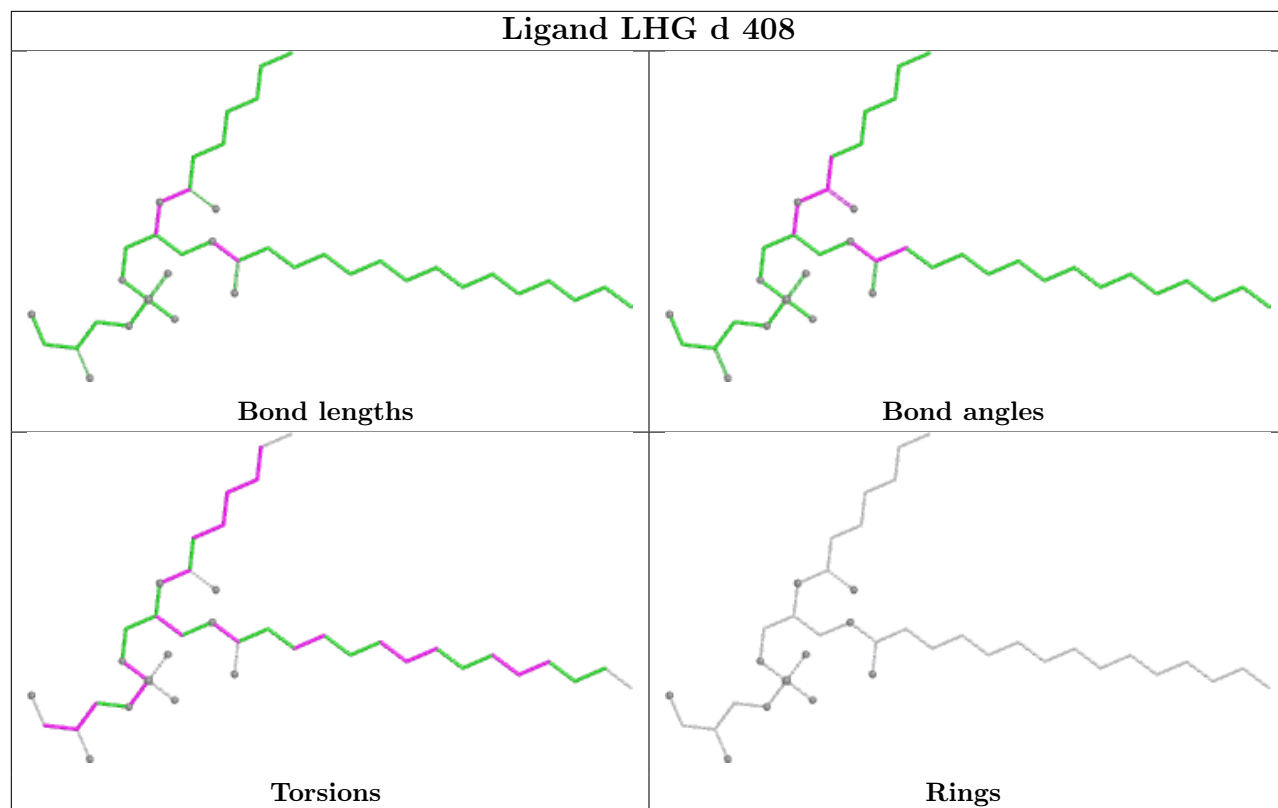


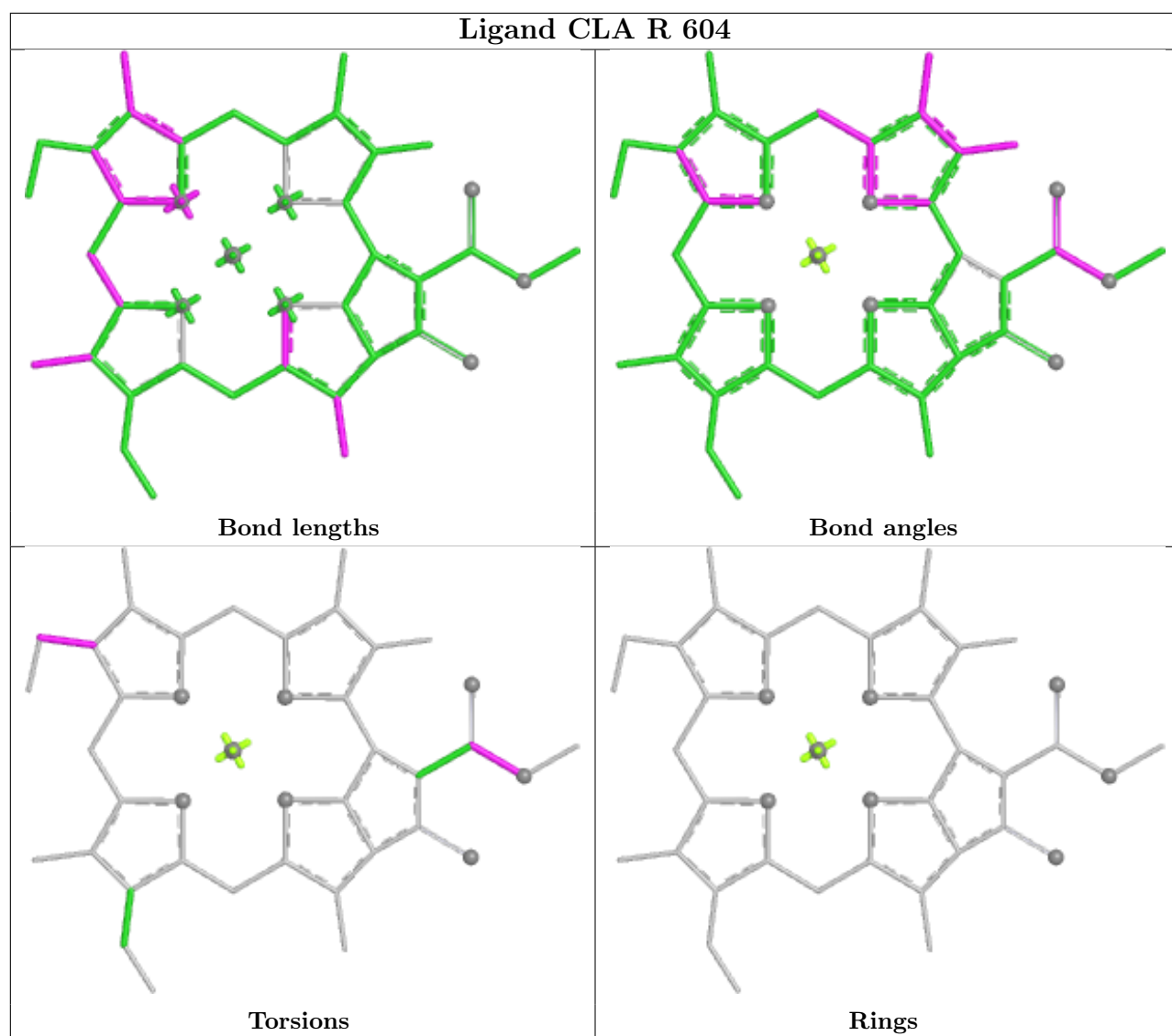
Ligand CHL r 307



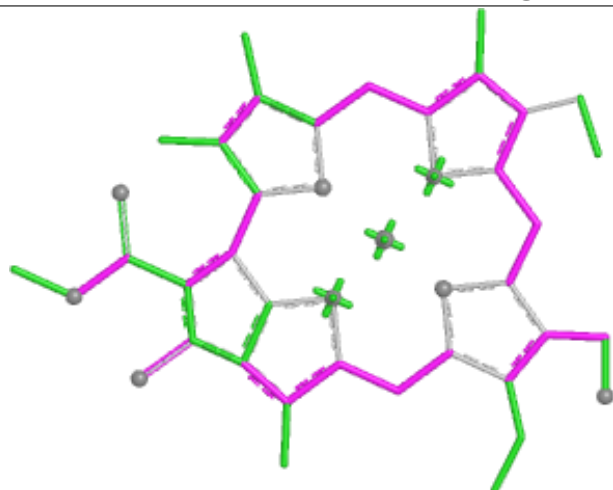
Ligand CHL 6 310



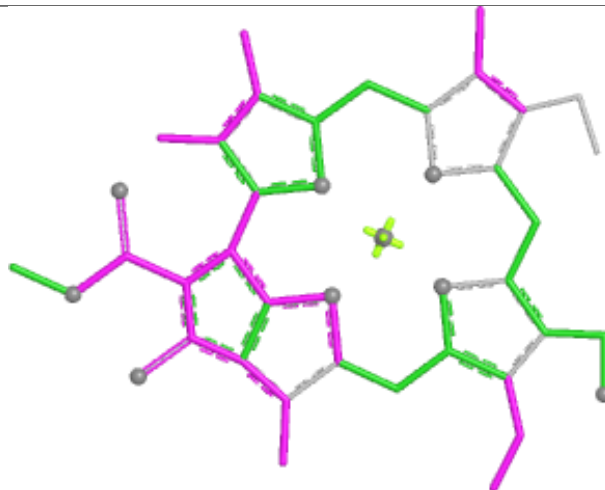




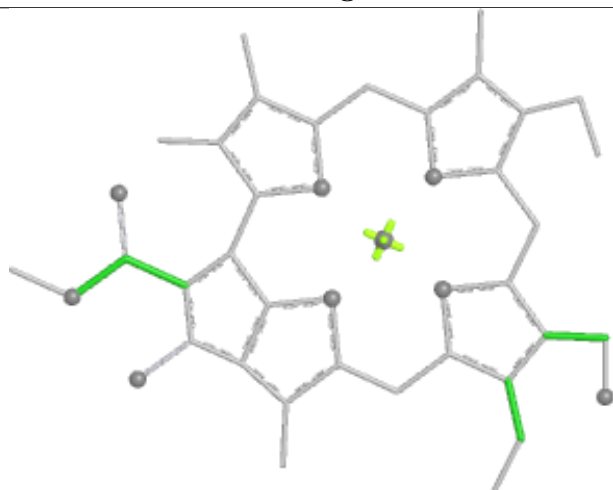
Ligand CHL 6 317



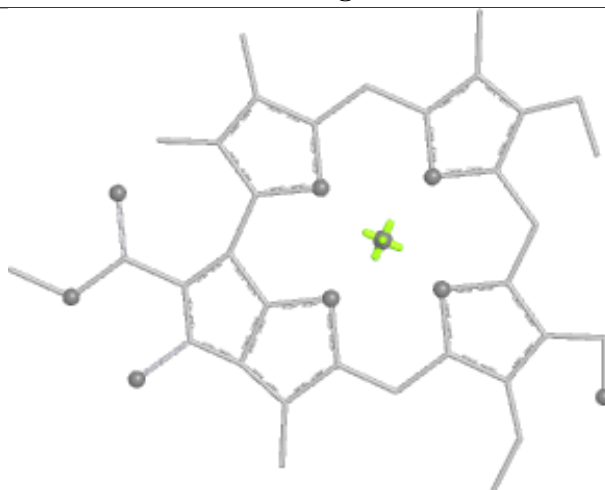
Bond lengths



Bond angles

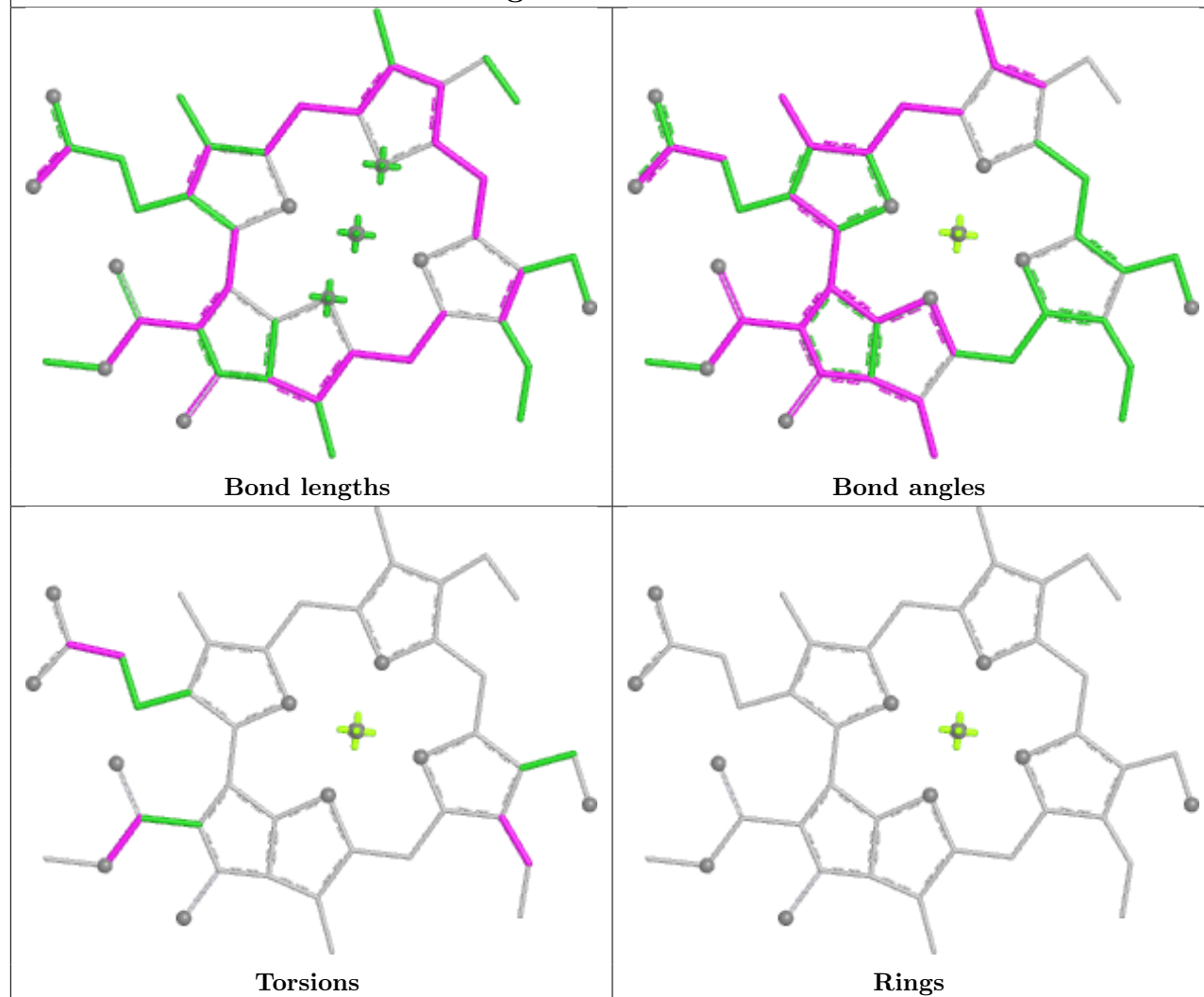


Torsions

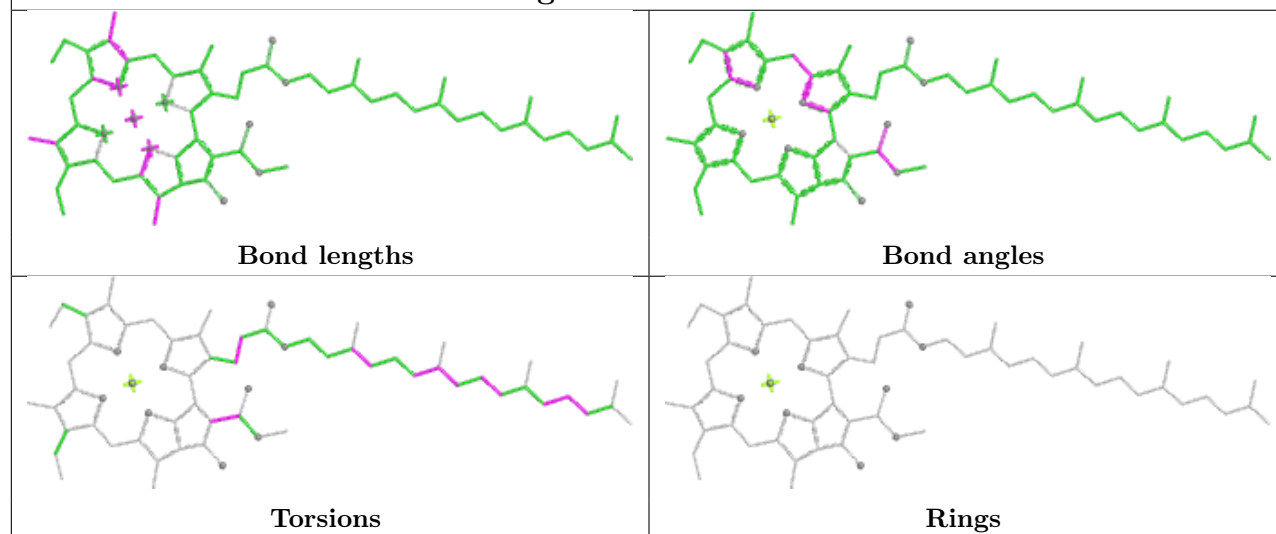


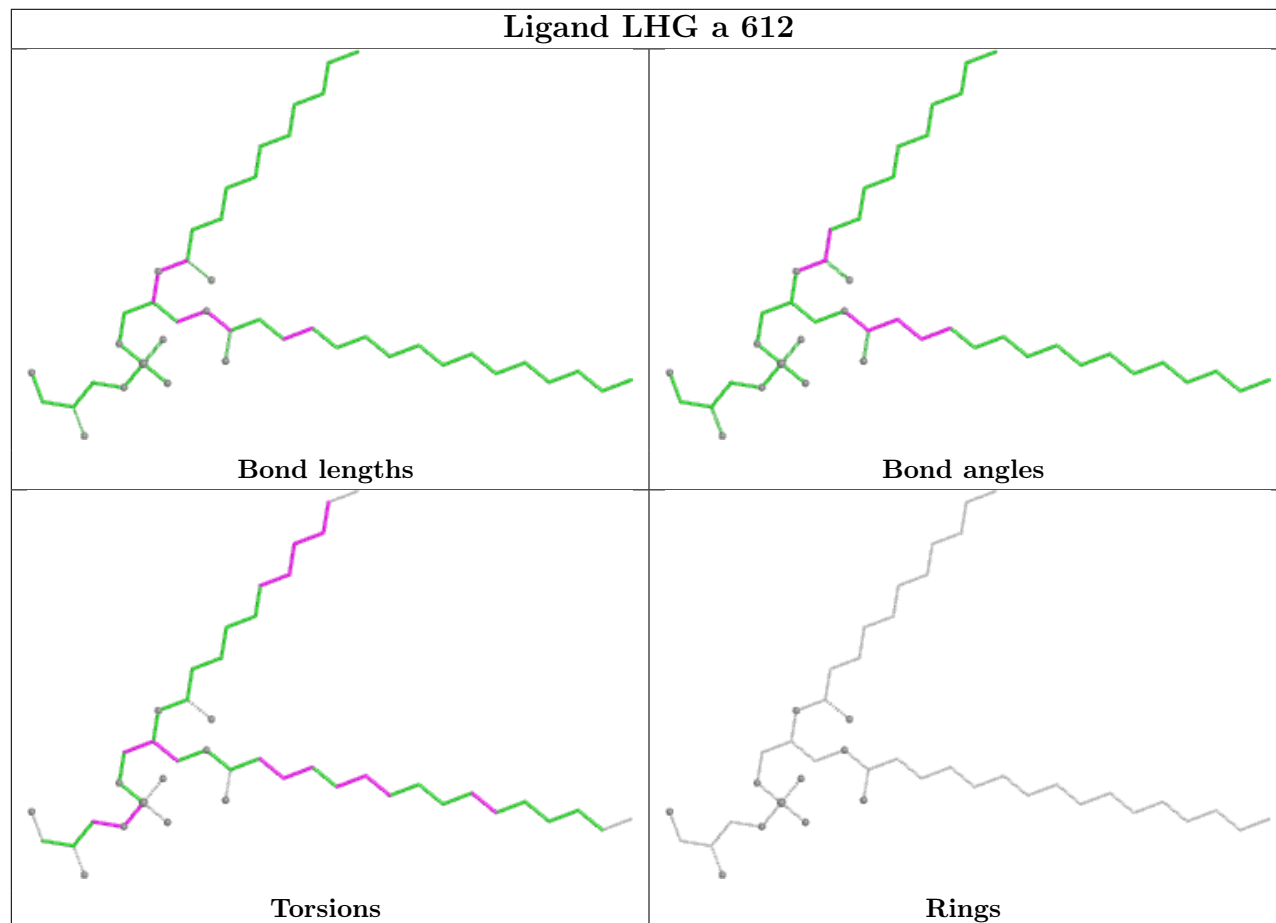
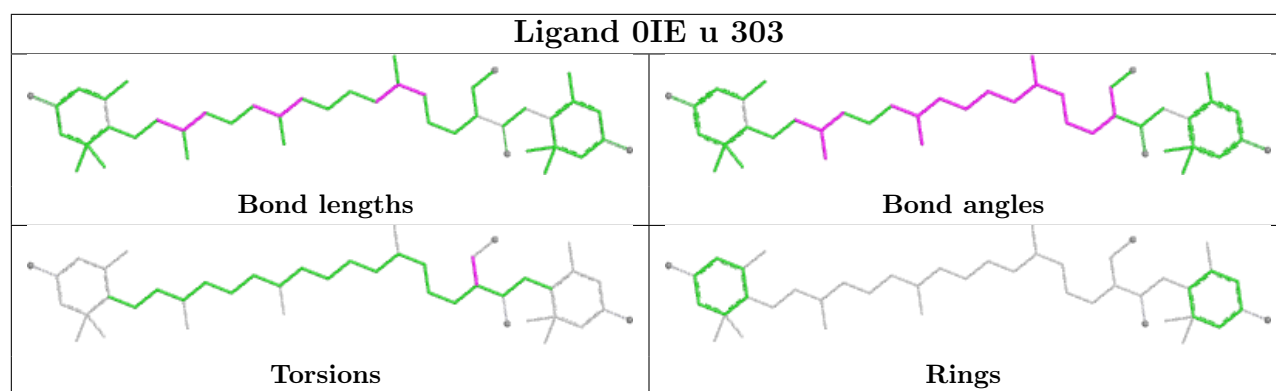
Rings

Ligand CHL r 309

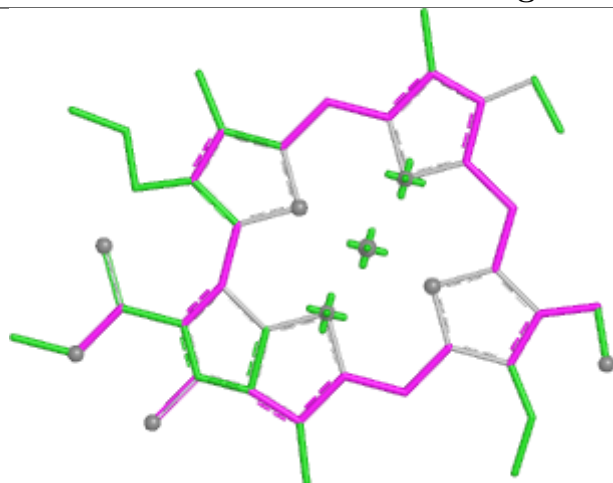


Ligand CLA c 607

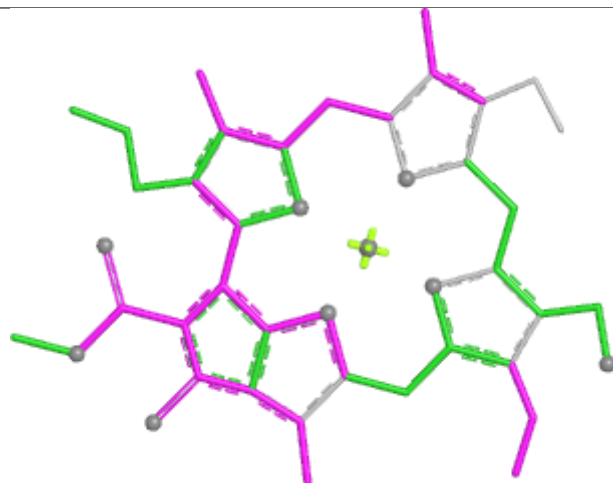




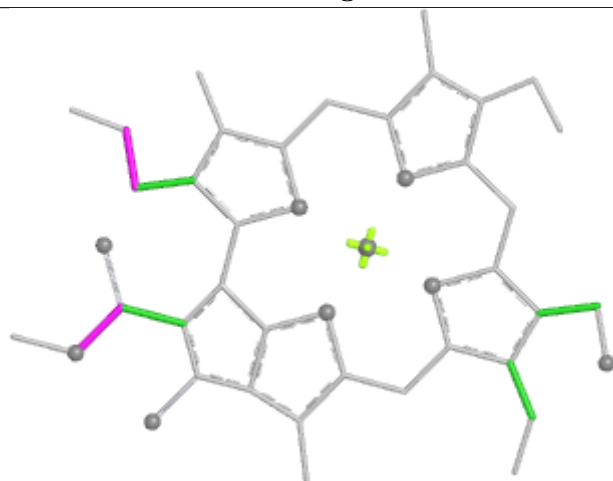
Ligand CHL 1 311



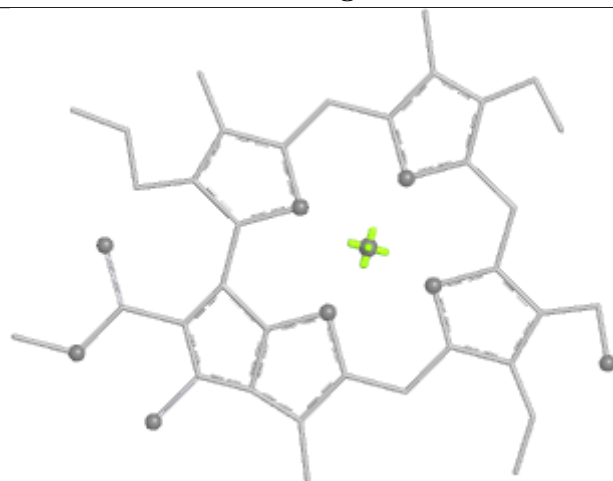
Bond lengths



Bond angles

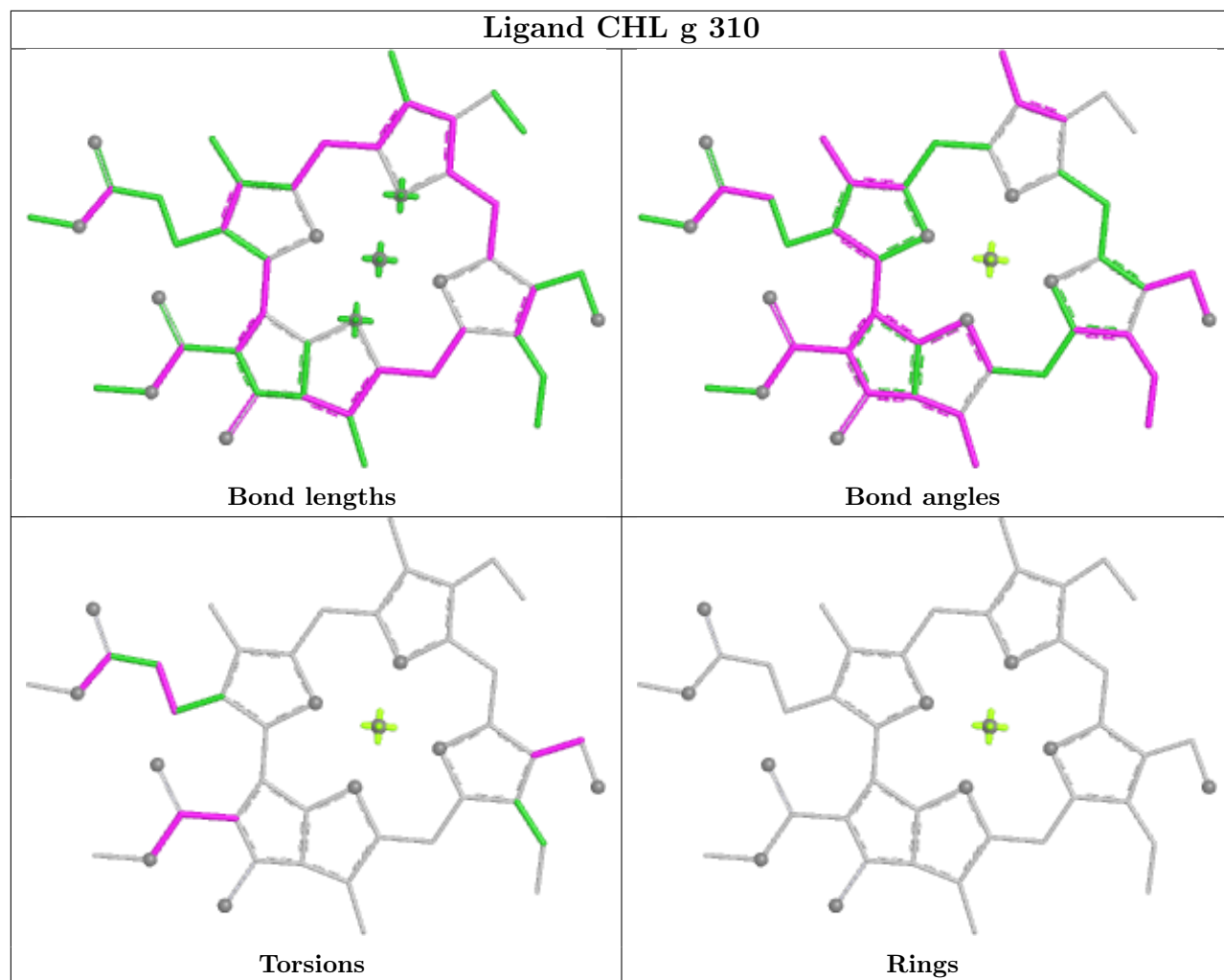


Torsions

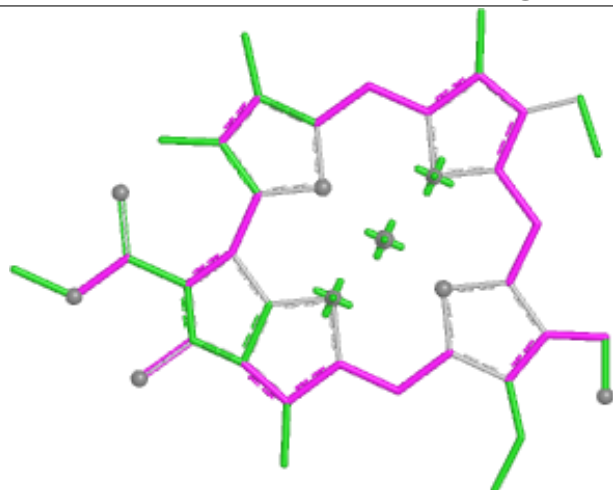


Rings

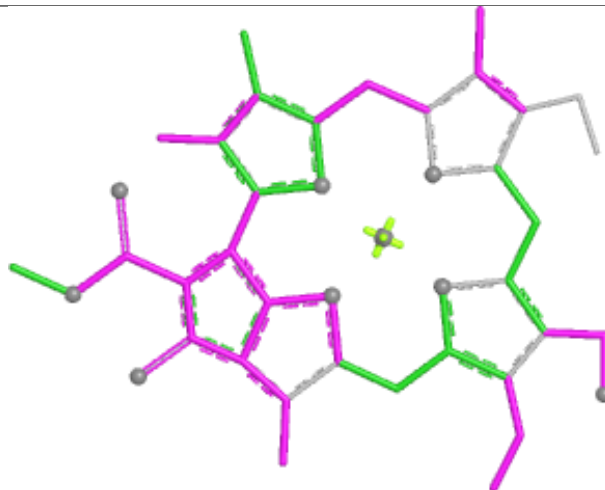
Ligand CHL g 310



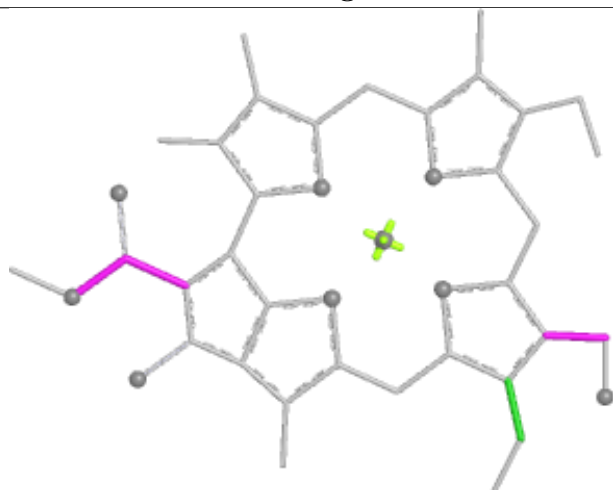
Ligand CHL n 317



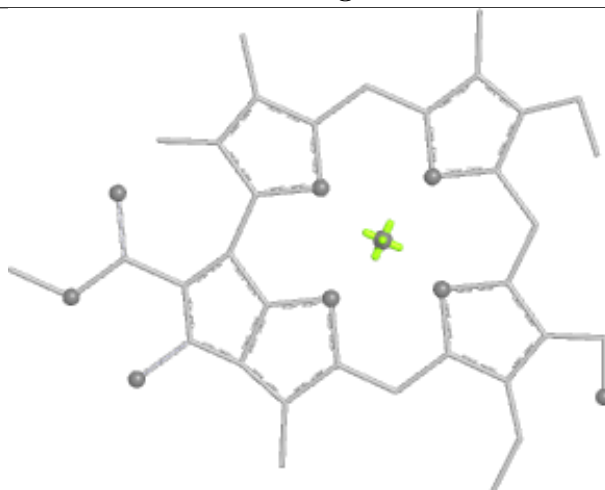
Bond lengths



Bond angles

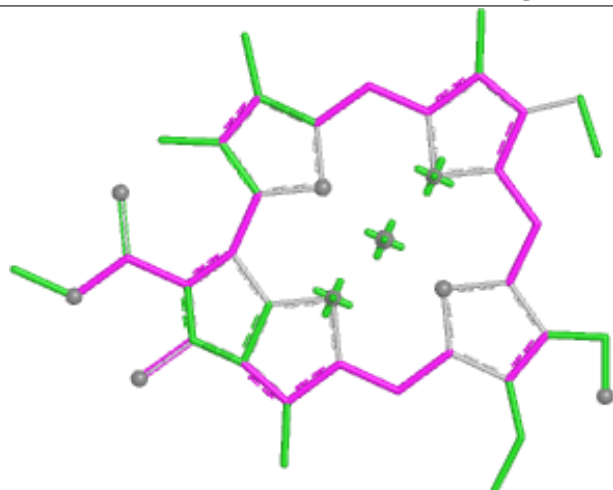


Torsions

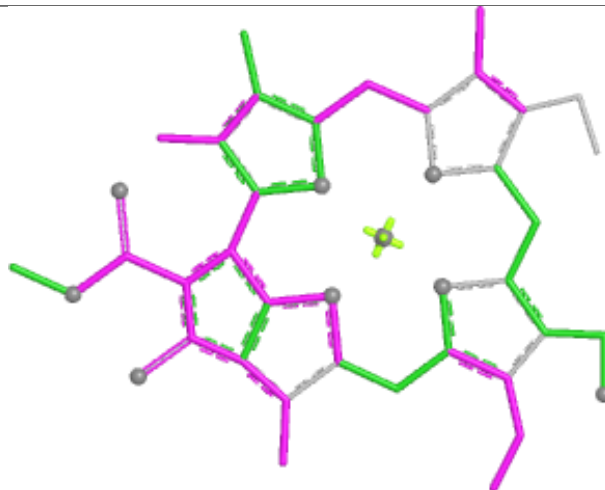


Rings

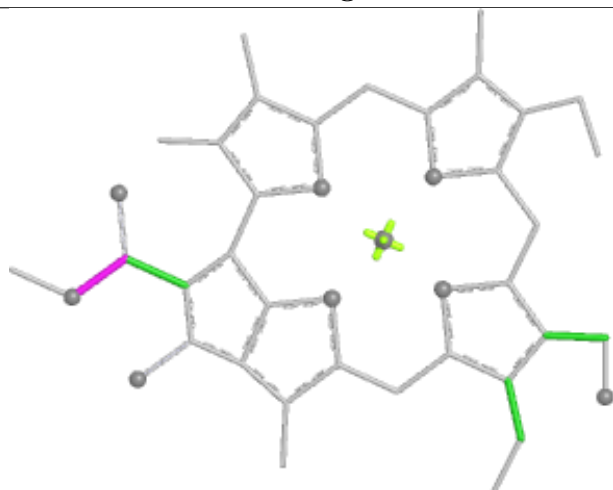
Ligand CHL 5 310



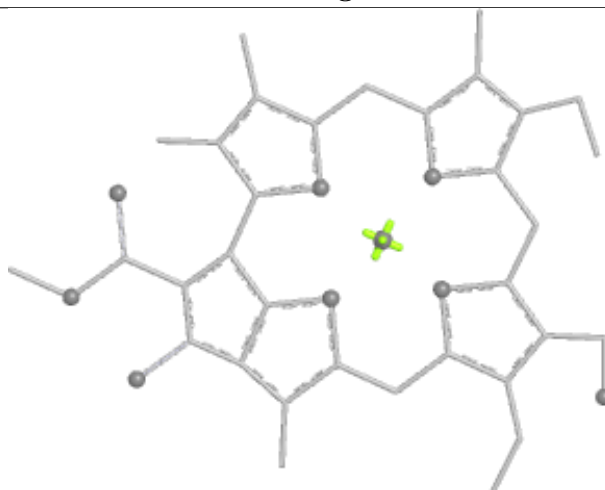
Bond lengths



Bond angles

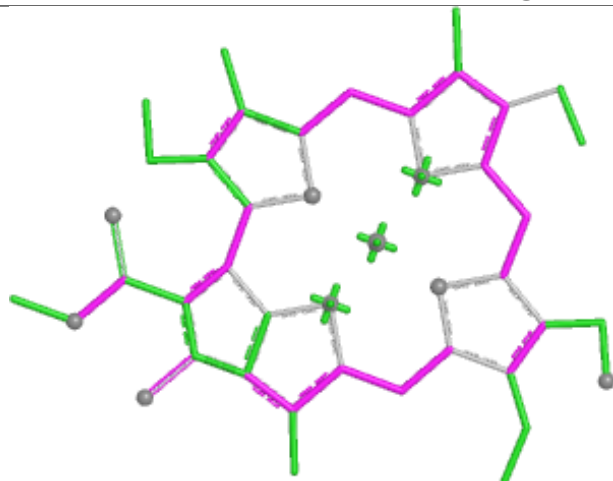


Torsions

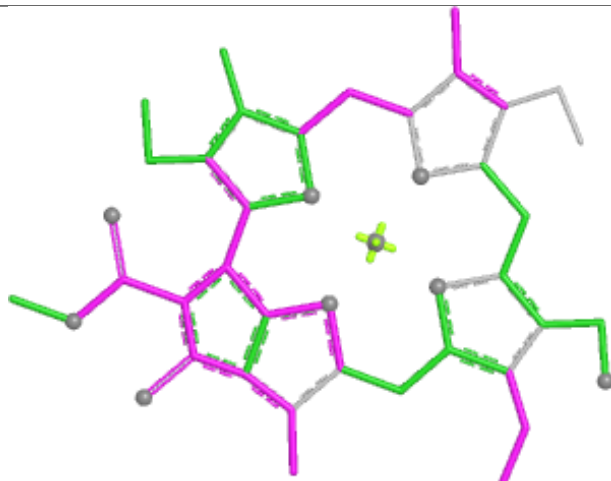


Rings

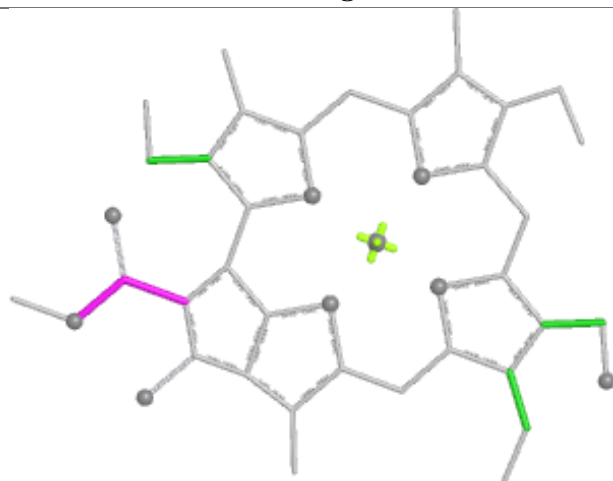
Ligand CHL 1 310



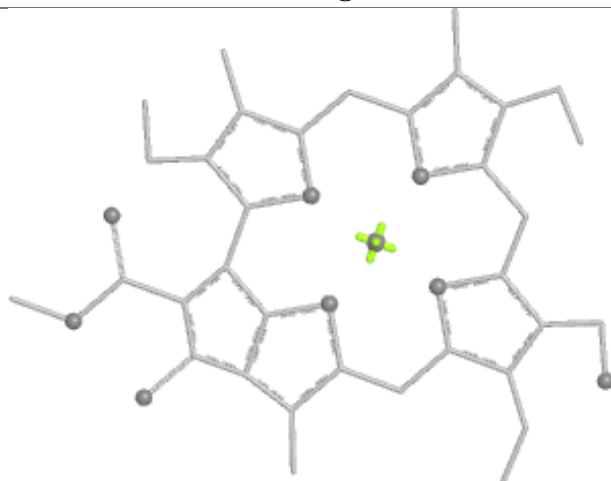
Bond lengths



Bond angles

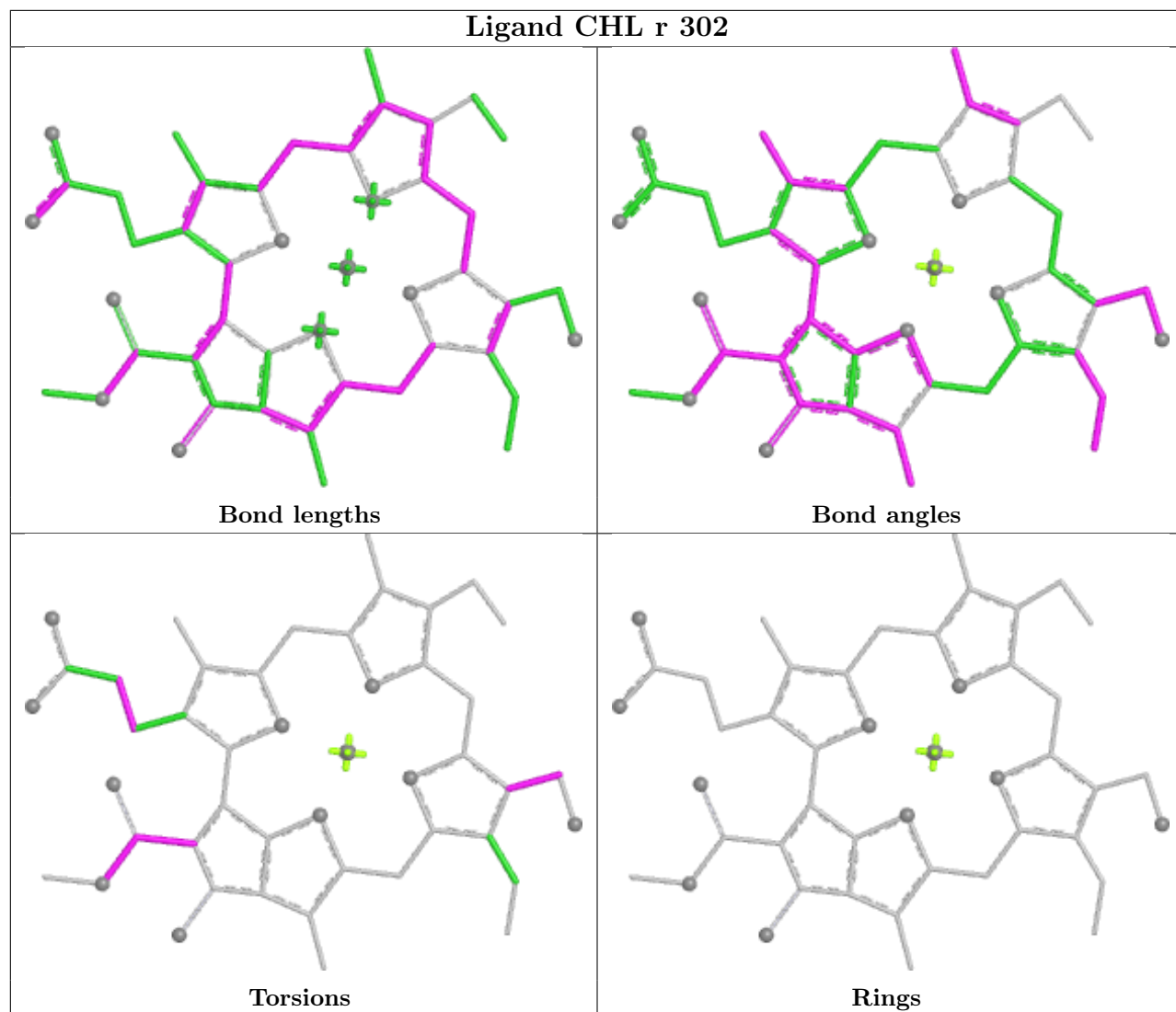


Torsions

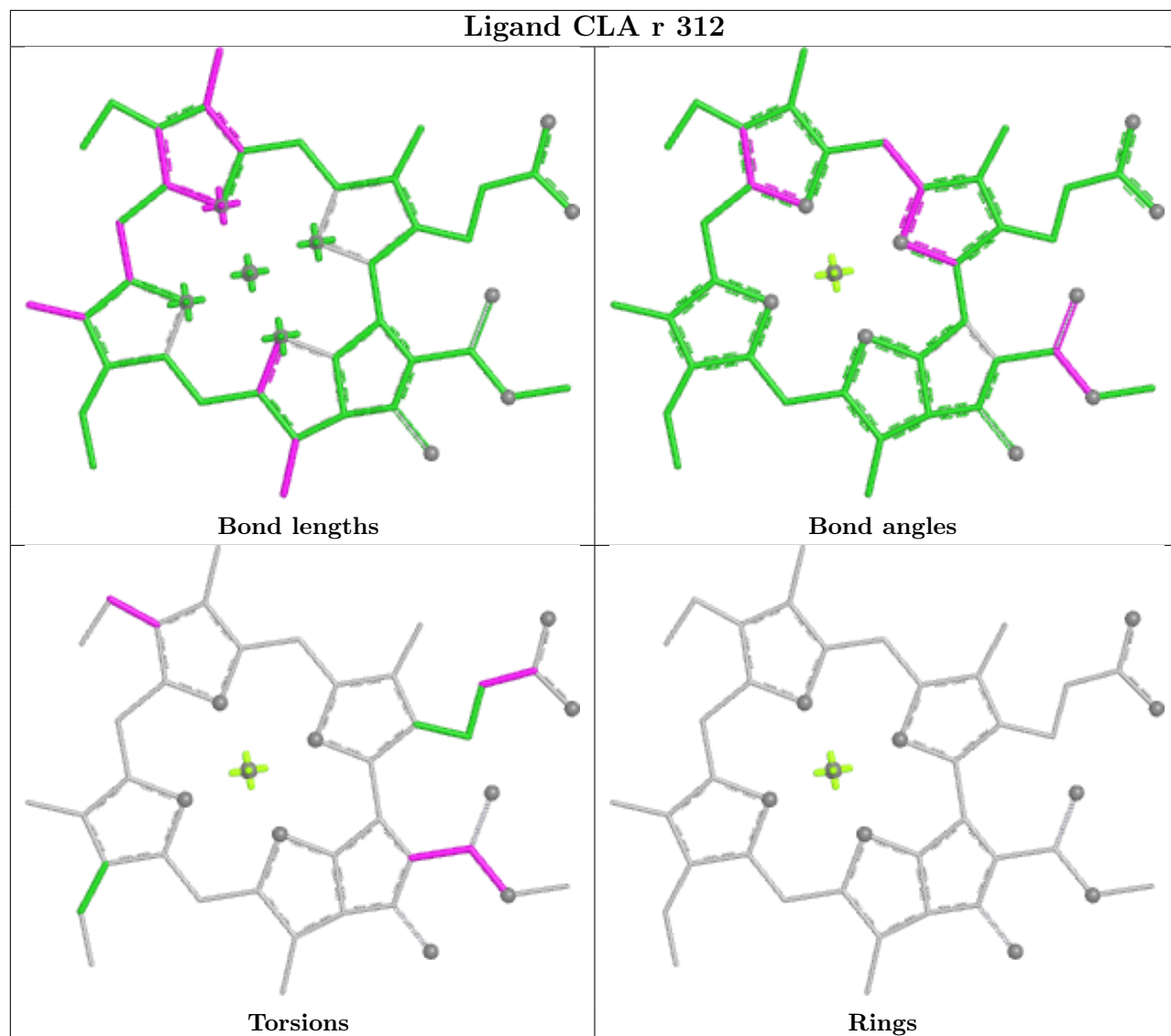


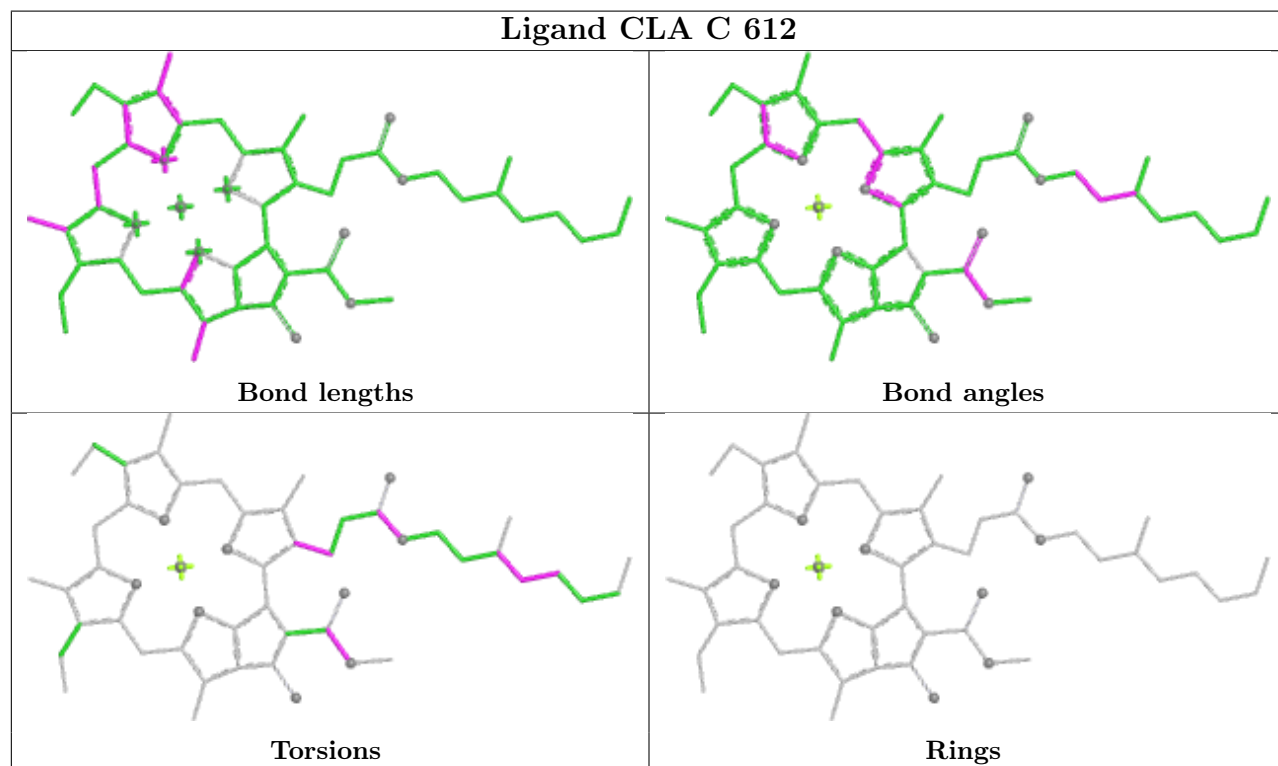
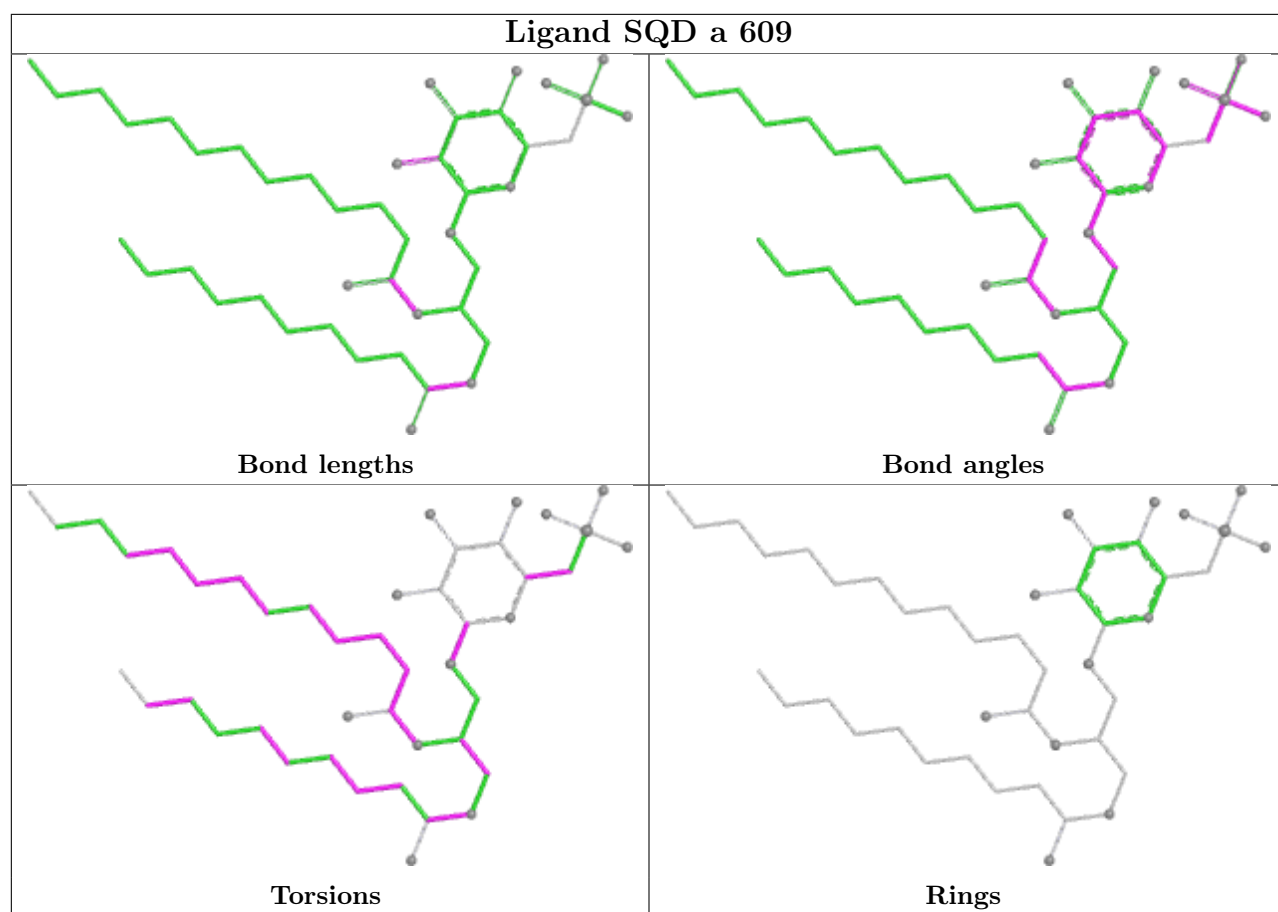
Rings

Ligand CHL r 302

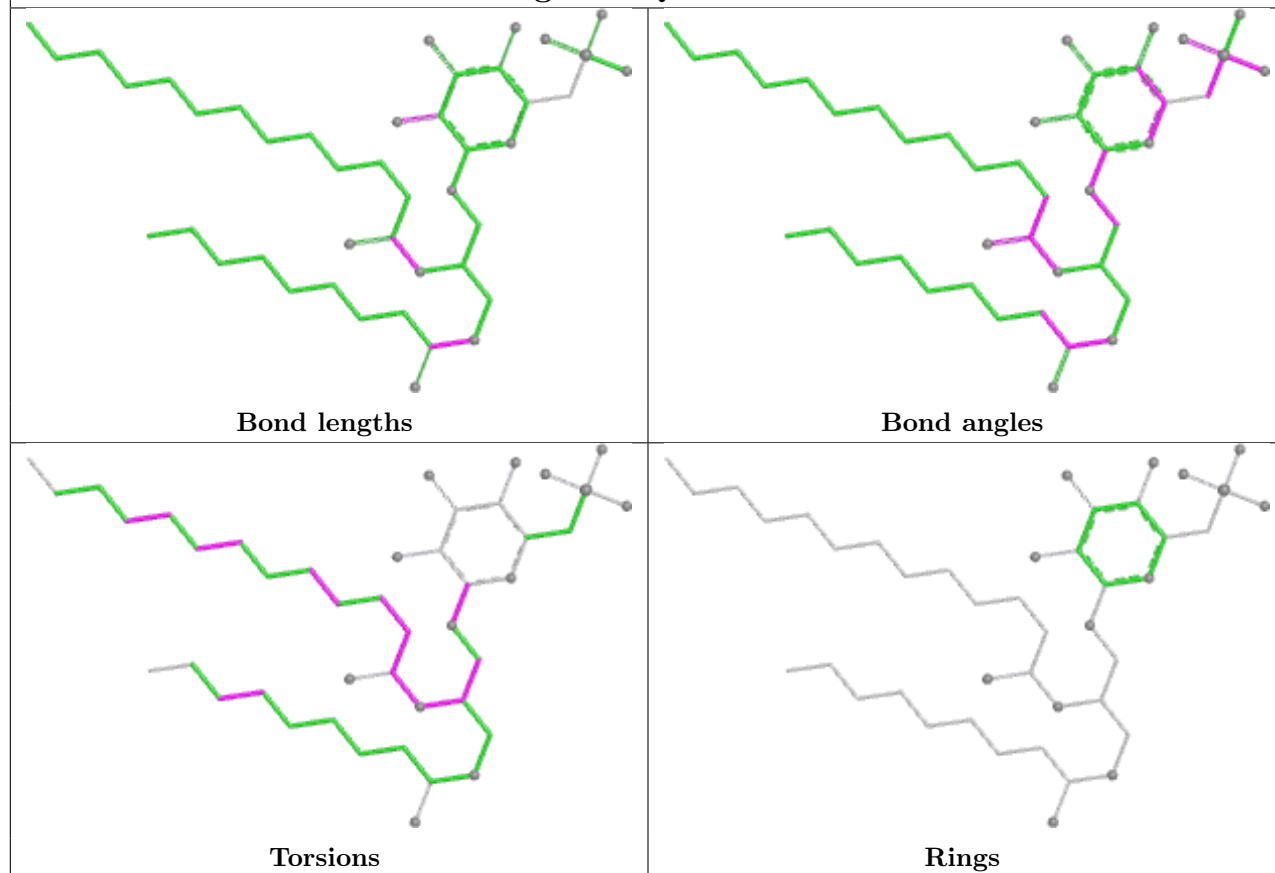


Ligand CLA r 312

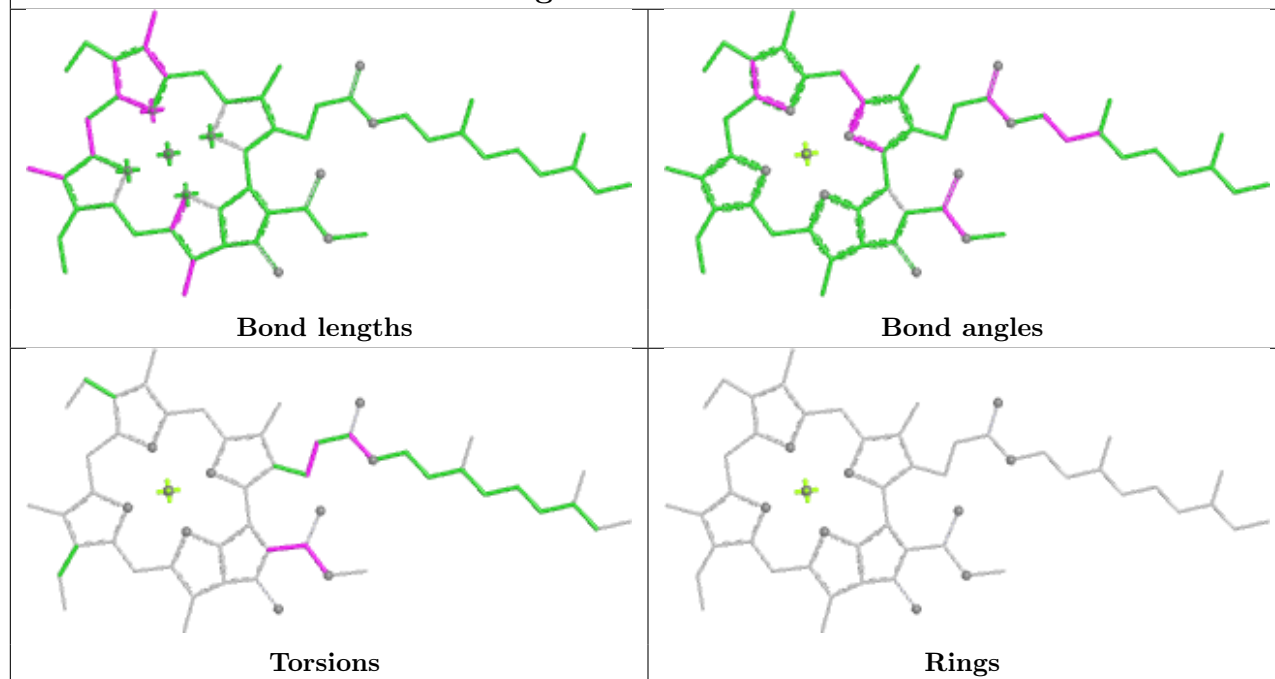


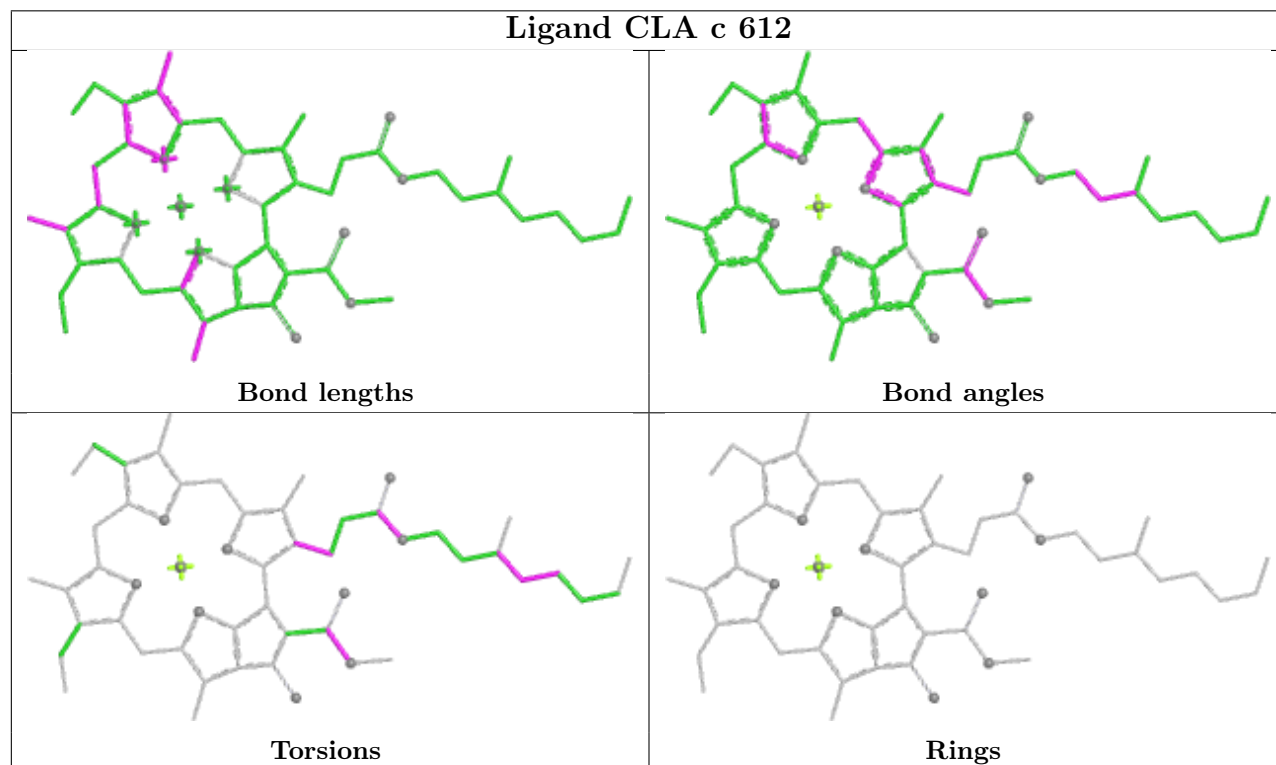
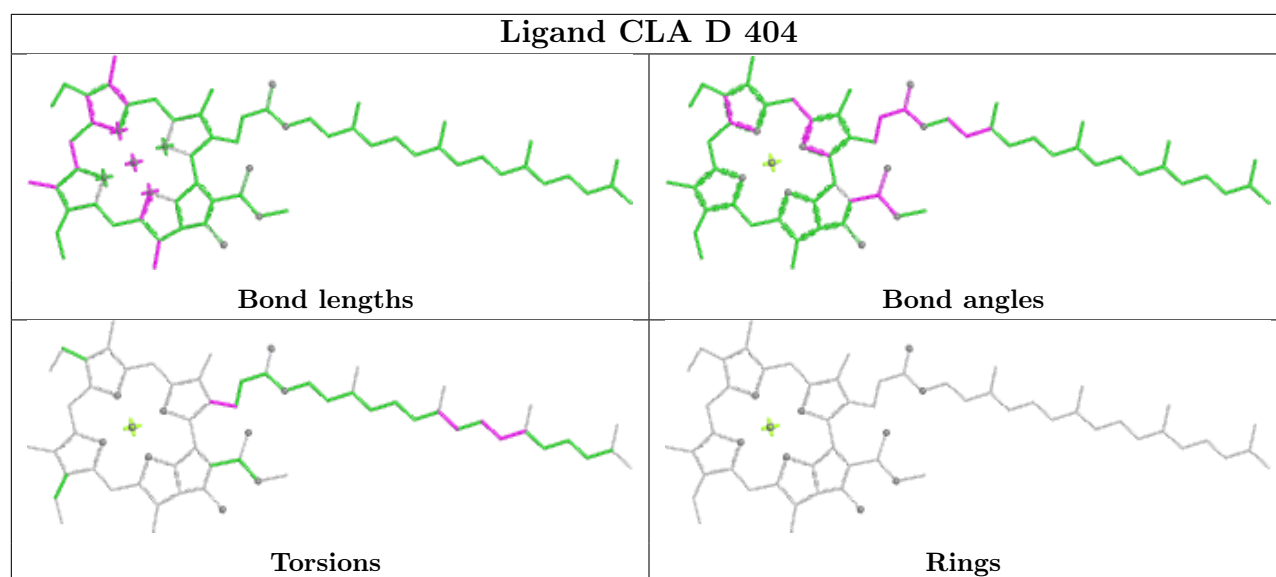


Ligand SQD d 409

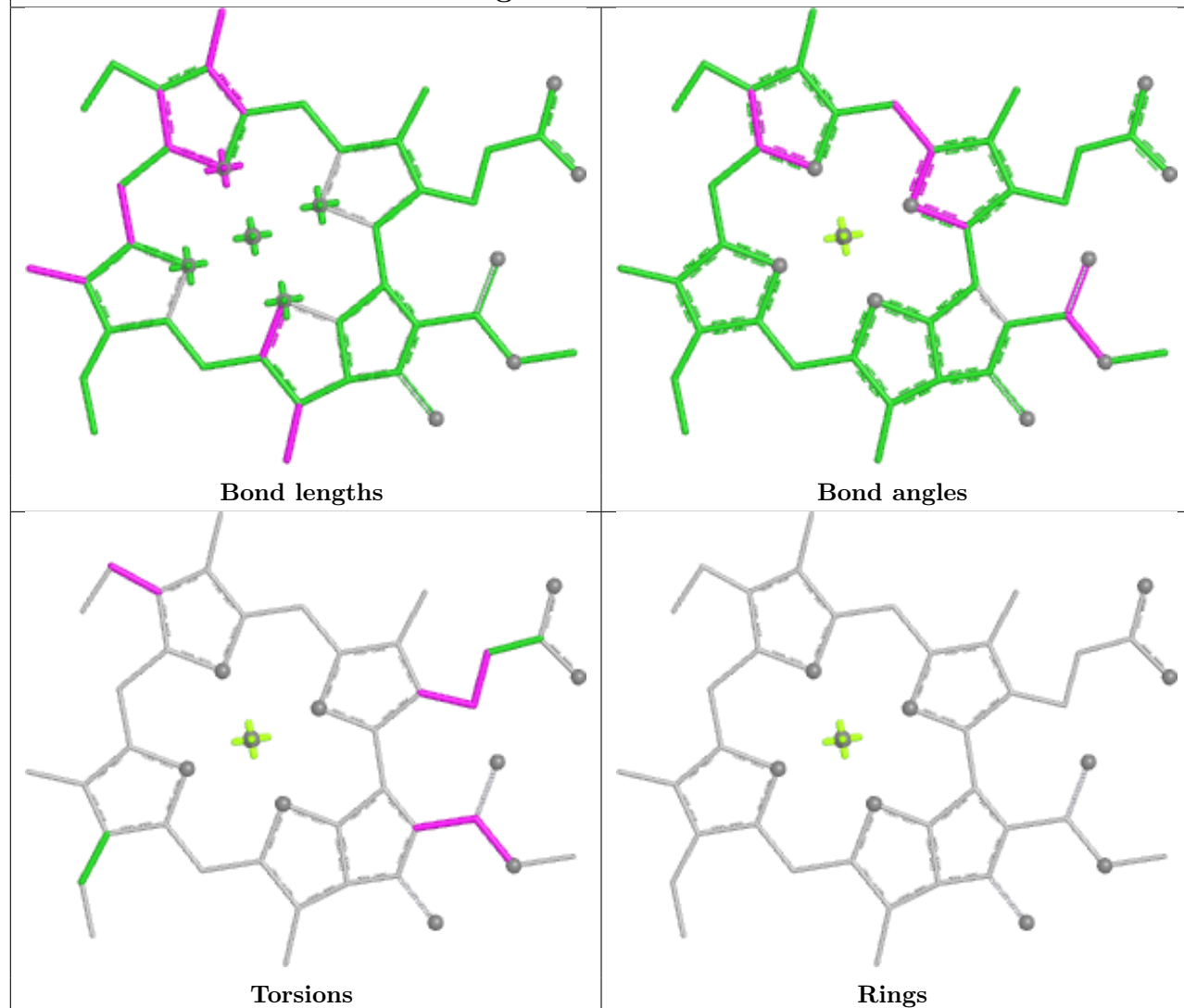


Ligand CLA 7 307

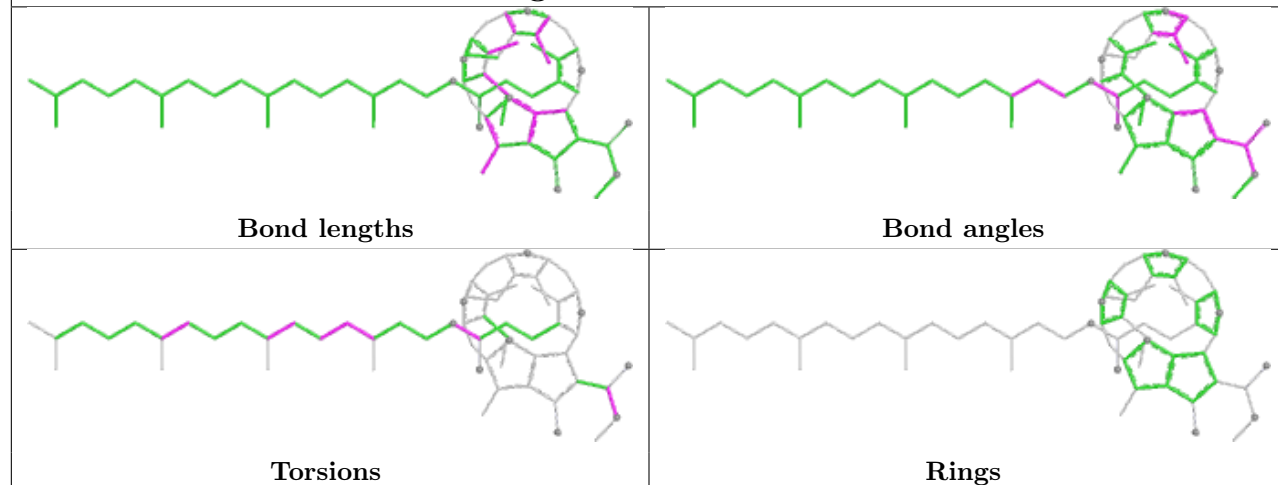




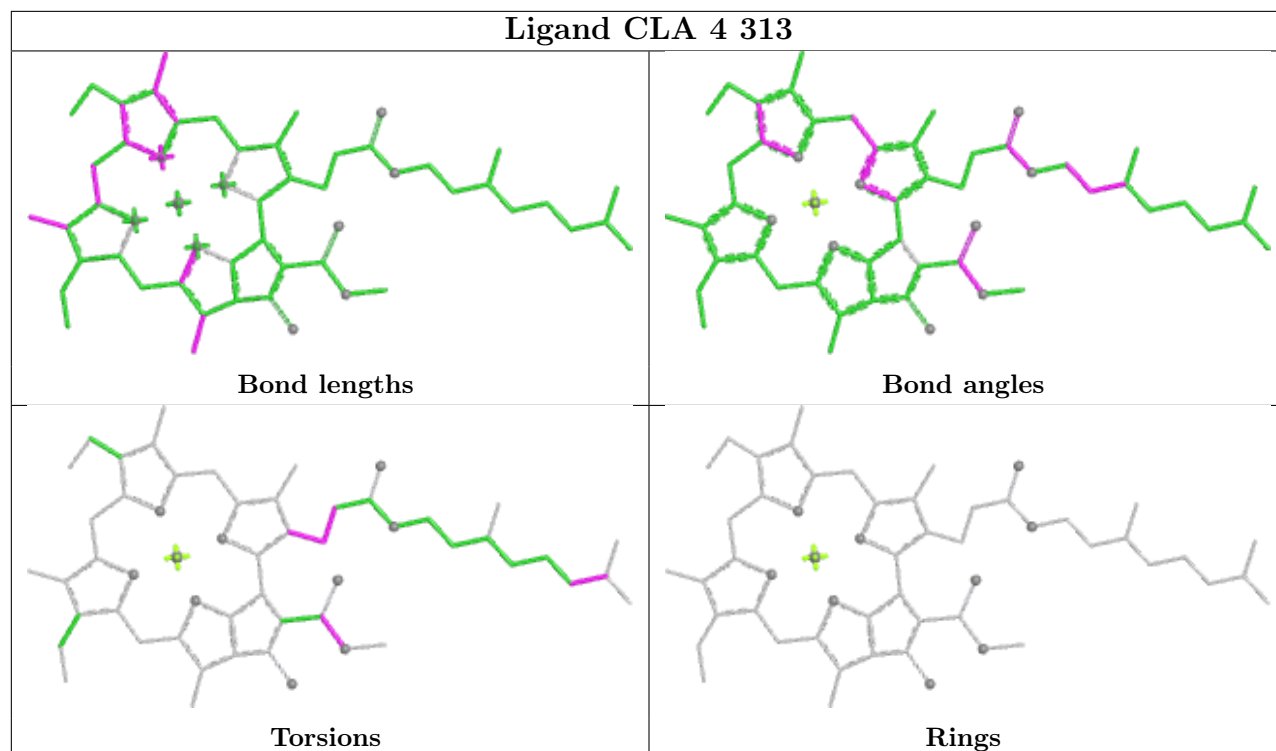
Ligand CLA b 601



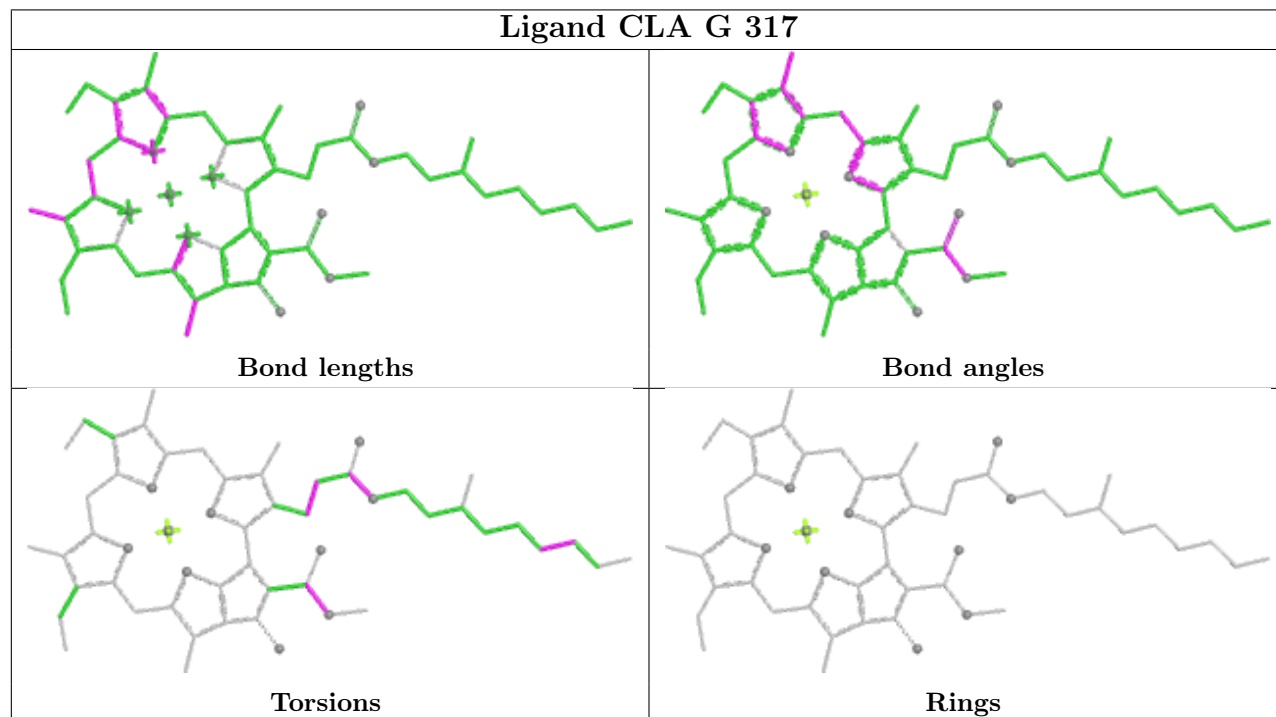
Ligand PHO D 403

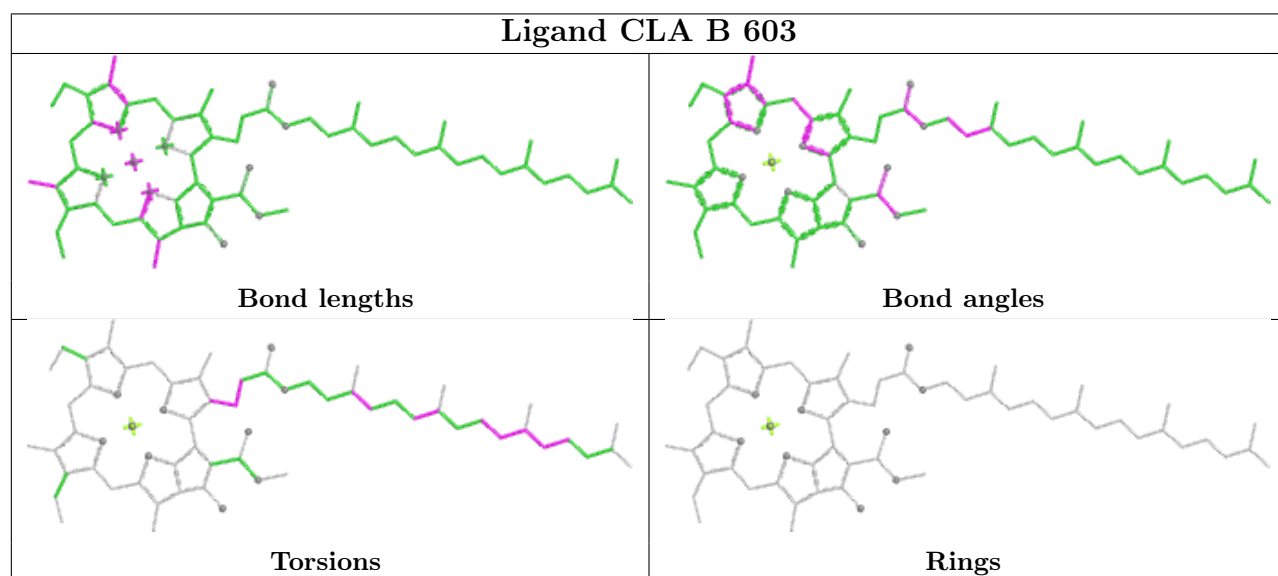
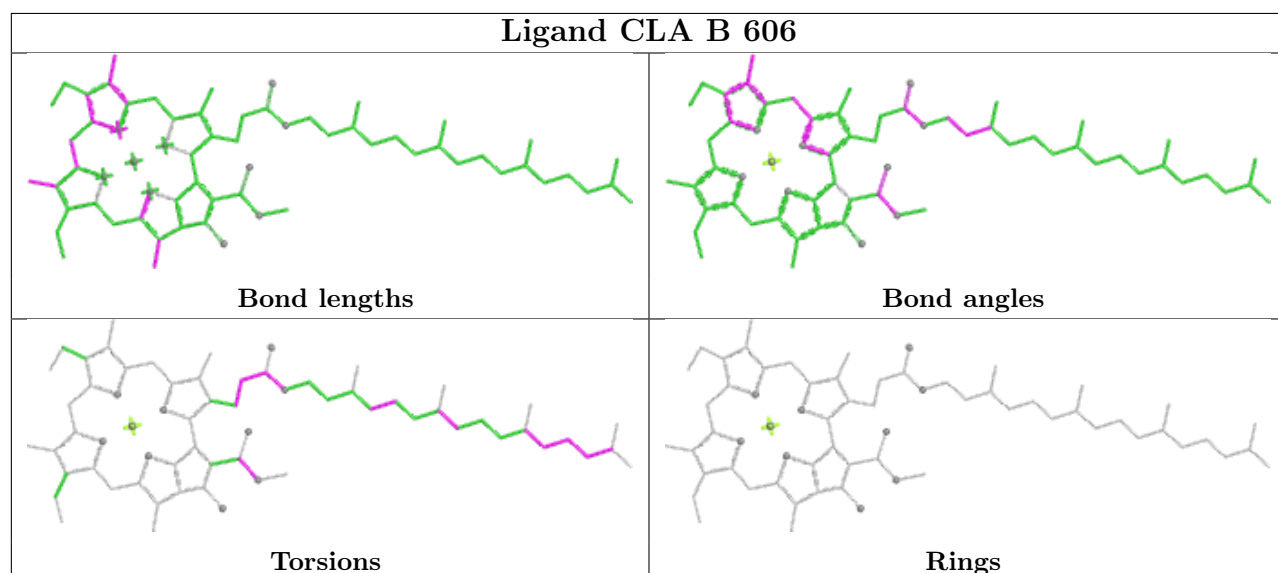
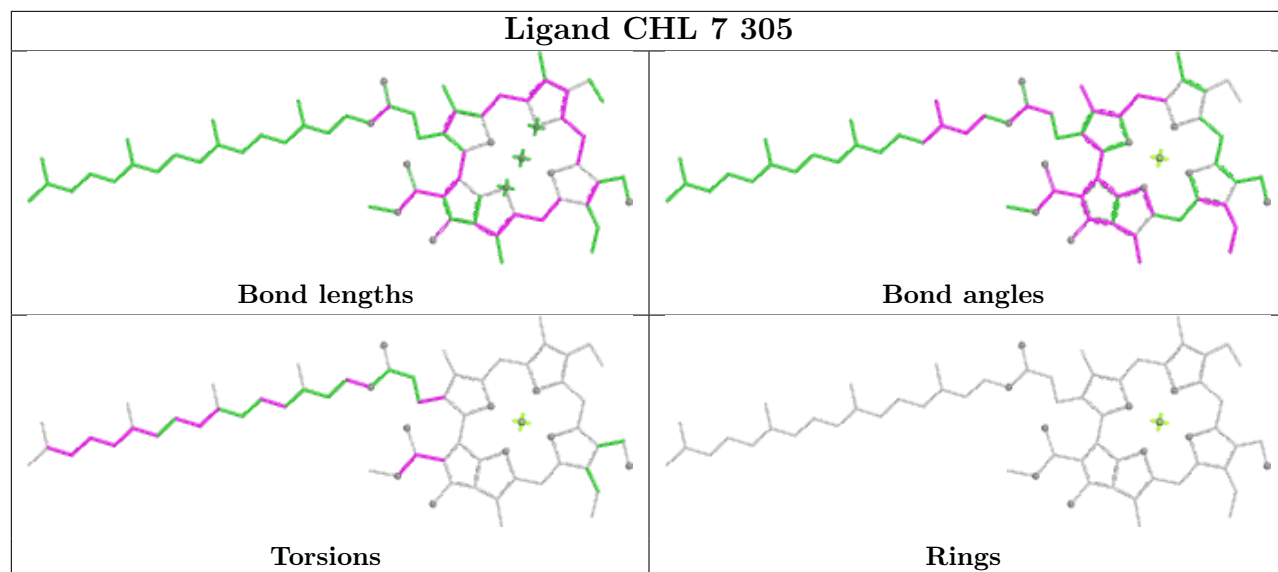


Ligand CLA 4 313

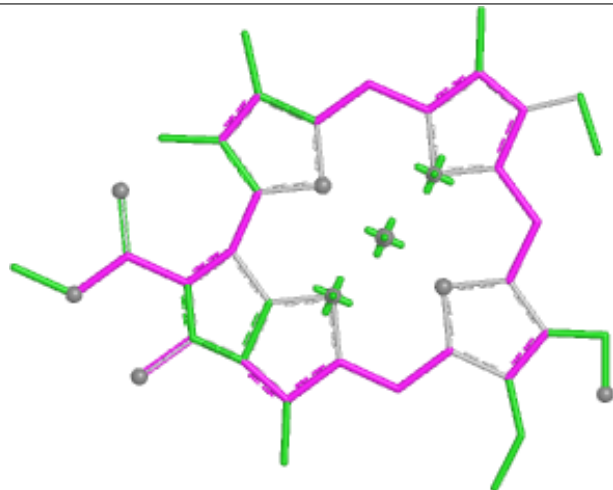


Ligand CLA G 317





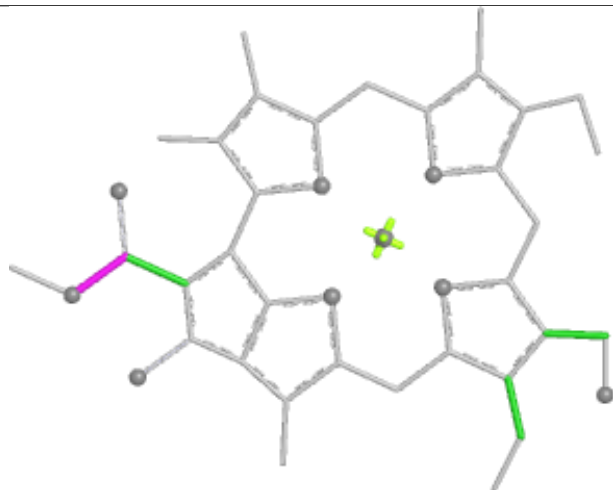
Ligand CHL 2 310



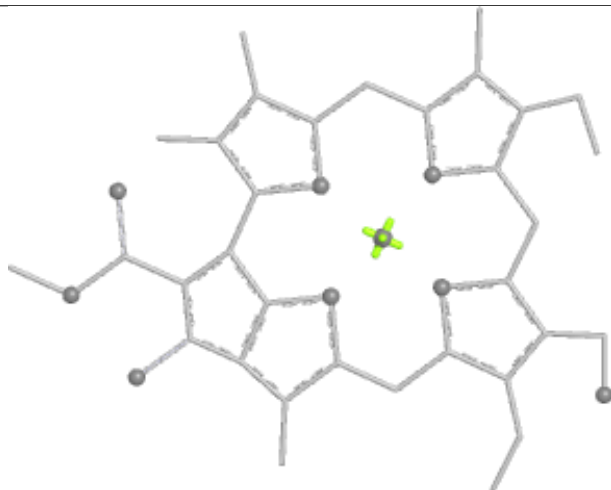
Bond lengths



Bond angles

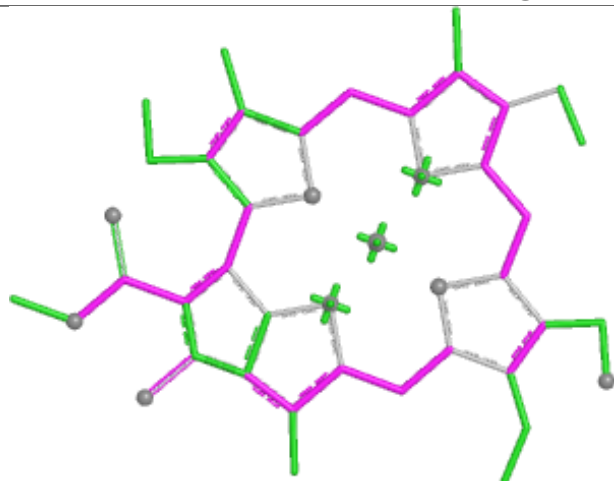


Torsions

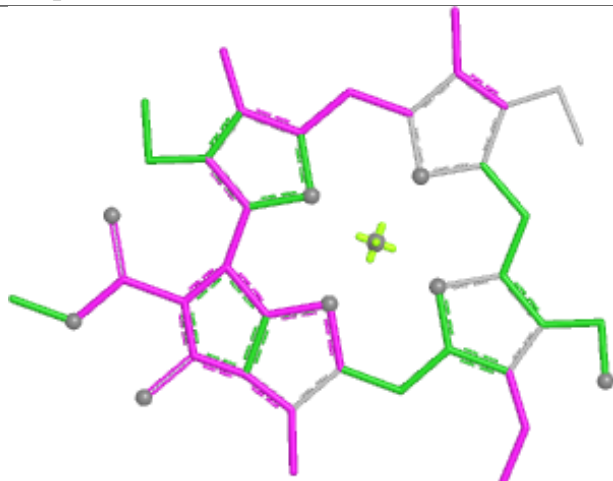


Rings

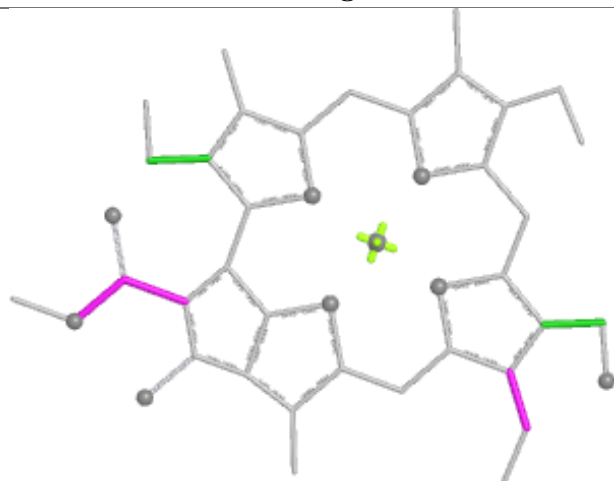
Ligand CHL p 313



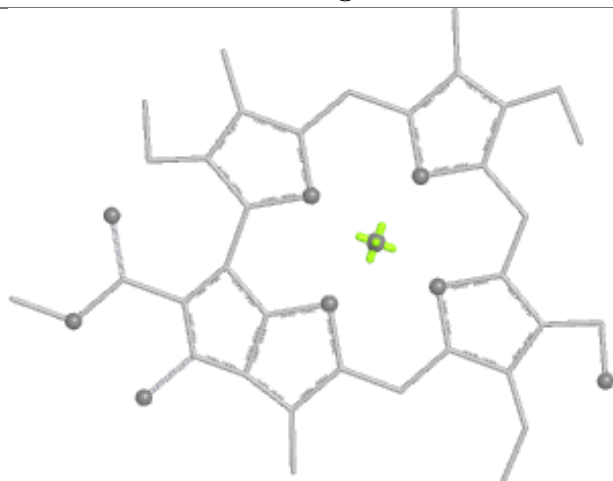
Bond lengths



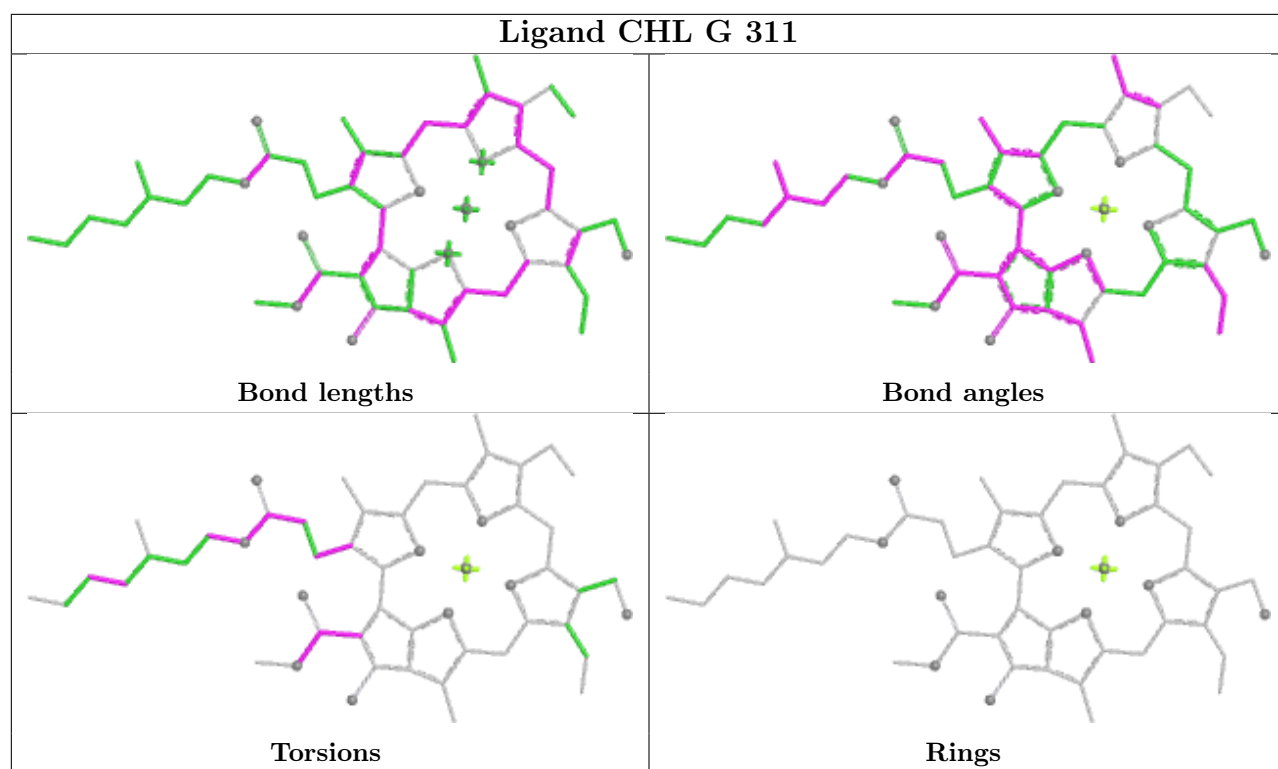
Bond angles



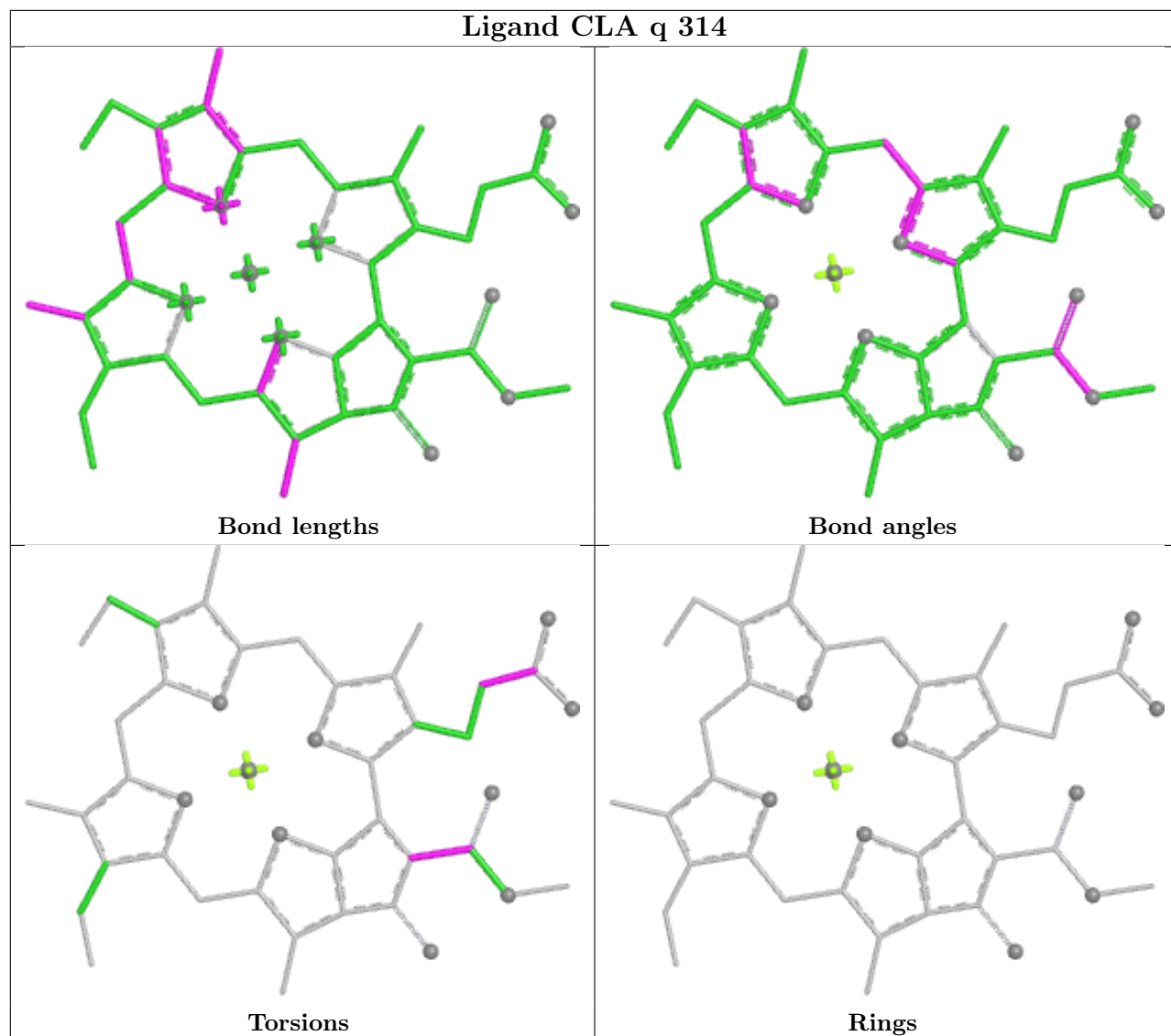
Torsions

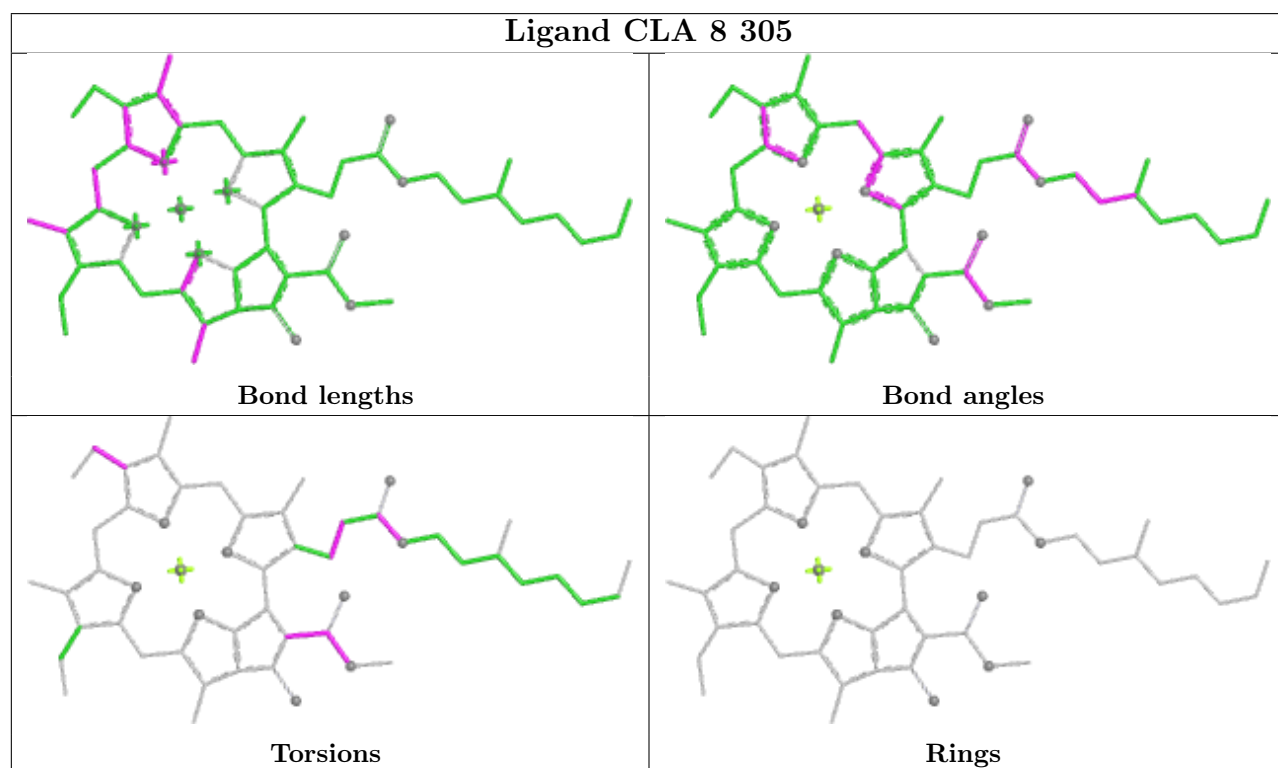
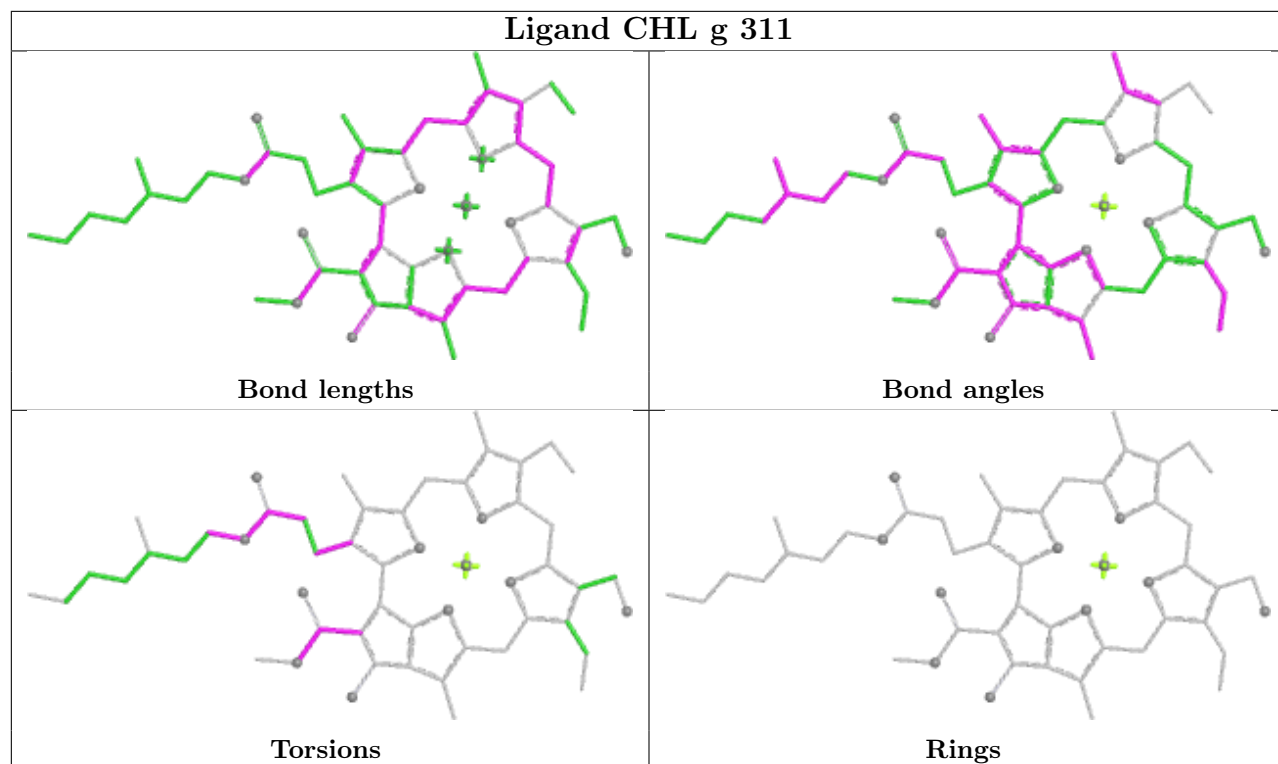


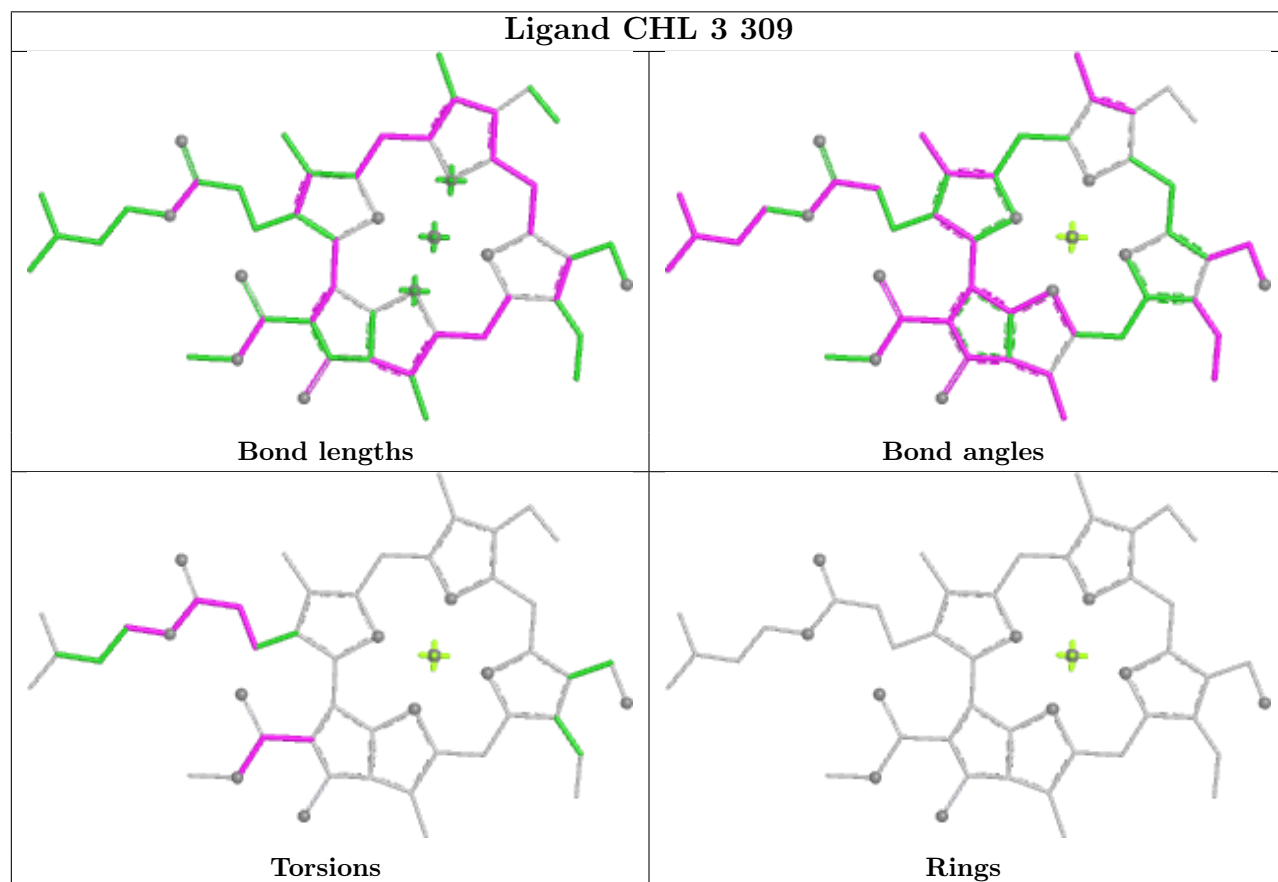
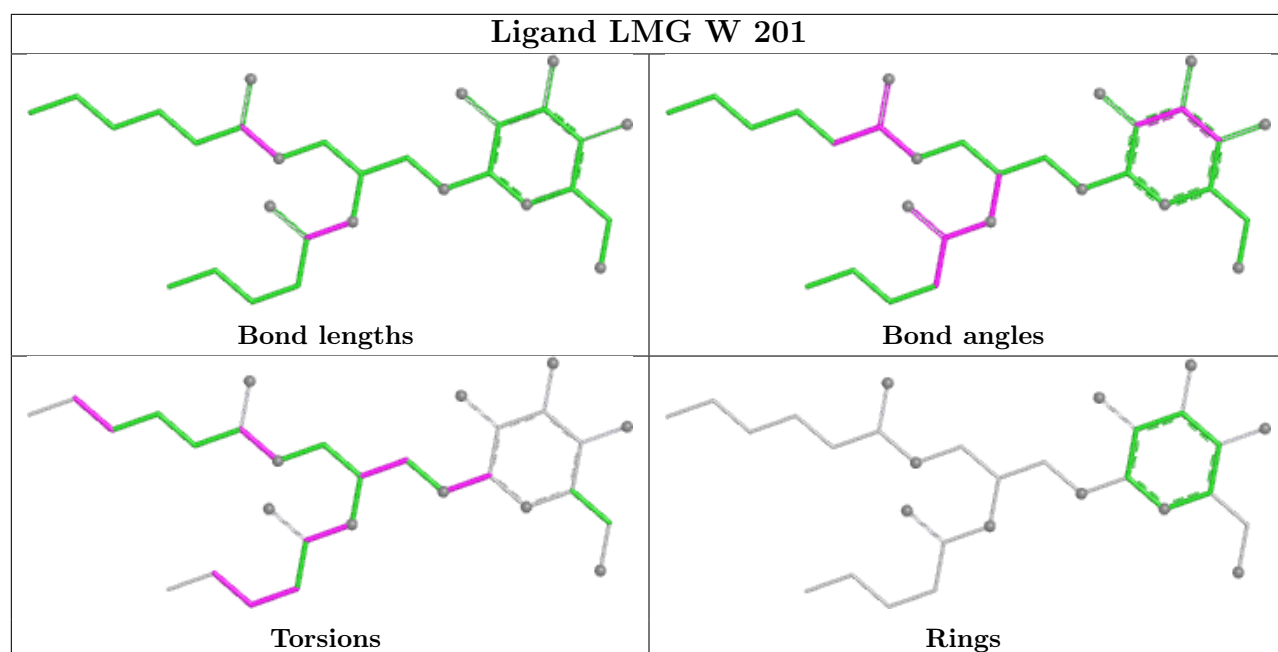
Rings

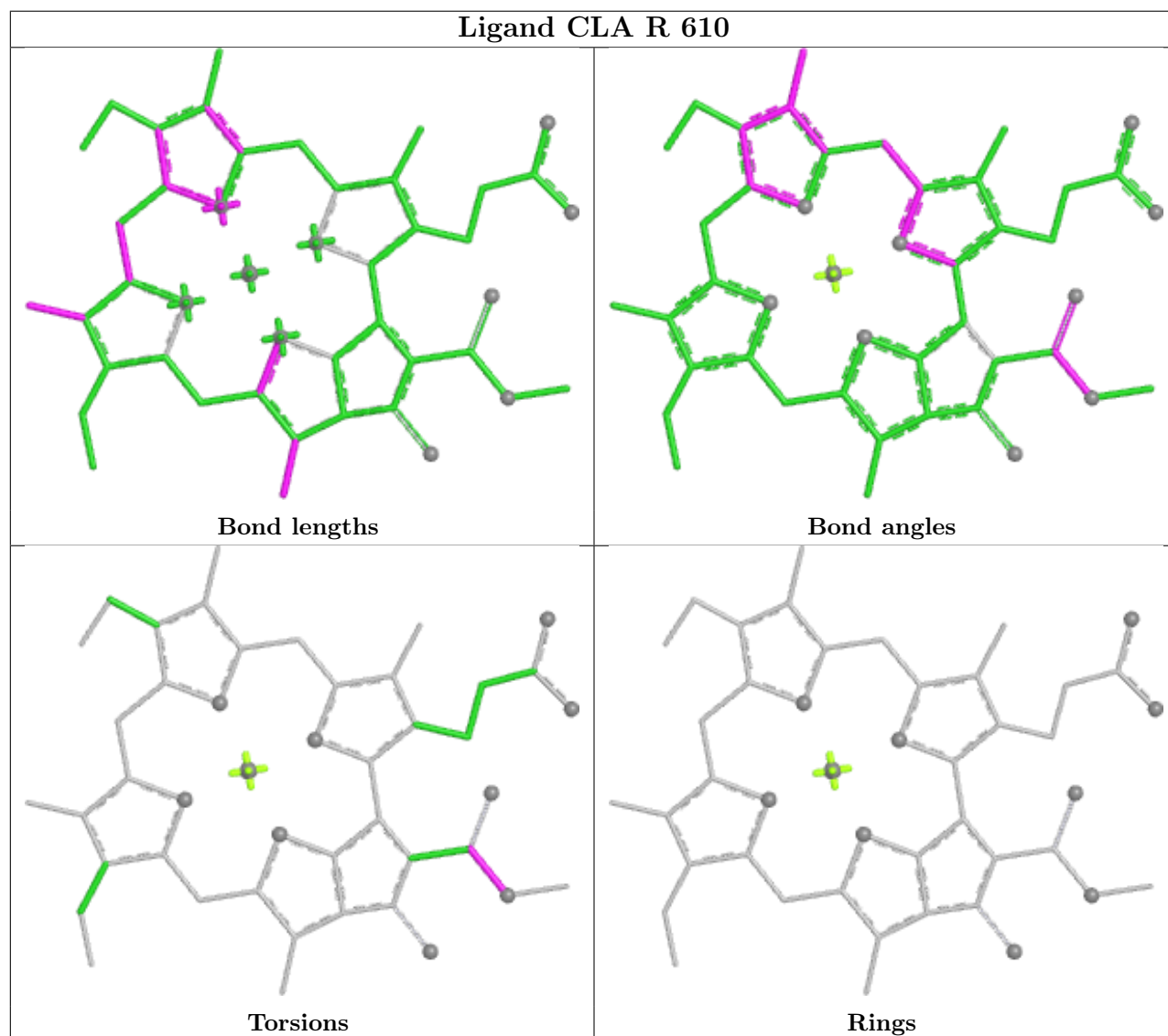
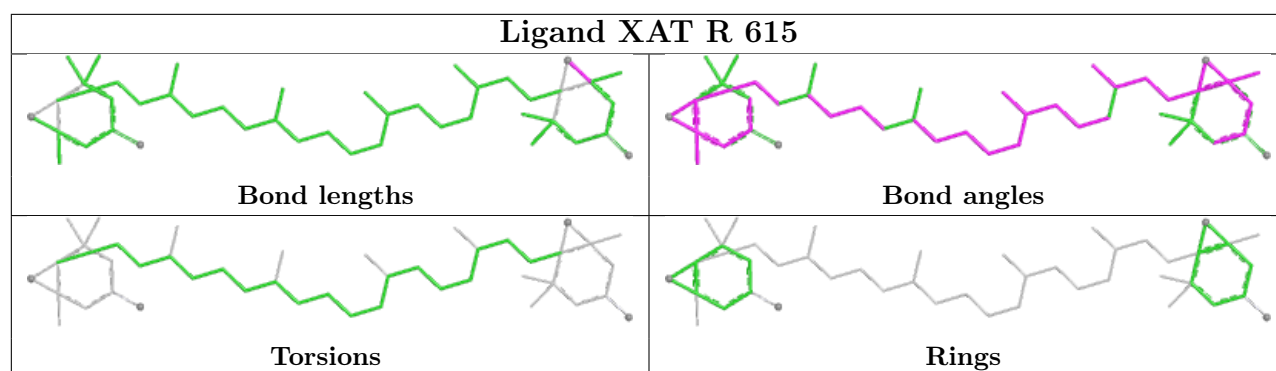


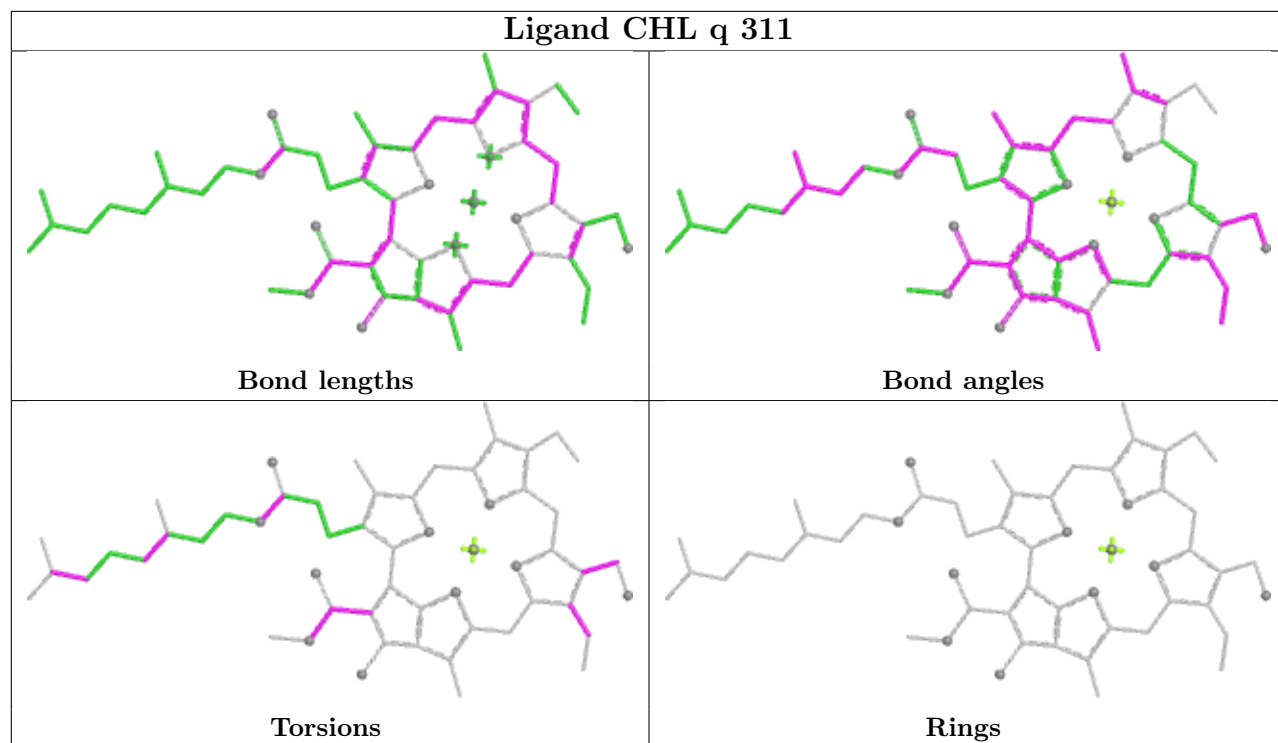
Ligand CLA q 314



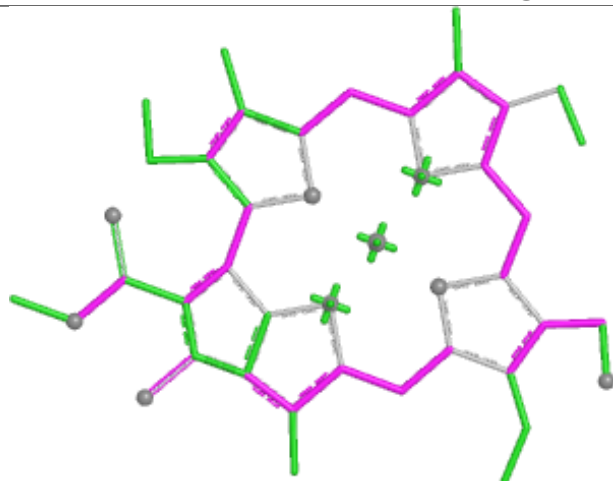




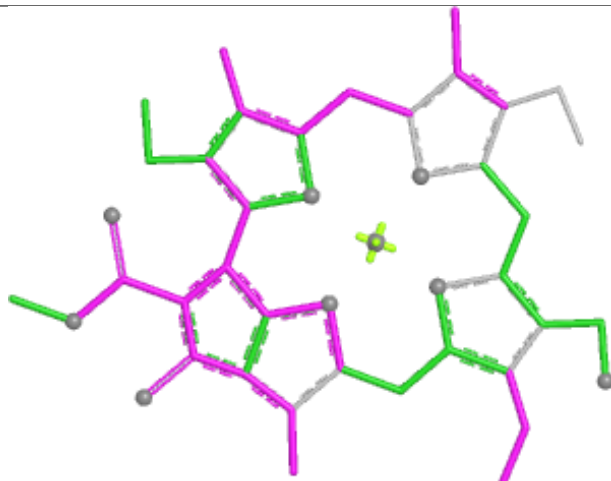




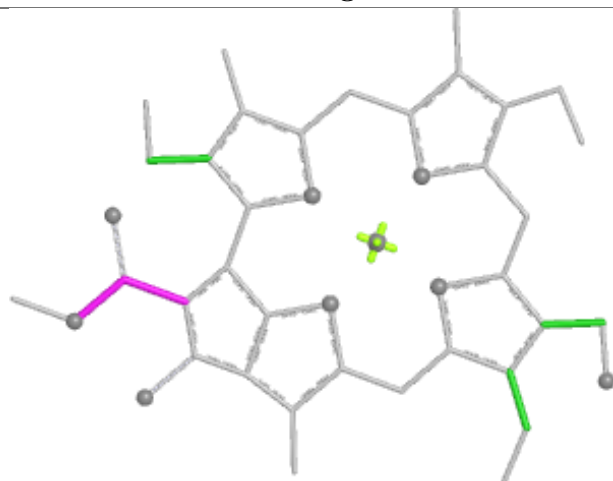
Ligand CHL 1 308



Bond lengths



Bond angles

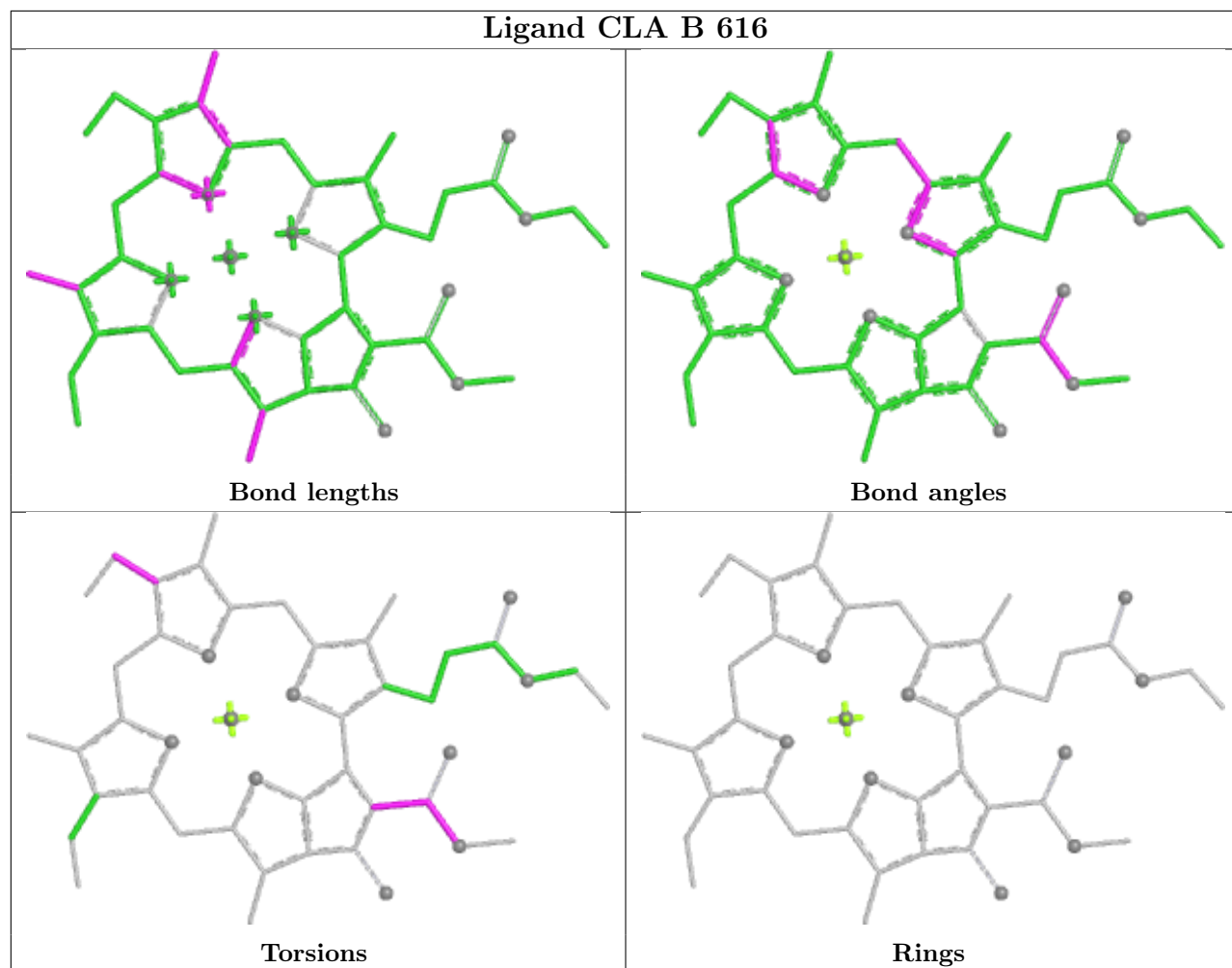


Torsions

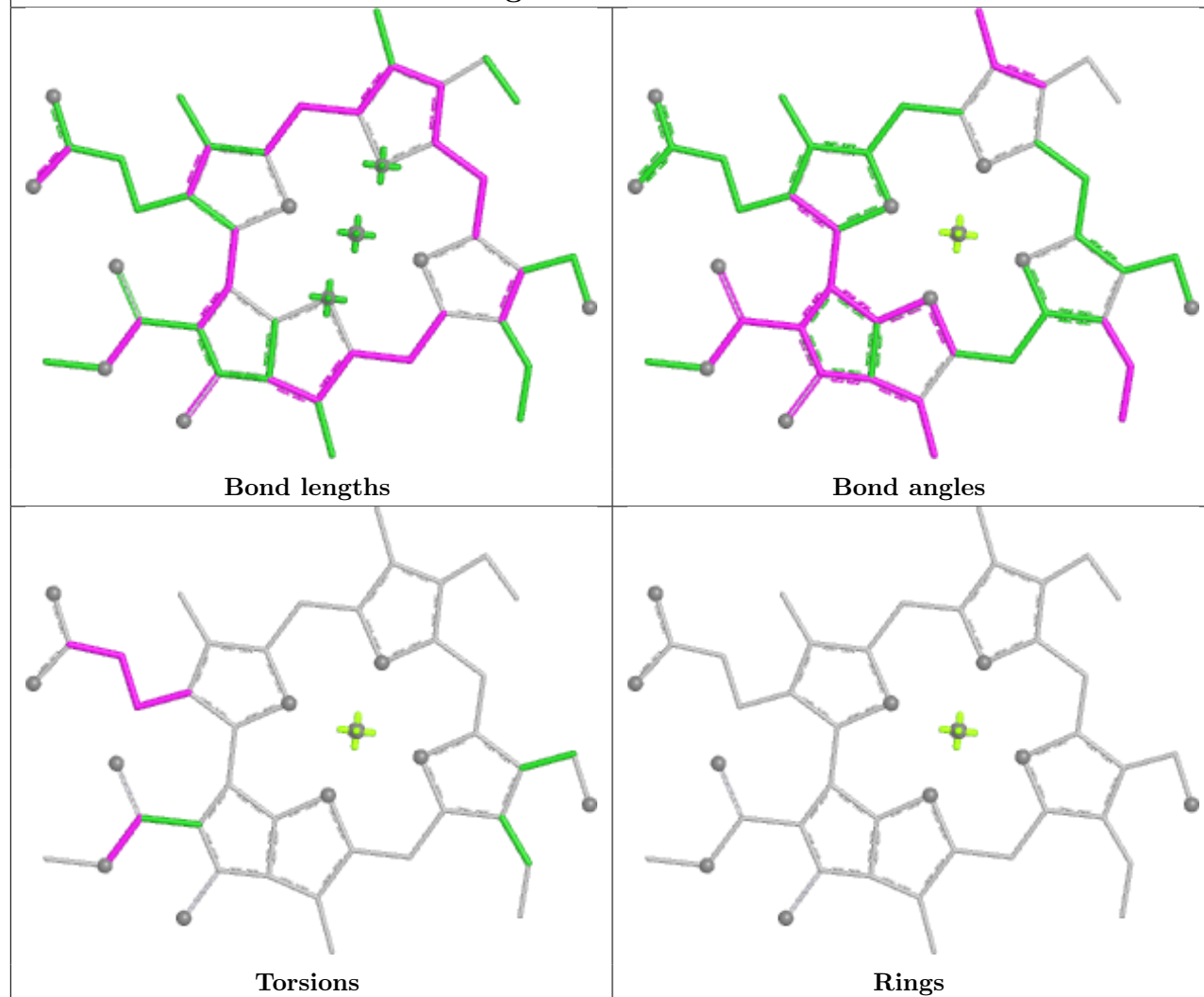


Rings

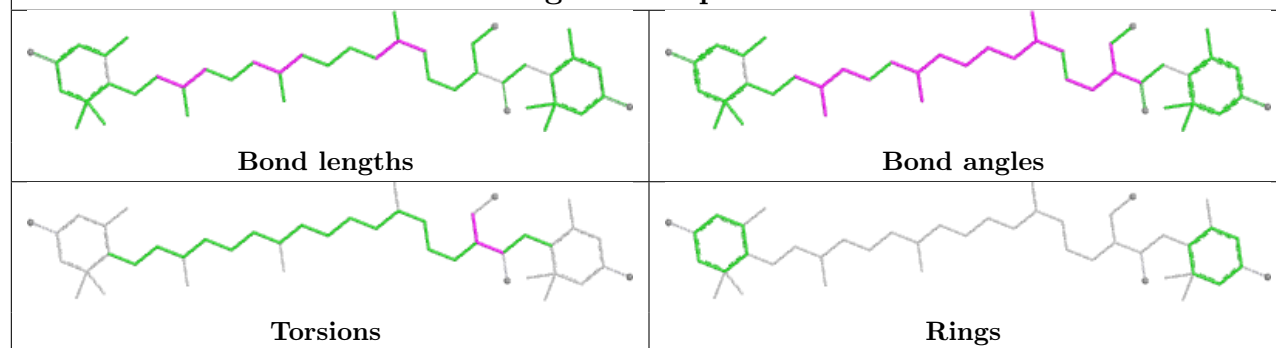
Ligand CLA B 616



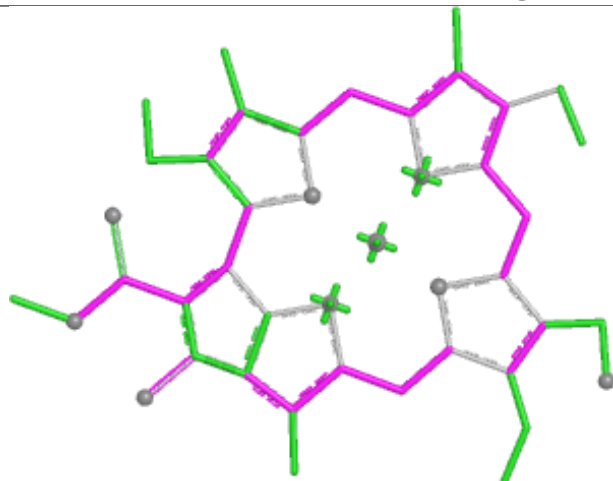
Ligand CHL 3 310



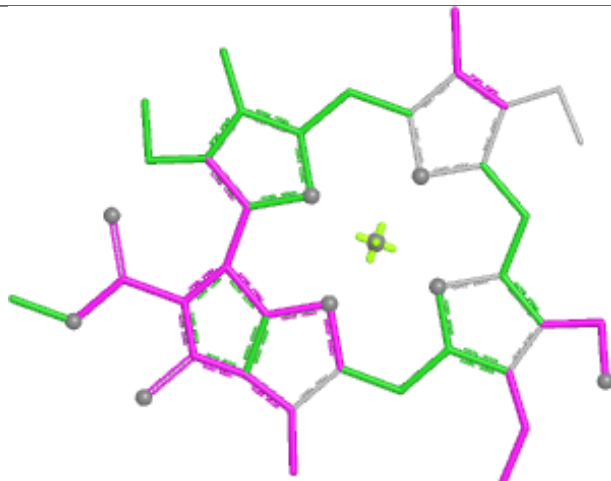
Ligand OIE p 302



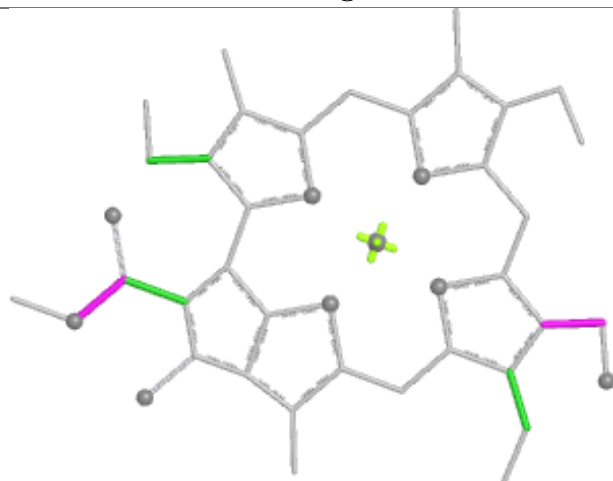
Ligand CHL Y 308



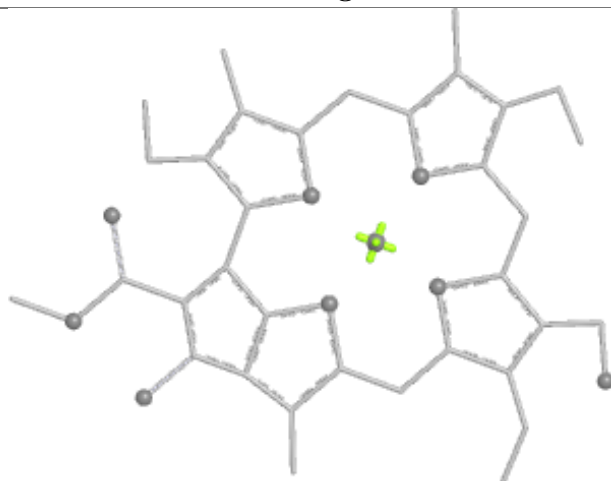
Bond lengths



Bond angles

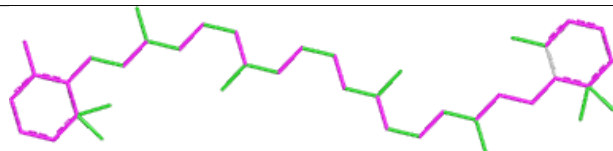


Torsions

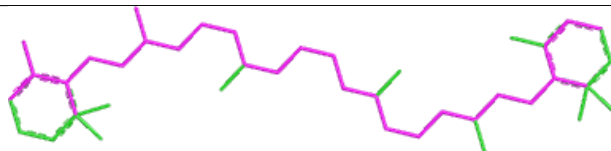


Rings

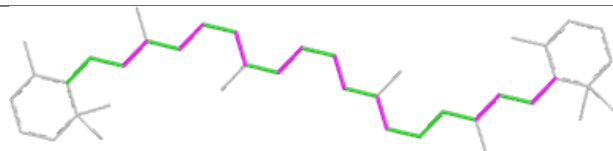
Ligand 8CT B 617



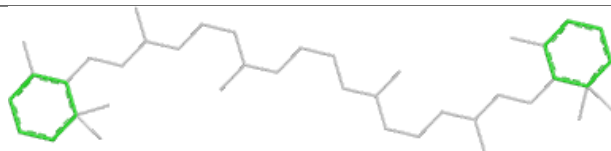
Bond lengths



Bond angles

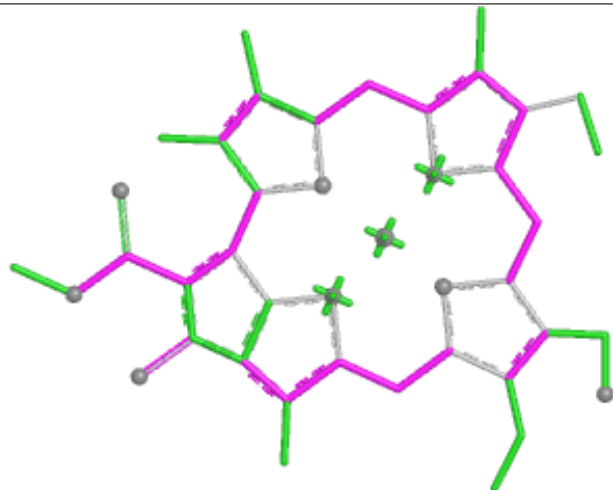


Torsions



Rings

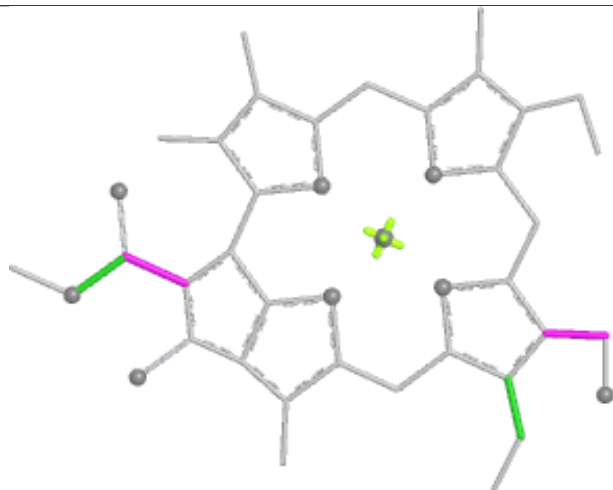
Ligand CHL y 318



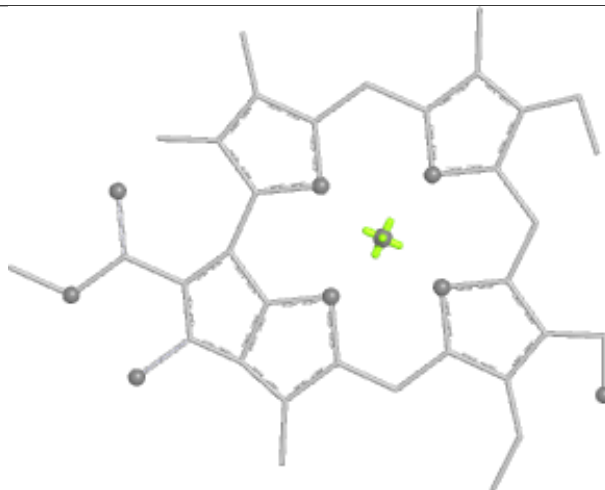
Bond lengths



Bond angles

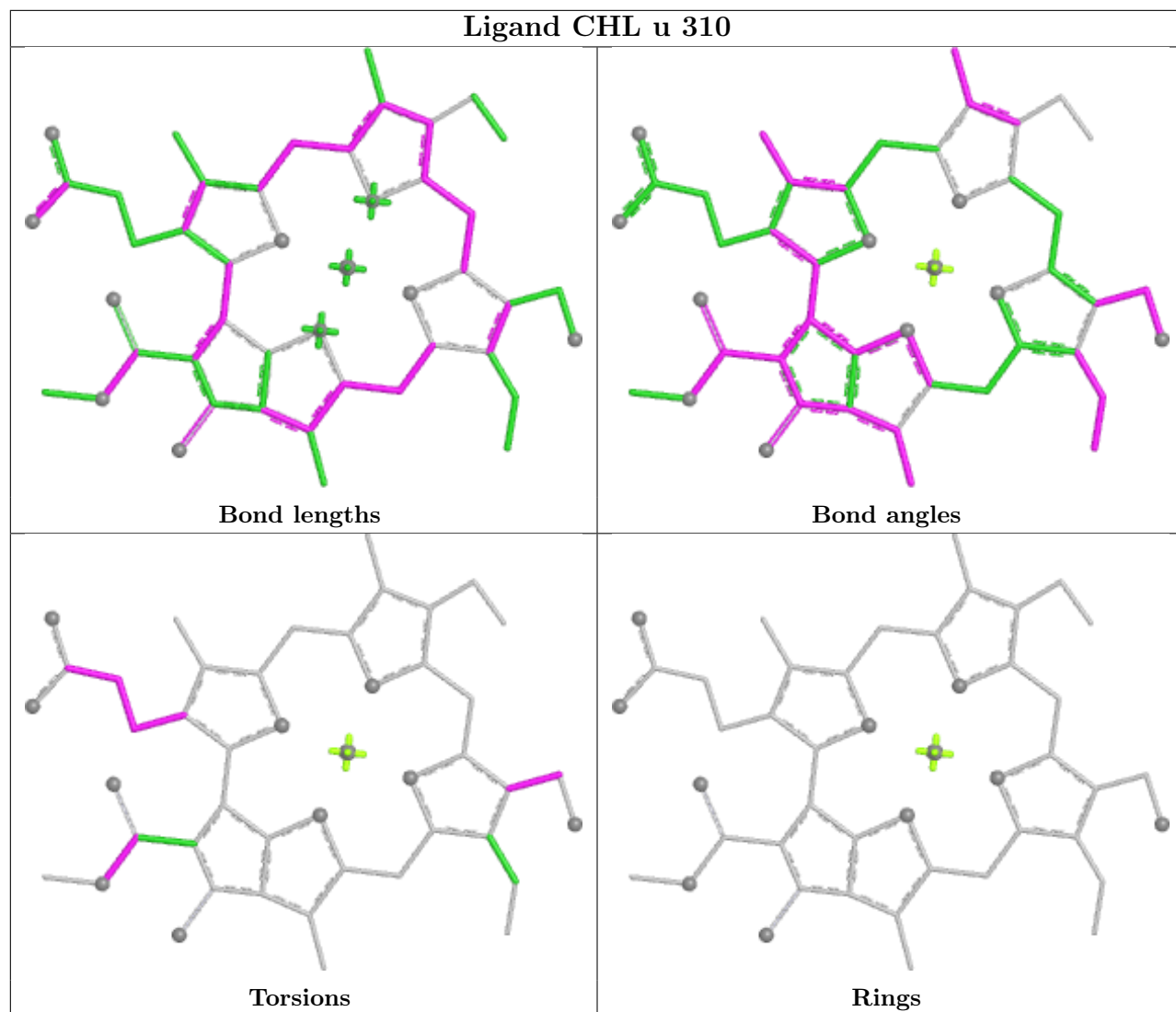


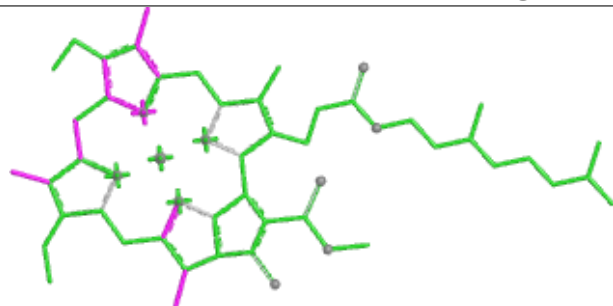
Torsions



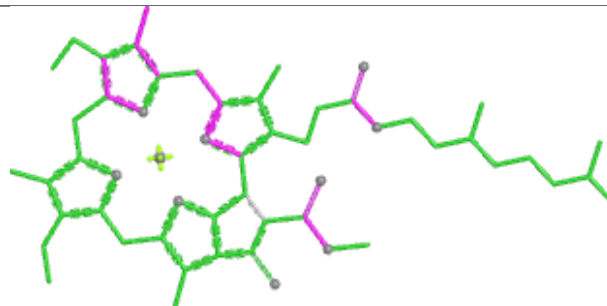
Rings

Ligand CHL u 310

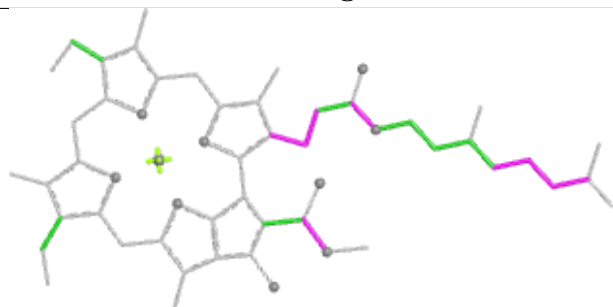


Ligand CLA B 608

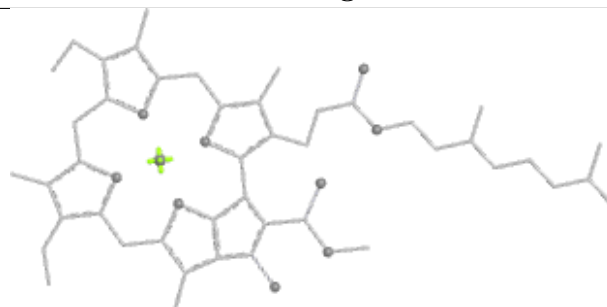
Bond lengths



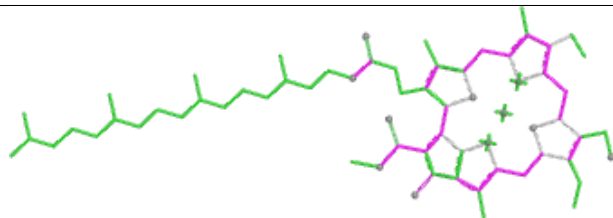
Bond angles



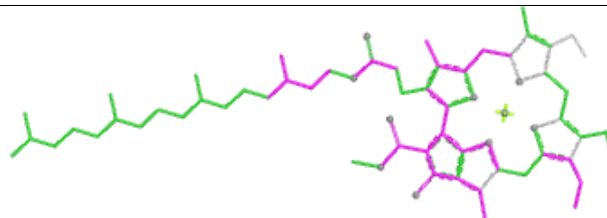
Torsions



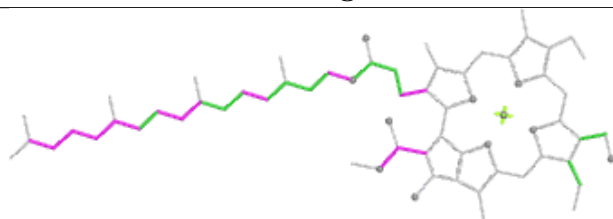
Rings

Ligand CHL p 305

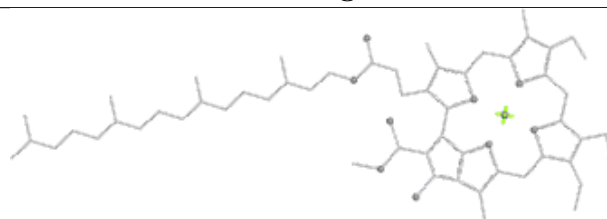
Bond lengths



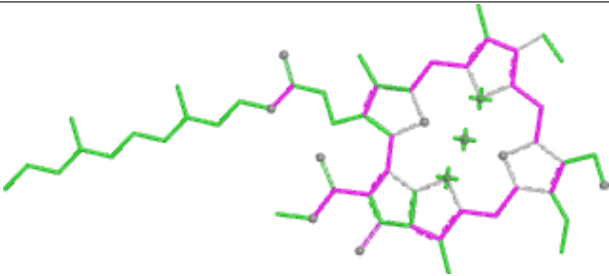
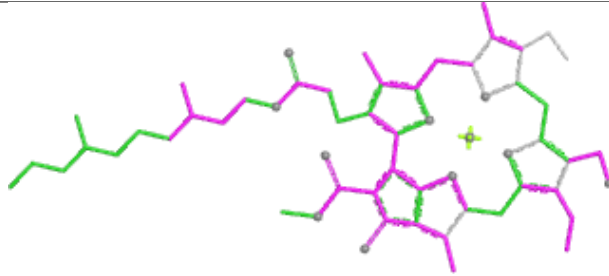
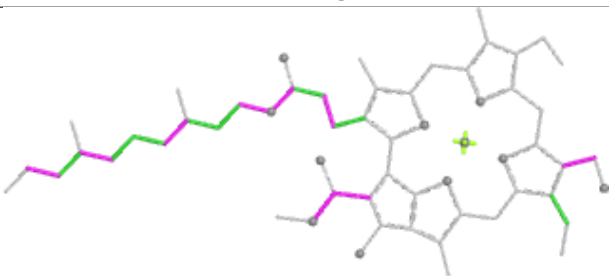
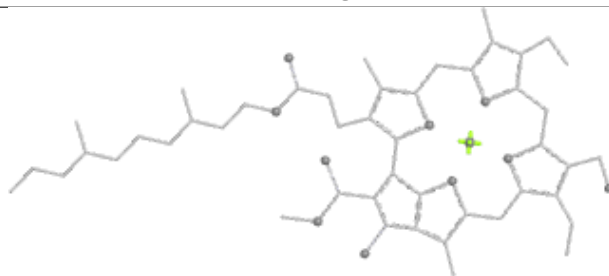
Bond angles



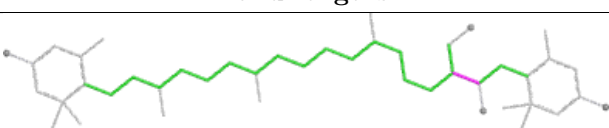
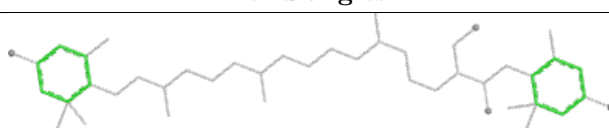


Torsions

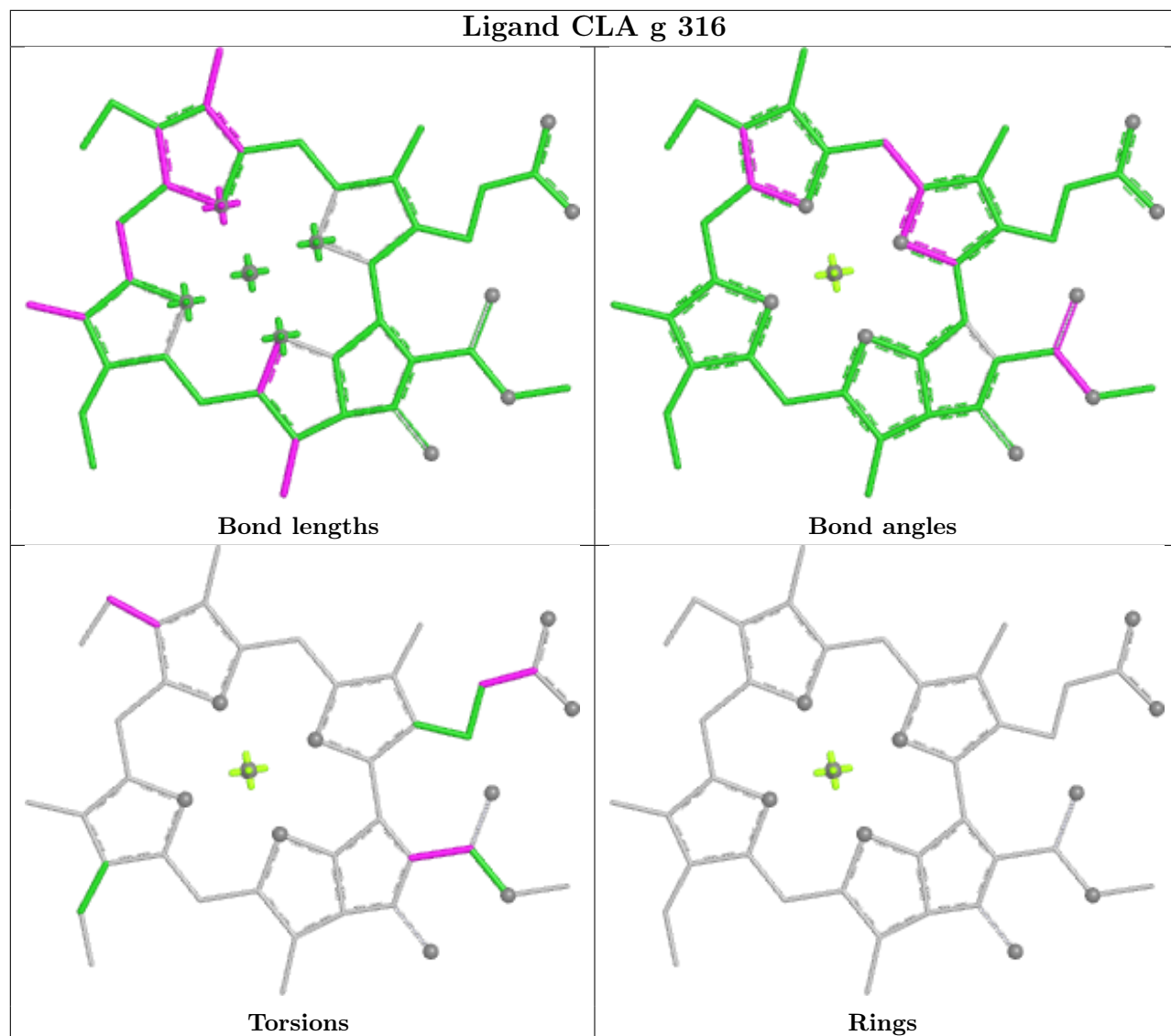


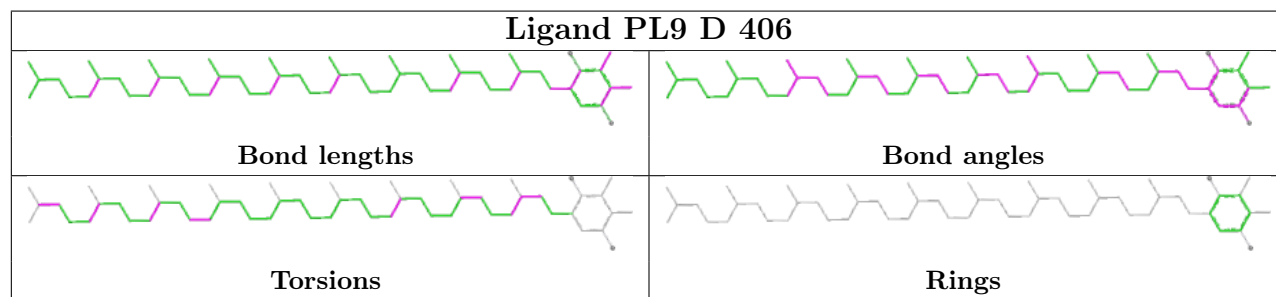
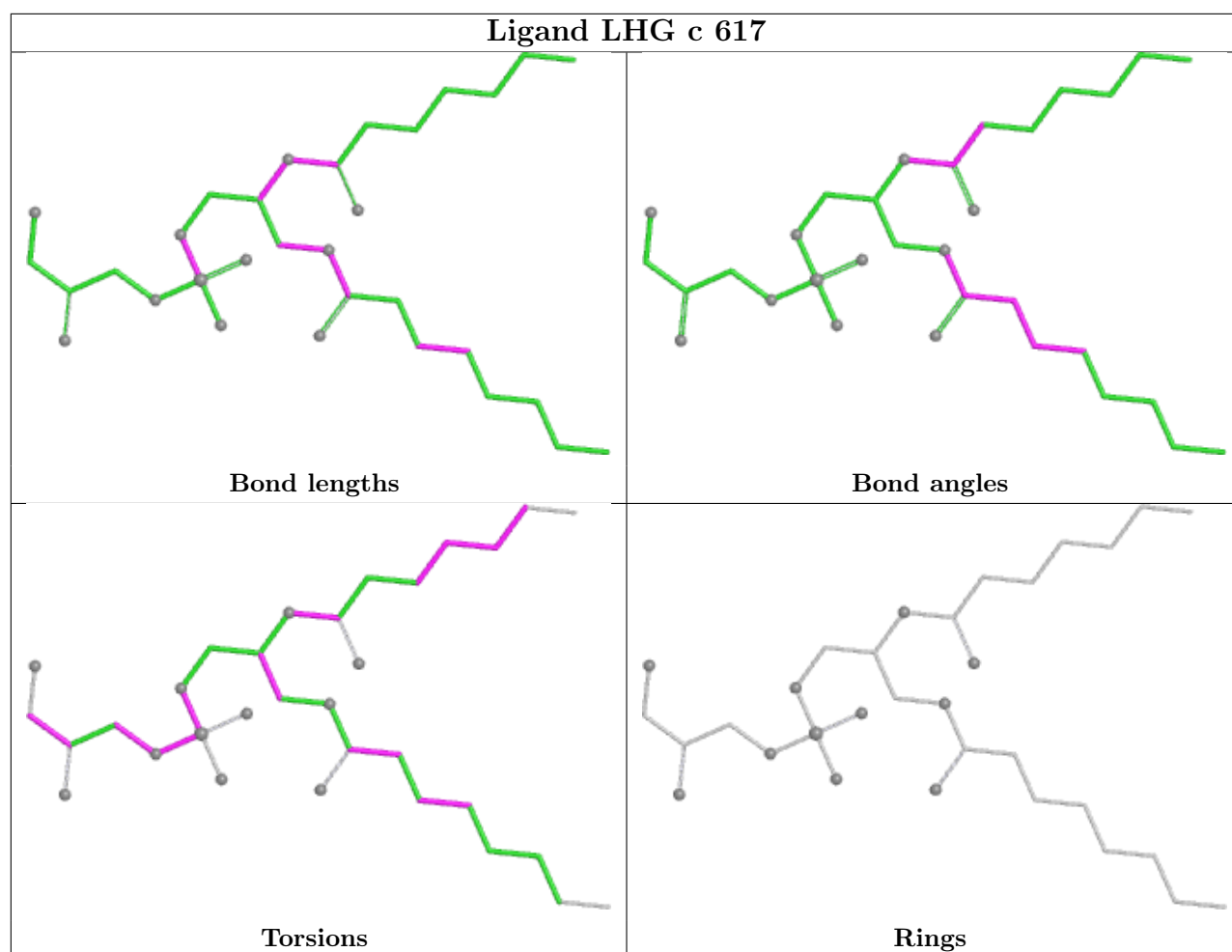
Rings

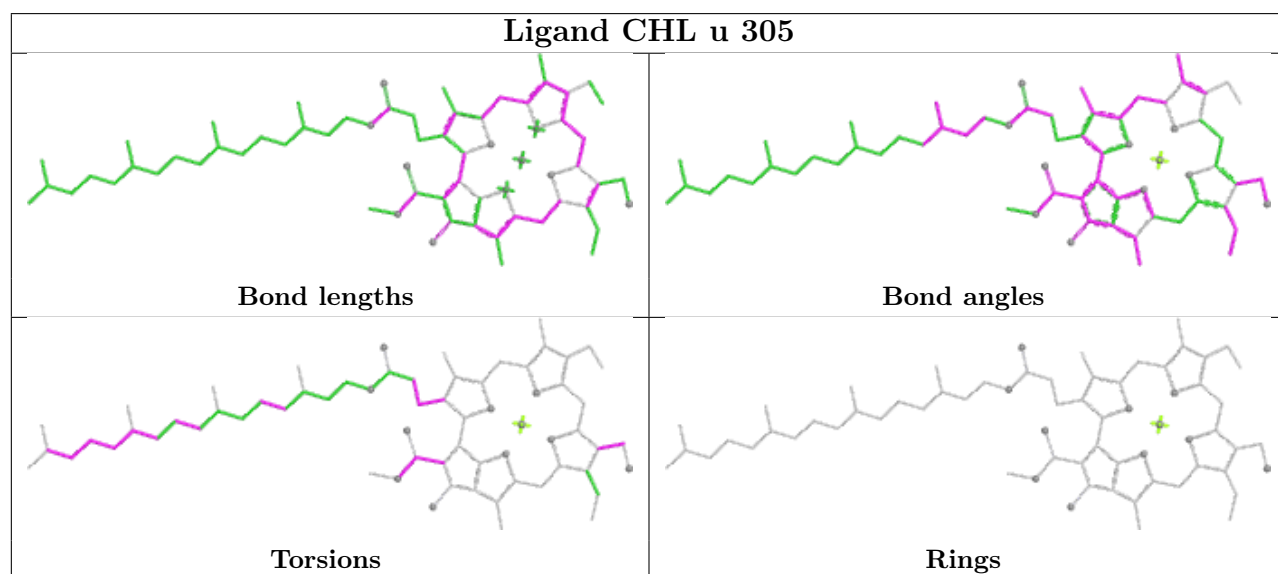
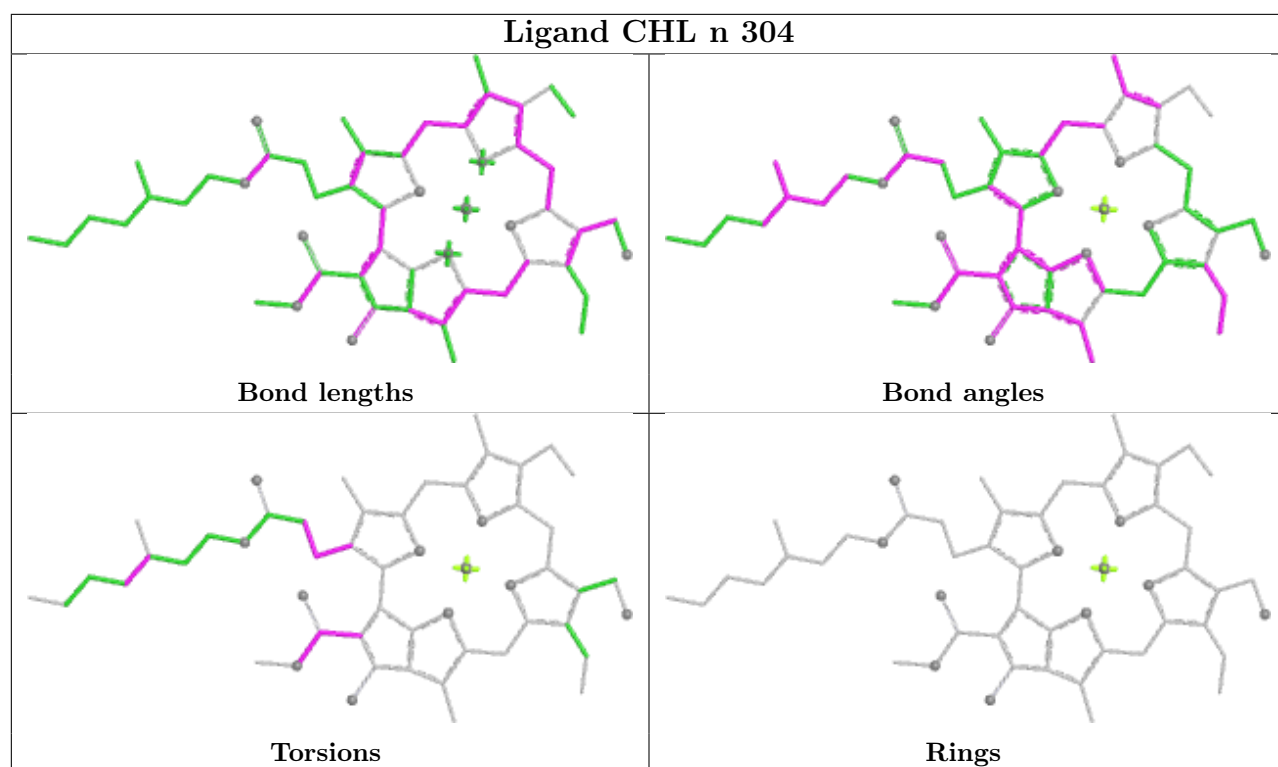
Ligand CHL s 403	
	
Bond lengths	Bond angles
	
Torsions	Rings

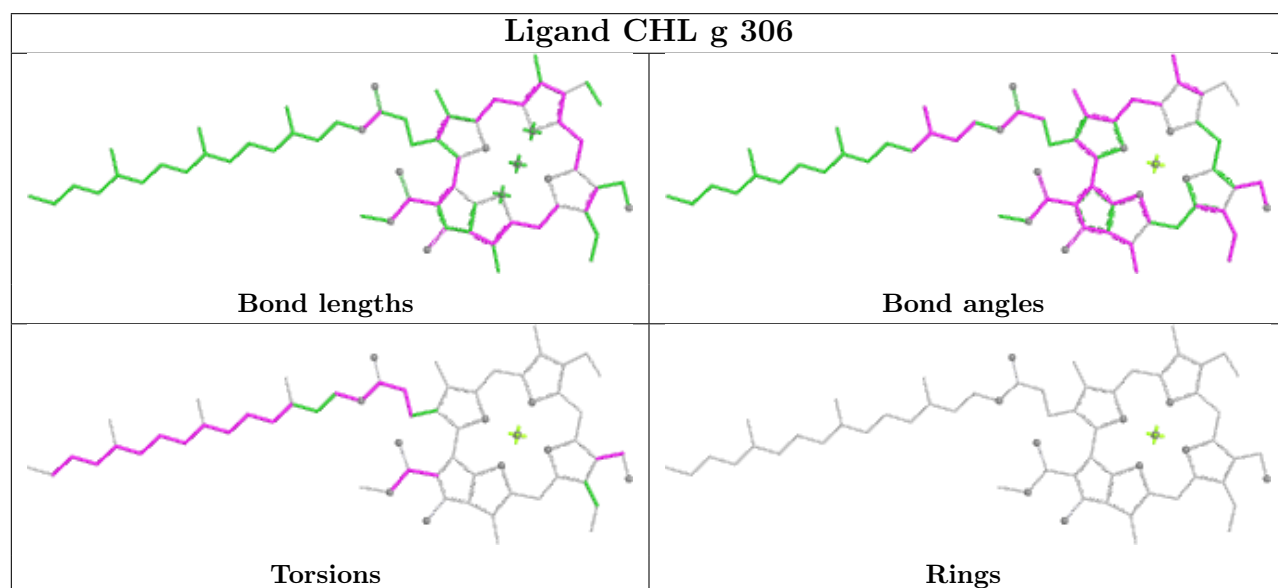
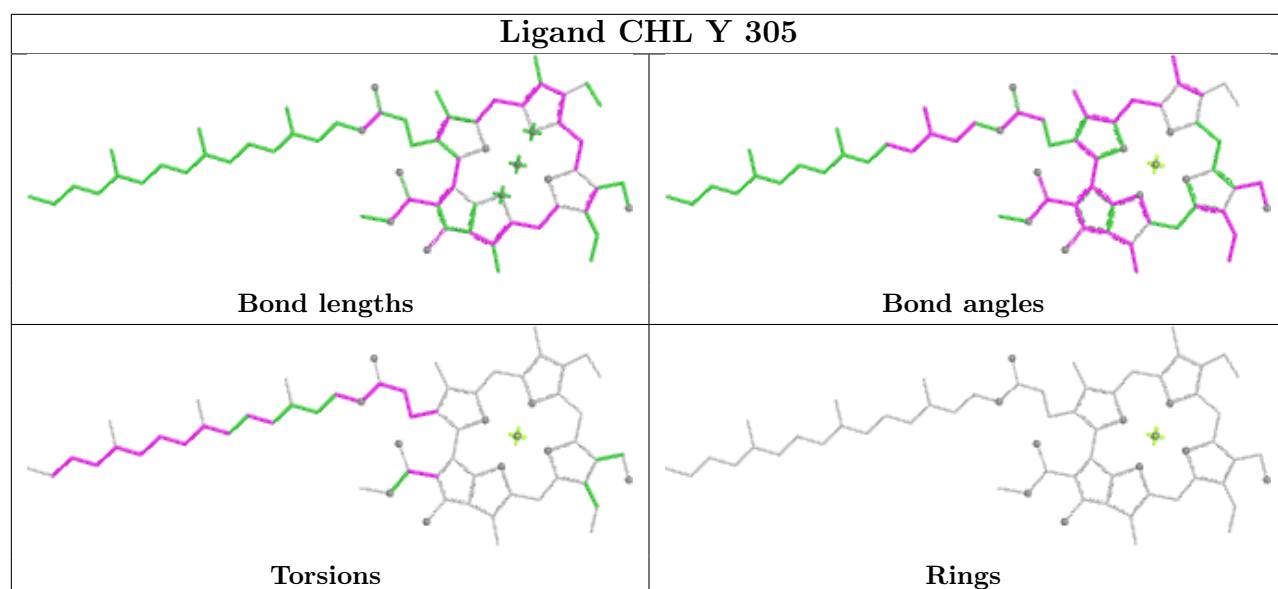
Ligand 0IE r 315	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA g 316

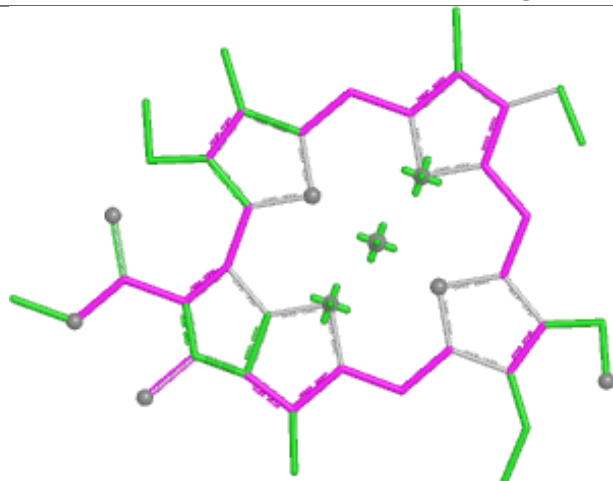




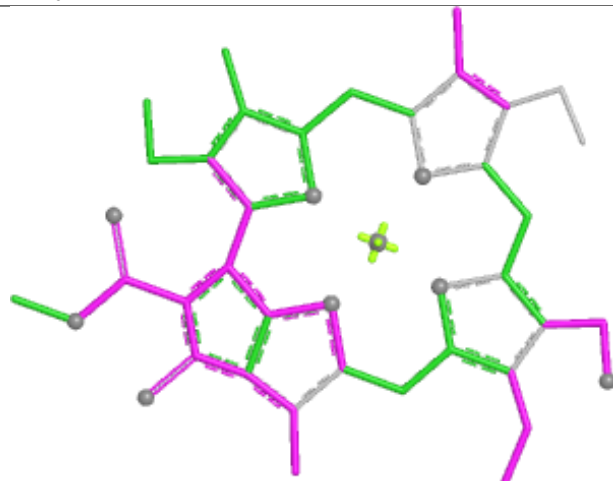




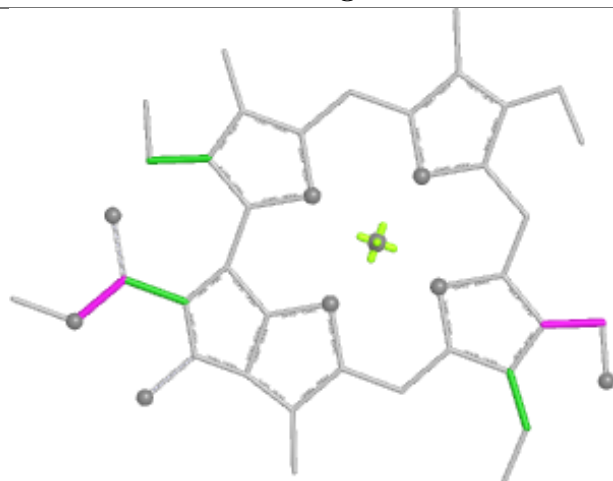
Ligand CHL y 309



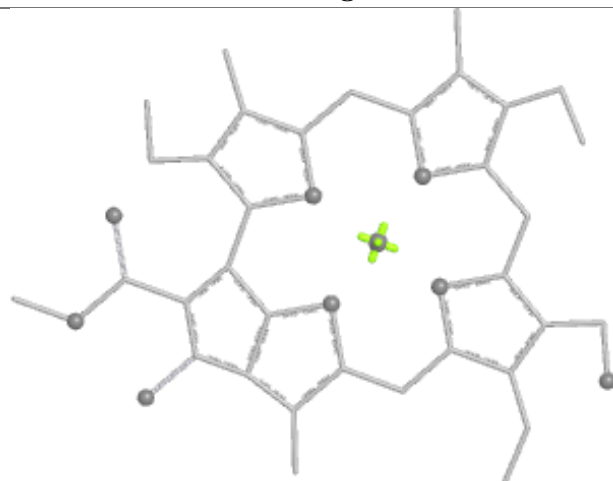
Bond lengths



Bond angles

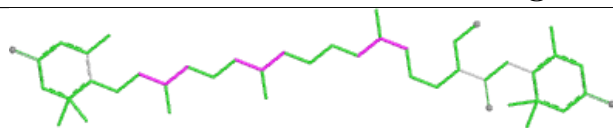


Torsions

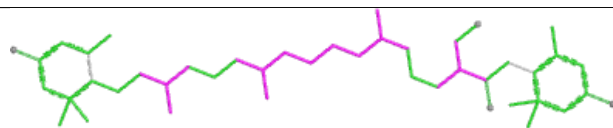


Rings

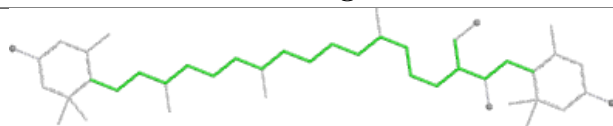
Ligand OIE 2 303



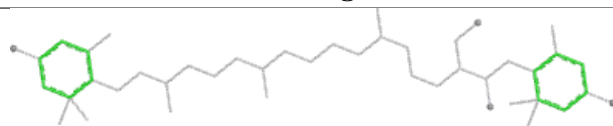
Bond lengths



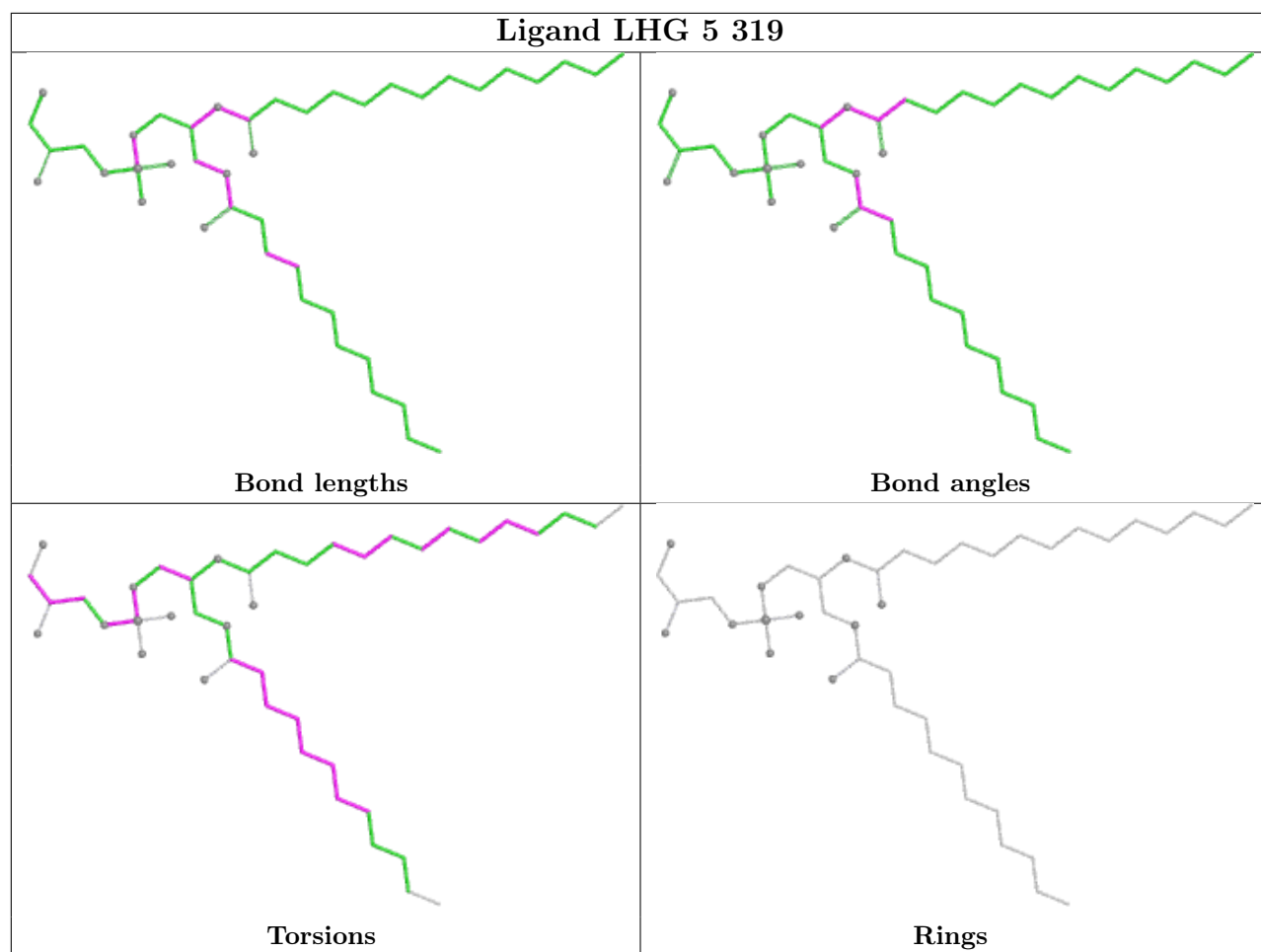
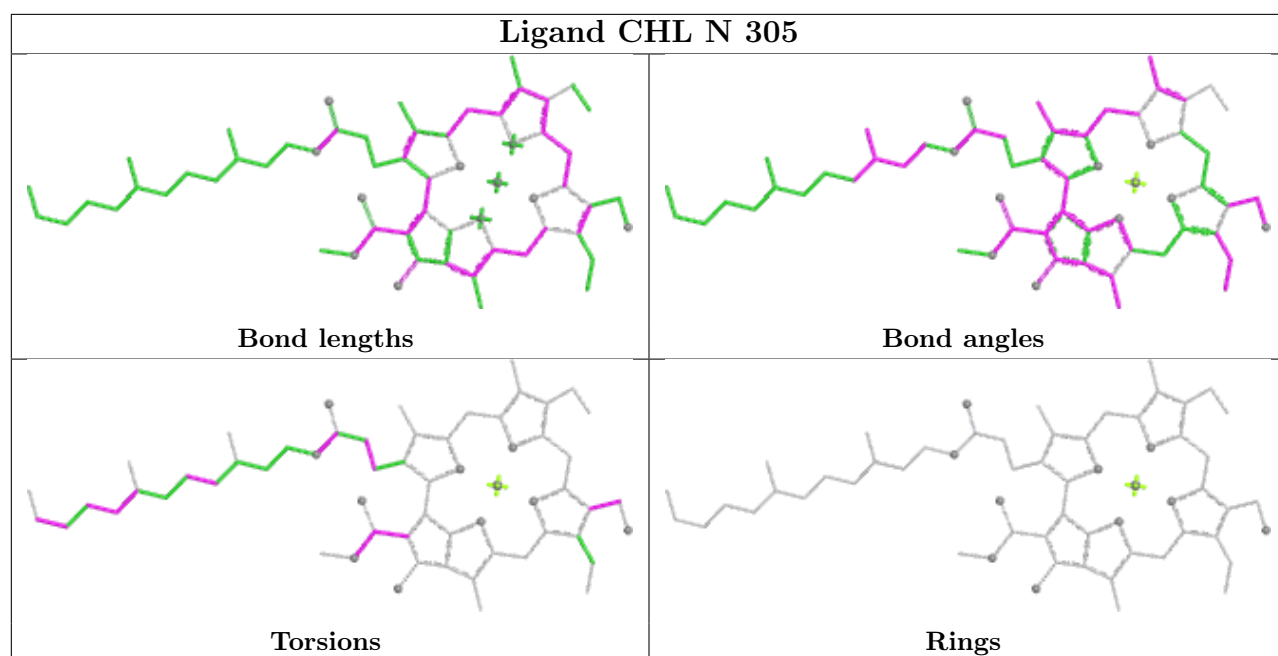
Bond angles

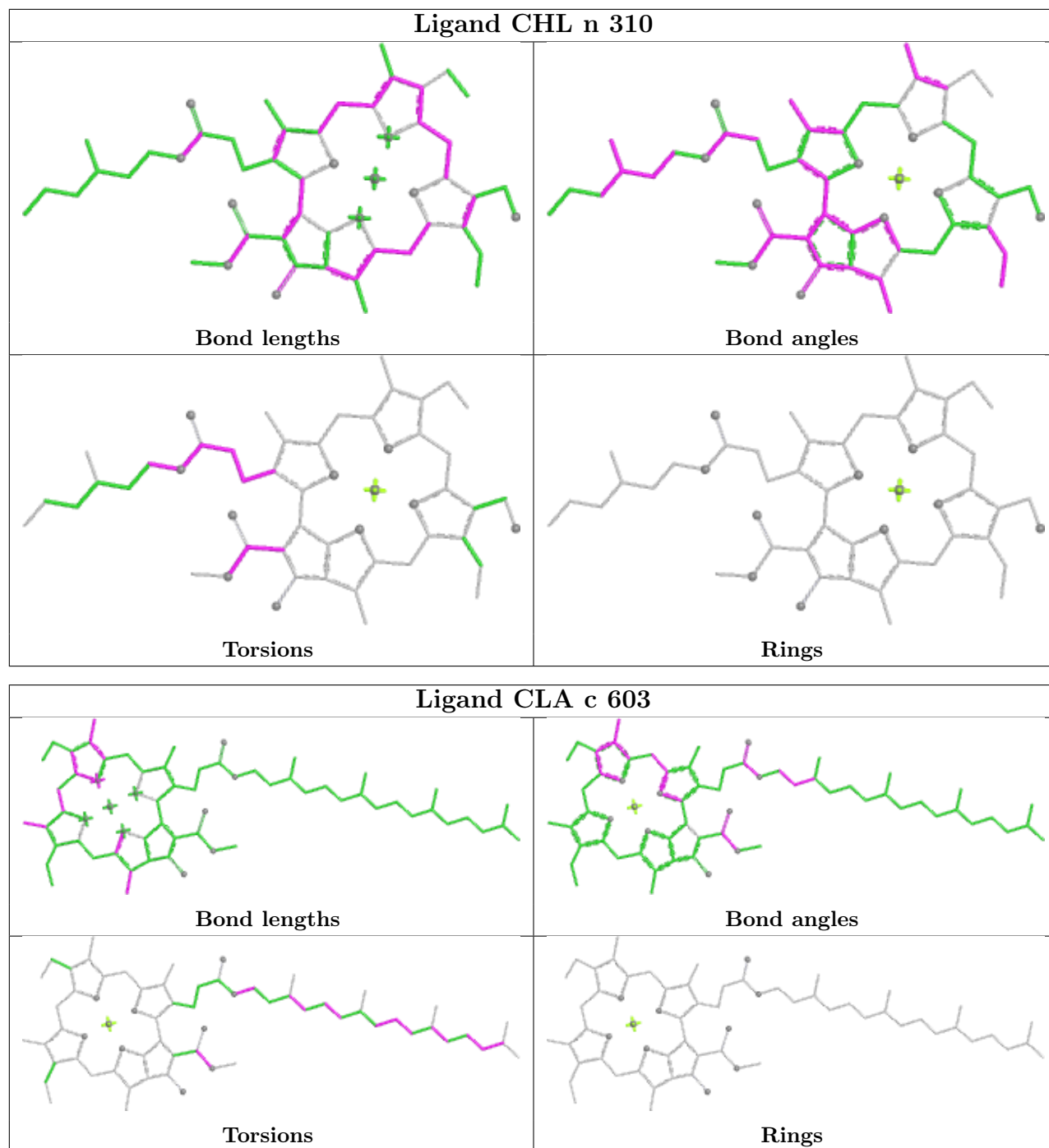


Torsions

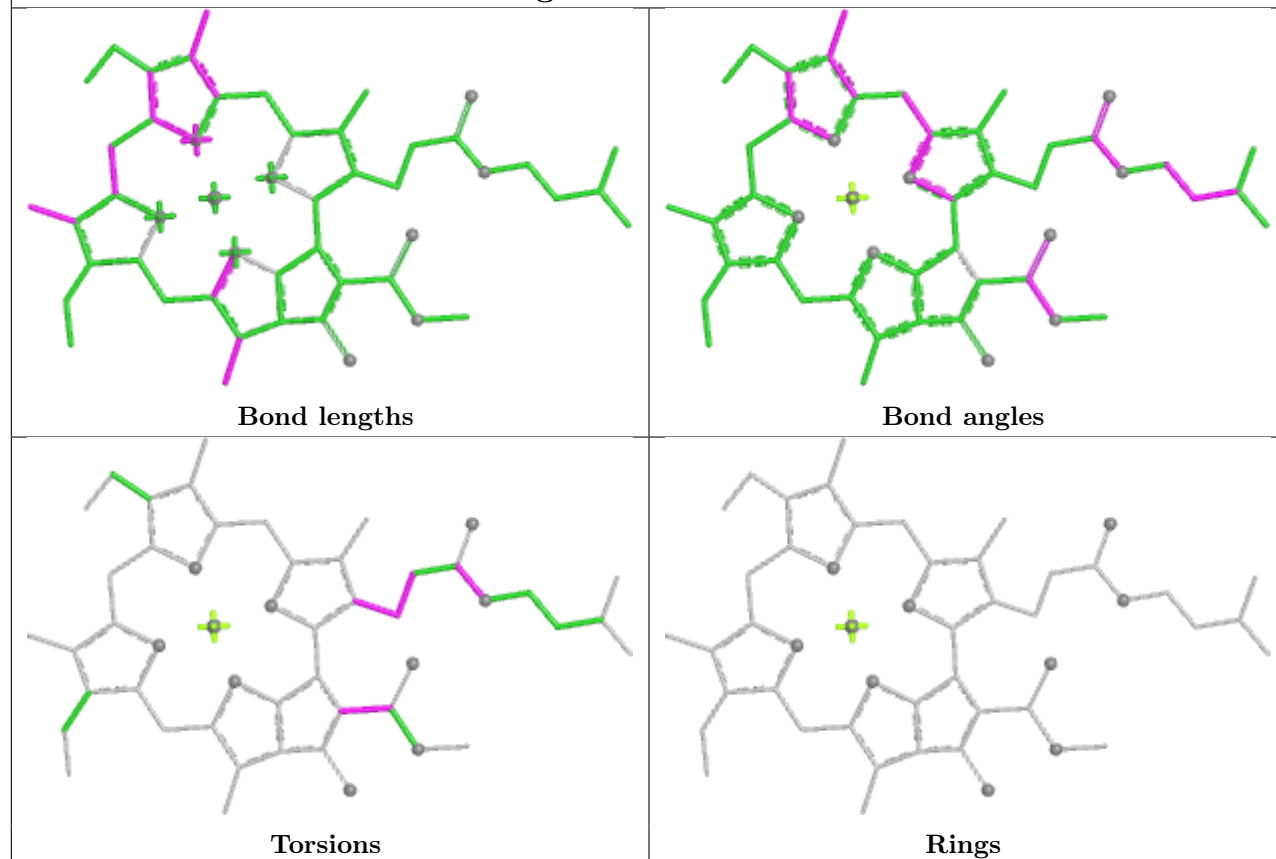


Rings

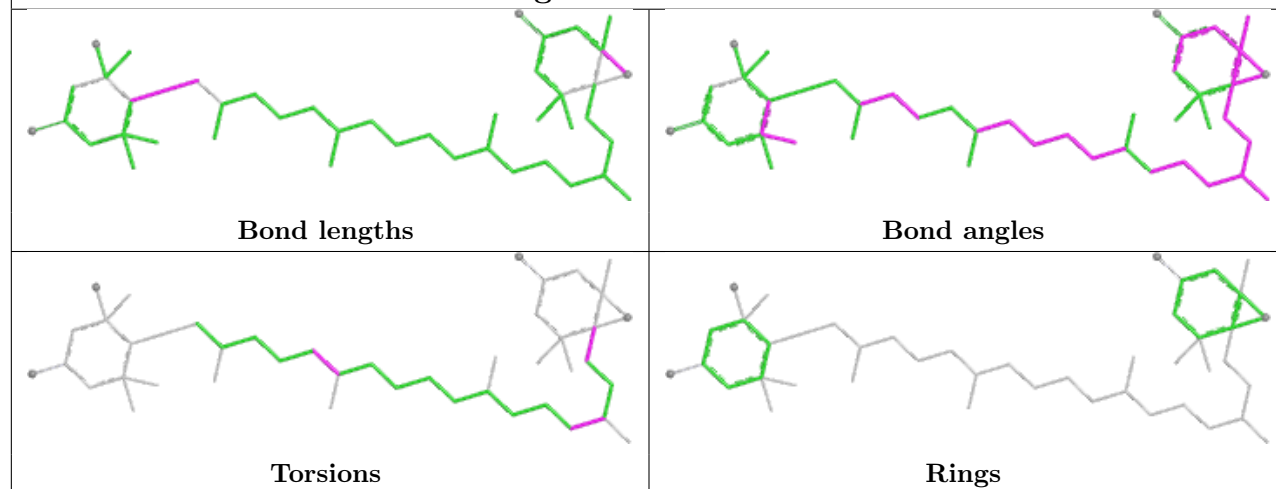




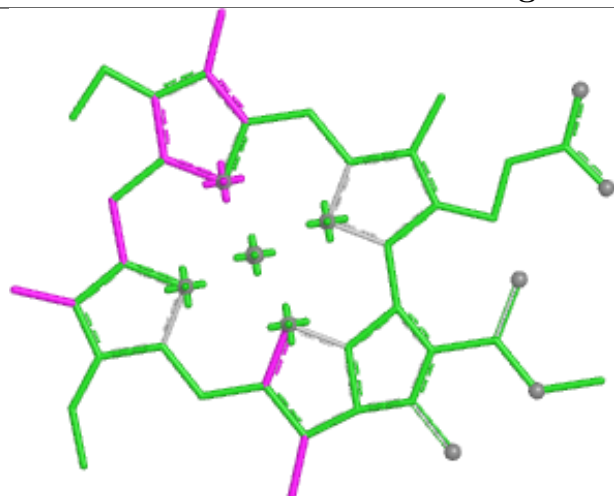
Ligand CLA 8 306



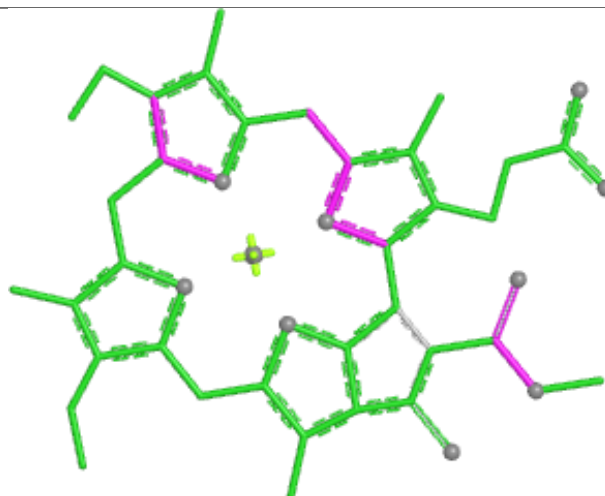
Ligand NEX 6 303



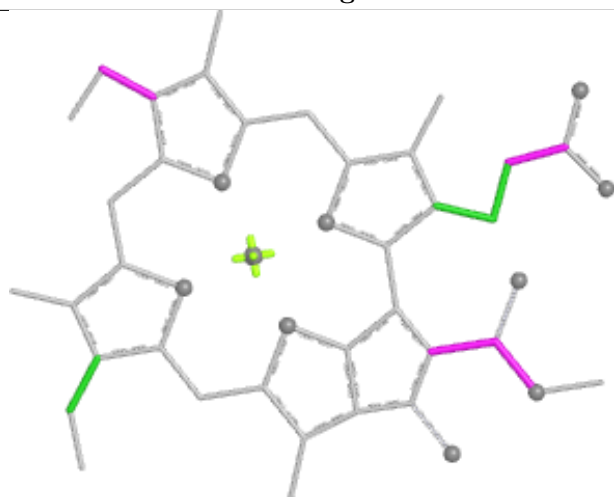
Ligand CLA 4 315



Bond lengths



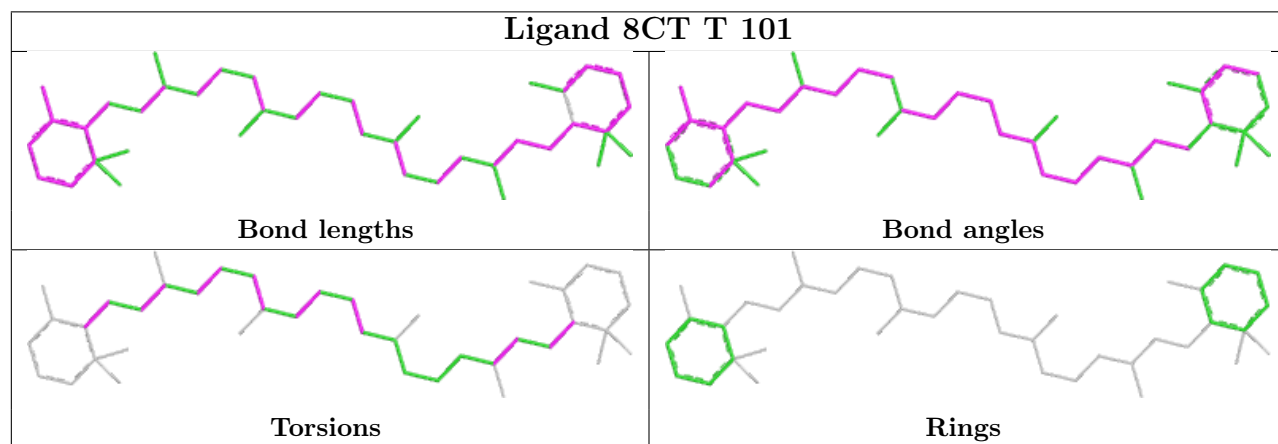
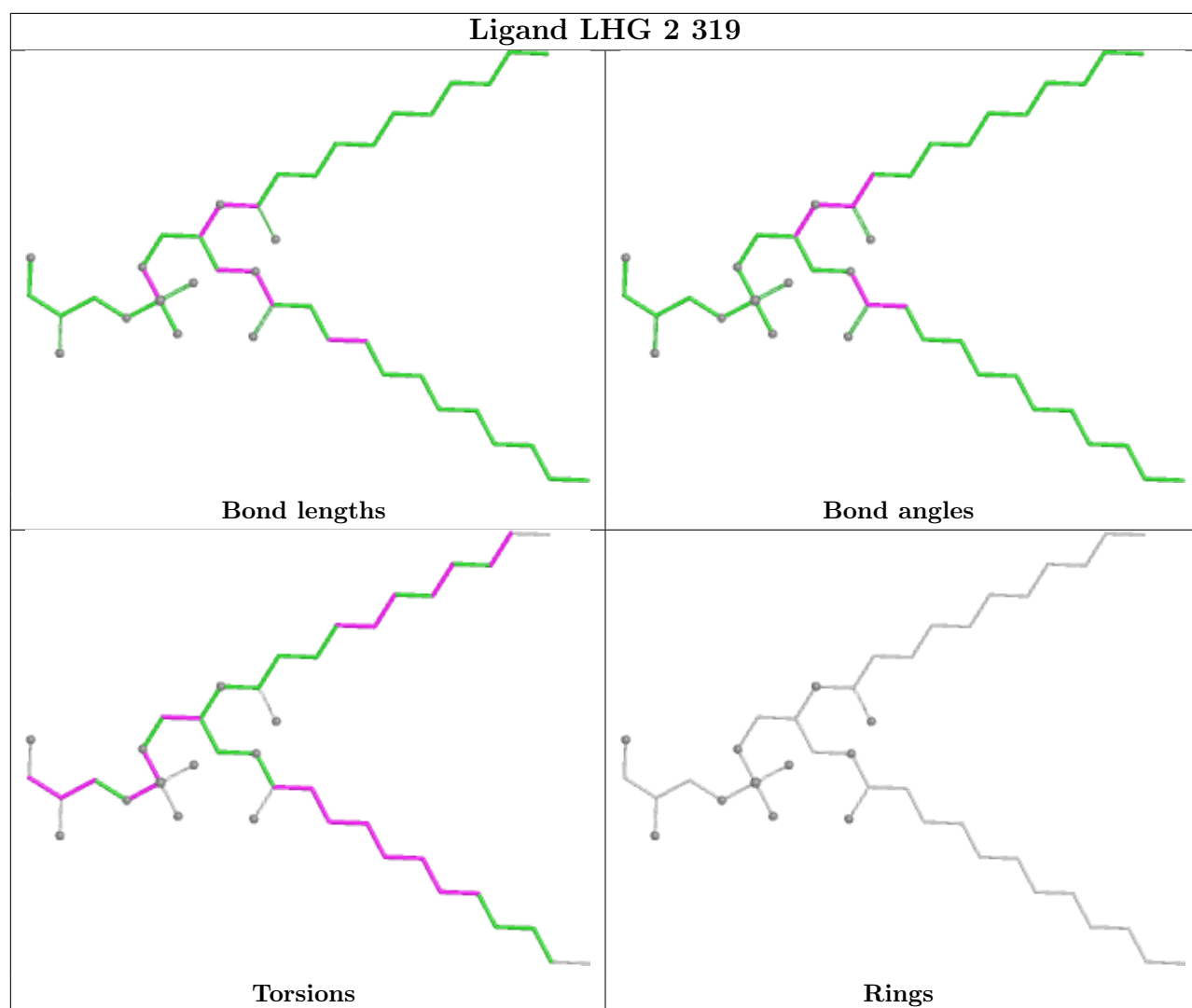
Bond angles



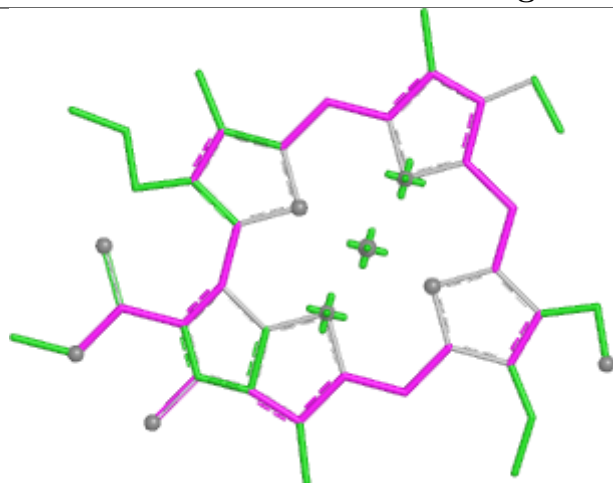
Torsions



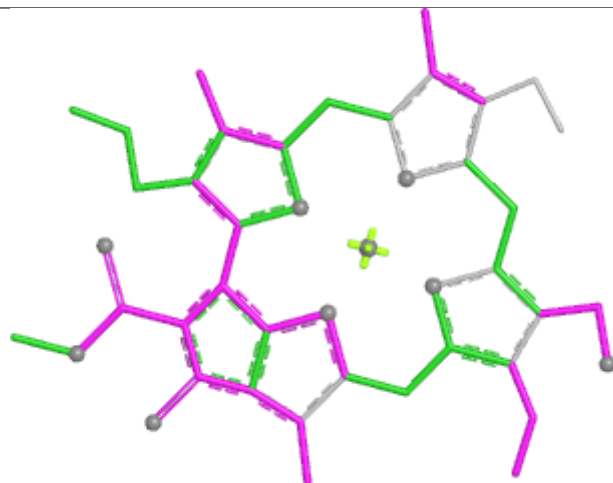
Rings



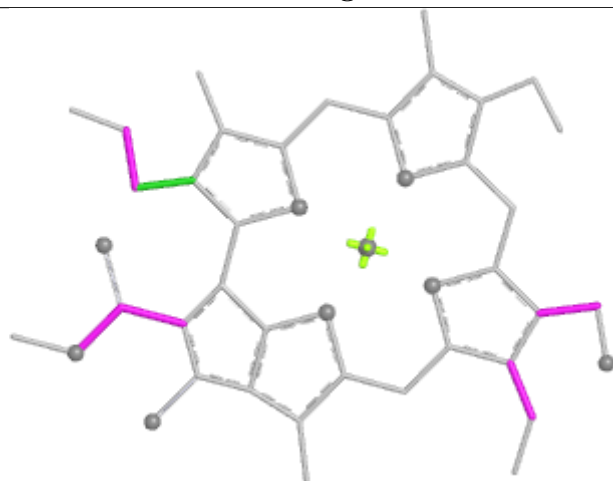
Ligand CHL 2 305



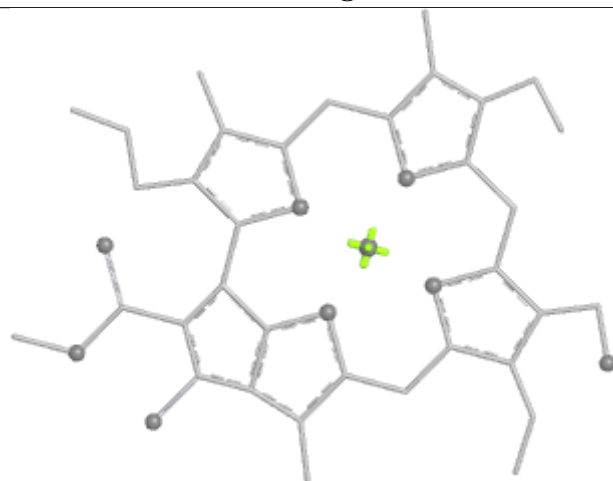
Bond lengths



Bond angles

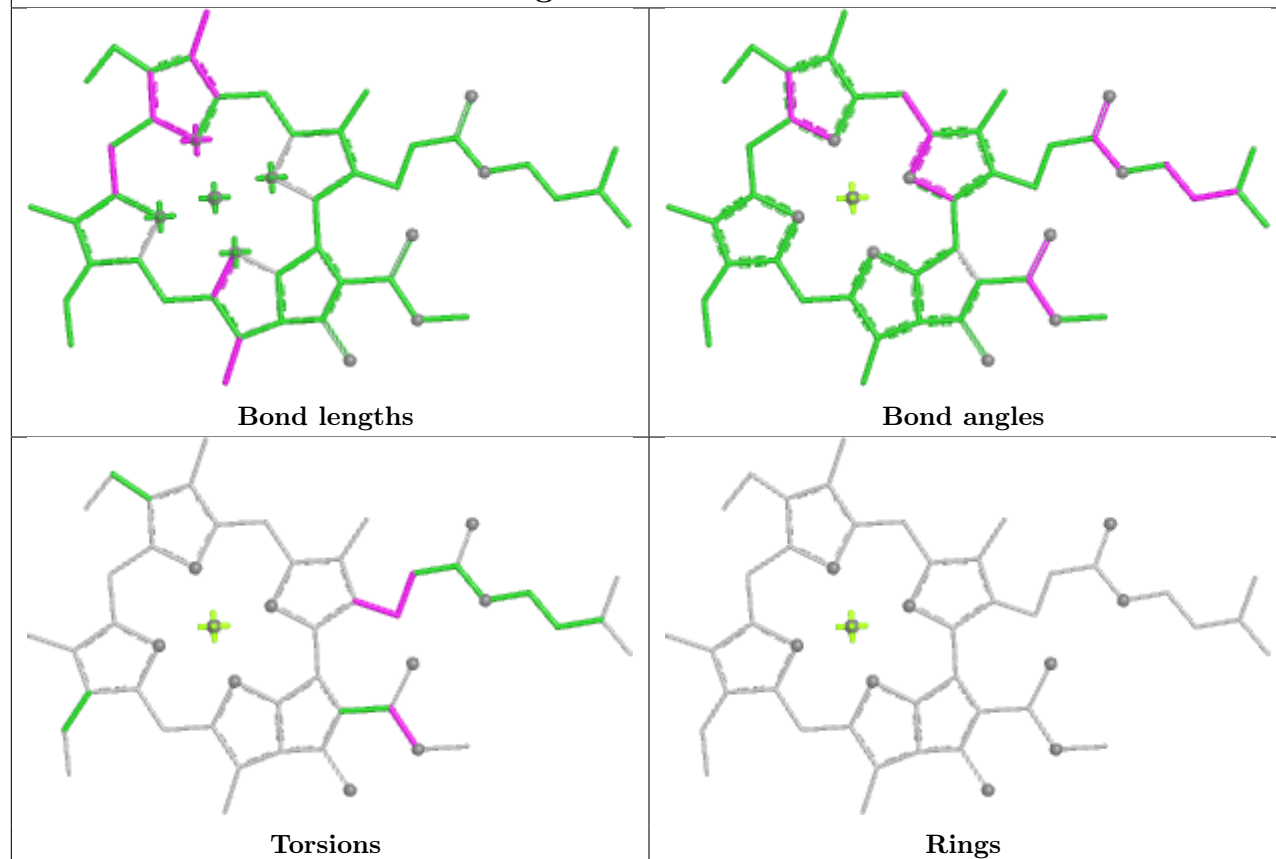


Torsions

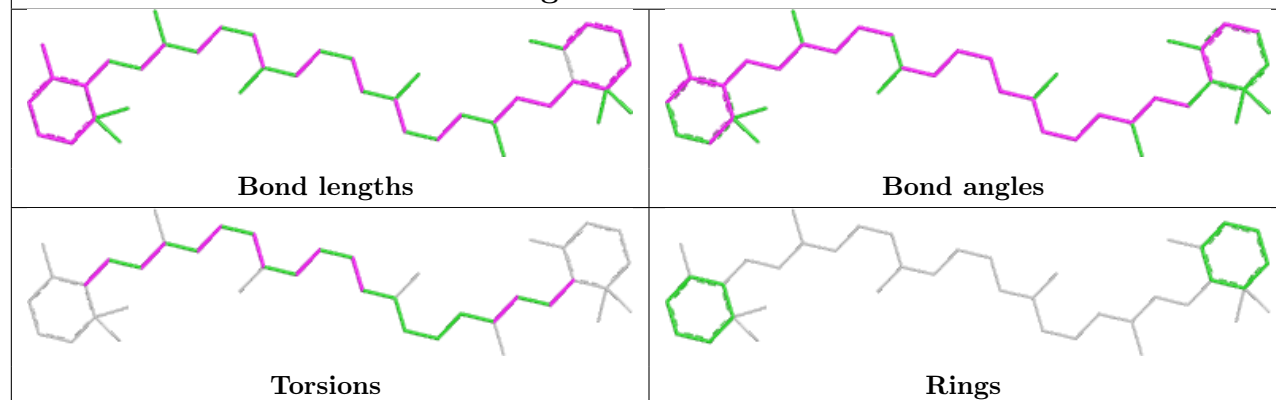


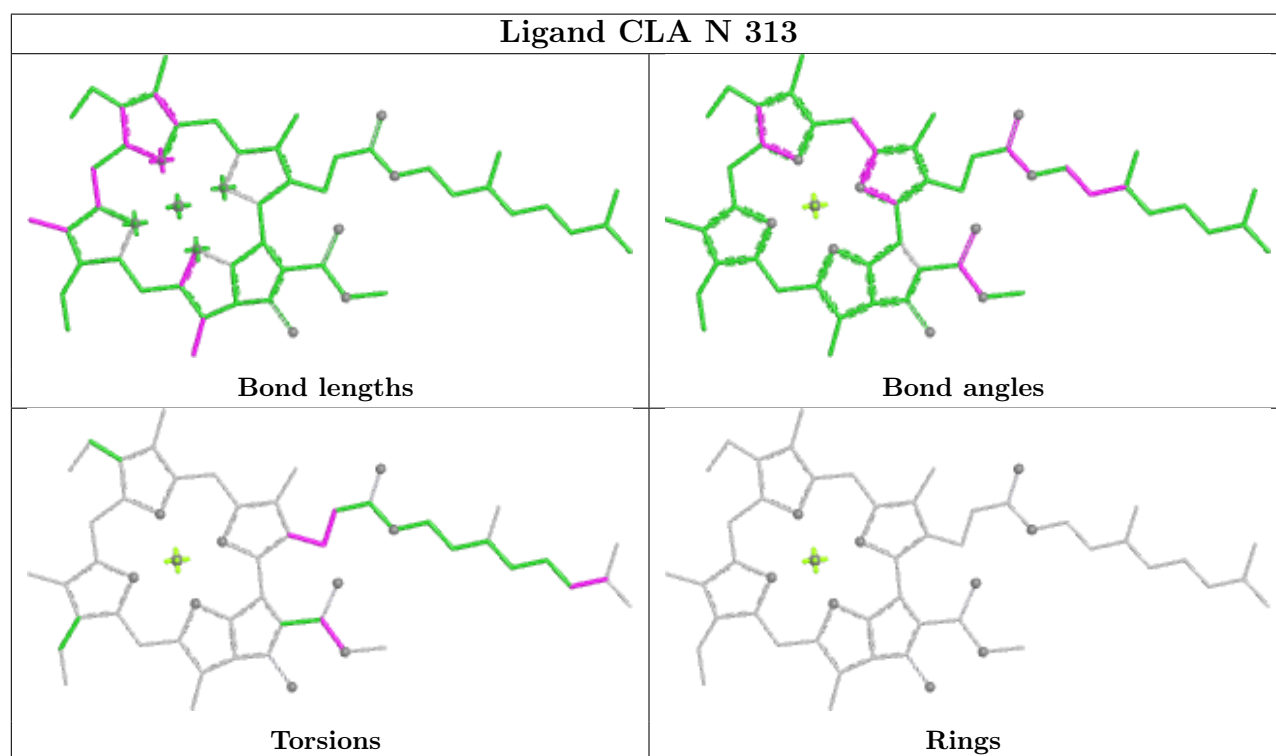
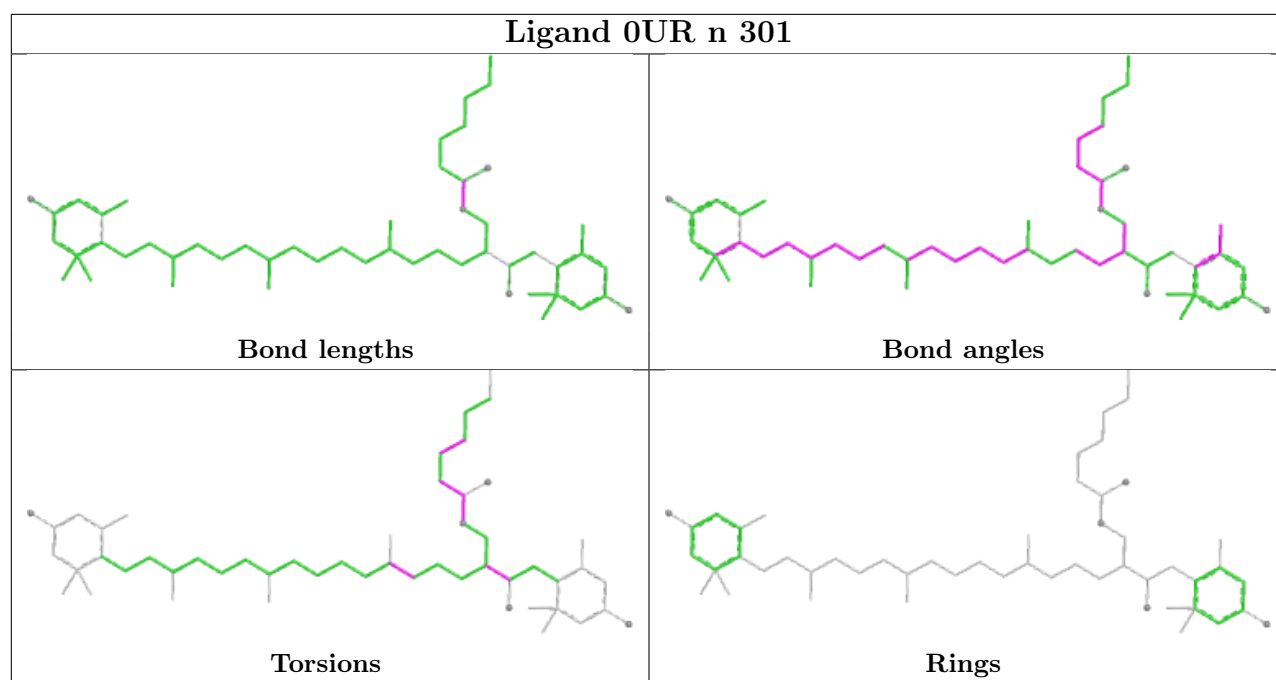
Rings

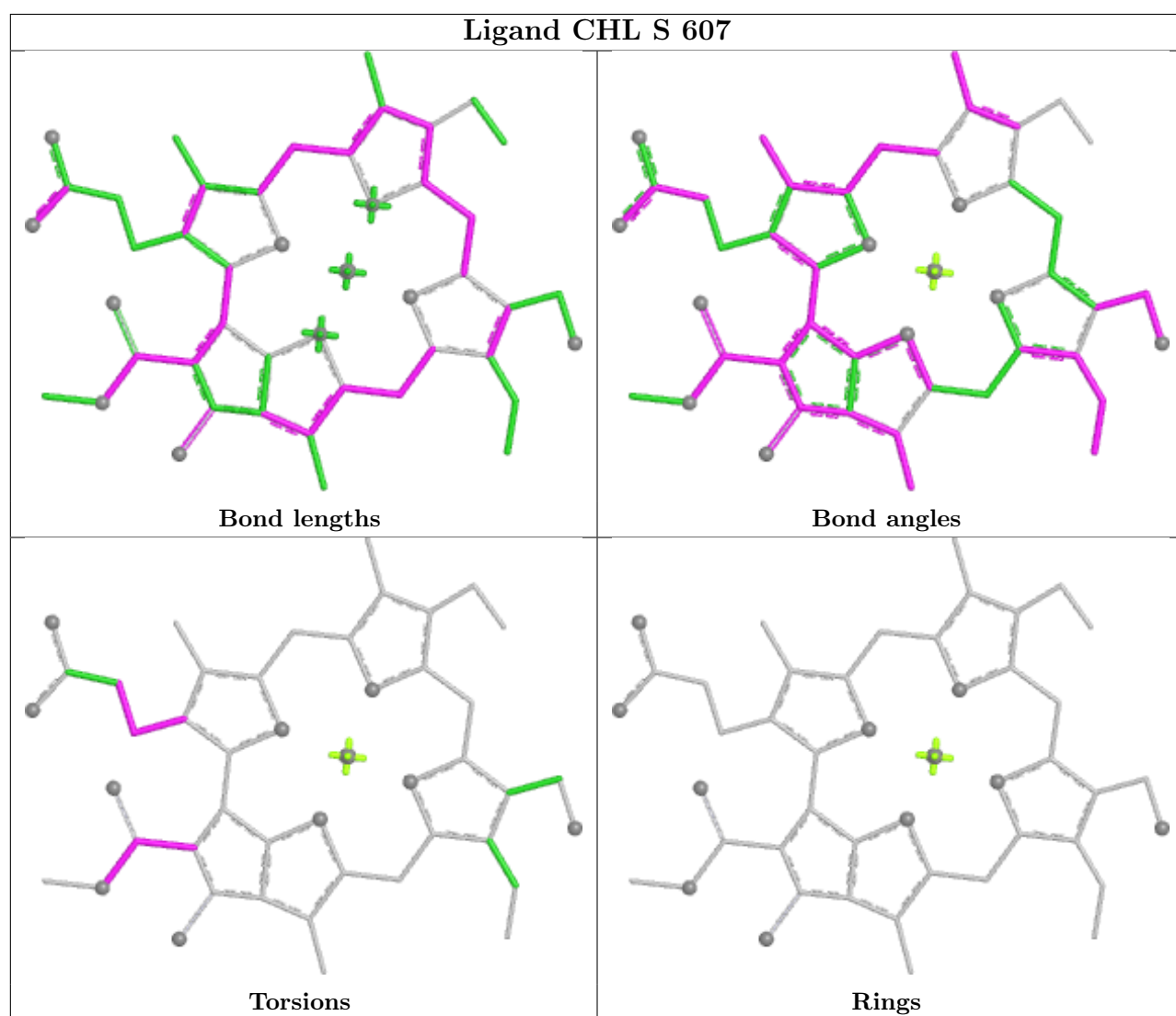
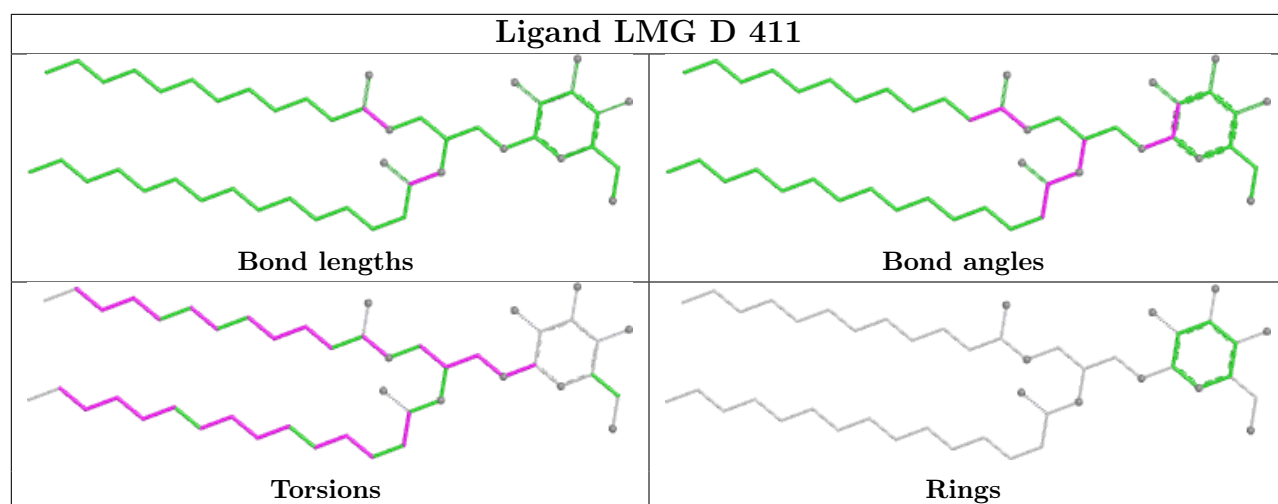
Ligand CLA u 308

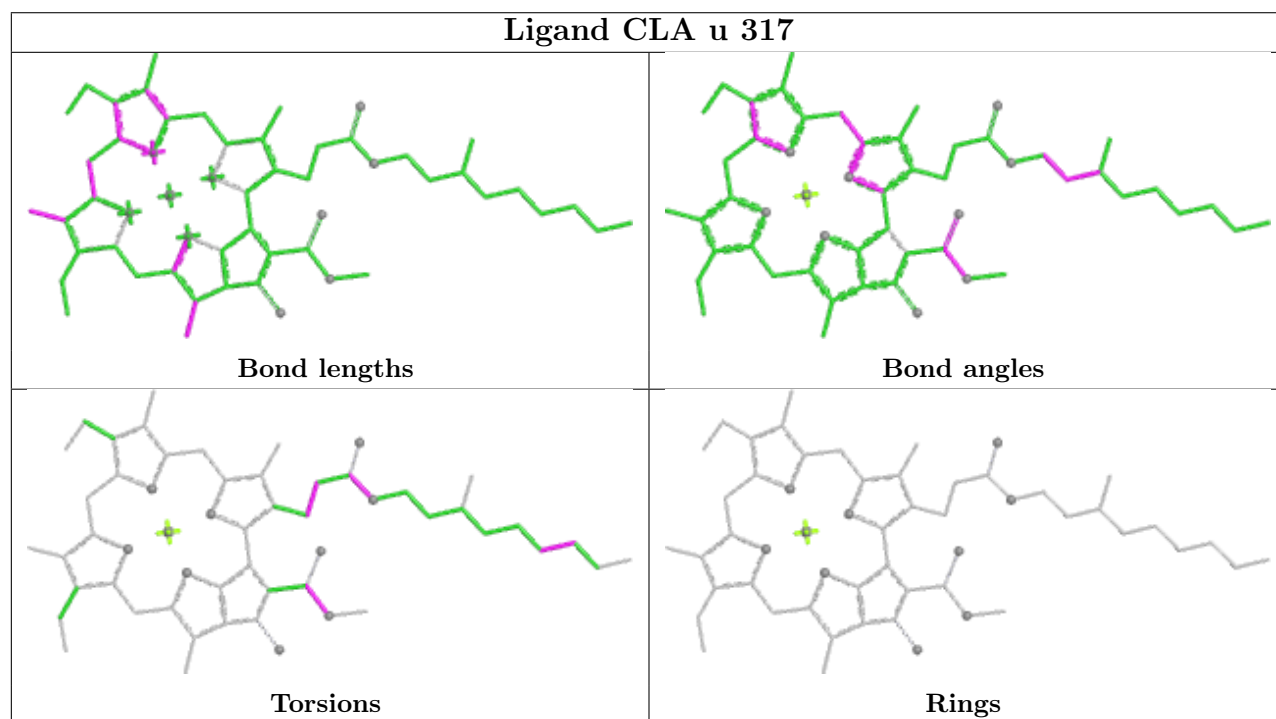
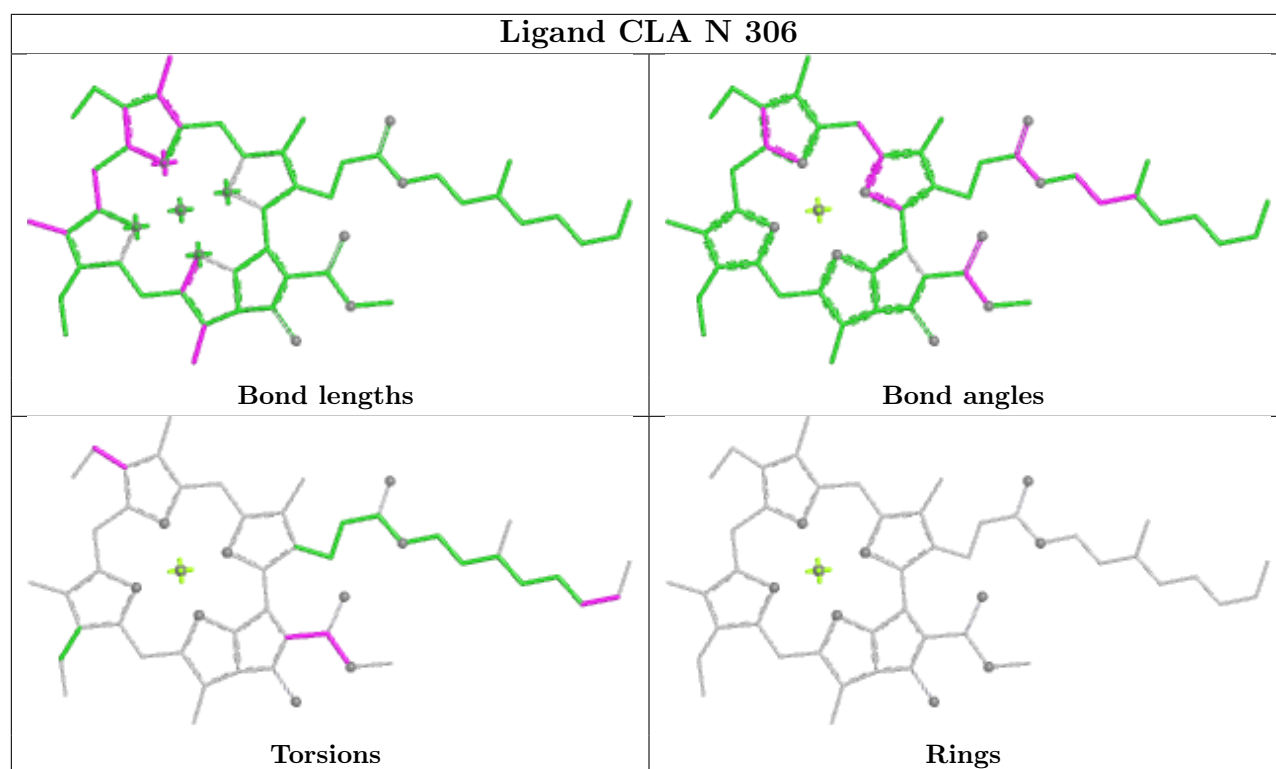


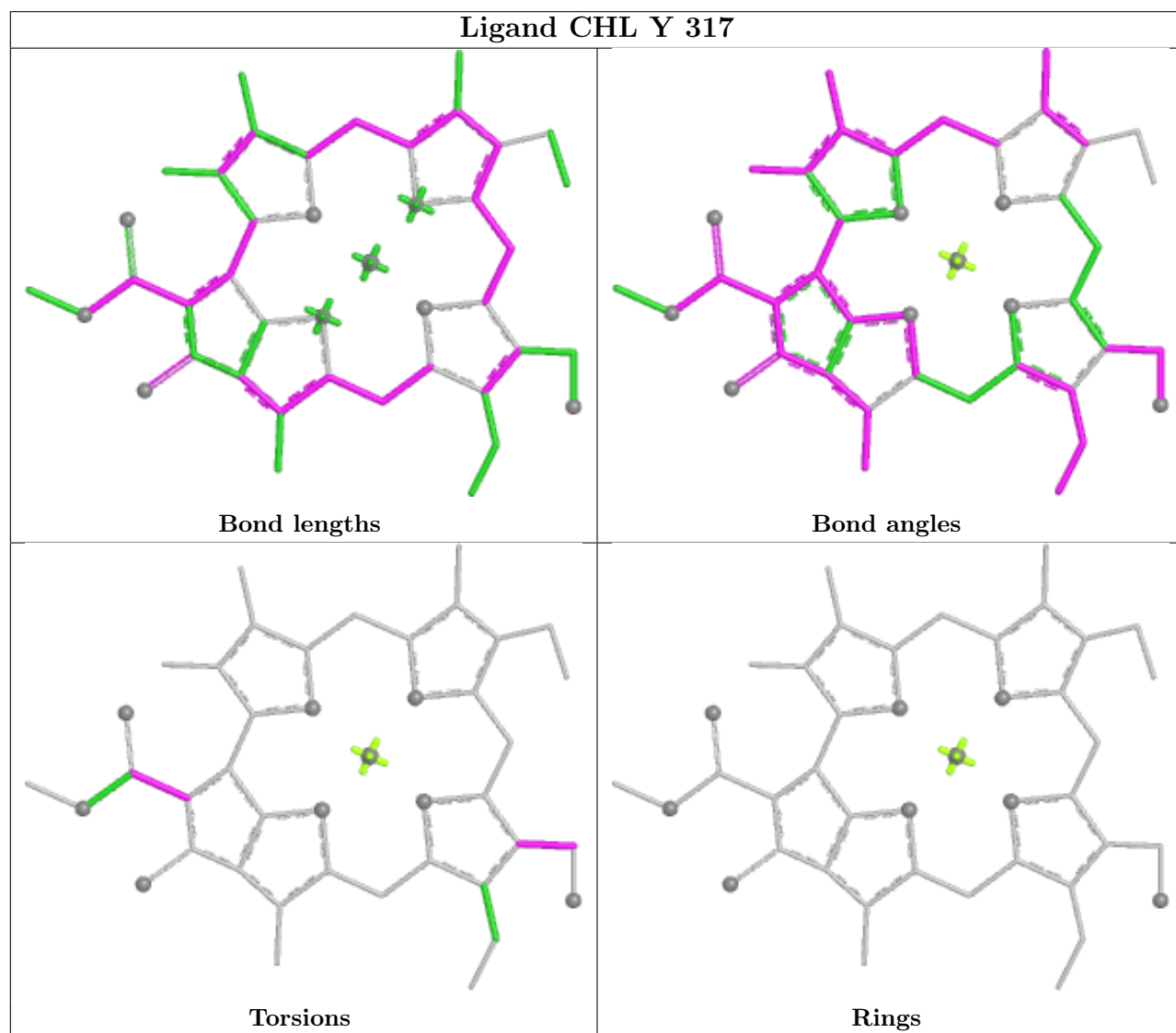
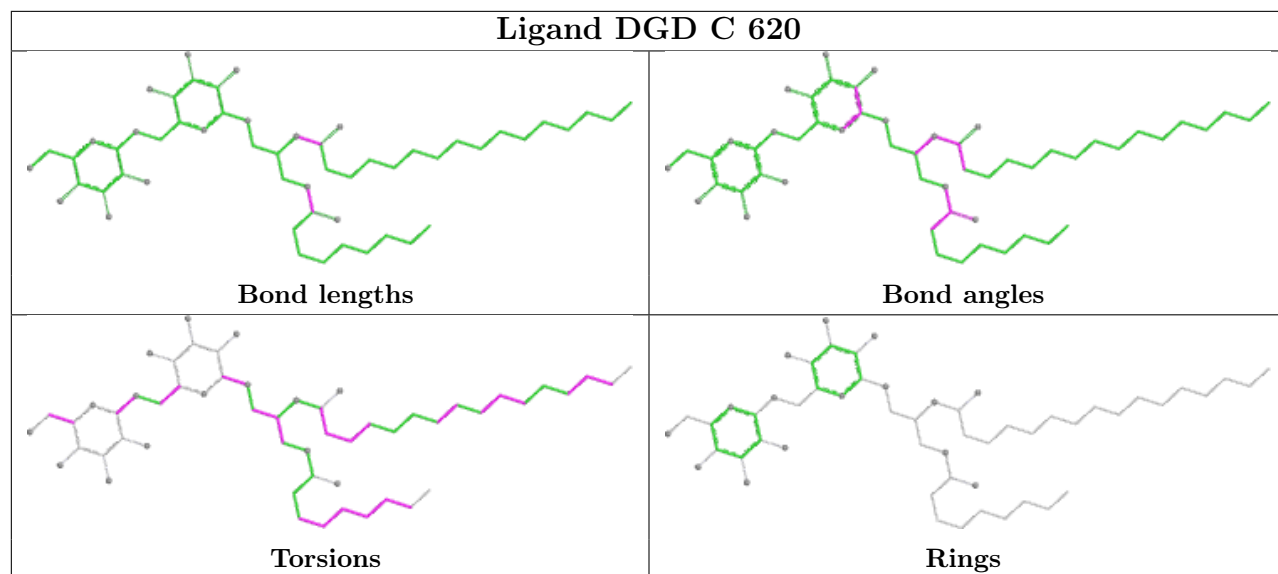
Ligand 8CT t 101



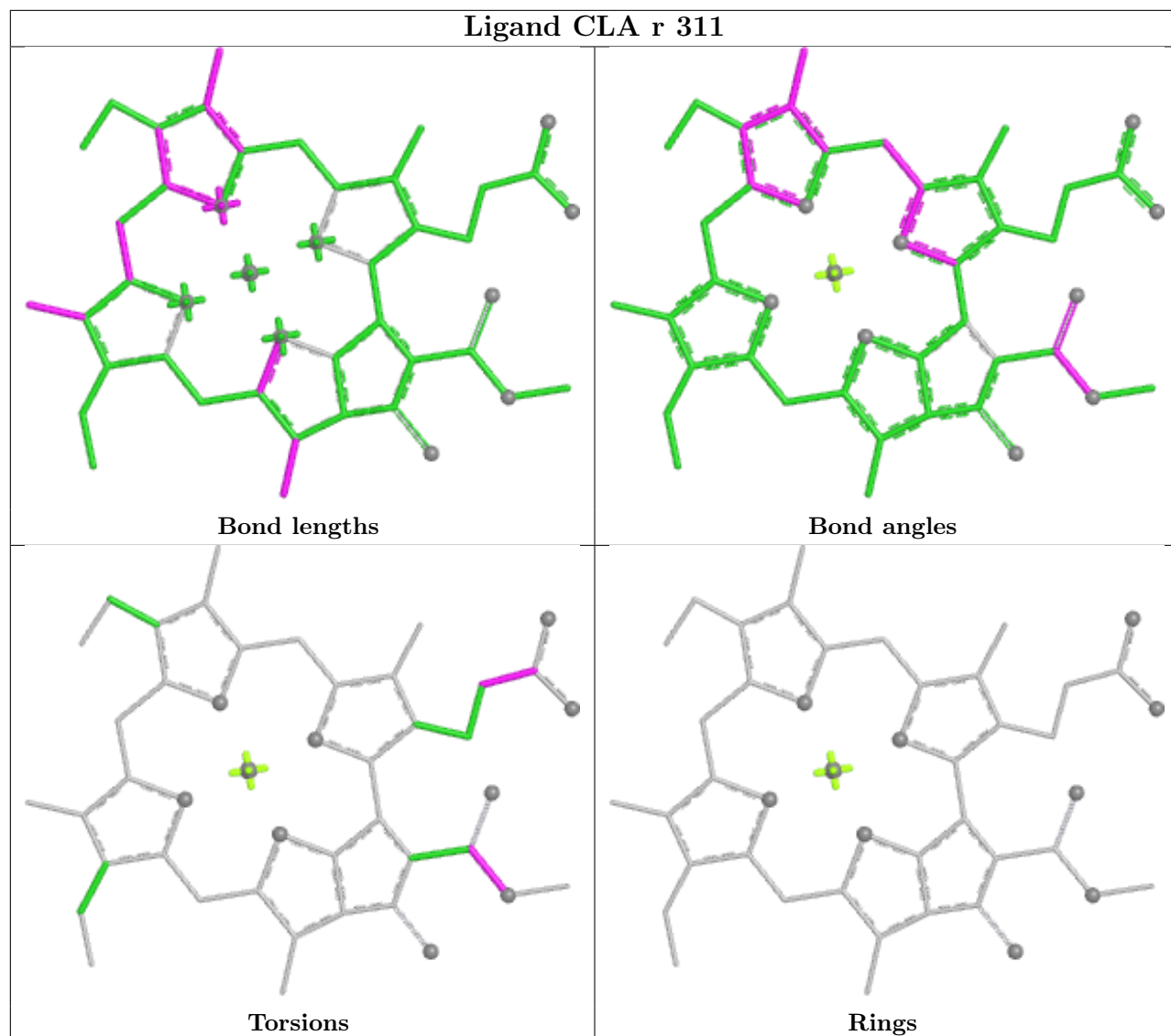


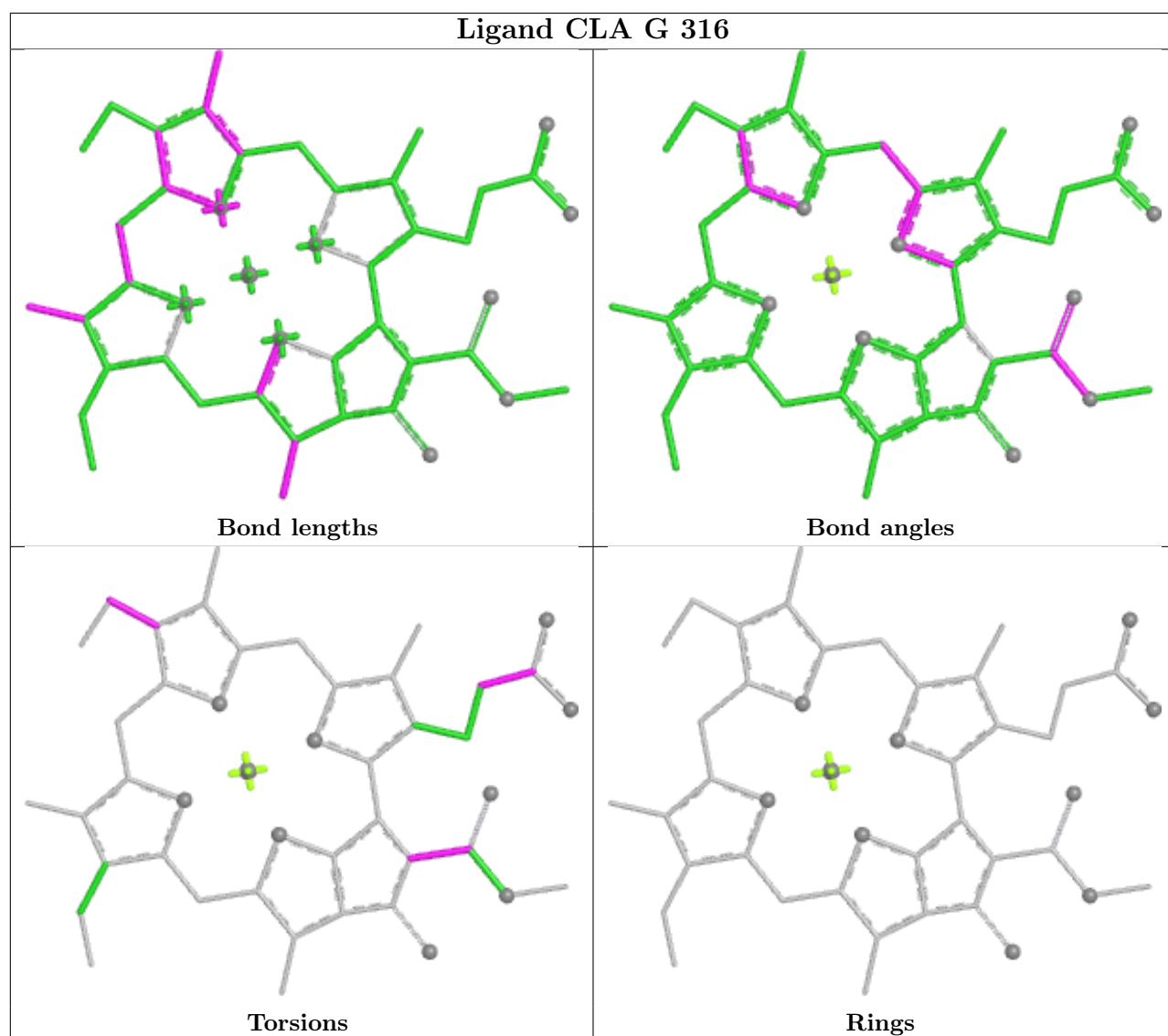




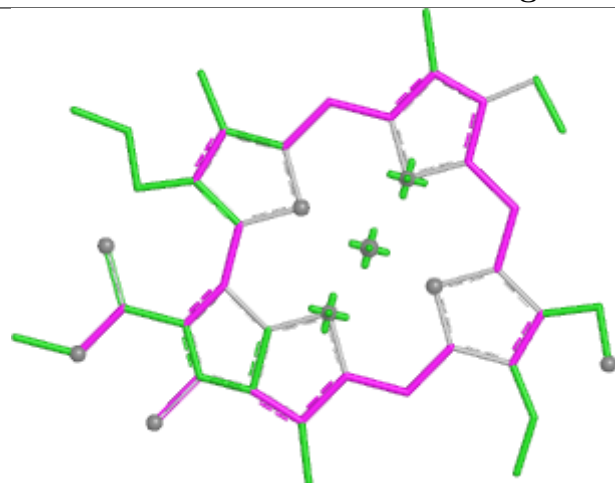


Ligand CLA r 311

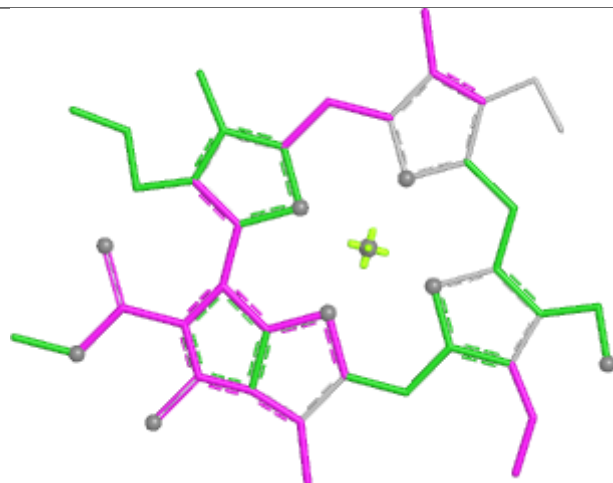




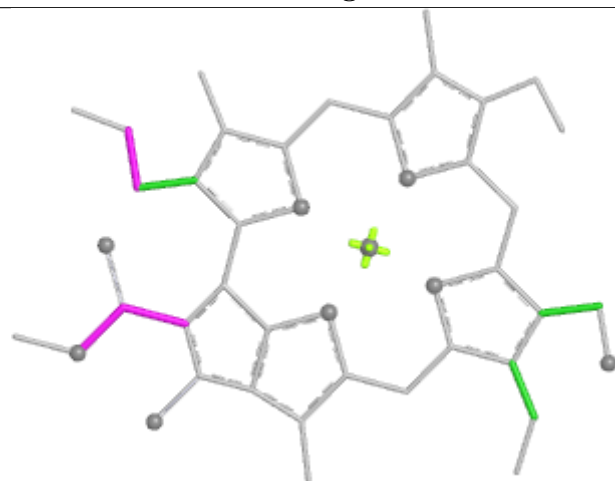
Ligand CHL 6 311



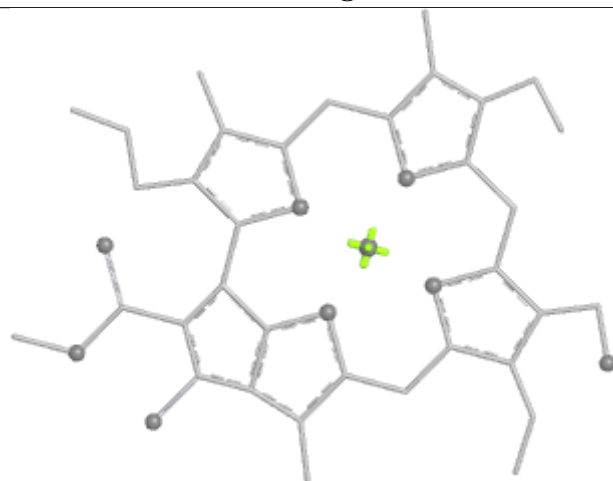
Bond lengths



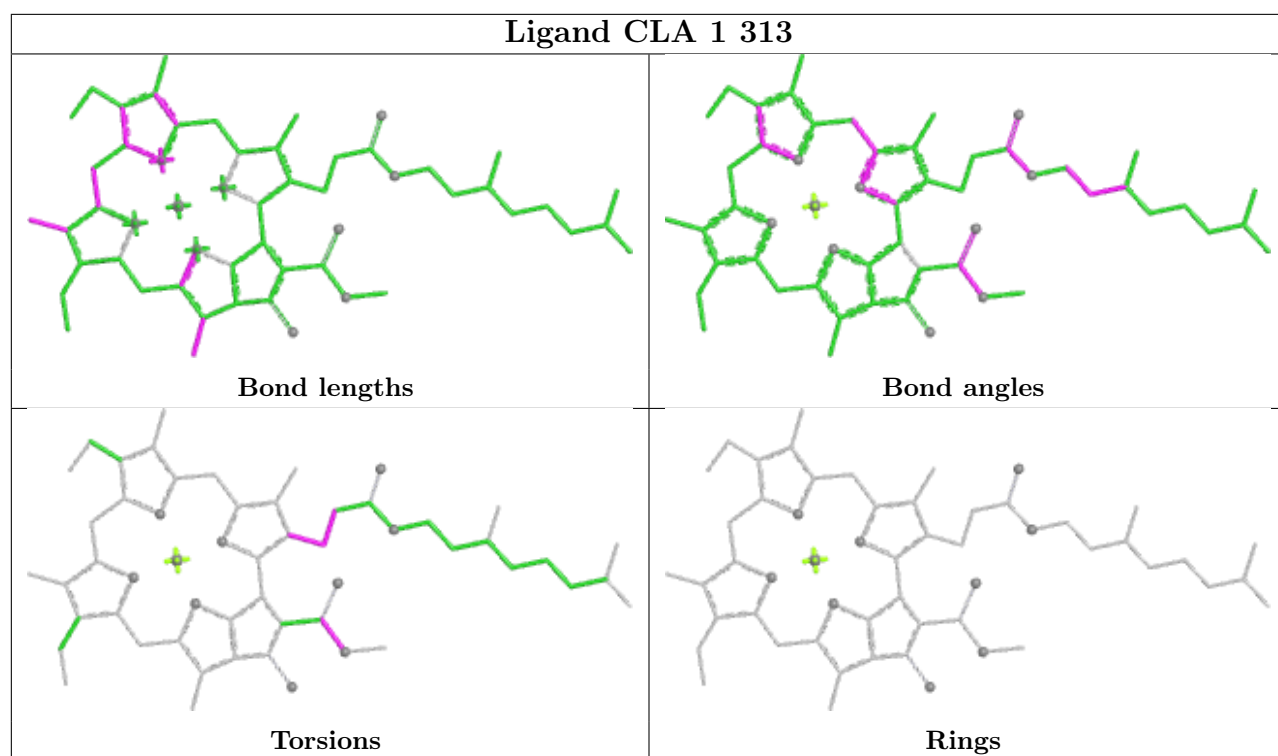
Bond angles



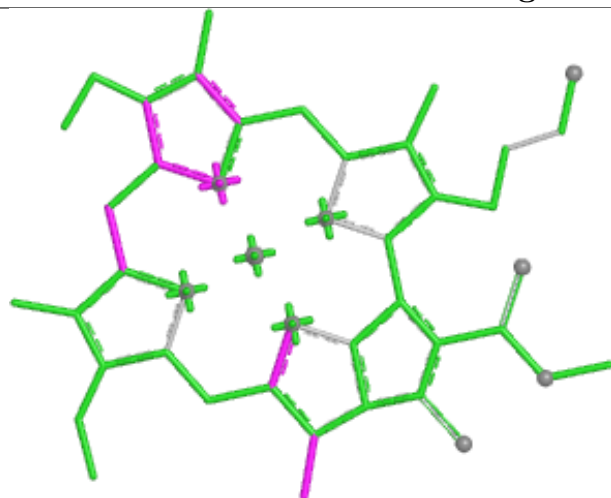
Torsions



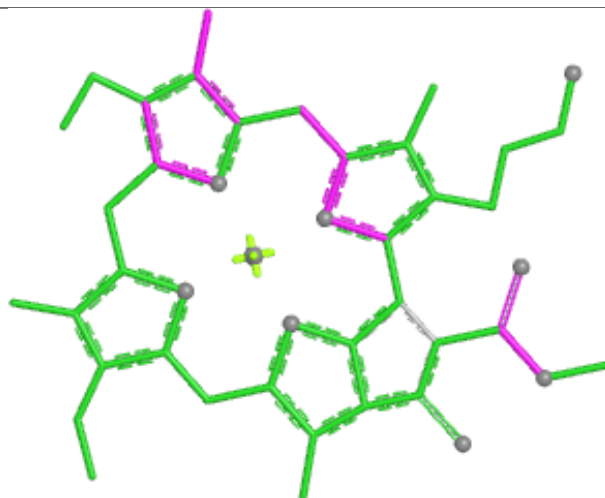
Rings



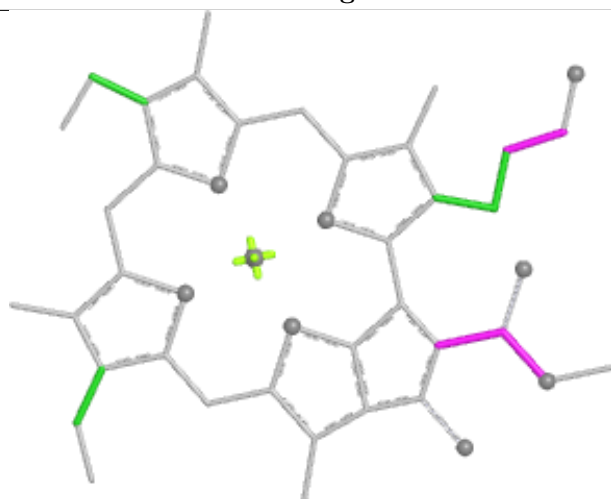
Ligand CLA 1 306



Bond lengths



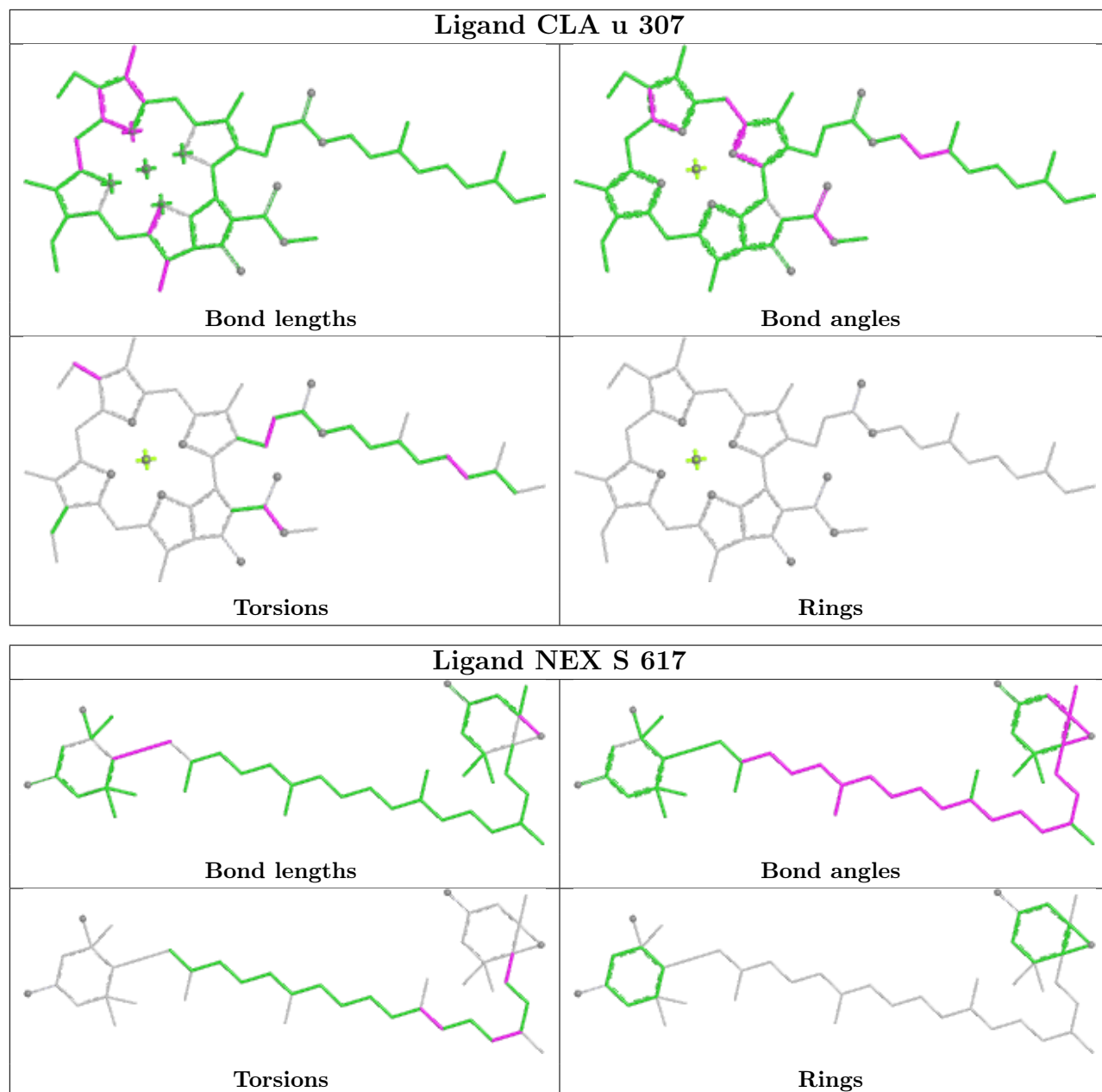
Bond angles

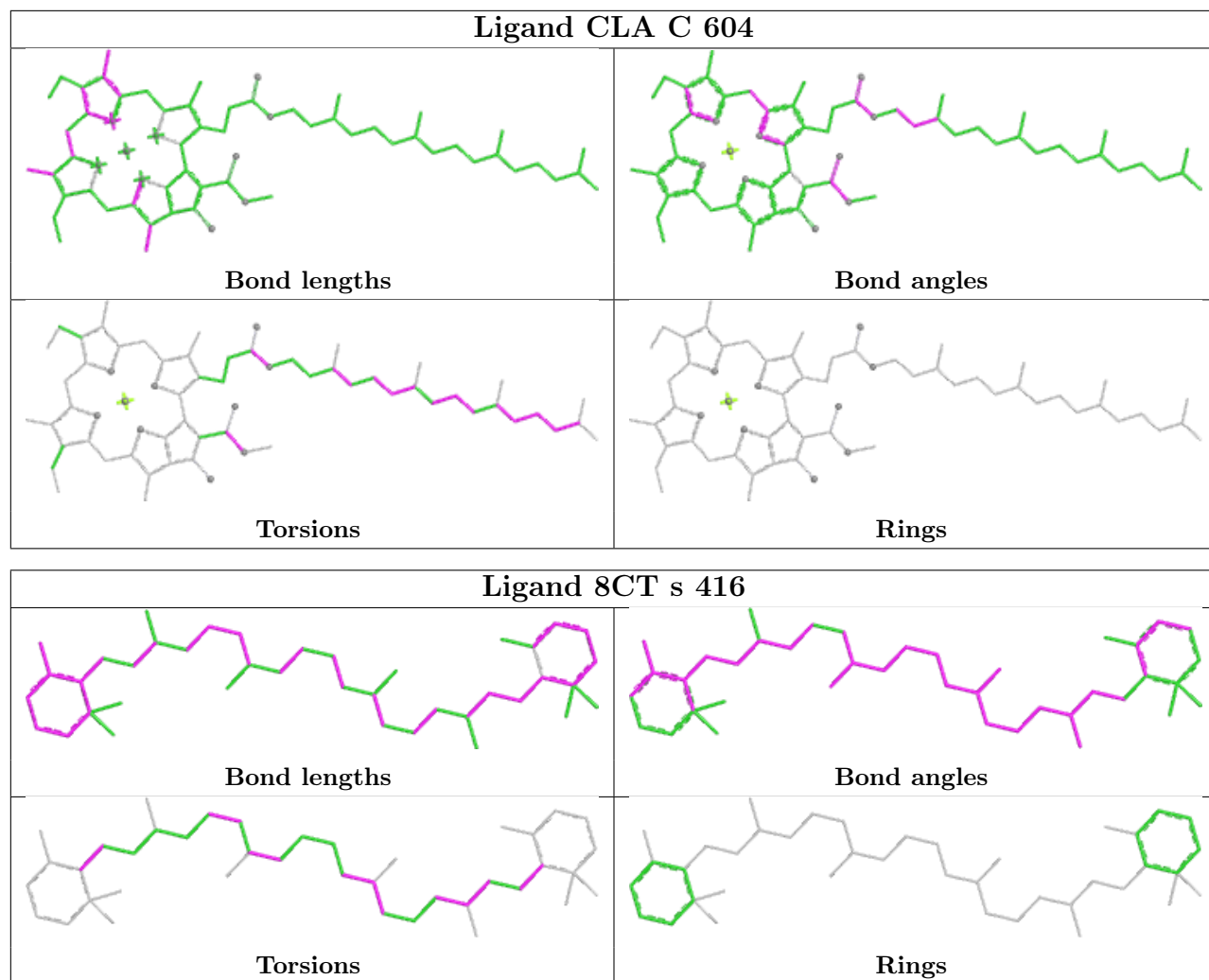


Torsions

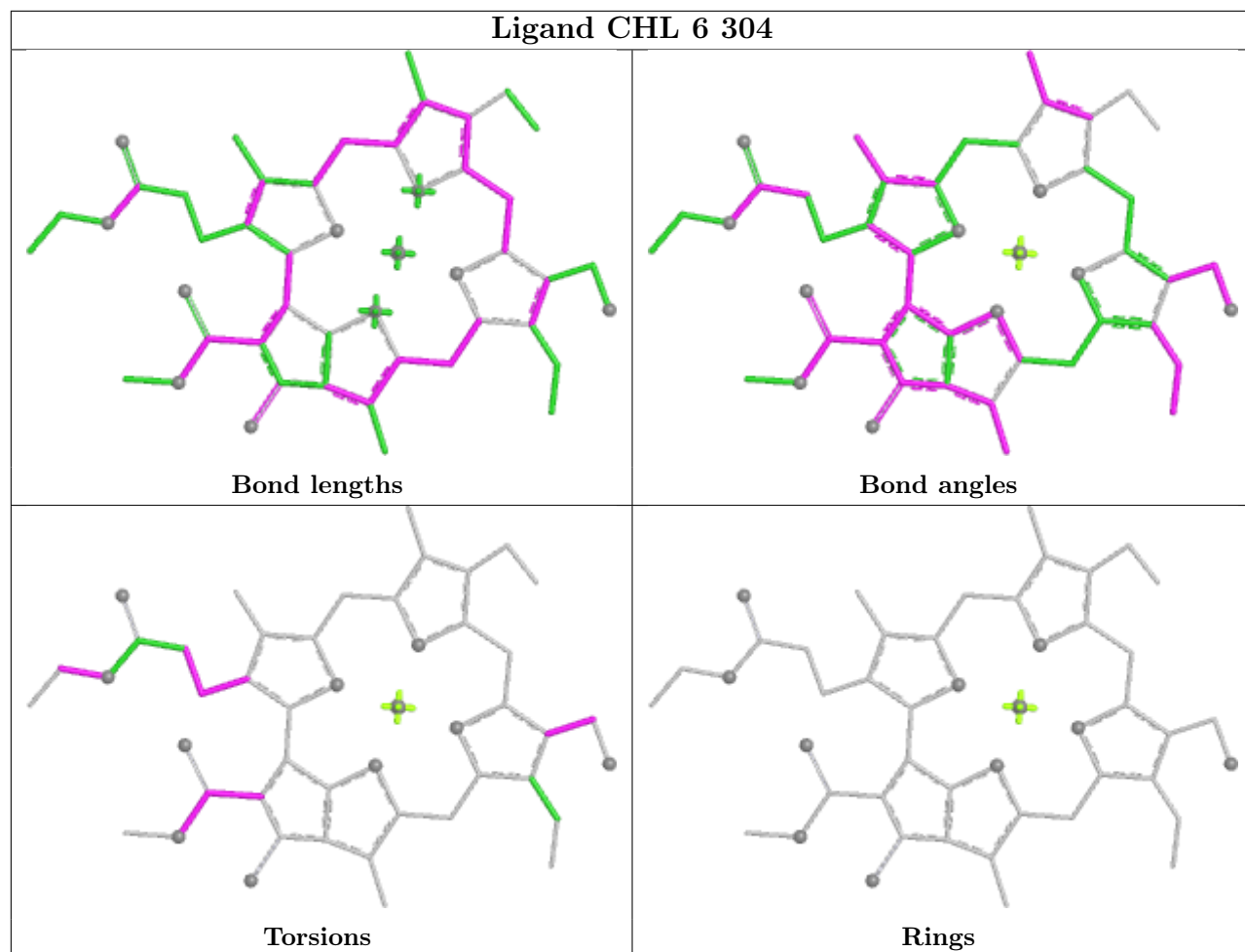


Rings

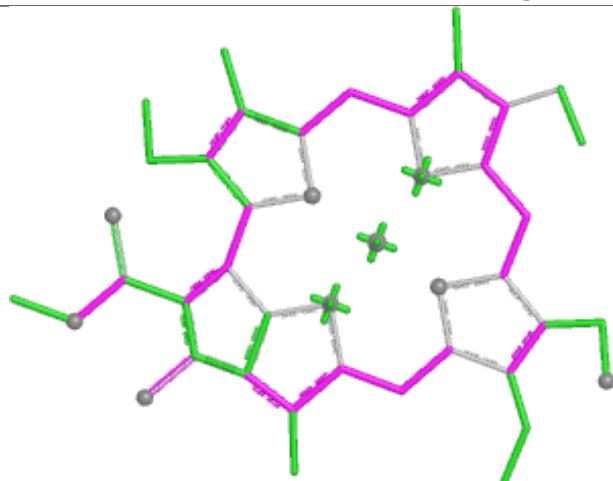




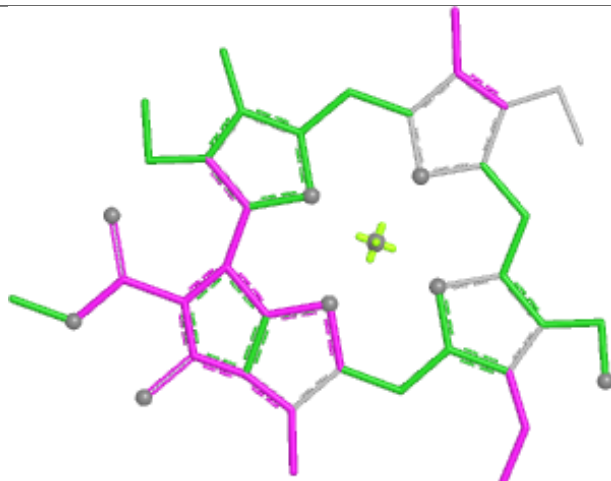
Ligand CHL 6 304



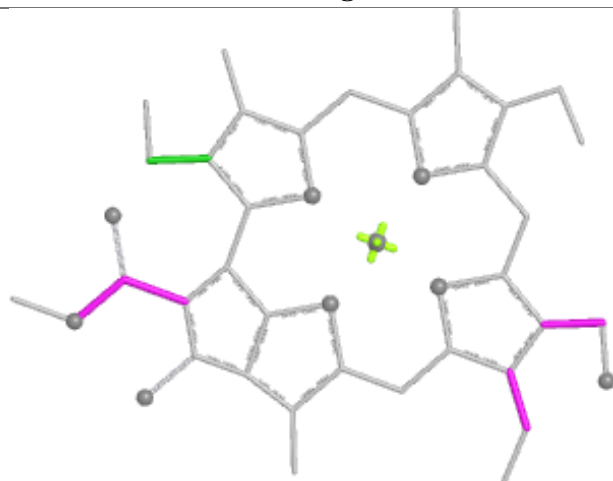
Ligand CHL 3 312



Bond lengths



Bond angles

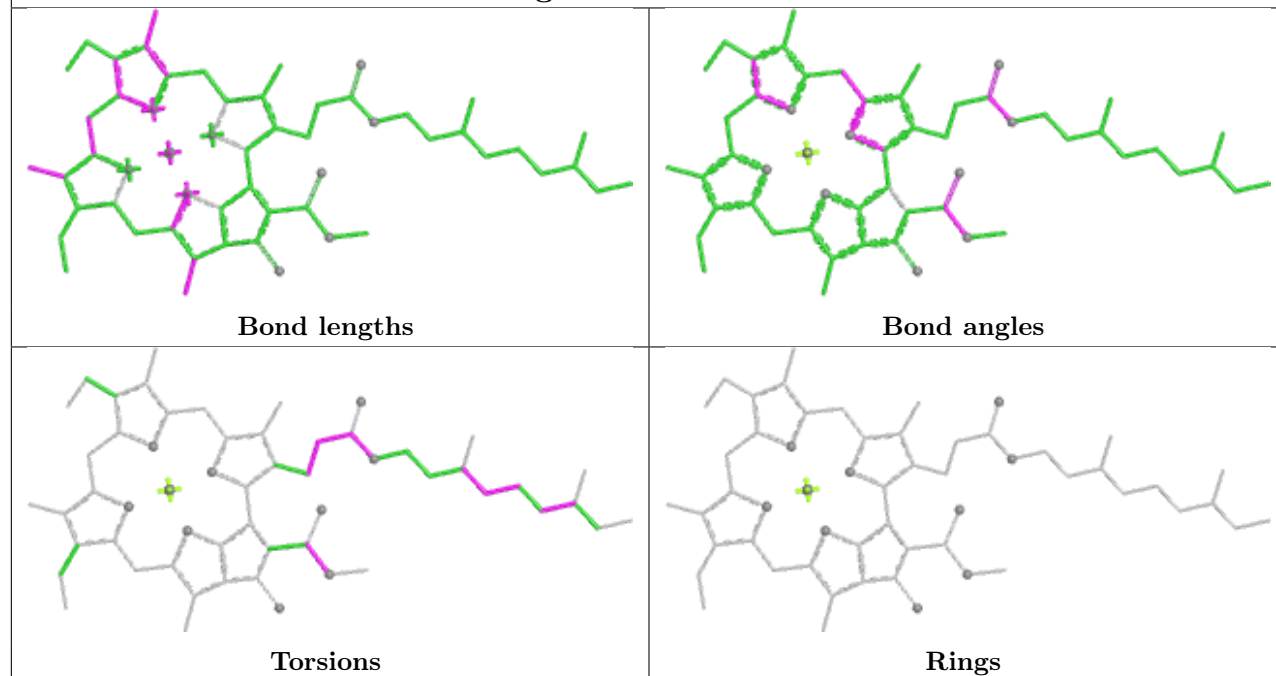


Torsions

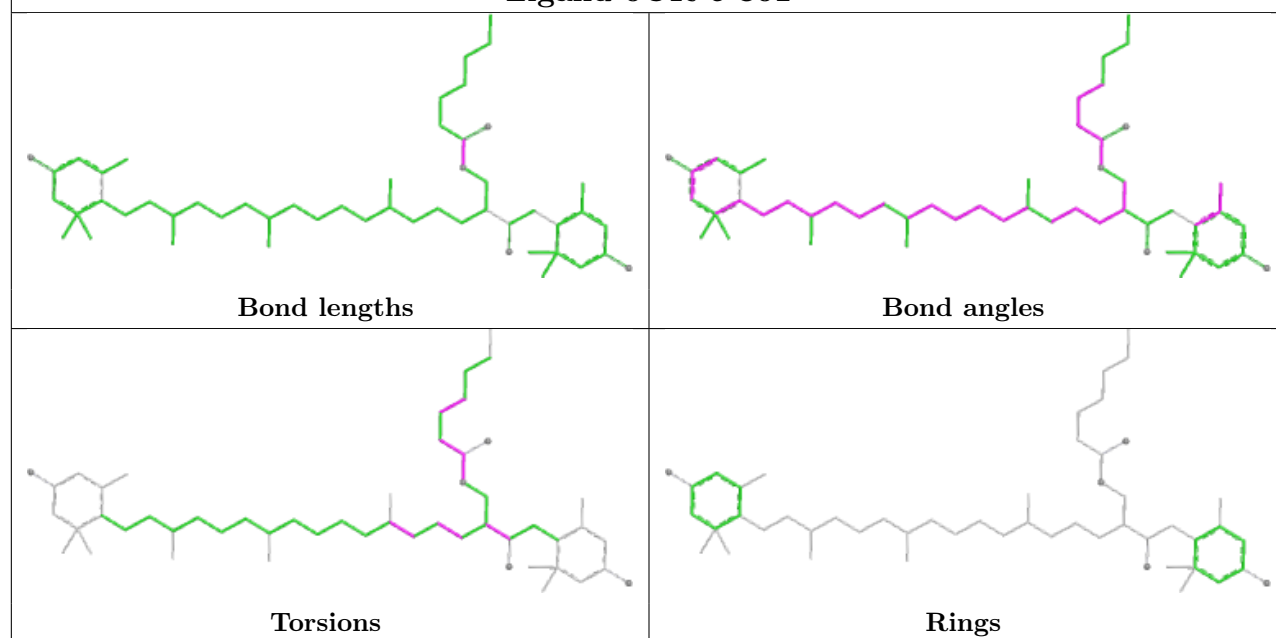


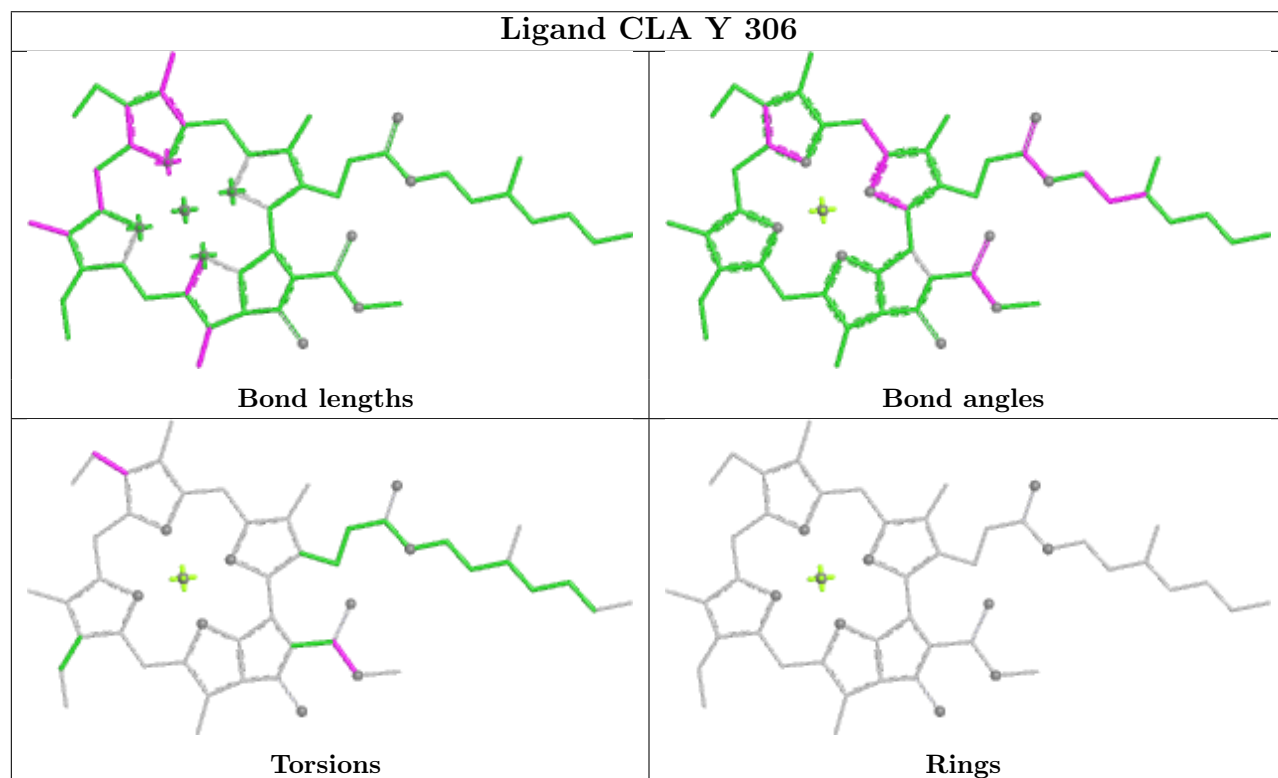
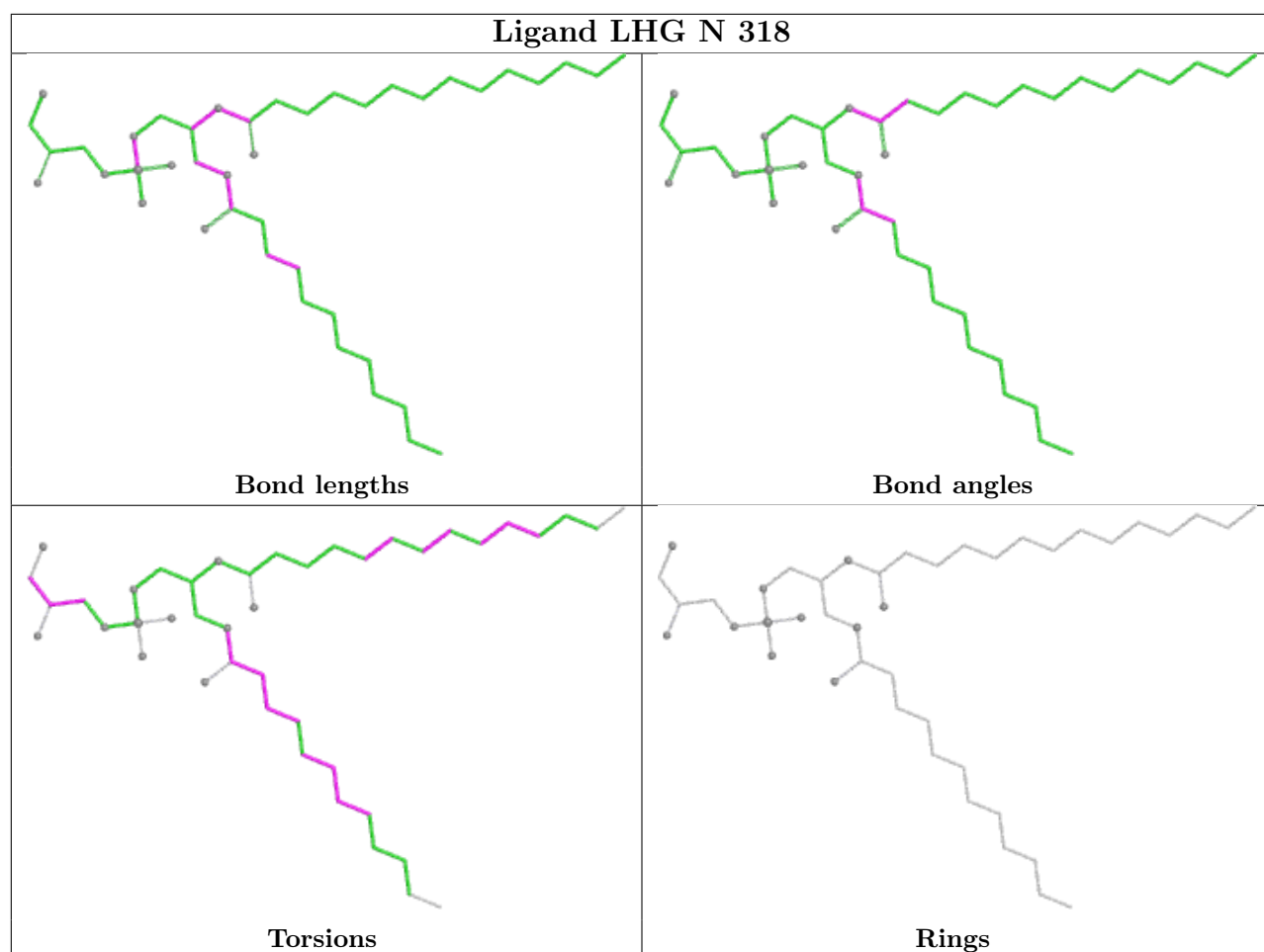
Rings

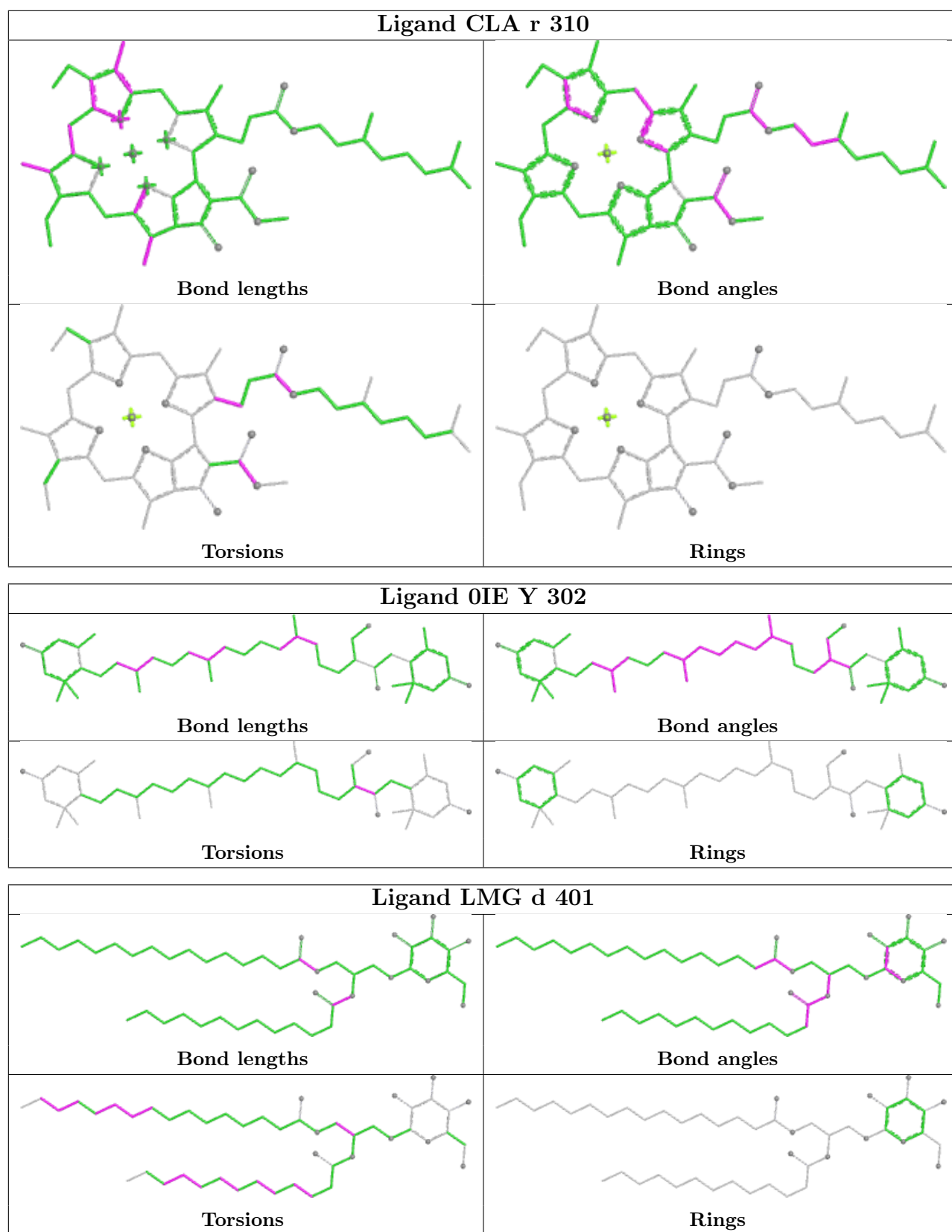
Ligand CLA b 614



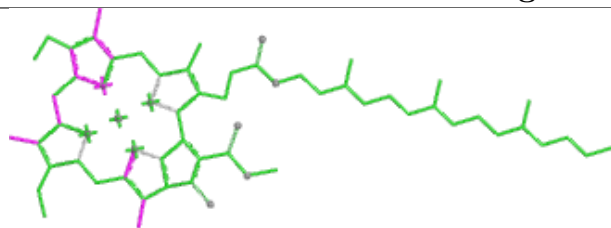
Ligand OUR 6 301



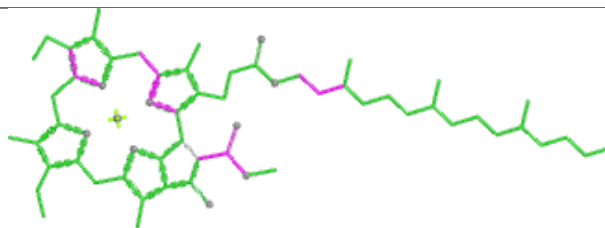




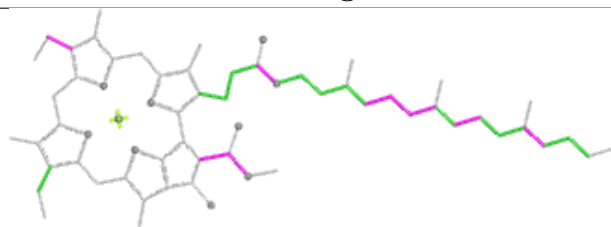
Ligand CLA 7 315



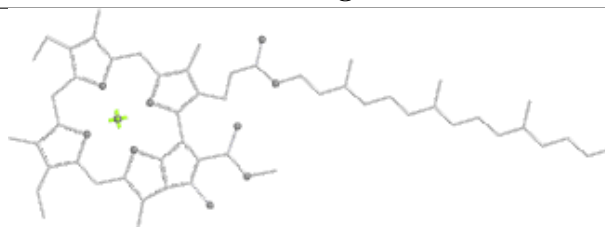
Bond lengths



Bond angles

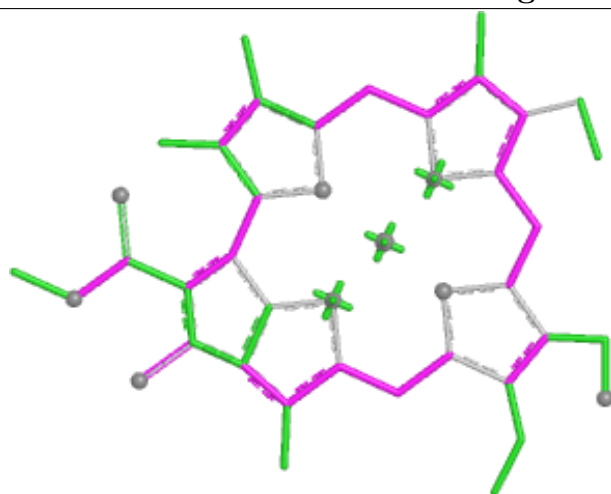


Torsions

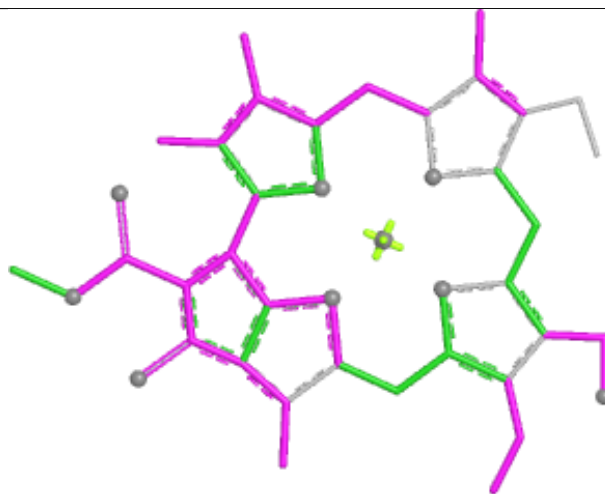


Rings

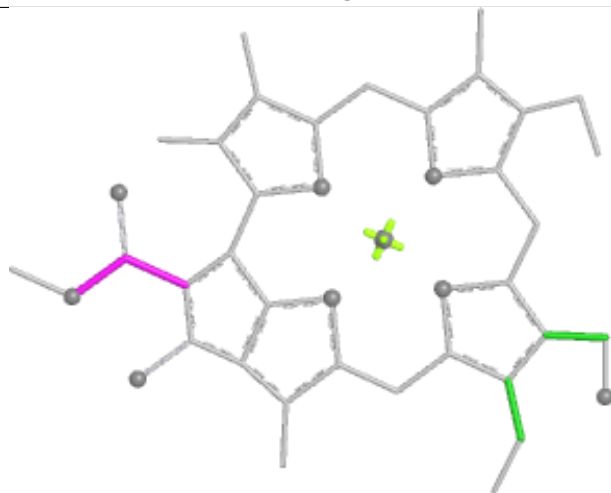
Ligand CHL 2 318



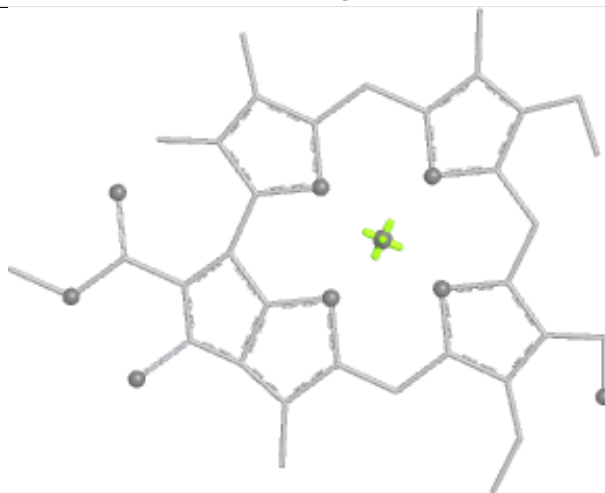
Bond lengths



Bond angles

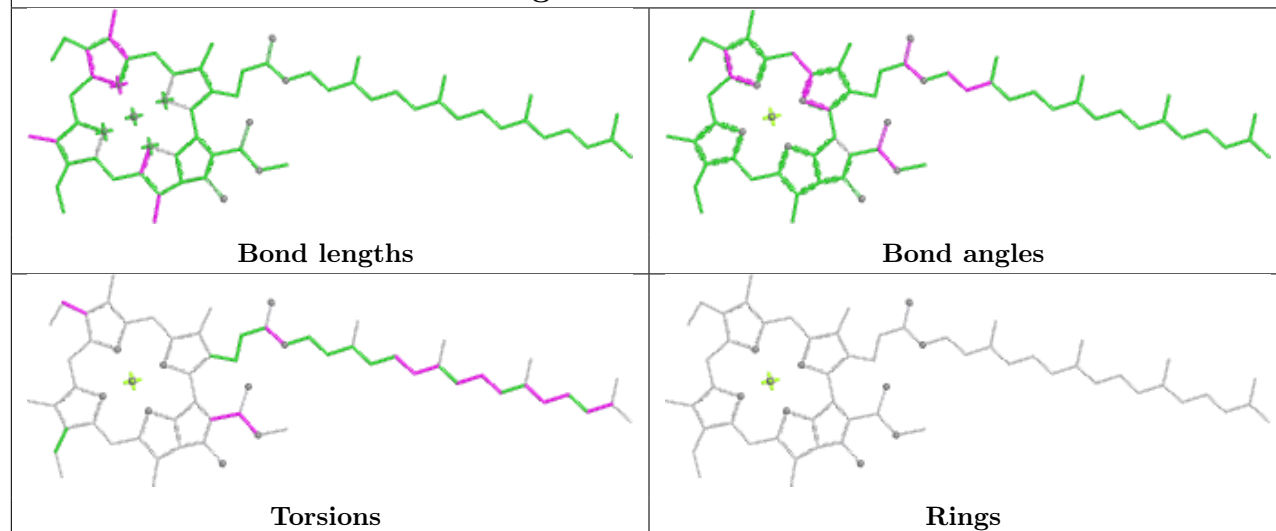


Torsions

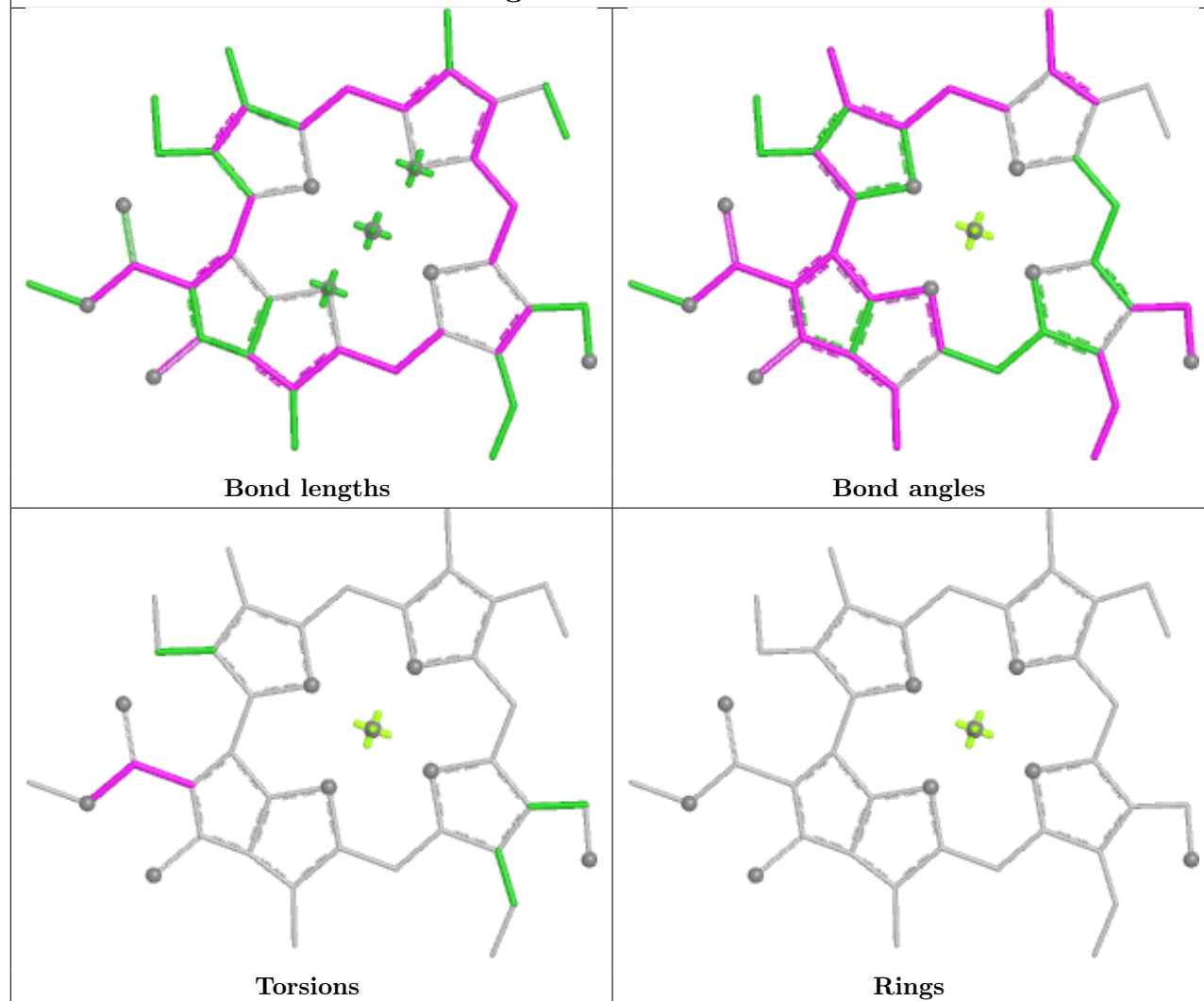


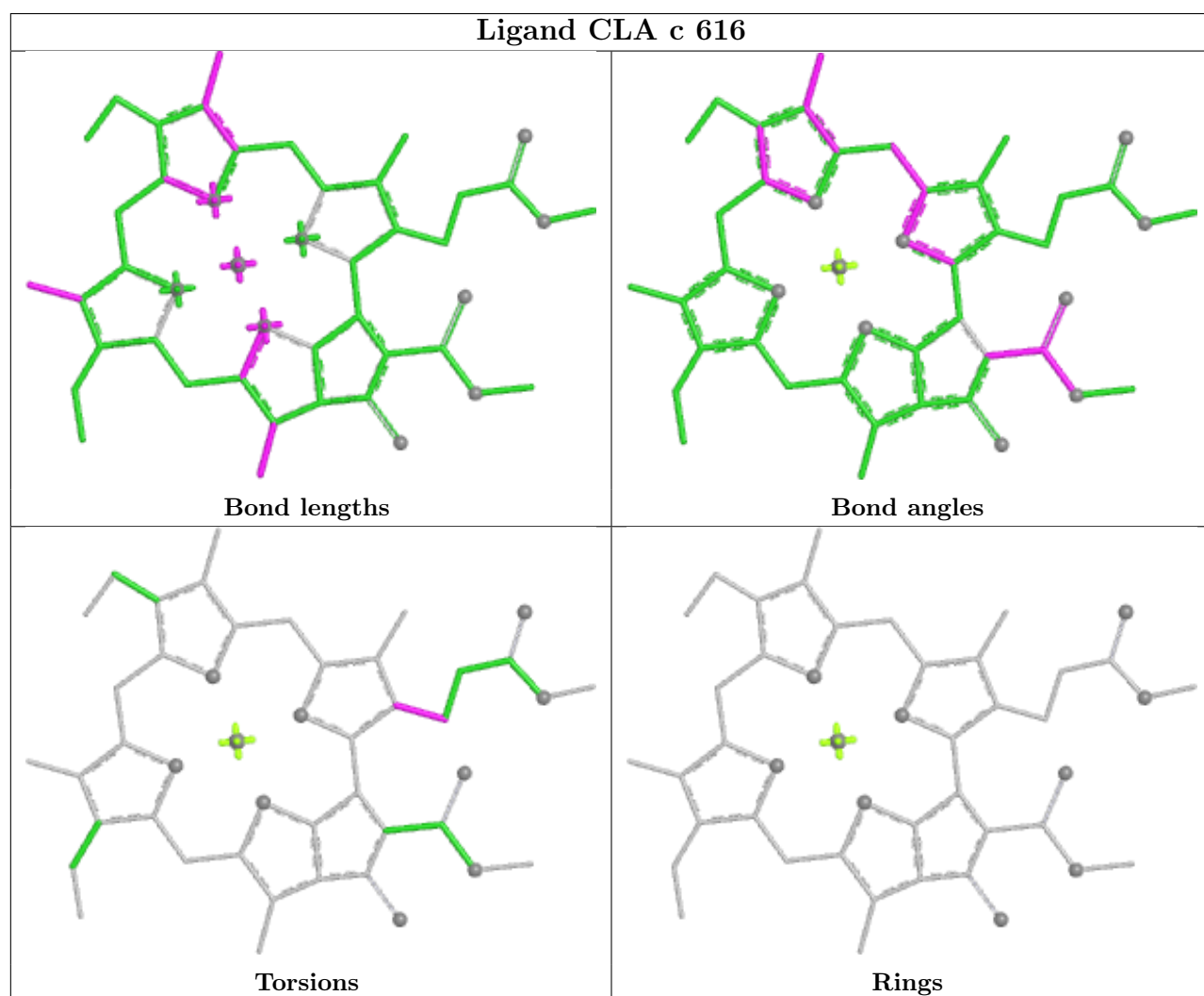
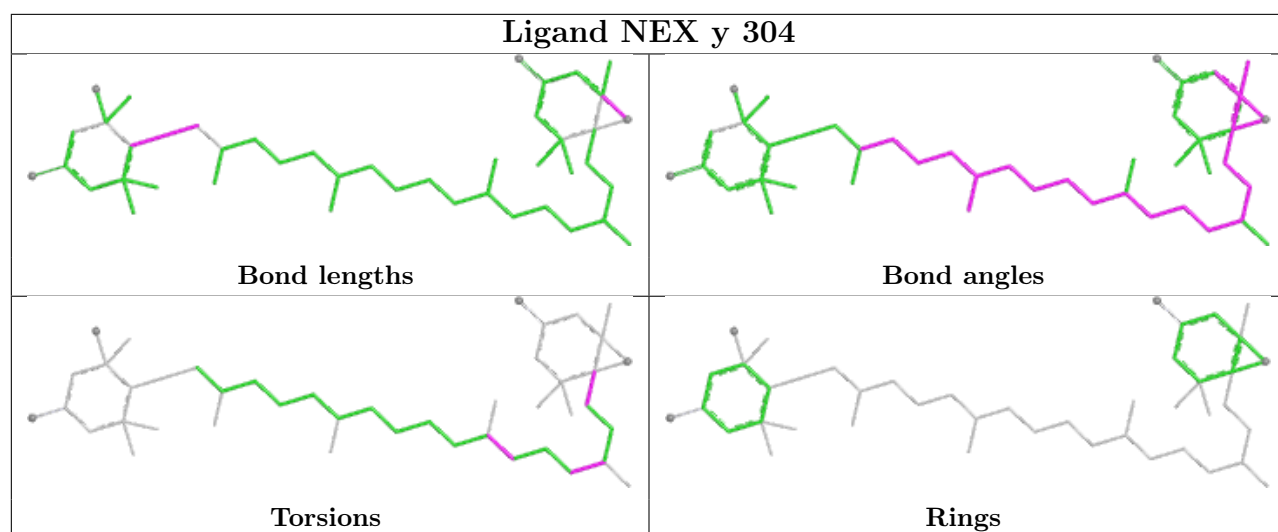
Rings

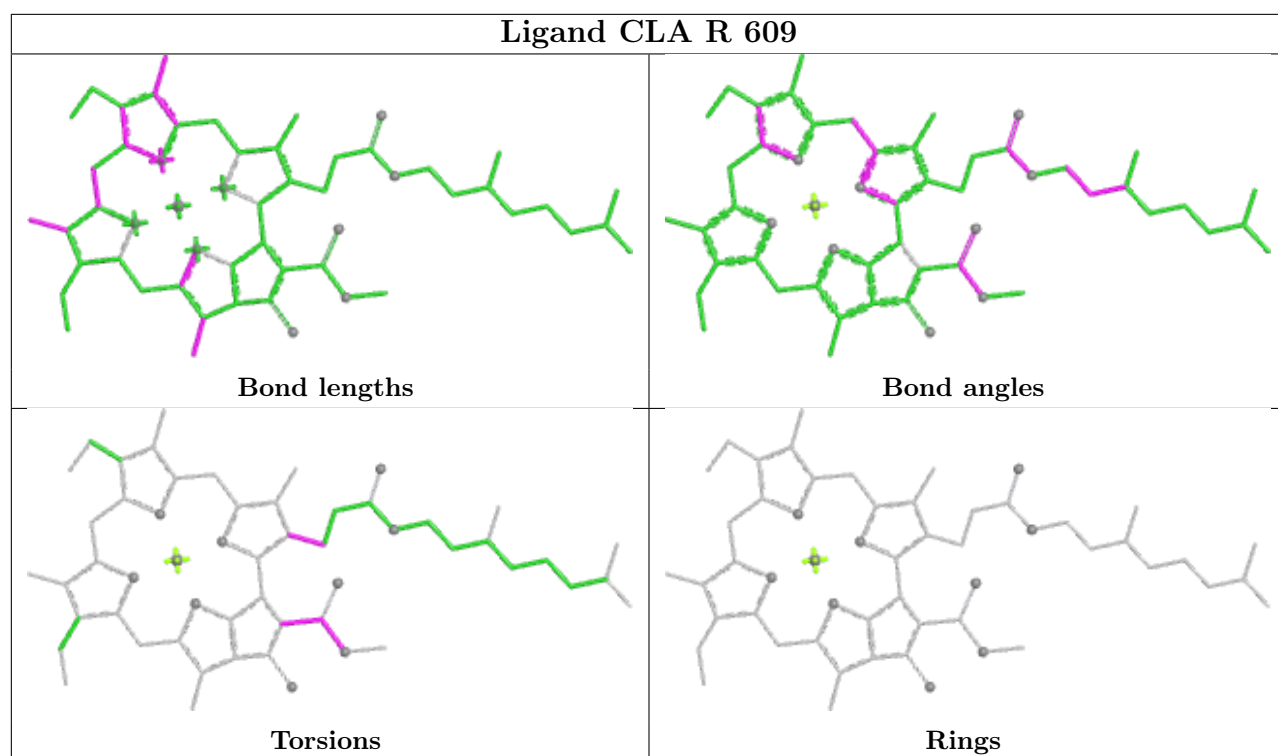
Ligand CLA C 602



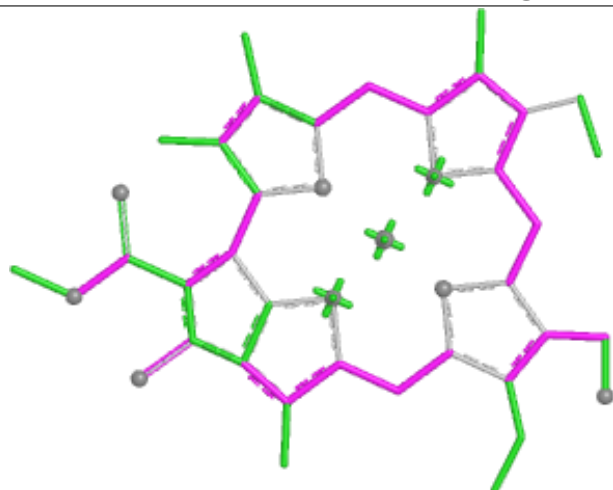
Ligand CHL 2 309



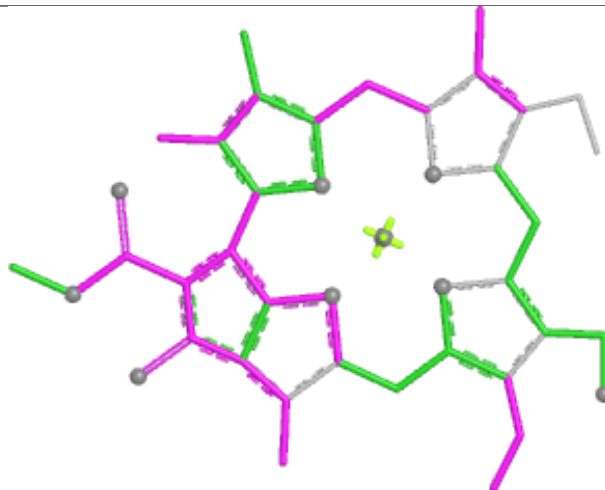




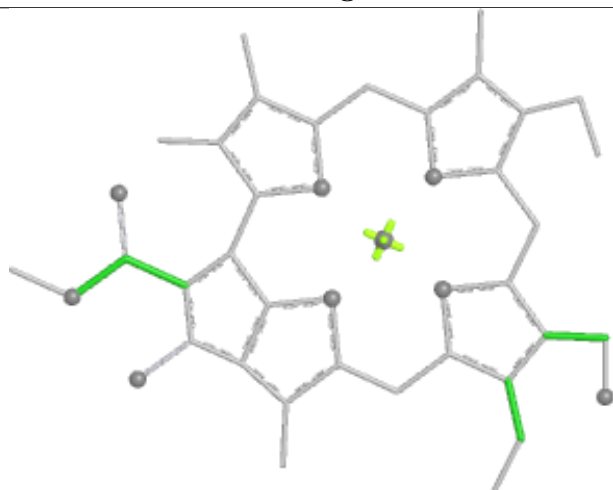
Ligand CHL 8 315



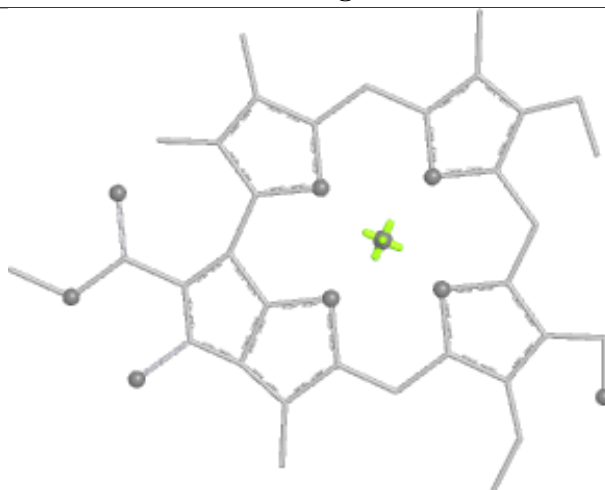
Bond lengths



Bond angles

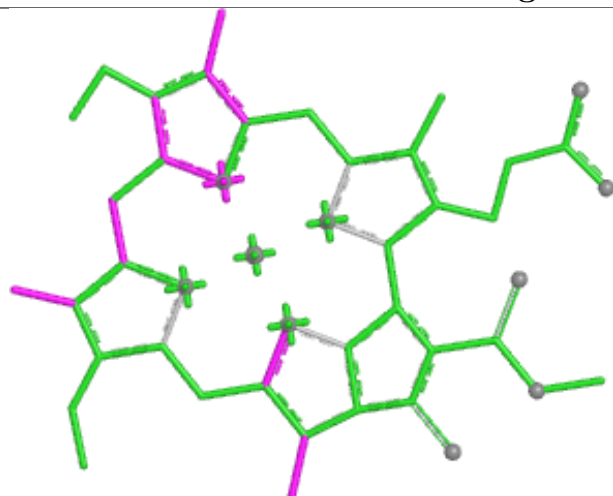


Torsions

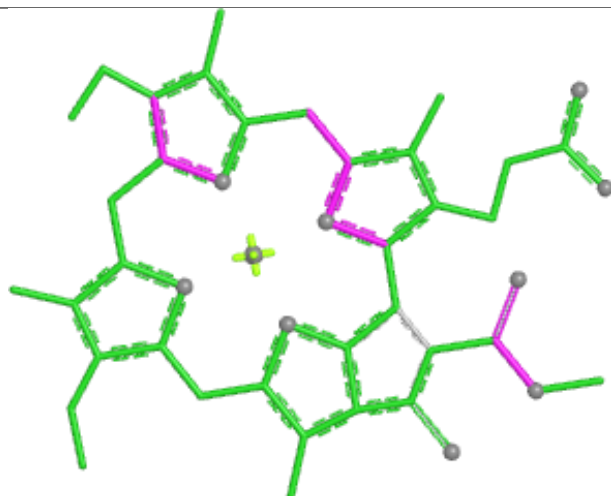


Rings

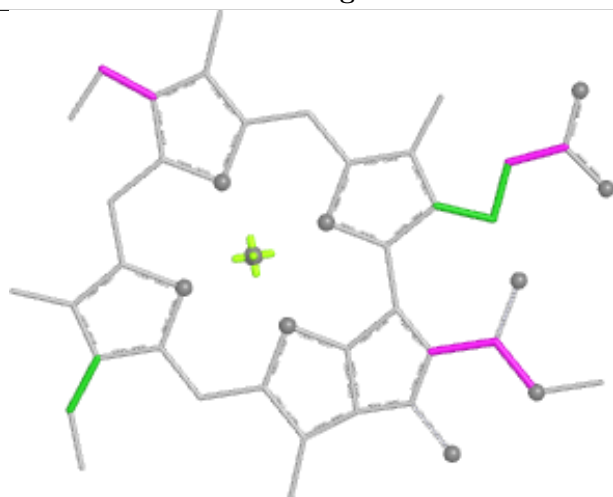
Ligand CLA 3 315



Bond lengths



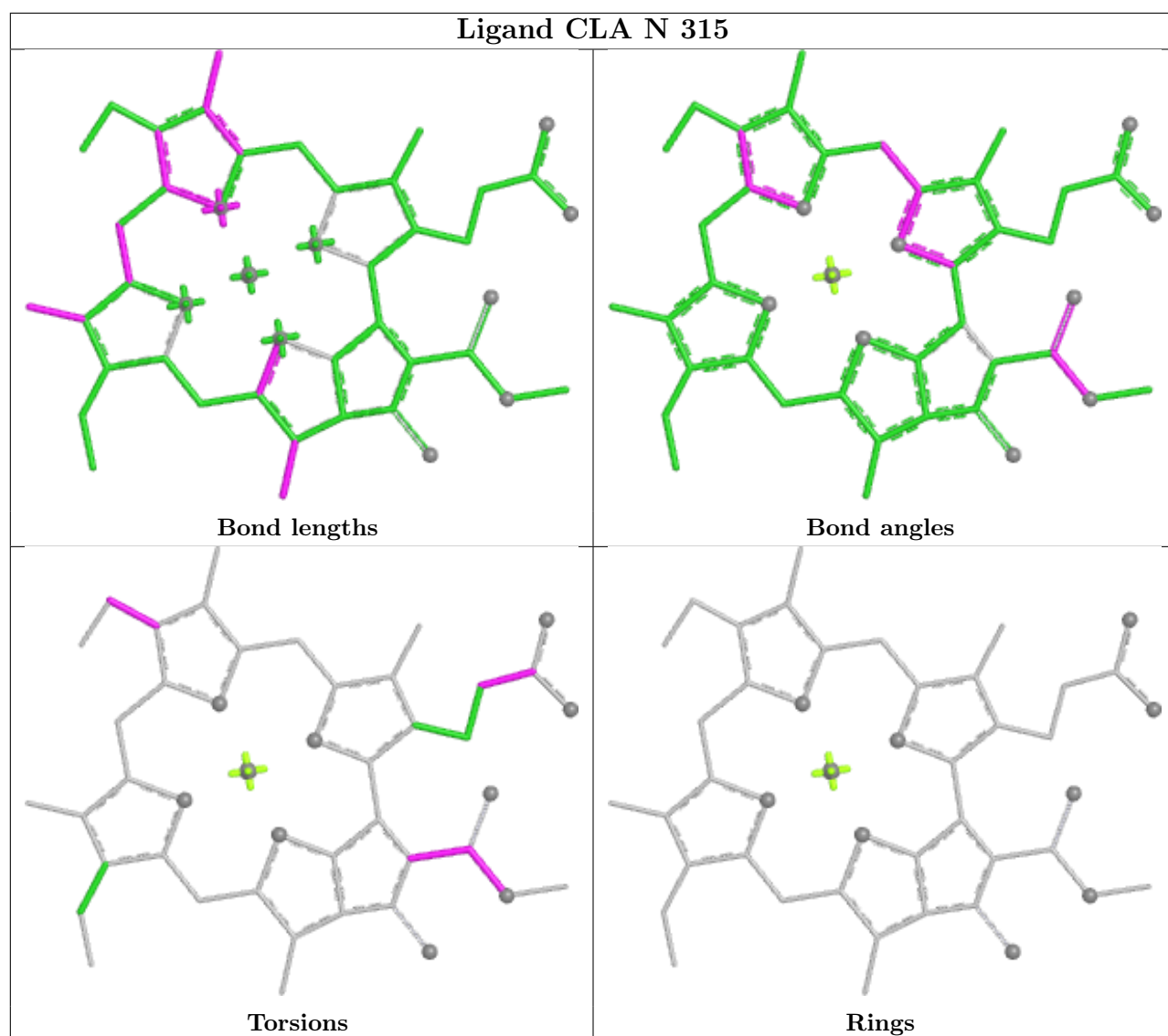
Bond angles

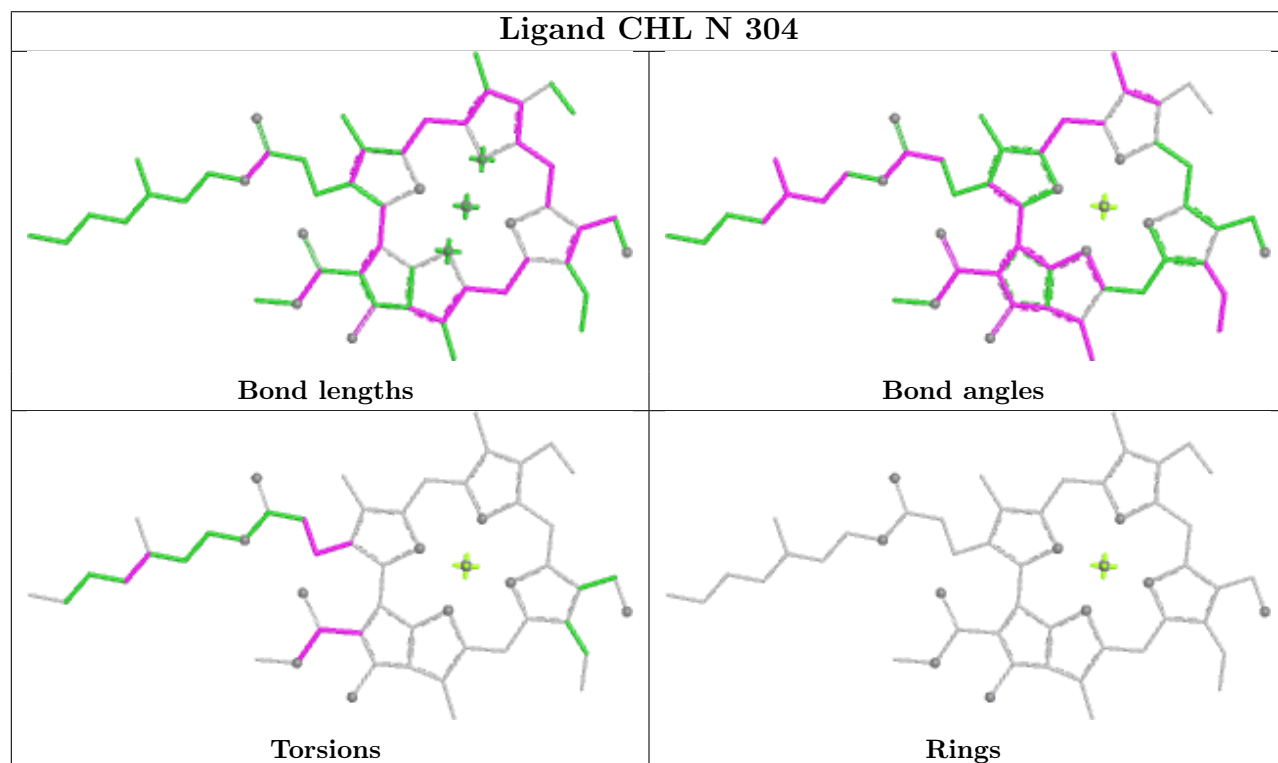
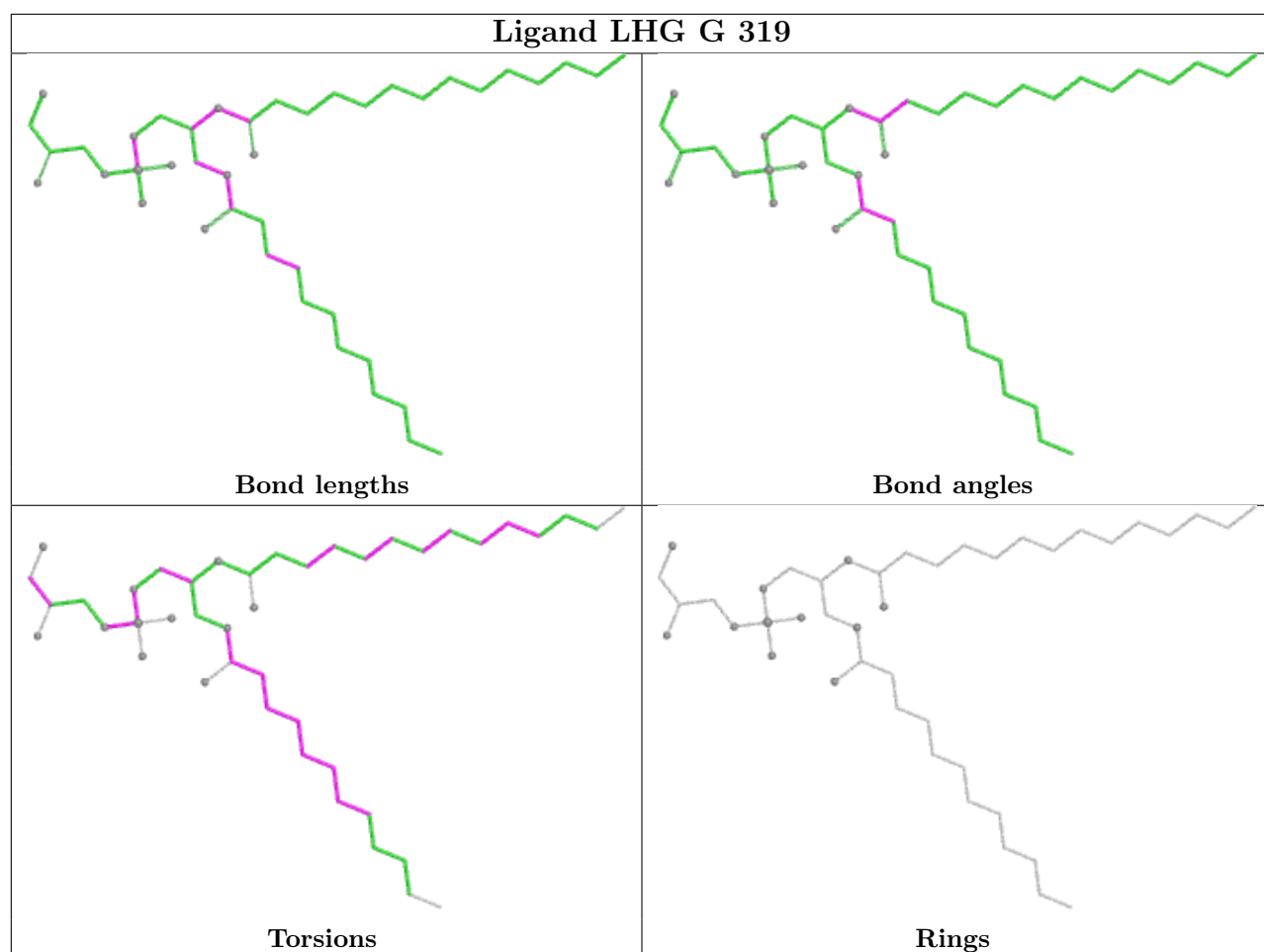


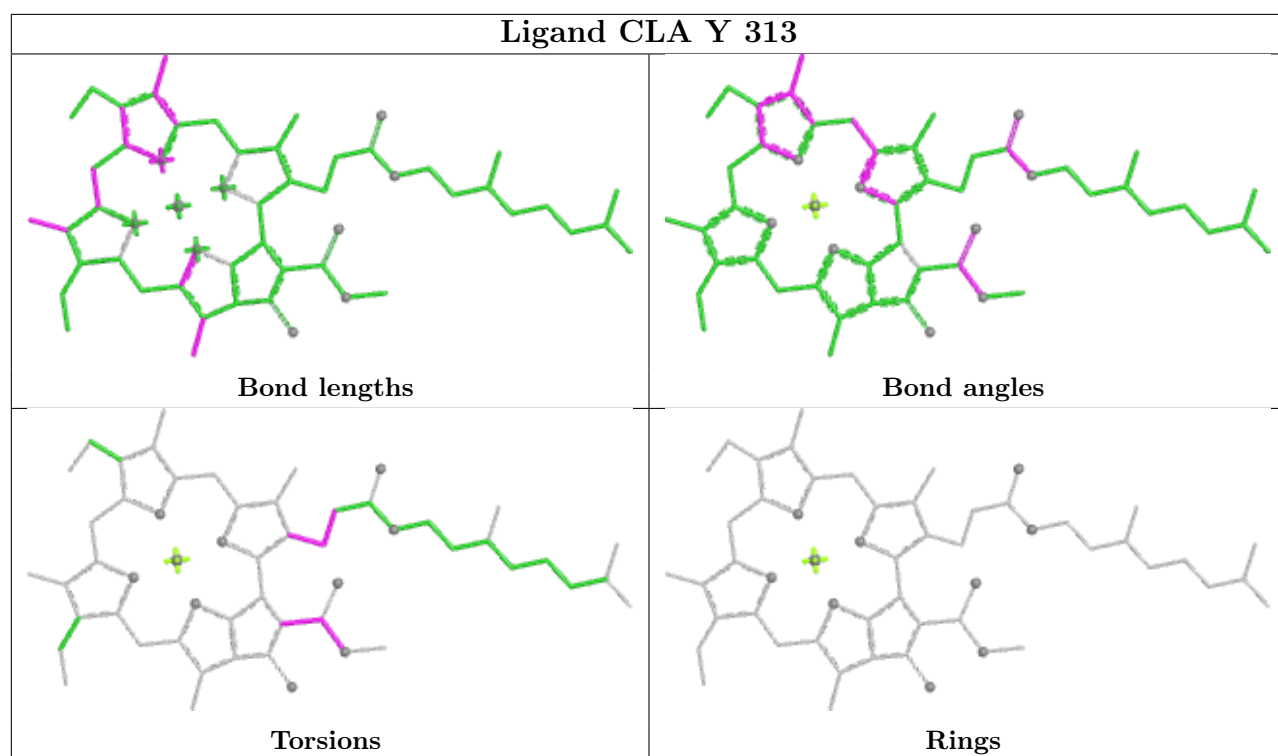
Torsions



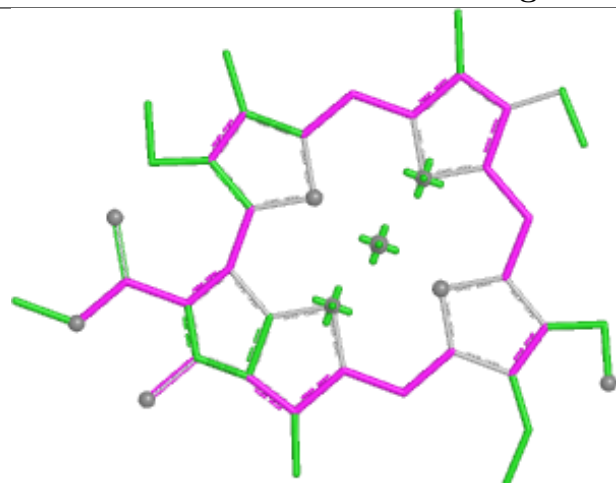
Rings



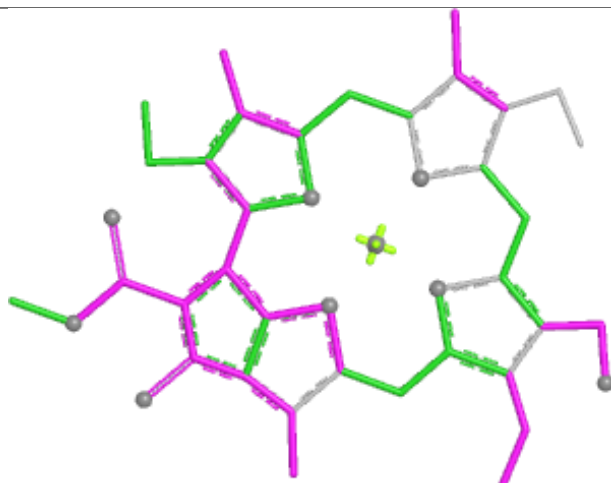




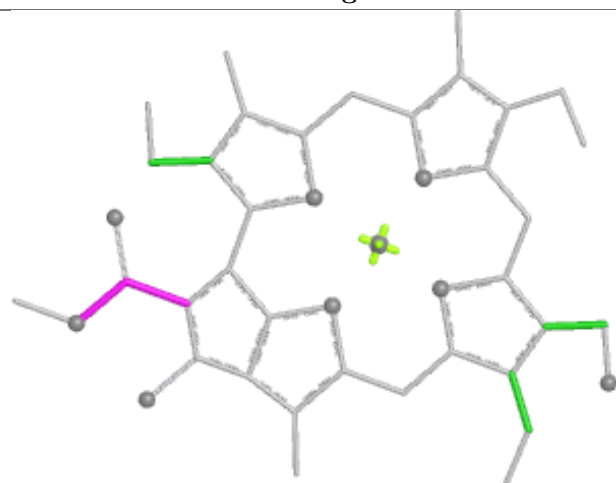
Ligand CHL 1 309



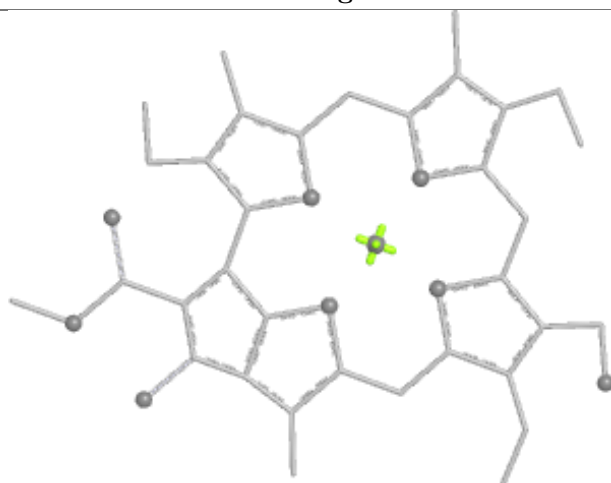
Bond lengths



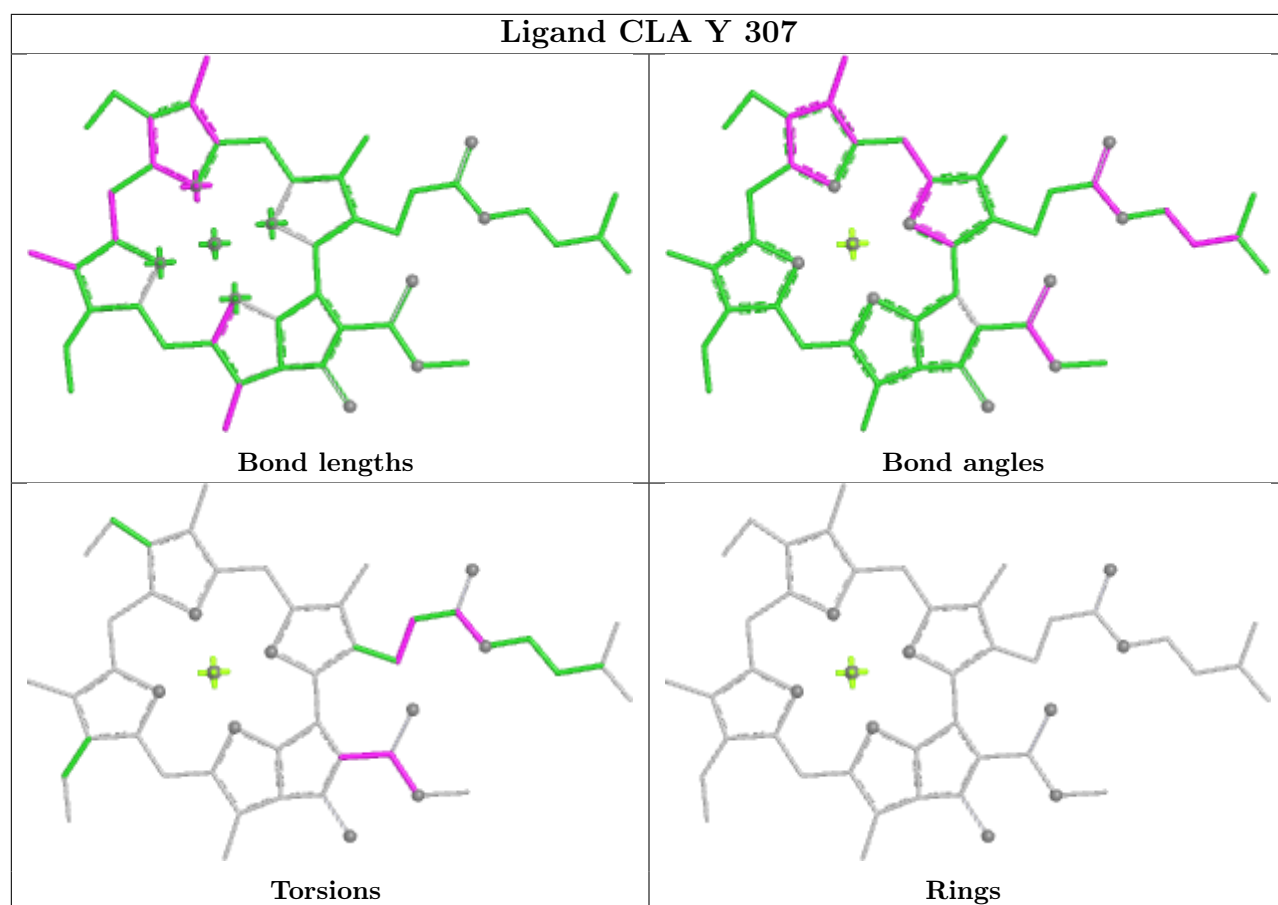
Bond angles



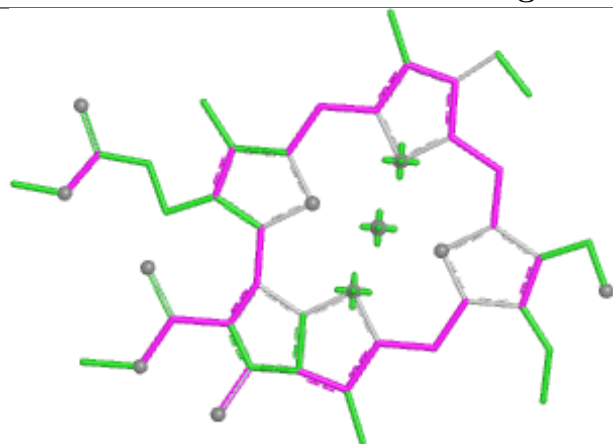
Torsions



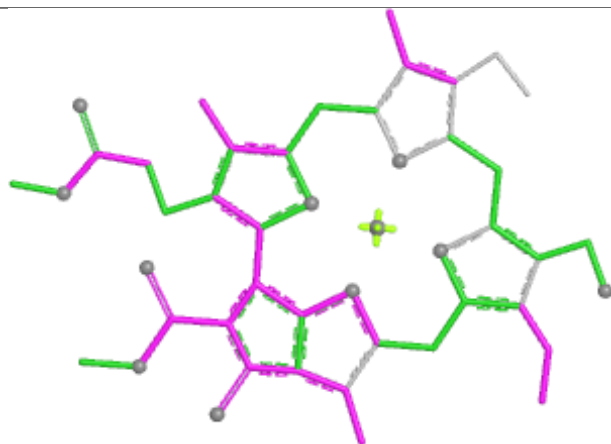
Rings



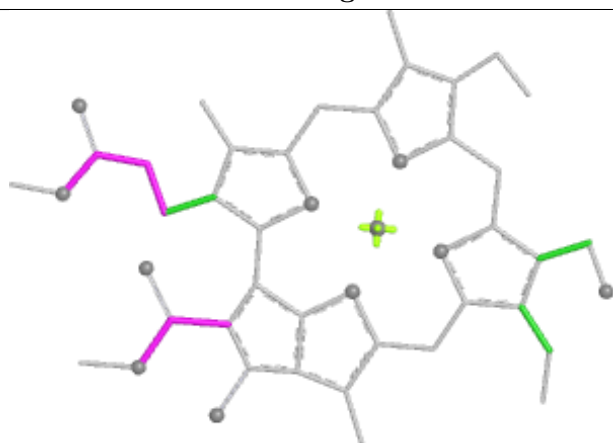
Ligand CHL 5 311



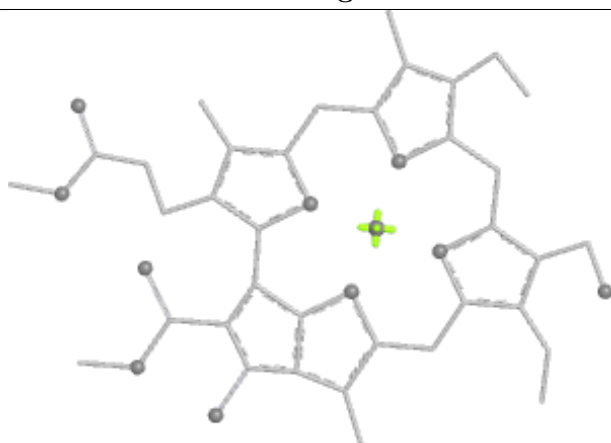
Bond lengths



Bond angles

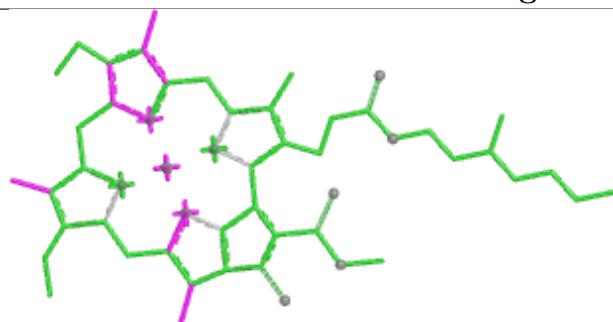


Torsions

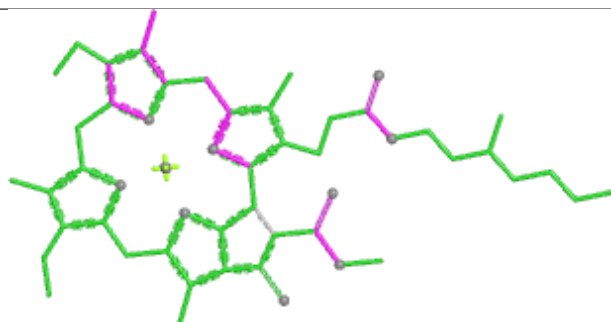


Rings

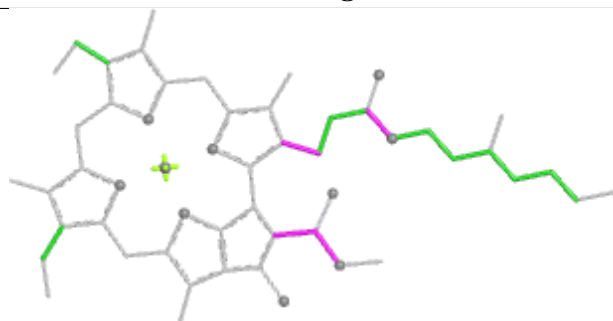
Ligand CLA c 606



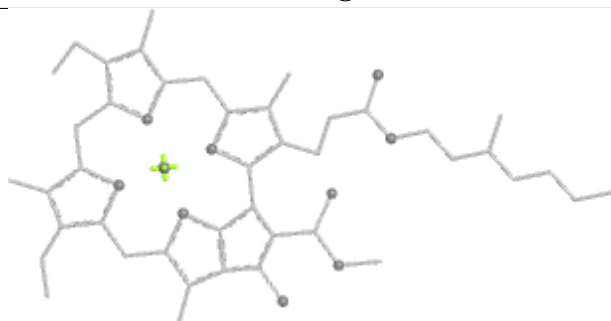
Bond lengths



Bond angles

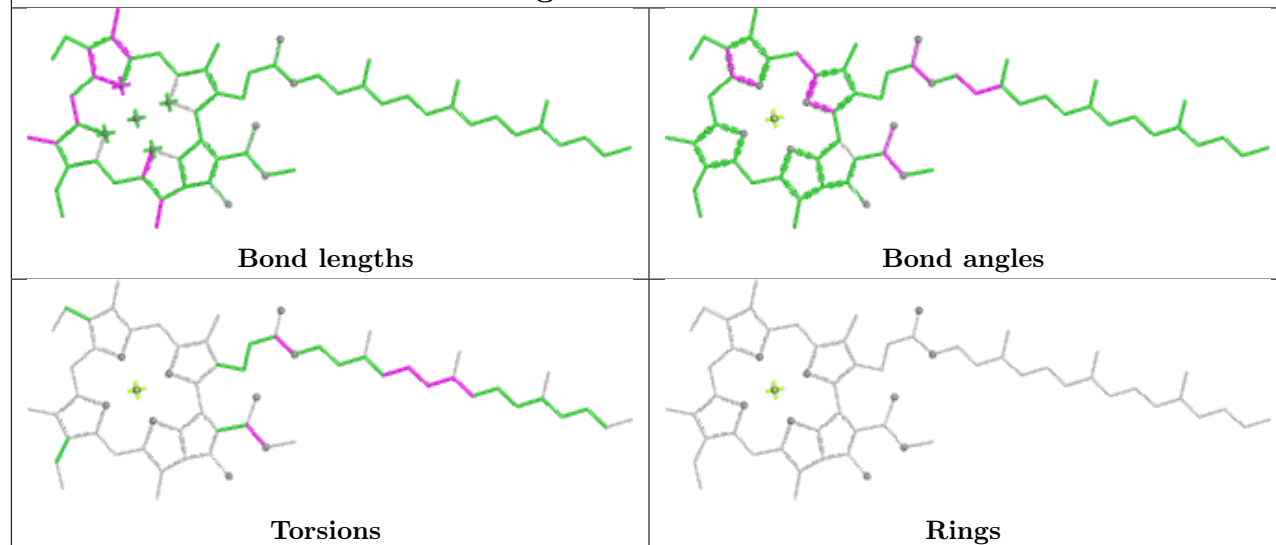


Torsions

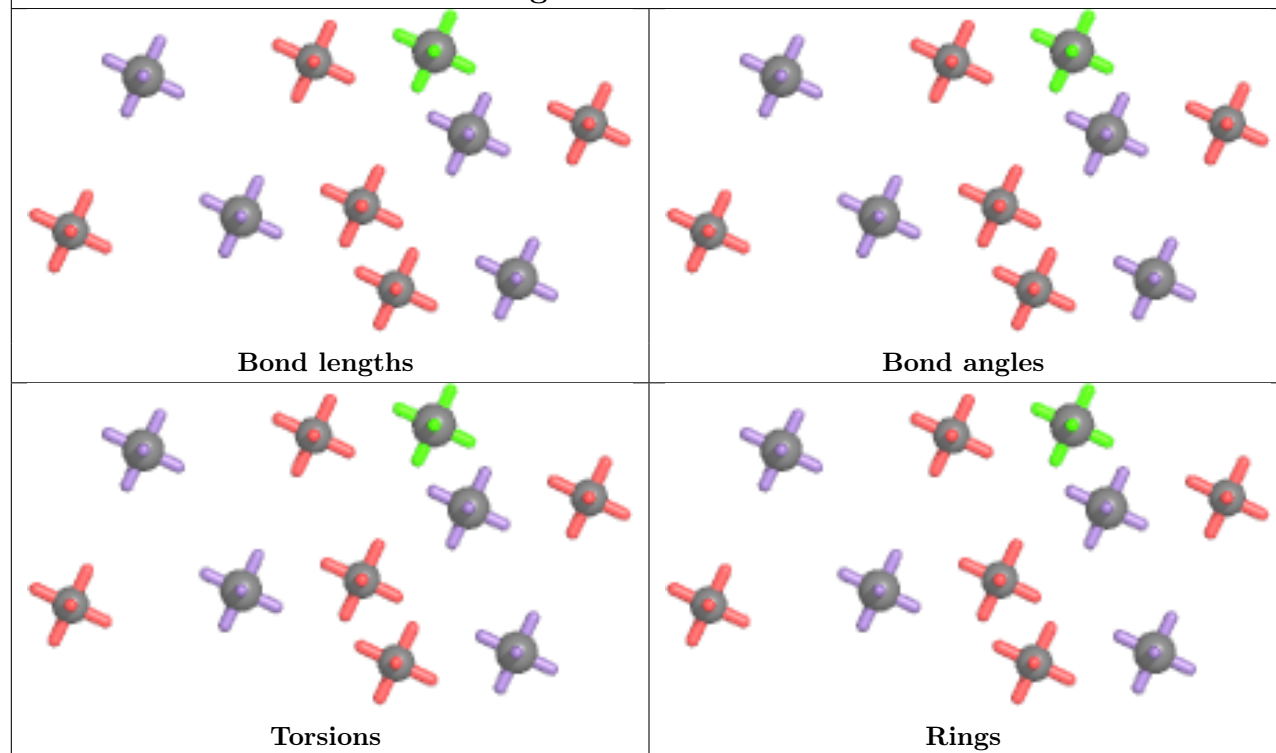


Rings

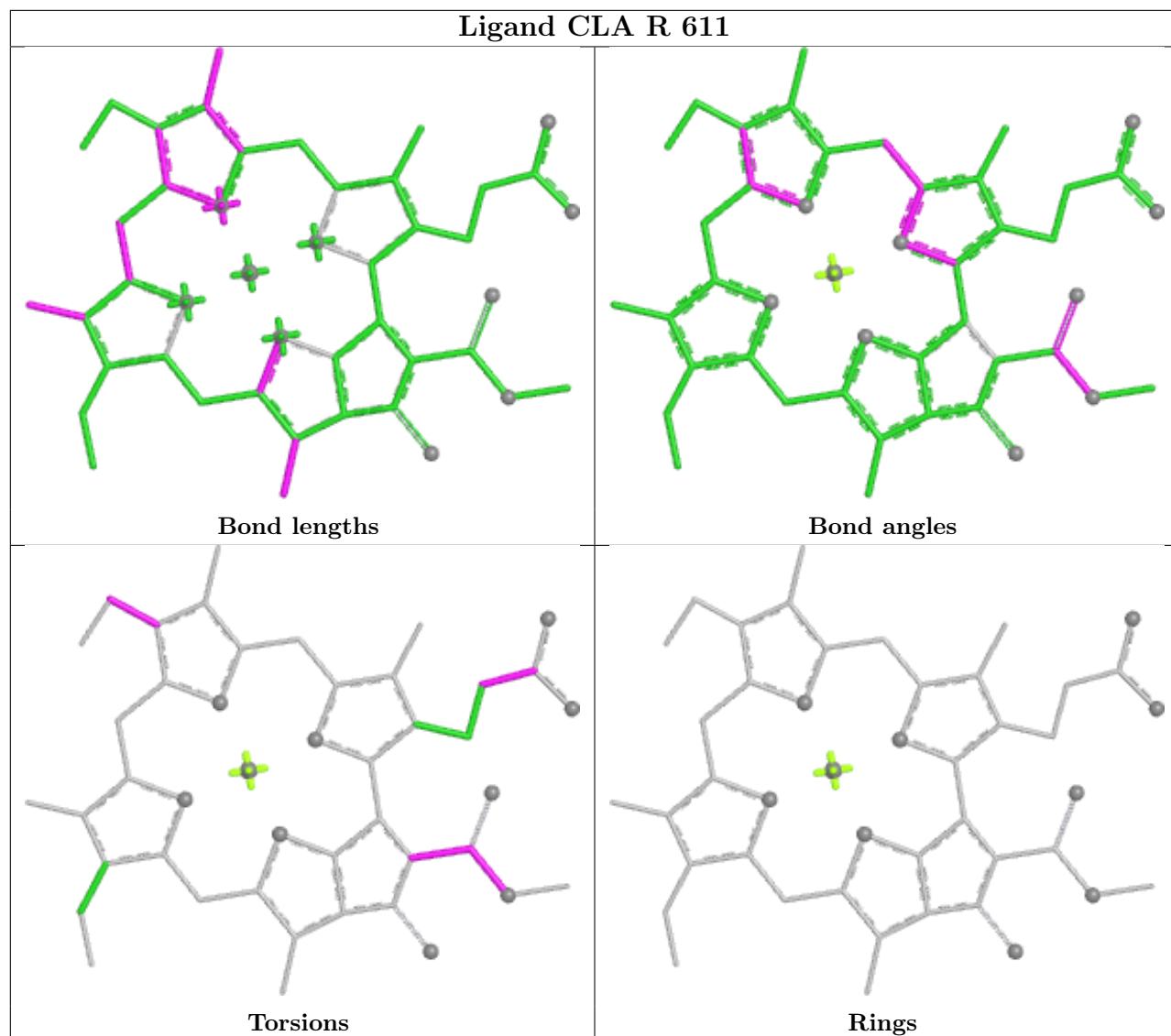
Ligand CLA 8 312



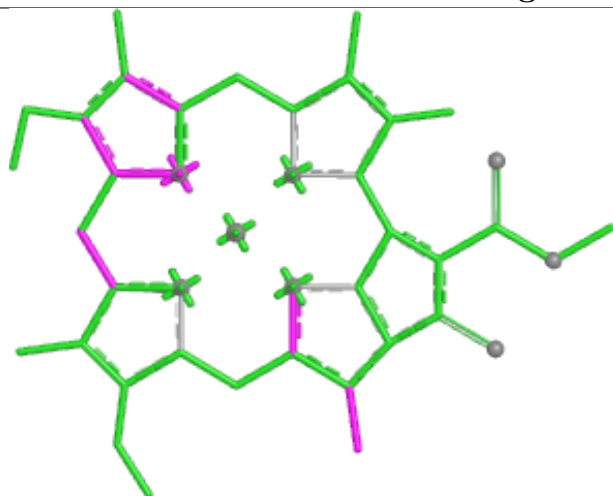
Ligand OEX A 602



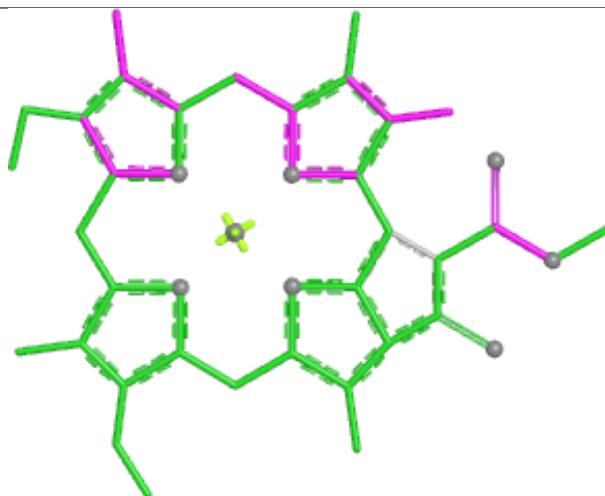
Ligand CLA R 611



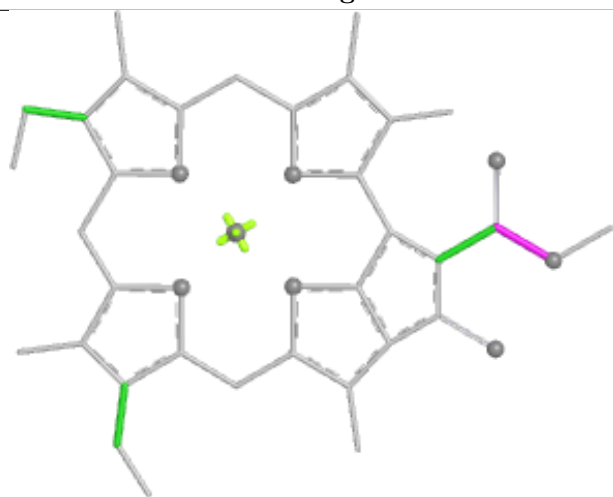
Ligand CLA a 610



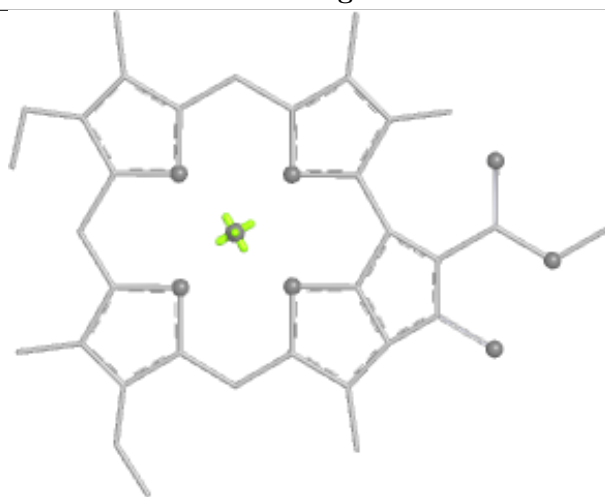
Bond lengths



Bond angles

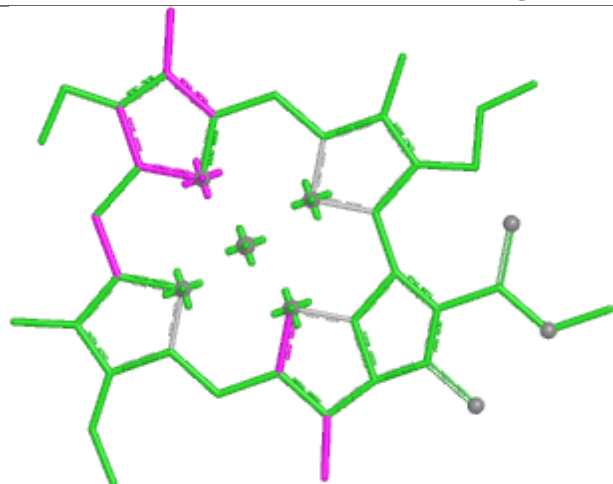


Torsions

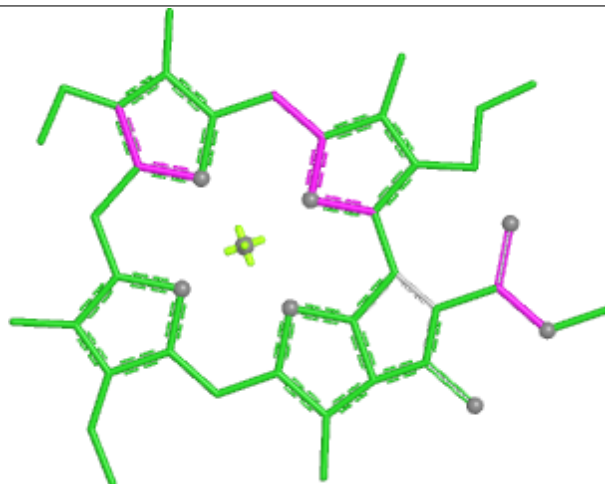


Rings

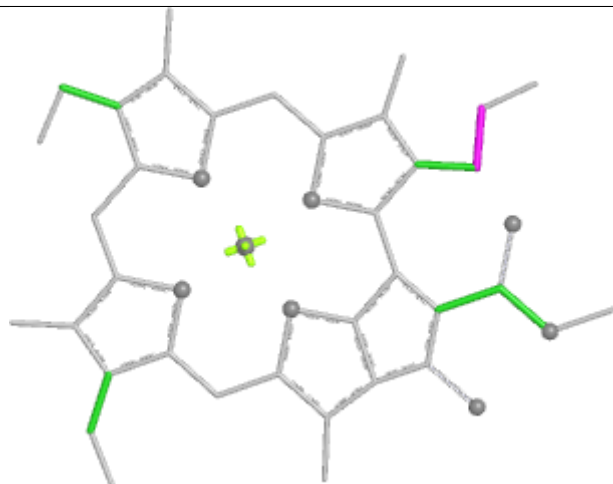
Ligand CLA N 316



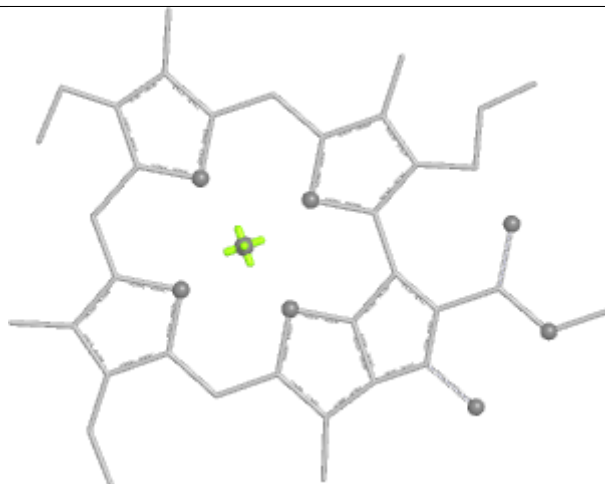
Bond lengths



Bond angles

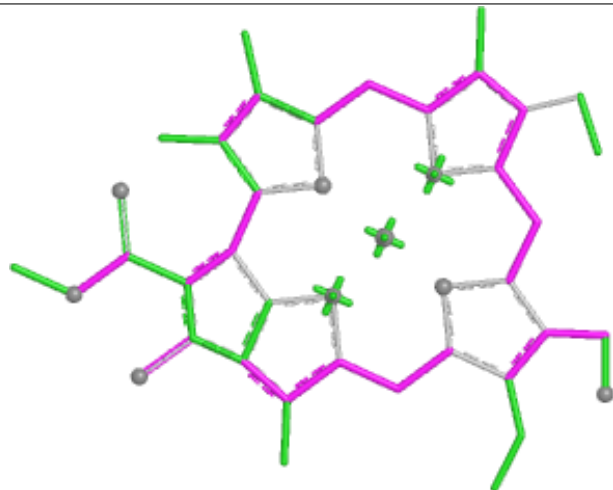


Torsions

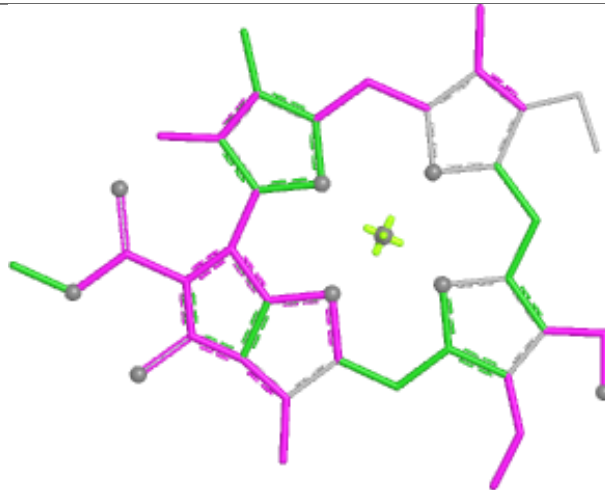


Rings

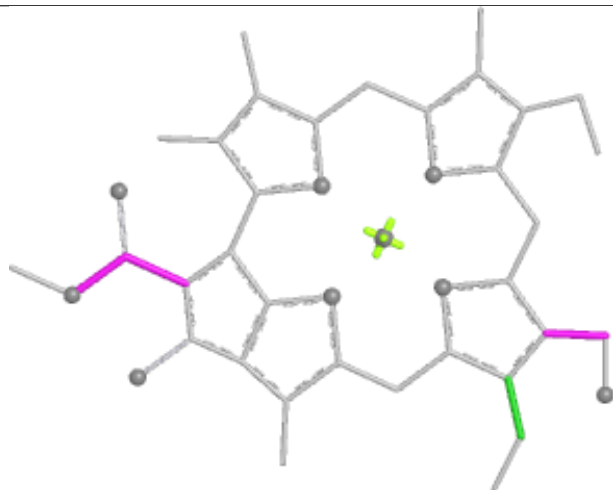
Ligand CHL N 317



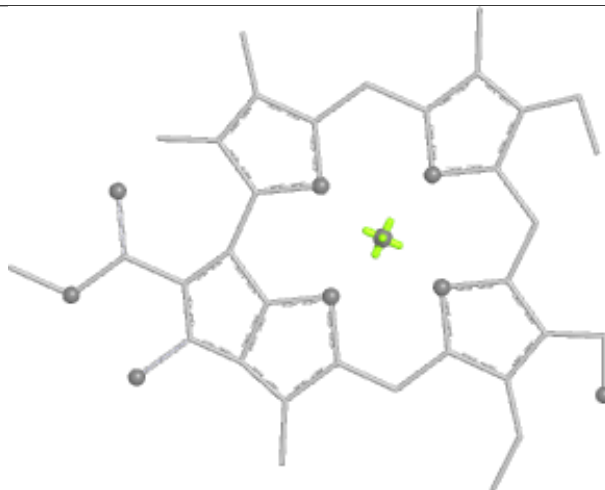
Bond lengths



Bond angles

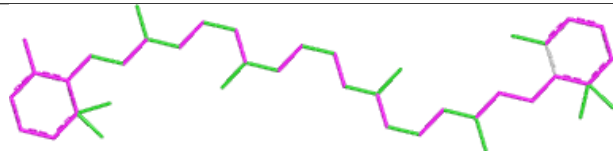


Torsions

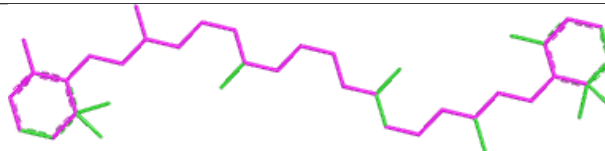


Rings

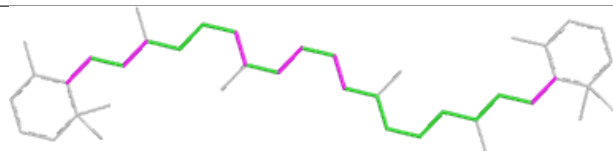
Ligand 8CT C 613



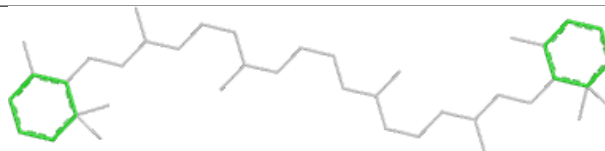
Bond lengths



Bond angles

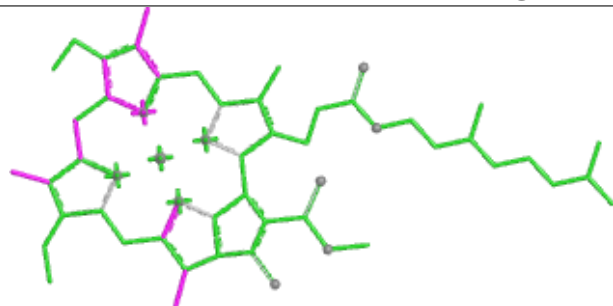


Torsions

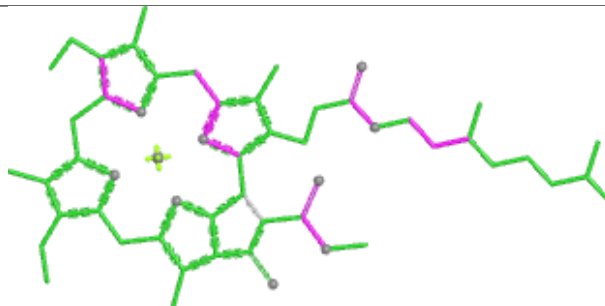


Rings

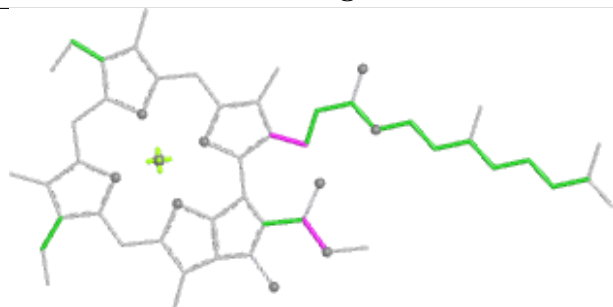
Ligand CLA G 314



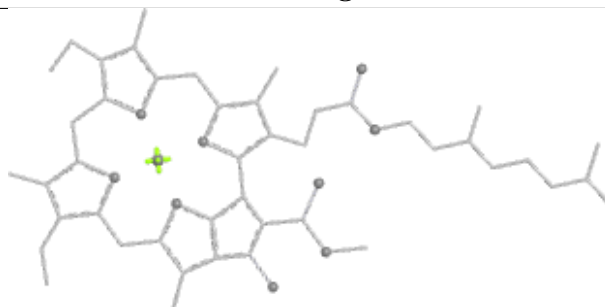
Bond lengths



Bond angles

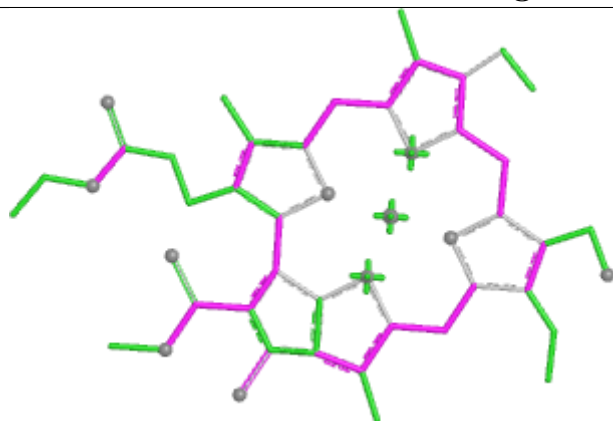


Torsions

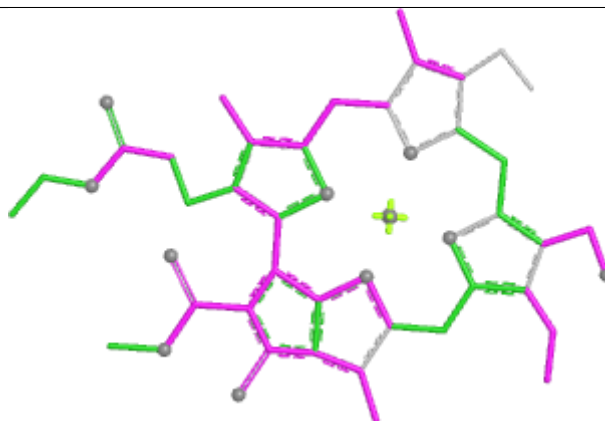


Rings

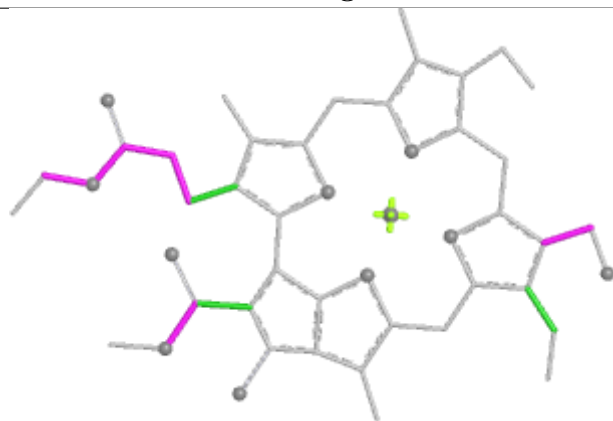
Ligand CHL R 607



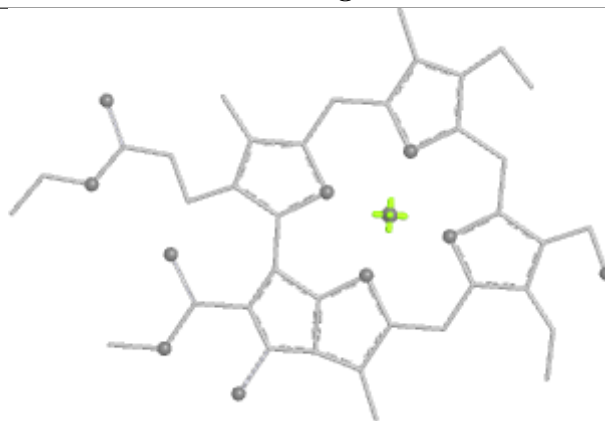
Bond lengths



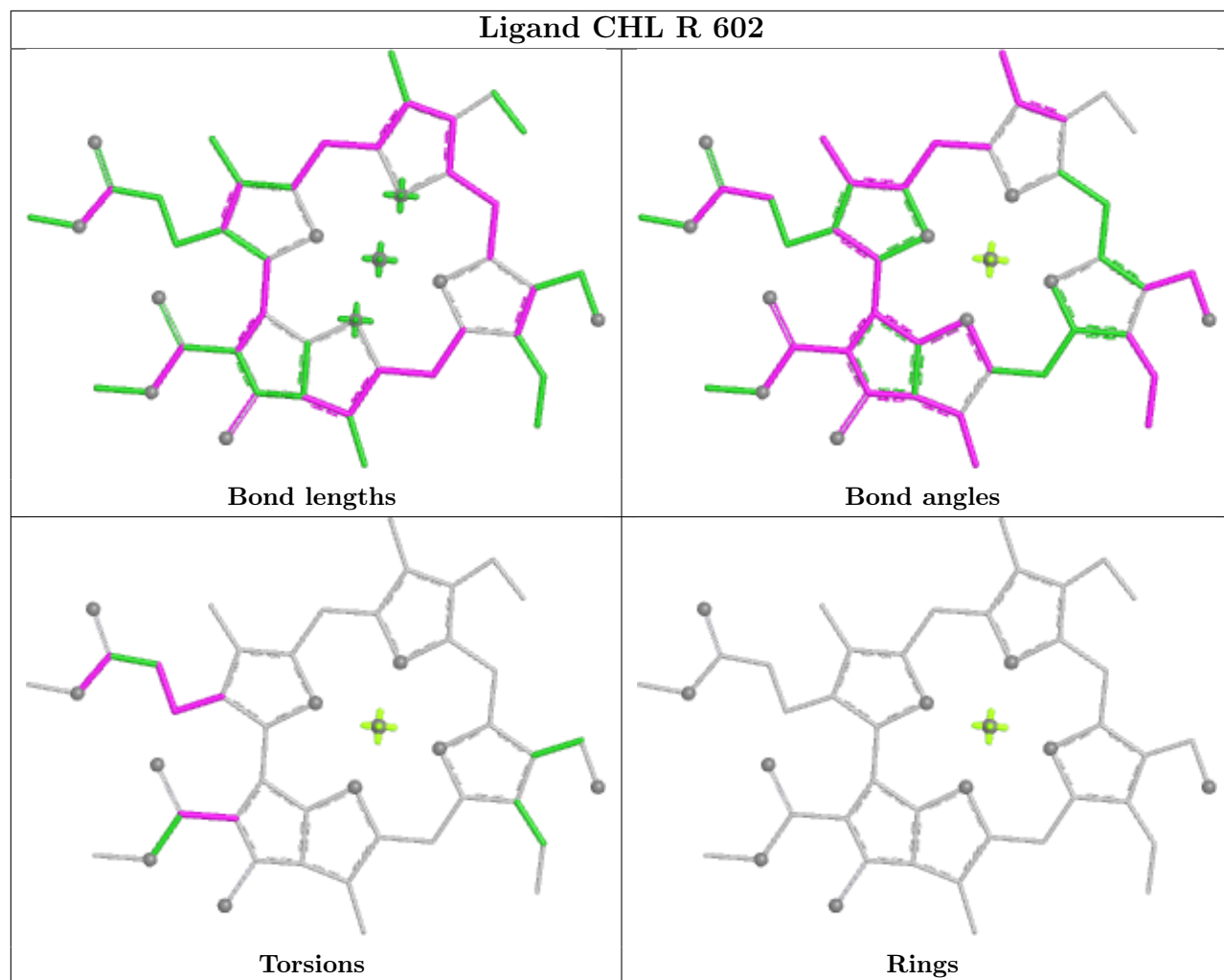
Bond angles



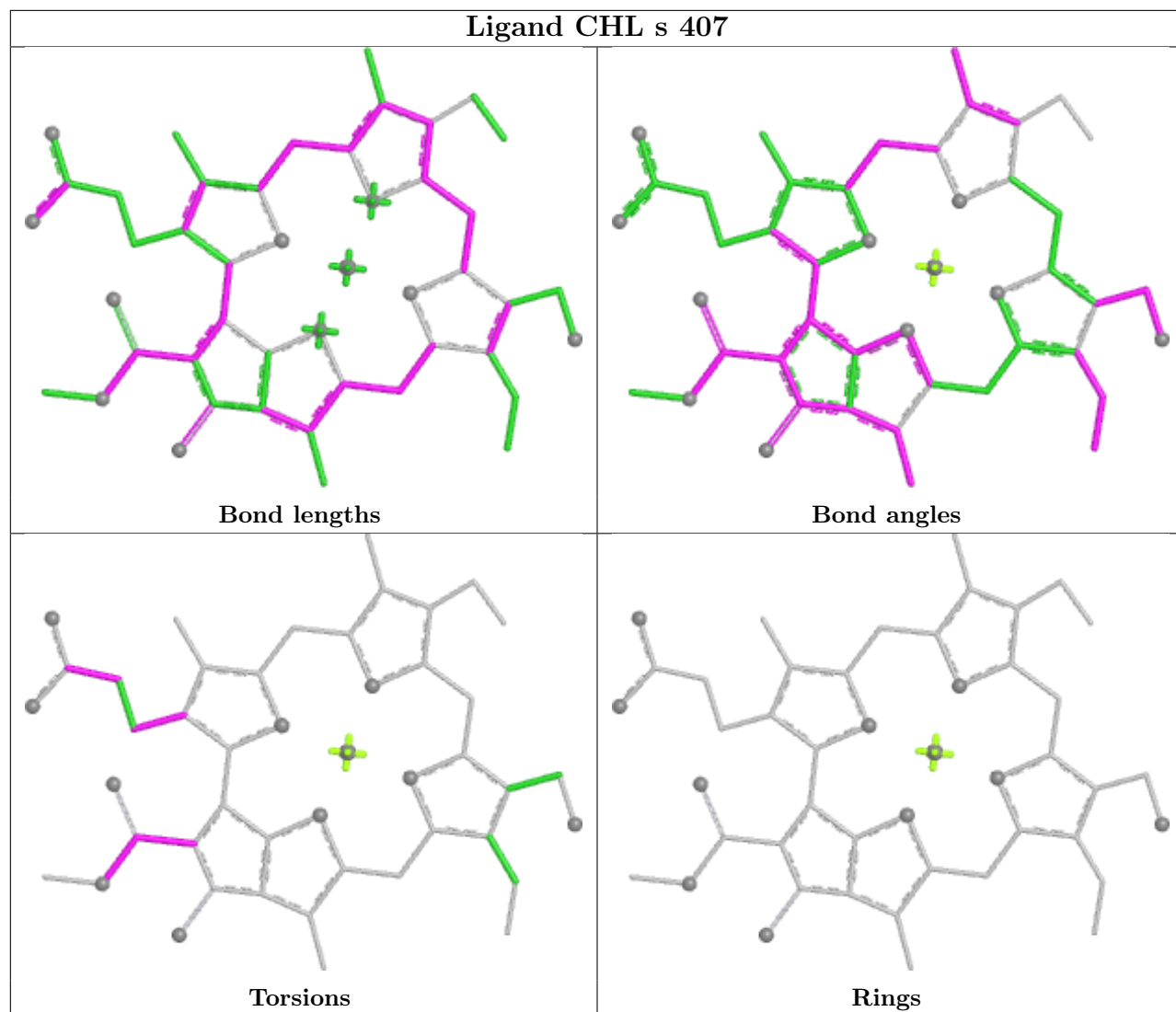
Torsions



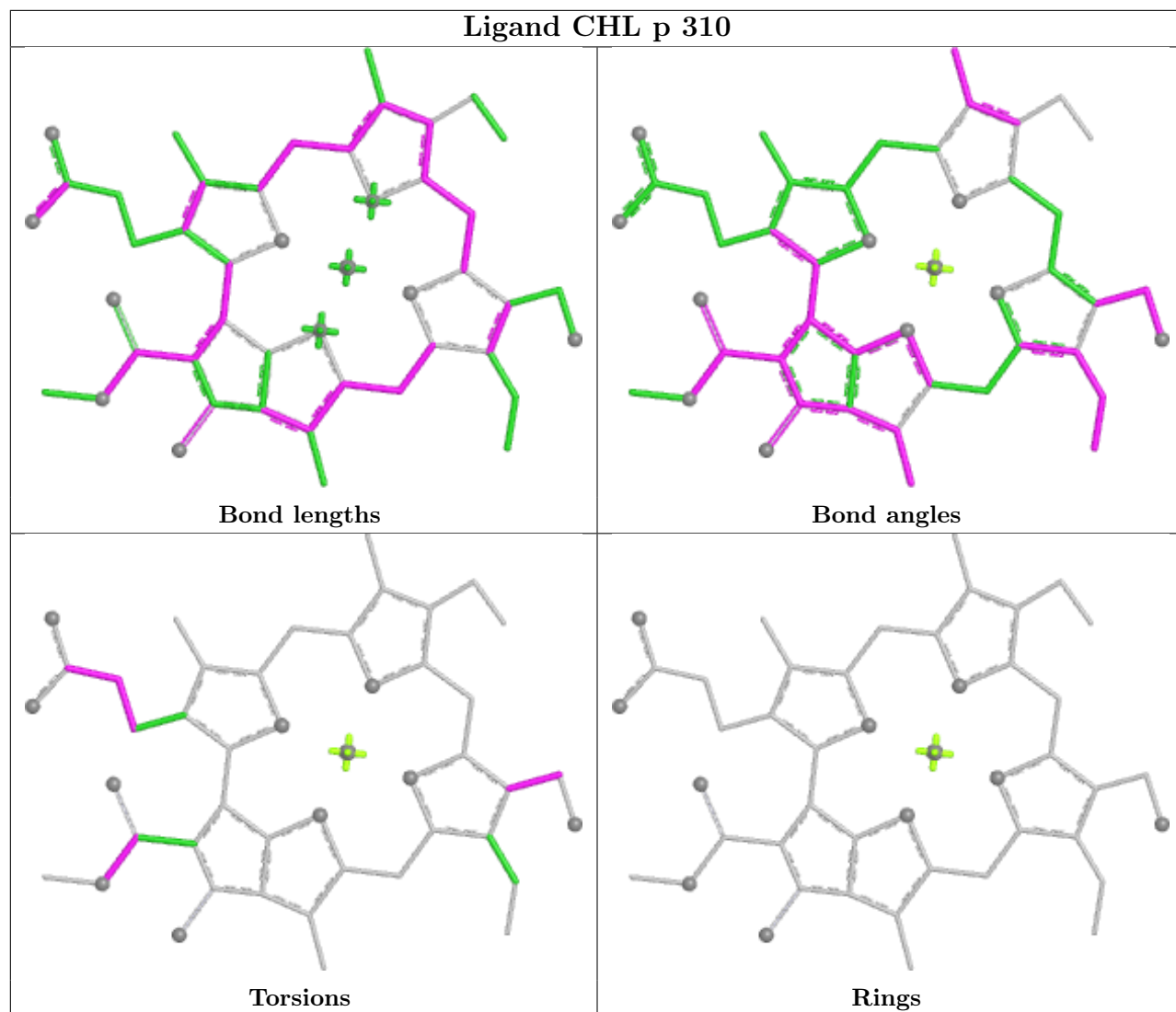
Rings



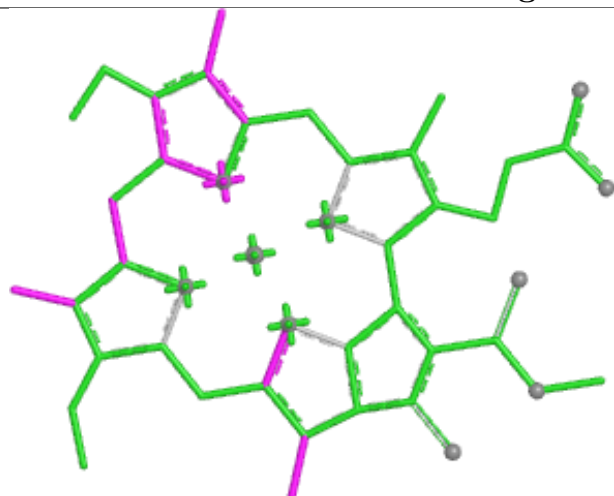
Ligand CHL s 407



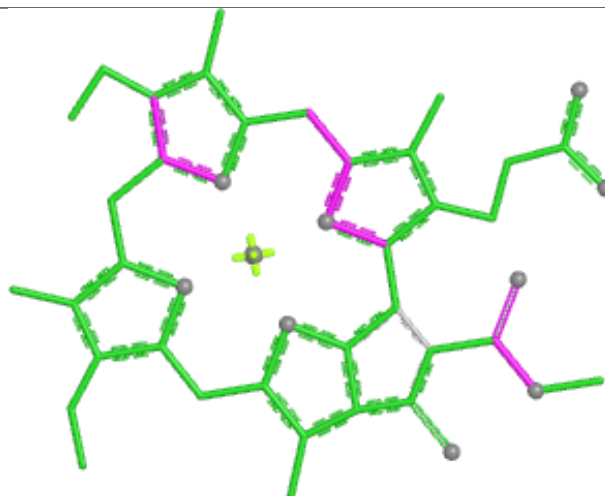
Ligand CHL p 310



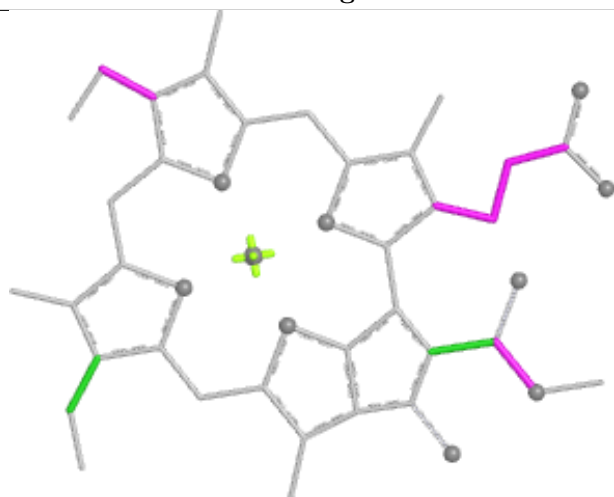
Ligand CLA 6 316



Bond lengths



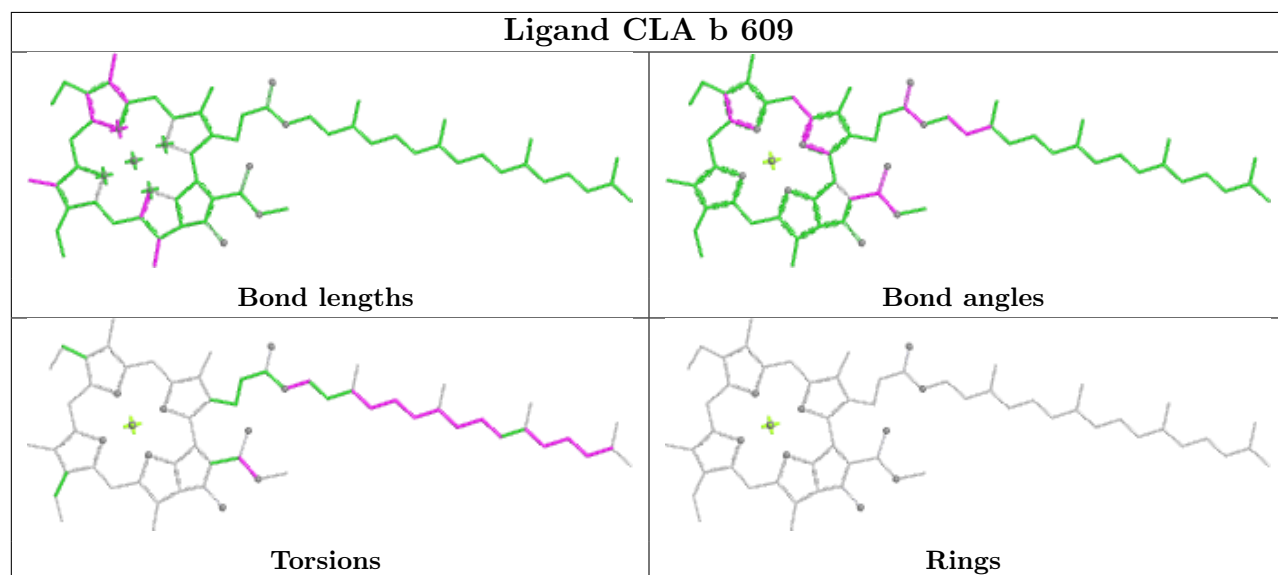
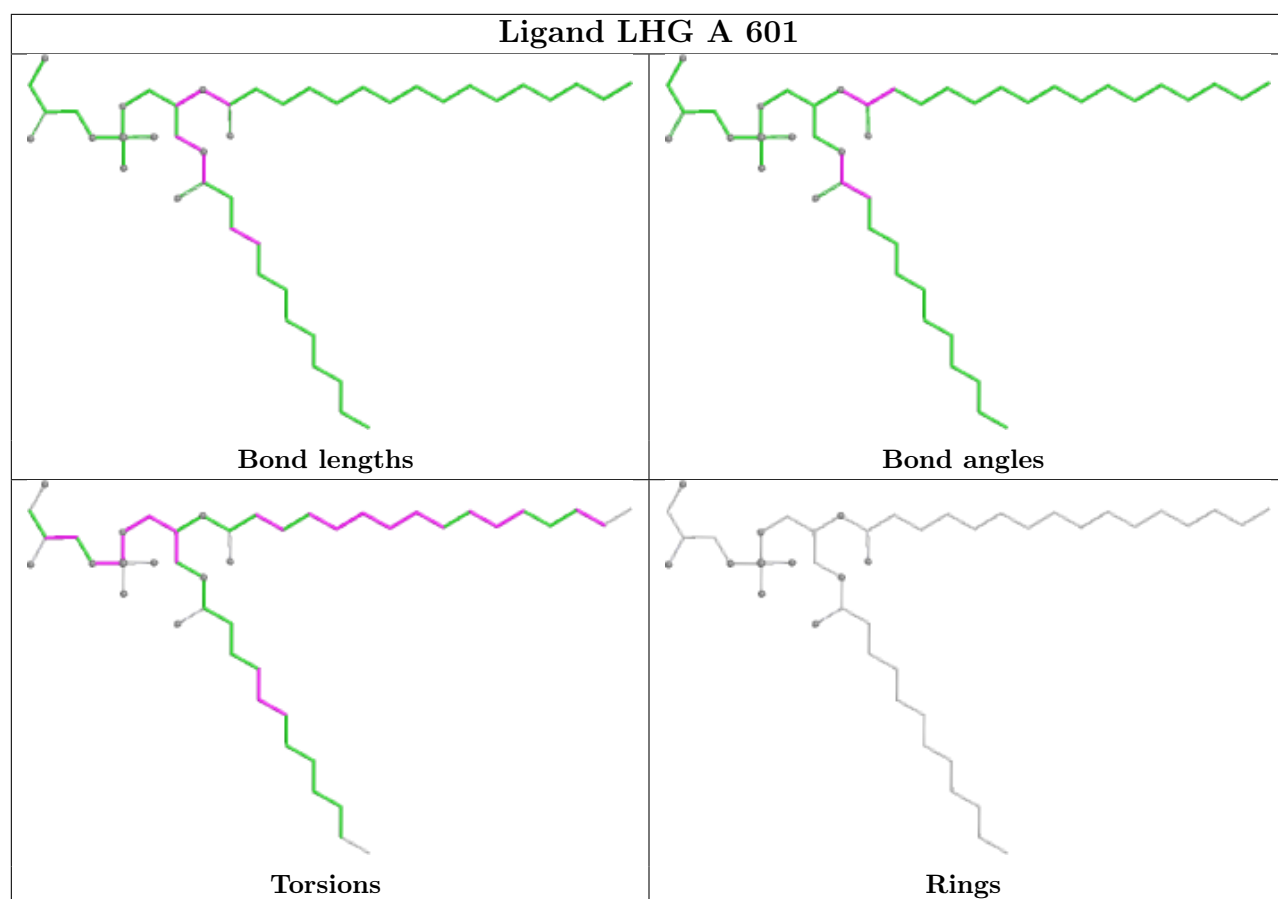
Bond angles



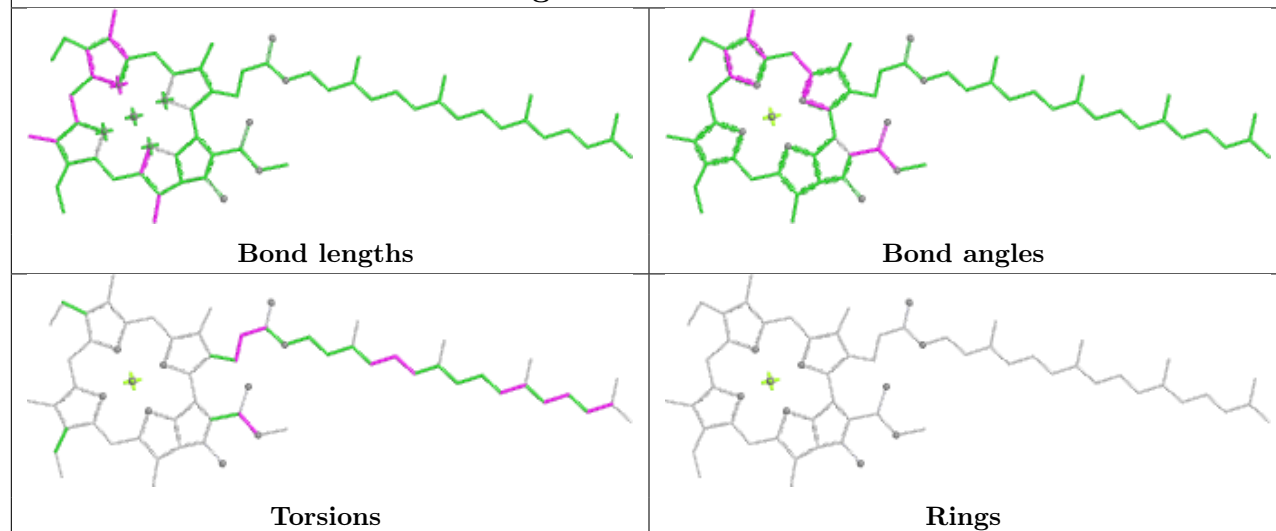
Torsions



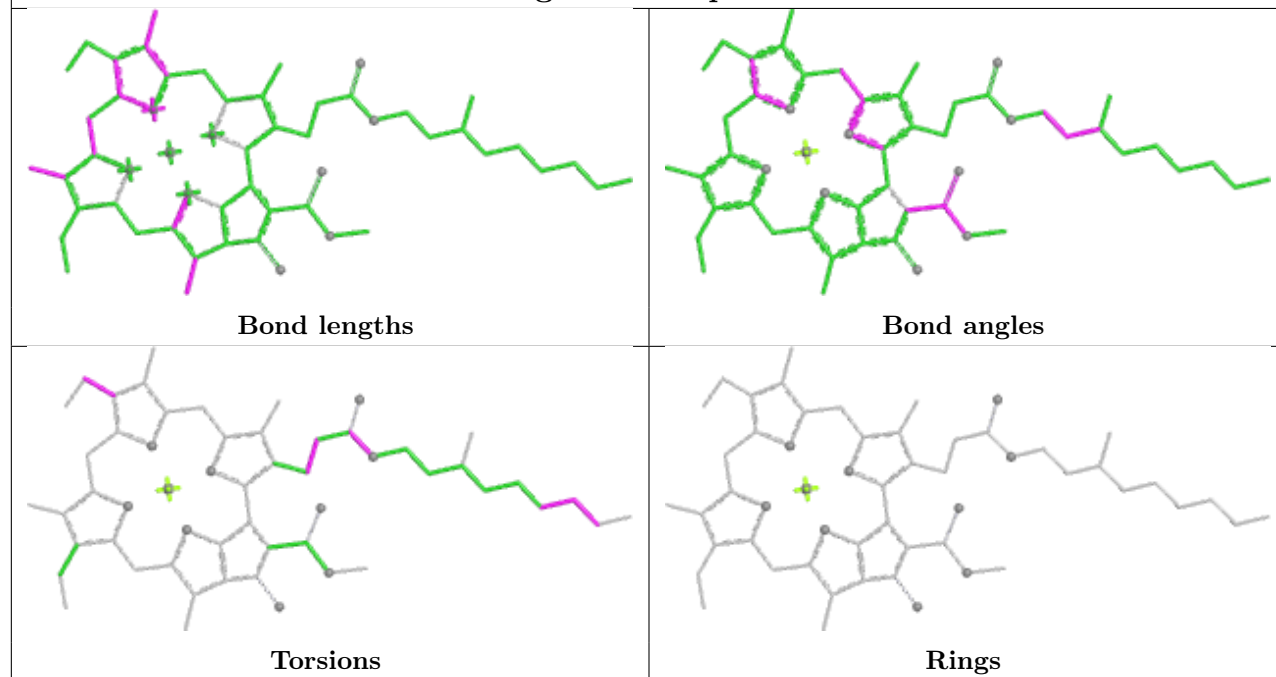
Rings



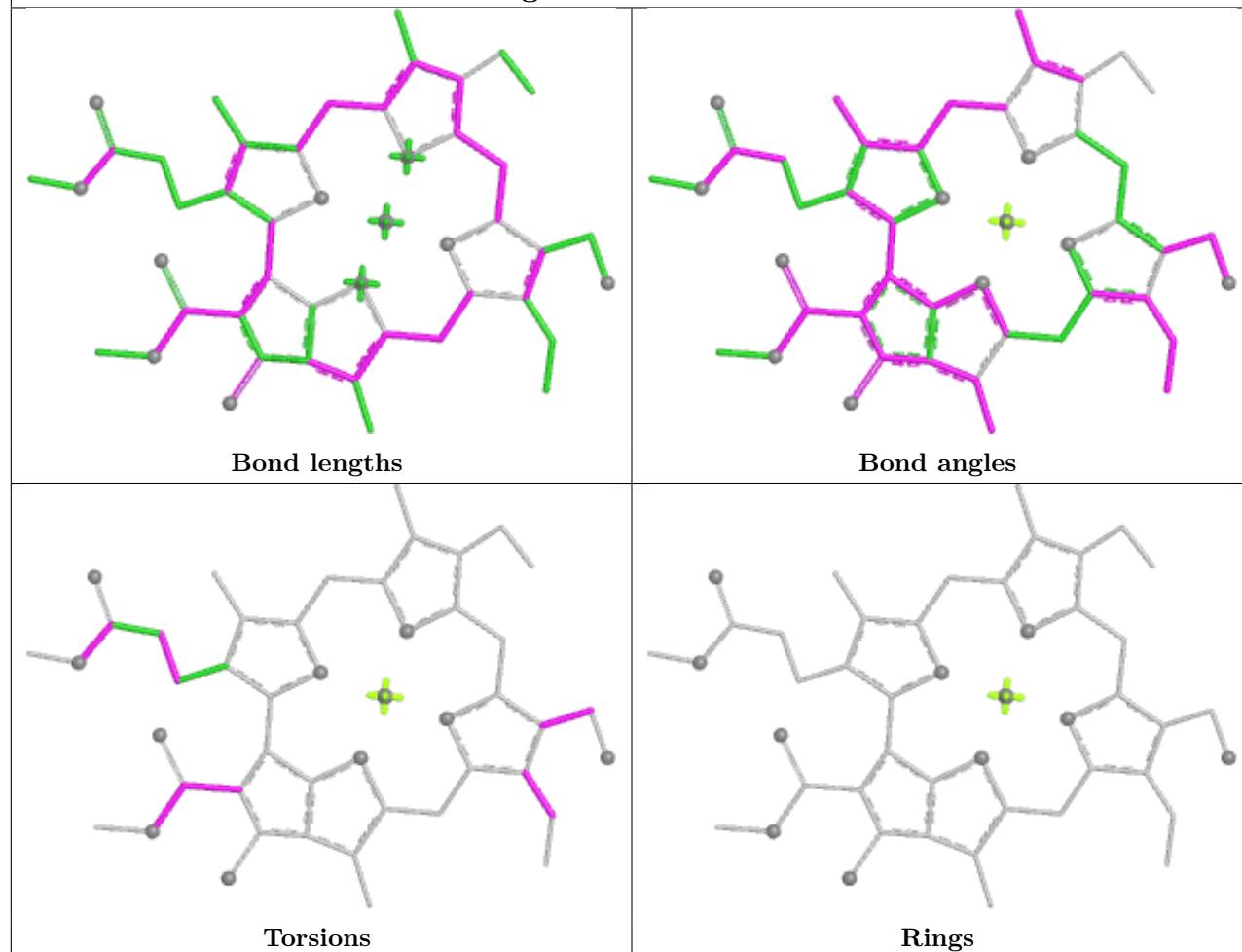
Ligand CLA B 602



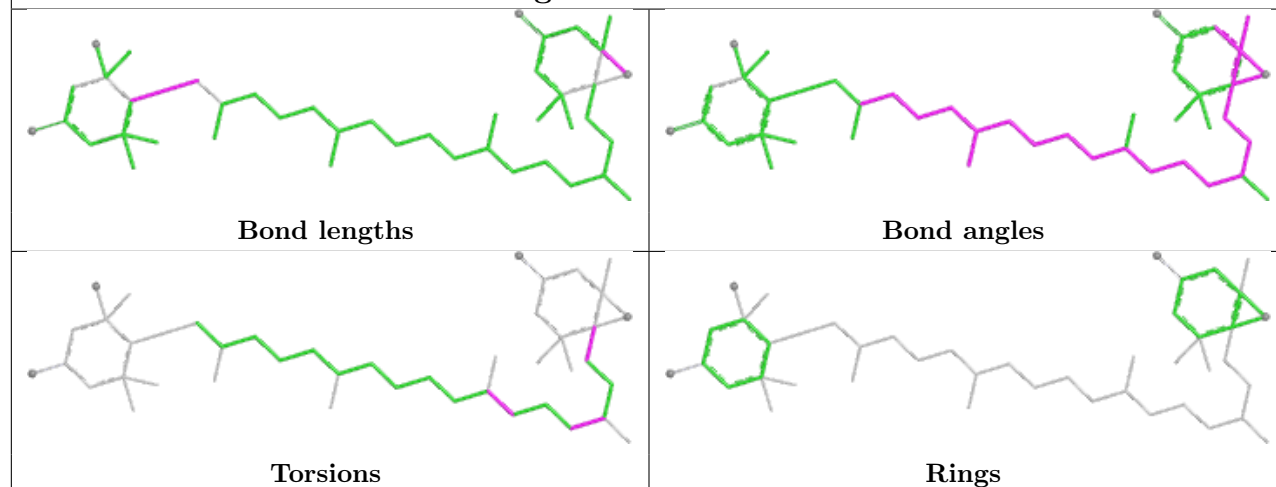
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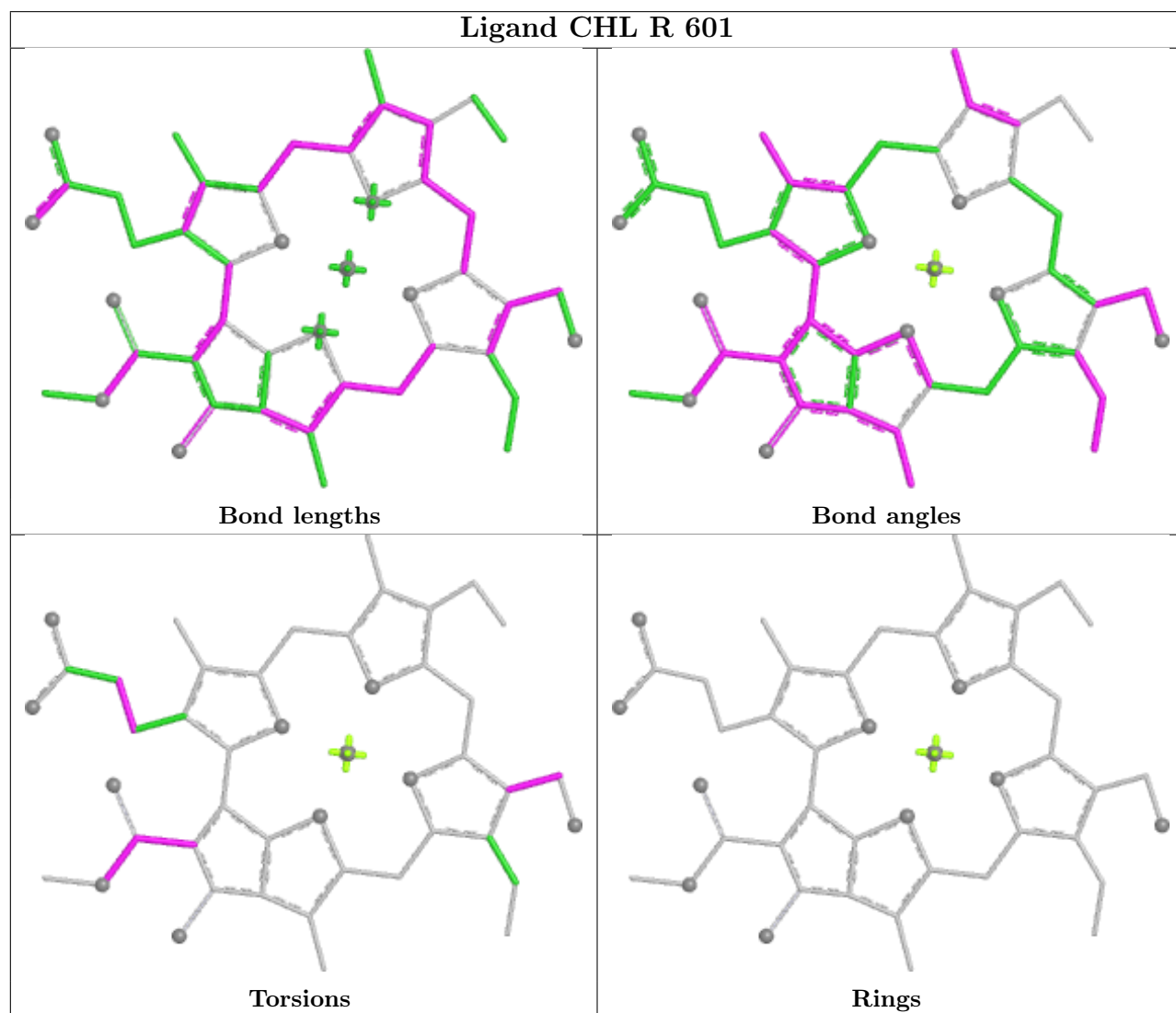
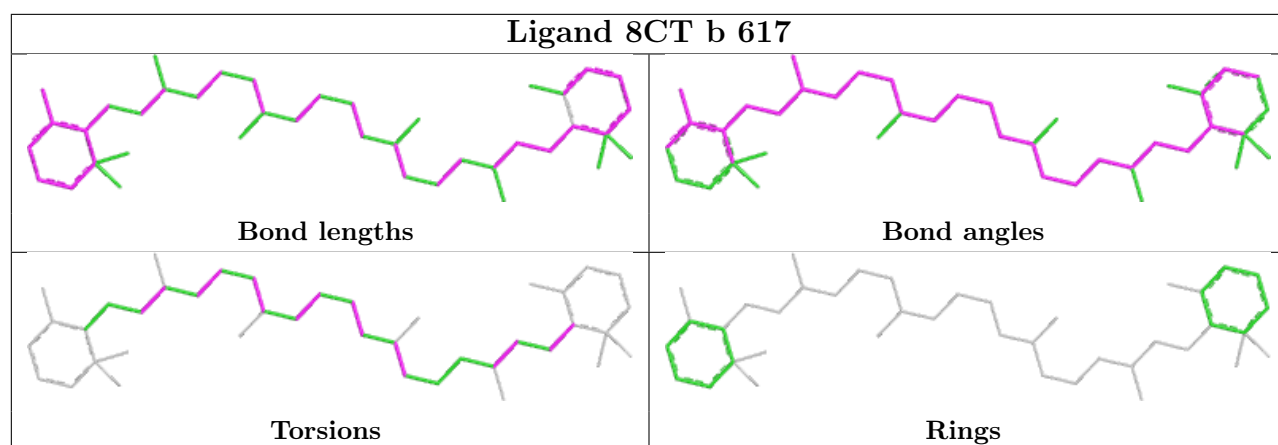


Ligand CHL 2 306

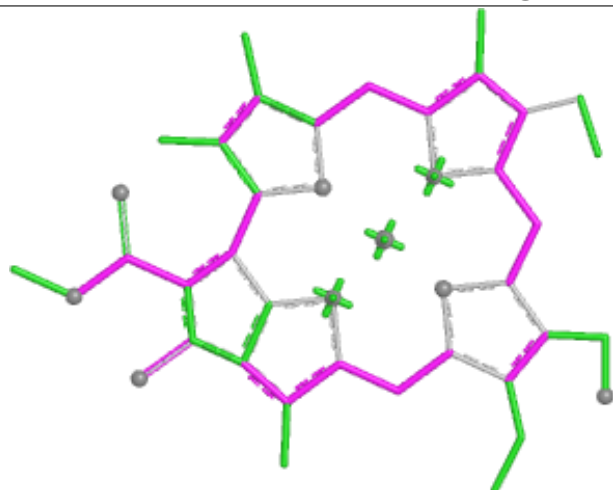


Ligand NEX 1 303

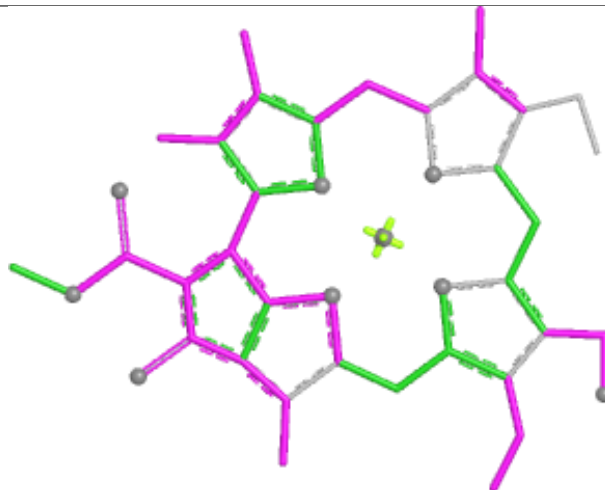




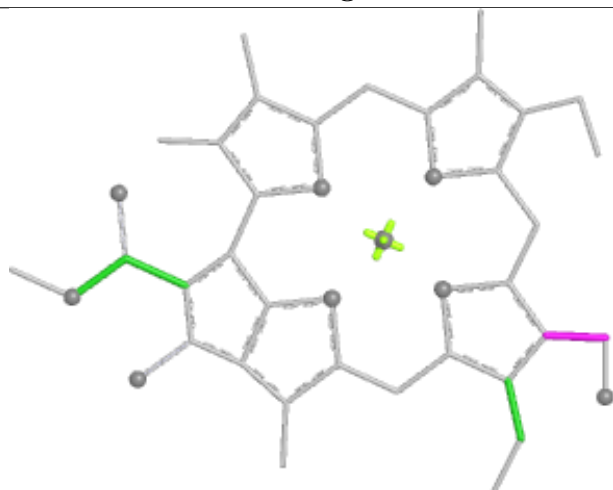
Ligand CHL S 613



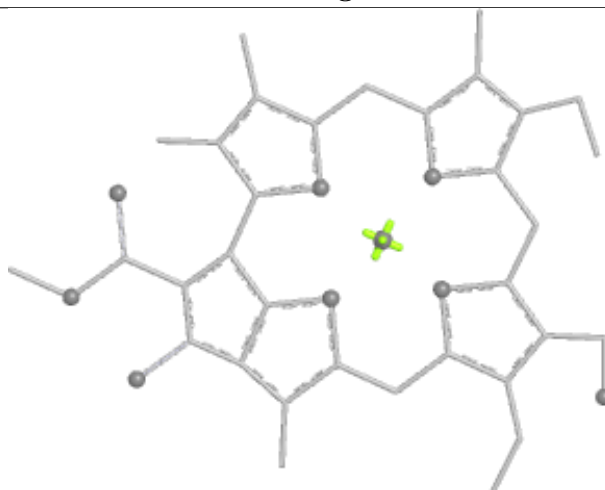
Bond lengths



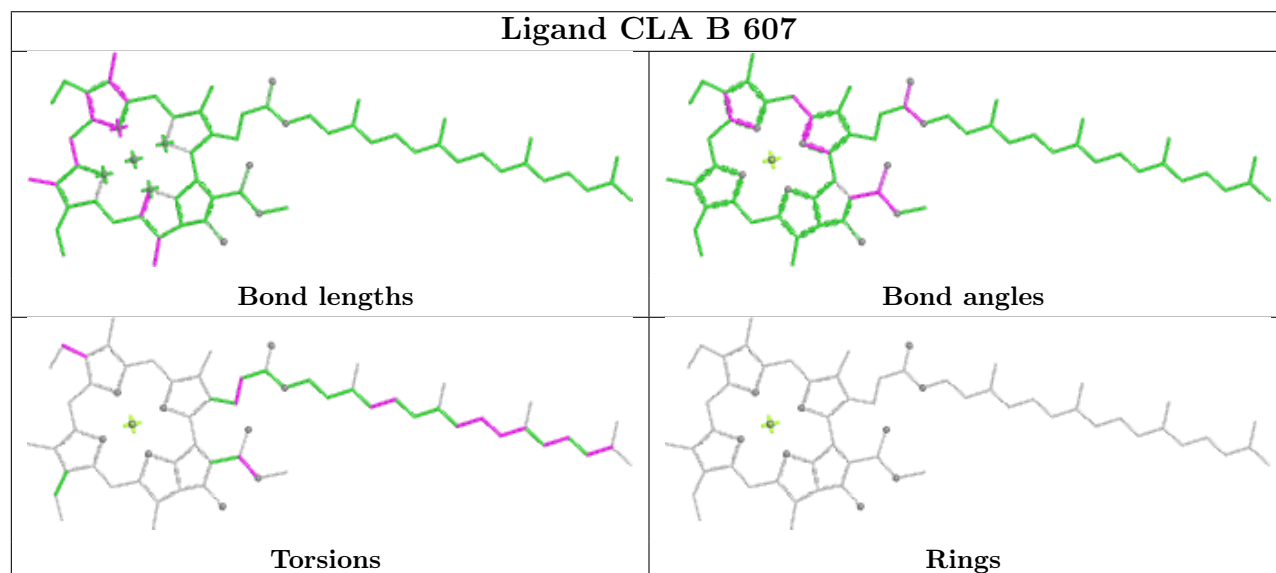
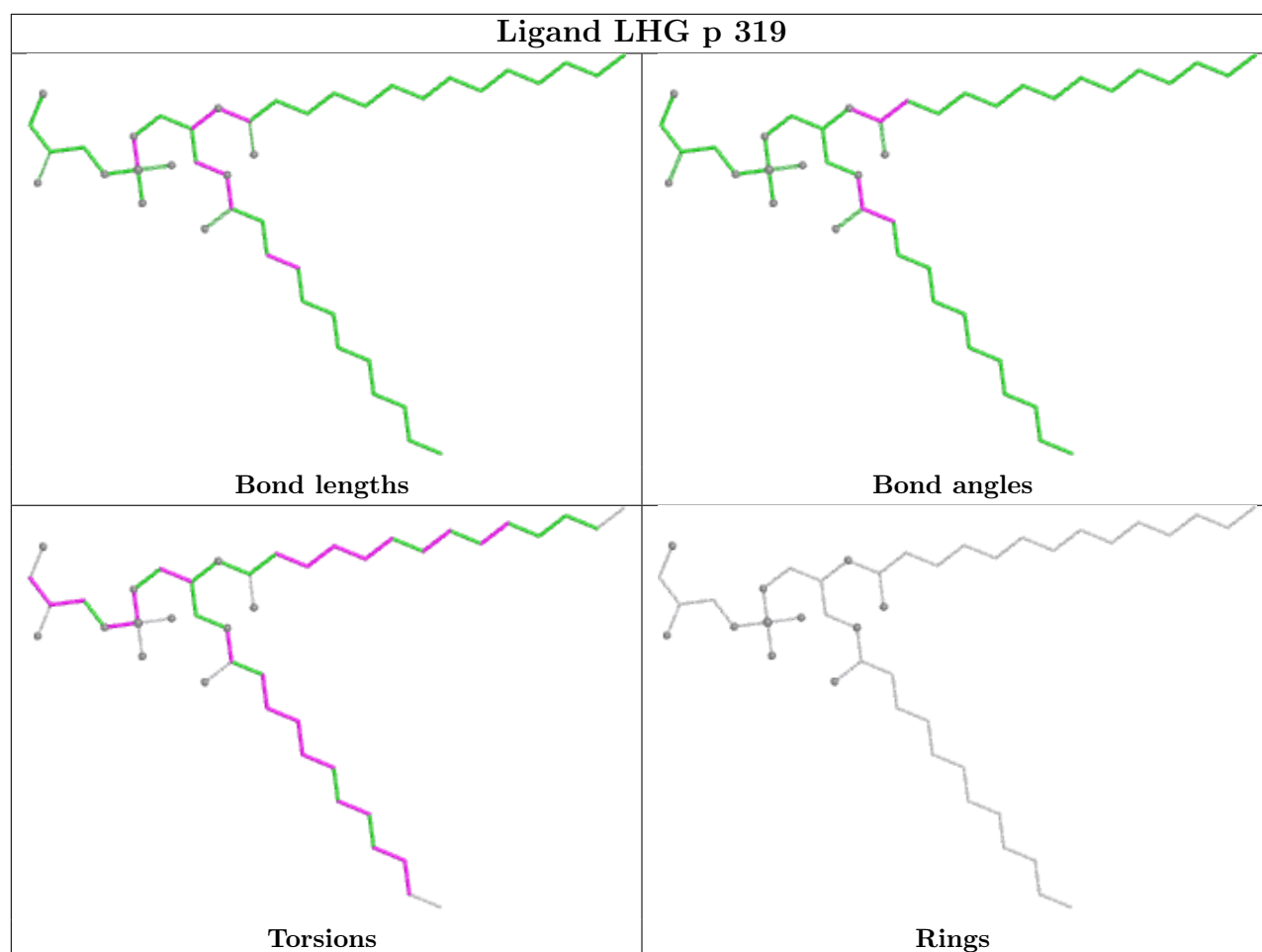
Bond angles

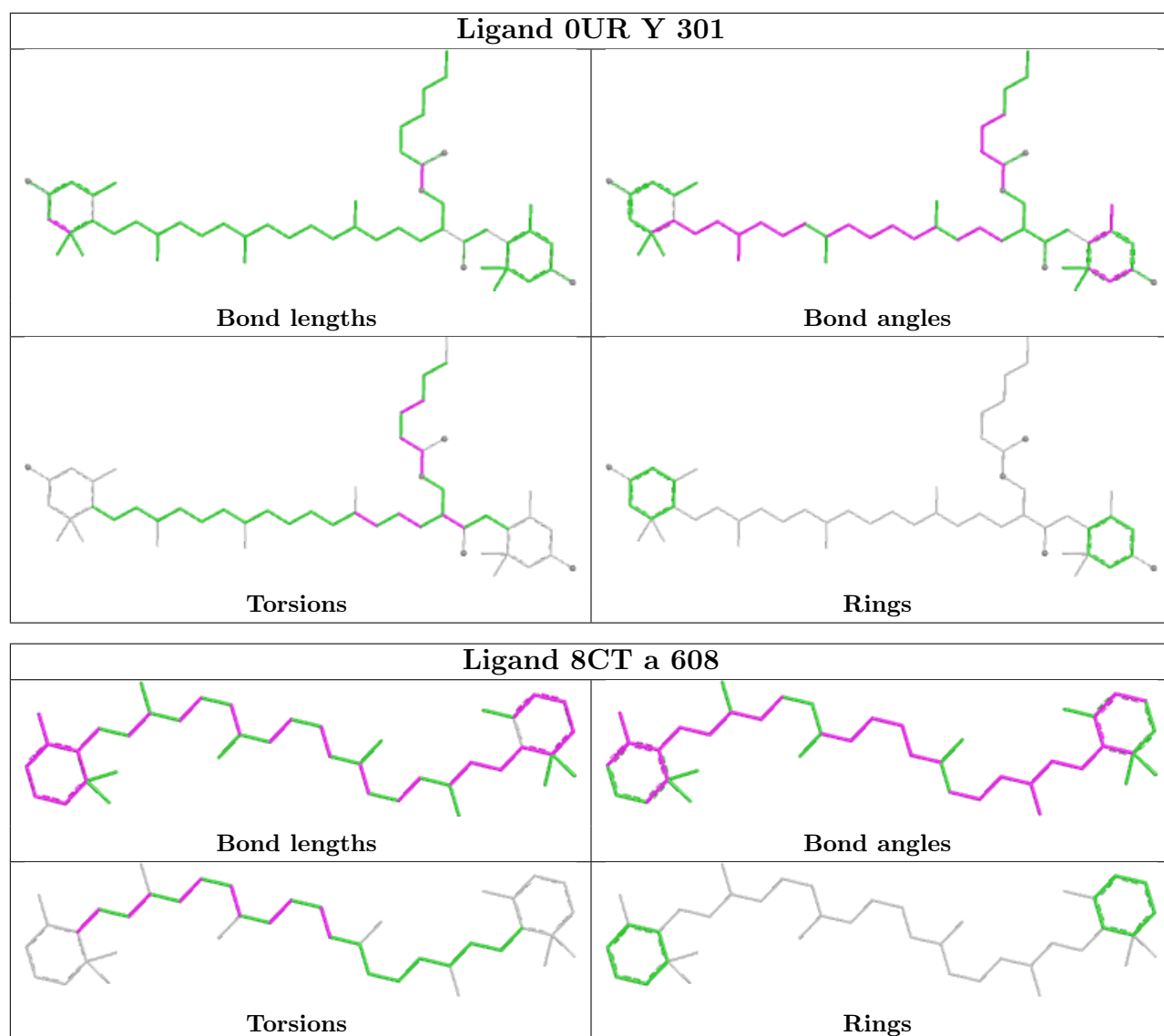


Torsions

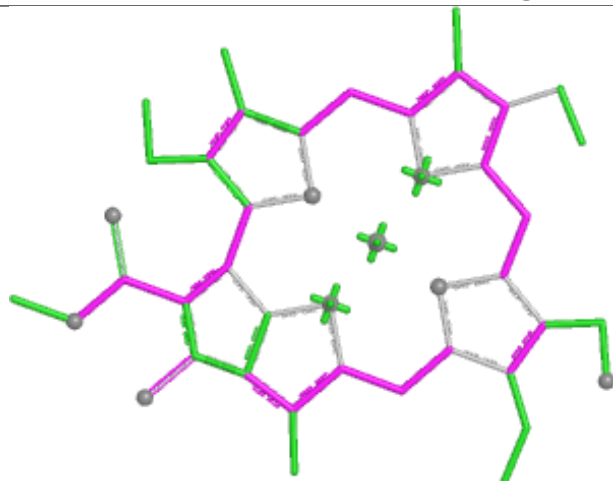


Rings

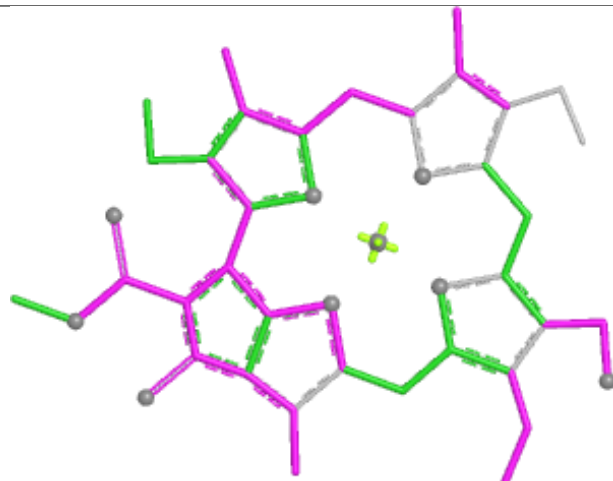




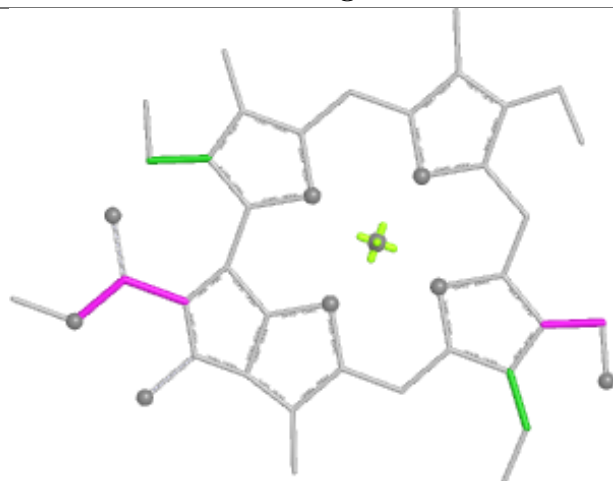
Ligand CHL 4 309



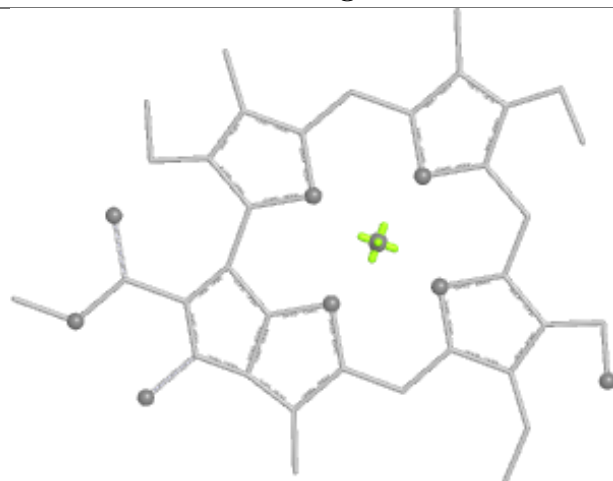
Bond lengths



Bond angles

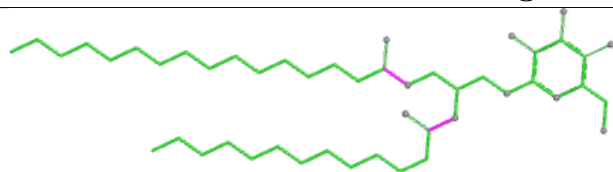


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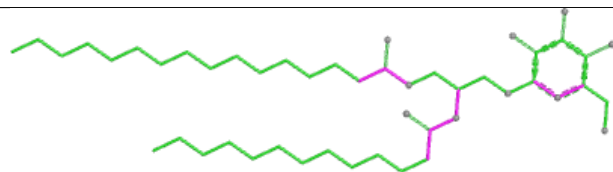


Rings

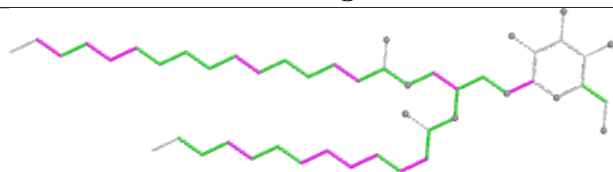
Ligand LMG i 101



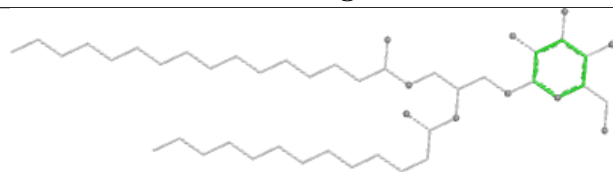
Bond lengths



Bond angles

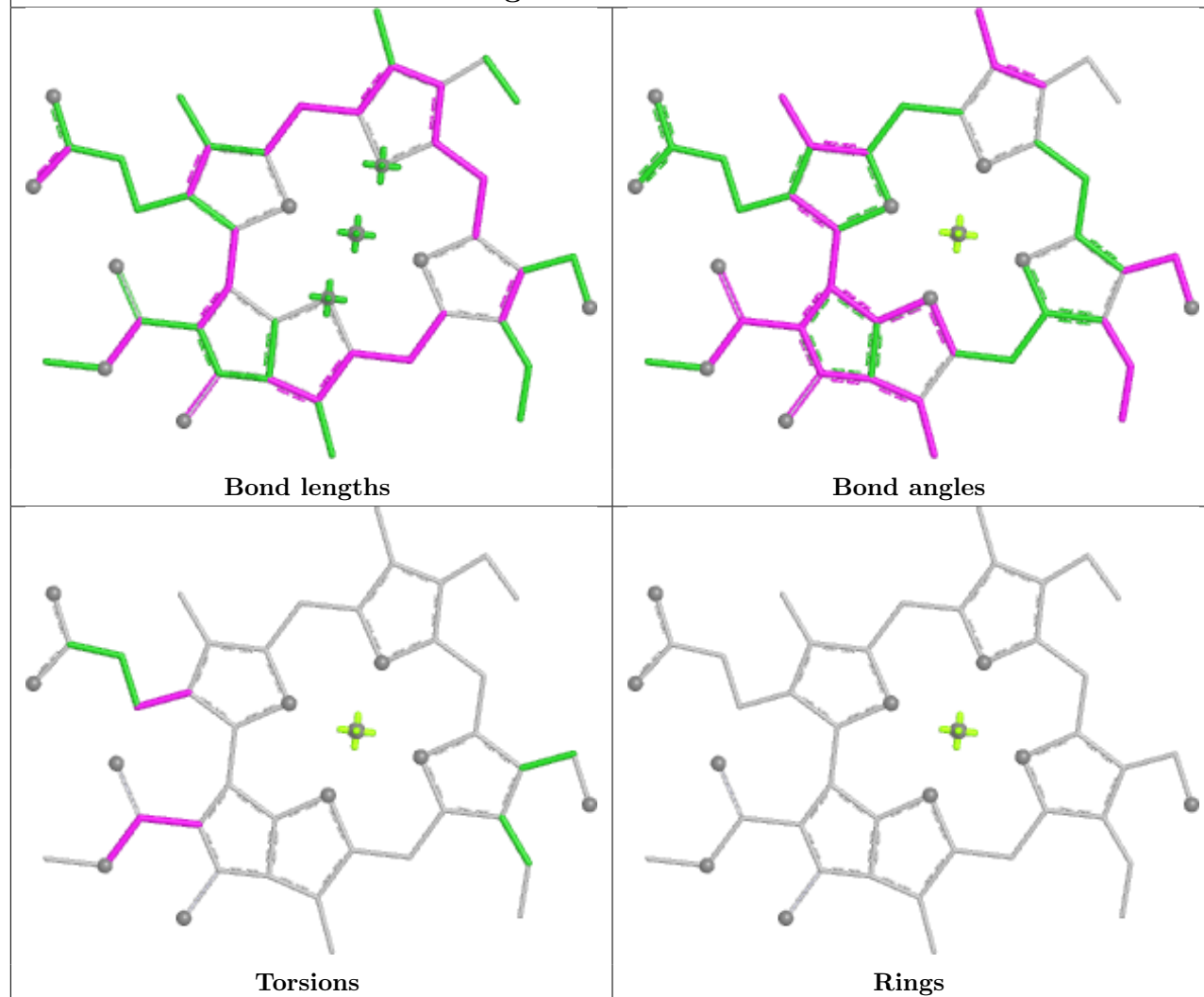


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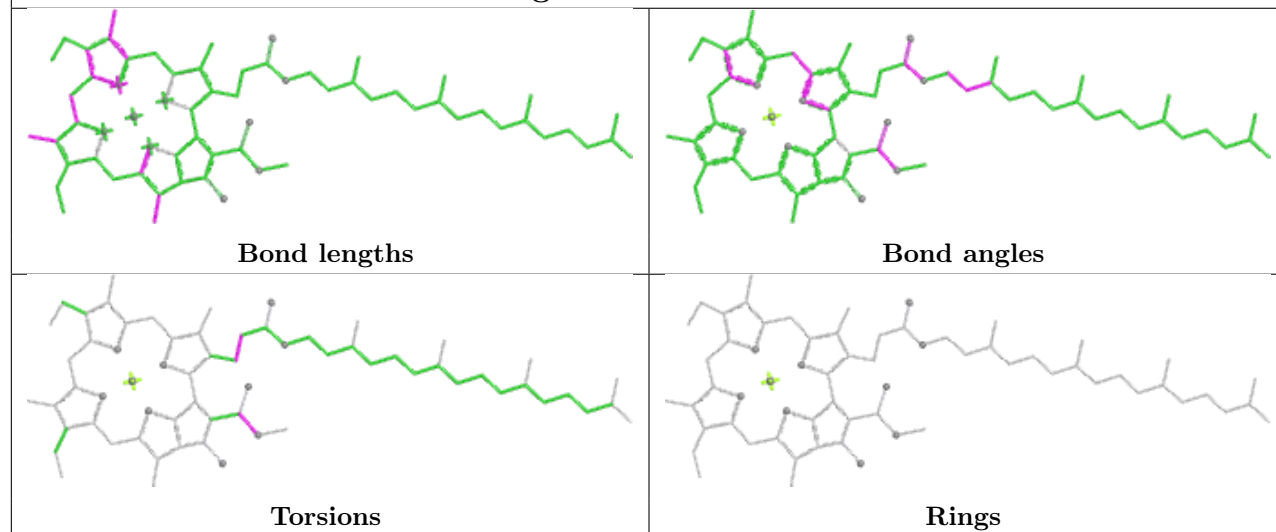


Rings

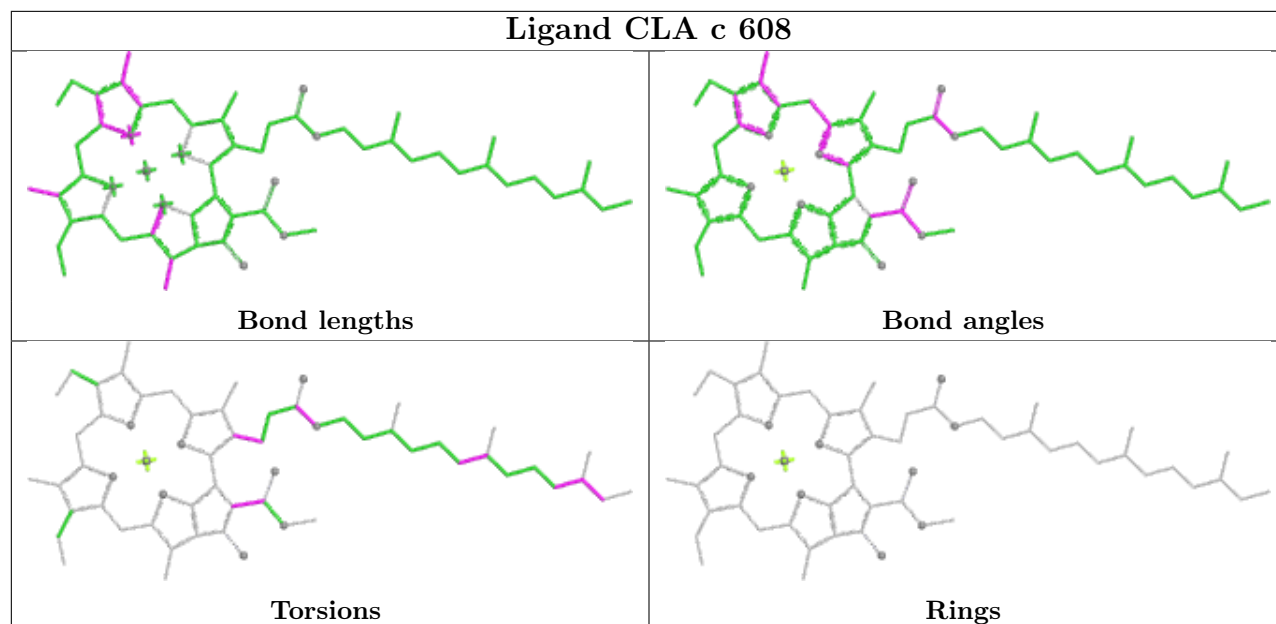
Ligand CHL u 311



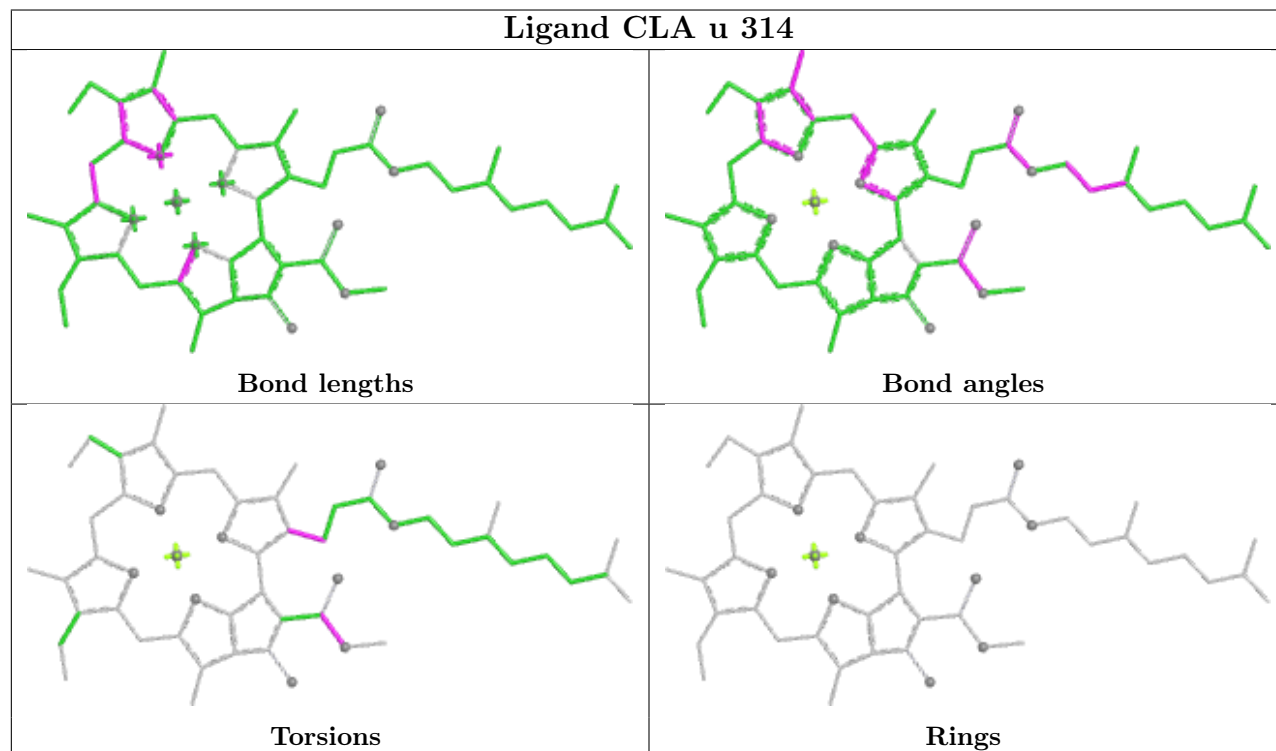
Ligand CLA B 610

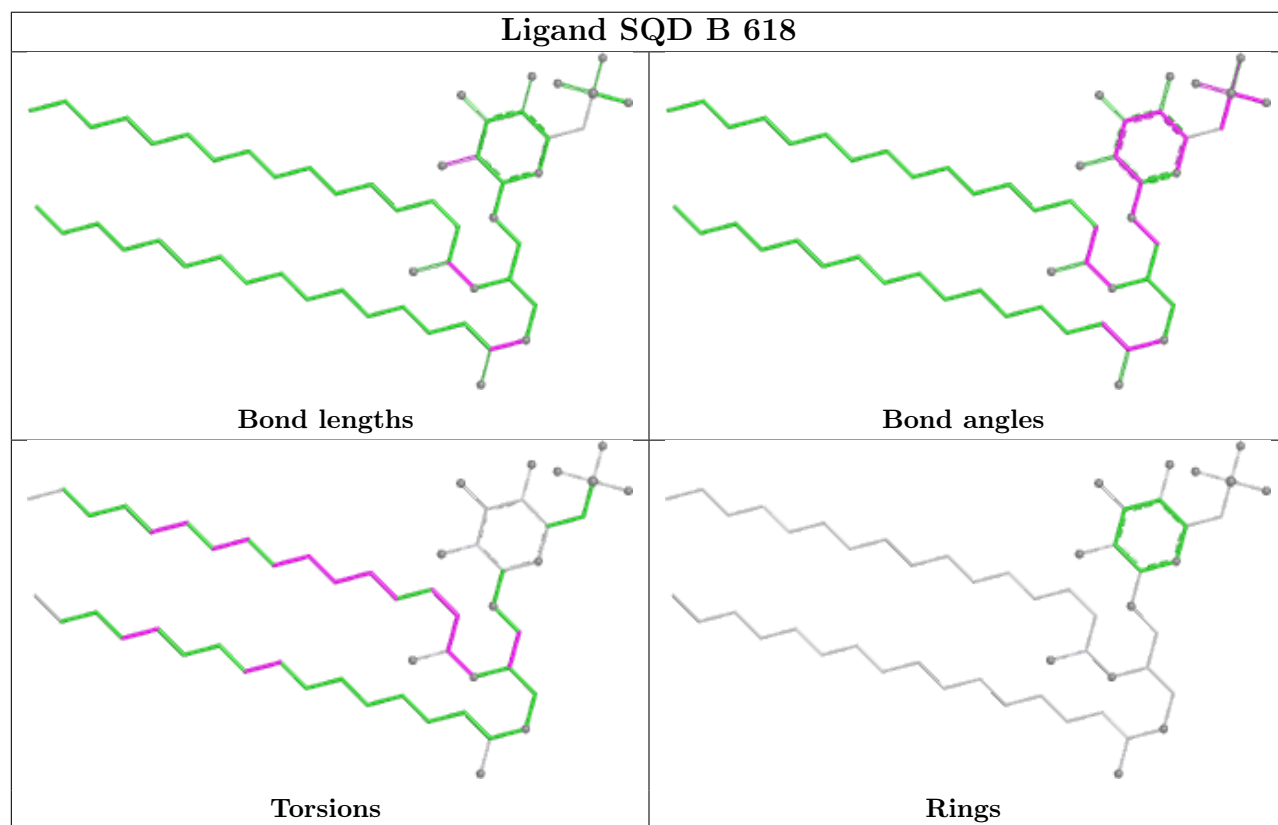
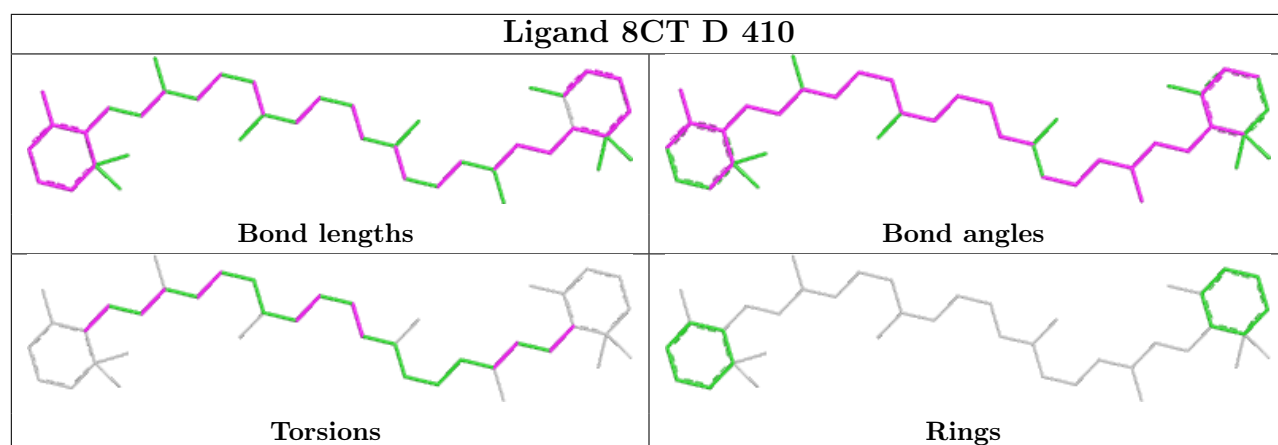


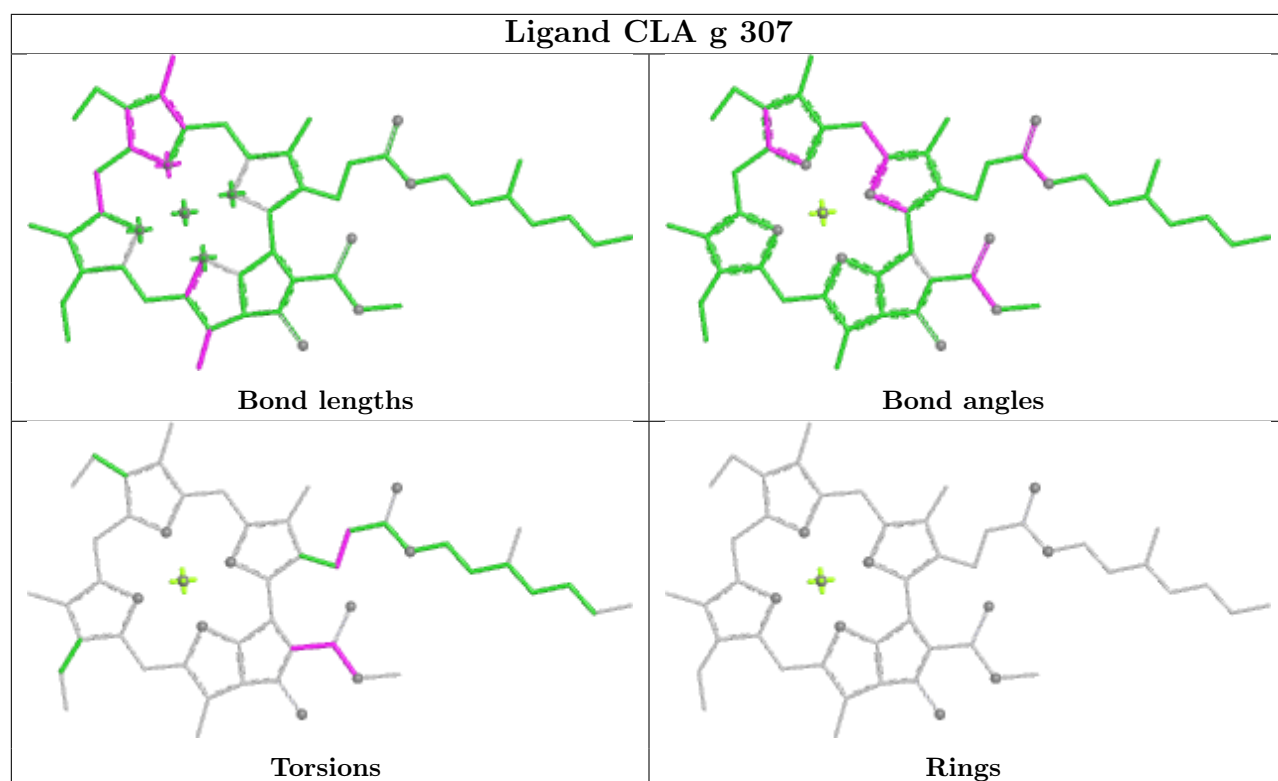
Ligand CLA c 608



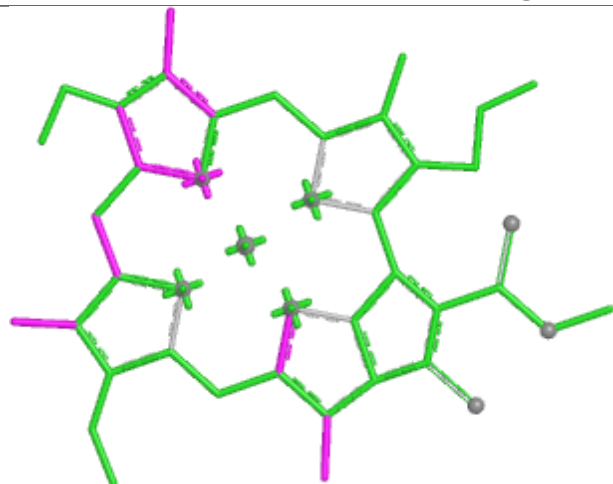
Ligand CLA u 314



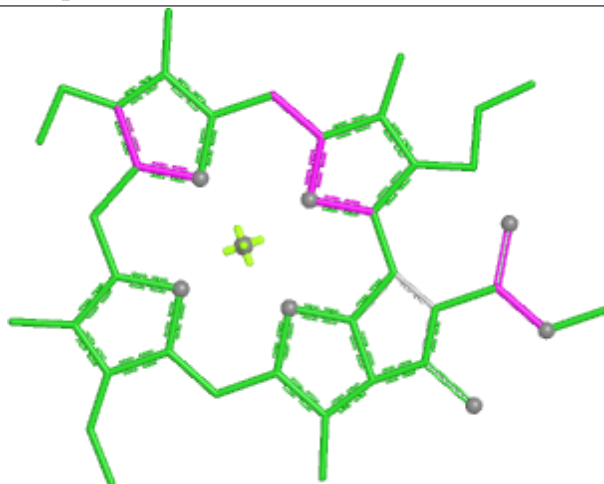




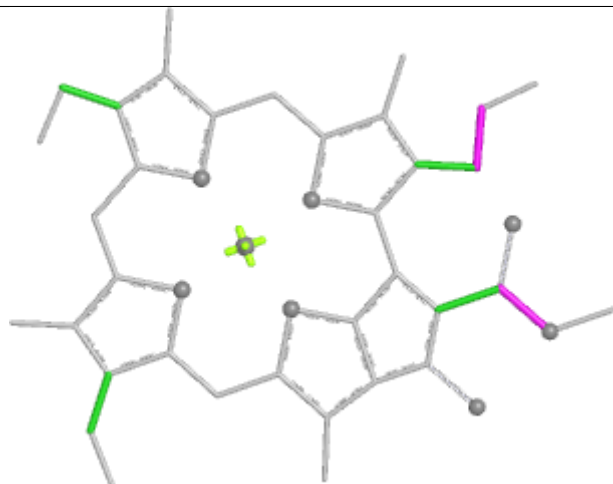
Ligand CLA q 315



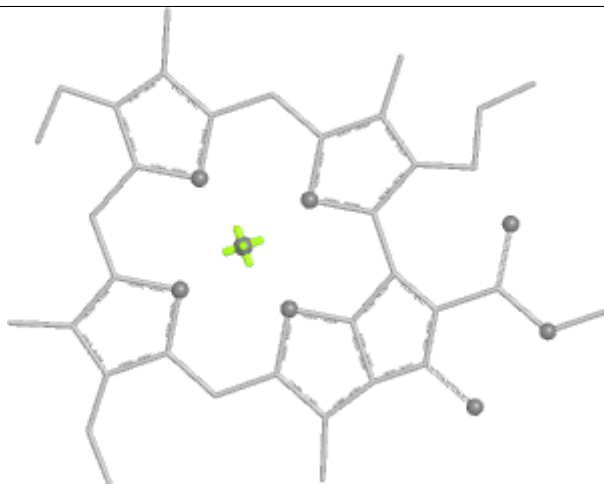
Bond lengths



Bond angles

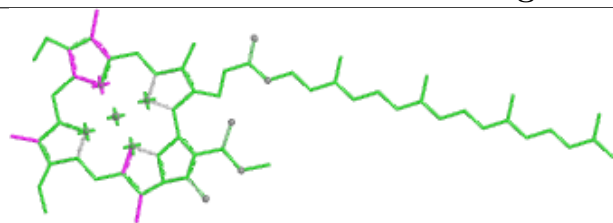


Torsions

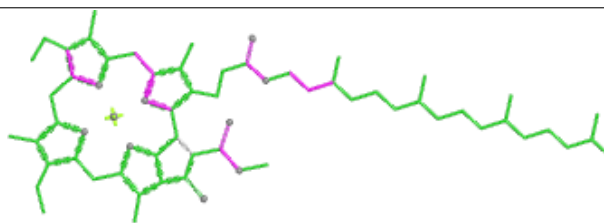


Rings

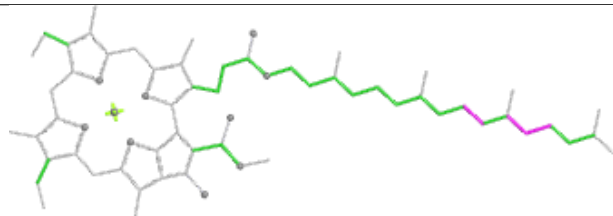
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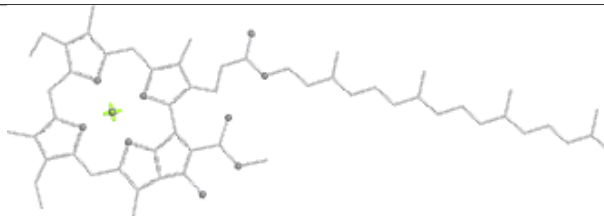
Bond lengths



Bond angles

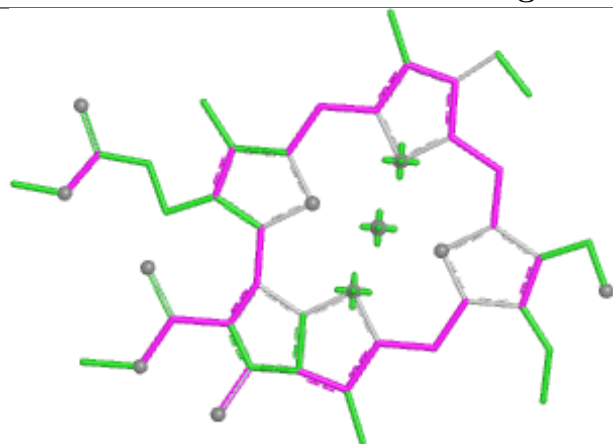


Torsions

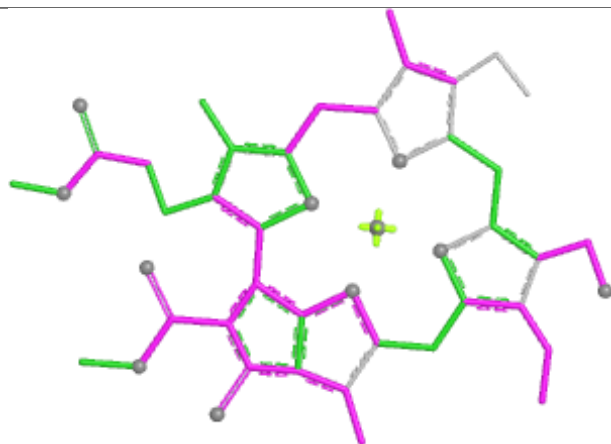


Rings

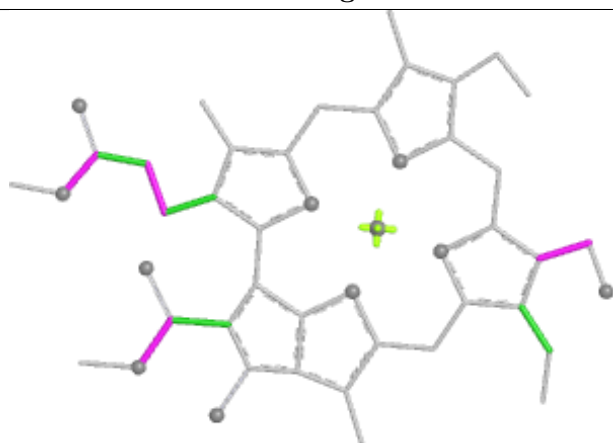
Ligand CHL 7 312



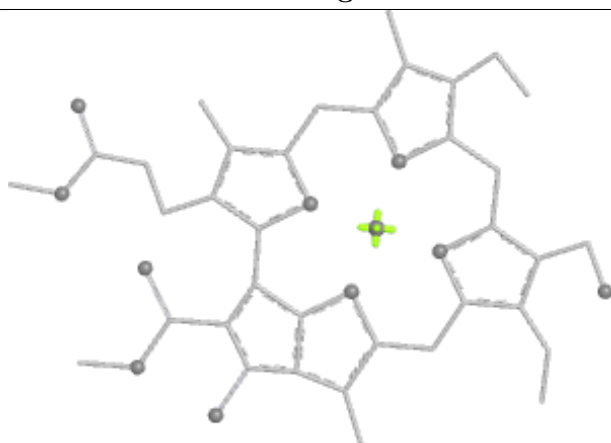
Bond lengths



Bond angles

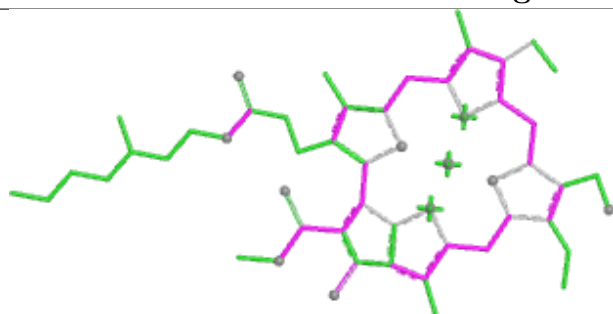


Torsions

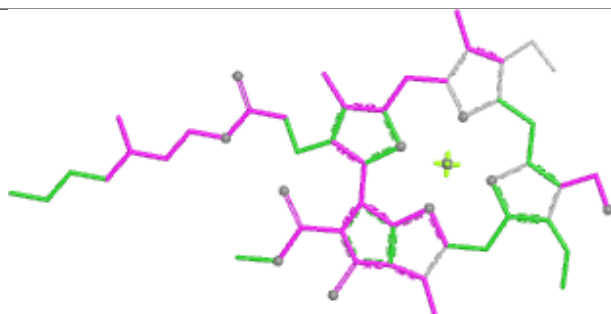


Rings

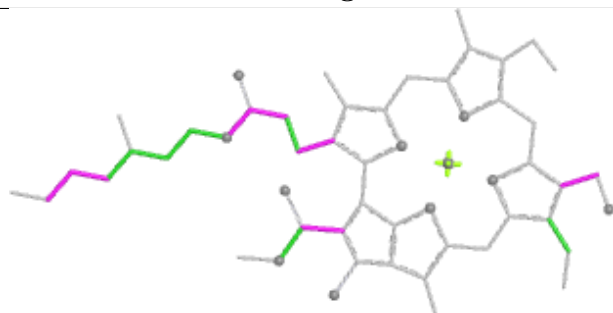
Ligand CHL Y 310



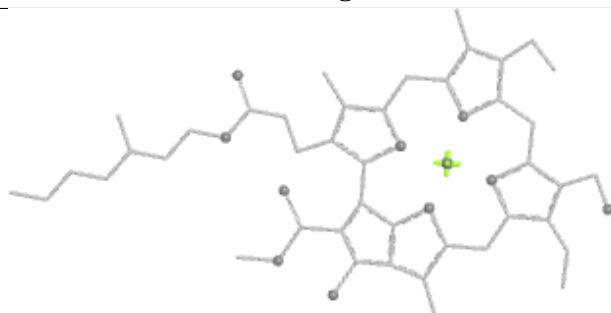
Bond lengths



Bond angles

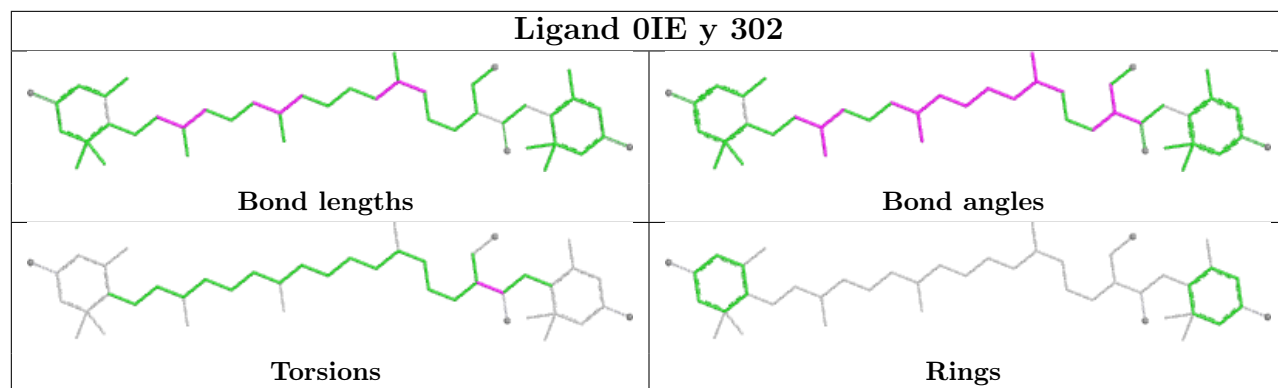


Torsions

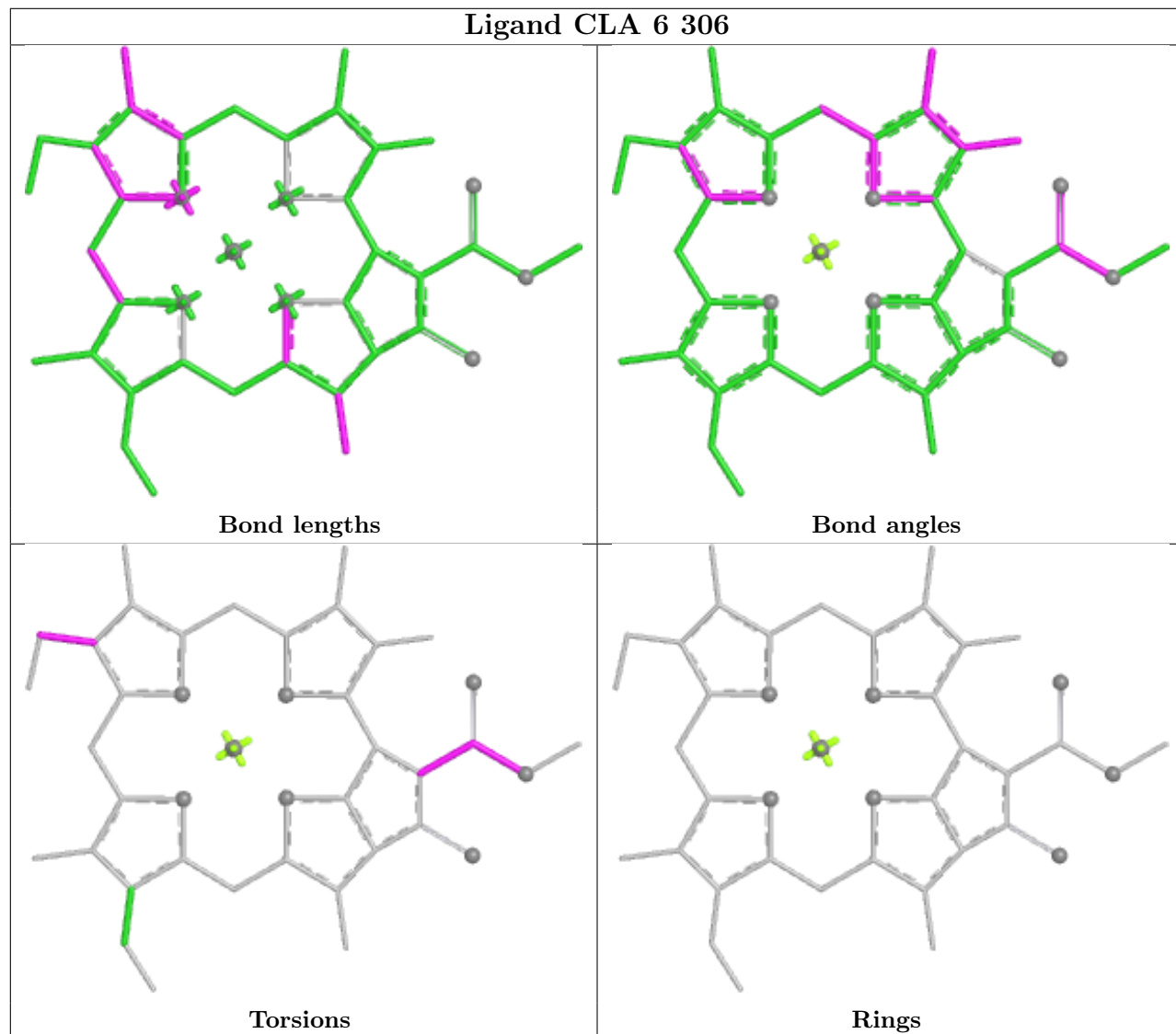


Rings

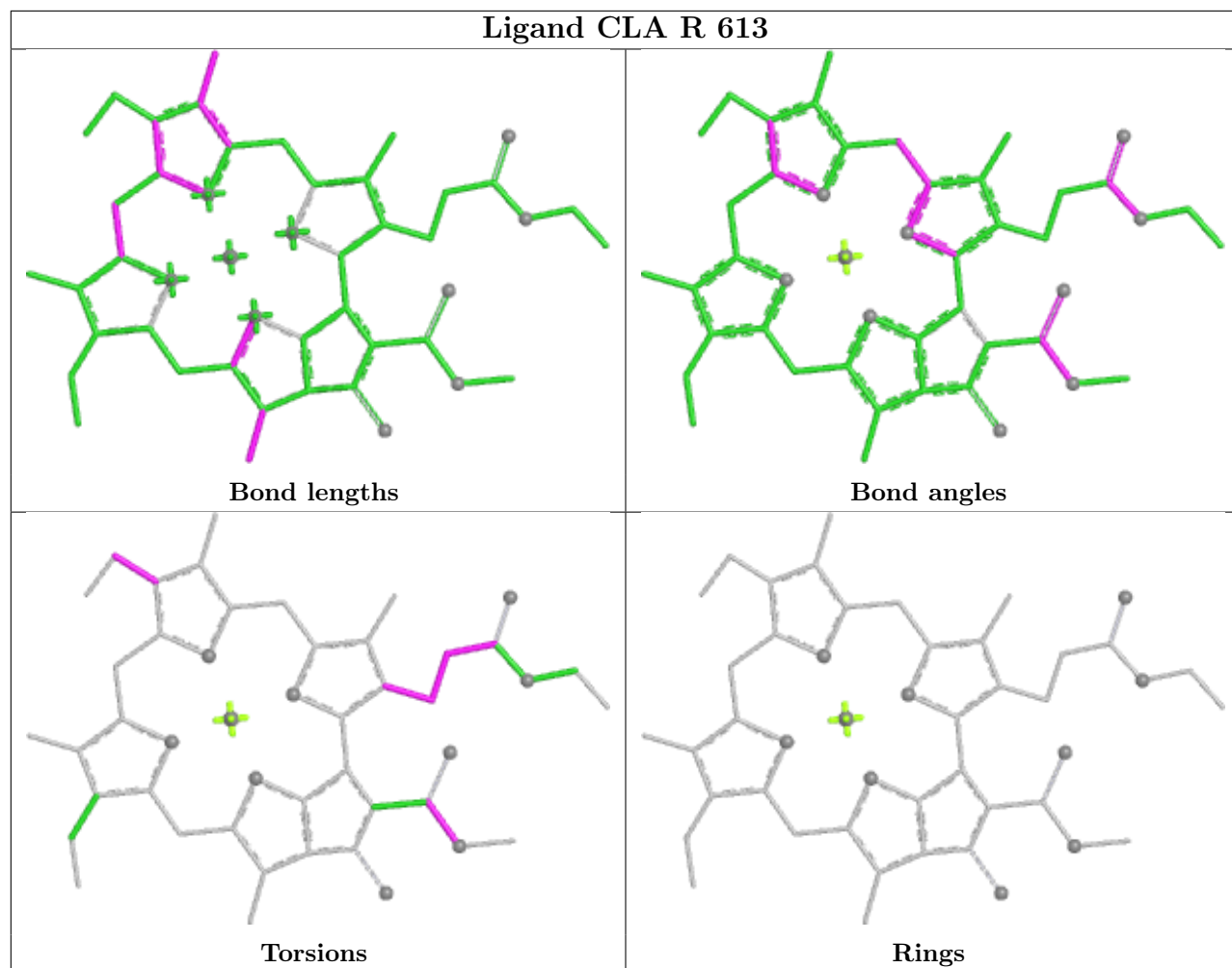
Ligand OIE y 302



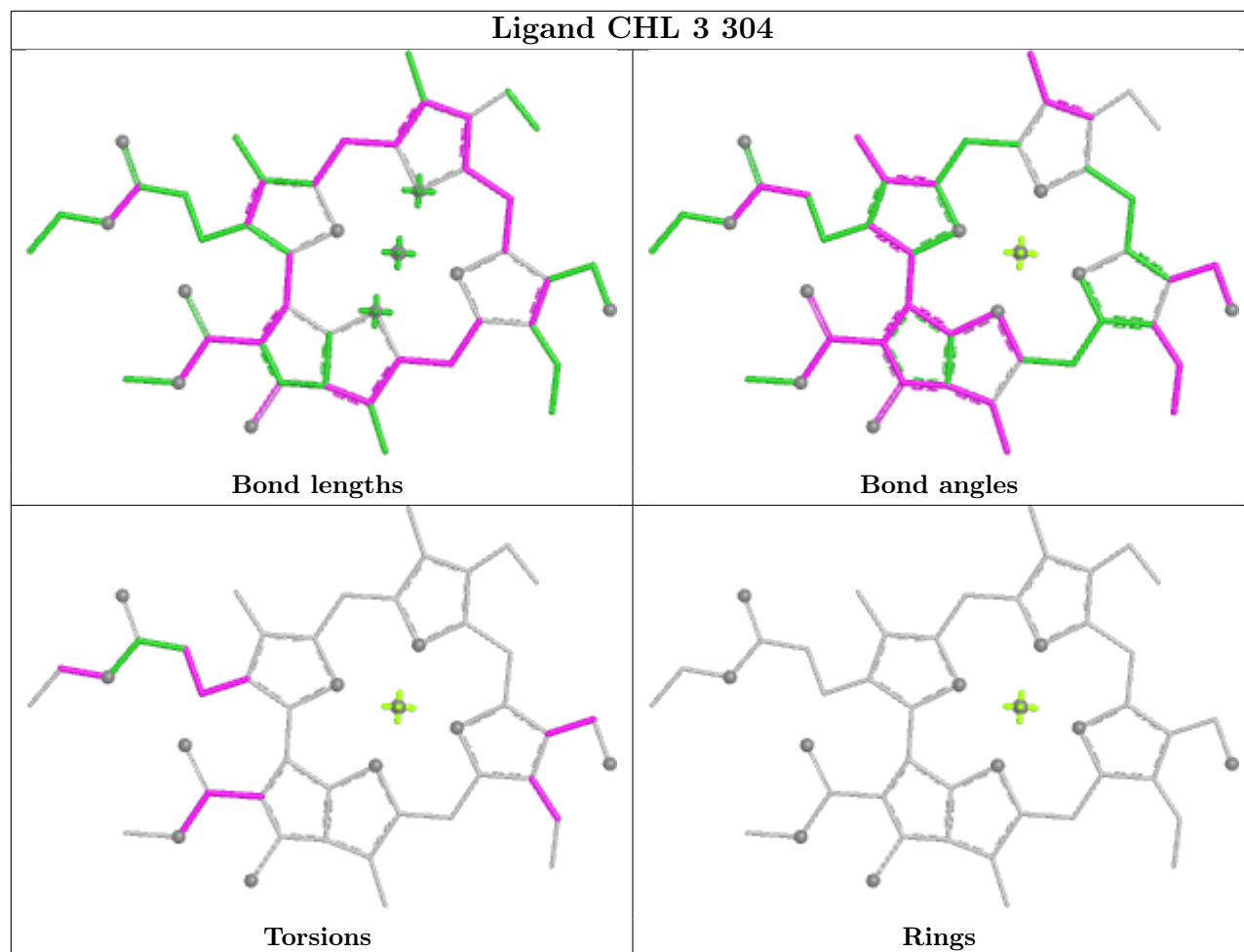
Ligand CLA 6 306



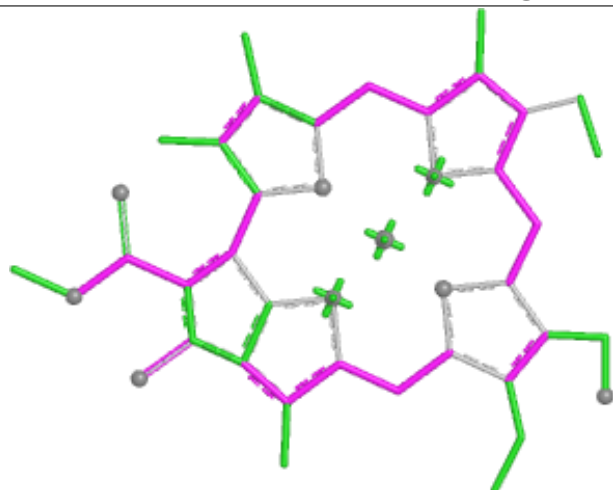
Ligand CLA R 613



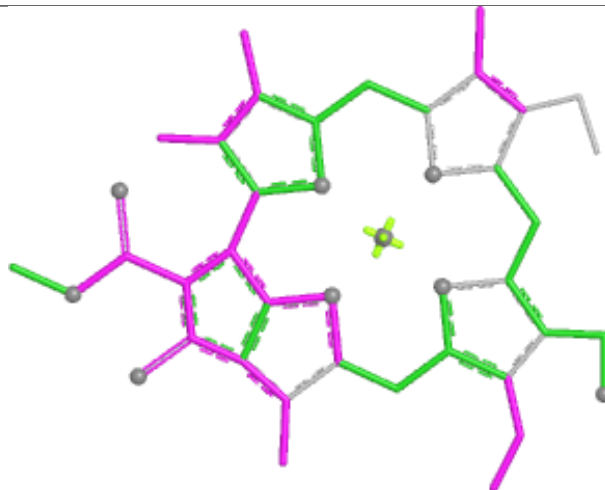
Ligand CHL 3 304



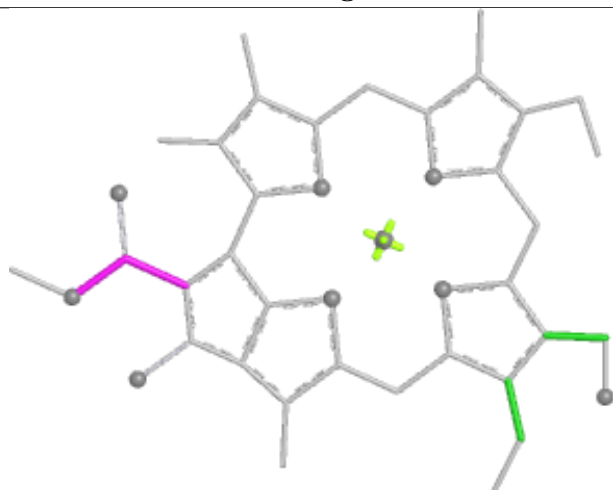
Ligand CHL 7 318



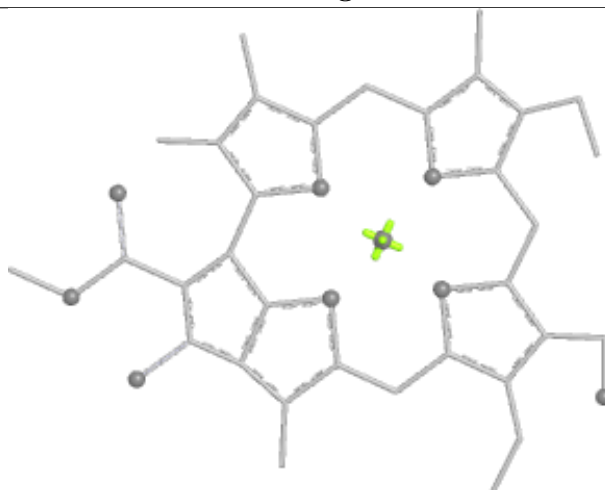
Bond lengths



Bond angles

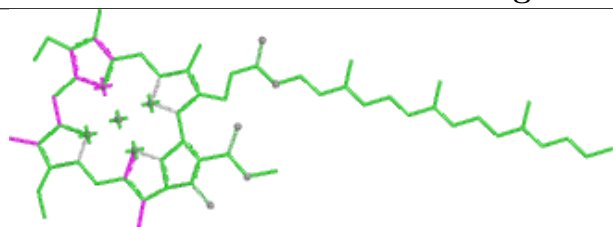


Torsions

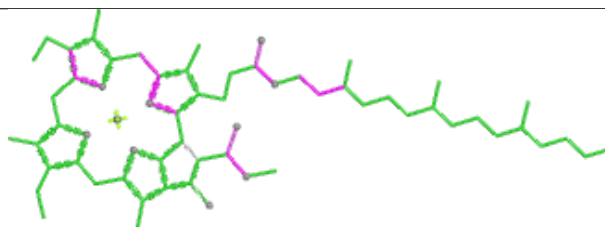


Rings

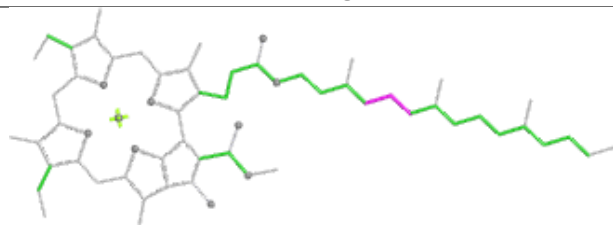
Ligand CLA N 314



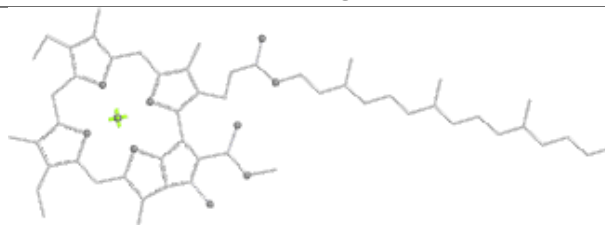
Bond lengths



Bond angles

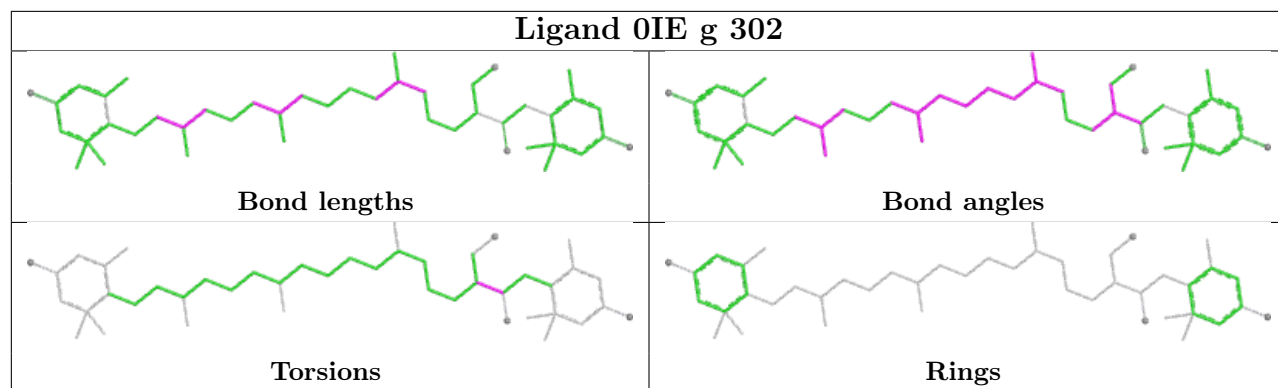


Torsions

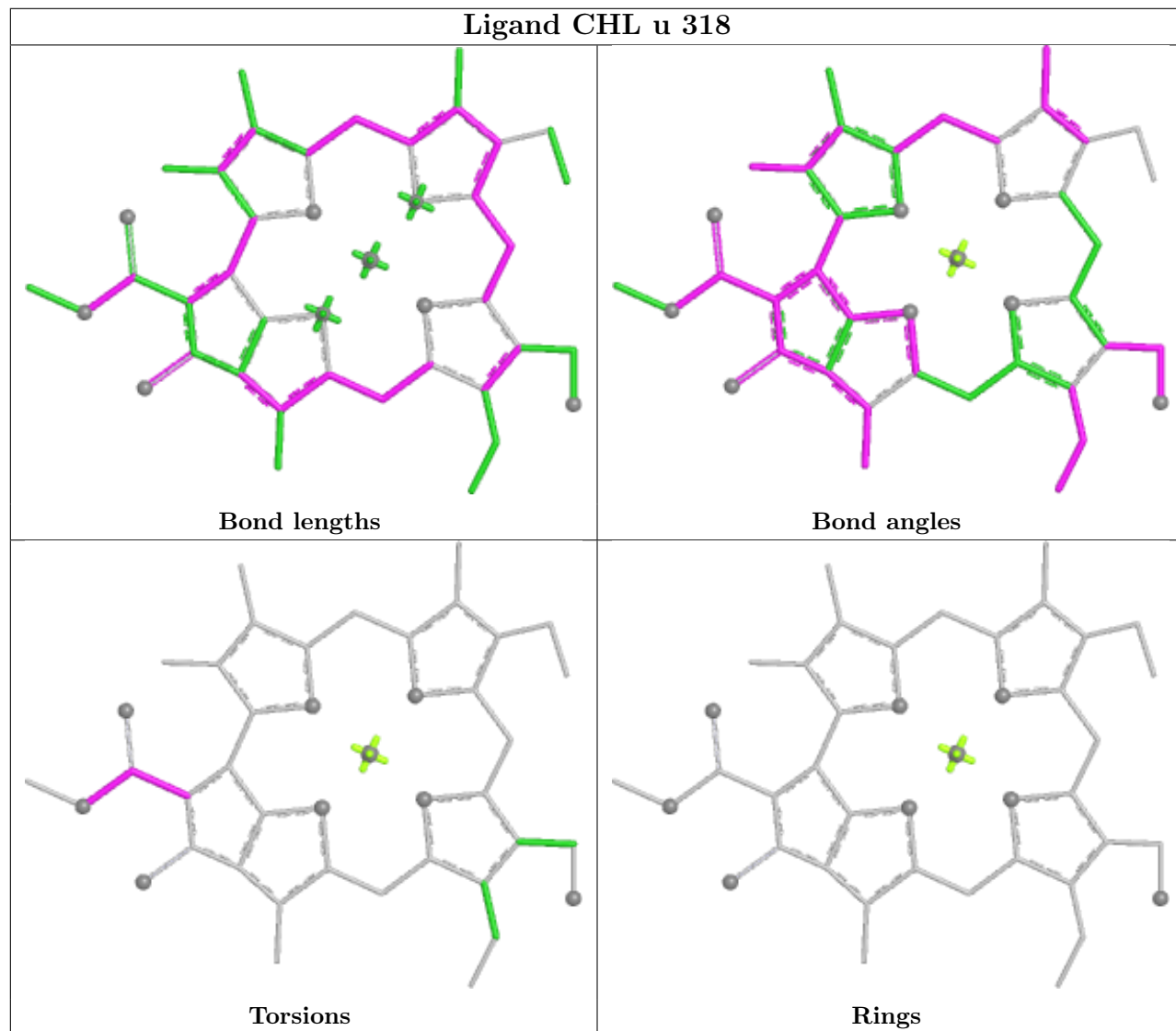


Rings

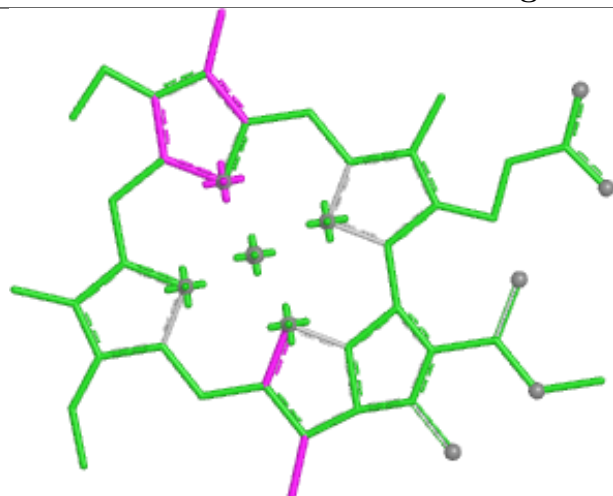
Ligand OIE g 302



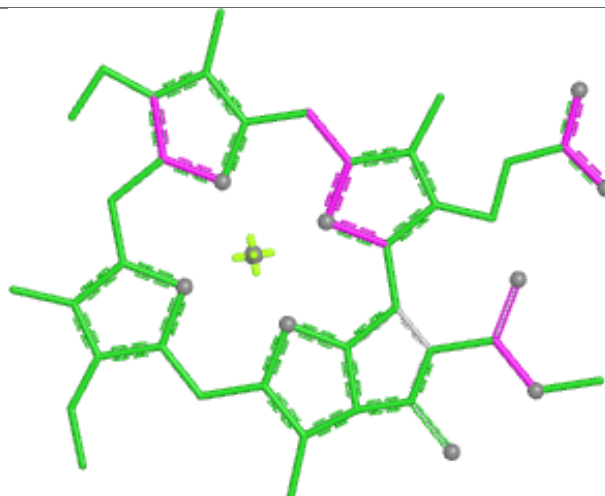
Ligand CHL u 318



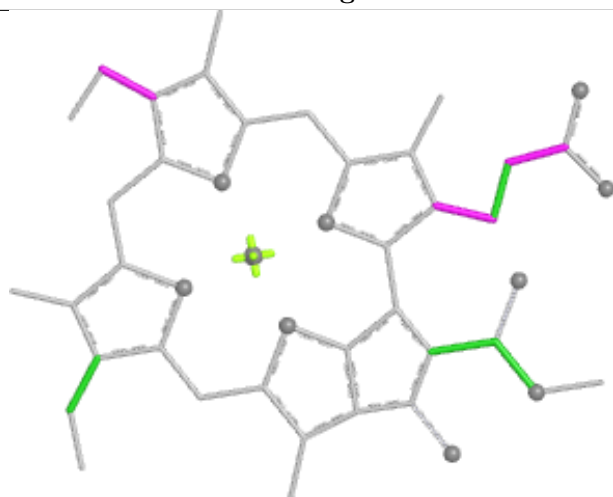
Ligand CLA r 313



Bond lengths



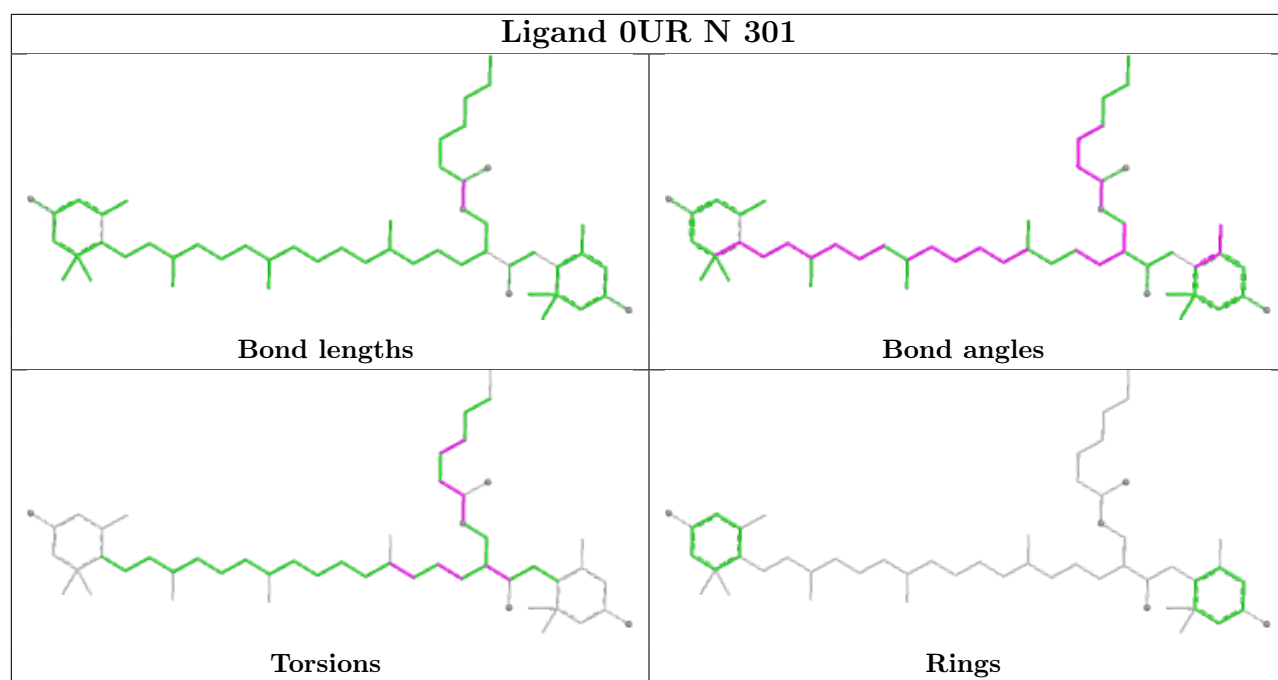
Bond angles



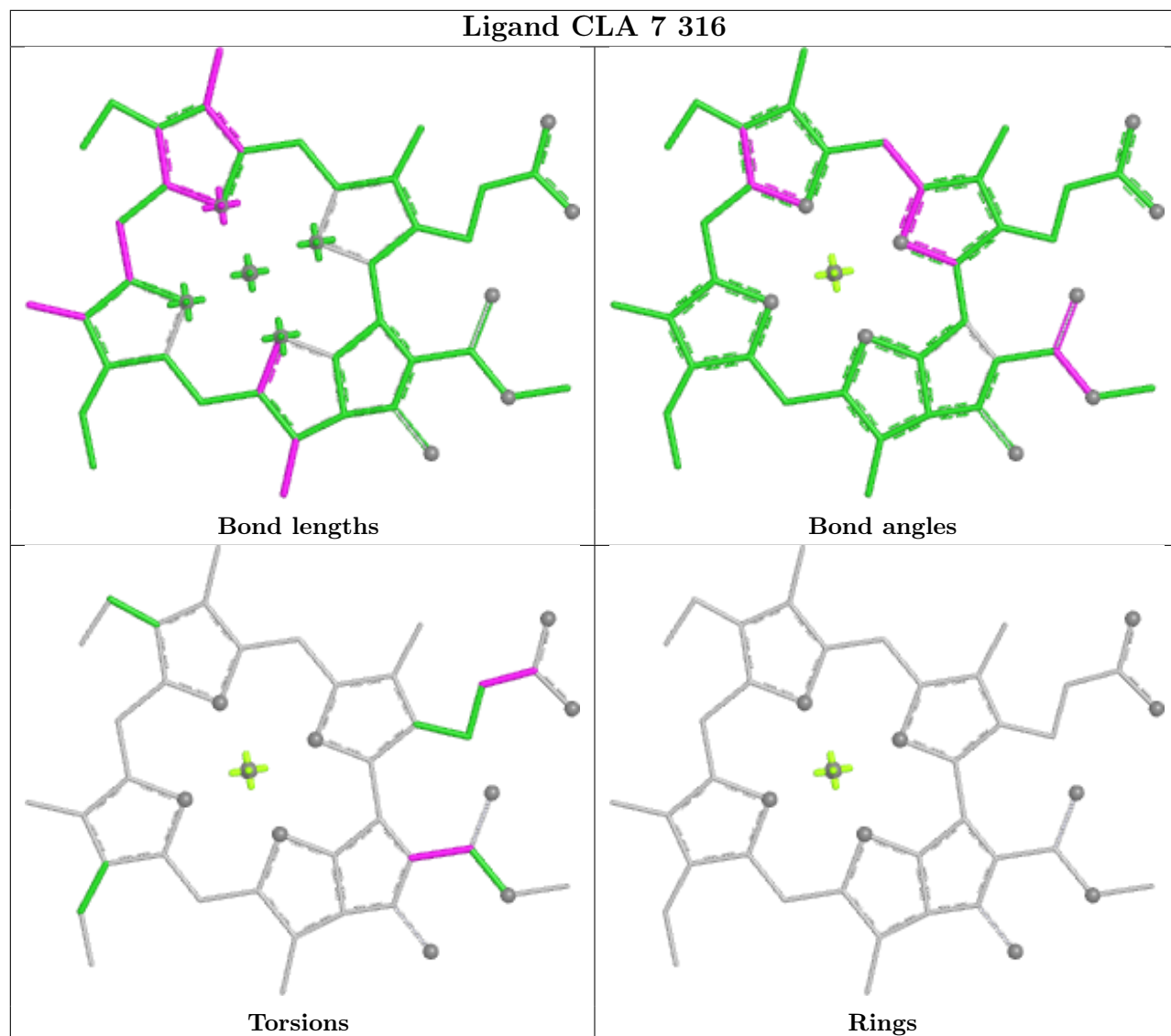
Torsions



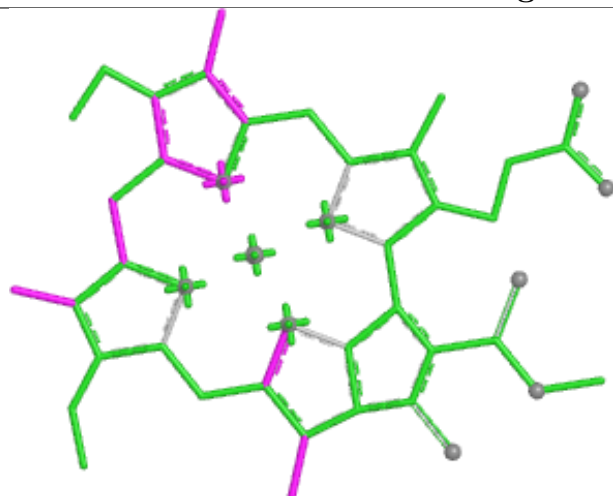
Rings



Ligand CLA 7 316



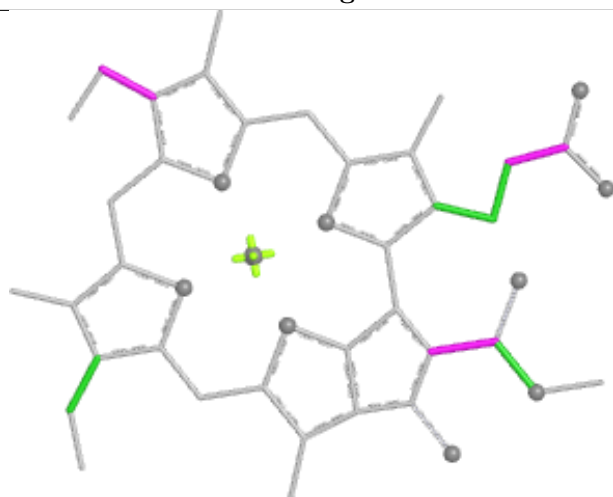
Ligand CLA u 316



Bond lengths



Bond angles

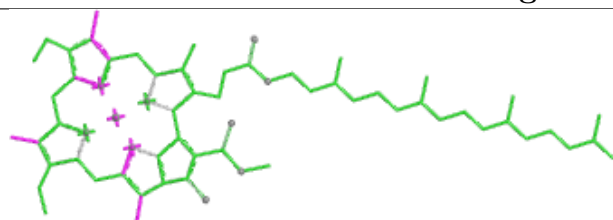


Torsions

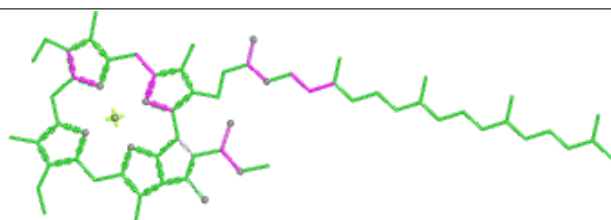


Rings

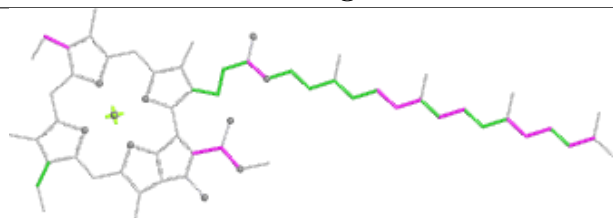
Ligand CLA c 602



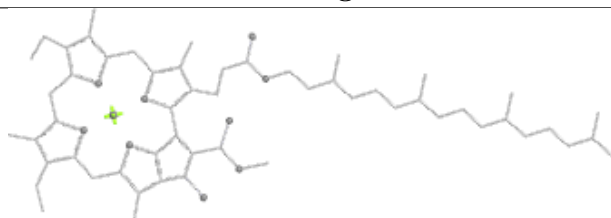
Bond lengths



Bond angles

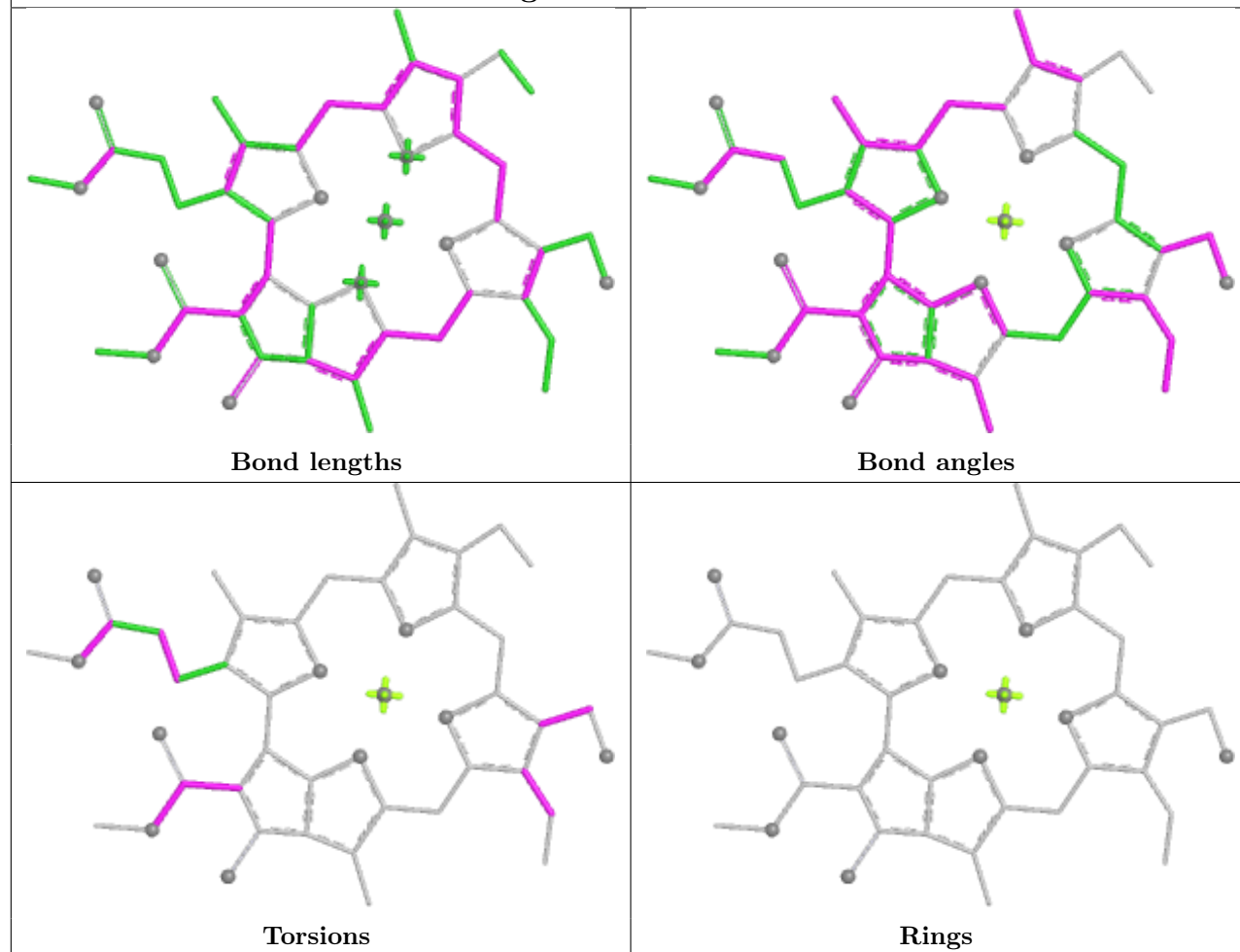


Torsions

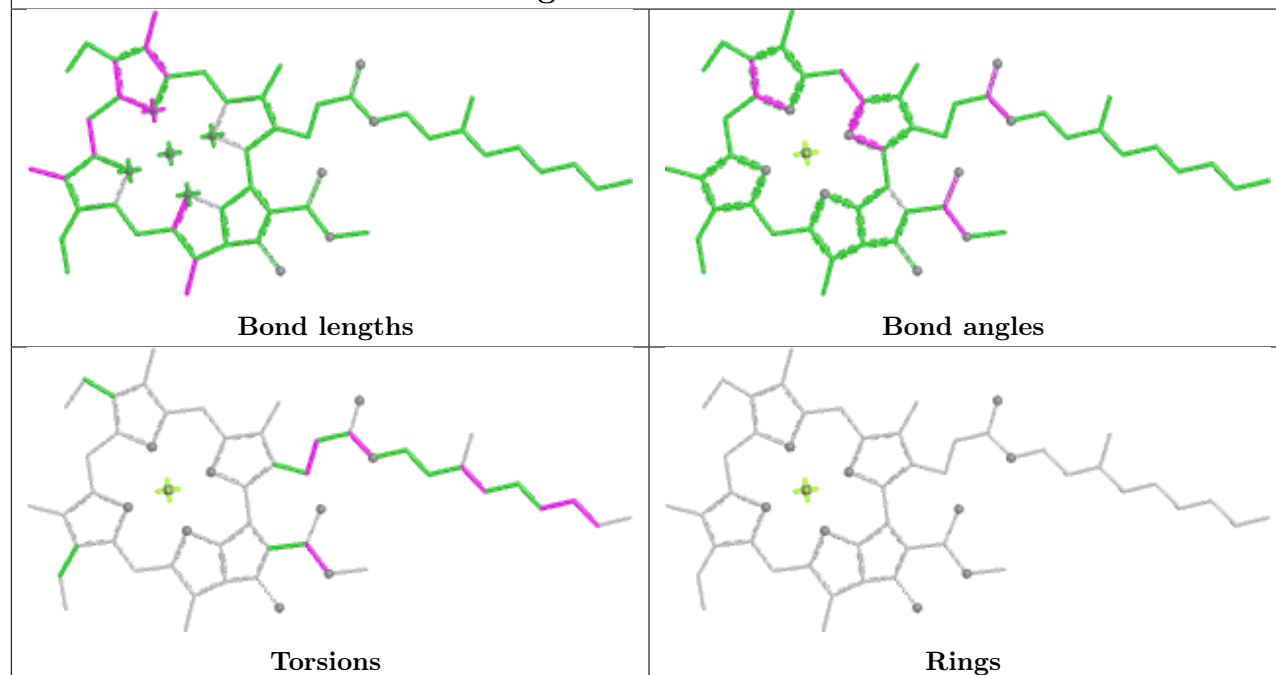


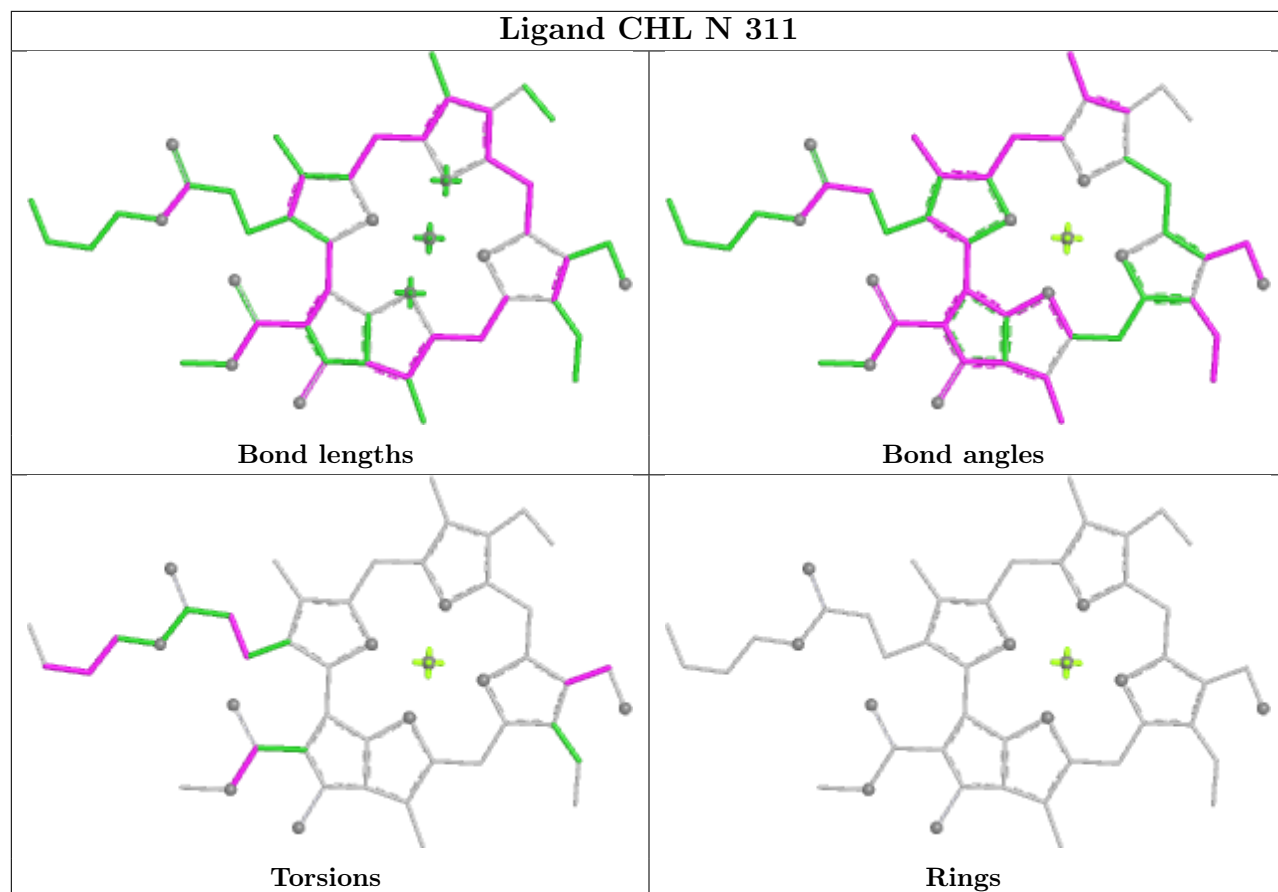
Rings

Ligand CHL 5 306

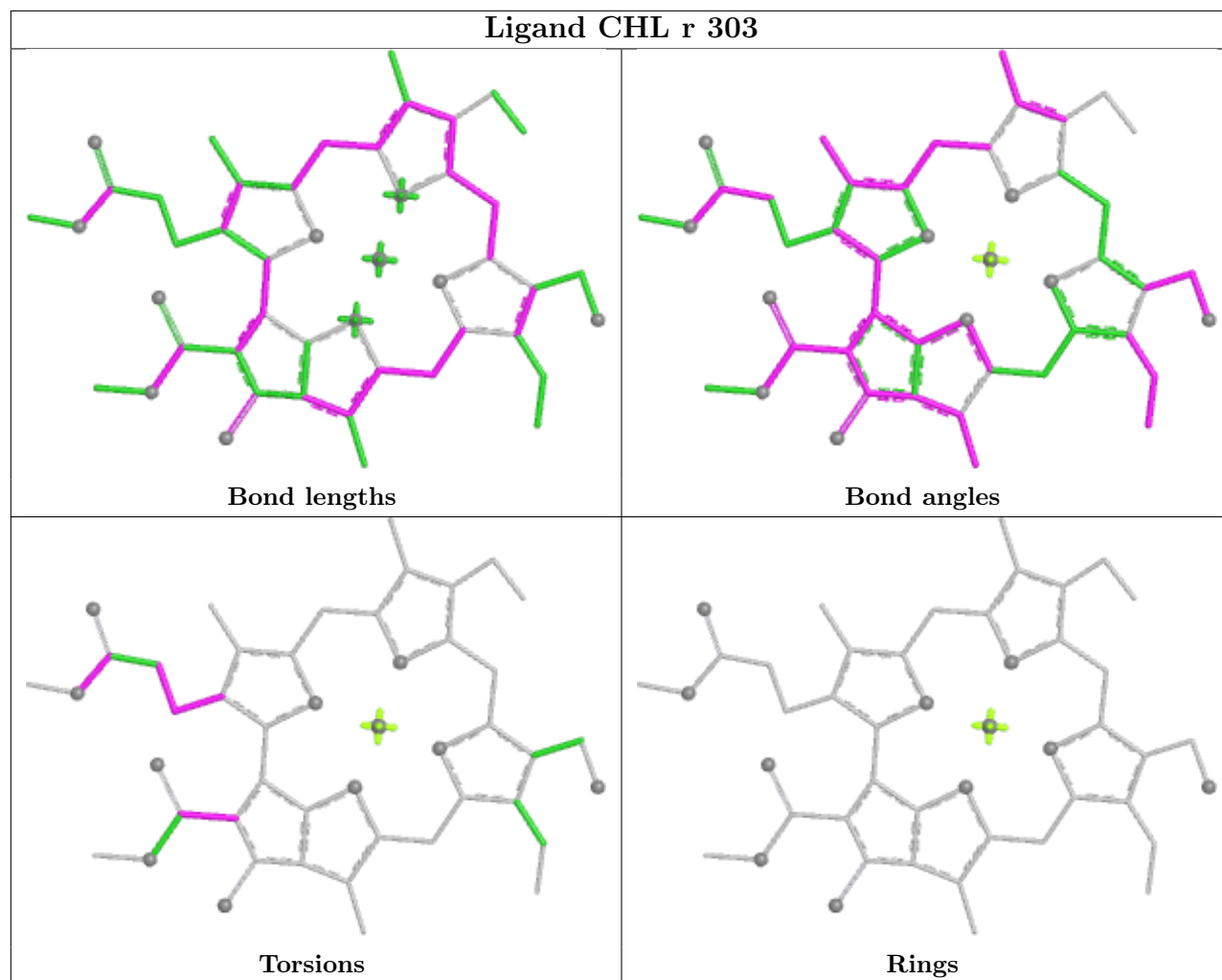


Ligand CLA s 413

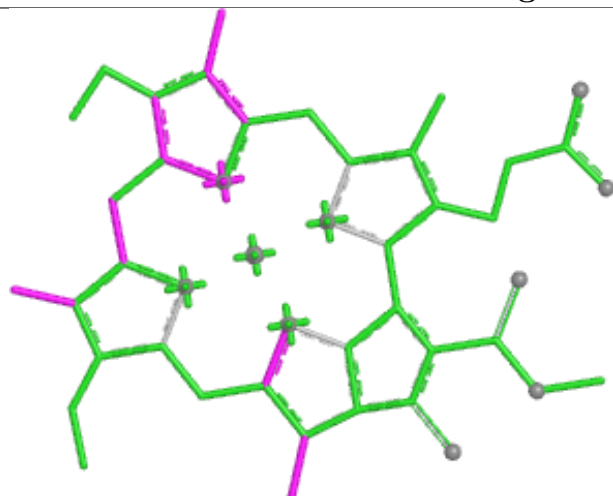




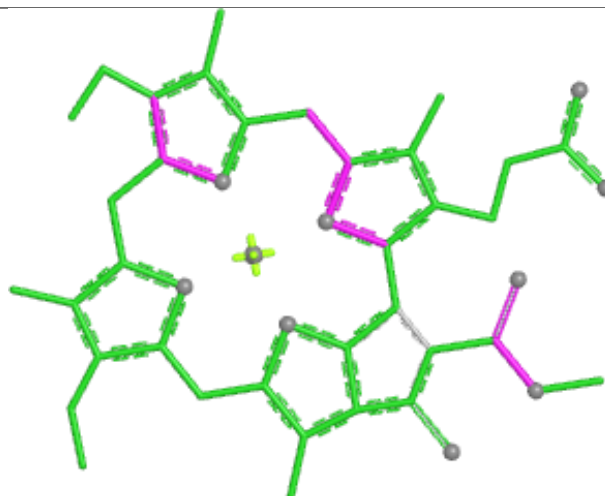
Ligand CHL r 303



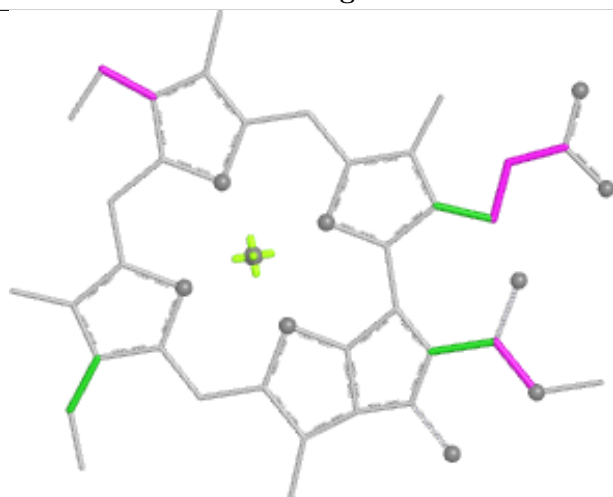
Ligand CLA 3 316



Bond lengths



Bond angles

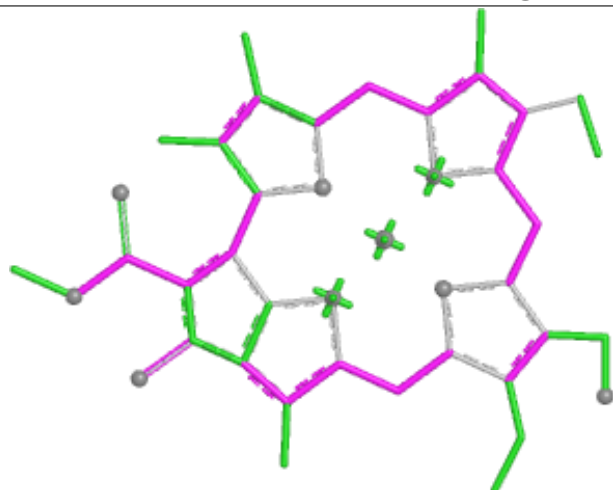


Torsions

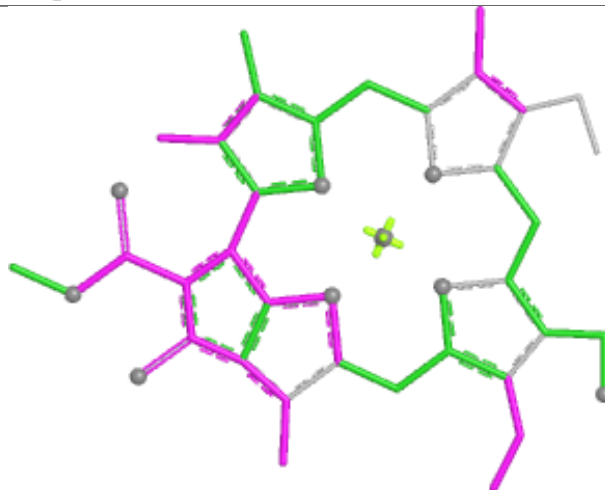


Rings

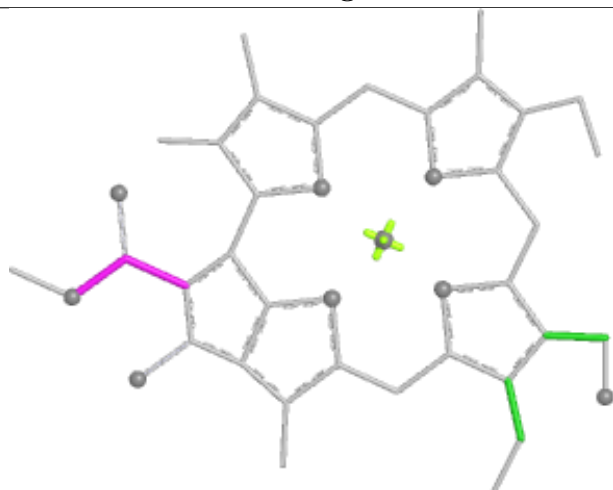
Ligand CHL p 318



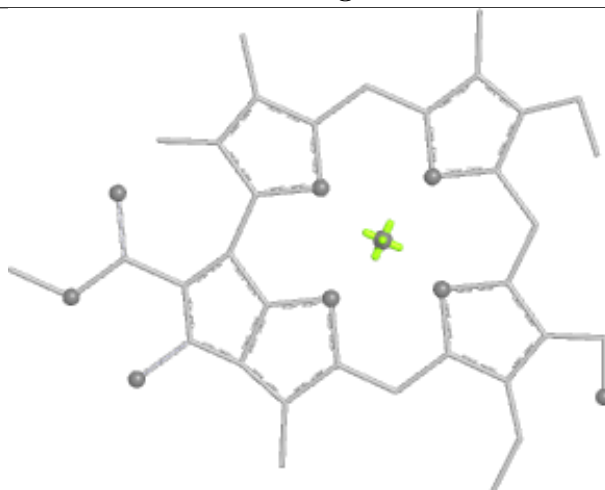
Bond lengths



Bond angles

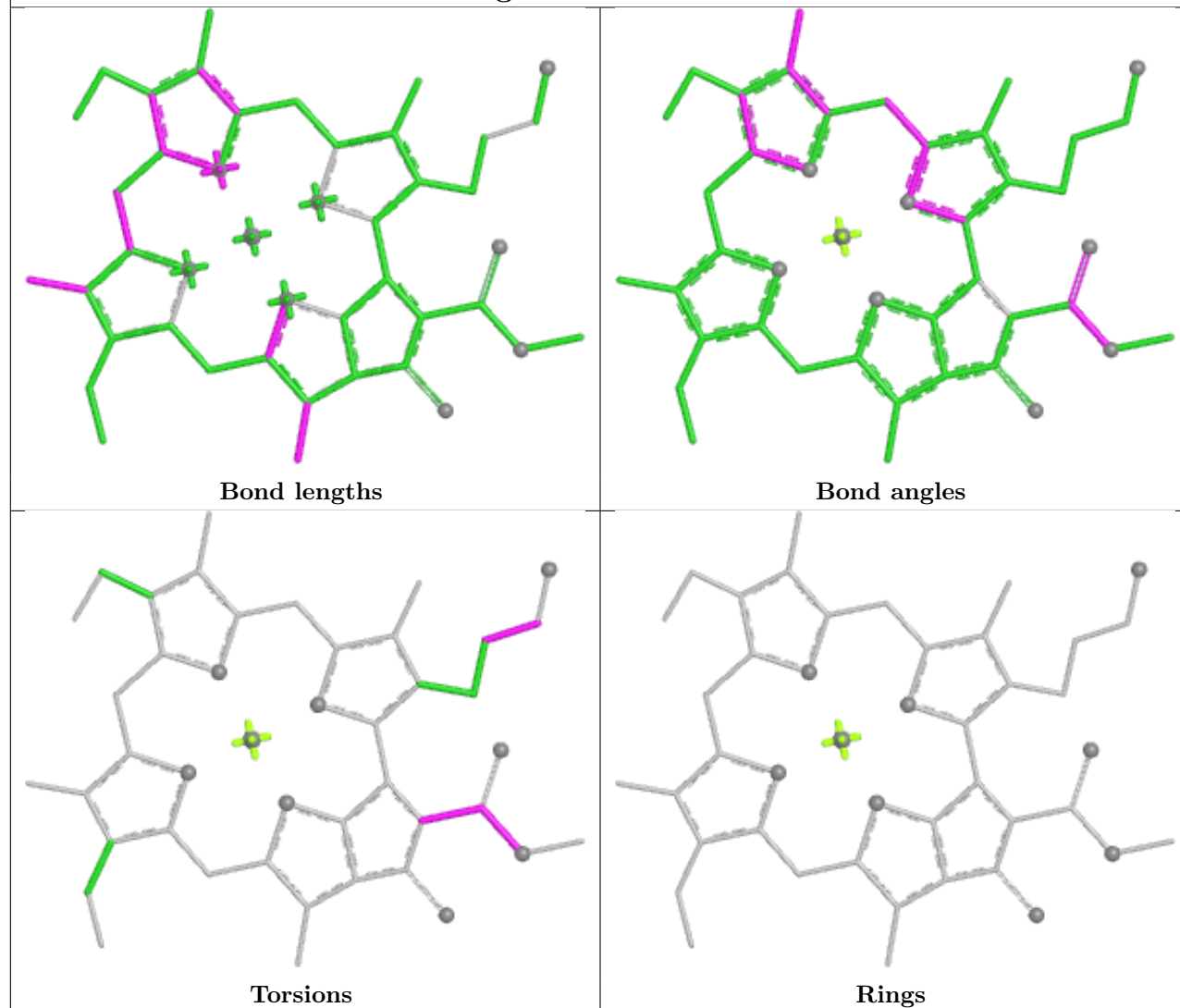


Torsions

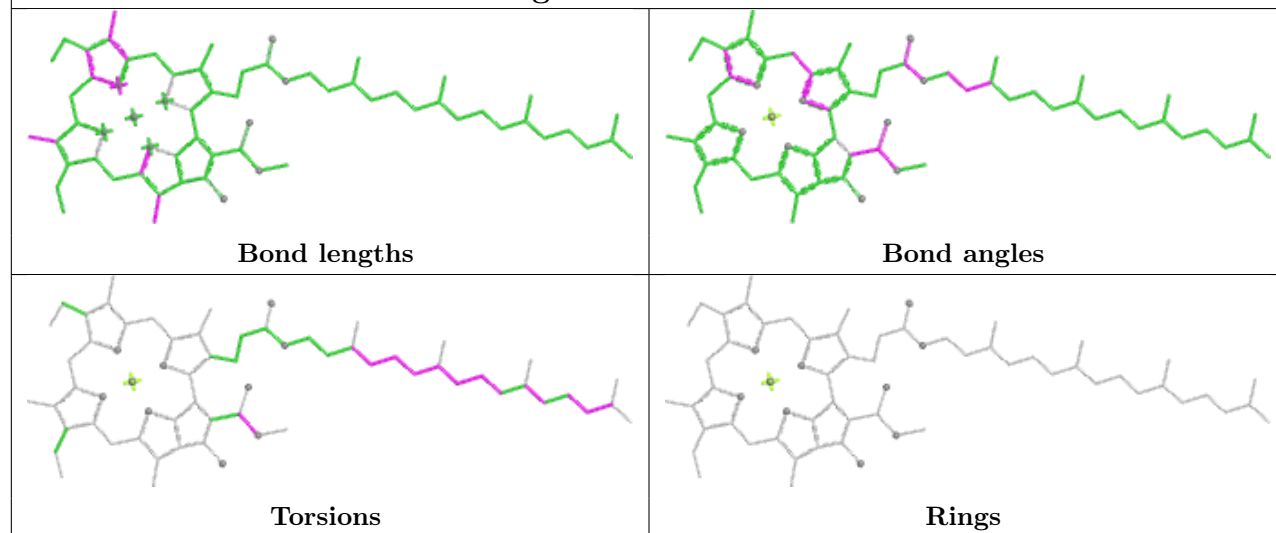


Rings

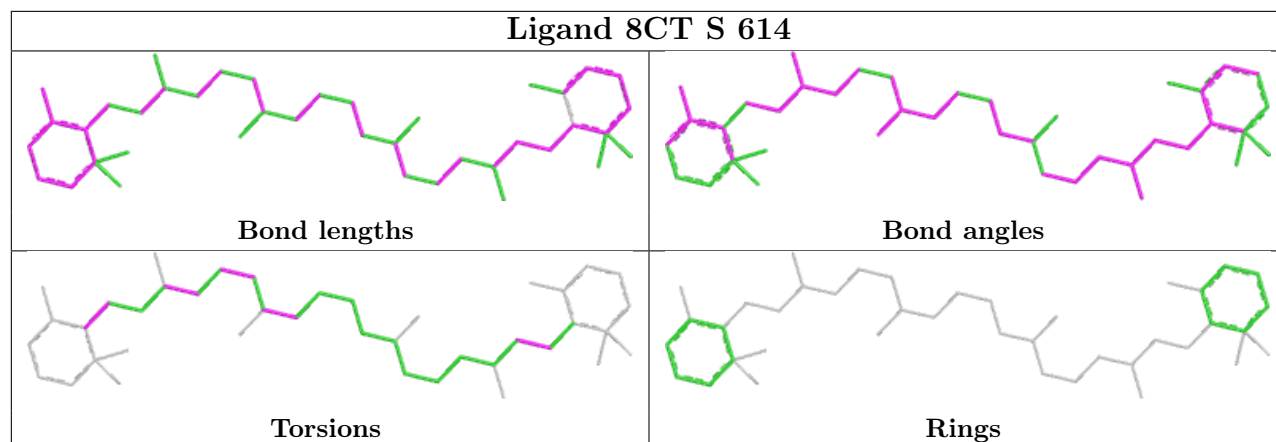
Ligand CLA 4 306



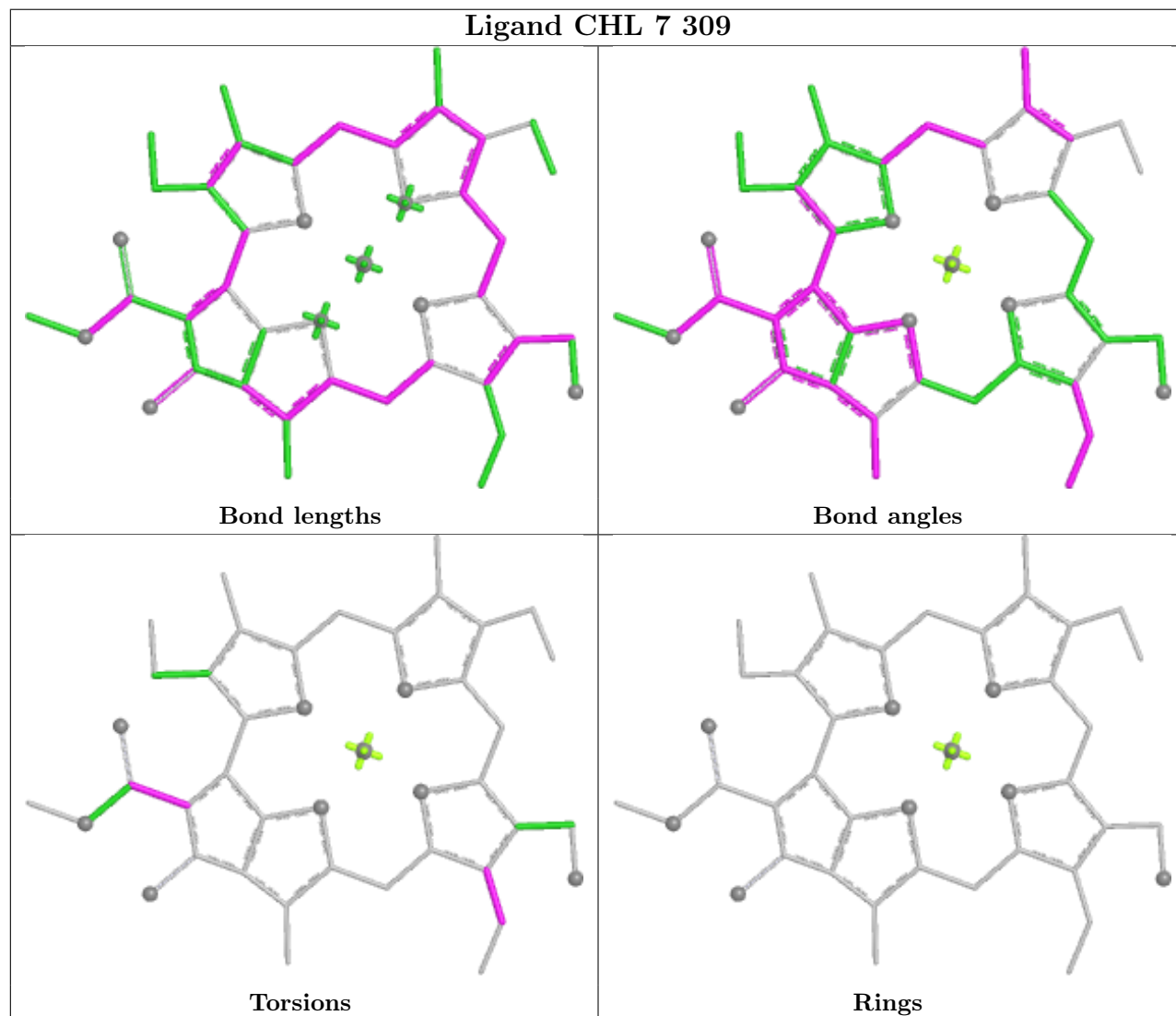
Ligand CLA B 609



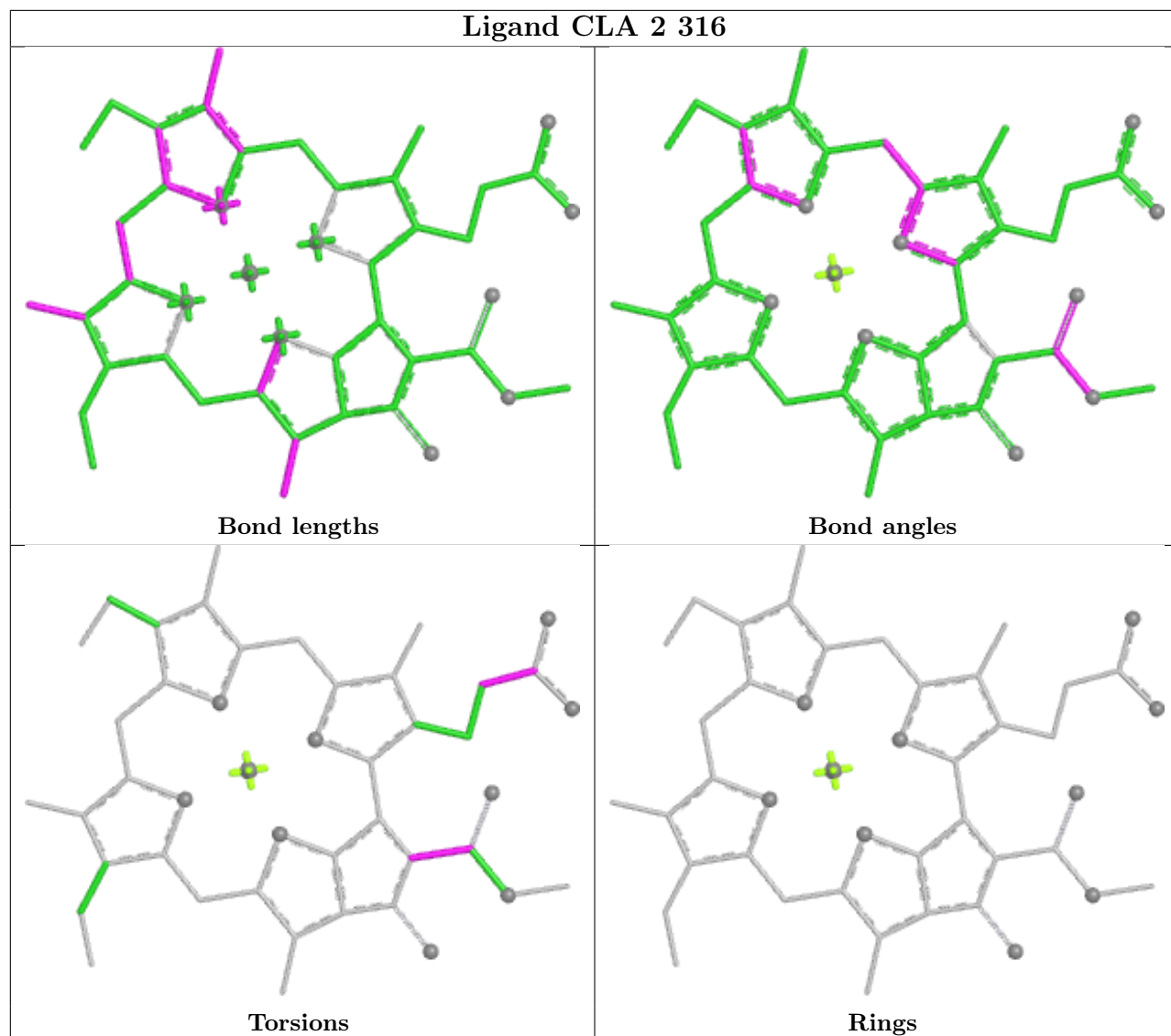
Ligand 8CT S 614



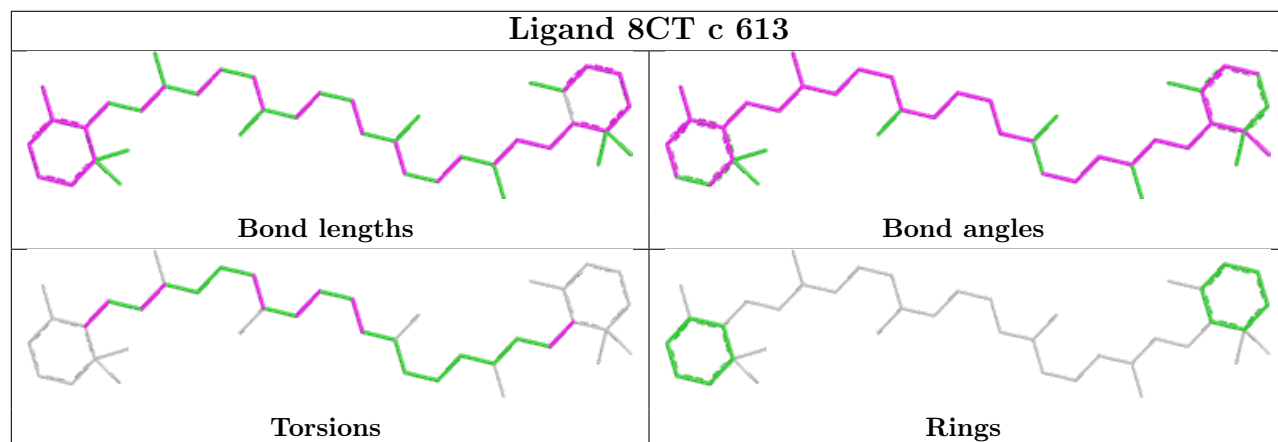
Ligand CHL 7 309

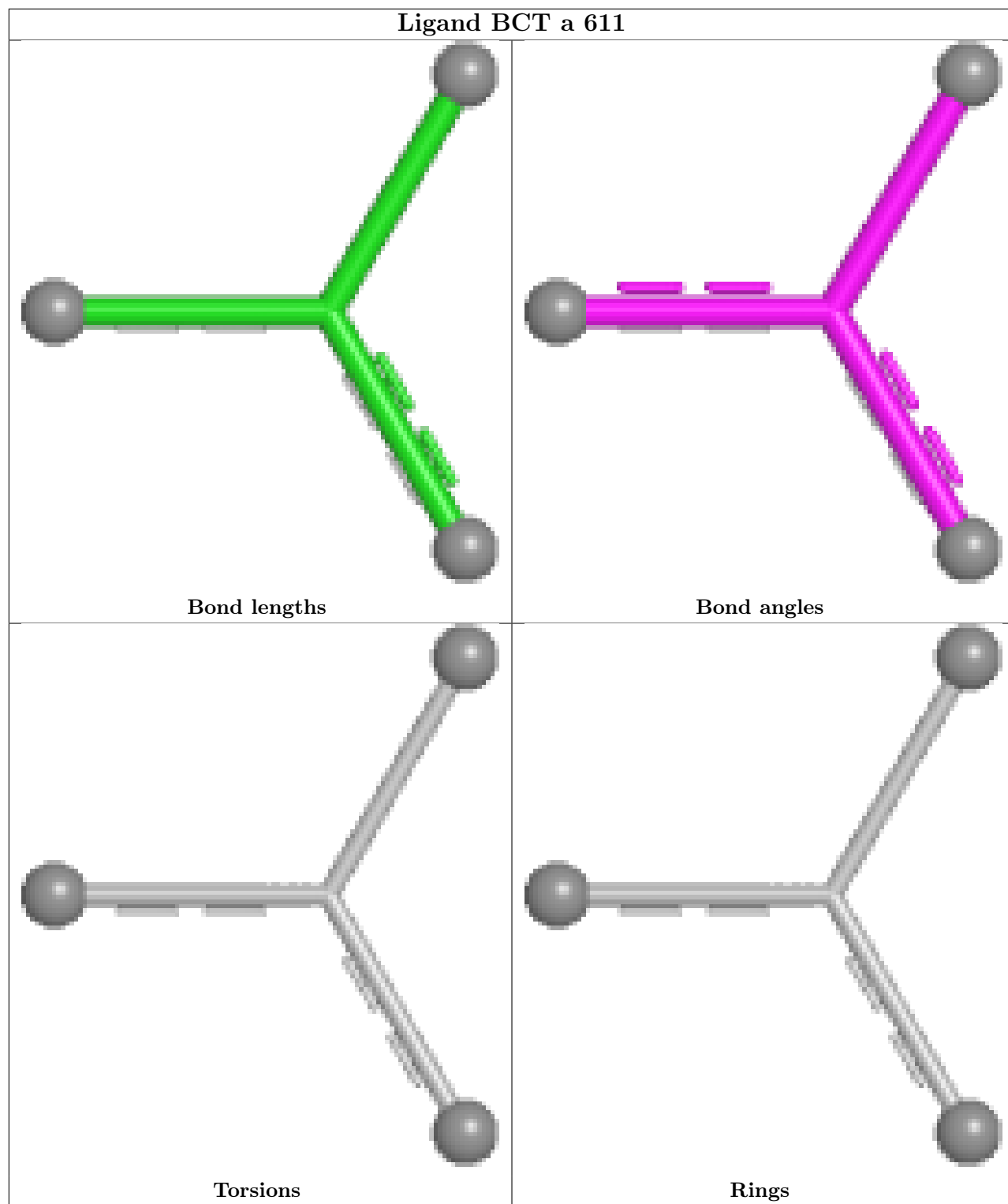


Ligand CLA 2 316

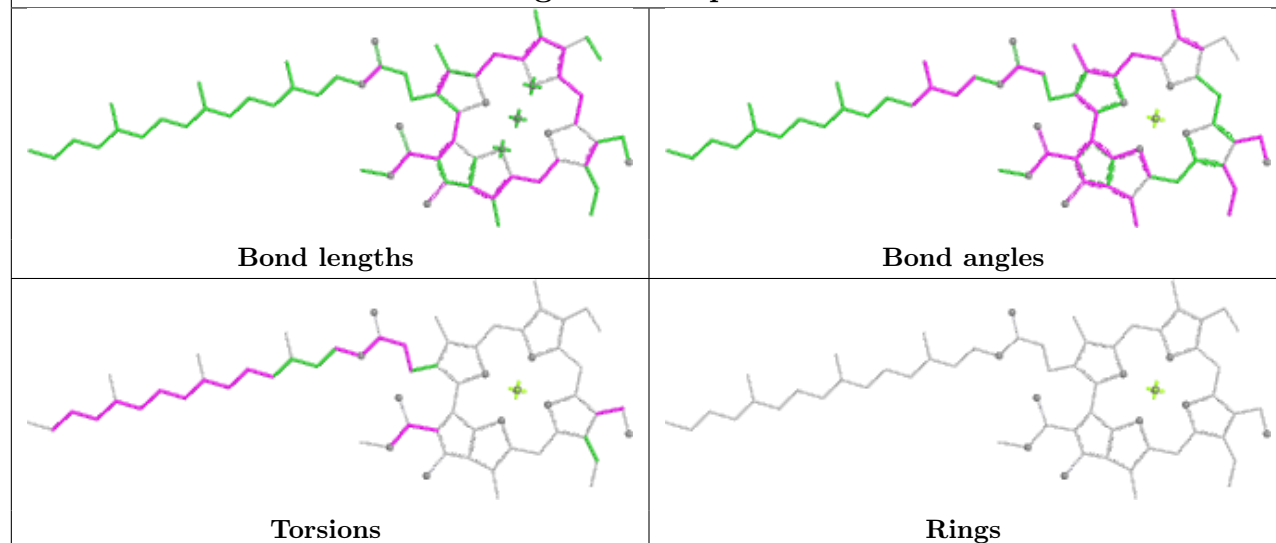


Ligand 8CT c 613

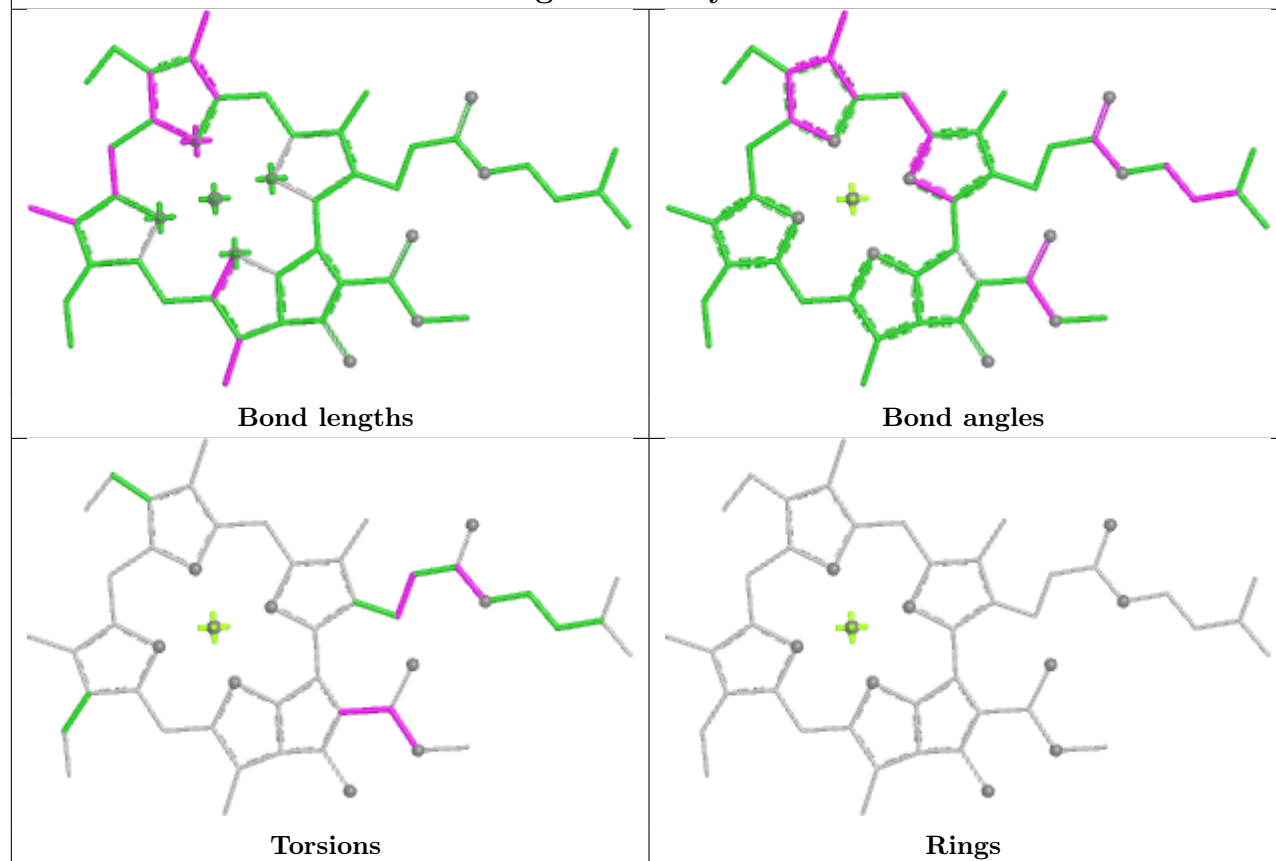




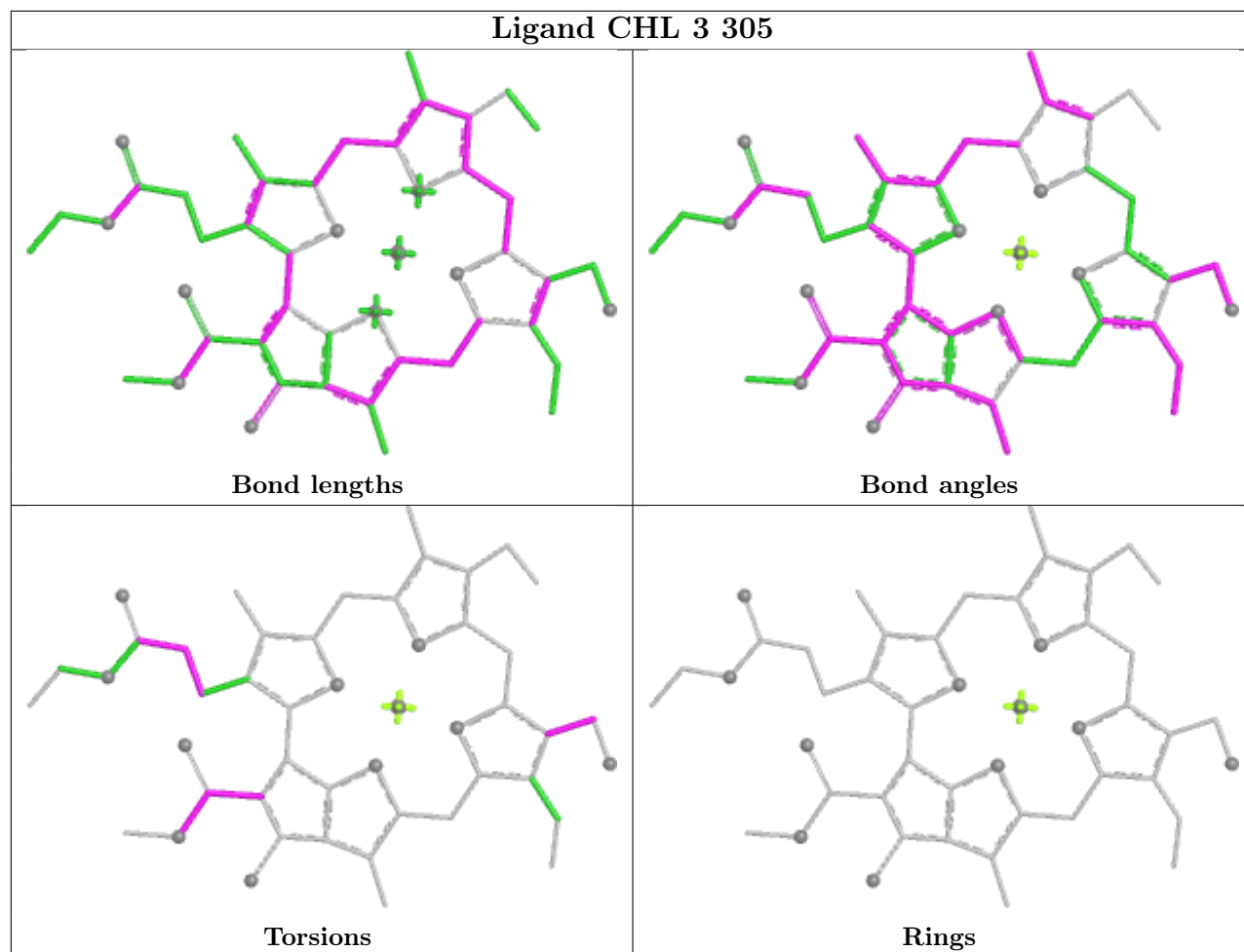
Ligand CHL p 306

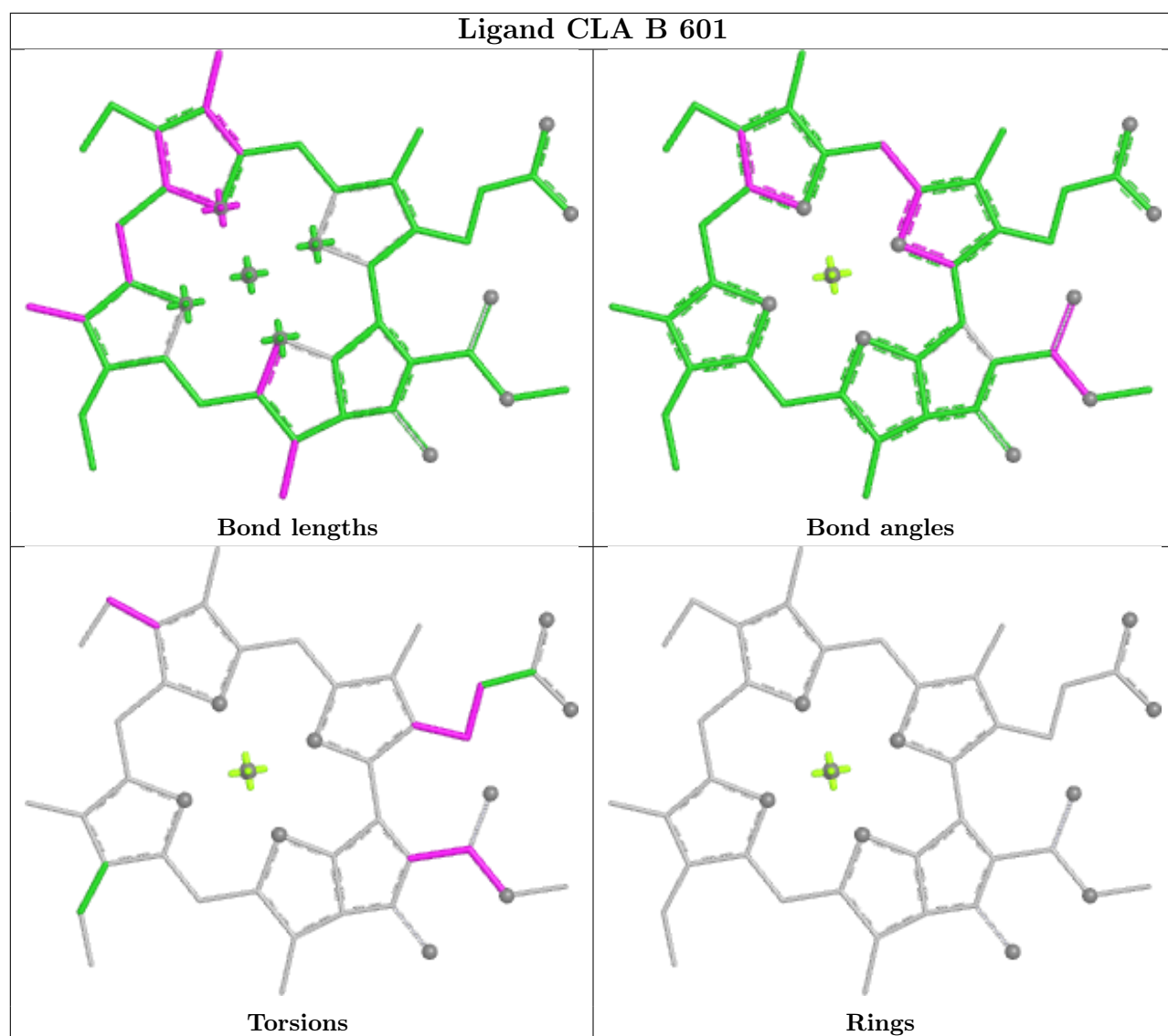


Ligand CLA y 308

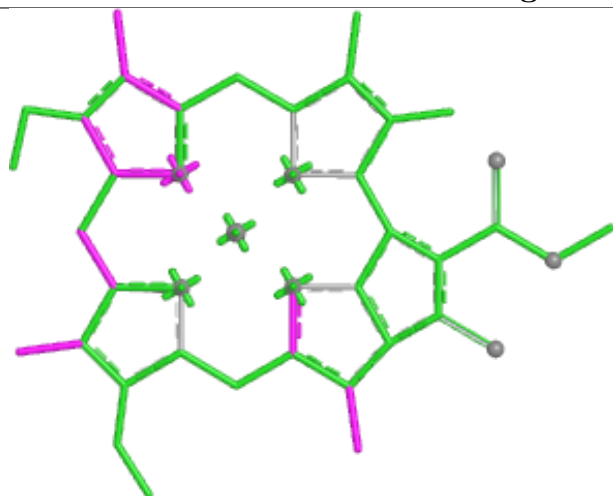


Ligand CHL 3 305

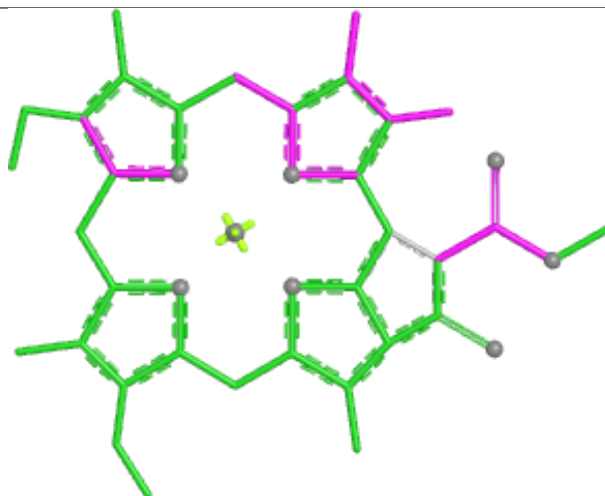




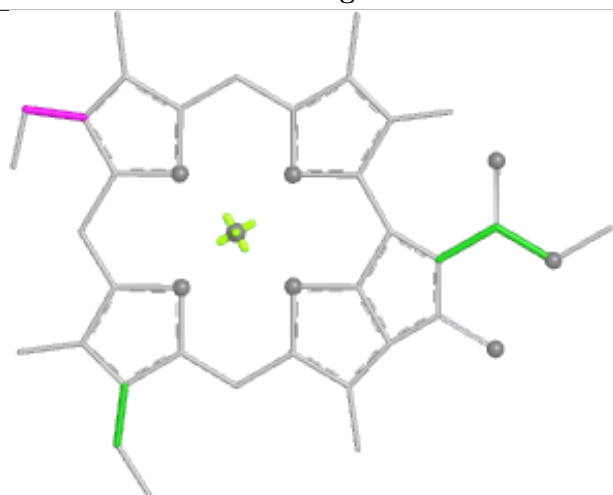
Ligand CLA r 305



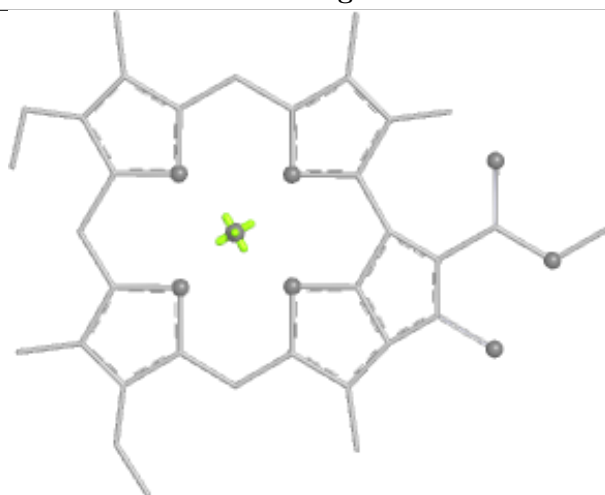
Bond lengths



Bond angles

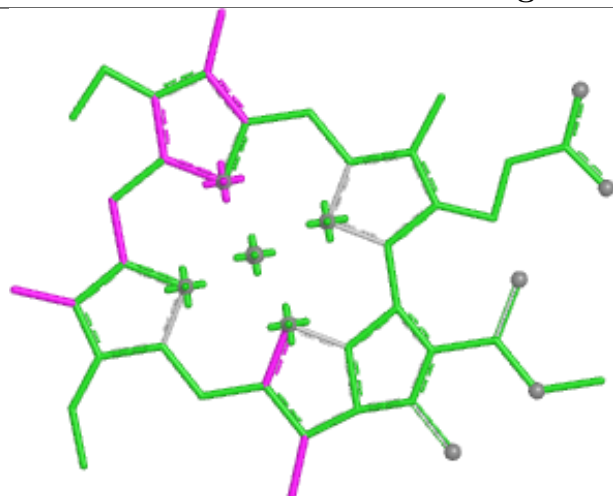


Torsions



Rings

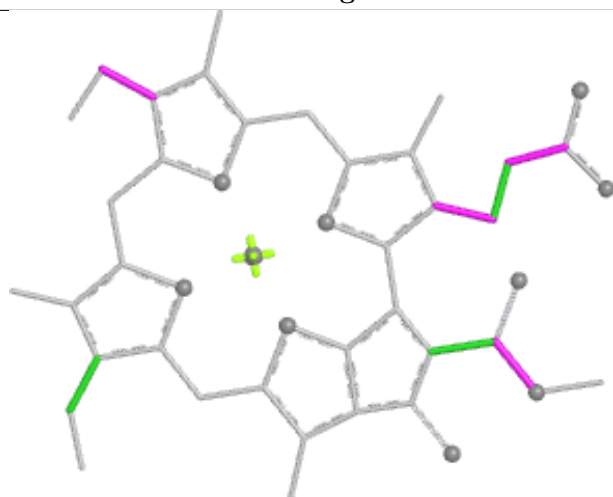
Ligand CLA S 616



Bond lengths



Bond angles

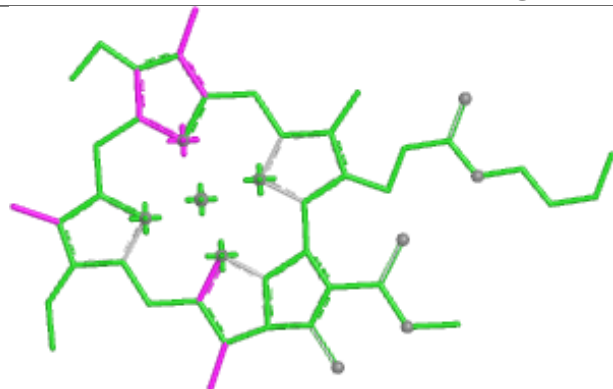


Torsions

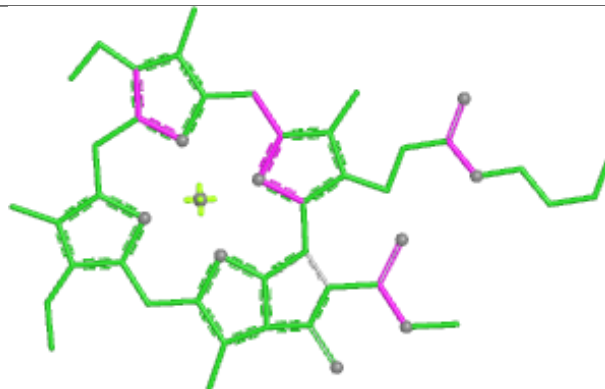


Rings

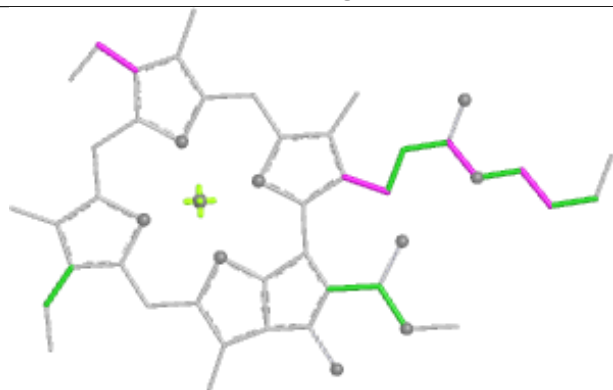
Ligand CLA A 605



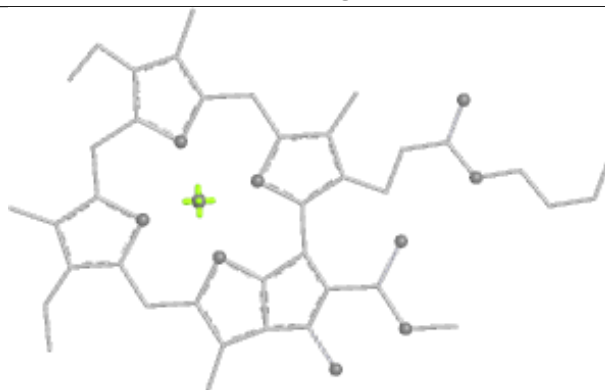
Bond lengths



Bond angles

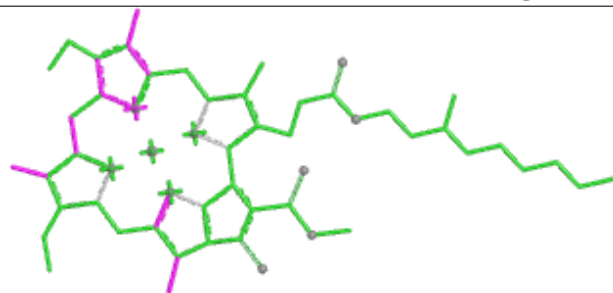


Torsions

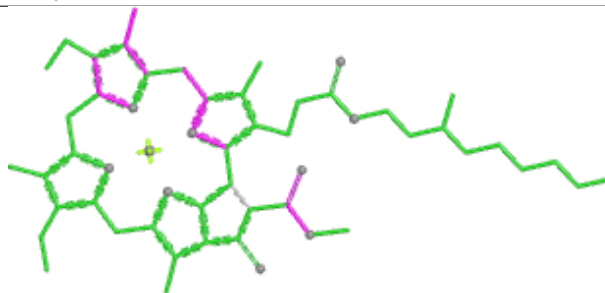


Rings

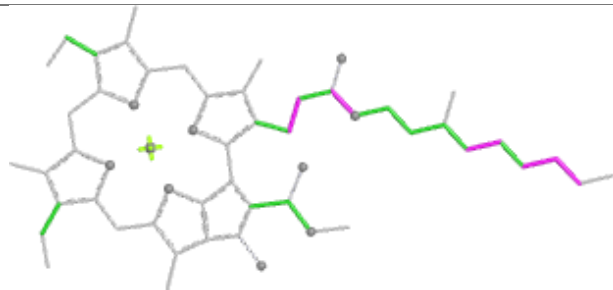
Ligand CLA y 317



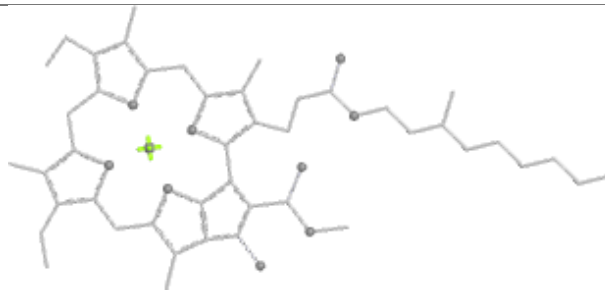
Bond lengths



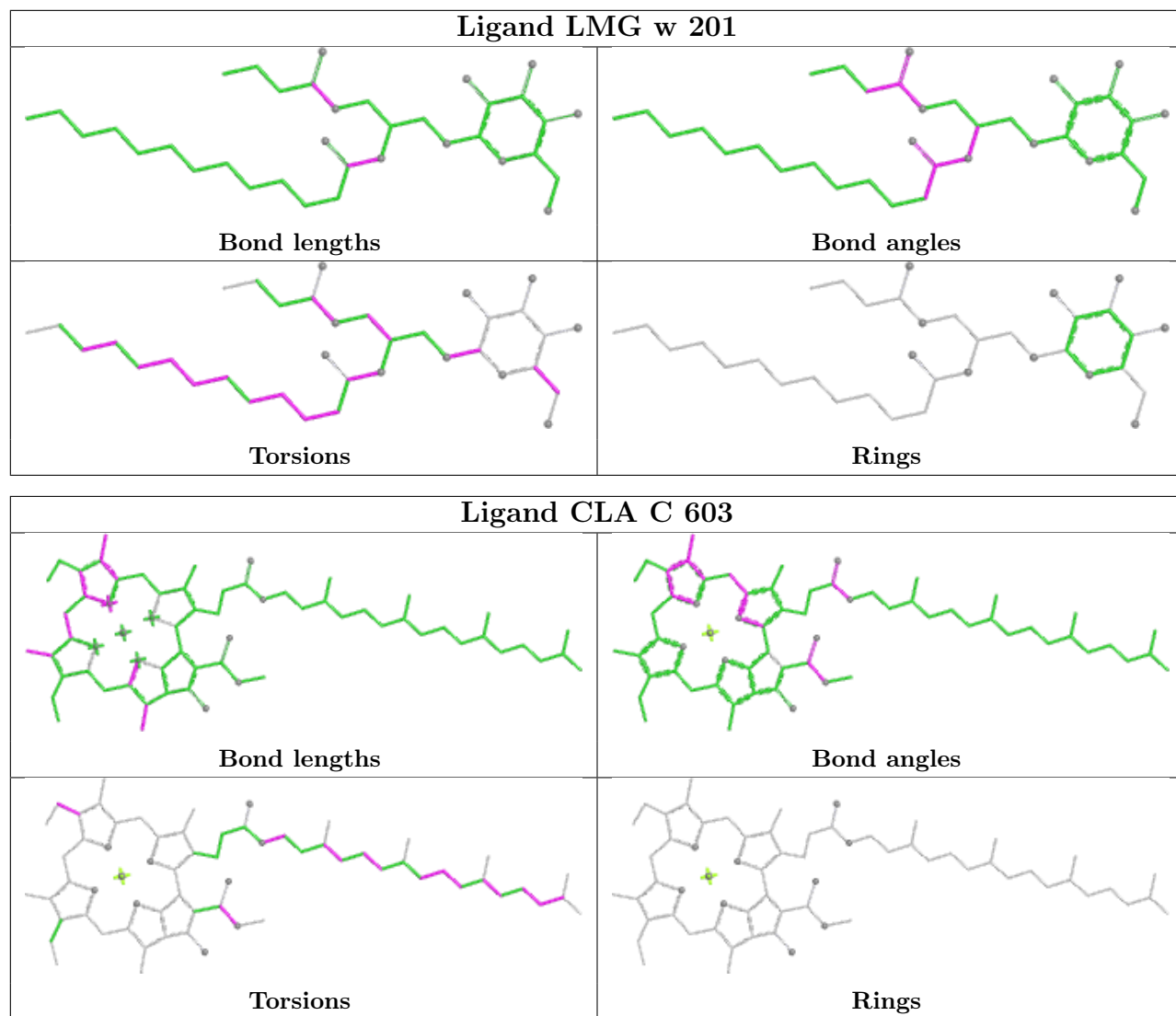
Bond angles

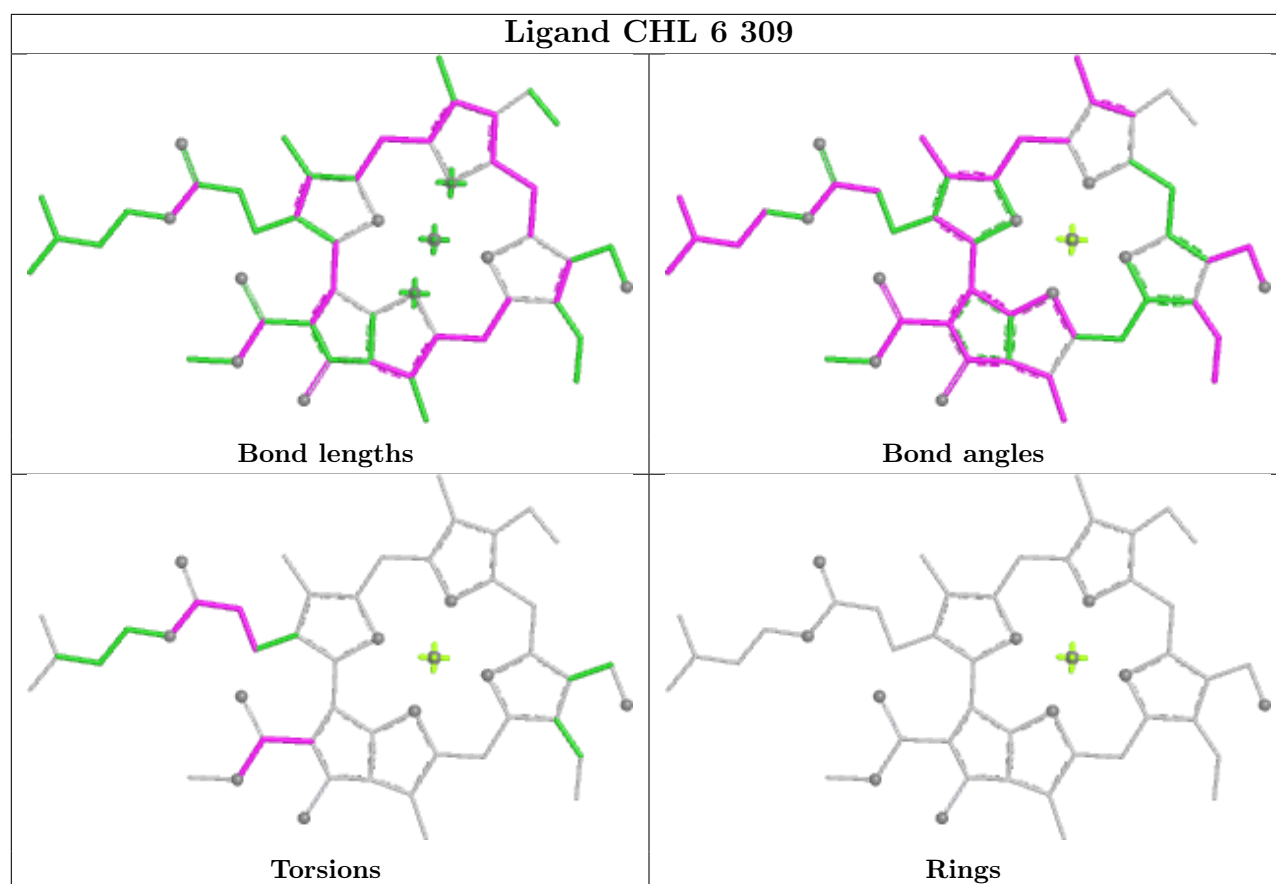


Torsions

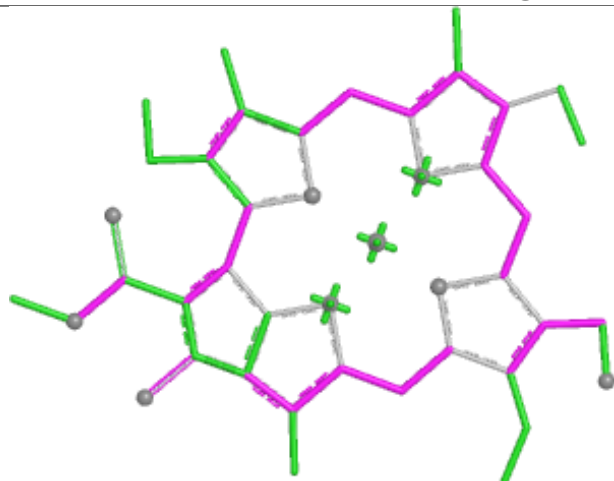


Rings

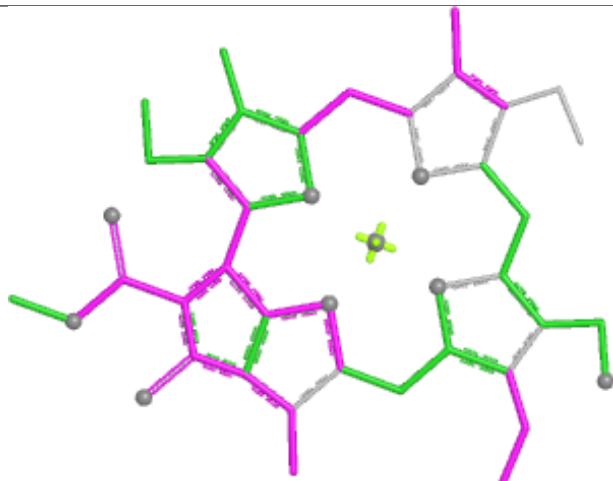




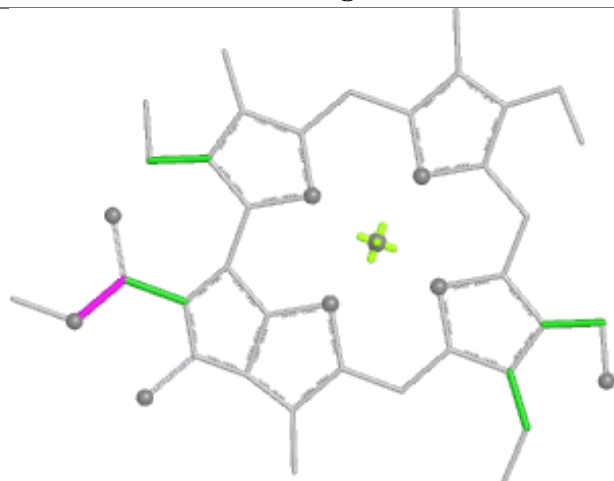
Ligand CHL u 309



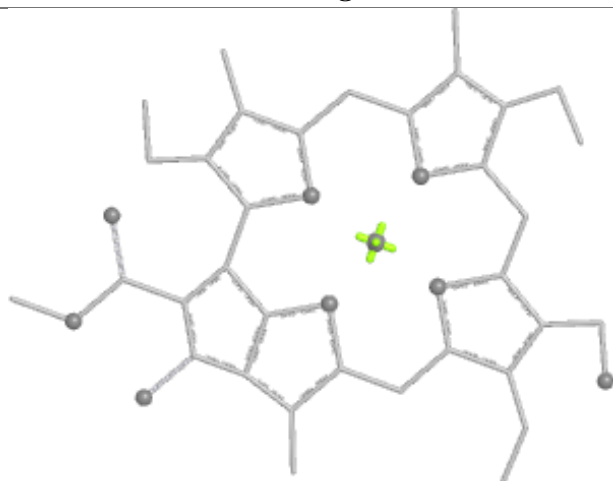
Bond lengths



Bond angles

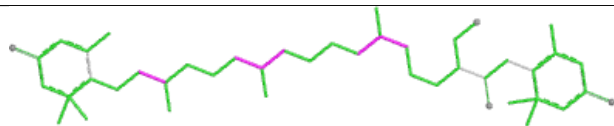


Torsions

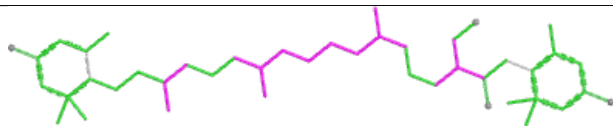


Rings

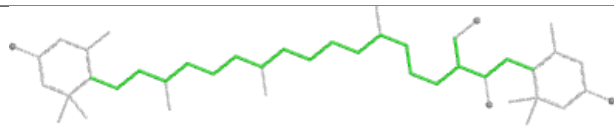
Ligand 0IE Y 303



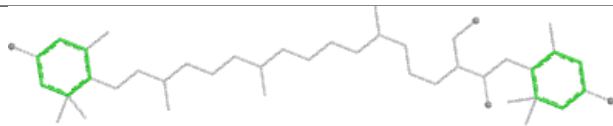
Bond lengths



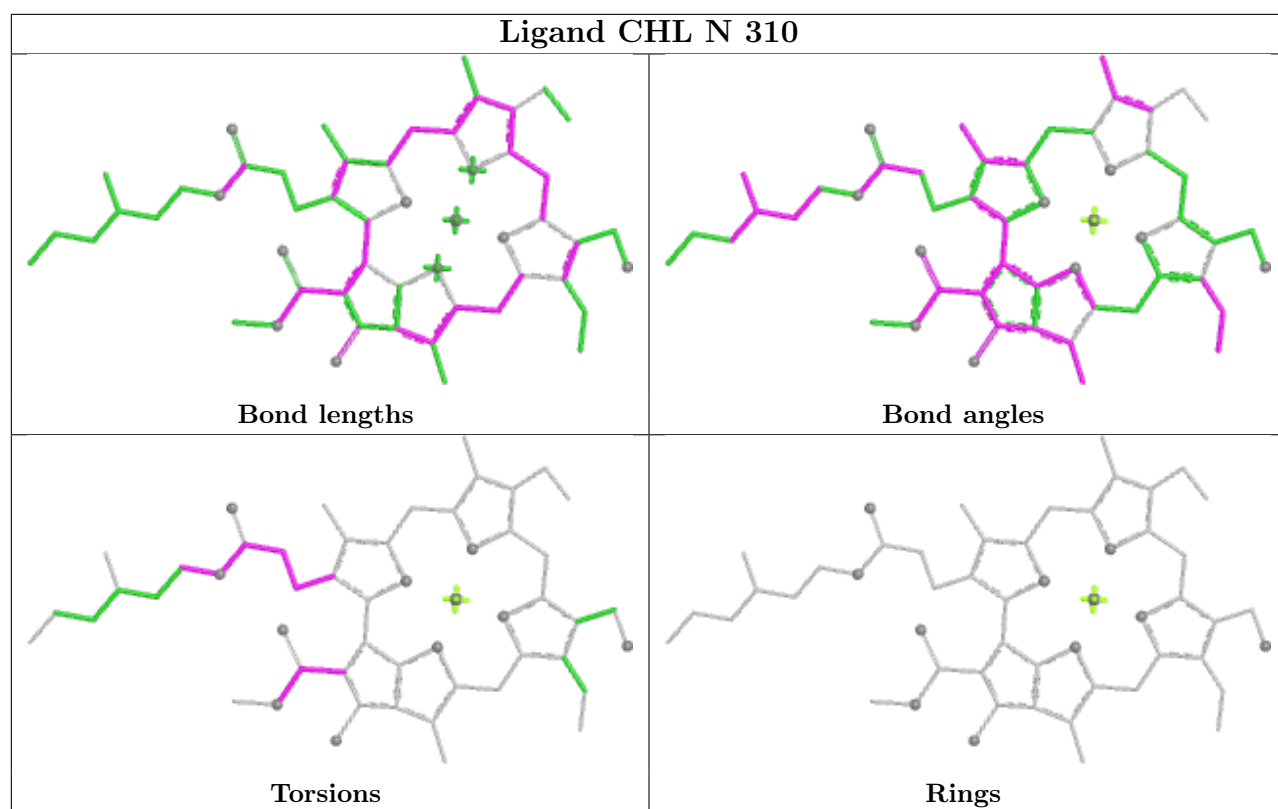
Bond angles



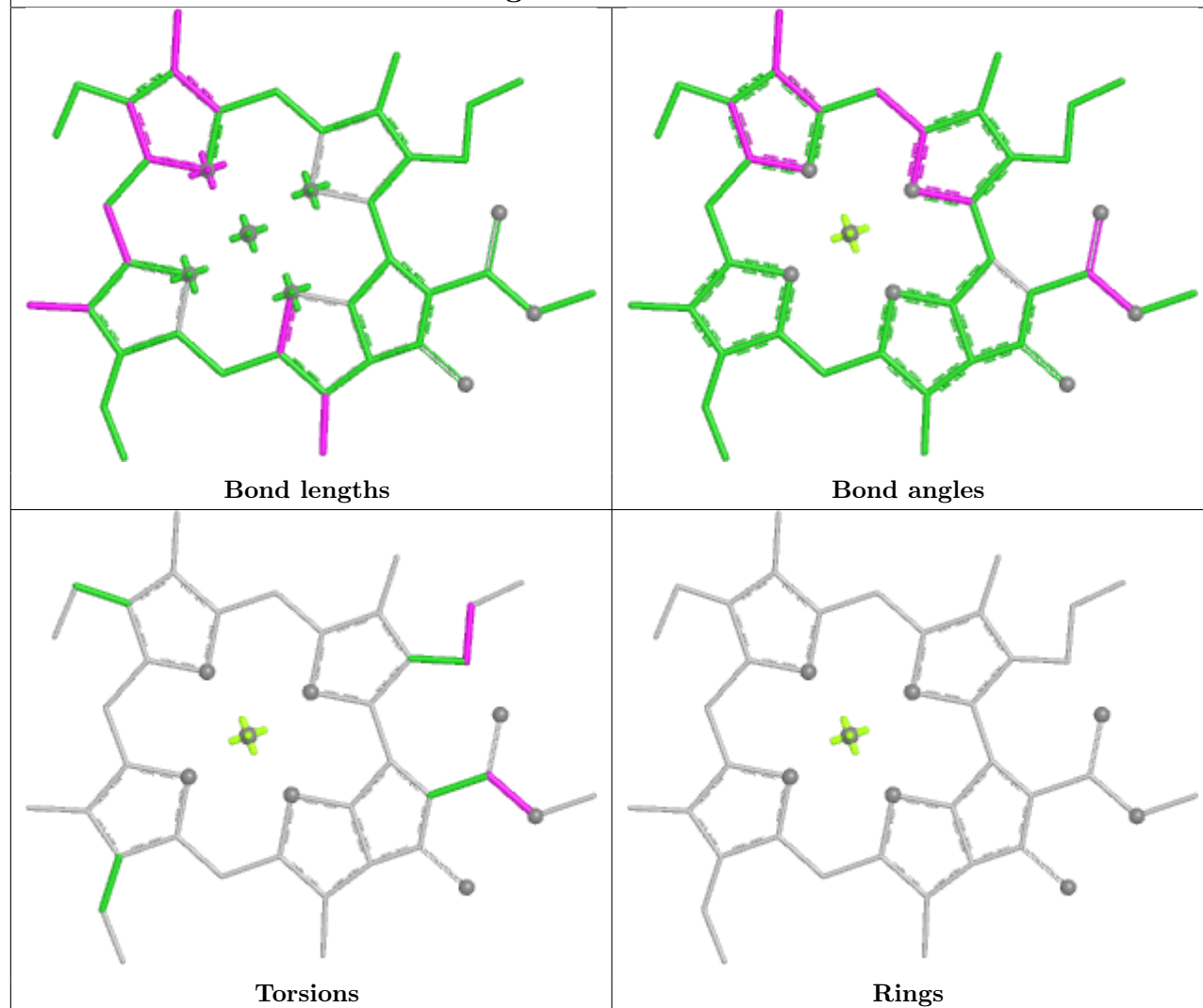
Torsions



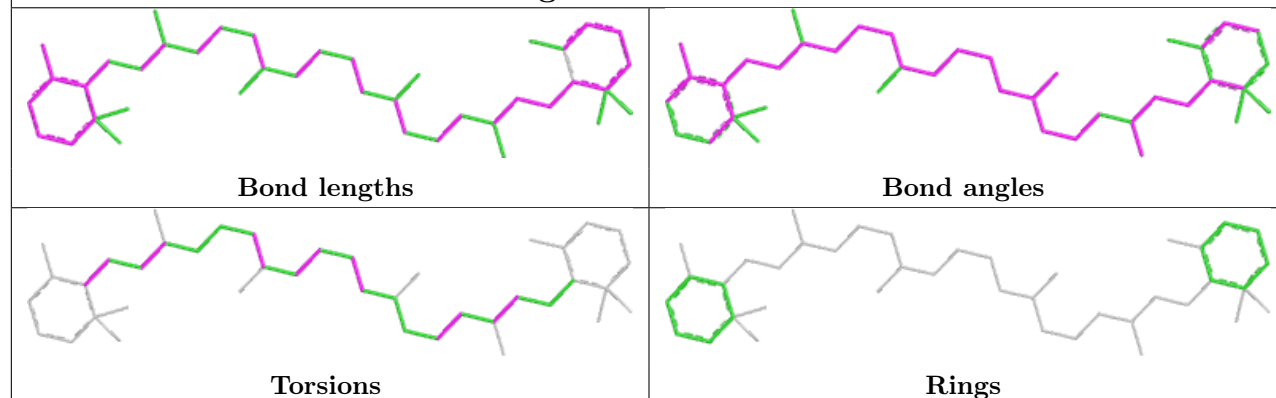
Rings



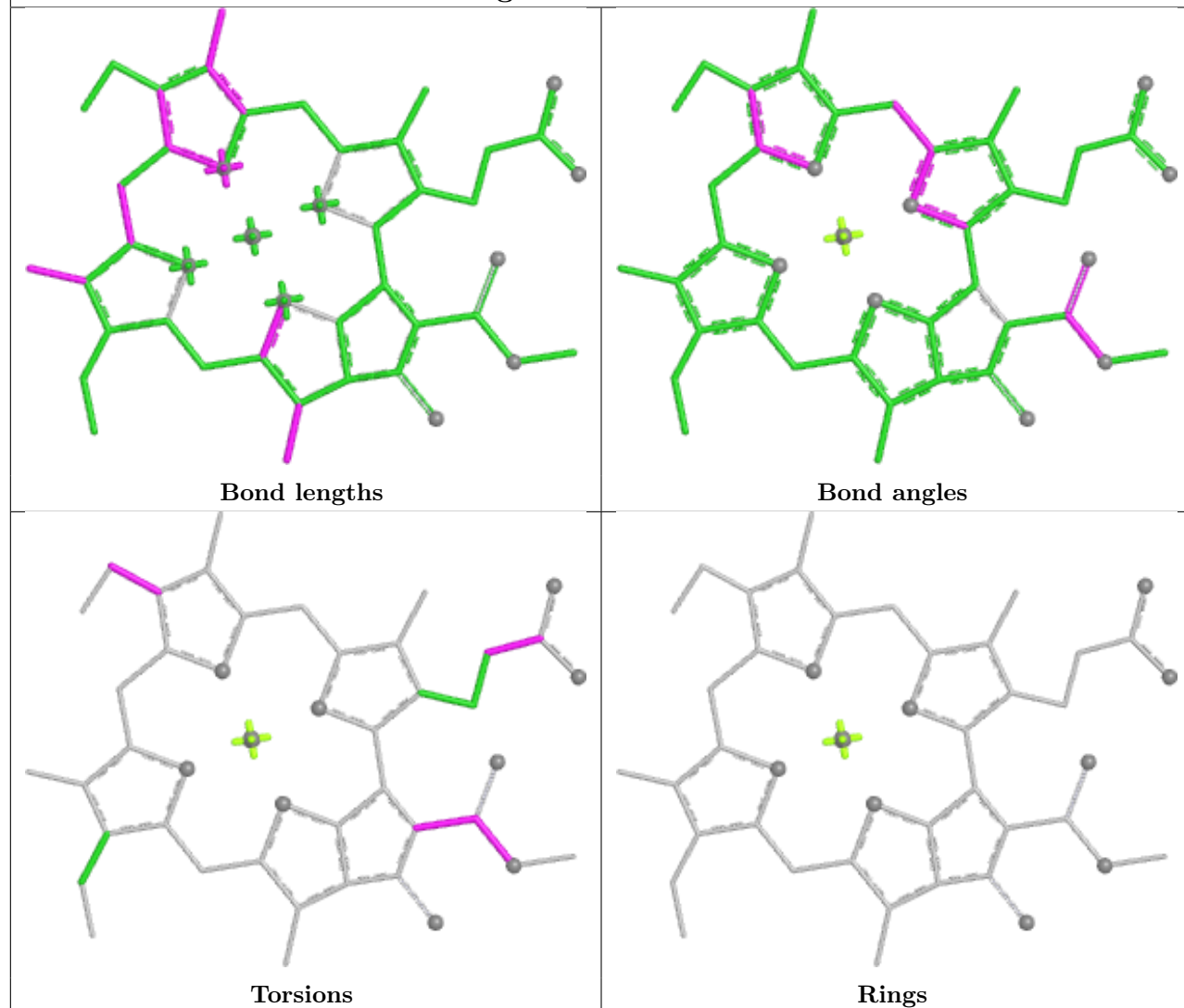
Ligand CLA 8 314



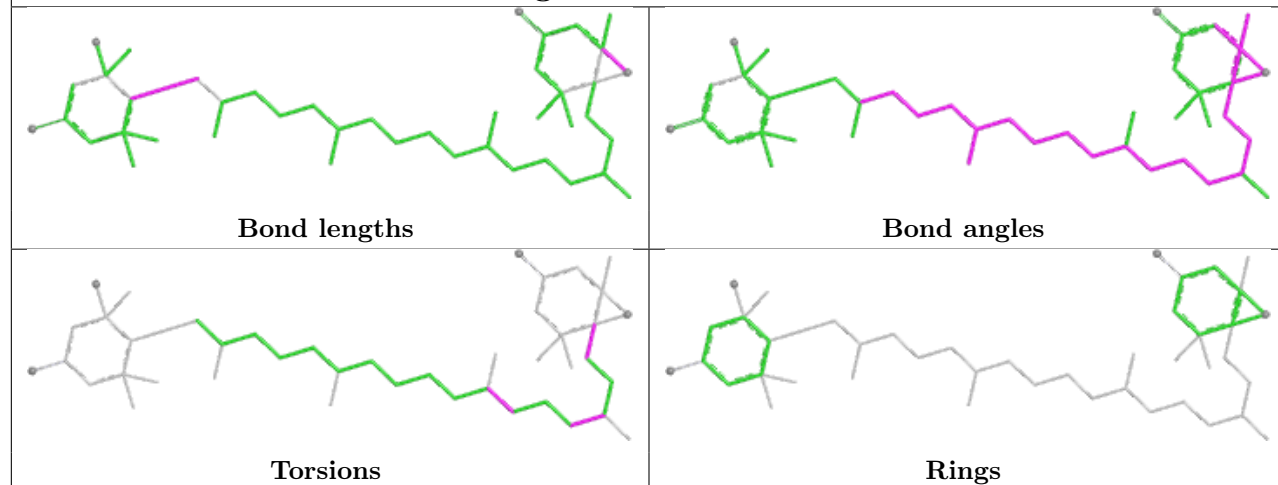
Ligand 8CT x 601

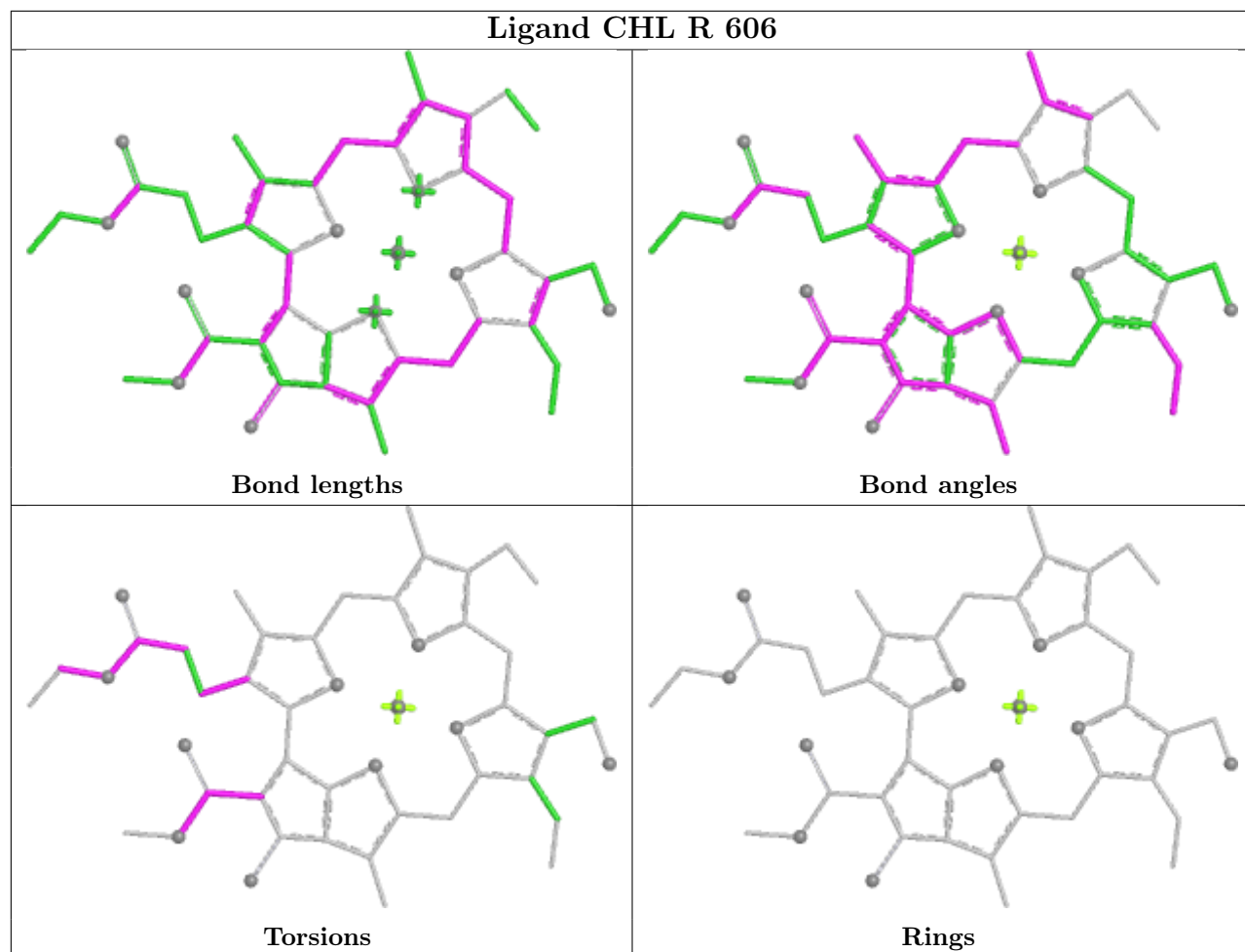


Ligand CLA 6 315

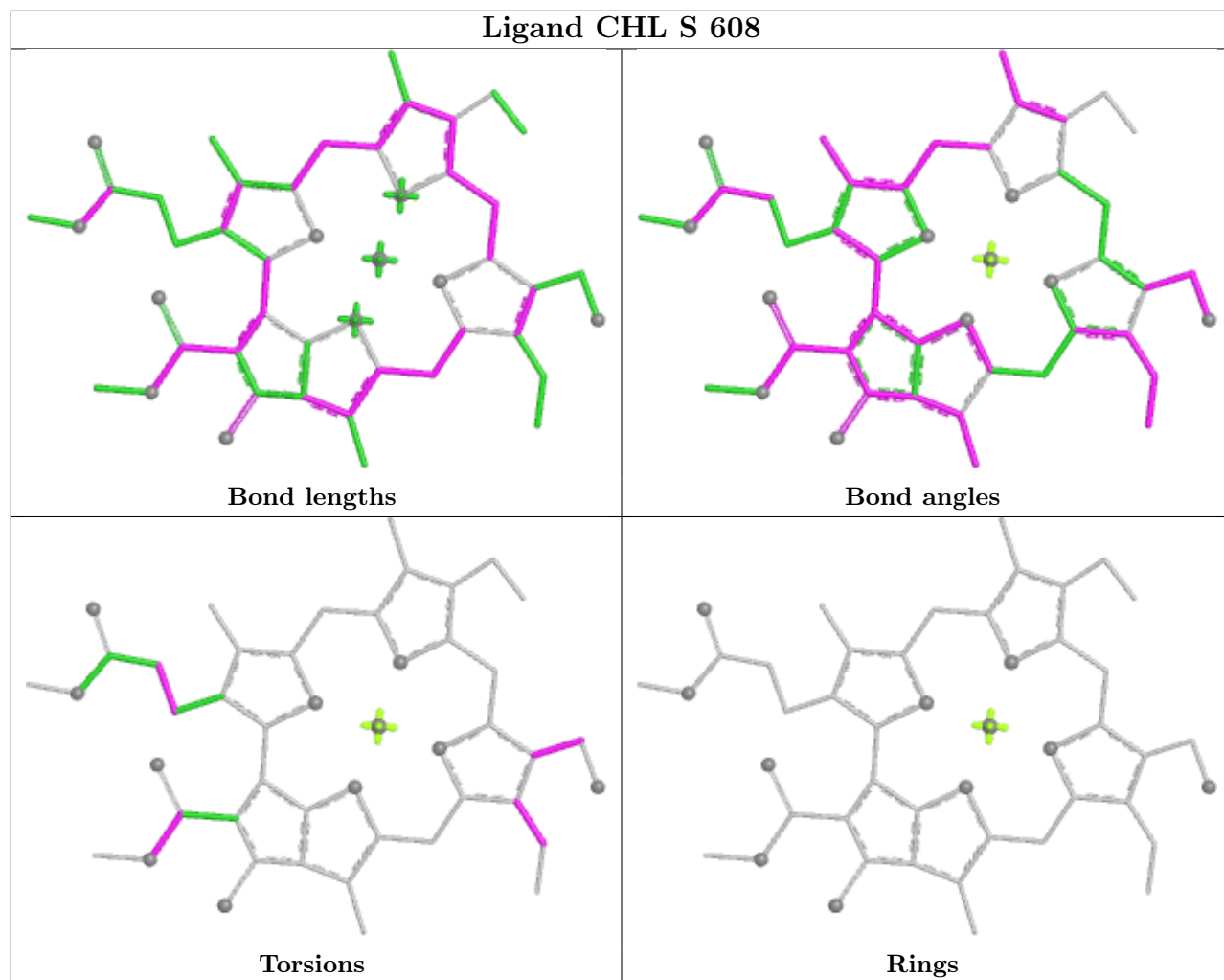


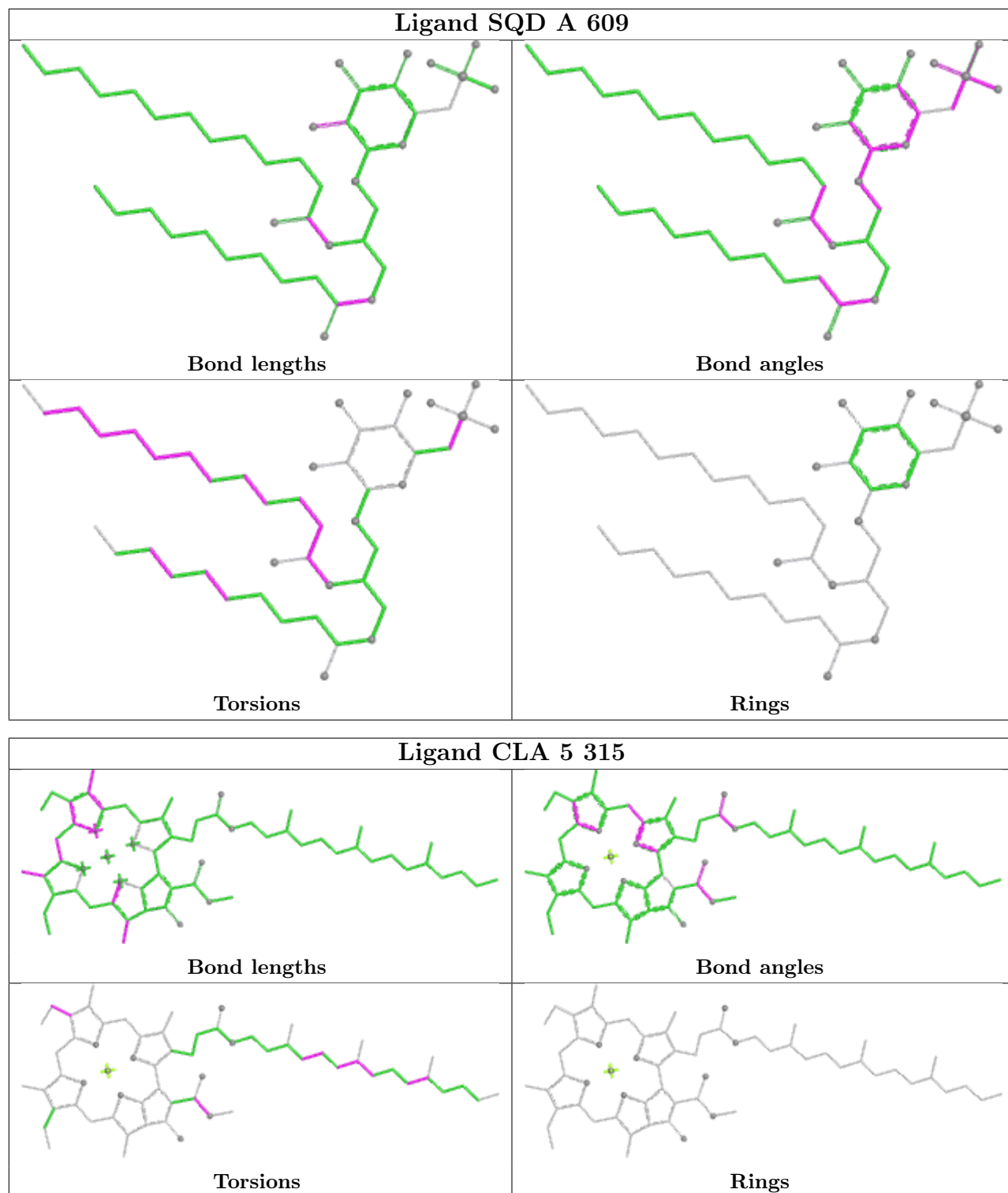
Ligand NEX 7 304

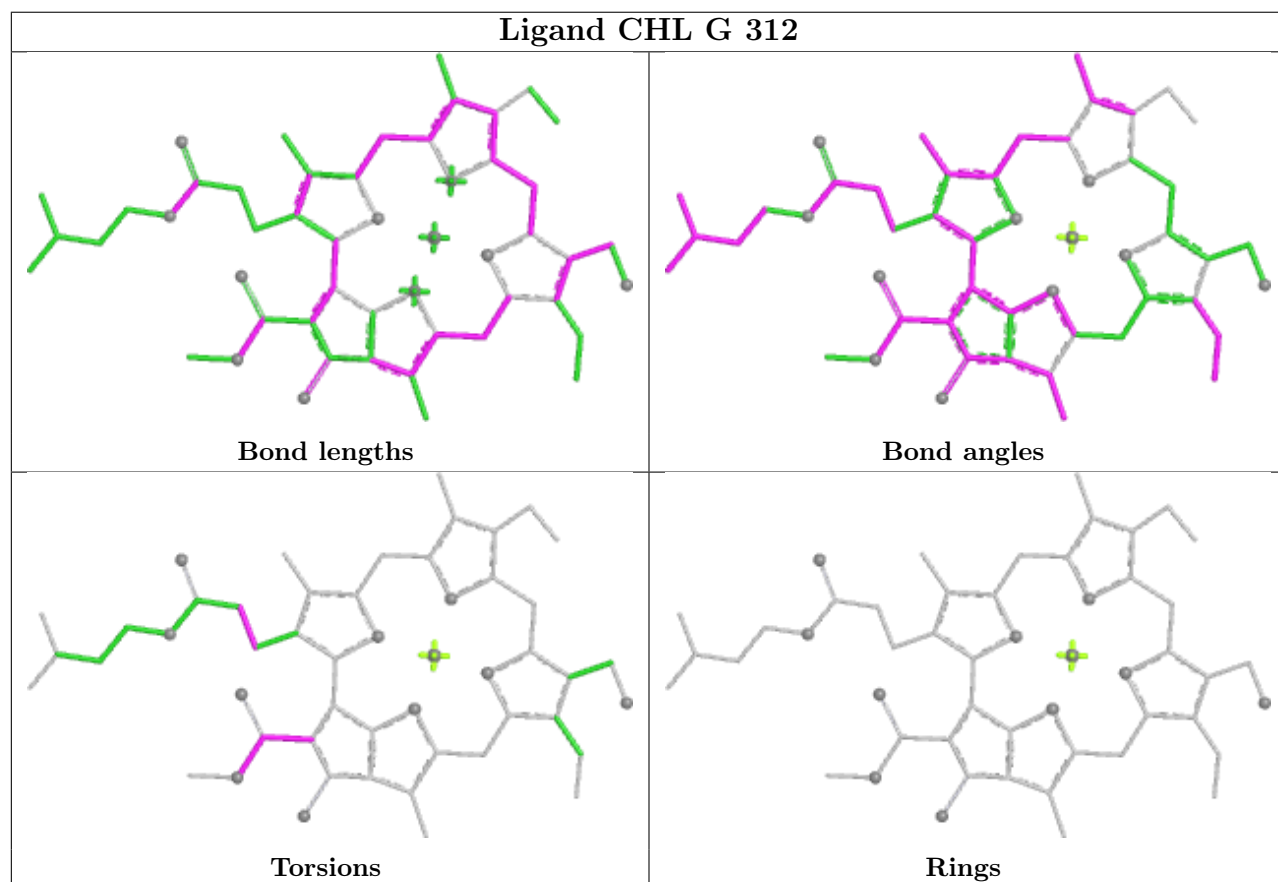
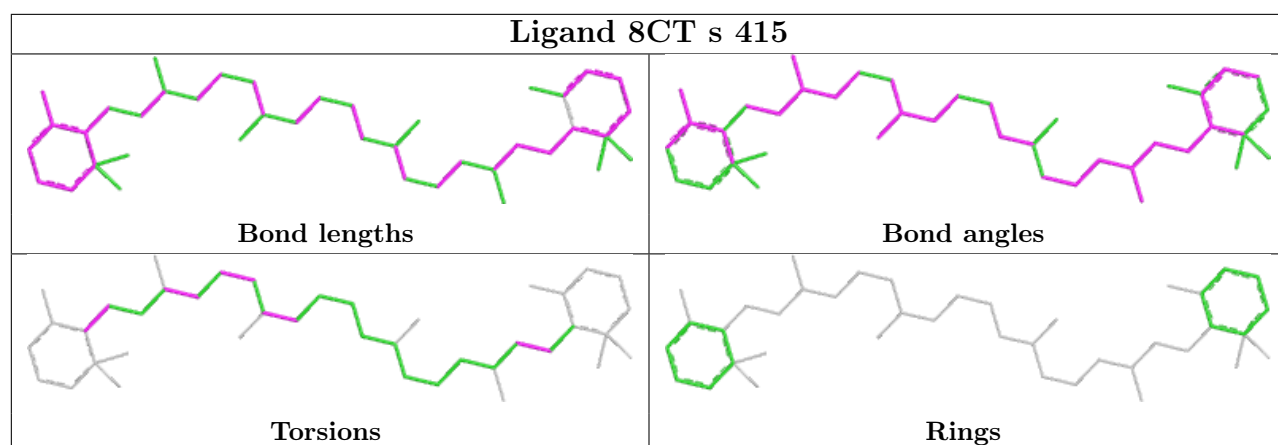




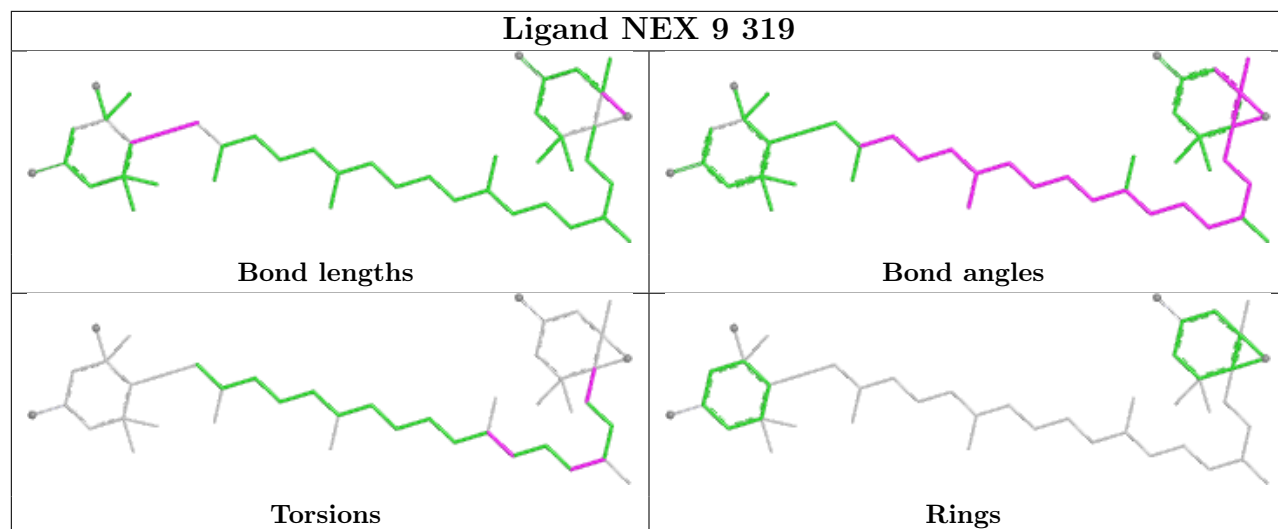
Ligand CHL S 608



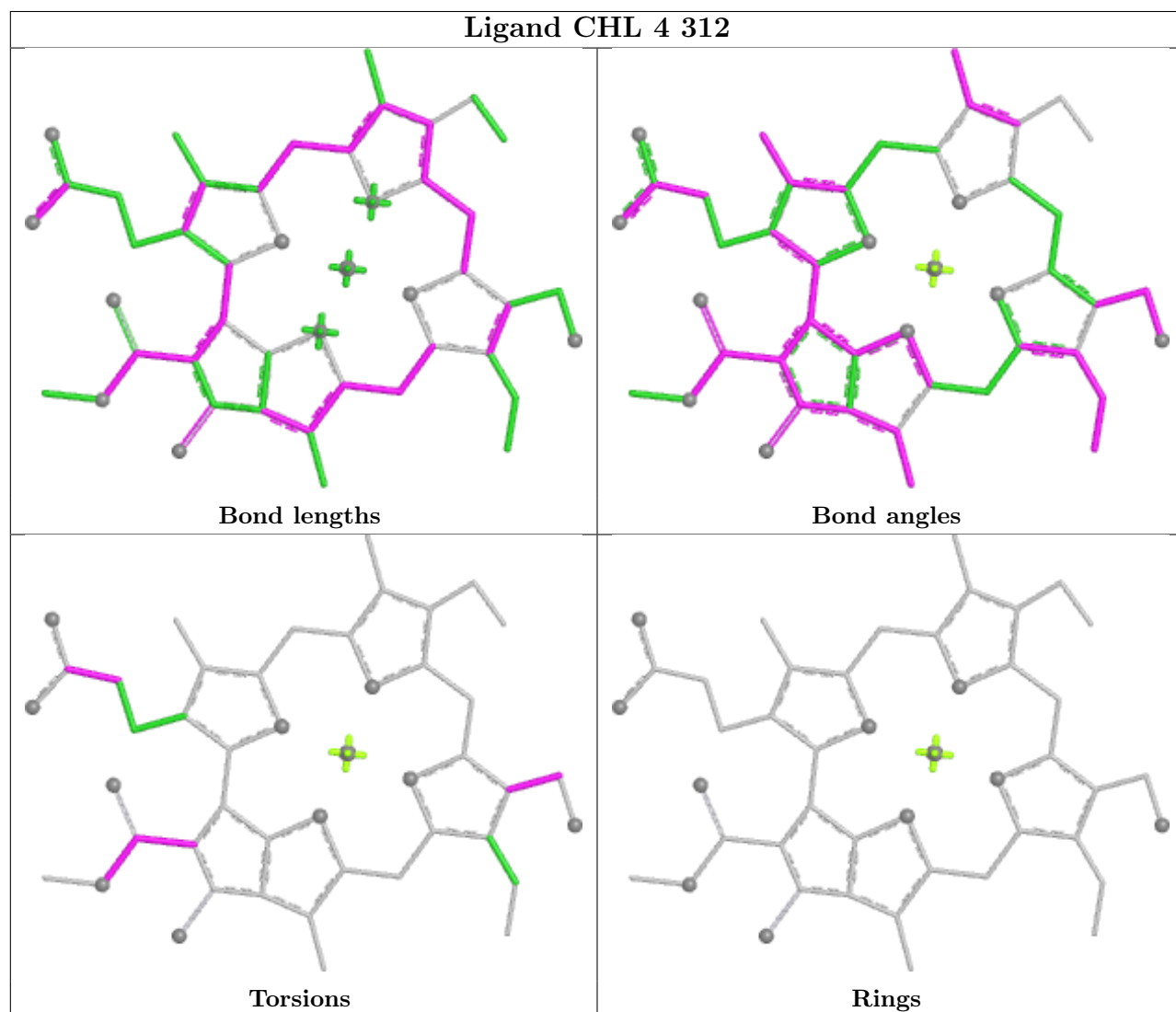




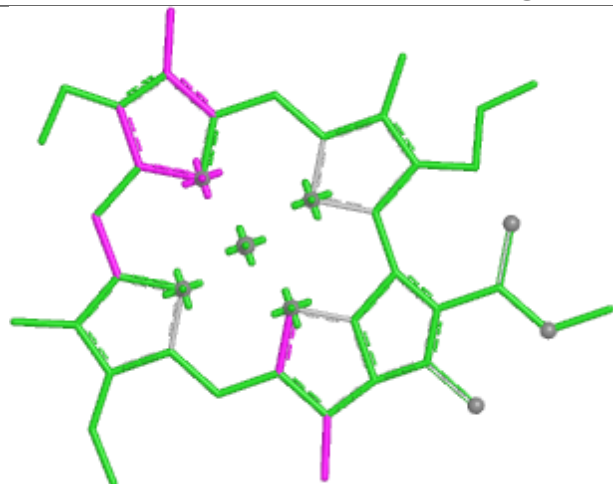
Ligand NEX 9 319



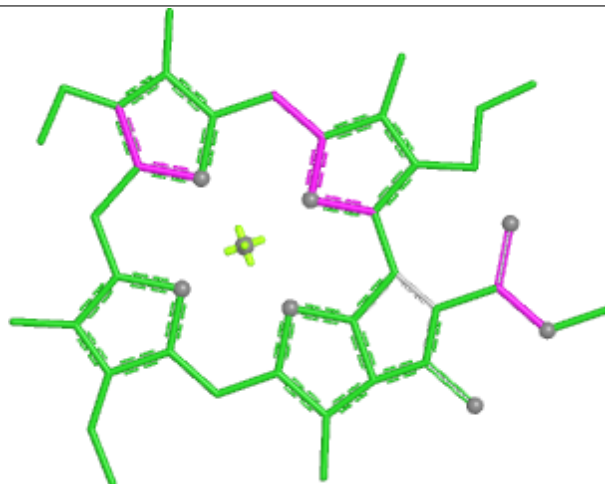
Ligand CHL 4 312



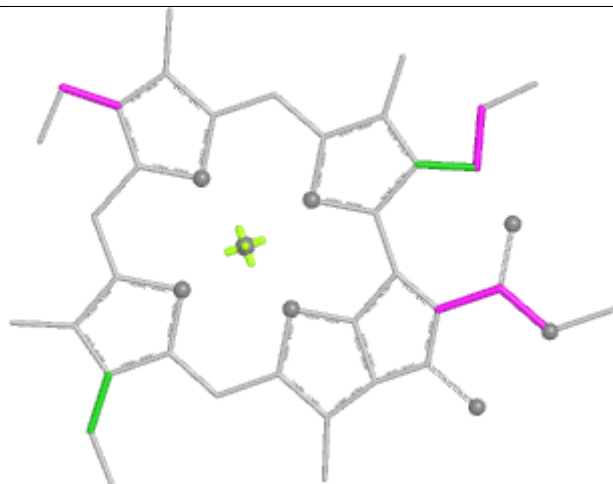
Ligand CLA 2 307



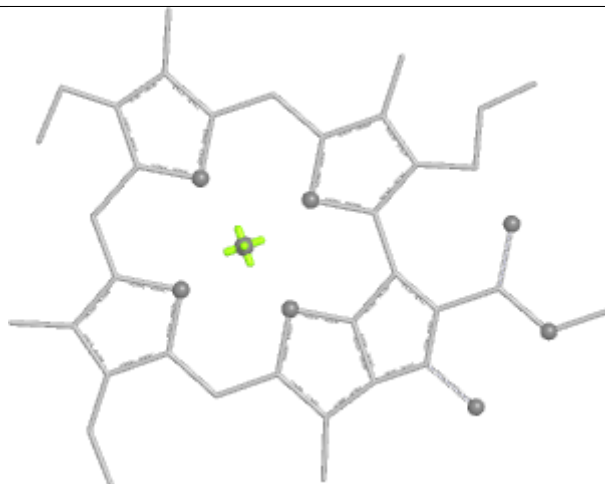
Bond lengths



Bond angles

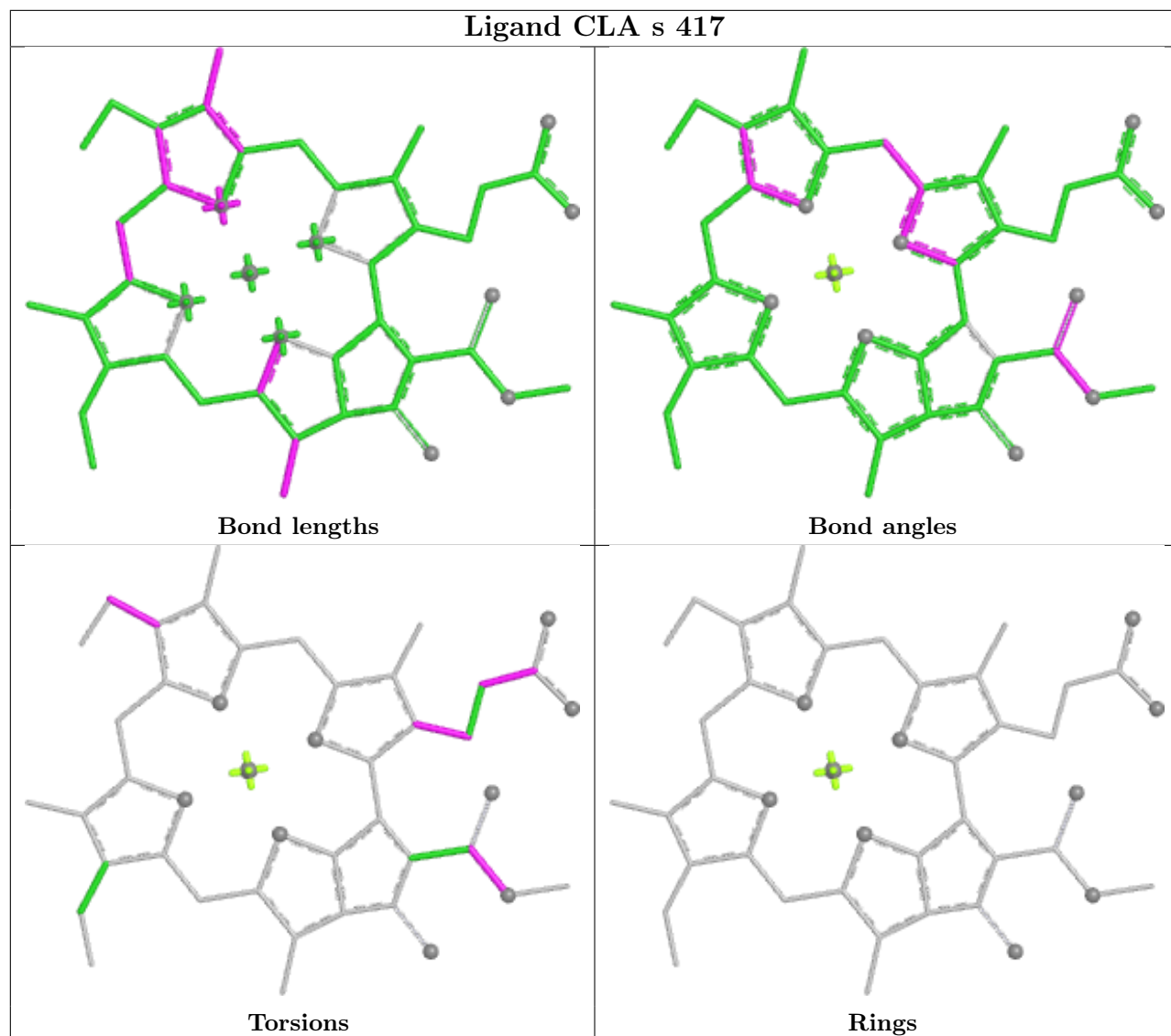


Torsions

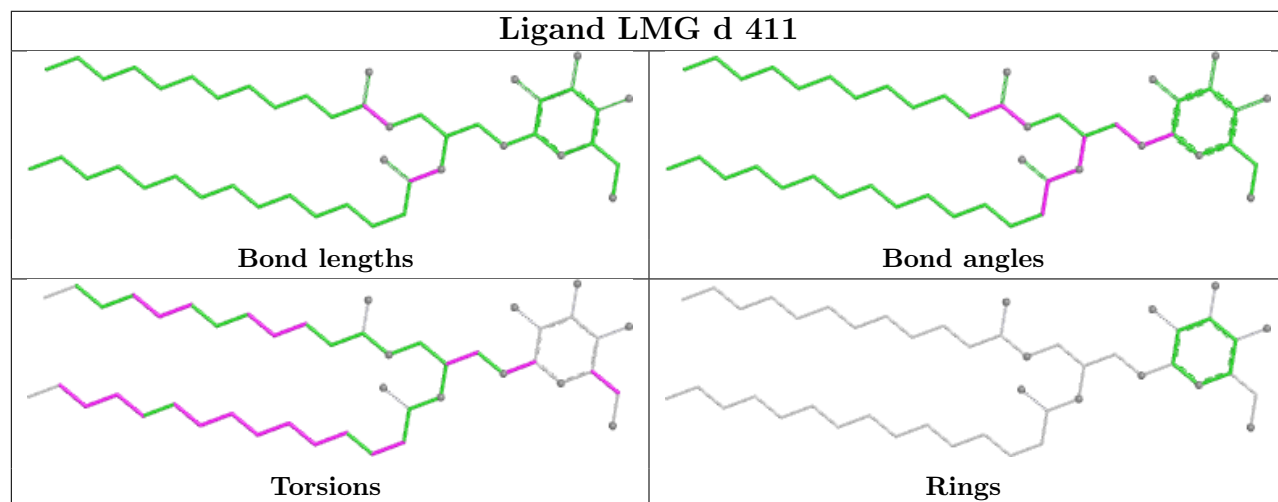


Rings

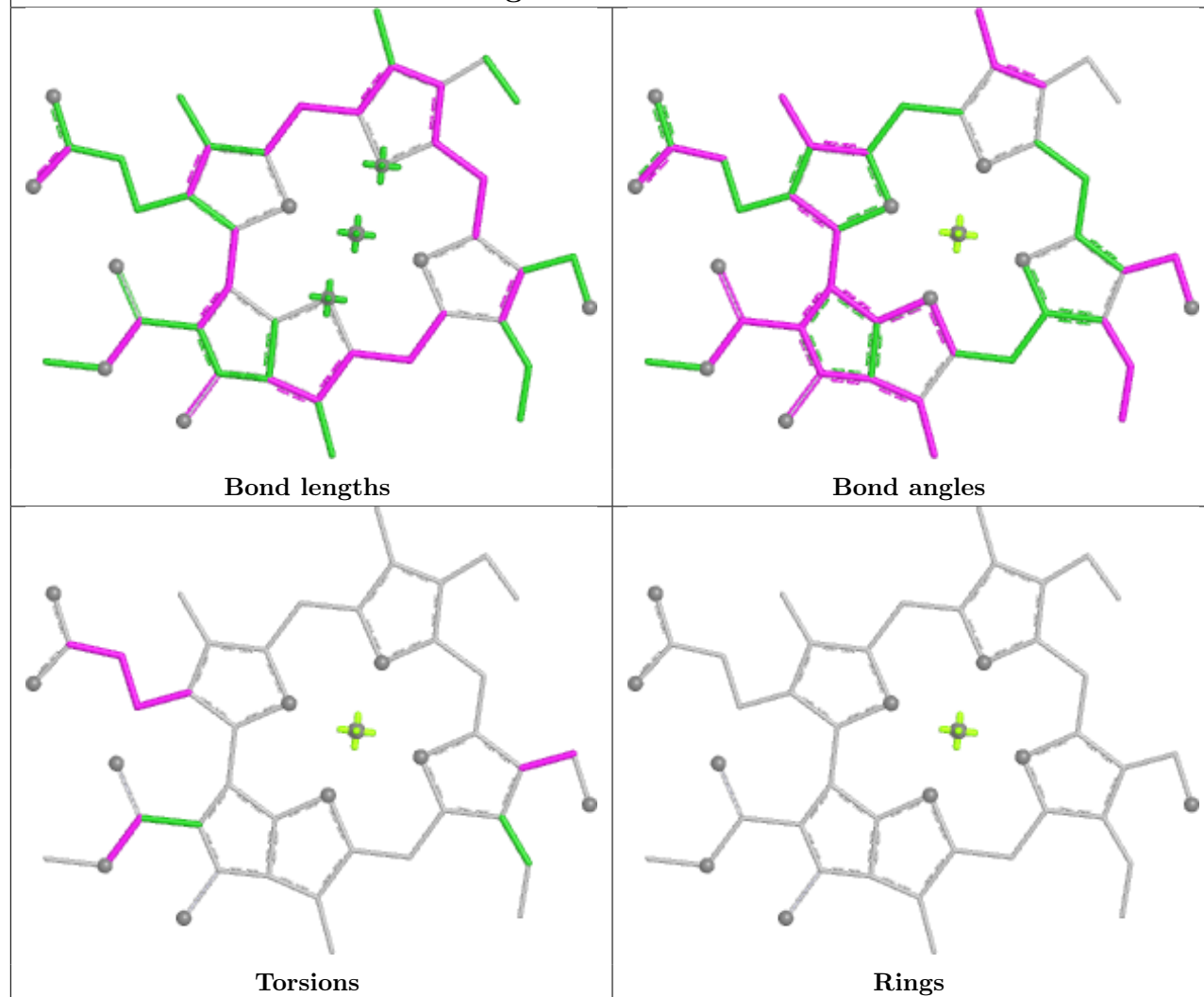
Ligand CLA s 417



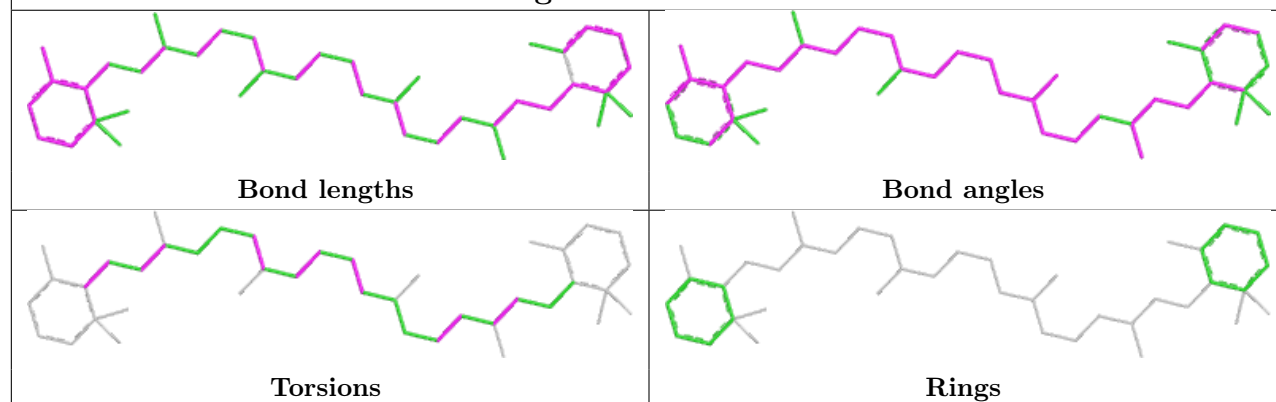
Ligand LMG d 411

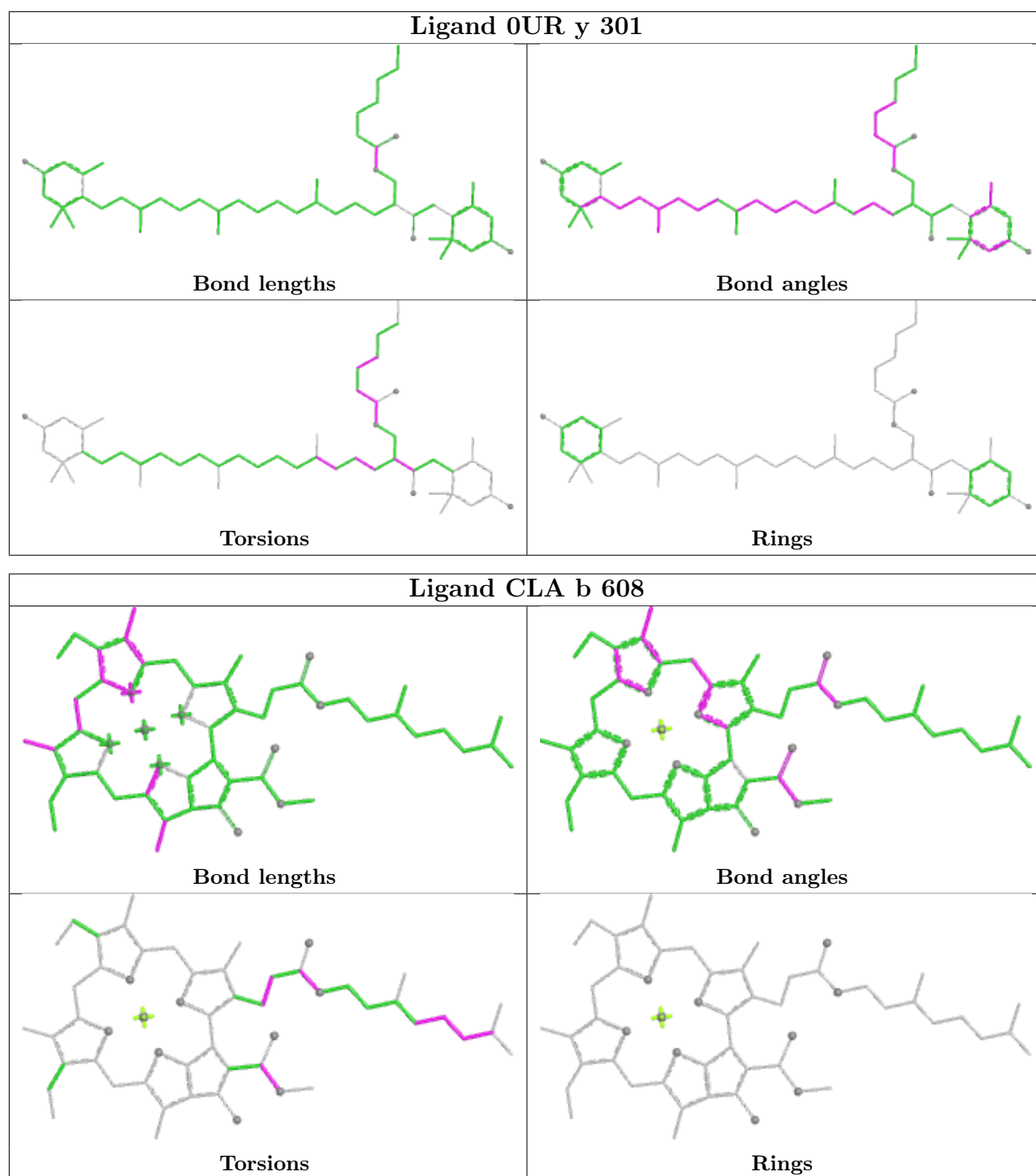


Ligand CHL 9 309



Ligand 8CT X 601





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

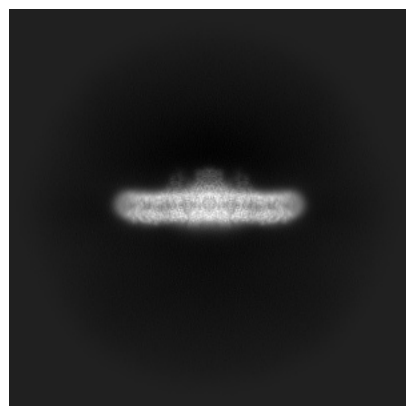
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62153. These allow visual inspection of the internal detail of the map and identification of artifacts.

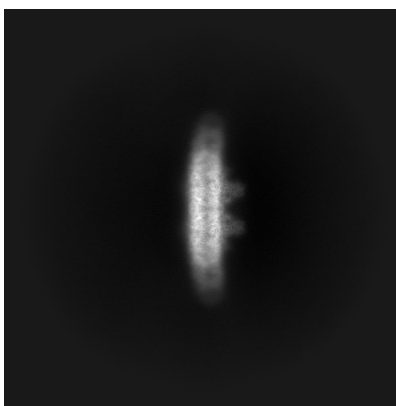
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

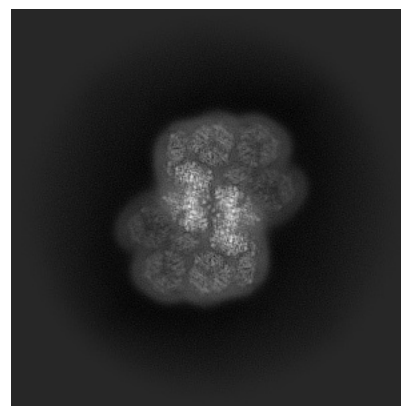
6.1.1 Primary map



X

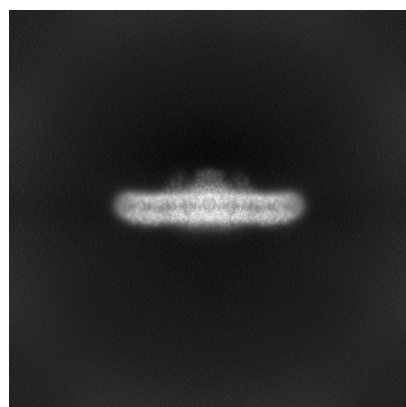


Y

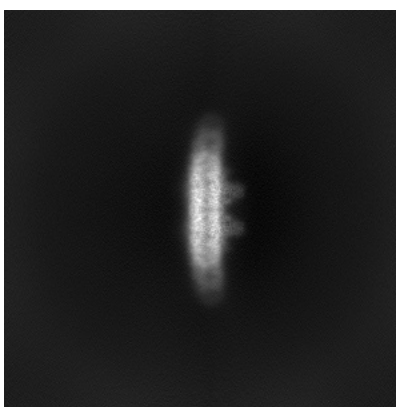


Z

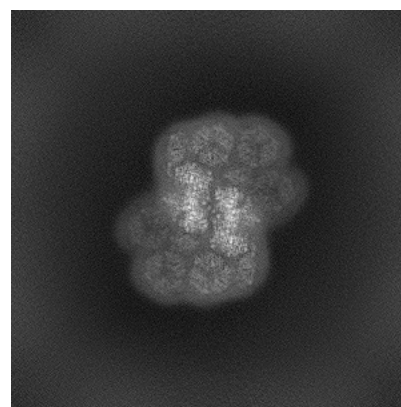
6.1.2 Raw map



X



Y

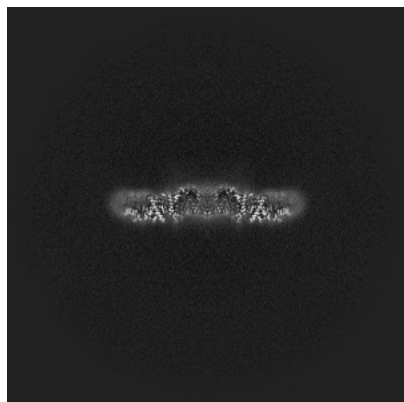


Z

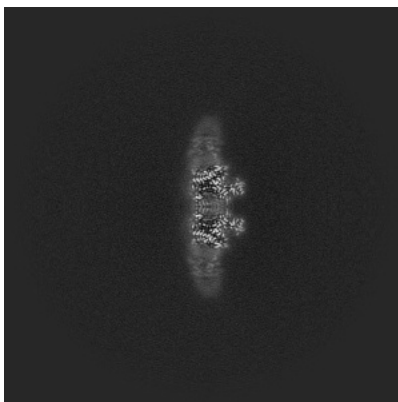
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

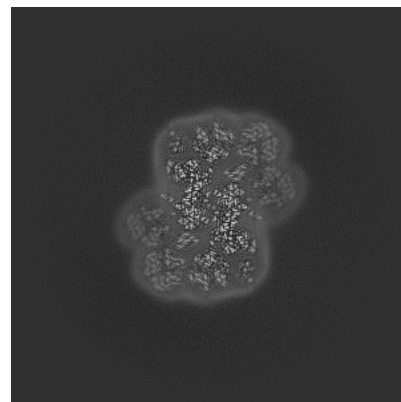
6.2.1 Primary map



X Index: 300

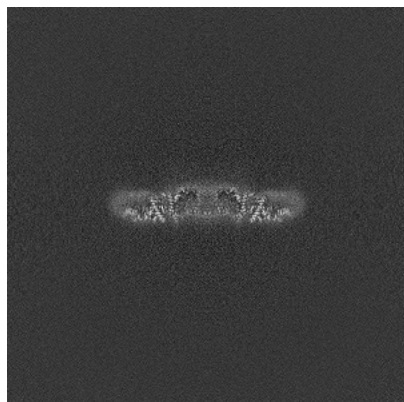


Y Index: 300

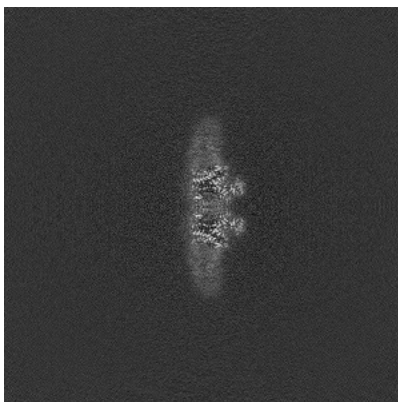


Z Index: 300

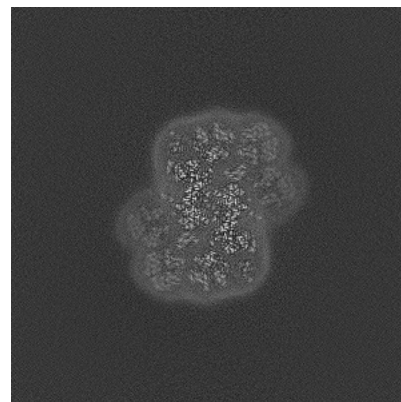
6.2.2 Raw map



X Index: 300



Y Index: 300

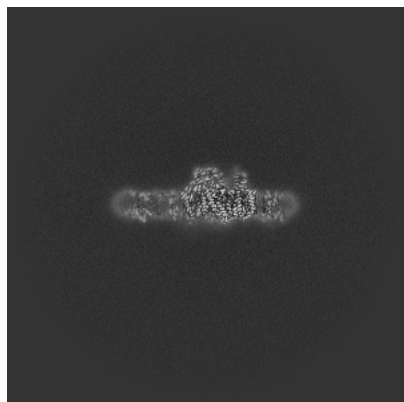


Z Index: 300

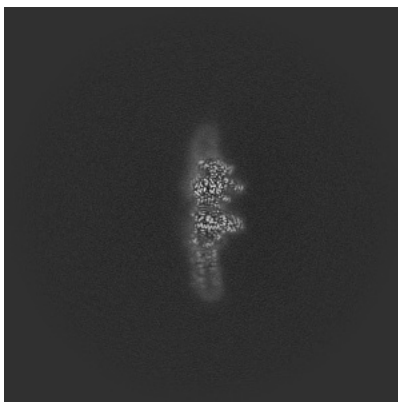
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

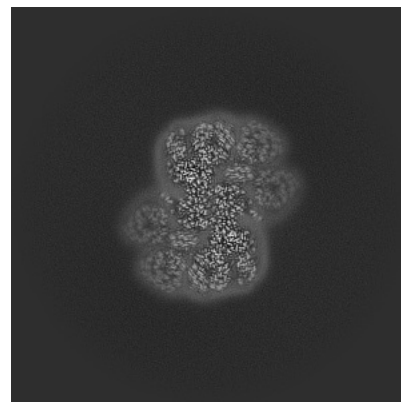
6.3.1 Primary map



X Index: 273

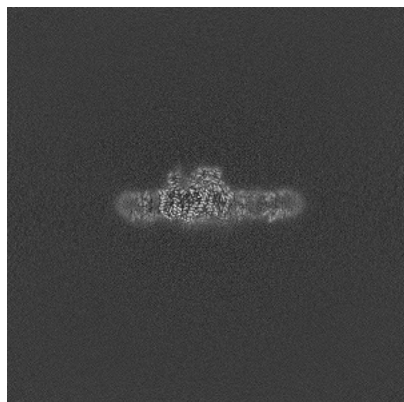


Y Index: 288

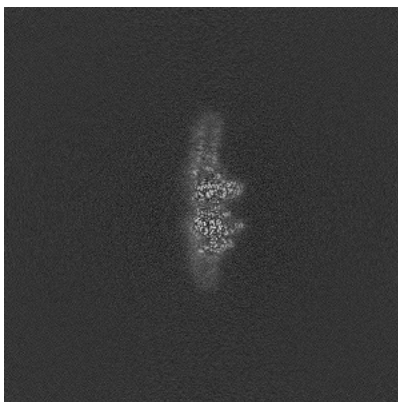


Z Index: 293

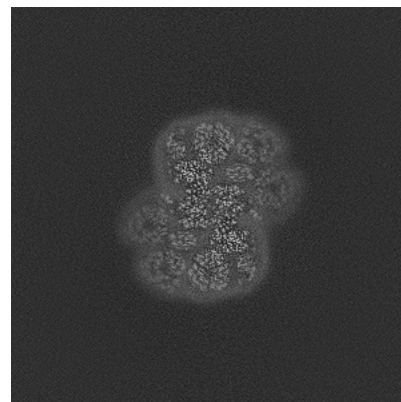
6.3.2 Raw map



X Index: 327



Y Index: 312

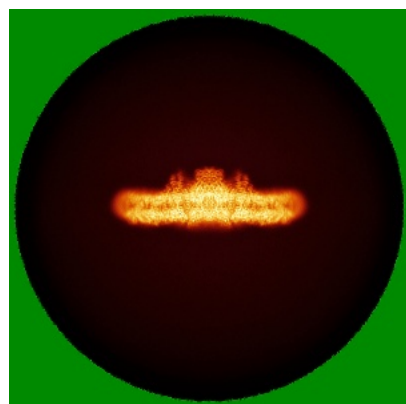


Z Index: 294

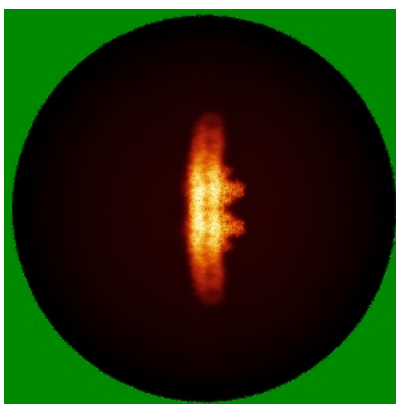
The images above show the largest variance slices of the map in three orthogonal directions.

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

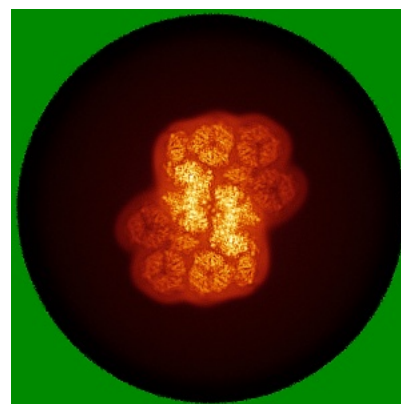
6.4.1 Primary map



X

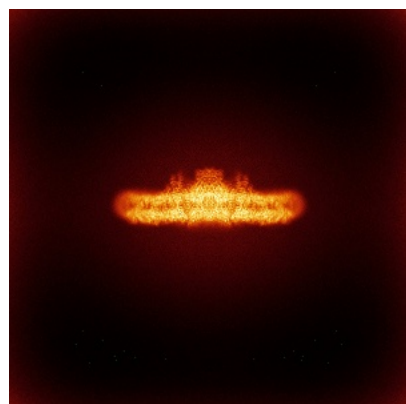


Y

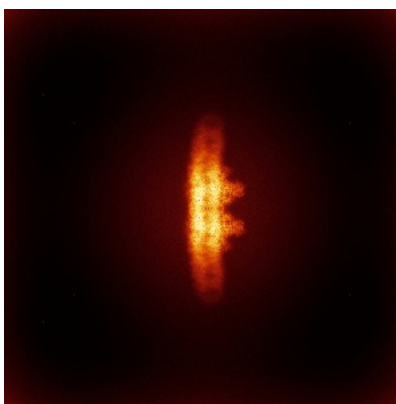


Z

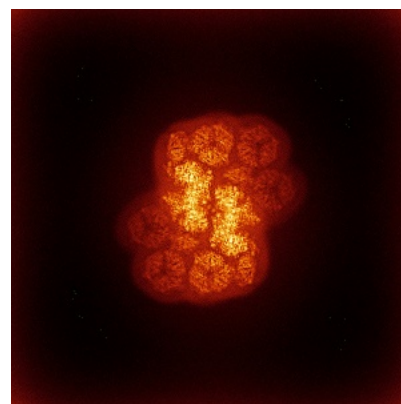
6.4.2 Raw map



X



Y

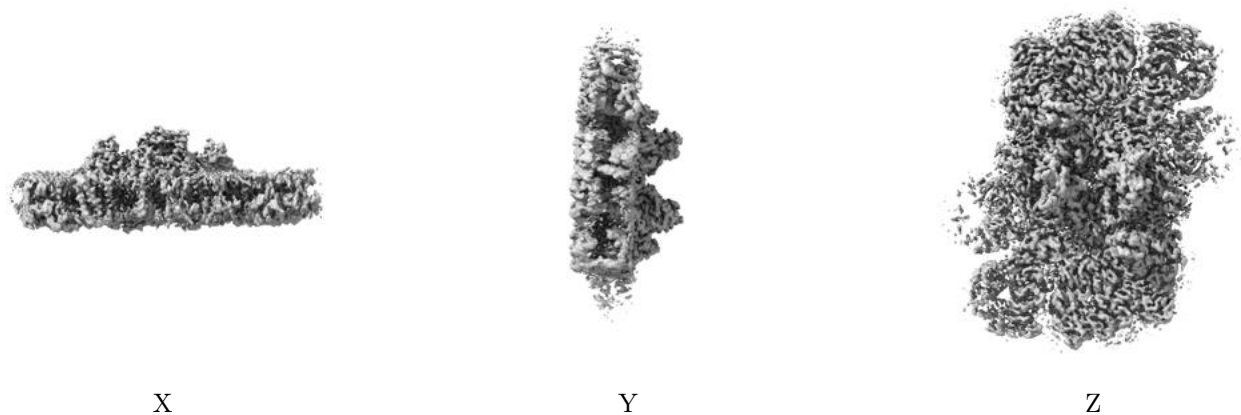


Z

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.

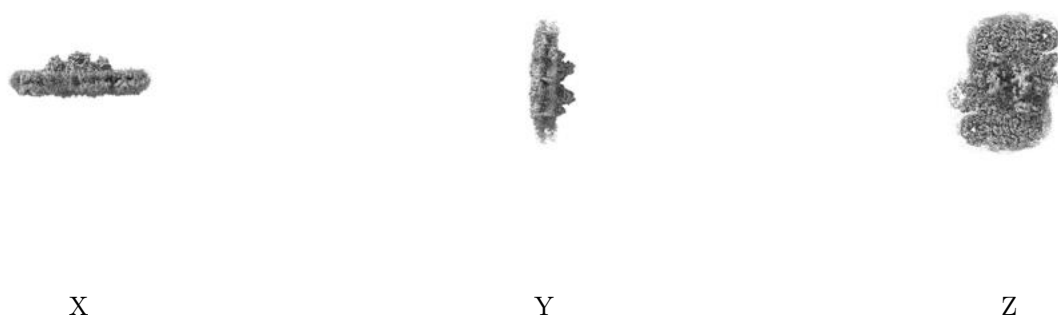
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.204. 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.

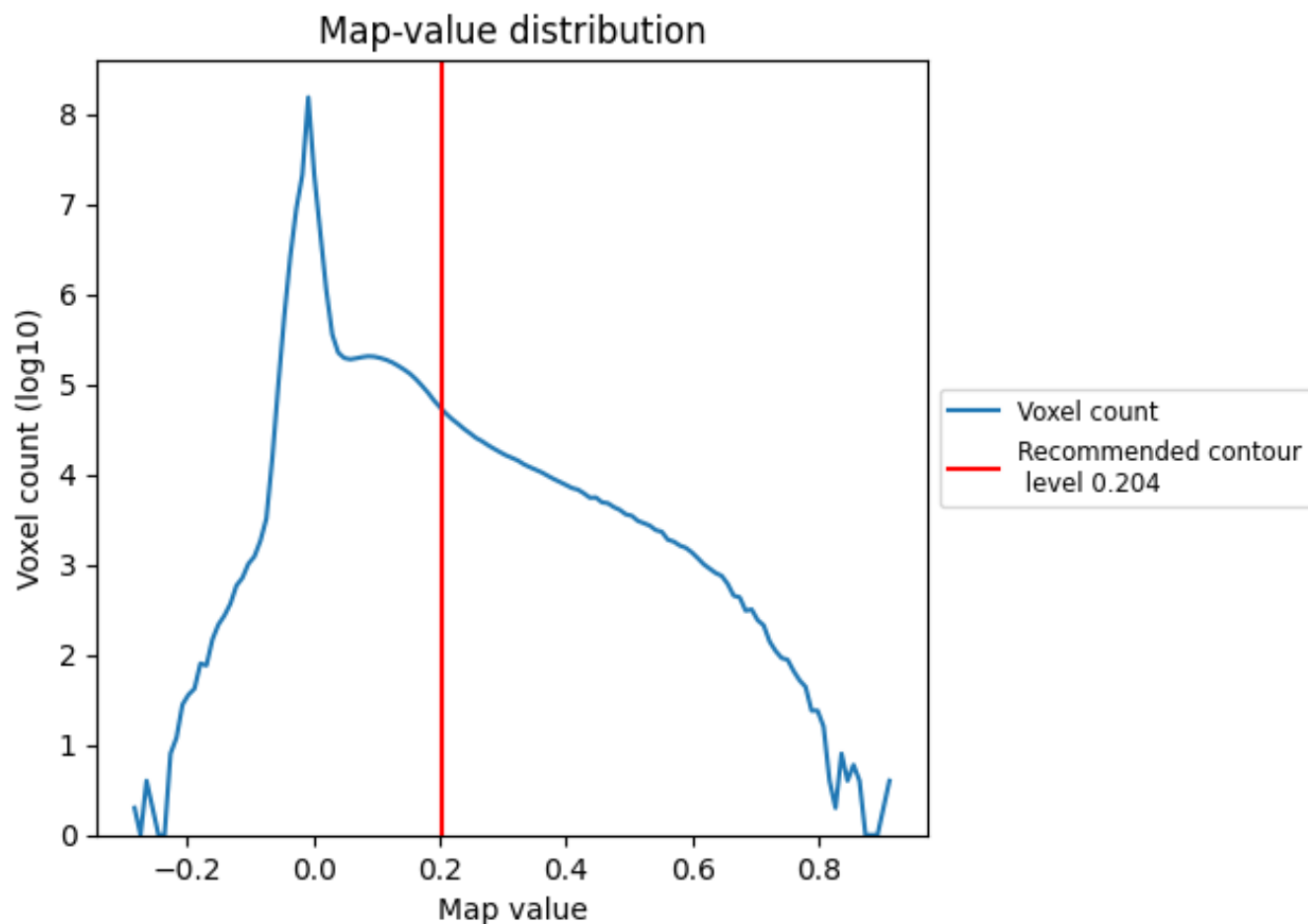
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

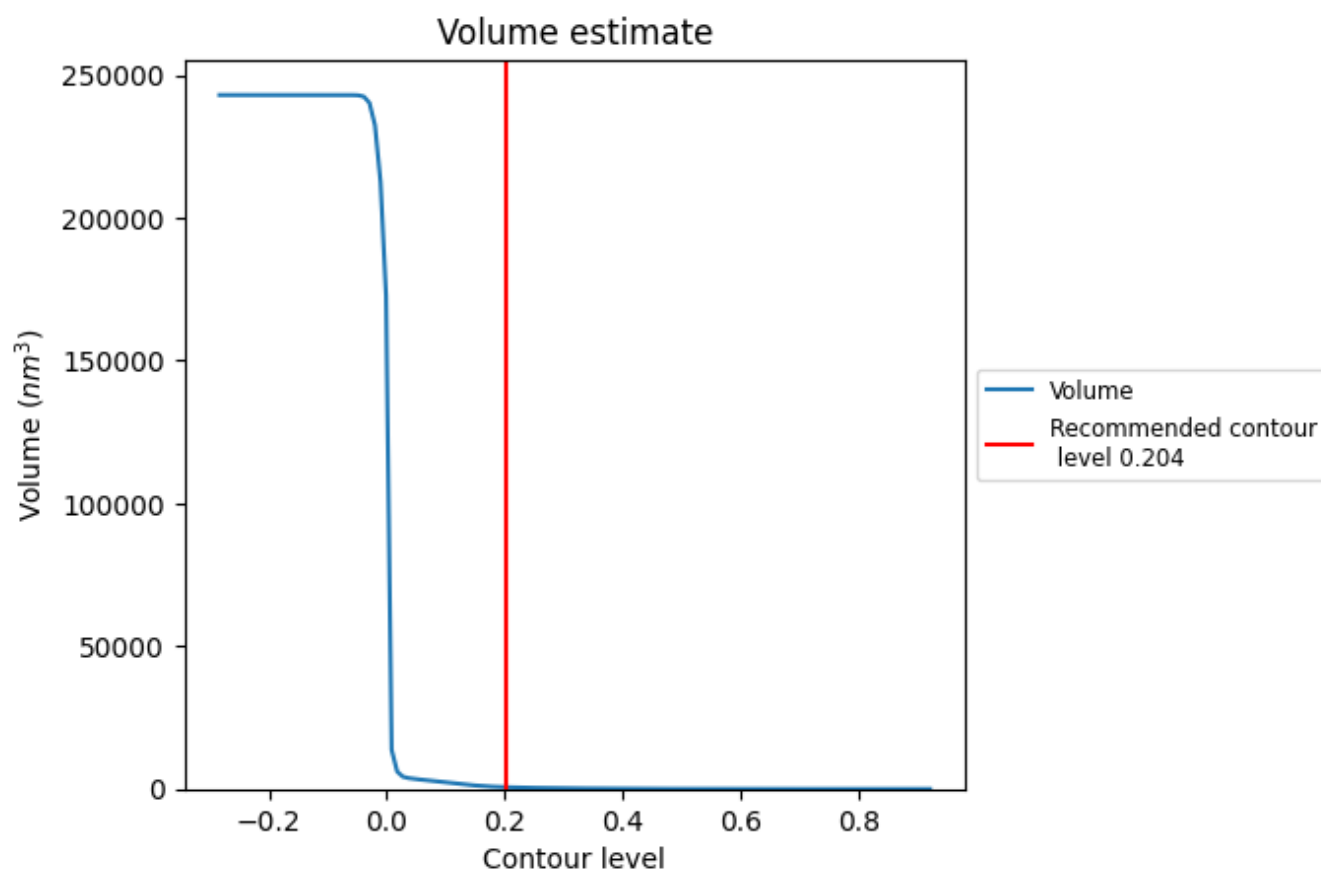
This section contains the results of statistical analysis of the map.

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.

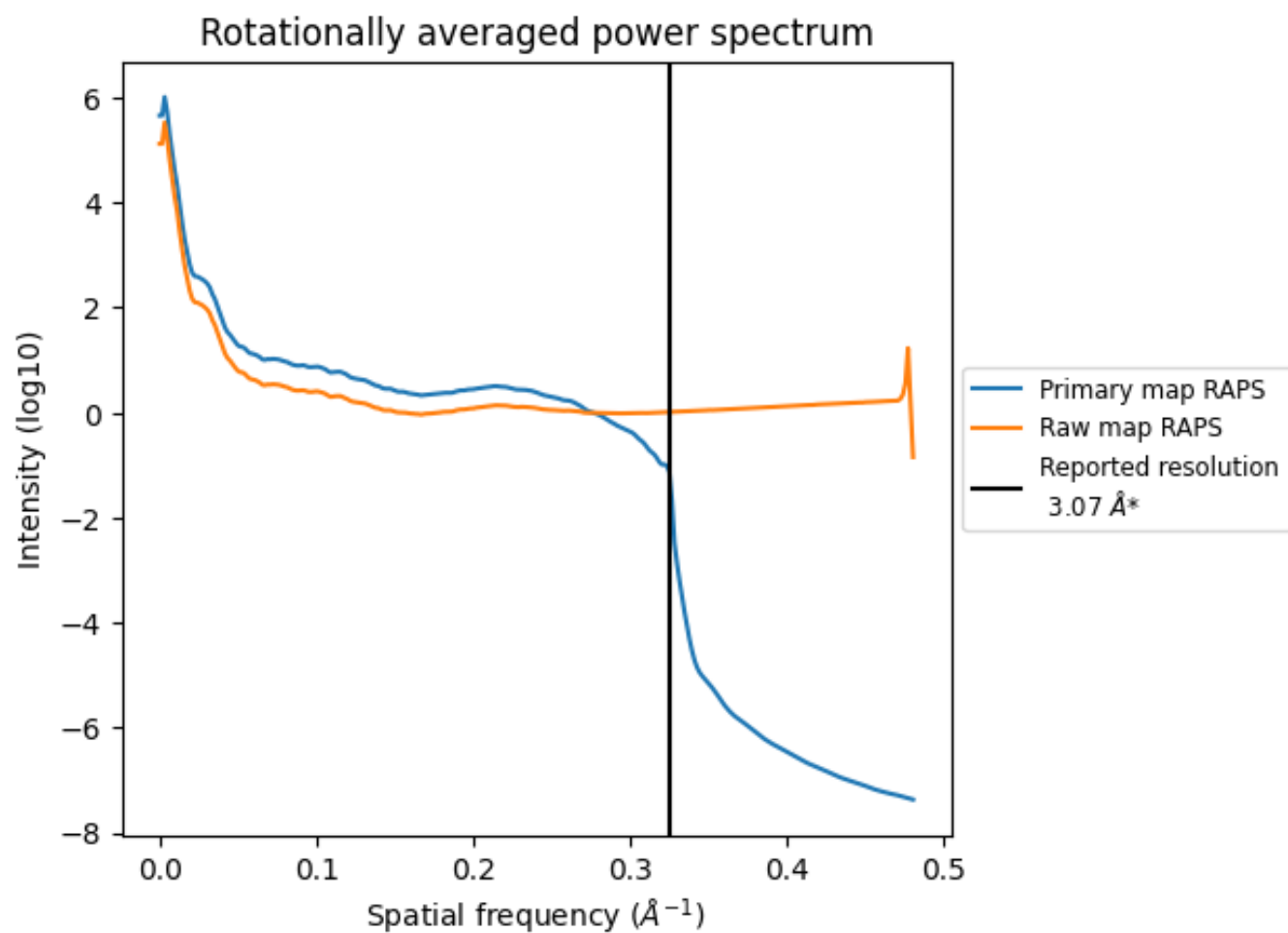
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 606 nm^3 ; this corresponds to an approximate mass of 548 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 ⓘ

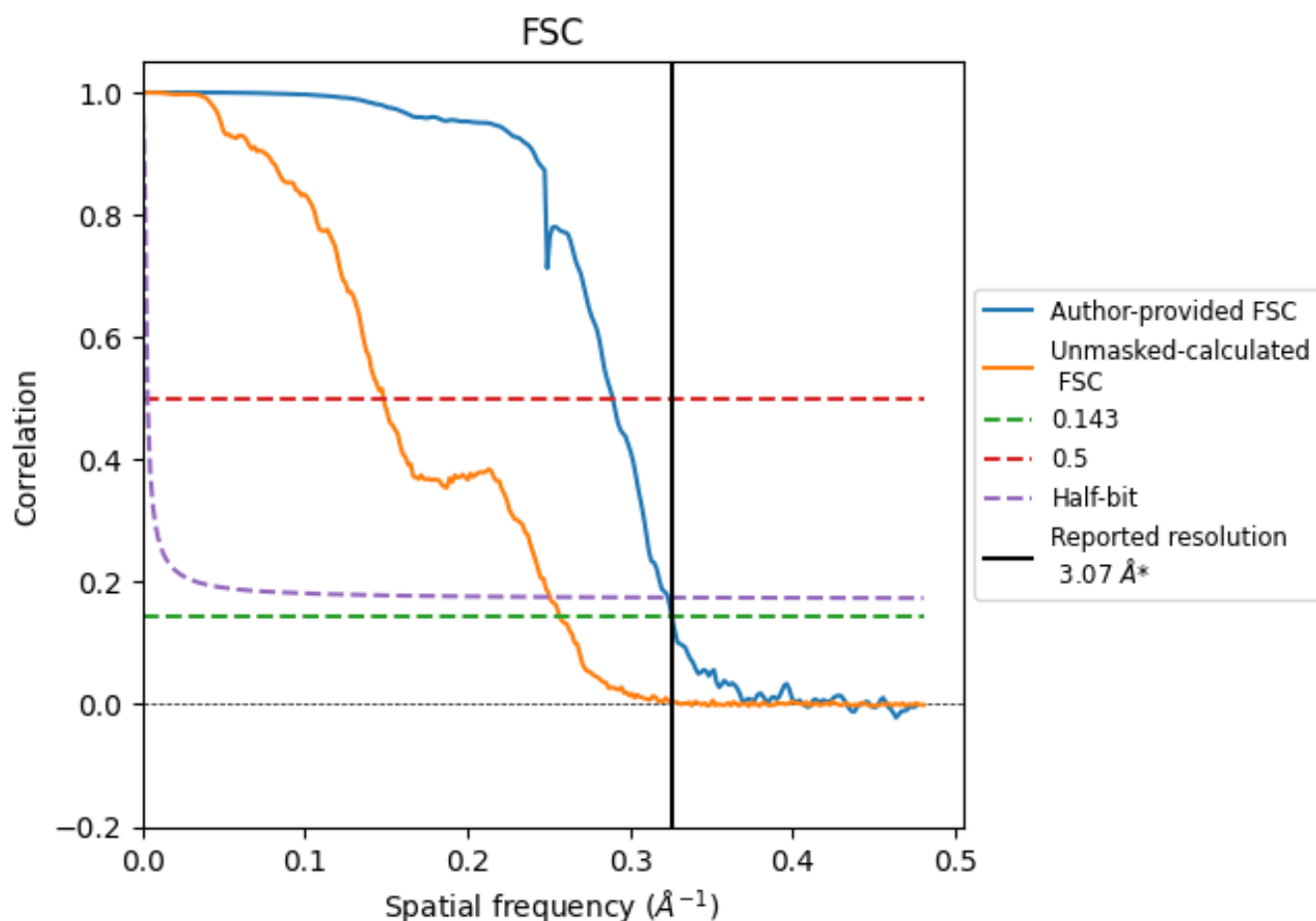


*Reported resolution corresponds to spatial frequency of 0.326 Å⁻¹

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 0.326 \AA^{-1}

8.2 Resolution estimates [i](#)

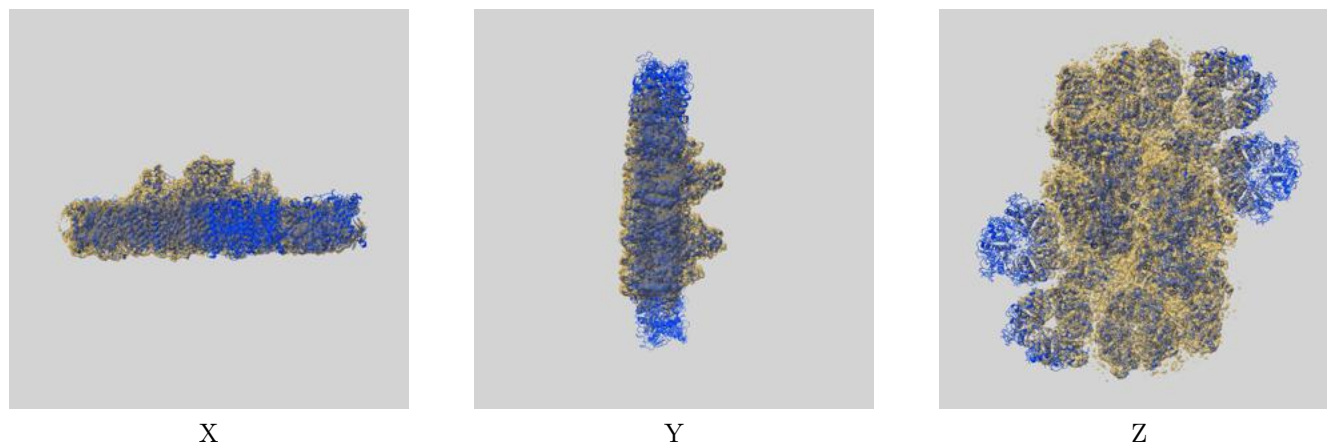
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.07	-	-
Author-provided FSC curve	3.07	3.45	3.09
Unmasked-calculated*	3.89	6.74	3.99

*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 3.89 differs from the reported value 3.07 by more than 10 %

9 Map-model fit [i](#)

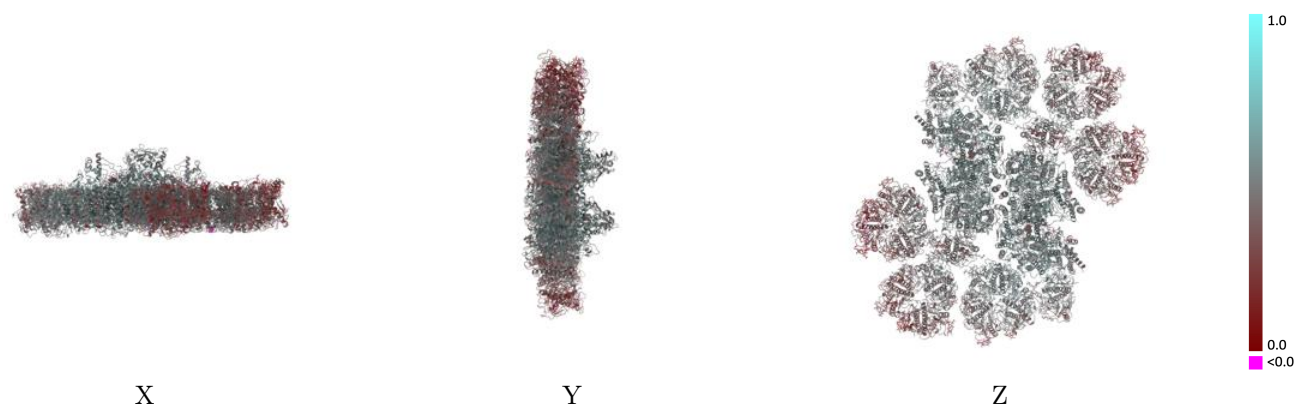
This section contains information regarding the fit between EMDB map EMD-62153 and PDB model 9K7V. Per-residue inclusion information can be found in [section 3](#) on [page 54](#).

9.1 Map-model overlay [i](#)



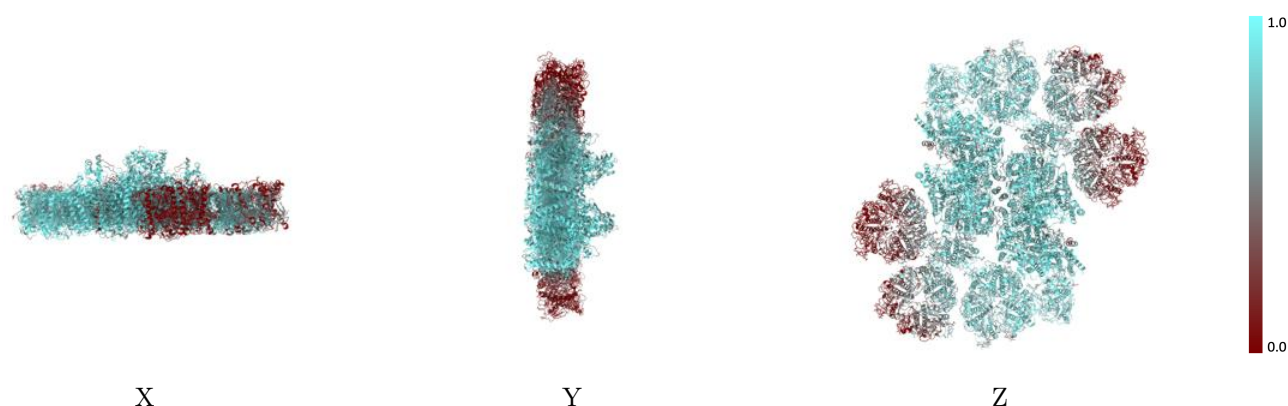
The images above show the 3D surface view of the map at the recommended contour level 0.204 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



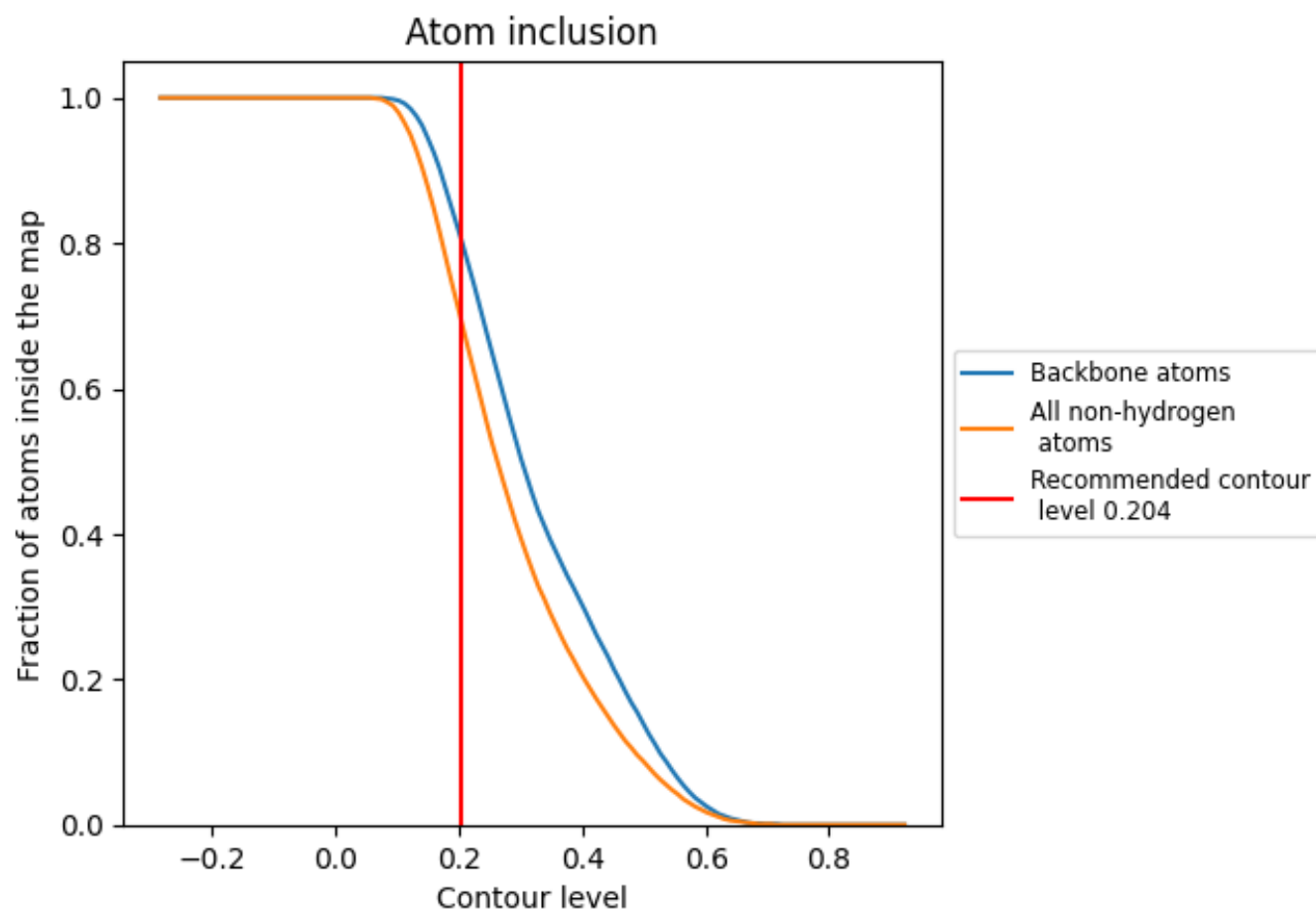
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.204).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 69% 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 (0.204) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6920	 0.4550
1	 0.3620	 0.3400
2	 0.6680	 0.4570
3	 0.3050	 0.3320
4	 0.3660	 0.3380
5	 0.6660	 0.4580
6	 0.3020	 0.3250
7	 0.7880	 0.4340
8	 0.8580	 0.4730
9	 0.0130	 0.2470
A	 0.9160	 0.5370
B	 0.9140	 0.5310
C	 0.9100	 0.5370
D	 0.9260	 0.5490
E	 0.8090	 0.4670
F	 0.8670	 0.4710
G	 0.2460	 0.3830
H	 0.8510	 0.5070
I	 0.9600	 0.5430
K	 0.9220	 0.5170
L	 0.9060	 0.5290
M	 0.7130	 0.4500
N	 0.3140	 0.3920
R	 0.7010	 0.4140
S	 0.8320	 0.4570
T	 0.8600	 0.5220
V	 0.4290	 0.3920
W	 0.9000	 0.5010
X	 0.8040	 0.4860
Y	 0.9010	 0.5210
Z	 0.8080	 0.4380
a	 0.9160	 0.5370
b	 0.9140	 0.5320
c	 0.9080	 0.5350
d	 0.9240	 0.5490



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Chain	Atom inclusion	Q-score
e	 0.8140	 0.4640
f	 0.8530	 0.4640
g	 0.2490	 0.3850
h	 0.8430	 0.5070
i	 0.9500	 0.5570
k	 0.9290	 0.5150
l	 0.9100	 0.5340
m	 0.7310	 0.4650
n	 0.3180	 0.3910
p	 0.7870	 0.4340
q	 0.8550	 0.4720
r	 0.7020	 0.4130
s	 0.8340	 0.4560
t	 0.8640	 0.5190
u	 0.0150	 0.2460
v	 0.4470	 0.3850
w	 0.8840	 0.4930
x	 0.7970	 0.4900
y	 0.8990	 0.5210
z	 0.8080	 0.4370