



Full wwPDB EM Validation Report ⓘ

Apr 6, 2026 – 01:23 AM UTC

PDB ID : 9V7T / pdb_00009v7t
EMDB ID : EMD-64823
Title : PSI-LHCE supercomplex from Euglena gracilis.
Authors : Bai, T.Y.; Mao, Z.Y.; Tian, L.R.
Deposited on : 2025-05-28
Resolution : 2.23 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:

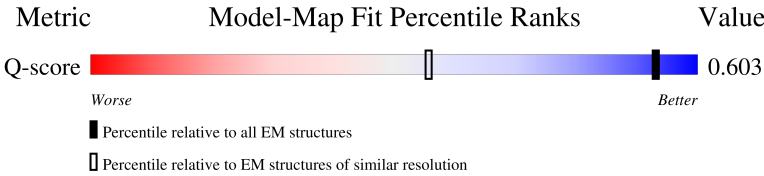
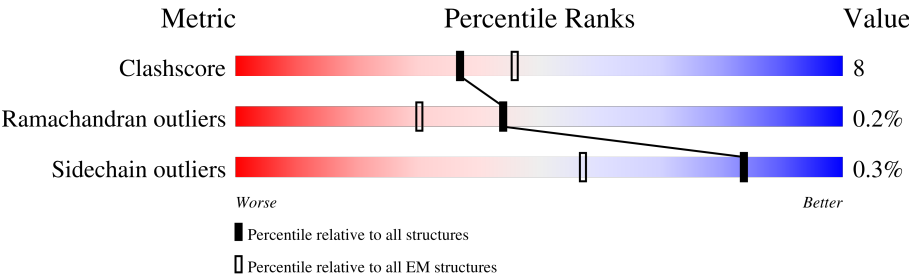
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.23 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	3335 (1.73 - 2.73)

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	A	751	
2	B	734	
3	C	81	
4	D	186	

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Mol	Chain	Length	Quality of chain
5	E	63	
6	F	168	
7	J	37	
8	M	31	
9	a	166	
10	b	169	
11	c	221	
12	d	220	
13	e	199	
14	h	174	
15	i	177	
16	j	183	
17	k	172	
18	l	167	
19	m	168	
20	f	174	
21	g	178	
22	n	184	
23	o	164	
24	p	148	

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
25	CLA	A	752	X	-	-	-
25	CLA	A	753	X	-	-	-
25	CLA	A	755	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	A	757	X	-	-	-
25	CLA	A	758	X	-	-	-
25	CLA	A	759	X	-	-	-
25	CLA	A	760	X	-	-	-
25	CLA	A	761	X	-	-	-
25	CLA	A	762	X	-	-	-
25	CLA	A	763	X	-	-	-
25	CLA	A	764	X	-	-	-
25	CLA	A	765	X	-	-	-
25	CLA	A	766	X	-	-	-
25	CLA	A	767	X	-	-	-
25	CLA	A	768	X	-	-	-
25	CLA	A	769	X	-	-	-
25	CLA	A	770	X	-	-	-
25	CLA	A	771	X	-	-	-
25	CLA	A	772	X	-	-	-
25	CLA	A	773	X	-	-	-
25	CLA	A	774	X	-	-	-
25	CLA	A	775	X	-	-	-
25	CLA	A	776	X	-	-	-
25	CLA	A	777	X	-	-	-
25	CLA	A	778	X	-	-	-
25	CLA	A	779	X	-	-	-
25	CLA	A	780	X	-	-	-
25	CLA	A	781	X	-	-	-
25	CLA	A	782	X	-	-	-
25	CLA	A	783	X	-	-	-
25	CLA	A	784	X	-	-	-
25	CLA	A	791	X	-	-	-
25	CLA	A	793	X	-	-	-
25	CLA	A	794	X	-	-	-
25	CLA	A	797	X	-	-	-
25	CLA	A	798	X	-	-	-
25	CLA	A	799	X	-	-	-
25	CLA	A	800	X	-	-	-
25	CLA	A	801	X	-	-	-
25	CLA	A	802	X	-	-	-
25	CLA	A	803	X	-	-	-
25	CLA	A	804	X	-	-	-
25	CLA	A	805	X	-	-	-
25	CLA	A	806	X	-	-	-
25	CLA	A	807	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	A	808	X	-	-	-
25	CLA	B	736	X	-	-	-
25	CLA	B	737	X	-	-	-
25	CLA	B	738	X	-	-	-
25	CLA	B	739	X	-	-	-
25	CLA	B	740	X	-	-	-
25	CLA	B	741	X	-	-	-
25	CLA	B	742	X	-	-	-
25	CLA	B	743	X	-	-	-
25	CLA	B	744	X	-	-	-
25	CLA	B	745	X	-	-	-
25	CLA	B	746	X	-	-	-
25	CLA	B	747	X	-	-	-
25	CLA	B	748	X	-	-	-
25	CLA	B	749	X	-	-	-
25	CLA	B	750	X	-	-	-
25	CLA	B	751	X	-	-	-
25	CLA	B	752	X	-	-	-
25	CLA	B	753	X	-	-	-
25	CLA	B	754	X	-	-	-
25	CLA	B	755	X	-	-	-
25	CLA	B	756	X	-	-	-
25	CLA	B	757	X	-	-	-
25	CLA	B	758	X	-	-	-
25	CLA	B	759	X	-	-	-
25	CLA	B	760	X	-	-	-
25	CLA	B	768	X	-	-	-
25	CLA	B	770	X	-	-	-
25	CLA	B	771	X	-	-	-
25	CLA	B	772	X	-	-	-
25	CLA	B	773	X	-	-	-
25	CLA	B	774	X	-	-	-
25	CLA	B	775	X	-	-	-
25	CLA	B	776	X	-	-	-
25	CLA	B	777	X	-	-	-
25	CLA	B	778	X	-	-	-
25	CLA	B	779	X	-	-	-
25	CLA	B	780	X	-	-	-
25	CLA	B	781	X	-	-	-
25	CLA	B	782	X	-	-	-
25	CLA	B	783	X	-	-	-
25	CLA	B	784	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	B	785	X	-	-	-
25	CLA	J	101	X	-	-	-
25	CLA	a	601	X	-	-	-
25	CLA	a	602	X	-	-	-
25	CLA	a	603	X	-	-	-
25	CLA	a	604	X	-	-	-
25	CLA	a	608	X	-	-	-
25	CLA	a	609	X	-	-	-
25	CLA	a	610	X	-	-	-
25	CLA	a	611	X	-	-	-
25	CLA	a	612	X	-	-	-
25	CLA	a	613	X	-	-	-
25	CLA	a	619	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	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	c	601	X	-	-	-
25	CLA	c	602	X	-	-	-
25	CLA	c	603	X	-	-	-
25	CLA	c	604	X	-	-	-
25	CLA	c	606	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	613	X	-	-	-
25	CLA	c	614	X	-	-	-
25	CLA	c	616	X	-	-	-
25	CLA	c	619	X	-	-	-
25	CLA	d	601	X	-	-	-
25	CLA	d	602	X	-	-	-
25	CLA	d	603	X	-	-	-
25	CLA	d	604	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	d	609	X	-	-	-
25	CLA	d	610	X	-	-	-
25	CLA	d	611	X	-	-	-
25	CLA	d	612	X	-	-	-
25	CLA	d	613	X	-	-	-
25	CLA	d	614	X	-	-	-
25	CLA	e	601	X	-	-	-
25	CLA	e	602	X	-	-	-
25	CLA	e	603	X	-	-	-
25	CLA	e	604	X	-	-	-
25	CLA	e	605	X	-	-	-
25	CLA	e	607	X	-	-	-
25	CLA	e	608	X	-	-	-
25	CLA	e	609	X	-	-	-
25	CLA	e	610	X	-	-	-
25	CLA	e	611	X	-	-	-
25	CLA	e	612	X	-	-	-
25	CLA	e	613	X	-	-	-
25	CLA	e	614	X	-	-	-
25	CLA	f	601	X	-	-	-
25	CLA	f	602	X	-	-	-
25	CLA	f	603	X	-	-	-
25	CLA	f	604	X	-	-	-
25	CLA	f	608	X	-	-	-
25	CLA	f	609	X	-	-	-
25	CLA	f	610	X	-	-	-
25	CLA	f	611	X	-	-	-
25	CLA	f	612	X	-	-	-
25	CLA	f	613	X	-	-	-
25	CLA	f	614	X	-	-	-
25	CLA	f	615	X	-	-	-
25	CLA	g	601	X	-	-	-
25	CLA	g	602	X	-	-	-
25	CLA	g	603	X	-	-	-
25	CLA	g	604	X	-	-	-
25	CLA	g	608	X	-	-	-
25	CLA	g	609	X	-	-	-
25	CLA	g	610	X	-	-	-
25	CLA	g	611	X	-	-	-
25	CLA	g	612	X	-	-	-
25	CLA	g	613	X	-	-	-
25	CLA	g	614	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	g	615	X	-	-	-
25	CLA	g	618	X	-	-	-
25	CLA	h	601	X	-	-	-
25	CLA	h	602	X	-	-	-
25	CLA	h	603	X	-	-	-
25	CLA	h	604	X	-	-	-
25	CLA	h	608	X	-	-	-
25	CLA	h	609	X	-	-	-
25	CLA	h	610	X	-	-	-
25	CLA	h	611	X	-	-	-
25	CLA	h	612	X	-	-	-
25	CLA	h	613	X	-	-	-
25	CLA	h	614	X	-	-	-
25	CLA	h	615	X	-	-	-
25	CLA	h	618	X	-	-	-
25	CLA	i	601	X	-	-	-
25	CLA	i	602	X	-	-	-
25	CLA	i	603	X	-	-	-
25	CLA	i	604	X	-	-	-
25	CLA	i	608	X	-	-	-
25	CLA	i	609	X	-	-	-
25	CLA	i	610	X	-	-	-
25	CLA	i	611	X	-	-	-
25	CLA	i	612	X	-	-	-
25	CLA	i	613	X	-	-	-
25	CLA	i	614	X	-	-	-
25	CLA	i	615	X	-	-	-
25	CLA	j	601	X	-	-	-
25	CLA	j	602	X	-	-	-
25	CLA	j	603	X	-	-	-
25	CLA	j	604	X	-	-	-
25	CLA	j	608	X	-	-	-
25	CLA	j	609	X	-	-	-
25	CLA	j	610	X	-	-	-
25	CLA	j	611	X	-	-	-
25	CLA	j	612	X	-	-	-
25	CLA	j	613	X	-	-	-
25	CLA	j	614	X	-	-	-
25	CLA	j	615	X	-	-	-
25	CLA	j	618	X	-	-	-
25	CLA	k	601	X	-	-	-
25	CLA	k	602	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	k	603	X	-	-	-
25	CLA	k	604	X	-	-	-
25	CLA	k	608	X	-	-	-
25	CLA	k	609	X	-	-	-
25	CLA	k	610	X	-	-	-
25	CLA	k	611	X	-	-	-
25	CLA	k	612	X	-	-	-
25	CLA	k	613	X	-	-	-
25	CLA	k	614	X	-	-	-
25	CLA	k	615	X	-	-	-
25	CLA	k	618	X	-	-	-
25	CLA	l	601	X	-	-	-
25	CLA	l	602	X	-	-	-
25	CLA	l	603	X	-	-	-
25	CLA	l	604	X	-	-	-
25	CLA	l	608	X	-	-	-
25	CLA	l	609	X	-	-	-
25	CLA	l	610	X	-	-	-
25	CLA	l	611	X	-	-	-
25	CLA	l	612	X	-	-	-
25	CLA	l	613	X	-	-	-
25	CLA	l	614	X	-	-	-
25	CLA	l	617	X	-	-	-
25	CLA	m	601	X	-	-	-
25	CLA	m	602	X	-	-	-
25	CLA	m	603	X	-	-	-
25	CLA	m	604	X	-	-	-
25	CLA	m	608	X	-	-	-
25	CLA	m	609	X	-	-	-
25	CLA	m	610	X	-	-	-
25	CLA	m	611	X	-	-	-
25	CLA	m	612	X	-	-	-
25	CLA	m	613	X	-	-	-
25	CLA	n	602	X	-	-	-
25	CLA	n	603	X	-	-	-
25	CLA	n	604	X	-	-	-
25	CLA	n	605	X	-	-	-
25	CLA	n	606	X	-	-	-
25	CLA	n	607	X	-	-	-
25	CLA	n	608	X	-	-	-
25	CLA	n	609	X	-	-	-
25	CLA	n	610	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	n	612	X	-	-	-
25	CLA	n	613	X	-	-	-
25	CLA	o	601	X	-	-	-
25	CLA	o	602	X	-	-	-
25	CLA	o	603	X	-	-	-
25	CLA	o	604	X	-	-	-
25	CLA	o	608	X	-	-	-
25	CLA	o	609	X	-	-	-
25	CLA	o	610	X	-	-	-
25	CLA	o	612	X	-	-	-
25	CLA	o	613	X	-	-	-
25	CLA	o	614	X	-	-	-
25	CLA	p	601	X	-	-	-
25	CLA	p	602	X	-	-	-
25	CLA	p	603	X	-	-	-
25	CLA	p	604	X	-	-	-
25	CLA	p	608	X	-	-	-
25	CLA	p	609	X	-	-	-
25	CLA	p	610	X	-	-	-
25	CLA	p	612	X	-	-	-
25	CLA	p	613	X	-	-	-
35	CHL	c	607	X	-	-	-
35	CHL	d	605	X	-	-	-
35	CHL	d	606	X	-	-	-
35	CHL	d	607	X	-	-	-
35	CHL	d	608	X	-	-	-
35	CHL	e	606	X	-	-	-

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 55406 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 I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	741	Total	C	N	O	S	0	0
			5878	3860	994	1003	21		

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	731	Total	C	N	O	S	0	0
			5861	3855	984	1007	15		

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			596	363	104	118	11		

- Molecule 4 is a protein called PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	186	Total	C	N	O	S	0	0
			1393	892	235	262	4		

- Molecule 5 is a protein called PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	63	Total	C	N	O	0	0
			481	311	81	89		

- Molecule 6 is a protein called PsaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	168	Total	C	N	O	S	0	0
			1250	801	206	239	4		

- Molecule 7 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	37	Total	C	N	O	S	0	0
			305	209	43	52	1		

- Molecule 8 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	M	31	Total	C	N	O	S	0	0
			243	162	37	43	1		

- Molecule 9 is a protein called Chloroplast light-harvesting complex I protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	a	166	Total	C	N	O	S	0	0
			1274	819	220	228	7		

- Molecule 10 is a protein called Chloroplast light-harvesting complex I protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	b	169	Total	C	N	O	S	0	0
			1302	842	213	243	4		

- Molecule 11 is a protein called LHCE 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	c	221	Total	C	N	O	S	0	0
			1676	1087	282	302	5		

- Molecule 12 is a protein called Light harvesting chlorophyll a /b binding protein of PSII.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	d	220	Total	C	N	O	S	0	0
			1669	1088	275	302	4		

- Molecule 13 is a protein called Chloroplast light-harvesting complex II protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	e	199	Total	C	N	O	S	0	0
			1517	981	256	275	5		

- Molecule 14 is a protein called LHCE 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	h	174	Total	C	N	O	S	0	0
			1350	865	233	247	5		

- Molecule 15 is a protein called LHCE 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	i	177	Total	C	N	O	S	0	0
			1355	865	242	244	4		

- Molecule 16 is a protein called Chloroplast light-harvesting complex I protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	j	183	Total	C	N	O	S	0	0
			1450	944	246	254	6		

- Molecule 17 is a protein called Chloroplast light-harvesting complex I protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	k	172	Total	C	N	O	S	0	0
			1338	860	232	241	5		

- Molecule 18 is a protein called Chloroplast light-harvesting complex I protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	l	167	Total	C	N	O	S	0	0
			1256	811	214	227	4		

- Molecule 19 is a protein called Chloroplast light-harvesting complex I protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	m	168	Total	C	N	O	S	0	0
			1260	813	215	228	4		

- Molecule 20 is a protein called Chloroplast light-harvesting complex I protein, Lhca7_2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	f	174	Total	C	N	O	S	0	0
			1332	851	236	241	4		

- Molecule 21 is a protein called Chloroplast light-harvesting complex I protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	g	178	Total	C	N	O	S	0	0
			1406	914	240	246	6		

- Molecule 22 is a protein called Chloroplast light-harvesting complex II protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	n	184	Total	C	N	O	S	0	0
			1411	921	232	254	4		

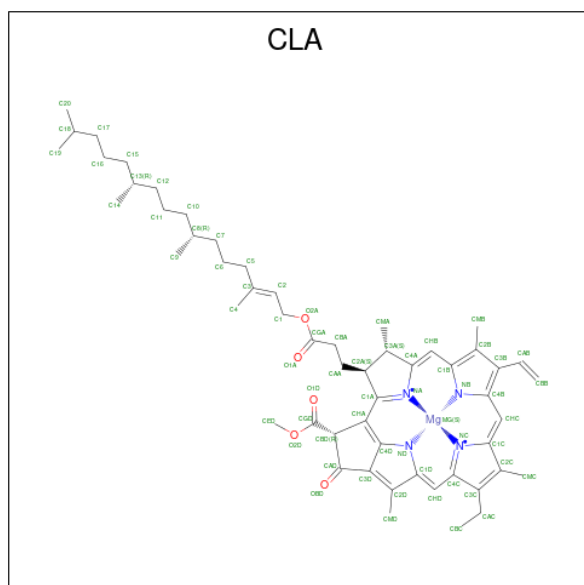
- Molecule 23 is a protein called Chloroplast light-harvesting complex I protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	o	164	Total	C	N	O	S	0	0
			1230	794	208	224	4		

- Molecule 24 is a protein called Chloroplast light-harvesting complex I protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	p	148	Total	C	N	O	S	0	0
			1126	727	188	207	4		

- Molecule 25 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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Mol	Chain	Residues	Atoms					AltConf
25	A	1	Total	C	Mg	N	O	0
			63	53	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
			45	35	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	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
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			64	55	1	4	4	
25	A	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			58	48	1	4	5	

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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
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	A	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	A	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	A	1	Total	C	Mg	N	O	0
			57	47	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
			52	42	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
			48	38	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	B	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			49	40	1	4	4	
25	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	B	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	B	1	Total 60	C 50	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 43	C 35	Mg 1	N 4	O 3	0
25	B	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	B	1	Total 53	C 43	Mg 1	N 4	O 5	0
25	B	1	Total 53	C 43	Mg 1	N 4	O 5	0
25	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	B	1	Total 61	C 51	Mg 1	N 4	O 5	0
25	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	B	1	Total 59	C 49	Mg 1	N 4	O 5	0
25	B	1	Total 53	C 43	Mg 1	N 4	O 5	0
25	B	1	Total 63	C 53	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 53	C 43	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 50	C 40	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	J	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			50	40	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
			53	43	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	b	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
25	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	b	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	b	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	b	1	Total 52	C 42	Mg 1	N 4	O 5	0
25	b	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	c	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	c	1	Total 59	C 49	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 48	C 38	Mg 1	N 4	O 5	0
25	c	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	c	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	c	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	c	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	c	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	c	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	c	1	Total 53	C 43	Mg 1	N 4	O 5	0
25	c	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	c	1	Total 47	C 37	Mg 1	N 4	O 5	0
25	c	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	d	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	d	1	Total 57	C 47	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	d	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	d	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
25	d	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	d	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
25	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	d	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	d	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	d	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	e	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	e	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	e	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	e	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	e	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
25	e	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
25	e	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	e	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	e	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	e	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	e	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
25	h	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	h	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	h	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	h	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	h	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
25	h	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	h	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
25	h	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	h	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
25	h	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
25	h	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	h	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	h	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	i	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
25	i	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
25	i	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	i	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	i	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	i	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	i	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	i	1	Total	C	Mg	N	O	0
			43	35	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
25	i	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	i	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
25	i	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	i	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	j	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	j	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	j	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	j	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
25	j	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
25	j	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	j	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
25	j	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	j	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	j	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
25	j	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	j	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	j	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	k	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	k	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
25	k	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	k	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	k	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	k	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	k	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
25	k	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	k	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	k	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
25	k	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	k	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	k	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	l	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	l	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
25	l	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	l	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	l	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	l	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	l	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
25	l	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	l	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	l	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
25	l	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	l	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
25	m	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	m	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	m	1	Total 54	C 44	Mg 1	N 4	O 5	0
25	m	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	m	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	m	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	m	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	m	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	m	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	m	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	f	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	f	1	Total 59	C 49	Mg 1	N 4	O 5	0
25	f	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	f	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	f	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	f	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	f	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	f	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	f	1	Total 59	C 49	Mg 1	N 4	O 5	0
25	f	1	Total 42	C 34	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
25	f	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	g	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	g	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
25	g	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	g	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	g	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	g	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	g	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	g	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	g	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	g	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	n	1	Total	C	Mg	N	O	0
			59	49	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
			48	38	1	4	5	
25	n	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	n	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	n	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	n	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

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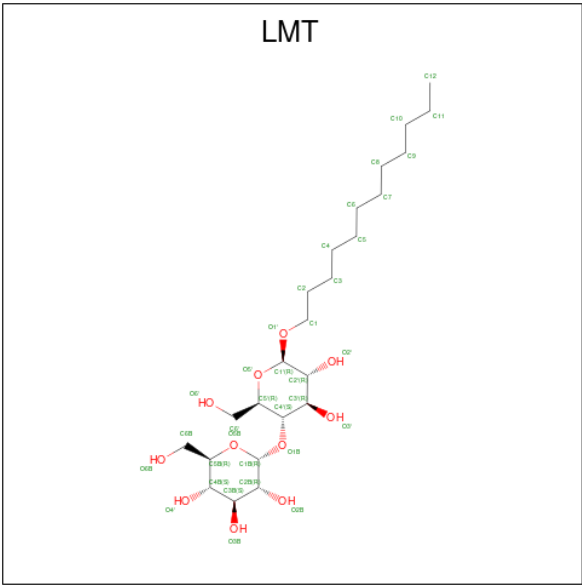
Mol	Chain	Residues	Atoms					AltConf
25	n	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	n	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	n	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	n	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	o	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	o	1	Total 47	C 37	Mg 1	N 4	O 5	0
25	o	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	o	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	o	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	o	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	o	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	o	1	Total 42	C 35	Mg 1	N 4	O 2	0
25	o	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	o	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	p	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	p	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	p	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	p	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	p	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	p	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	p	1	Total 45	C 35	Mg 1	N 4	O 5	0

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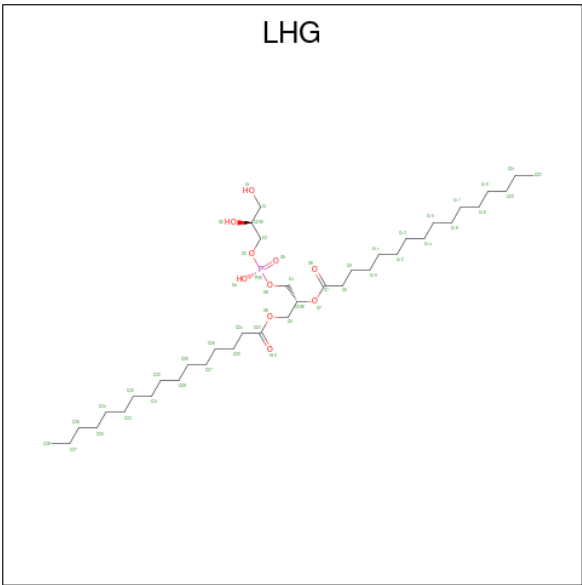
Mol	Chain	Residues	Atoms					AltConf
25	p	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	p	1	Total	C	Mg	N	O	0
			43	35	1	4	3	

- Molecule 26 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



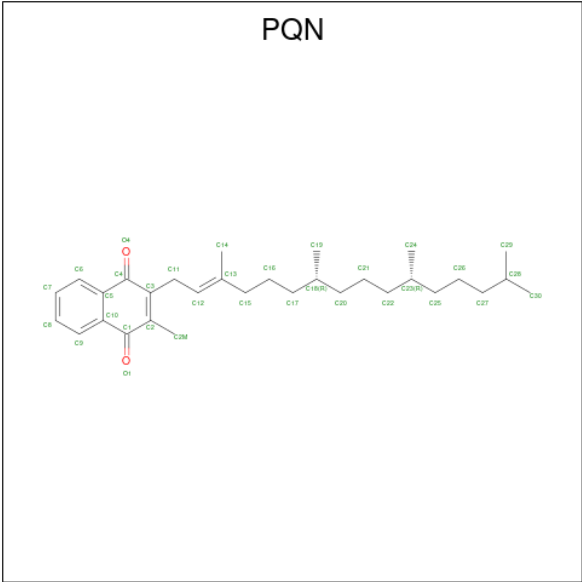
Mol	Chain	Residues	Atoms			AltConf
26	A	1	Total	C	O	0
			35	24	11	

- Molecule 27 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



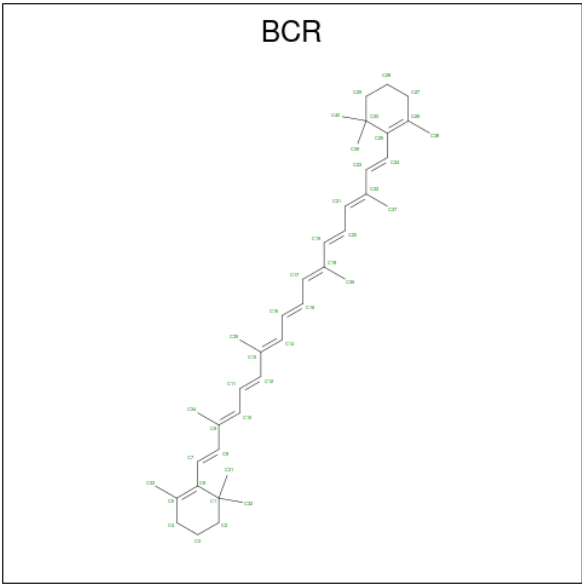
Mol	Chain	Residues	Atoms				AltConf
27	A	1	Total	C	O	P	0
			38	27	10	1	
27	A	1	Total	C	O	P	0
			49	38	10	1	
27	a	1	Total	C	O	P	0
			26	15	10	1	
27	b	1	Total	C	O	P	0
			31	20	10	1	
27	c	1	Total	C	O	P	0
			30	19	10	1	
27	d	1	Total	C	O	P	0
			29	18	10	1	
27	h	1	Total	C	O	P	0
			30	19	10	1	
27	h	1	Total	C	O	P	0
			31	20	10	1	
27	i	1	Total	C	O	P	0
			36	25	10	1	
27	j	1	Total	C	O	P	0
			37	26	10	1	
27	m	1	Total	C	O	P	0
			32	21	10	1	
27	g	1	Total	C	O	P	0
			35	24	10	1	

- Molecule 28 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂).



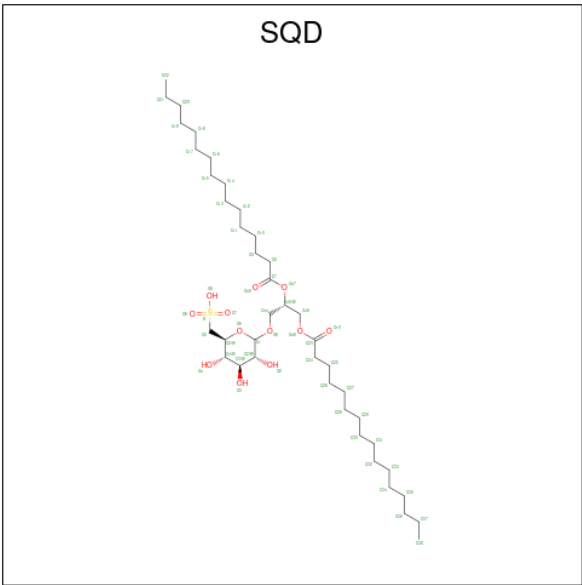
Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	C	O	0
			33	31	2	
28	B	1	Total	C	O	0
			33	31	2	
28	B	1	Total	C	O	0
			27	25	2	
28	d	1	Total	C	O	0
			26	24	2	

- Molecule 29 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



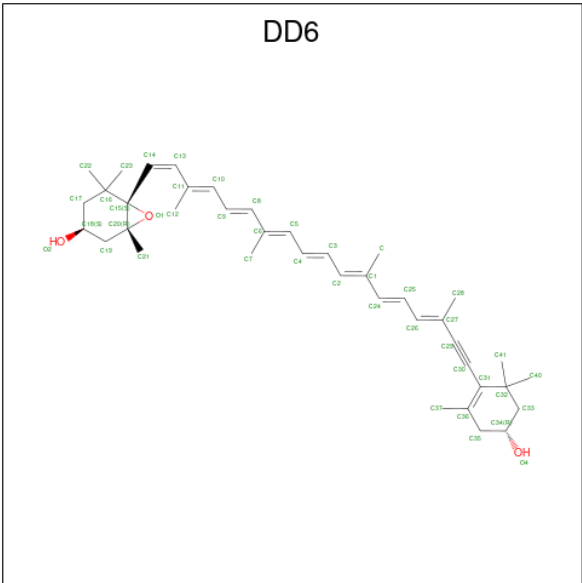
Mol	Chain	Residues	Atoms	AltConf
29	A	1	Total C 40 40	0
29	A	1	Total C 40 40	0
29	A	1	Total C 40 40	0
29	A	1	Total C 40 40	0
29	A	1	Total C 40 40	0
29	A	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	M	1	Total C 40 40	0

- Molecule 30 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



Mol	Chain	Residues	Atoms				AltConf
30	A	1	Total	C	O	S	0
			27	14	12	1	
30	c	1	Total	C	O	S	0
			39	26	12	1	
30	j	1	Total	C	O	S	0
			36	23	12	1	
30	g	1	Total	C	O	S	0
			32	19	12	1	

- Molecule 31 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene -3,3'-diol (CCD ID: DD6) (formula: C₄₀H₅₄O₃).



Mol	Chain	Residues	Atoms			AltConf
31	A	1	Total 43	C 40	O 3	0
31	A	1	Total 43	C 40	O 3	0
31	F	1	Total 43	C 40	O 3	0
31	J	1	Total 43	C 40	O 3	0
31	a	1	Total 43	C 40	O 3	0
31	a	1	Total 43	C 40	O 3	0
31	b	1	Total 43	C 40	O 3	0
31	b	1	Total 43	C 40	O 3	0
31	c	1	Total 43	C 40	O 3	0
31	c	1	Total 43	C 40	O 3	0
31	c	1	Total 43	C 40	O 3	0
31	c	1	Total 43	C 40	O 3	0
31	d	1	Total 43	C 40	O 3	0
31	d	1	Total 43	C 40	O 3	0
31	d	1	Total 43	C 40	O 3	0
31	e	1	Total 43	C 40	O 3	0
31	e	1	Total 43	C 40	O 3	0
31	e	1	Total 43	C 40	O 3	0
31	h	1	Total 43	C 40	O 3	0
31	h	1	Total 43	C 40	O 3	0
31	i	1	Total 43	C 40	O 3	0
31	i	1	Total 43	C 40	O 3	0

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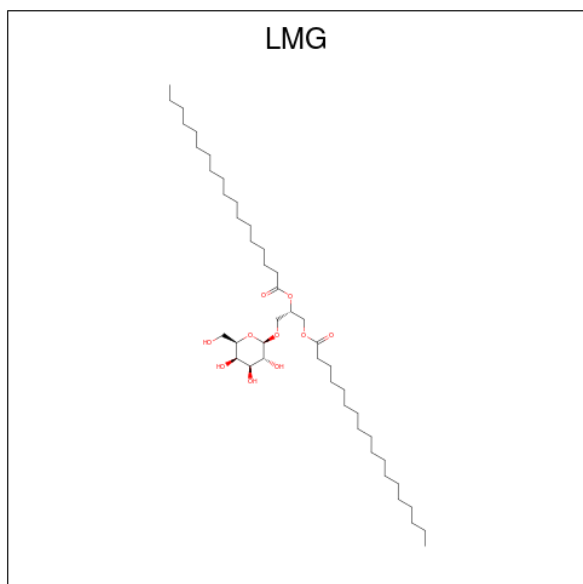
Mol	Chain	Residues	Atoms			AltConf
31	i	1	Total	C	O	0
			43	40	3	
31	j	1	Total	C	O	0
			43	40	3	
31	j	1	Total	C	O	0
			43	40	3	
31	k	1	Total	C	O	0
			43	40	3	
31	k	1	Total	C	O	0
			43	40	3	
31	l	1	Total	C	O	0
			43	40	3	
31	l	1	Total	C	O	0
			43	40	3	
31	m	1	Total	C	O	0
			43	40	3	
31	m	1	Total	C	O	0
			43	40	3	
31	f	1	Total	C	O	0
			43	40	3	
31	f	1	Total	C	O	0
			43	40	3	
31	g	1	Total	C	O	0
			43	40	3	
31	g	1	Total	C	O	0
			43	40	3	
31	n	1	Total	C	O	0
			43	40	3	
31	n	1	Total	C	O	0
			43	40	3	
31	n	1	Total	C	O	0
			43	40	3	
31	o	1	Total	C	O	0
			43	40	3	
31	o	1	Total	C	O	0
			43	40	3	
31	p	1	Total	C	O	0
			43	40	3	

- Molecule 32 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



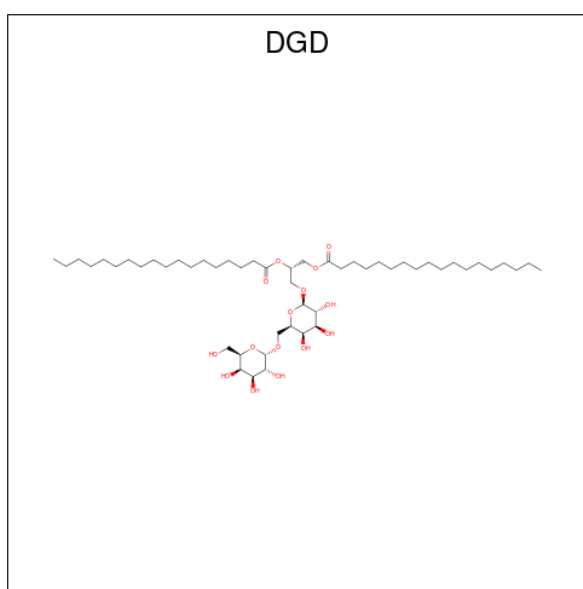
Mol	Chain	Residues	Atoms			AltConf
32	B	1	Total	Fe	S	0
			8	4	4	
32	C	1	Total	Fe	S	0
			8	4	4	
32	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



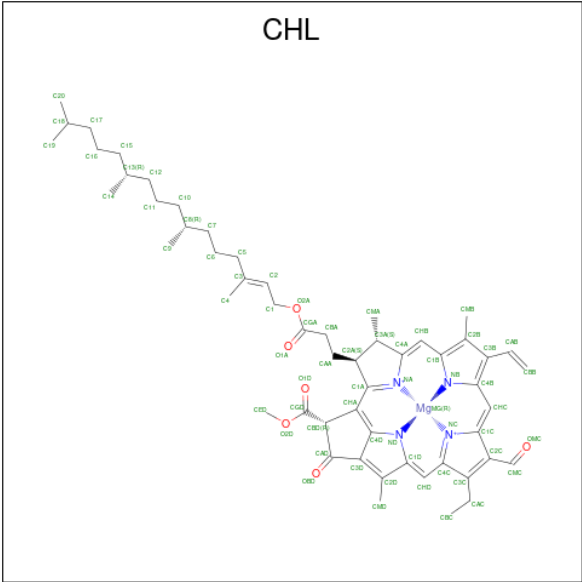
Mol	Chain	Residues	Atoms			AltConf
33	B	1	Total	C	O	0
			52	42	10	
33	a	1	Total	C	O	0
			43	33	10	
33	i	1	Total	C	O	0
			44	34	10	
33	k	1	Total	C	O	0
			36	26	10	

- Molecule 34 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
34	B	1	Total	C	O	0
			54	39	15	
34	b	1	Total	C	O	0
			48	33	15	
34	e	1	Total	C	O	0
			36	21	15	

- Molecule 35 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).

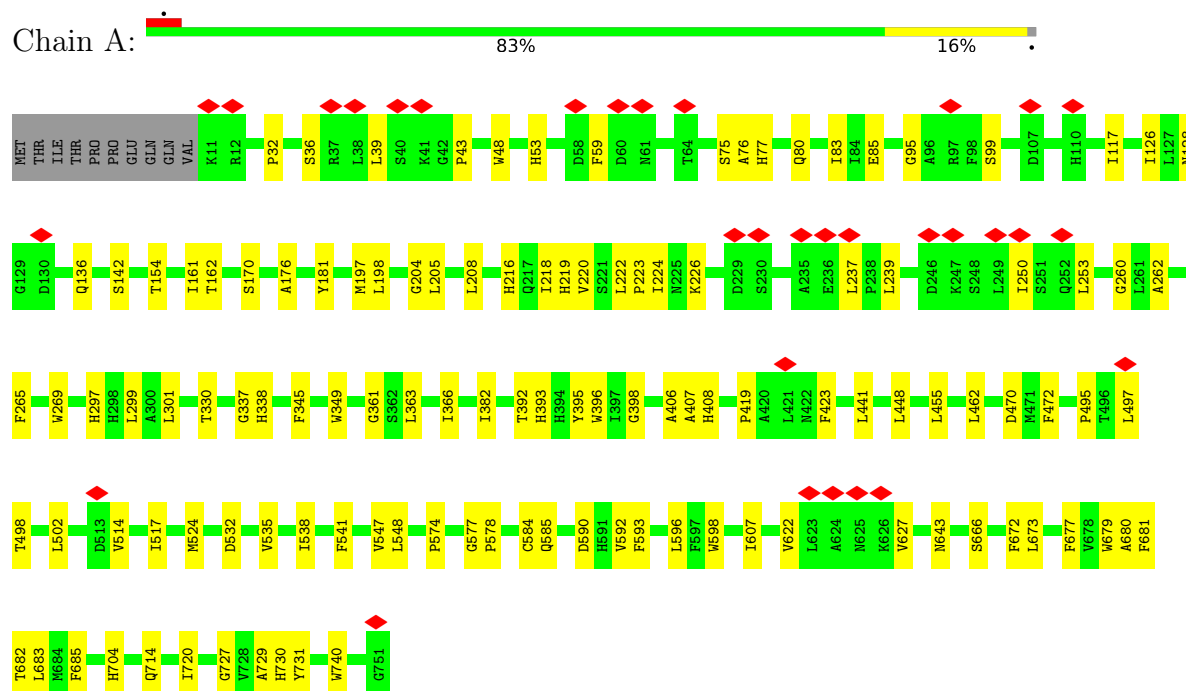


Mol	Chain	Residues	Atoms					AltConf
35	c	1	Total	C	Mg	N	O	0
			49	38	1	4	6	
35	d	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
35	d	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
35	d	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
35	d	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
35	e	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

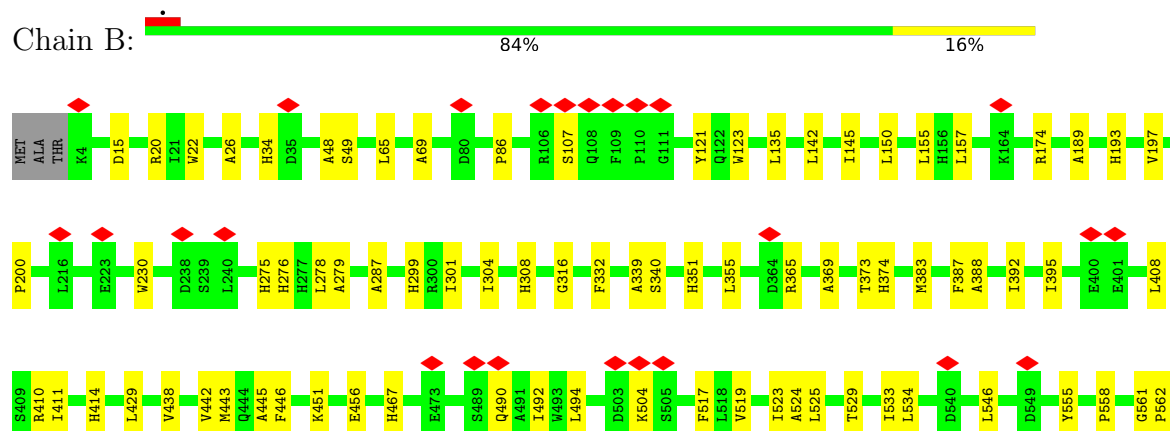
3 Residue-property plots

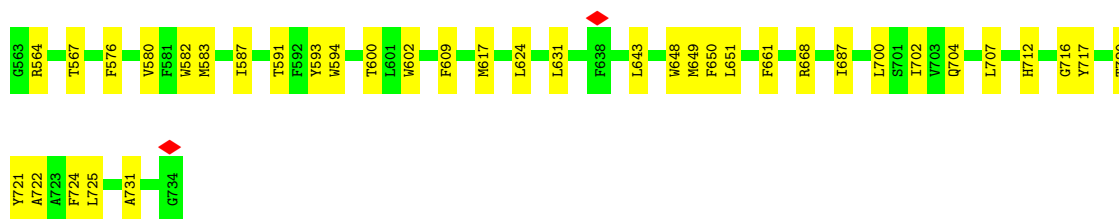
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 I P700 chlorophyll a apoprotein A1

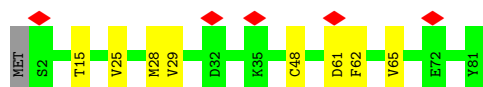
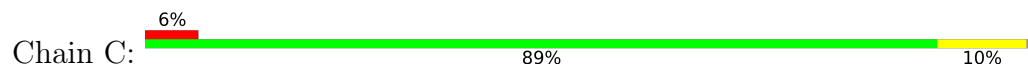


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

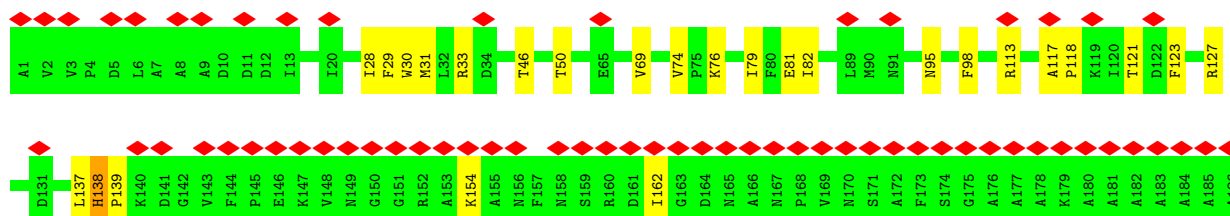
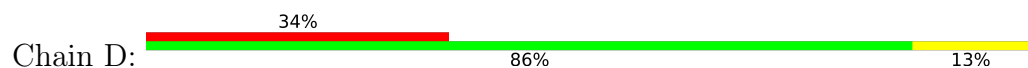




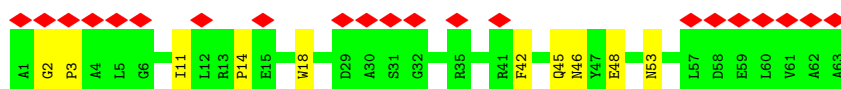
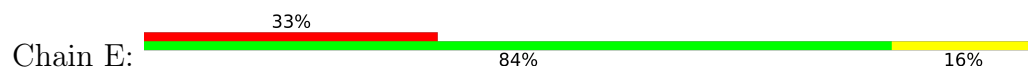
• Molecule 3: Photosystem I iron-sulfur center



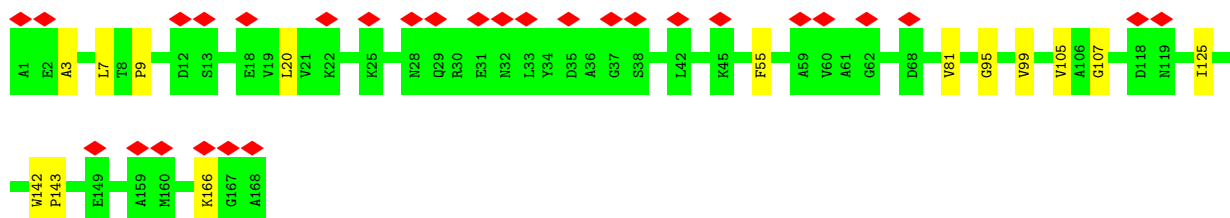
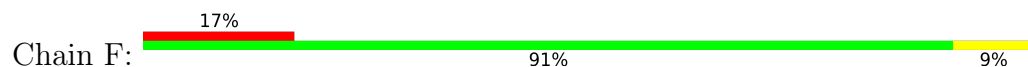
• Molecule 4: PsaD



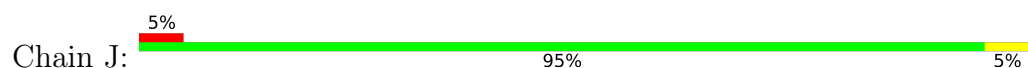
• Molecule 5: PsaE

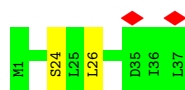


• Molecule 6: PsaF

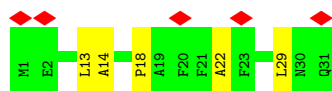
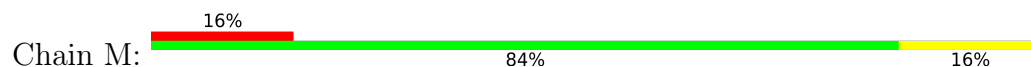


• Molecule 7: Photosystem I reaction center subunit IX

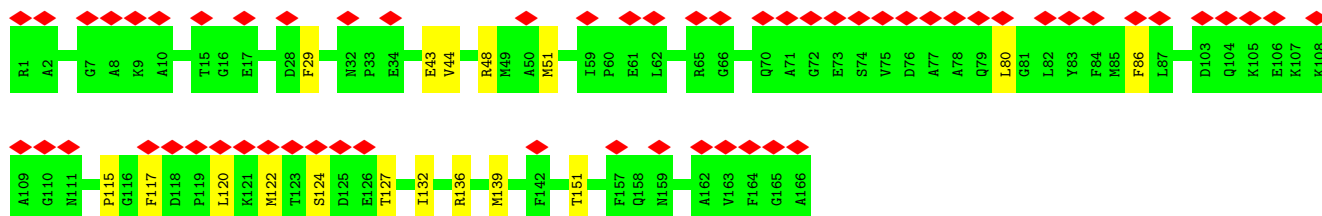
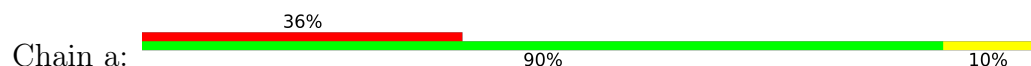




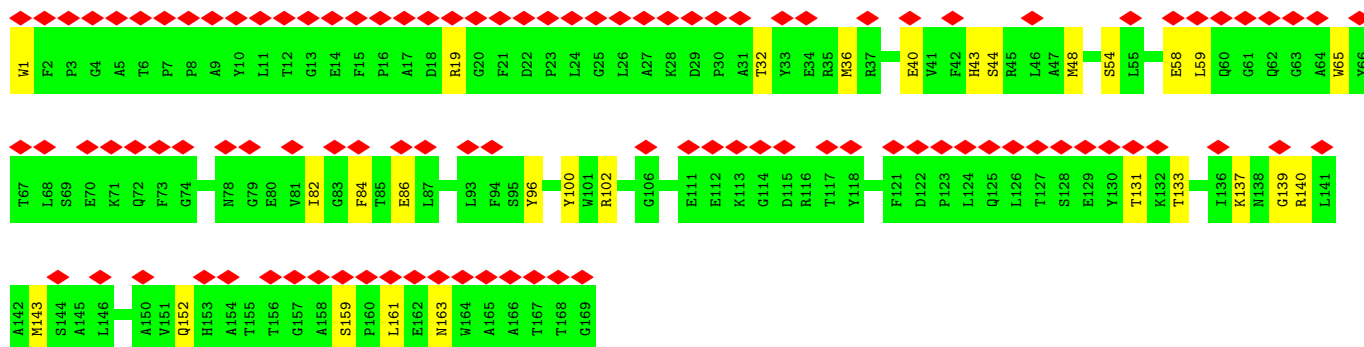
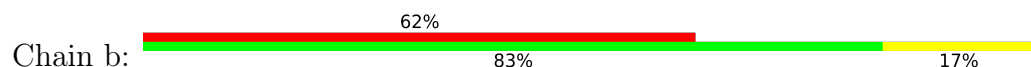
- Molecule 8: Photosystem I reaction center subunit XII



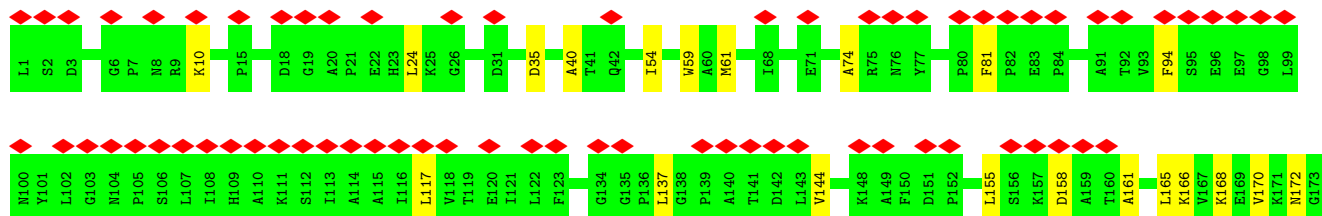
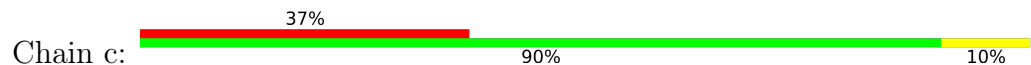
- Molecule 9: Chloroplast light-harvesting complex I protein

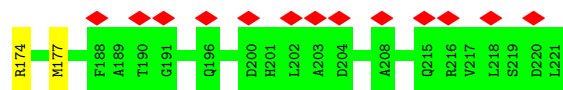


- Molecule 10: Chloroplast light-harvesting complex I protein

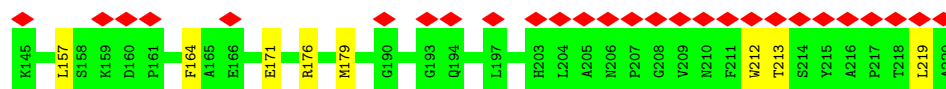
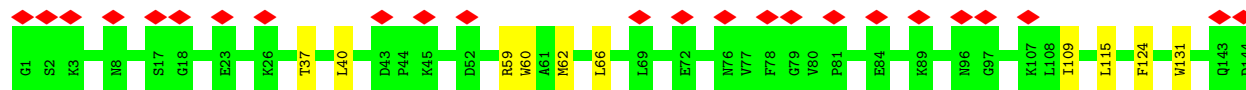


- Molecule 11: LHCE 3

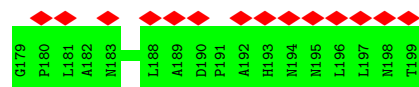
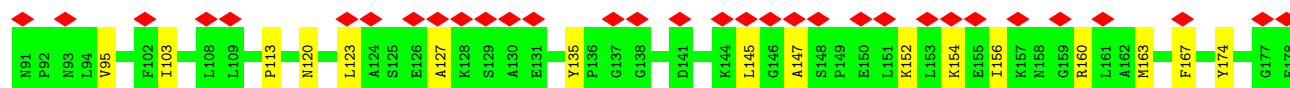
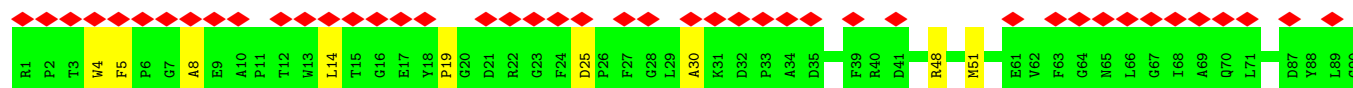
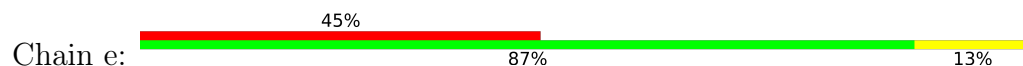




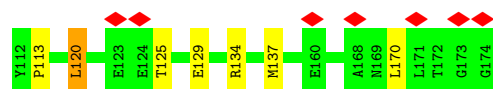
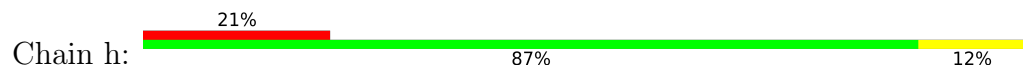
- Molecule 12: Light harvesting chlorophyll a /b binding protein of PSII



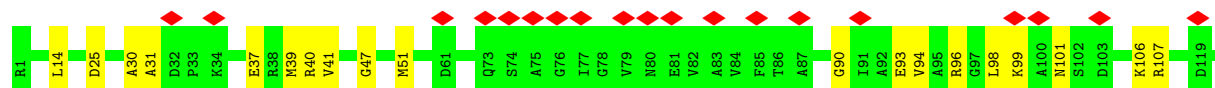
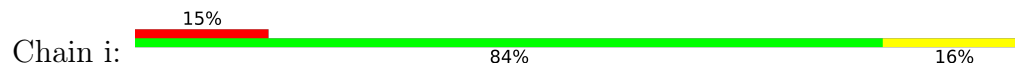
- Molecule 13: Chloroplast light-harvesting complex II protein

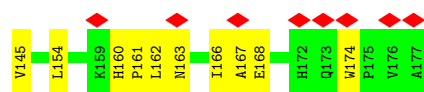


- Molecule 14: LHCE 8

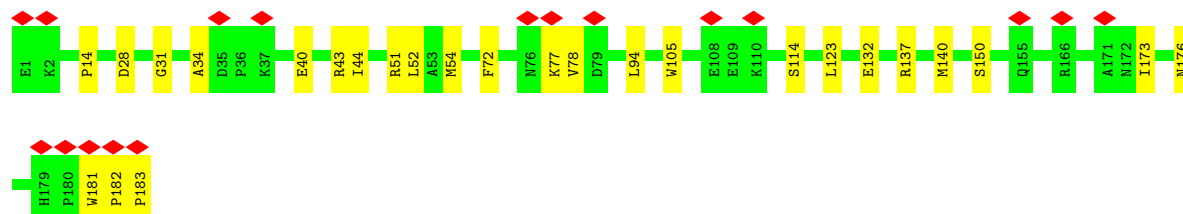
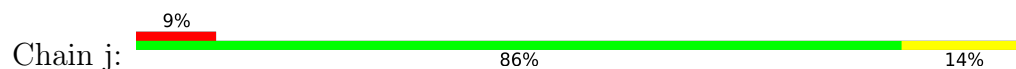


- Molecule 15: LHCE 9

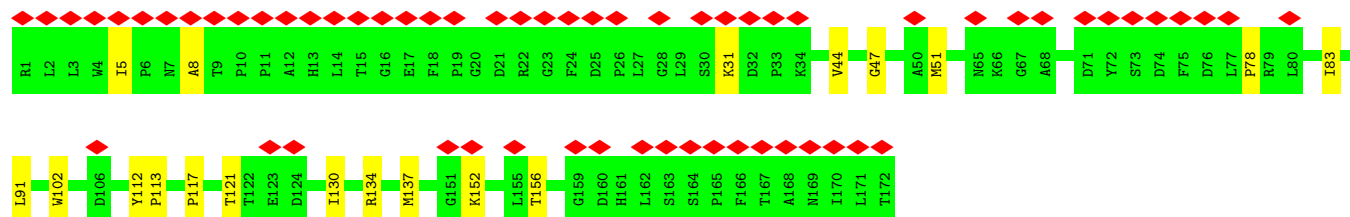
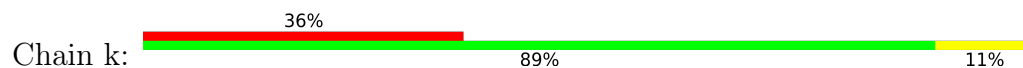




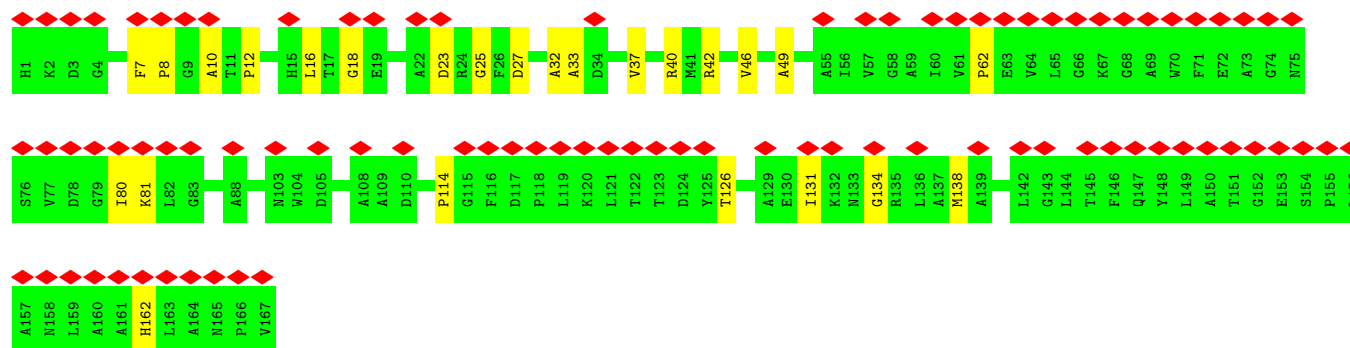
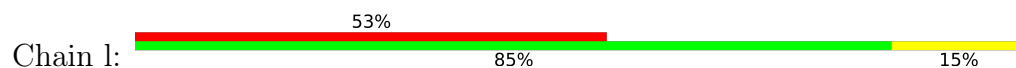
- Molecule 16: Chloroplast light-harvesting complex I protein



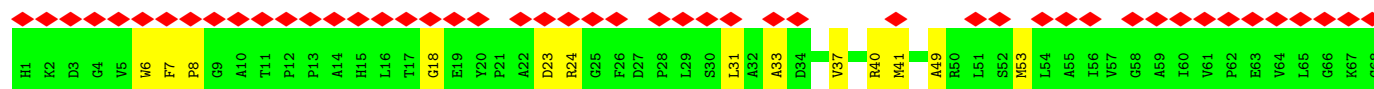
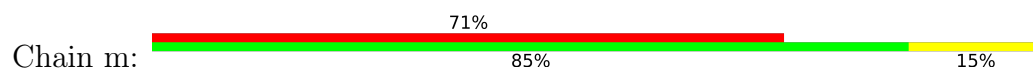
- Molecule 17: Chloroplast light-harvesting complex I protein

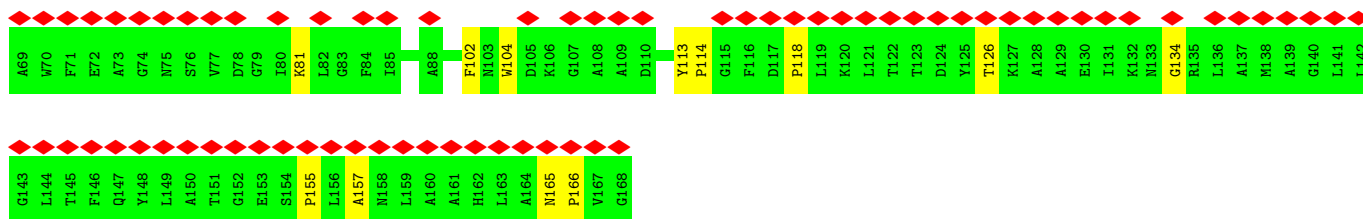


- Molecule 18: Chloroplast light-harvesting complex I protein

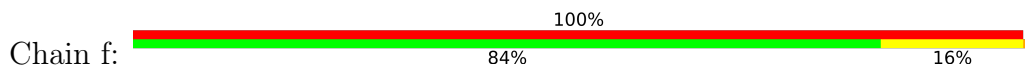


- Molecule 19: Chloroplast light-harvesting complex I protein

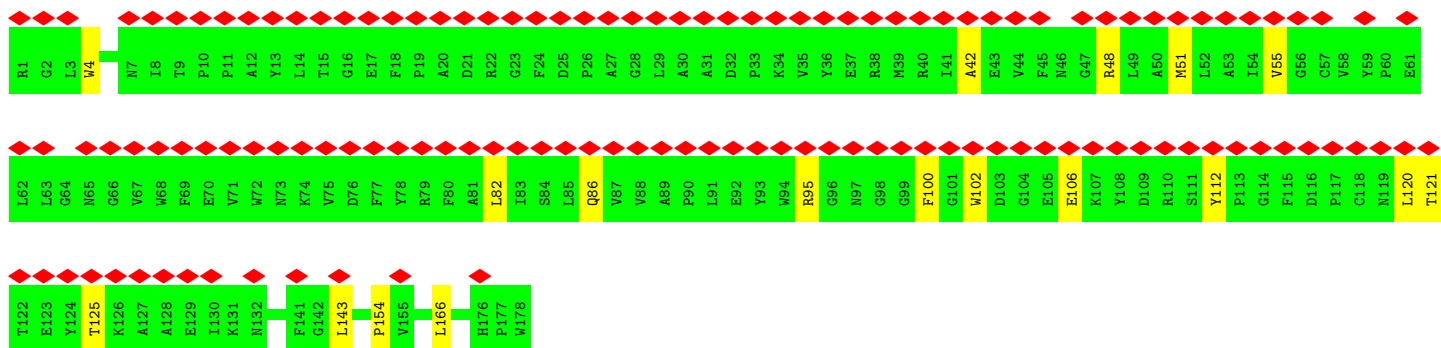
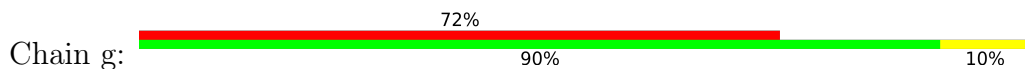




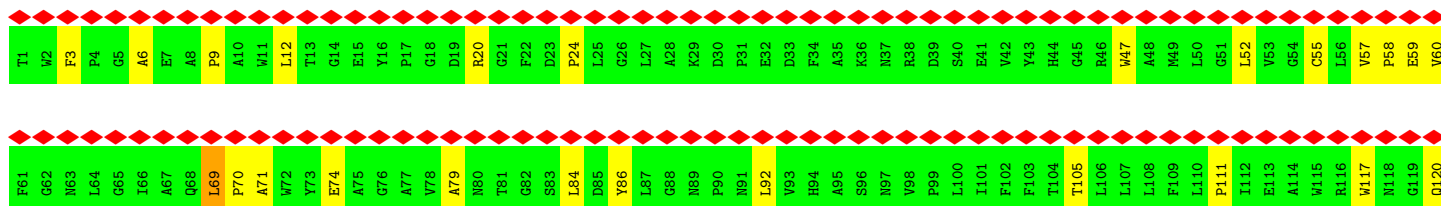
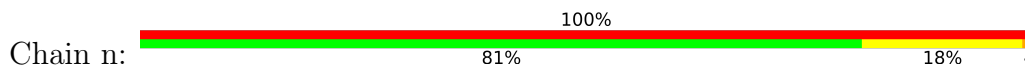
• Molecule 20: Chloroplast light-harvesting complex I protein, Lhca7_2

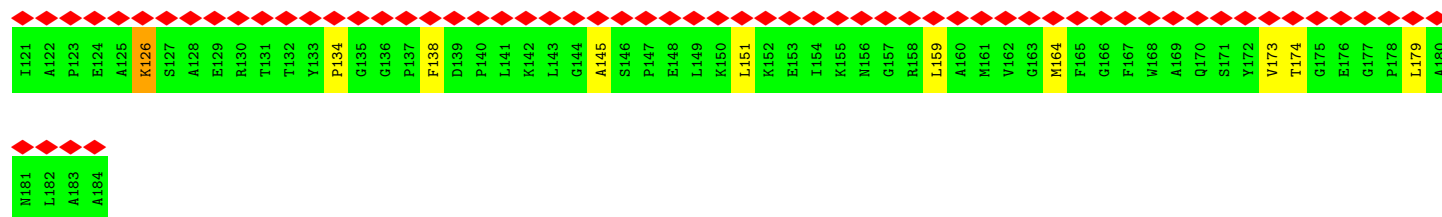


• Molecule 21: Chloroplast light-harvesting complex I protein

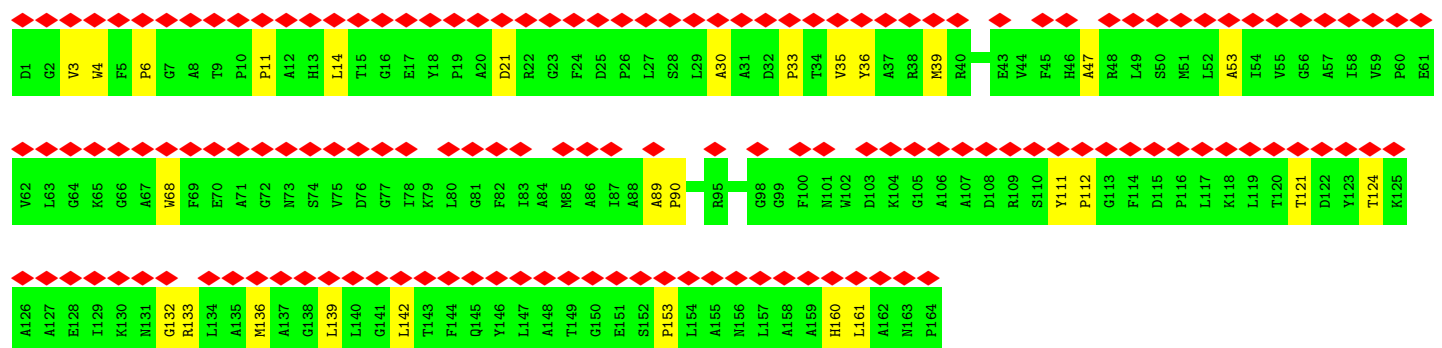
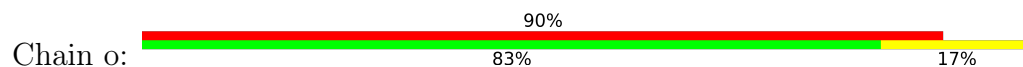


• Molecule 22: Chloroplast light-harvesting complex II protein

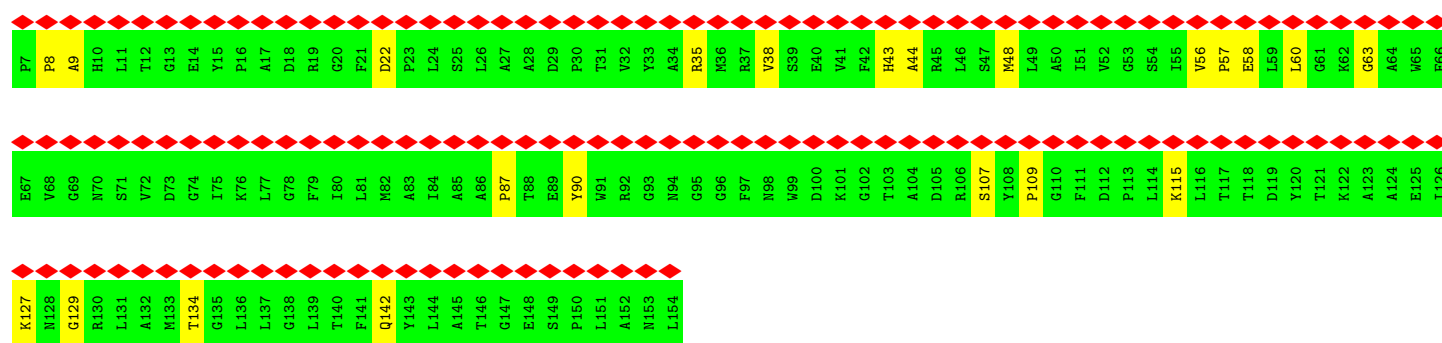
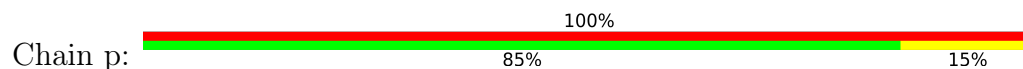




• Molecule 23: Chloroplast light-harvesting complex I protein



• Molecule 24: Chloroplast light-harvesting complex I protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	562173	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI POLARA 300	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 (6k x 4k)	Depositor
Maximum map value	1.741	Depositor
Minimum map value	-0.575	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.5	Depositor
Map size (\AA)	532.48, 532.48, 532.48	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CLA, LHG, DD6, PQN, BCR, CHL, LMG, SF4, DGD, LMT, SQD

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	A	0.17	0/6079	0.28	0/8287
2	B	0.17	0/6071	0.28	0/8277
3	C	0.16	0/606	0.30	0/819
4	D	0.13	0/1426	0.27	0/1941
5	E	0.13	0/491	0.25	0/669
6	F	0.14	0/1275	0.26	0/1739
7	J	0.14	0/314	0.24	0/429
8	M	0.16	0/247	0.24	0/332
9	a	0.14	0/1311	0.25	0/1772
10	b	0.13	0/1344	0.28	0/1829
11	c	0.14	0/1719	0.25	0/2336
12	d	0.15	0/1719	0.27	0/2343
13	e	0.13	0/1566	0.25	0/2141
14	h	0.14	0/1388	0.28	0/1886
15	i	0.16	0/1391	0.30	0/1894
16	j	0.16	0/1499	0.27	0/2045
17	k	0.14	0/1377	0.26	0/1871
18	l	0.13	0/1293	0.26	0/1763
19	m	0.14	0/1297	0.30	0/1768
20	f	0.10	0/1367	0.26	0/1861
21	g	0.12	0/1452	0.25	0/1980
22	n	0.11	0/1458	0.26	0/1993
23	o	0.12	0/1266	0.28	0/1727
24	p	0.11	0/1156	0.26	0/1572
All	All	0.15	0/39112	0.27	0/53274

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	138	HIS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5878	0	5745	99	0
2	B	5861	0	5659	102	0
3	C	596	0	571	6	0
4	D	1393	0	1371	17	0
5	E	481	0	479	9	0
6	F	1250	0	1259	13	0
7	J	305	0	317	2	0
8	M	243	0	258	4	0
9	a	1274	0	1235	13	0
10	b	1302	0	1244	19	0
11	c	1676	0	1689	16	0
12	d	1669	0	1650	16	0
13	e	1517	0	1468	19	0
14	h	1350	0	1324	18	0
15	i	1355	0	1336	24	0
16	j	1450	0	1401	20	0
17	k	1338	0	1314	13	0
18	l	1256	0	1234	20	0
19	m	1260	0	1236	24	0
20	f	1332	0	1312	16	0
21	g	1406	0	1358	15	0
22	n	1411	0	1372	24	0
23	o	1230	0	1205	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	p	1126	0	1115	13	0
25	A	2588	0	2466	120	0
25	B	2333	0	2201	117	0
25	J	50	0	39	2	0
25	a	571	0	488	24	0
25	b	492	0	373	14	0
25	c	679	0	556	22	0
25	d	480	0	389	11	0
25	e	623	0	506	16	0
25	f	553	0	448	10	0
25	g	598	0	467	22	0
25	h	642	0	533	27	0
25	i	603	0	527	15	0
25	j	667	0	568	19	0
25	k	631	0	520	14	0
25	l	562	0	459	17	0
25	m	461	0	369	15	0
25	n	499	0	389	14	0
25	o	429	0	320	12	0
25	p	393	0	297	9	0
26	A	35	0	46	0	0
27	A	87	0	123	7	0
27	a	26	0	22	1	0
27	b	31	0	32	3	0
27	c	30	0	29	3	0
27	d	29	0	28	3	0
27	g	35	0	40	0	0
27	h	61	0	62	3	0
27	i	36	0	42	2	0
27	j	37	0	44	4	0
27	m	32	0	34	2	0
28	A	33	0	46	5	0
28	B	60	0	78	2	0
28	d	26	0	29	0	0
29	A	240	0	336	14	0
29	B	240	0	336	24	0
29	M	40	0	56	2	0
30	A	27	0	18	0	0
30	c	39	0	42	0	0
30	g	32	0	28	2	0
30	j	36	0	36	0	0
31	A	86	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	F	43	0	0	0	0
31	J	43	0	0	0	0
31	a	86	0	0	1	0
31	b	86	0	0	0	0
31	c	172	0	0	0	0
31	d	129	0	0	1	0
31	e	129	0	0	0	0
31	f	86	0	0	0	0
31	g	86	0	0	0	0
31	h	86	0	0	0	0
31	i	129	0	0	1	0
31	j	86	0	0	0	0
31	k	86	0	0	0	0
31	l	86	0	0	0	0
31	m	86	0	0	2	0
31	n	129	0	0	1	0
31	o	86	0	0	0	0
31	p	43	0	0	0	0
32	B	8	0	0	0	0
32	C	16	0	0	0	0
33	B	52	0	77	5	0
33	a	43	0	56	0	0
33	i	44	0	61	0	0
33	k	36	0	42	3	0
34	B	54	0	66	2	0
34	b	48	0	54	3	0
34	e	36	0	30	2	0
35	c	49	0	34	3	0
35	d	186	0	128	7	0
35	e	46	0	31	0	0
All	All	55406	0	51153	806	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 8.

All (806) 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)
19:m:7:PHE:HA	25:m:601:CLA:NB	1.93	0.82
13:e:30:ALA:HB2	25:e:602:CLA:HBA1	1.63	0.81
23:o:47:ALA:HB1	23:o:132:GLY:HA3	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:775:CLA:HBA1	25:A:775:CLA:HBD	1.67	0.76
1:A:740:TRP:HB2	25:A:775:CLA:HBB1	1.69	0.74
1:A:204:GLY:O	1:A:208:LEU:HB2	1.86	0.74
19:m:49:ALA:HB1	19:m:134:GLY:HA3	1.69	0.74
27:a:181:LHG:HC42	25:a:601:CLA:HBD	1.70	0.73
25:a:602:CLA:HBB1	25:a:602:CLA:H51	1.70	0.73
18:l:49:ALA:HB1	18:l:134:GLY:HA3	1.71	0.72
20:f:149:SER:HB2	20:f:152:LEU:HB2	1.72	0.72
23:o:160:HIS:HE1	25:o:614:CLA:NA	1.87	0.72
18:l:46:VAL:HG22	18:l:131:ILE:HD11	1.72	0.70
25:A:784:CLA:HBA2	27:A:786:LHG:H161	1.73	0.69
28:A:785:PQN:H162	29:A:796:BCR:H382	1.74	0.69
25:B:753:CLA:H41	25:B:771:CLA:HBC3	1.73	0.69
14:h:5:ILE:HG22	14:h:8:ALA:HB2	1.74	0.69
23:o:36:TYR:H	23:o:39:MET:HG2	1.59	0.68
3:C:62:PHE:HD2	4:D:162:ILE:HG21	1.59	0.68
1:A:76:ALA:HB1	25:A:760:CLA:HBB1	1.76	0.68
5:E:14:PRO:HB2	6:F:166:LYS:HG3	1.77	0.67
20:f:39:MET:HB3	25:f:602:CLA:H3A	1.75	0.67
25:A:753:CLA:HBB1	25:A:791:CLA:NB	2.10	0.67
2:B:721:TYR:HB2	25:B:736:CLA:HED2	1.77	0.67
29:A:792:BCR:H12C	25:A:798:CLA:H12	1.77	0.66
1:A:223:PRO:HG3	1:A:250:ILE:HD13	1.77	0.66
25;j:601:CLA:HBB1	33:k:179:LMG:H331	1.76	0.66
1:A:83:ILE:HD12	25:A:797:CLA:HAB	1.76	0.66
4:D:74:VAL:HG22	4:D:76:LYS:H	1.59	0.66
6:F:105:VAL:HG21	6:F:142:TRP:HB2	1.77	0.66
23:o:121:THR:H	23:o:124:THR:HG22	1.61	0.66
25:B:751:CLA:H2	25:B:757:CLA:HBB2	1.78	0.65
14:h:120:LEU:HB2	25:h:610:CLA:HBA1	1.77	0.65
1:A:729:ALA:HA	27:A:786:LHG:H342	1.78	0.65
15:i:90:GLY:HA3	25:i:609:CLA:HAB	1.76	0.65
18:l:114:PRO:HB3	25:l:608:CLA:HBC2	1.78	0.65
25:B:777:CLA:H3A	25:B:784:CLA:HED3	1.79	0.65
10:b:44:SER:HB3	10:b:139:GLY:HA3	1.78	0.64
25:i:603:CLA:HBC2	25:i:615:CLA:HBB2	1.79	0.64
2:B:339:ALA:HB2	29:B:766:BCR:H372	1.80	0.64
1:A:265:PHE:HB2	25:a:619:CLA:H41	1.81	0.63
13:e:145:LEU:HB2	25:e:610:CLA:HBA1	1.80	0.63
10:b:59:LEU:HD12	10:b:161:LEU:HD11	1.81	0.63
25:e:608:CLA:HBA1	25:e:608:CLA:HBD	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:n:3:PHE:HD2	22:n:6:ALA:HB2	1.64	0.62
25:B:775:CLA:HAB	33:B:786:LMG:H342	1.80	0.62
25:e:602:CLA:H43	25:e:603:CLA:HBA1	1.81	0.62
27:h:190:LHG:HC82	25:h:611:CLA:HBC3	1.82	0.62
35:c:607:CHL:HBA2	12:d:219:LEU:HB2	1.82	0.61
35:d:607:CHL:HHC	35:d:607:CHL:HBB1	1.82	0.61
14:h:113:PRO:HB3	25:h:608:CLA:HBC2	1.80	0.61
2:B:722:ALA:HB2	25:B:778:CLA:HBB1	1.80	0.61
17:k:113:PRO:HB3	25:k:608:CLA:HBC2	1.82	0.61
20:f:160:HIS:HB2	20:f:164:HIS:HD2	1.66	0.61
2:B:369:ALA:HB1	2:B:725:LEU:HD11	1.83	0.61
1:A:269:TRP:CH2	25:A:767:CLA:HBB1	2.36	0.60
1:A:498:THR:HG21	25:A:780:CLA:HMD3	1.83	0.60
2:B:490:GLN:HB2	25:B:780:CLA:HED1	1.82	0.60
2:B:69:ALA:HB2	2:B:135:LEU:HB2	1.83	0.60
21:g:143:LEU:HD22	21:g:154:PRO:HB3	1.82	0.60
22:n:120:GLN:HB3	22:n:126:LYS:HE2	1.83	0.60
27:j:198:LHG:HC42	25:j:601:CLA:HBD	1.84	0.60
1:A:226:LYS:HD3	1:A:253:LEU:HB3	1.83	0.60
1:A:538:ILE:HD12	25:A:752:CLA:H171	1.84	0.60
25:i:601:CLA:H2A	25:i:601:CLA:HED3	1.81	0.60
23:o:161:LEU:HD21	25:o:614:CLA:HAC1	1.83	0.59
25:d:613:CLA:HMB2	25:d:614:CLA:HAB	1.84	0.59
4:D:33:ARG:HD2	25:j:611:CLA:HAA2	1.83	0.59
1:A:598:TRP:HH2	25:A:758:CLA:HAB	1.68	0.59
29:B:765:BCR:H332	33:B:786:LMG:H141	1.84	0.59
15:i:160:HIS:HB3	15:i:163:ASN:HD22	1.67	0.59
12:d:60:TRP:CE2	35:d:608:CHL:HED2	2.38	0.58
9:a:124:SER:H	9:a:127:THR:HG22	1.68	0.58
10:b:1:TRP:HB2	10:b:19:ARG:HB3	1.84	0.58
27:A:756:LHG:H292	25:A:804:CLA:HBB1	1.84	0.58
29:B:765:BCR:H373	25:B:781:CLA:H111	1.85	0.58
18:l:7:PHE:HB3	18:l:10:ALA:HB2	1.83	0.58
13:e:123:LEU:HD21	25:e:608:CLA:HBB1	1.84	0.58
10:b:32:THR:O	10:b:36:MET:HG2	2.03	0.58
11:c:40:ALA:HB2	25:c:602:CLA:HBA1	1.86	0.58
23:o:160:HIS:CD2	25:o:614:CLA:NC	2.70	0.58
25:A:773:CLA:H12	25:A:781:CLA:HAA1	1.86	0.58
1:A:682:THR:HG21	1:A:731:TYR:HB2	1.85	0.58
25:B:751:CLA:HED2	25:B:781:CLA:HBD	1.86	0.58
25:l:614:CLA:C1D	25:l:617:CLA:HBB2	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:11:ILE:HD12	5:E:18:TRP:HB2	1.85	0.57
2:B:395:ILE:HD13	2:B:555:TYR:HA	1.86	0.57
10:b:84:PHE:HE2	34:b:182:DGD:HD1	1.69	0.57
25:A:755:CLA:HAC2	25:A:766:CLA:HAB	1.86	0.57
29:B:762:BCR:HC8	25:B:775:CLA:HMD1	1.85	0.57
25:B:751:CLA:HBB1	29:B:766:BCR:H19C	1.85	0.57
25:A:776:CLA:H61	29:A:787:BCR:H342	1.86	0.57
25:A:758:CLA:C1B	25:B:737:CLA:HBB1	2.35	0.57
2:B:49:SER:HB3	25:B:738:CLA:HBB1	1.86	0.57
25:p:603:CLA:HAA2	25:p:603:CLA:HBD	1.85	0.57
13:e:147:ALA:HB2	25:e:610:CLA:H2A	1.87	0.57
25:A:758:CLA:H143	25:B:742:CLA:HAB	1.85	0.56
25:A:770:CLA:HBB1	25:A:774:CLA:H72	1.86	0.56
27:i:194:LHG:HC91	27:i:194:LHG:H281	1.88	0.56
17:k:83:ILE:HG23	25:k:618:CLA:HMD2	1.87	0.56
21:g:48:ARG:HA	21:g:51:MET:HE3	1.87	0.56
25:A:761:CLA:H3A	25:A:777:CLA:HAB	1.87	0.56
25:B:773:CLA:H42	25:B:781:CLA:HBB2	1.87	0.56
15:i:101:ASN:HA	15:i:106:LYS:HG2	1.87	0.56
25:A:770:CLA:H151	25:A:804:CLA:HBC1	1.87	0.56
12:d:59:ARG:HA	12:d:62:MET:HE3	1.87	0.56
2:B:332:PHE:HE2	2:B:408:LEU:HD11	1.70	0.56
2:B:649:MET:HE1	25:B:741:CLA:H41	1.87	0.56
25:j:601:CLA:HMB2	33:k:179:LMG:H292	1.88	0.56
1:A:673:LEU:HD11	2:B:617:MET:HB2	1.88	0.55
1:A:338:HIS:CD2	25:A:771:CLA:ND	2.73	0.55
1:A:392:THR:HG22	25:A:775:CLA:HAB	1.88	0.55
25:B:739:CLA:H3A	25:B:753:CLA:HAB	1.89	0.55
6:F:81:VAL:HG21	12:d:115:LEU:HD13	1.88	0.55
2:B:442:VAL:HG21	25:B:756:CLA:HAC2	1.88	0.55
12:d:176:ARG:HA	12:d:179:MET:HE3	1.88	0.55
21:g:82:LEU:HG	21:g:86:GLN:HE21	1.71	0.55
25:B:738:CLA:HBD	25:B:738:CLA:H122	1.89	0.55
25:B:755:CLA:HBC2	25:B:783:CLA:HMC2	1.87	0.55
22:n:105:THR:HG22	25:n:606:CLA:C4A	2.29	0.55
25:c:603:CLA:HBC1	35:c:607:CHL:HBB2	1.88	0.55
19:m:8:PRO:HD3	25:m:601:CLA:C1B	2.37	0.55
19:m:165:ASN:HB3	19:m:166:PRO:HD3	1.87	0.55
9:a:136:ARG:HA	9:a:139:MET:HE3	1.88	0.55
25:j:613:CLA:H122	25:j:613:CLA:HAB	1.88	0.55
25:g:608:CLA:HAA1	25:g:608:CLA:HBD	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:LEU:HB3	1:A:541:PHE:HB2	1.88	0.55
13:e:5:PHE:HB3	13:e:8:ALA:HB2	1.88	0.55
15:i:30:ALA:HB2	25:i:602:CLA:HBA1	1.89	0.55
16:j:51:ARG:HA	16:j:54:MET:HE3	1.88	0.55
21:g:112:TYR:HB3	25:g:610:CLA:HED2	1.89	0.55
1:A:162:THR:OG1	25:A:799:CLA:HBA1	2.07	0.54
2:B:155:LEU:HD13	25:h:612:CLA:H41	1.89	0.54
13:e:120:ASN:HA	13:e:127:ALA:HA	1.89	0.54
1:A:85:GLU:HB3	1:A:170:SER:HB2	1.89	0.54
1:A:714:GLN:HE22	5:E:45:GLN:H	1.55	0.54
23:o:11:PRO:HD2	23:o:14:LEU:HD12	1.89	0.54
14:h:5:ILE:HG12	14:h:6:PRO:HD2	1.89	0.54
1:A:363:LEU:HD11	25:A:769:CLA:H71	1.89	0.54
25:B:750:CLA:HHC	25:B:777:CLA:HMD3	1.89	0.54
16:j:105:TRP:HB2	19:m:40:ARG:HG3	1.90	0.54
25:f:613:CLA:HAA1	25:f:613:CLA:HBD	1.89	0.54
25:p:610:CLA:HAB	25:p:612:CLA:HAC2	1.90	0.54
1:A:330:THR:HG22	1:A:337:GLY:HA3	1.90	0.54
2:B:301:ILE:HG21	25:B:750:CLA:HAC1	1.90	0.54
11:c:165:LEU:HD23	11:c:168:LYS:HD3	1.89	0.54
29:B:764:BCR:H343	25:B:772:CLA:H3A	1.90	0.54
8:M:13:LEU:HD21	29:M:201:BCR:HC32	1.88	0.54
14:h:134:ARG:HA	14:h:137:MET:HE3	1.89	0.54
4:D:127:ARG:HB2	4:D:137:LEU:HD11	1.89	0.54
13:e:160:ARG:HA	13:e:163:MET:HE3	1.90	0.54
22:n:145:ALA:HB2	25:n:610:CLA:HED3	1.90	0.54
25:A:752:CLA:HAB	25:B:736:CLA:HAA1	1.90	0.53
25:B:750:CLA:H142	25:B:777:CLA:H51	1.89	0.53
25:B:776:CLA:H52	13:e:113:PRO:HG3	1.90	0.53
17:k:5:ILE:HG23	17:k:8:ALA:HB2	1.91	0.53
25:B:752:CLA:H203	29:B:764:BCR:H15C	1.90	0.53
19:m:102:PHE:H	27:m:182:LHG:HC12	1.73	0.53
25:B:753:CLA:H141	25:B:778:CLA:H141	1.90	0.53
19:m:8:PRO:HD3	25:m:601:CLA:C2B	2.39	0.53
25:A:793:CLA:HMB2	7:J:26:LEU:HD21	1.91	0.53
9:a:115:PRO:HB3	25:a:608:CLA:HBC2	1.91	0.53
13:e:19:PRO:HB2	13:e:156:ILE:HD12	1.91	0.53
1:A:32:PRO:HB2	1:A:48:TRP:HH2	1.74	0.53
1:A:75:SER:OG	1:A:181:TYR:HB2	2.08	0.53
1:A:83:ILE:HD11	25:A:765:CLA:H112	1.90	0.53
25:B:758:CLA:H72	25:B:758:CLA:HBB1	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:760:CLA:H72	25:A:766:CLA:H12	1.90	0.52
2:B:524:ALA:HB2	25:B:758:CLA:HMA1	1.90	0.52
25:n:603:CLA:HAC2	25:n:607:CLA:HBB2	1.90	0.52
1:A:730:HIS:HE1	25:A:784:CLA:ND	2.08	0.52
25:B:774:CLA:H71	25:B:781:CLA:H11	1.91	0.52
25:i:603:CLA:HBB1	31:i:621:DD6:C6	2.38	0.52
21:g:102:TRP:HB2	24:p:35:ARG:HD3	1.91	0.52
10:b:140:ARG:HA	10:b:143:MET:HE3	1.91	0.52
25:i:613:CLA:HBD	25:i:613:CLA:HBA1	1.90	0.52
16:j:77:LYS:HG3	16:j:78:VAL:HG23	1.91	0.52
1:A:361:GLY:HA2	1:A:398:GLY:HA2	1.92	0.52
1:A:495:PRO:HG3	1:A:502:LEU:HD23	1.92	0.52
25:A:784:CLA:HBD	25:A:784:CLA:HBA1	1.91	0.52
2:B:373:THR:HG22	25:B:778:CLA:HAB	1.89	0.52
27:d:237:LHG:HC5	25:d:601:CLA:HMD3	1.92	0.52
25:A:775:CLA:HBC3	29:A:790:BCR:H313	1.91	0.52
14:h:2:LEU:HB3	25:h:601:CLA:HED3	1.91	0.52
2:B:668:ARG:HB2	28:B:761:PQN:H7	1.90	0.52
21:g:120:LEU:HB2	25:g:610:CLA:HBA1	1.92	0.52
16:j:181:TRP:HB2	16:j:182:PRO:HD3	1.92	0.52
17:k:134:ARG:HA	17:k:137:MET:HE3	1.91	0.52
2:B:631:LEU:HD22	2:B:724:PHE:HA	1.92	0.51
18:l:32:ALA:HB2	25:l:602:CLA:HBA1	1.91	0.51
25:l:613:CLA:HBD	25:l:613:CLA:HBA1	1.92	0.51
20:f:157:HIS:CD2	25:f:614:CLA:NC	2.78	0.51
1:A:142:SER:HA	25:A:775:CLA:HMA2	1.92	0.51
1:A:622:VAL:HG22	1:A:627:VAL:HG22	1.91	0.51
13:e:48:ARG:HA	13:e:51:MET:HE3	1.91	0.51
22:n:159:LEU:HD21	25:n:612:CLA:HAA1	1.91	0.51
1:A:349:TRP:HB3	25:A:760:CLA:HAC1	1.91	0.51
10:b:43:HIS:CE1	25:b:609:CLA:HMD3	2.45	0.51
1:A:598:TRP:CH2	25:A:758:CLA:HAB	2.45	0.51
2:B:174:ARG:HB2	25:B:745:CLA:HBC2	1.92	0.51
2:B:564:ARG:HG2	5:E:48:GLU:HG2	1.93	0.51
15:i:31:ALA:HB3	19:m:33:ALA:HB3	1.93	0.51
25:A:774:CLA:HMB1	25:A:780:CLA:HAA2	1.93	0.51
25:B:759:CLA:HBB2	28:B:761:PQN:H141	1.93	0.51
5:E:11:ILE:HD11	5:E:42:PHE:CZ	2.46	0.51
25:k:610:CLA:H43	25:k:612:CLA:HBA1	1.91	0.51
25:n:604:CLA:HAA1	25:n:604:CLA:HBD	1.91	0.51
19:m:126:THR:HG22	25:m:610:CLA:H3A	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:B:764:BCR:H313	25:B:772:CLA:H12	1.92	0.51
17:k:78:PRO:HB2	18:l:80:ILE:HG22	1.93	0.51
23:o:4:TRP:H	23:o:4:TRP:CD1	2.29	0.51
24:p:44:ALA:HB1	24:p:129:GLY:HA3	1.93	0.51
25:A:753:CLA:HMD3	2:B:533:ILE:HG12	1.93	0.51
2:B:411:ILE:HA	2:B:414:HIS:CE1	2.46	0.51
15:i:94:VAL:HG11	22:n:111:PRO:HD3	1.93	0.51
17:k:44:VAL:HG22	17:k:130:ILE:HD11	1.93	0.51
19:m:118:PRO:HD2	31:m:620:DD6:O2	2.11	0.51
2:B:189:ALA:HA	25:B:772:CLA:HAB	1.92	0.50
6:F:20:LEU:HB2	6:F:55:PHE:CD2	2.45	0.50
25:h:610:CLA:H12	25:h:610:CLA:HMB1	1.93	0.50
2:B:519:VAL:HG21	2:B:593:TYR:HB2	1.93	0.50
25:h:613:CLA:HBA1	25:h:613:CLA:HBD	1.92	0.50
16:j:34:ALA:HB3	18:l:33:ALA:HB3	1.93	0.50
19:m:6:TRP:HA	25:m:601:CLA:C4D	2.41	0.50
19:m:18:GLY:HA2	19:m:23:ASP:HB3	1.93	0.50
29:M:201:BCR:H382	29:M:201:BCR:H23C	1.93	0.50
27:c:243:LHG:HC32	25:c:601:CLA:HAC1	1.94	0.50
14:h:46:HIS:CE1	25:h:609:CLA:HMD3	2.46	0.50
10:b:54:SER:HB2	10:b:65:TRP:HB3	1.92	0.50
24:p:38:VAL:HG22	24:p:107:SER:HB2	1.93	0.50
15:i:90:GLY:HA2	15:i:93:GLU:HB2	1.91	0.50
25:A:791:CLA:H51	2:B:438:VAL:HG13	1.94	0.50
22:n:71:ALA:HB3	22:n:74:GLU:HG2	1.92	0.50
15:i:161:PRO:O	15:i:162:LEU:HB2	2.11	0.50
1:A:154:THR:HG21	1:A:237:LEU:HD12	1.94	0.50
25:B:737:CLA:HED3	25:B:737:CLA:HBA2	1.94	0.50
17:k:121:THR:HG21	25:k:610:CLA:HED3	1.94	0.50
21:g:42:ALA:HB2	25:g:609:CLA:HED2	1.92	0.50
25:g:610:CLA:HBB2	25:g:612:CLA:CHB	2.41	0.50
12:d:66:LEU:HD23	25:d:604:CLA:HMC1	1.94	0.50
25:j:609:CLA:H2	27:m:182:LHG:H132	1.94	0.49
2:B:123:TRP:HH2	25:B:752:CLA:H12	1.77	0.49
2:B:340:SER:HA	25:B:781:CLA:H51	1.93	0.49
25:B:785:CLA:HAA1	25:B:785:CLA:HBD	1.93	0.49
15:i:41:VAL:HG22	15:i:107:ARG:HG3	1.94	0.49
22:n:20:ARG:HH21	22:n:151:LEU:HD21	1.76	0.49
25:l:602:CLA:H43	25:l:603:CLA:HBA1	1.94	0.49
1:A:574:PRO:HB3	1:A:720:ILE:HB	1.94	0.49
1:A:683:LEU:HB2	25:A:753:CLA:HMC2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:279:ALA:HB2	25:B:773:CLA:HBB1	1.94	0.49
2:B:687:ILE:HD11	16:j:123:LEU:HD21	1.95	0.49
25:a:613:CLA:H11	25:a:619:CLA:H52	1.95	0.49
25:c:609:CLA:HBA1	12:d:37:THR:HG21	1.95	0.49
27:j:198:LHG:H262	25:j:601:CLA:HMD2	1.93	0.49
9:a:29:PHE:CD2	25:a:602:CLA:H12	2.47	0.49
16:j:44:ILE:HG12	16:j:114:SER:HB2	1.94	0.49
18:l:42:ARG:O	18:l:46:VAL:HG23	2.13	0.49
25:A:776:CLA:H12	29:A:787:BCR:H311	1.94	0.49
23:o:89:ALA:HB3	23:o:90:PRO:HD3	1.94	0.49
25:A:758:CLA:NB	25:B:737:CLA:HBB1	2.27	0.49
25:A:783:CLA:HBB2	6:F:107:GLY:HA3	1.94	0.49
27:d:237:LHG:HC61	27:d:237:LHG:H111	1.95	0.49
1:A:677:PHE:CG	29:A:790:BCR:H363	2.47	0.49
25:a:602:CLA:H3A	25:a:602:CLA:CGA	2.43	0.49
25:f:608:CLA:HAA2	25:f:608:CLA:HBD	1.94	0.49
25:n:602:CLA:H43	25:n:603:CLA:HBA1	1.94	0.49
1:A:197:MET:HE2	25:A:766:CLA:HHD	1.94	0.49
12:d:164:PHE:CZ	25:d:610:CLA:HED3	2.48	0.49
15:i:145:VAL:HA	15:i:174:TRP:HB2	1.95	0.49
23:o:142:LEU:HD13	23:o:153:PRO:HB3	1.94	0.49
1:A:59:PHE:CD2	25:A:760:CLA:HMC2	2.48	0.48
19:m:7:PHE:HA	25:m:601:CLA:C1B	2.43	0.48
1:A:198:LEU:HG	25:A:772:CLA:HMD2	1.95	0.48
1:A:345:PHE:HZ	29:A:788:BCR:H24C	1.78	0.48
2:B:355:LEU:HD11	25:B:781:CLA:HBB1	1.95	0.48
22:n:105:THR:HA	25:n:606:CLA:HMA3	1.96	0.48
1:A:218:ILE:HA	1:A:222:LEU:HD12	1.94	0.48
1:A:679:TRP:O	1:A:682:THR:HB	2.14	0.48
25:o:610:CLA:HBB2	25:o:612:CLA:CHB	2.44	0.48
1:A:77:HIS:CE1	25:A:760:CLA:ND	2.81	0.48
25:i:604:CLA:HAB	25:i:608:CLA:H52	1.95	0.48
22:n:47:TRP:CD2	25:n:608:CLA:HED3	2.48	0.48
1:A:682:THR:HG23	1:A:727:GLY:O	2.13	0.48
25:A:791:CLA:HMB3	25:B:736:CLA:H191	1.96	0.48
2:B:643:LEU:HD11	2:B:731:ALA:HB2	1.94	0.48
25:B:741:CLA:O1A	25:B:778:CLA:HBD	2.13	0.48
25:B:756:CLA:HBB1	25:B:779:CLA:C2B	2.44	0.48
9:a:48:ARG:HA	9:a:51:MET:HE3	1.95	0.48
14:h:48:ARG:HA	14:h:51:MET:HE3	1.94	0.48
27:h:189:LHG:H101	27:h:189:LHG:H131	1.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:j:137:ARG:HA	16:j:140:MET:HE3	1.96	0.48
17:k:47:GLY:O	17:k:51:MET:HG3	2.13	0.48
1:A:419:PRO:HG2	4:D:81:GLU:HB2	1.96	0.48
25:A:777:CLA:H101	27:A:786:LHG:H331	1.94	0.48
17:k:91:LEU:HD13	25:k:608:CLA:HMA1	1.95	0.48
23:o:6:PRO:HD3	25:o:601:CLA:HMA1	1.96	0.48
25:h:615:CLA:HBD	25:h:615:CLA:HAA2	1.95	0.48
15:i:37:GLU:HG3	15:i:40:ARG:HH12	1.78	0.48
25:B:775:CLA:HBB2	33:B:786:LMG:H362	1.96	0.48
25:c:603:CLA:H43	12:d:40:LEU:HD21	1.94	0.48
25:c:610:CLA:H3A	25:c:610:CLA:HBA2	1.45	0.48
25:k:618:CLA:HBB2	25:l:609:CLA:H101	1.96	0.48
1:A:408:HIS:HE1	25:A:777:CLA:NA	2.11	0.47
25:B:738:CLA:HBC2	25:B:753:CLA:HMA1	1.96	0.47
1:A:681:PHE:N	25:A:753:CLA:HAB	2.28	0.47
25:A:755:CLA:H62	25:A:755:CLA:H41	1.56	0.47
25:g:613:CLA:HAA1	25:g:613:CLA:HBD	1.96	0.47
23:o:35:VAL:O	23:o:36:TYR:HB3	2.12	0.47
24:p:58:GLU:HG3	24:p:63:GLY:C	2.40	0.47
2:B:230:TRP:CH2	25:B:747:CLA:HBB1	2.50	0.47
25:B:752:CLA:H192	29:B:763:BCR:H352	1.95	0.47
12:d:157:LEU:HB2	25:d:610:CLA:HBA1	1.94	0.47
25:d:603:CLA:HBC1	35:d:607:CHL:HBB2	1.96	0.47
13:e:174:TYR:CD1	34:e:205:DGD:HG11	2.49	0.47
25:e:602:CLA:H3A	25:e:602:CLA:HBA2	1.55	0.47
20:f:155:VAL:O	20:f:159:LYS:HG2	2.14	0.47
25:A:784:CLA:HAC1	28:A:785:PQN:H192	1.96	0.47
25:c:602:CLA:H3A	25:c:602:CLA:HBA2	1.56	0.47
23:o:112:PRO:HD3	25:o:608:CLA:HMD2	1.97	0.47
25:B:751:CLA:HBB1	29:B:766:BCR:C19	2.44	0.47
14:h:129:GLU:HB2	25:h:610:CLA:CHB	2.45	0.47
25:h:608:CLA:H3A	25:h:608:CLA:HBA2	1.56	0.47
18:l:126:THR:HG22	25:l:610:CLA:HBB	1.96	0.47
21:g:4:TRP:O	25:g:601:CLA:NA	2.48	0.47
2:B:373:THR:HG23	2:B:591:THR:HG21	1.97	0.47
14:h:93:TYR:CE2	25:o:609:CLA:HBA1	2.50	0.47
23:o:30:ALA:HB1	23:o:36:TYR:HB2	1.97	0.47
25:A:763:CLA:H162	25:A:763:CLA:H122	1.71	0.47
2:B:150:LEU:HD22	8:M:22:ALA:HA	1.96	0.47
2:B:299:HIS:HB3	2:B:304:ILE:HD11	1.96	0.47
2:B:661:PHE:HB3	25:B:737:CLA:HMC2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:c:74:ALA:HB2	11:c:81:PHE:HD2	1.80	0.47
25:c:608:CLA:HBD	25:c:608:CLA:HAA1	1.97	0.47
13:e:103:ILE:HG12	25:e:605:CLA:HBC2	1.97	0.47
14:h:75:TYR:OH	25:h:604:CLA:H2A	2.14	0.47
15:i:174:TRP:HE1	25:j:618:CLA:CAD	2.27	0.47
25:j:610:CLA:H61	25:j:610:CLA:H41	1.72	0.47
19:m:113:TYR:HB3	25:m:610:CLA:HED2	1.96	0.47
20:f:48:ARG:HA	20:f:51:MET:HE3	1.94	0.47
25:p:602:CLA:H3A	25:p:602:CLA:HBA2	1.66	0.47
1:A:382:ILE:HG21	1:A:517:ILE:HB	1.96	0.47
25:A:799:CLA:H3A	25:A:799:CLA:HBA2	1.49	0.47
25:l:602:CLA:H61	25:l:602:CLA:H41	1.80	0.47
22:n:79:ALA:HB2	22:n:84:LEU:HD11	1.96	0.47
1:A:80:GLN:HG2	25:A:760:CLA:H3A	1.97	0.47
2:B:22:TRP:CG	2:B:704:GLN:HE22	2.33	0.47
25:B:784:CLA:HAC2	33:B:786:LMG:HC71	1.96	0.47
11:c:10:LYS:HE2	27:c:243:LHG:HC2	1.97	0.47
11:c:155:LEU:HB2	25:c:610:CLA:HBA1	1.97	0.47
25:h:608:CLA:HBD	25:h:608:CLA:HAA1	1.97	0.47
16:j:31:GLY:HA3	18:l:37:VAL:HG21	1.96	0.47
25:f:613:CLA:H62	25:f:613:CLA:H92	1.70	0.47
22:n:117:TRP:HZ3	25:n:609:CLA:HED3	1.80	0.47
23:o:133:ARG:HA	23:o:136:MET:HE3	1.97	0.47
25:A:767:CLA:HBD	25:A:767:CLA:HAA1	1.97	0.47
25:A:784:CLA:H61	25:A:784:CLA:H41	1.77	0.47
13:e:14:LEU:HD11	13:e:25:ASP:HB2	1.97	0.47
14:h:125:THR:HG22	25:h:610:CLA:H3A	1.97	0.47
25:o:602:CLA:HBA2	25:o:602:CLA:H3A	1.76	0.47
25:A:775:CLA:H61	25:A:775:CLA:H41	1.69	0.46
3:C:29:VAL:HG21	4:D:154:LYS:HG3	1.97	0.46
25:d:602:CLA:HBB2	25:d:603:CLA:CHB	2.45	0.46
27:j:198:LHG:HC82	27:j:198:LHG:H281	1.97	0.46
18:l:162:HIS:CD2	25:l:614:CLA:NB	2.83	0.46
19:m:31:LEU:HD12	25:m:602:CLA:H12	1.97	0.46
1:A:441:LEU:HG	1:A:548:LEU:HB2	1.97	0.46
25:A:770:CLA:H62	25:A:770:CLA:H92	1.83	0.46
25:B:756:CLA:H51	25:B:756:CLA:H8	1.51	0.46
11:c:24:LEU:HD11	11:c:35:ASP:HB2	1.96	0.46
20:f:68:TRP:HD1	20:f:150:PRO:HG3	1.80	0.46
25:g:602:CLA:H3A	25:g:602:CLA:HBA2	1.72	0.46
25:A:768:CLA:HBA2	25:A:768:CLA:H3A	1.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:785:CLA:HMD3	12:d:115:LEU:HD23	1.97	0.46
25:h:601:CLA:H3A	25:h:601:CLA:HBA2	1.47	0.46
15:i:166:ILE:HD13	25:j:604:CLA:H101	1.97	0.46
27:i:194:LHG:H302	27:i:194:LHG:H112	1.98	0.46
25:i:610:CLA:HMB3	25:i:612:CLA:HAA1	1.98	0.46
21:g:166:LEU:HD12	30:g:190:SQD:H5	1.96	0.46
22:n:86:TYR:HD2	22:n:92:LEU:HD13	1.80	0.46
1:A:704:HIS:HE1	25:A:783:CLA:C4D	2.27	0.46
2:B:26:ALA:HB2	34:B:787:DGD:HB42	1.97	0.46
25:a:602:CLA:H11	31:a:621:DD6:O1	2.15	0.46
25:a:609:CLA:HMB1	10:b:100:TYR:HB2	1.97	0.46
15:i:47:GLY:O	15:i:51:MET:HG3	2.15	0.46
25:i:610:CLA:H41	25:i:610:CLA:H61	1.74	0.46
25:f:610:CLA:H41	25:f:610:CLA:H61	1.56	0.46
25:A:765:CLA:H41	25:A:765:CLA:H62	1.49	0.46
2:B:712:HIS:HE1	25:B:760:CLA:ND	2.12	0.46
9:a:120:LEU:HD12	9:a:122:MET:HE2	1.97	0.46
25:h:602:CLA:H41	25:h:602:CLA:H61	1.58	0.46
16:j:72:PHE:CD2	16:j:150:SER:HB2	2.51	0.46
18:l:126:THR:HG21	25:l:610:CLA:HBA2	1.97	0.46
15:i:167:ALA:O	25:j:604:CLA:H11	2.16	0.46
16:j:173:ILE:HD11	25:k:604:CLA:H161	1.98	0.46
23:o:68:TRP:HE1	23:o:142:LEU:HD11	1.81	0.46
2:B:365:ARG:HB3	2:B:602:TRP:CZ3	2.51	0.46
25:B:780:CLA:H62	25:B:780:CLA:H41	1.56	0.46
6:F:142:TRP:CG	6:F:143:PRO:HD3	2.50	0.46
25:e:610:CLA:HBB2	25:e:612:CLA:CHB	2.45	0.46
17:k:117:PRO:HB3	33:k:179:LMG:H142	1.98	0.46
25:g:613:CLA:H62	25:g:613:CLA:H41	1.70	0.46
22:n:58:PRO:HA	22:n:69:LEU:HB3	1.97	0.46
1:A:36:SER:HB3	1:A:39:LEU:HB2	1.98	0.46
25:A:784:CLA:H142	29:A:796:BCR:H363	1.98	0.46
25:A:794:CLA:H112	6:F:129:VAL:HG13	1.98	0.46
22:n:173:VAL:HG23	22:n:174:THR:HG23	1.97	0.46
24:p:57:PRO:O	24:p:58:GLU:HB2	2.15	0.46
25:A:763:CLA:HAB	29:A:792:BCR:H352	1.98	0.46
2:B:15:ASP:HB3	2:B:20:ARG:HB2	1.98	0.46
2:B:707:LEU:HD23	34:B:787:DGD:HB31	1.98	0.46
25:B:776:CLA:HAB	33:B:786:LMG:H132	1.97	0.46
4:D:28:ILE:HD12	4:D:30:TRP:HD1	1.80	0.46
4:D:123:PHE:CE2	4:D:138:HIS:HD2	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:p:8:PRO:HG2	24:p:22:ASP:H	1.80	0.46
1:A:216:HIS:HB2	25:A:799:CLA:C1C	2.46	0.46
1:A:301:LEU:HD11	25:A:769:CLA:HBB1	1.97	0.46
2:B:279:ALA:CB	25:B:773:CLA:HBB1	2.46	0.46
2:B:351:HIS:CD2	25:B:781:CLA:NC	2.85	0.46
2:B:648:TRP:CE3	29:B:767:BCR:HC41	2.51	0.46
18:l:134:GLY:O	18:l:138:MET:HG3	2.16	0.46
20:f:144:HIS:HB2	25:f:615:CLA:HED1	1.97	0.46
25:A:772:CLA:HBB2	29:A:788:BCR:H361	1.98	0.45
4:D:113:ARG:HG2	4:D:121:THR:HG22	1.98	0.45
25:l:614:CLA:HAA1	25:l:614:CLA:HBD	1.97	0.45
21:g:125:THR:HG22	25:g:610:CLA:H3A	1.97	0.45
25:g:613:CLA:H3A	25:g:613:CLA:HBA2	1.78	0.45
2:B:278:LEU:HD11	25:B:747:CLA:HAB	1.96	0.45
2:B:301:ILE:HG23	25:B:774:CLA:HED3	1.97	0.45
25:B:785:CLA:H3A	25:B:785:CLA:HBA2	1.65	0.45
25:i:601:CLA:H3A	25:i:601:CLA:HBA2	1.60	0.45
20:f:40:ARG:HB2	20:f:107:ARG:HH21	1.82	0.45
1:A:262:ALA:HA	25:a:619:CLA:H43	1.98	0.45
1:A:643:ASN:HB2	2:B:651:LEU:HD11	1.98	0.45
25:B:758:CLA:HBA2	25:B:782:CLA:CGA	2.47	0.45
29:B:765:BCR:H363	25:B:774:CLA:H2	1.97	0.45
25:h:610:CLA:HMB3	25:h:612:CLA:HAA1	1.96	0.45
15:i:93:GLU:OE1	15:i:96:ARG:HD3	2.16	0.45
20:f:81:GLU:HA	20:f:84:VAL:HG22	1.97	0.45
2:B:523:ILE:CG2	25:B:782:CLA:HBB1	2.45	0.45
11:c:61:MET:HE3	11:c:172:ASN:HB3	1.97	0.45
25:k:608:CLA:HAA1	25:k:608:CLA:HBD	1.99	0.45
18:l:7:PHE:CG	18:l:8:PRO:HD2	2.52	0.45
2:B:276:HIS:HB2	25:B:773:CLA:CHB	2.45	0.45
11:c:137:LEU:HB2	25:c:608:CLA:HMC2	1.98	0.45
11:c:174:ARG:HA	11:c:177:MET:HE3	1.97	0.45
1:A:406:ALA:HB2	29:A:789:BCR:H323	1.98	0.45
2:B:65:LEU:HD11	29:B:764:BCR:H281	1.97	0.45
29:B:767:BCR:H383	25:B:770:CLA:HMD3	1.99	0.45
25:l:610:CLA:HBA2	25:l:610:CLA:H3A	1.49	0.45
1:A:197:MET:HB2	25:A:766:CLA:HBC2	1.98	0.45
25:A:805:CLA:CAD	4:D:29:PHE:HB2	2.47	0.45
2:B:594:TRP:CD1	25:B:782:CLA:HBC2	2.52	0.45
25:h:604:CLA:HBA1	25:h:604:CLA:H3A	1.73	0.45
23:o:160:HIS:HE1	25:o:614:CLA:C4A	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:523:ILE:HG23	25:B:782:CLA:HBB1	1.99	0.45
25:B:748:CLA:HBA2	25:B:748:CLA:H3A	1.86	0.45
3:C:15:THR:HG22	3:C:28:MET:HG3	1.97	0.45
25:B:741:CLA:H203	25:B:741:CLA:H162	1.70	0.45
25:B:756:CLA:H91	6:F:99:VAL:HG21	1.98	0.45
25:j:610:CLA:HBA2	25:j:610:CLA:H3A	1.50	0.45
25:k:613:CLA:HAA1	25:k:613:CLA:HBD	1.98	0.45
1:A:297:HIS:HB2	25:A:768:CLA:C1B	2.47	0.45
25:A:768:CLA:H102	25:A:768:CLA:HBC3	1.99	0.45
25:B:758:CLA:HBD	25:B:758:CLA:HBA1	1.99	0.45
10:b:152:GLN:HB3	10:b:163:ASN:ND2	2.32	0.45
25:i:610:CLA:H3A	25:i:610:CLA:HBA2	1.45	0.45
21:g:121:THR:HG21	25:g:610:CLA:HED3	1.98	0.45
25:g:615:CLA:HAA2	25:g:615:CLA:HBD	1.99	0.45
22:n:59:GLU:HB2	22:n:179:LEU:HD12	2.00	0.45
1:A:53:HIS:HB3	27:A:786:LHG:H111	1.99	0.44
2:B:576:PHE:O	2:B:580:VAL:HG23	2.16	0.44
3:C:61:ASP:HB2	5:E:53:ASN:ND2	2.31	0.44
25:b:605:CLA:HAA1	25:b:605:CLA:HBD	1.99	0.44
35:d:606:CHL:HBA2	35:d:606:CHL:HBD	1.99	0.44
21:g:95:ARG:HA	25:g:608:CLA:HBC2	2.00	0.44
2:B:308:HIS:HE1	25:B:776:CLA:ND	2.12	0.44
25:B:739:CLA:H112	25:B:739:CLA:H152	1.77	0.44
25:B:739:CLA:H191	25:B:778:CLA:H151	2.00	0.44
22:n:70:PRO:HD2	25:n:604:CLA:HED3	1.99	0.44
23:o:36:TYR:HA	23:o:39:MET:HB2	1.99	0.44
25:A:772:CLA:H193	25:A:772:CLA:H162	1.89	0.44
25:A:783:CLA:HBB1	25:A:794:CLA:HMD3	2.00	0.44
25:A:798:CLA:H62	25:A:798:CLA:H41	1.79	0.44
2:B:123:TRP:CH2	25:B:752:CLA:H12	2.52	0.44
2:B:287:ALA:HB2	25:B:774:CLA:HBC2	1.99	0.44
2:B:443:MET:SD	2:B:451:LYS:HE3	2.57	0.44
25:m:602:CLA:H41	25:m:603:CLA:H3A	2.00	0.44
1:A:532:ASP:HA	1:A:535:VAL:HG12	2.00	0.44
2:B:230:TRP:HB2	25:B:747:CLA:HBA1	2.00	0.44
25:g:610:CLA:H3A	25:g:610:CLA:HBA2	1.68	0.44
1:A:578:PRO:HD3	2:B:561:GLY:HA2	1.99	0.44
25:A:752:CLA:HAA2	25:A:752:CLA:CGD	2.48	0.44
25:B:771:CLA:HAA1	25:B:771:CLA:HBD	1.99	0.44
25:a:619:CLA:HED2	25:a:619:CLA:HBD	1.86	0.44
25:b:612:CLA:H62	25:b:612:CLA:H41	1.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:e:123:LEU:HD21	25:e:608:CLA:CBB	2.48	0.44
25:k:602:CLA:H72	25:k:603:CLA:HMB3	1.98	0.44
25:l:610:CLA:H61	25:l:610:CLA:H41	1.66	0.44
2:B:712:HIS:HE1	25:B:760:CLA:C4D	2.31	0.44
29:B:766:BCR:H11C	25:B:783:CLA:H43	2.00	0.44
7:J:24:SER:HB3	25:J:101:CLA:HHC	1.99	0.44
25:b:604:CLA:HBA1	25:b:604:CLA:HBD	1.98	0.44
14:h:10:PRO:HA	14:h:11:PRO:HD3	1.82	0.44
16:j:44:ILE:HD13	19:m:104:TRP:NE1	2.33	0.44
25:l:602:CLA:H3A	25:l:602:CLA:HBA2	1.54	0.44
1:A:176:ALA:HB2	25:A:764:CLA:HBC2	1.99	0.44
25:A:765:CLA:H11	25:A:797:CLA:HBD	1.99	0.44
2:B:583:MET:O	2:B:587:ILE:HG12	2.18	0.44
11:c:59:TRP:CE2	25:c:608:CLA:HED2	2.53	0.44
16:j:94:LEU:HD13	25:j:608:CLA:HMA2	2.00	0.44
25:c:613:CLA:H2	25:c:614:CLA:HMD1	1.99	0.44
13:e:4:TRP:H	13:e:4:TRP:CD1	2.35	0.44
19:m:114:PRO:HB3	25:m:608:CLA:HBC2	1.99	0.44
1:A:117:ILE:O	25:A:798:CLA:HED2	2.18	0.44
25:A:769:CLA:H72	25:A:769:CLA:H112	1.67	0.44
25:A:783:CLA:H92	25:A:783:CLA:H62	1.77	0.44
25:A:793:CLA:HAA1	6:F:99:VAL:HG13	2.00	0.44
25:a:608:CLA:H41	25:a:608:CLA:H62	1.76	0.44
25:c:603:CLA:H11	25:c:603:CLA:HMA2	2.00	0.44
25:c:613:CLA:HAA1	25:c:613:CLA:HBD	1.99	0.44
25:m:602:CLA:H41	25:m:602:CLA:H62	1.92	0.44
2:B:456:GLU:HG3	6:F:7:LEU:HD11	2.00	0.43
11:c:94:PHE:CE1	12:d:213:THR:HG22	2.53	0.43
25:d:611:CLA:HBD	25:d:611:CLA:HAA1	2.00	0.43
16:j:52:LEU:HD22	25:j:609:CLA:HHH	1.99	0.43
24:p:109:PRO:HB3	25:p:608:CLA:HBC2	1.99	0.43
1:A:680:ALA:C	25:A:753:CLA:HAB	2.43	0.43
2:B:48:ALA:HB3	8:M:29:LEU:HD21	2.00	0.43
2:B:387:PHE:HB3	2:B:534:LEU:HB3	2.00	0.43
29:B:766:BCR:H17C	25:B:781:CLA:H112	2.00	0.43
16:j:40:GLU:HG2	16:j:43:ARG:HH22	1.83	0.43
22:n:55:CYS:O	22:n:58:PRO:HD2	2.18	0.43
1:A:392:THR:HG23	1:A:607:ILE:HG21	1.99	0.43
1:A:498:THR:HG21	25:A:780:CLA:CMD	2.48	0.43
25:A:800:CLA:HBA1	25:A:800:CLA:H3A	1.87	0.43
2:B:383:MET:HE1	29:B:766:BCR:H361	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:J:101:CLA:H3A	25:J:101:CLA:HBA2	1.47	0.43
15:i:14:LEU:HD11	15:i:25:ASP:HB2	1.99	0.43
23:o:53:ALA:HB3	23:o:139:LEU:HD11	2.00	0.43
1:A:666:SER:HB2	2:B:445:ALA:HB1	1.99	0.43
2:B:275:HIS:HE1	25:B:747:CLA:C4D	2.31	0.43
25:B:746:CLA:HBB2	25:B:752:CLA:H143	2.00	0.43
1:A:95:GLY:O	1:A:99:SER:HB2	2.19	0.43
1:A:366:ILE:HA	25:A:773:CLA:HED2	2.00	0.43
25:a:603:CLA:H11	25:a:603:CLA:HBA1	1.72	0.43
15:i:99:LYS:HB2	15:i:106:LYS:HD3	1.99	0.43
1:A:393:HIS:HE2	25:A:776:CLA:C1B	2.32	0.43
1:A:455:LEU:HD22	1:A:472:PHE:CE2	2.53	0.43
2:B:86:PRO:HB3	2:B:121:TYR:CG	2.54	0.43
2:B:600:THR:HG21	2:B:609:PHE:HB2	2.00	0.43
25:B:739:CLA:H3A	25:B:753:CLA:CAB	2.48	0.43
25:B:777:CLA:HBD	25:B:777:CLA:HBA1	1.99	0.43
18:l:18:GLY:HA2	18:l:23:ASP:HB3	2.00	0.43
1:A:161:ILE:HG22	25:A:799:CLA:H12	2.00	0.43
25:A:791:CLA:C1D	25:B:736:CLA:H2	2.49	0.43
2:B:142:LEU:HG	29:B:764:BCR:H382	1.99	0.43
25:b:612:CLA:H2	25:c:611:CLA:C1B	2.48	0.43
12:d:124:PHE:HB3	31:d:623:DD6:C3	2.48	0.43
13:e:174:TYR:HD1	34:e:205:DGD:HG11	1.84	0.43
25:f:613:CLA:H3A	25:f:613:CLA:HBA2	1.86	0.43
25:A:752:CLA:C1A	25:B:736:CLA:HAB	2.47	0.43
2:B:145:ILE:HD12	25:B:746:CLA:H152	2.01	0.43
25:B:745:CLA:H152	29:B:763:BCR:H271	2.01	0.43
25:a:611:CLA:H3A	25:a:611:CLA:HBA2	1.69	0.43
10:b:133:THR:HG22	10:b:137:LYS:HD2	2.01	0.43
27:b:181:LHG:HC32	34:b:182:DGD:HA82	2.00	0.43
11:c:166:LYS:O	11:c:170:VAL:HG23	2.19	0.43
25:c:609:CLA:HBA2	25:c:609:CLA:H3A	1.55	0.43
25:h:603:CLA:HBB1	25:h:615:CLA:HMB2	2.01	0.43
25:a:613:CLA:H62	25:a:613:CLA:H41	1.73	0.43
25:m:613:CLA:HED3	25:m:613:CLA:H2A	2.01	0.43
22:n:57:VAL:HA	22:n:60:VAL:HG12	2.01	0.43
24:p:56:VAL:HG13	24:p:60:LEU:HD13	2.01	0.43
2:B:558:PRO:HB3	2:B:702:ILE:HB	2.00	0.43
11:c:54:ILE:HG21	11:c:144:VAL:HG13	2.01	0.43
25:e:604:CLA:HBD	25:e:604:CLA:HAA1	2.00	0.43
25:h:609:CLA:HHC	25:h:609:CLA:HBB1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:h:610:CLA:H92	25:h:610:CLA:H61	1.76	0.43
1:A:585:GLN:HA	1:A:590:ASP:OD2	2.19	0.42
25:A:761:CLA:H202	25:A:761:CLA:H162	1.82	0.42
4:D:28:ILE:HG13	4:D:31:MET:H	1.83	0.42
9:a:44:VAL:HG22	9:a:132:ILE:HD11	2.01	0.42
11:c:158:ASP:HB3	11:c:161:ALA:HB3	2.01	0.42
27:h:190:LHG:H112	25:h:601:CLA:HMD2	2.00	0.42
25:h:610:CLA:H12	25:h:610:CLA:CMB	2.47	0.42
21:g:166:LEU:HG	30:g:190:SQD:H81	2.01	0.42
2:B:276:HIS:HB2	25:B:773:CLA:C1B	2.49	0.42
25:B:749:CLA:H3A	25:B:749:CLA:HBA2	1.50	0.42
9:a:86:PHE:HZ	34:b:182:DGD:HG11	1.85	0.42
12:d:131:TRP:CZ3	35:d:608:CHL:HAB	2.53	0.42
17:k:102:TRP:HB2	18:l:40:ARG:HG3	2.01	0.42
18:l:81:LYS:HE2	18:l:81:LYS:HB3	1.83	0.42
22:n:134:PRO:HB3	25:n:608:CLA:HBC2	2.01	0.42
25:A:763:CLA:H192	25:A:763:CLA:H161	1.76	0.42
28:A:785:PQN:H303	28:A:785:PQN:H261	1.79	0.42
2:B:374:HIS:HE2	25:B:752:CLA:C1B	2.33	0.42
23:o:21:ASP:HA	25:o:602:CLA:O1D	2.19	0.42
24:p:43:HIS:HE1	25:p:603:CLA:NA	2.16	0.42
24:p:142:GLN:HE22	25:p:613:CLA:C4C	2.32	0.42
25:A:772:CLA:H93	25:A:772:CLA:H62	1.75	0.42
25:A:783:CLA:H12	25:B:779:CLA:H42	2.00	0.42
2:B:467:HIS:CD2	25:B:757:CLA:ND	2.87	0.42
29:B:762:BCR:HC8	25:B:775:CLA:CMD	2.50	0.42
25:B:778:CLA:HBA2	25:B:778:CLA:H3A	1.78	0.42
5:E:2:GLY:HA2	5:E:3:PRO:HD3	1.90	0.42
17:k:112:TYR:HB3	25:k:610:CLA:HED2	2.00	0.42
25:m:602:CLA:H61	25:m:602:CLA:H92	1.80	0.42
25:g:602:CLA:H62	25:g:603:CLA:HMB1	2.02	0.42
22:n:9:PRO:HG2	22:n:12:LEU:HB3	2.01	0.42
29:B:766:BCR:C17	25:B:781:CLA:H112	2.49	0.42
25:b:612:CLA:H42	25:c:611:CLA:NC	2.35	0.42
15:i:39:MET:HB3	25:i:602:CLA:H3A	2.01	0.42
25:g:601:CLA:HAA1	25:g:601:CLA:HBD	2.01	0.42
23:o:124:THR:HG23	25:o:610:CLA:H3A	2.01	0.42
24:p:48:MET:HE2	24:p:48:MET:HB3	1.93	0.42
25:p:602:CLA:HBB2	25:p:603:CLA:CHD	2.50	0.42
1:A:95:GLY:HA2	1:A:99:SER:OG	2.18	0.42
1:A:126:ILE:HG21	2:B:446:PHE:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:A:792:BCR:H20C	29:A:792:BCR:H361	1.92	0.42
2:B:494:LEU:HD23	2:B:494:LEU:HA	1.81	0.42
10:b:131:THR:HG22	25:b:610:CLA:HBB	2.02	0.42
19:m:37:VAL:O	19:m:41:MET:HG2	2.19	0.42
25:g:609:CLA:H42	24:p:87:PRO:HG3	2.00	0.42
2:B:374:HIS:HB2	25:B:778:CLA:C1B	2.50	0.42
2:B:388:ALA:O	2:B:392:ILE:HG13	2.19	0.42
25:B:774:CLA:HAA1	25:B:777:CLA:OBD	2.20	0.42
14:h:14:LEU:HD11	14:h:25:ASP:HB2	2.02	0.42
25:k:610:CLA:HBA2	25:k:610:CLA:H3A	1.46	0.42
25:k:613:CLA:H62	25:k:613:CLA:H41	1.76	0.42
25:A:782:CLA:H2A	25:A:782:CLA:HED3	2.02	0.42
2:B:624:LEU:HD22	25:B:736:CLA:HMD3	2.02	0.42
2:B:716:GLY:O	2:B:720:THR:HG22	2.20	0.42
2:B:720:THR:HG23	25:B:736:CLA:O1D	2.20	0.42
25:a:610:CLA:HBA2	25:a:610:CLA:H3A	1.85	0.42
25:b:610:CLA:HBB2	25:b:612:CLA:CHB	2.50	0.42
35:d:605:CHL:HHC	35:d:605:CHL:HBB1	2.01	0.42
13:e:154:LYS:HD3	25:e:612:CLA:HAA2	2.01	0.42
25:l:609:CLA:H92	25:l:609:CLA:H61	1.78	0.42
20:f:59:VAL:N	20:f:60:PRO:HD2	2.34	0.42
15:i:154:LEU:HD13	25:i:614:CLA:HBC2	2.01	0.42
19:m:126:THR:CG2	25:m:610:CLA:H3A	2.49	0.42
20:f:37:GLU:HG3	20:f:40:ARG:NH2	2.35	0.42
25:g:609:CLA:HMB1	24:p:90:TYR:HB2	2.02	0.42
1:A:128:ASN:HB3	1:A:136:GLN:HB3	2.02	0.42
1:A:260:GLY:HA3	9:a:151:THR:HG23	2.01	0.42
1:A:301:LEU:CD1	25:A:769:CLA:HBB1	2.50	0.42
4:D:117:ALA:HB3	4:D:118:PRO:HD3	2.01	0.42
25:c:606:CLA:HMC3	35:c:607:CHL:C1C	2.50	0.42
14:h:125:THR:CG2	25:h:610:CLA:H3A	2.50	0.42
20:f:19:PHE:HE1	20:f:119:ASP:HB2	1.84	0.42
1:A:220:VAL:C	1:A:223:PRO:HD2	2.44	0.41
1:A:577:GLY:HA2	2:B:562:PRO:HD3	2.01	0.41
27:A:756:LHG:HC31	25:A:808:CLA:C1C	2.50	0.41
2:B:339:ALA:HB1	29:B:766:BCR:H20C	2.02	0.41
2:B:546:LEU:HD21	2:B:567:THR:HG22	2.01	0.41
25:B:739:CLA:H61	25:B:739:CLA:H41	1.49	0.41
10:b:102:ARG:HH22	25:b:609:CLA:CHA	2.33	0.41
27:c:243:LHG:H112	27:c:243:LHG:HC82	1.79	0.41
25:c:610:CLA:H43	25:c:612:CLA:HBA1	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:l:62:PRO:HG3	25:l:604:CLA:C1D	2.50	0.41
19:m:6:TRP:O	19:m:7:PHE:HB3	2.20	0.41
19:m:155:PRO:C	19:m:157:ALA:H	2.28	0.41
1:A:441:LEU:HD21	1:A:547:VAL:HG12	2.02	0.41
25:A:773:CLA:HBB1	25:A:782:CLA:HBB	2.01	0.41
2:B:197:VAL:C	2:B:200:PRO:HD2	2.45	0.41
15:i:166:ILE:O	15:i:167:ALA:HB3	2.21	0.41
25:i:613:CLA:HBC1	25:i:615:CLA:H43	2.02	0.41
16:j:182:PRO:HA	16:j:183:PRO:HD3	1.91	0.41
25:f:602:CLA:H3A	25:f:602:CLA:HBA2	1.70	0.41
25:p:602:CLA:HBB2	25:p:603:CLA:C1D	2.50	0.41
25:A:753:CLA:CGA	25:A:753:CLA:H3A	2.50	0.41
11:c:168:LYS:HE2	25:c:612:CLA:HBD	2.02	0.41
25:c:611:CLA:HBD	25:c:612:CLA:OBD	2.20	0.41
14:h:110:ARG:O	14:h:111:SER:HB3	2.20	0.41
16:j:14:PRO:HG2	16:j:28:ASP:HB3	2.02	0.41
25:l:609:CLA:HHC	25:l:609:CLA:HBB1	2.02	0.41
25:g:608:CLA:H3A	25:g:608:CLA:HBA2	1.58	0.41
29:B:767:BCR:H382	29:B:767:BCR:H23C	2.02	0.41
11:c:117:LEU:HD11	12:d:212:TRP:CE2	2.55	0.41
16:j:132:GLU:HB2	25:j:610:CLA:CHB	2.50	0.41
19:m:81:LYS:HE2	19:m:81:LYS:HB3	1.84	0.41
1:A:224:ILE:HG23	1:A:237:LEU:HD13	2.03	0.41
25:A:752:CLA:HAA2	25:A:752:CLA:O1D	2.21	0.41
25:A:800:CLA:HHC	25:A:800:CLA:HBB1	2.02	0.41
4:D:69:VAL:HG22	4:D:98:PHE:CD1	2.55	0.41
9:a:43:GLU:HB2	25:a:602:CLA:CHB	2.51	0.41
13:e:135:TYR:CE2	13:e:152:LYS:HE3	2.56	0.41
14:h:66:LYS:HD3	14:h:66:LYS:HA	1.85	0.41
23:o:121:THR:H	23:o:124:THR:CG2	2.29	0.41
25:A:771:CLA:CMB	25:A:808:CLA:HBB1	2.50	0.41
25:A:805:CLA:HBA1	4:D:28:ILE:HB	2.03	0.41
2:B:429:LEU:HB3	2:B:525:LEU:HB2	2.03	0.41
25:B:775:CLA:HBA1	25:B:776:CLA:H2	2.02	0.41
4:D:46:THR:O	4:D:50:THR:HG23	2.20	0.41
12:d:171:GLU:HB2	25:d:610:CLA:CHB	2.51	0.41
25:e:611:CLA:HBD	25:e:612:CLA:OBD	2.20	0.41
25:i:608:CLA:HBD	25:i:608:CLA:HAA2	2.01	0.41
25:p:609:CLA:H3A	25:p:609:CLA:HBA1	1.89	0.41
1:A:299:LEU:HD11	25:A:767:CLA:HAB	2.03	0.41
27:A:786:LHG:H272	27:A:786:LHG:H242	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:61:ASP:HB2	5:E:53:ASN:CG	2.45	0.41
25:a:610:CLA:H62	25:a:610:CLA:H41	1.75	0.41
10:b:44:SER:O	10:b:48:MET:HG3	2.20	0.41
10:b:44:SER:CB	10:b:139:GLY:HA3	2.48	0.41
10:b:102:ARG:HG2	25:b:608:CLA:CHD	2.50	0.41
27:b:181:LHG:H281	25:b:604:CLA:CAD	2.51	0.41
25:d:610:CLA:HBA2	25:d:610:CLA:H3A	1.83	0.41
13:e:167:PHE:CE2	25:e:602:CLA:H161	2.56	0.41
25:j:613:CLA:H92	25:j:613:CLA:H61	1.72	0.41
25:g:608:CLA:CAD	25:g:610:CLA:HMD3	2.50	0.41
22:n:52:LEU:HG	22:n:164:MET:HG2	2.03	0.41
1:A:462:LEU:HD13	1:A:470:ASP:HB2	2.02	0.41
1:A:590:ASP:HA	1:A:593:PHE:HB3	2.02	0.41
29:A:787:BCR:H292	25:a:602:CLA:H111	2.02	0.41
2:B:517:PHE:HE2	25:B:758:CLA:C1D	2.34	0.41
2:B:529:THR:HG21	2:B:582:TRP:CE2	2.55	0.41
2:B:687:ILE:HD11	16:j:123:LEU:HD11	2.03	0.41
25:B:745:CLA:H3A	25:B:745:CLA:HBA1	1.64	0.41
4:D:74:VAL:HG12	4:D:95:ASN:HD21	1.86	0.41
9:a:80:LEU:HD13	25:a:604:CLA:HBA1	2.03	0.41
10:b:40:GLU:HB2	25:b:602:CLA:CHB	2.51	0.41
25:d:604:CLA:HBA1	35:d:606:CHL:C1D	2.51	0.41
25:h:610:CLA:H3A	25:h:610:CLA:HBA2	1.72	0.41
15:i:94:VAL:O	15:i:98:LEU:HG	2.20	0.41
25:k:609:CLA:HHC	25:k:609:CLA:HBB1	2.03	0.41
19:m:24:ARG:HA	19:m:24:ARG:HD3	1.91	0.41
25:m:602:CLA:H11	31:m:621:DD6:O1	2.20	0.41
22:n:138:PHE:CE2	25:n:608:CLA:NC	2.89	0.41
1:A:208:LEU:HD23	1:A:208:LEU:HA	1.88	0.41
1:A:219:HIS:HE1	25:A:757:CLA:C4D	2.34	0.41
1:A:396:TRP:CD1	25:A:775:CLA:HAB	2.56	0.41
1:A:407:ALA:HB2	1:A:592:VAL:HG11	2.03	0.41
1:A:423:PHE:HB2	4:D:79:ILE:HD13	2.03	0.41
1:A:596:LEU:HD21	25:A:777:CLA:HBC1	2.03	0.41
1:A:672:PHE:HZ	25:A:752:CLA:CHD	2.34	0.41
25:A:761:CLA:H162	25:A:761:CLA:H122	1.76	0.41
25:A:781:CLA:HBA1	25:A:781:CLA:HBD	2.03	0.41
25:A:793:CLA:HBD	25:A:793:CLA:HAA2	2.02	0.41
25:A:801:CLA:HBA2	25:A:801:CLA:H3A	1.60	0.41
2:B:650:PHE:HZ	25:B:736:CLA:C1D	2.33	0.41
3:C:25:VAL:HG21	3:C:48:CYS:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:3:ALA:HB2	6:F:9:PRO:HD3	2.03	0.41
8:M:14:ALA:O	8:M:18:PRO:HD2	2.21	0.41
9:a:122:MET:HE3	25:a:610:CLA:O2A	2.20	0.41
25:a:619:CLA:H12	25:a:619:CLA:HBA1	1.73	0.41
27:j:198:LHG:H252	25:j:611:CLA:HBC3	2.03	0.41
20:f:77:ILE:HG13	25:f:604:CLA:HMA2	2.03	0.41
21:g:100:PHE:H	21:g:106:GLU:CD	2.28	0.41
25:g:602:CLA:H61	25:g:602:CLA:H41	1.62	0.41
22:n:24:PRO:O	31:n:621:DD6:O2	2.38	0.41
25:n:602:CLA:HBA2	25:n:602:CLA:H3A	1.84	0.41
25:n:603:CLA:H62	25:n:603:CLA:H41	1.81	0.41
1:A:216:HIS:HB2	25:A:799:CLA:CHC	2.51	0.41
1:A:685:PHE:HA	28:A:785:PQN:H9	2.03	0.41
27:b:181:LHG:HC41	25:b:604:CLA:HBB1	2.03	0.41
25:c:603:CLA:H11	25:c:603:CLA:H2A	2.03	0.41
21:g:51:MET:O	21:g:55:VAL:HG22	2.20	0.41
1:A:43:PRO:HG3	6:F:125:ILE:HG21	2.03	0.40
25:A:753:CLA:HBB1	25:A:791:CLA:C1B	2.49	0.40
2:B:34:HIS:HE1	25:B:771:CLA:HED1	1.85	0.40
25:a:602:CLA:CHB	25:a:602:CLA:H2	2.51	0.40
18:l:12:PRO:HB3	18:l:25:GLY:HA3	2.03	0.40
18:l:16:LEU:HD11	18:l:27:ASP:HB2	2.02	0.40
1:A:239:LEU:HD23	1:A:239:LEU:HA	1.91	0.40
1:A:297:HIS:HE2	25:A:769:CLA:C1B	2.33	0.40
25:A:752:CLA:H161	25:A:758:CLA:HMA1	2.03	0.40
25:A:766:CLA:H41	25:A:766:CLA:H62	1.53	0.40
28:A:785:PQN:H141	25:A:794:CLA:HBB2	2.02	0.40
2:B:717:TYR:CZ	25:B:736:CLA:HED1	2.56	0.40
5:E:46:ASN:C	5:E:48:GLU:H	2.29	0.40
10:b:58:GLU:OE2	10:b:159:SER:HB3	2.21	0.40
19:m:53:MET:HE2	19:m:134:GLY:N	2.37	0.40
20:f:46:HIS:HB3	20:f:133:LEU:HD21	2.03	0.40
20:f:55:VAL:HA	20:f:58:VAL:HG22	2.02	0.40
1:A:514:VAL:HG13	1:A:524:MET:HB3	2.03	0.40
25:A:770:CLA:HBB1	25:A:774:CLA:C7	2.51	0.40
2:B:193:HIS:HB2	25:B:746:CLA:C1C	2.51	0.40
2:B:576:PHE:CE1	25:B:753:CLA:HAC2	2.56	0.40
25:B:755:CLA:HMC1	25:B:783:CLA:HAC1	2.04	0.40
9:a:117:PHE:HB2	25:a:608:CLA:H43	2.03	0.40
25:b:601:CLA:HED3	25:b:601:CLA:H2A	2.02	0.40
25:e:613:CLA:HBD	25:e:613:CLA:HAA1	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:h:170:LEU:HD13	25:h:613:CLA:HMD3	2.04	0.40
15:i:145:VAL:HG22	15:i:174:TRP:CE3	2.56	0.40
25:j:613:CLA:C1C	25:j:613:CLA:H51	2.51	0.40
17:k:152:LYS:HD2	17:k:156:THR:HG21	2.03	0.40
25:A:784:CLA:H93	25:A:784:CLA:H62	1.86	0.40
2:B:316:GLY:HA3	2:B:410:ARG:HD2	2.03	0.40
2:B:492:ILE:H	2:B:492:ILE:HG12	1.66	0.40
2:B:700:LEU:HD22	2:B:704:GLN:NE2	2.37	0.40
25:B:750:CLA:HBD	25:B:750:CLA:HAA2	2.04	0.40
25:B:760:CLA:HHC	25:B:760:CLA:HBB1	2.04	0.40
10:b:82:ILE:HB	10:b:86:GLU:HB2	2.02	0.40
27:d:237:LHG:H131	27:d:237:LHG:H102	1.68	0.40
25:e:610:CLA:HBA2	25:e:610:CLA:H3A	1.77	0.40
25:h:613:CLA:H41	25:h:613:CLA:H62	1.55	0.40
15:i:166:ILE:C	15:i:168:GLU:H	2.29	0.40
29:A:788:BCR:H24C	29:A:788:BCR:H371	1.87	0.40
25:A:791:CLA:HAB	2:B:582:TRP:HH2	1.86	0.40
2:B:48:ALA:HB2	2:B:157:LEU:HG	2.02	0.40
2:B:504:LYS:HB2	2:B:504:LYS:HE2	1.82	0.40
25:B:744:CLA:H3A	25:B:744:CLA:HBA2	1.87	0.40
29:B:765:BCR:H24C	29:B:765:BCR:H371	1.84	0.40
6:F:95:GLY:O	6:F:99:VAL:HG23	2.21	0.40
16:j:176:ASN:HD21	25:j:613:CLA:HED2	1.87	0.40
23:o:111:TYR:HB3	25:o:610:CLA:HED2	2.04	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	A	739/751 (98%)	713 (96%)	24 (3%)	2 (0%)	36 38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	729/734 (99%)	705 (97%)	23 (3%)	1 (0%)	48	54
3	C	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
4	D	184/186 (99%)	173 (94%)	10 (5%)	1 (0%)	24	23
5	E	61/63 (97%)	57 (93%)	4 (7%)	0	100	100
6	F	166/168 (99%)	163 (98%)	3 (2%)	0	100	100
7	J	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
8	M	29/31 (94%)	29 (100%)	0	0	100	100
9	a	164/166 (99%)	158 (96%)	6 (4%)	0	100	100
10	b	167/169 (99%)	158 (95%)	9 (5%)	0	100	100
11	c	219/221 (99%)	208 (95%)	11 (5%)	0	100	100
12	d	218/220 (99%)	207 (95%)	10 (5%)	1 (0%)	24	23
13	e	197/199 (99%)	190 (96%)	6 (3%)	1 (0%)	24	23
14	h	172/174 (99%)	166 (96%)	6 (4%)	0	100	100
15	i	175/177 (99%)	166 (95%)	9 (5%)	0	100	100
16	j	181/183 (99%)	179 (99%)	2 (1%)	0	100	100
17	k	170/172 (99%)	162 (95%)	8 (5%)	0	100	100
18	l	165/167 (99%)	162 (98%)	3 (2%)	0	100	100
19	m	166/168 (99%)	155 (93%)	11 (7%)	0	100	100
20	f	172/174 (99%)	151 (88%)	20 (12%)	1 (1%)	21	20
21	g	176/178 (99%)	173 (98%)	3 (2%)	0	100	100
22	n	182/184 (99%)	155 (85%)	25 (14%)	2 (1%)	11	7
23	o	162/164 (99%)	150 (93%)	11 (7%)	1 (1%)	21	20
24	p	146/148 (99%)	131 (90%)	14 (10%)	1 (1%)	18	16
All	All	4853/4915 (99%)	4619 (95%)	223 (5%)	11 (0%)	44	48

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
20	f	77	ILE
1	A	205	LEU
1	A	497	LEU
2	B	107	SER
13	e	95	VAL
22	n	126	LYS

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Mol	Chain	Res	Type
24	p	9	ALA
22	n	69	LEU
4	D	139	PRO
23	o	33	PRO
12	d	109	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	621/632 (98%)	619 (100%)	2 (0%)	86	90
2	B	607/609 (100%)	607 (100%)	0	100	100
3	C	69/70 (99%)	68 (99%)	1 (1%)	59	69
4	D	140/140 (100%)	139 (99%)	1 (1%)	76	81
5	E	49/49 (100%)	49 (100%)	0	100	100
6	F	127/127 (100%)	127 (100%)	0	100	100
7	J	34/34 (100%)	34 (100%)	0	100	100
8	M	26/26 (100%)	26 (100%)	0	100	100
9	a	125/125 (100%)	125 (100%)	0	100	100
10	b	130/130 (100%)	129 (99%)	1 (1%)	73	80
11	c	172/172 (100%)	172 (100%)	0	100	100
12	d	167/167 (100%)	167 (100%)	0	100	100
13	e	152/152 (100%)	152 (100%)	0	100	100
14	h	142/142 (100%)	140 (99%)	2 (1%)	59	69
15	i	137/137 (100%)	137 (100%)	0	100	100
16	j	145/145 (100%)	145 (100%)	0	100	100
17	k	141/141 (100%)	140 (99%)	1 (1%)	76	81
18	l	122/122 (100%)	122 (100%)	0	100	100
19	m	122/122 (100%)	122 (100%)	0	100	100
20	f	135/135 (100%)	134 (99%)	1 (1%)	76	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	g	140/140 (100%)	140 (100%)	0	100	100
22	n	140/140 (100%)	140 (100%)	0	100	100
23	o	119/119 (100%)	118 (99%)	1 (1%)	73	80
24	p	114/114 (100%)	111 (97%)	3 (3%)	40	48
All	All	3876/3890 (100%)	3863 (100%)	13 (0%)	84	90

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	395	TYR
1	A	584	CYS
3	C	65	VAL
4	D	82	ILE
10	b	96	TYR
14	h	5	ILE
14	h	120	LEU
17	k	31	LYS
20	f	127	LYS
23	o	3	VAL
24	p	115	LYS
24	p	127	LYS
24	p	134	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	A	225	ASN
1	A	252	GLN
1	A	714	GLN
2	B	294	ASN
2	B	444	GLN
2	B	452	GLN
2	B	475	ASN
2	B	627	ASN
2	B	630	GLN
4	D	138	HIS
4	D	170	ASN
5	E	21	GLN
9	a	70	GLN

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Mol	Chain	Res	Type
9	a	158	GLN
9	a	159	ASN
10	b	60	GLN
10	b	78	ASN
11	c	51	GLN
12	d	143	GLN
13	e	198	ASN
14	h	37	GLN
14	h	97	ASN
14	h	164	HIS
15	i	63	GLN
15	i	163	ASN
15	i	164	HIS
16	j	49	ASN
16	j	89	GLN
16	j	179	HIS
19	m	165	ASN
20	f	140	GLN
20	f	164	HIS
21	g	152	GLN
22	n	37	ASN
22	n	63	ASN
24	p	70	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

367 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
25	CLA	h	618	-	47,51,73	1.39	7 (14%)	55,86,113	1.76	5 (9%)
25	CLA	m	604	-	47,51,73	1.39	6 (12%)	55,86,113	1.89	5 (9%)
25	CLA	e	602	-	69,73,73	1.22	7 (10%)	82,113,113	1.57	10 (12%)
25	CLA	d	609	-	53,57,73	1.36	7 (13%)	61,93,113	1.85	5 (8%)
25	CLA	B	742	-	47,51,73	1.39	7 (14%)	55,86,113	1.79	4 (7%)
25	CLA	A	760	-	69,73,73	1.21	6 (8%)	82,113,113	1.65	7 (8%)
35	CHL	e	606	-	40,54,74	2.22	12 (30%)	34,90,114	3.24	17 (50%)
25	CLA	l	617	-	46,50,73	1.41	7 (15%)	53,85,113	1.97	5 (9%)
25	CLA	A	797	-	53,57,73	1.35	6 (11%)	61,93,113	1.80	6 (9%)
25	CLA	k	613	-	56,60,73	1.34	7 (12%)	65,97,113	1.79	8 (12%)
25	CLA	B	778	-	67,71,73	1.22	6 (8%)	79,110,113	1.58	9 (11%)
25	CLA	B	757	-	64,68,73	1.26	5 (7%)	76,107,113	1.57	12 (15%)
25	CLA	B	782	-	54,58,73	1.36	6 (11%)	64,95,113	1.89	10 (15%)
25	CLA	g	602	-	57,61,73	1.33	7 (12%)	67,98,113	1.67	8 (11%)
25	CLA	d	613	-	46,50,73	1.39	7 (15%)	53,85,113	1.83	5 (9%)
31	DD6	g	620	-	40,45,45	1.35	4 (10%)	51,67,67	2.15	14 (27%)
25	CLA	o	602	-	51,55,73	1.38	6 (11%)	60,91,113	1.80	7 (11%)
25	CLA	l	609	-	64,68,73	1.26	7 (10%)	76,107,113	1.72	8 (10%)
25	CLA	c	613	-	57,61,73	1.33	7 (12%)	67,98,113	1.72	10 (14%)
25	CLA	B	736	-	69,73,73	1.20	6 (8%)	82,113,113	1.54	10 (12%)
25	CLA	B	783	-	54,58,73	1.37	7 (12%)	64,95,113	1.79	7 (10%)
25	CLA	B	738	-	69,73,73	1.21	6 (8%)	82,113,113	1.68	6 (7%)
32	SF4	C	83	-	0,12,12	-	-	-	-	-
28	PQN	A	785	-	34,34,34	1.03	2 (5%)	43,45,45	1.75	10 (23%)
32	SF4	B	735	-	0,12,12	-	-	-	-	-
30	SQD	A	795	-	25,27,54	1.83	7 (28%)	35,38,65	1.56	7 (20%)
25	CLA	A	803	-	55,59,73	1.34	6 (10%)	64,96,113	1.83	9 (14%)
25	CLA	k	615	-	46,50,73	1.40	7 (15%)	53,85,113	1.88	6 (11%)
25	CLA	c	612	-	47,51,73	1.39	7 (14%)	55,86,113	1.82	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	A	781	-	56,60,73	1.35	6 (10%)	65,97,113	1.71	10 (15%)
31	DD6	l	621	-	40,45,45	1.48	6 (15%)	51,67,67	2.01	14 (27%)
25	CLA	A	753	-	67,71,73	1.23	5 (7%)	79,110,113	1.61	9 (11%)
25	CLA	d	602	-	61,65,73	1.29	6 (9%)	72,103,113	1.72	9 (12%)
25	CLA	d	610	-	63,67,73	1.28	6 (9%)	74,105,113	1.74	8 (10%)
27	LHG	a	181	-	25,25,48	1.91	2 (8%)	28,31,54	1.43	5 (17%)
30	SQD	g	190	-	30,32,54	1.87	7 (23%)	40,43,65	1.51	6 (15%)
25	CLA	o	603	-	47,51,73	1.44	7 (14%)	55,86,113	1.78	5 (9%)
25	CLA	a	611	-	49,53,73	1.41	6 (12%)	58,89,113	1.80	7 (12%)
25	CLA	A	774	-	68,72,73	1.22	6 (8%)	80,111,113	1.79	6 (7%)
25	CLA	a	613	-	59,63,73	1.32	6 (10%)	70,101,113	1.73	8 (11%)
25	CLA	n	602	-	63,67,73	1.26	6 (9%)	74,105,113	1.79	8 (10%)
25	CLA	a	610	-	58,62,73	1.31	5 (8%)	68,99,113	1.79	8 (11%)
31	DD6	j	620	-	40,45,45	1.55	6 (15%)	51,67,67	2.06	12 (23%)
25	CLA	e	608	-	52,56,73	1.36	7 (13%)	61,92,113	1.72	6 (9%)
27	LHG	m	182	-	31,31,48	1.77	2 (6%)	34,37,54	1.35	5 (14%)
25	CLA	i	609	-	47,51,73	1.37	6 (12%)	55,86,113	1.84	5 (9%)
25	CLA	d	612	-	46,50,73	1.40	7 (15%)	53,85,113	1.88	3 (5%)
25	CLA	A	804	-	54,58,73	1.37	6 (11%)	64,95,113	1.74	9 (14%)
29	BCR	A	792	-	41,41,41	1.42	7 (17%)	56,56,56	1.49	11 (19%)
25	CLA	b	602	-	57,61,73	1.35	7 (12%)	67,98,113	1.74	9 (13%)
25	CLA	m	613	-	46,50,73	1.40	6 (13%)	53,85,113	1.79	7 (13%)
25	CLA	e	604	-	54,58,73	1.37	7 (12%)	64,95,113	1.75	10 (15%)
25	CLA	k	602	-	57,61,73	1.34	7 (12%)	67,98,113	1.71	9 (13%)
25	CLA	k	610	-	61,65,73	1.28	6 (9%)	72,103,113	1.68	9 (12%)
25	CLA	B	781	-	69,73,73	1.22	6 (8%)	82,113,113	1.69	6 (7%)
25	CLA	A	801	-	69,73,73	1.21	7 (10%)	82,113,113	1.67	11 (13%)
25	CLA	B	753	-	69,73,73	1.22	7 (10%)	82,113,113	1.51	7 (8%)
31	DD6	o	620	-	40,45,45	1.32	4 (10%)	51,67,67	2.02	11 (21%)
25	CLA	A	762	-	54,58,73	1.39	7 (12%)	64,95,113	1.81	10 (15%)
25	CLA	A	808	-	57,61,73	1.33	7 (12%)	67,98,113	1.85	10 (14%)
25	CLA	B	756	-	64,68,73	1.26	7 (10%)	76,107,113	1.70	10 (13%)
25	CLA	a	612	-	47,51,73	1.39	7 (14%)	55,86,113	1.84	4 (7%)
25	CLA	g	601	-	46,50,73	1.39	7 (15%)	53,85,113	1.80	6 (11%)
25	CLA	o	608	-	47,51,73	1.38	7 (14%)	55,86,113	1.78	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	i	610	-	59,63,73	1.30	5 (8%)	70,101,113	1.69	9 (12%)
35	CHL	d	607	-	37,51,74	2.21	10 (27%)	30,86,114	3.23	14 (46%)
31	DD6	f	620	-	40,45,45	1.30	4 (10%)	51,67,67	2.15	12 (23%)
25	CLA	l	612	-	47,51,73	1.39	6 (12%)	55,86,113	1.81	4 (7%)
25	CLA	g	611	-	46,50,73	1.39	6 (13%)	53,85,113	1.86	6 (11%)
31	DD6	n	623	-	40,45,45	1.35	7 (17%)	51,67,67	1.64	10 (19%)
25	CLA	B	774	-	64,68,73	1.28	7 (10%)	76,107,113	1.74	9 (11%)
25	CLA	f	614	-	46,50,73	1.40	6 (13%)	53,85,113	1.75	7 (13%)
25	CLA	B	776	-	63,67,73	1.29	7 (11%)	74,105,113	1.73	7 (9%)
25	CLA	h	609	-	54,58,73	1.37	7 (12%)	64,95,113	1.75	7 (10%)
25	CLA	g	608	-	49,53,73	1.43	7 (14%)	58,89,113	1.83	4 (6%)
25	CLA	J	101	-	54,58,73	1.38	7 (12%)	64,95,113	1.78	9 (14%)
31	DD6	e	623	-	40,45,45	1.37	8 (20%)	51,67,67	1.59	8 (15%)
25	CLA	k	614	-	46,50,73	1.39	6 (13%)	53,85,113	1.79	5 (9%)
28	PQN	B	769	-	28,28,34	1.06	2 (7%)	35,37,45	1.94	10 (28%)
25	CLA	d	604	-	56,60,73	1.36	7 (12%)	65,97,113	1.74	8 (12%)
25	CLA	i	612	-	47,51,73	1.38	7 (14%)	55,86,113	1.82	5 (9%)
25	CLA	h	602	-	59,63,73	1.34	7 (11%)	70,101,113	1.73	9 (12%)
25	CLA	B	760	-	47,51,73	1.37	6 (12%)	55,86,113	1.79	4 (7%)
25	CLA	j	609	-	54,58,73	1.37	7 (12%)	64,95,113	1.80	7 (10%)
25	CLA	A	761	-	69,73,73	1.21	6 (8%)	82,113,113	1.69	8 (9%)
25	CLA	k	618	-	54,58,73	1.36	6 (11%)	64,95,113	1.77	7 (10%)
29	BCR	A	789	-	41,41,41	0.79	1 (2%)	56,56,56	1.07	5 (8%)
25	CLA	f	609	-	46,50,73	1.41	7 (15%)	53,85,113	1.79	6 (11%)
25	CLA	A	805	-	59,63,73	1.30	6 (10%)	70,101,113	1.64	9 (12%)
25	CLA	h	615	-	46,50,73	1.39	7 (15%)	53,85,113	1.89	4 (7%)
25	CLA	f	610	-	59,63,73	1.34	7 (11%)	70,101,113	1.72	10 (14%)
25	CLA	B	758	-	69,73,73	1.21	7 (10%)	82,113,113	1.59	10 (12%)
25	CLA	B	754	-	47,51,73	1.38	8 (17%)	55,86,113	1.79	5 (9%)
31	DD6	m	621	-	40,45,45	1.43	5 (12%)	51,67,67	2.03	13 (25%)
25	CLA	j	611	-	54,58,73	1.37	7 (12%)	64,95,113	1.78	8 (12%)
25	CLA	A	767	-	47,51,73	1.38	7 (14%)	55,86,113	1.77	4 (7%)
25	CLA	B	745	-	67,71,73	1.22	7 (10%)	79,110,113	1.71	9 (11%)
25	CLA	A	779	-	47,51,73	1.39	6 (12%)	55,86,113	1.82	7 (12%)
25	CLA	c	608	-	54,58,73	1.37	7 (12%)	64,95,113	1.70	9 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	j	613	-	66,70,73	1.23	5 (7%)	78,109,113	1.67	9 (11%)
25	CLA	A	769	-	69,73,73	1.22	7 (10%)	82,113,113	1.56	11 (13%)
31	DD6	j	621	-	40,45,45	1.49	5 (12%)	51,67,67	2.04	12 (23%)
25	CLA	f	615	-	47,51,73	1.40	7 (14%)	55,86,113	1.81	5 (9%)
25	CLA	j	610	-	68,72,73	1.21	5 (7%)	80,111,113	1.56	8 (10%)
25	CLA	A	757	-	49,53,73	1.39	7 (14%)	58,89,113	1.83	7 (12%)
33	LMG	i	195	-	44,44,55	0.85	1 (2%)	52,52,63	1.07	2 (3%)
31	DD6	f	621	-	40,45,45	1.29	4 (10%)	51,67,67	2.29	17 (33%)
29	BCR	B	766	-	41,41,41	1.49	4 (9%)	56,56,56	1.32	9 (16%)
25	CLA	c	606	-	47,51,73	1.39	6 (12%)	55,86,113	1.78	6 (10%)
25	CLA	A	791	-	67,71,73	1.23	7 (10%)	79,110,113	1.60	9 (11%)
25	CLA	h	611	-	47,51,73	1.38	6 (12%)	55,86,113	1.78	6 (10%)
25	CLA	g	612	-	46,50,73	1.41	7 (15%)	53,85,113	1.87	3 (5%)
25	CLA	a	604	-	49,53,73	1.41	7 (14%)	58,89,113	1.74	7 (12%)
25	CLA	h	613	-	57,61,73	1.33	6 (10%)	67,98,113	1.76	9 (13%)
28	PQN	d	223	-	27,27,34	1.07	2 (7%)	34,36,45	1.92	9 (26%)
29	BCR	A	788	-	41,41,41	1.46	4 (9%)	56,56,56	1.41	12 (21%)
25	CLA	h	610	-	58,62,73	1.31	6 (10%)	68,99,113	1.75	9 (13%)
25	CLA	n	613	-	46,50,73	1.41	8 (17%)	53,85,113	1.72	4 (7%)
25	CLA	A	802	-	47,51,73	1.38	5 (10%)	55,86,113	1.67	4 (7%)
25	CLA	A	763	-	69,73,73	1.21	6 (8%)	82,113,113	1.60	8 (9%)
25	CLA	f	613	-	63,67,73	1.28	6 (9%)	74,105,113	1.67	8 (10%)
31	DD6	i	621	-	40,45,45	1.51	7 (17%)	51,67,67	2.01	13 (25%)
25	CLA	n	609	-	49,53,73	1.41	7 (14%)	58,89,113	1.85	4 (6%)
25	CLA	k	601	-	47,51,73	1.39	7 (14%)	55,86,113	1.75	6 (10%)
25	CLA	n	607	-	46,50,73	1.41	7 (15%)	53,85,113	1.80	5 (9%)
35	CHL	d	606	-	40,54,74	2.23	12 (30%)	34,90,114	3.26	17 (50%)
25	CLA	A	759	-	64,68,73	1.25	6 (9%)	76,107,113	1.74	9 (11%)
31	DD6	g	621	-	40,45,45	1.43	5 (12%)	51,67,67	2.10	12 (23%)
25	CLA	n	612	-	46,50,73	1.41	7 (15%)	53,85,113	1.90	3 (5%)
25	CLA	n	603	-	59,63,73	1.34	7 (11%)	70,101,113	1.73	6 (8%)
27	LHG	d	237	-	28,28,48	1.80	2 (7%)	31,34,54	1.36	5 (16%)
25	CLA	j	618	-	54,58,73	1.37	7 (12%)	64,95,113	1.81	6 (9%)
25	CLA	A	806	-	49,53,73	1.39	7 (14%)	58,89,113	1.80	8 (13%)
25	CLA	i	603	-	47,51,73	1.39	7 (14%)	55,86,113	1.72	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	f	612	-	46,50,73	1.44	6 (13%)	53,85,113	1.60	4 (7%)
25	CLA	i	611	-	47,51,73	1.38	6 (12%)	55,86,113	1.84	6 (10%)
25	CLA	c	610	-	59,63,73	1.31	8 (13%)	70,101,113	1.72	9 (12%)
25	CLA	b	609	-	49,53,73	1.39	7 (14%)	58,89,113	1.79	7 (12%)
25	CLA	h	608	-	52,56,73	1.37	7 (13%)	61,92,113	1.81	5 (8%)
31	DD6	p	621	-	40,45,45	1.29	4 (10%)	51,67,67	2.16	14 (27%)
25	CLA	A	766	-	62,66,73	1.27	6 (9%)	73,104,113	1.84	8 (10%)
27	LHG	c	243	-	29,29,48	1.80	2 (6%)	32,35,54	1.38	5 (15%)
25	CLA	m	611	-	47,51,73	1.39	7 (14%)	55,86,113	1.73	5 (9%)
25	CLA	B	771	-	57,61,73	1.35	7 (12%)	67,98,113	1.73	8 (11%)
27	LHG	h	190	-	30,30,48	1.73	2 (6%)	33,36,54	1.39	5 (15%)
25	CLA	h	604	-	64,68,73	1.27	7 (10%)	76,107,113	1.70	8 (10%)
25	CLA	B	747	-	53,57,73	1.41	7 (13%)	62,93,113	1.71	7 (11%)
25	CLA	B	770	-	57,61,73	1.34	7 (12%)	67,98,113	1.69	7 (10%)
27	LHG	A	786	-	48,48,48	1.38	2 (4%)	51,54,54	1.19	5 (9%)
25	CLA	b	610	-	46,50,73	1.39	6 (13%)	53,85,113	1.82	6 (11%)
29	BCR	M	201	-	41,41,41	0.77	1 (2%)	56,56,56	1.17	5 (8%)
25	CLA	m	609	-	54,58,73	1.37	7 (12%)	64,95,113	1.78	7 (10%)
25	CLA	p	610	-	49,53,73	1.44	7 (14%)	58,89,113	1.70	5 (8%)
27	LHG	j	198	-	36,36,48	1.58	2 (5%)	39,42,54	1.29	5 (12%)
25	CLA	n	604	-	52,56,73	1.38	7 (13%)	61,92,113	1.79	7 (11%)
31	DD6	e	620	-	40,45,45	1.40	6 (15%)	51,67,67	1.43	9 (17%)
34	DGD	e	205	-	37,37,67	1.22	1 (2%)	51,51,81	1.09	1 (1%)
25	CLA	A	780	-	62,66,73	1.29	6 (9%)	73,104,113	1.66	6 (8%)
25	CLA	b	604	-	49,53,73	1.40	7 (14%)	58,89,113	1.80	5 (8%)
25	CLA	g	609	-	54,58,73	1.38	7 (12%)	64,95,113	1.74	6 (9%)
31	DD6	o	621	-	40,45,45	1.38	4 (10%)	51,67,67	2.03	13 (25%)
34	DGD	b	182	-	49,49,67	1.22	6 (12%)	63,63,81	1.07	3 (4%)
25	CLA	A	777	-	69,73,73	1.23	7 (10%)	82,113,113	1.72	8 (9%)
25	CLA	A	773	-	57,61,73	1.34	7 (12%)	67,98,113	1.73	8 (11%)
25	CLA	l	614	-	46,50,73	1.42	6 (13%)	53,85,113	1.88	6 (11%)
25	CLA	b	612	-	56,60,73	1.35	8 (14%)	65,97,113	1.80	8 (12%)
25	CLA	l	602	-	63,67,73	1.28	8 (12%)	74,105,113	1.66	10 (13%)
31	DD6	n	620	-	40,45,45	1.30	4 (10%)	51,67,67	2.37	13 (25%)
25	CLA	p	609	-	54,58,73	1.41	8 (14%)	64,95,113	1.77	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	B	739	-	69,73,73	1.20	6 (8%)	82,113,113	1.67	10 (12%)
25	CLA	l	610	-	58,62,73	1.32	5 (8%)	68,99,113	1.69	7 (10%)
31	DD6	J	4002	-	40,45,45	1.54	6 (15%)	51,67,67	2.10	14 (27%)
33	LMG	k	179	-	36,36,55	0.96	2 (5%)	44,44,63	1.12	3 (6%)
25	CLA	B	785	-	49,53,73	1.39	6 (12%)	58,89,113	1.75	7 (12%)
25	CLA	h	601	-	54,58,73	1.38	6 (11%)	64,95,113	1.78	9 (14%)
25	CLA	p	602	-	47,51,73	1.42	9 (19%)	55,86,113	1.93	8 (14%)
25	CLA	f	604	-	46,50,73	1.41	7 (15%)	53,85,113	1.80	6 (11%)
29	BCR	B	763	-	41,41,41	0.76	1 (2%)	56,56,56	1.09	4 (7%)
25	CLA	k	604	-	69,73,73	1.22	6 (8%)	82,113,113	1.61	8 (9%)
25	CLA	B	755	-	64,68,73	1.27	7 (10%)	76,107,113	1.70	9 (11%)
25	CLA	b	605	-	49,53,73	1.40	7 (14%)	58,89,113	1.81	5 (8%)
25	CLA	p	613	-	47,51,73	1.41	7 (14%)	55,86,113	1.86	8 (14%)
31	DD6	c	620	-	40,45,45	1.54	7 (17%)	51,67,67	2.05	14 (27%)
25	CLA	i	613	-	63,67,73	1.28	7 (11%)	74,105,113	1.72	10 (13%)
25	CLA	n	605	-	46,50,73	1.40	6 (13%)	53,85,113	1.81	6 (11%)
25	CLA	B	768	-	59,63,73	1.32	6 (10%)	70,101,113	1.73	8 (11%)
25	CLA	A	799	-	64,68,73	1.28	7 (10%)	76,107,113	1.74	11 (14%)
31	DD6	d	623	-	40,45,45	1.35	4 (10%)	51,67,67	2.21	16 (31%)
31	DD6	k	620	-	40,45,45	1.46	5 (12%)	51,67,67	2.04	12 (23%)
25	CLA	e	605	-	46,50,73	1.40	6 (13%)	53,85,113	1.88	5 (9%)
25	CLA	f	608	-	46,50,73	1.40	7 (15%)	53,85,113	1.91	5 (9%)
27	LHG	A	756	-	37,37,48	1.52	2 (5%)	40,43,54	1.25	5 (12%)
25	CLA	B	780	-	57,61,73	1.35	7 (12%)	67,98,113	1.80	7 (10%)
25	CLA	k	603	-	46,50,73	1.39	7 (15%)	53,85,113	2.00	4 (7%)
25	CLA	e	607	-	47,51,73	1.38	6 (12%)	55,86,113	1.85	5 (9%)
25	CLA	e	609	-	56,60,73	1.35	6 (10%)	65,97,113	1.77	7 (10%)
25	CLA	d	603	-	46,50,73	1.38	7 (15%)	53,85,113	1.90	4 (7%)
25	CLA	B	773	-	65,69,73	1.26	8 (12%)	77,108,113	1.72	8 (10%)
25	CLA	B	772	-	54,58,73	1.38	7 (12%)	64,95,113	1.78	6 (9%)
25	CLA	l	613	-	52,56,73	1.37	6 (11%)	61,92,113	1.73	7 (11%)
33	LMG	B	786	-	52,52,55	0.81	2 (3%)	60,60,63	1.07	2 (3%)
32	SF4	C	82	-	0,12,12	-	-	-	-	-
25	CLA	g	610	-	59,63,73	1.30	6 (10%)	70,101,113	1.68	8 (11%)
25	CLA	f	601	-	46,50,73	1.41	6 (13%)	53,85,113	1.74	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	a	609	-	54,58,73	1.38	7 (12%)	64,95,113	1.78	7 (10%)
25	CLA	e	601	-	45,49,73	1.41	6 (13%)	52,84,113	1.84	7 (13%)
25	CLA	b	611	-	46,50,73	1.40	6 (13%)	53,85,113	1.83	4 (7%)
25	CLA	m	608	-	46,50,73	1.40	7 (15%)	53,85,113	1.84	4 (7%)
31	DD6	b	621	-	40,45,45	1.44	5 (12%)	51,67,67	2.03	14 (27%)
25	CLA	a	602	-	64,68,73	1.26	5 (7%)	76,107,113	1.58	13 (17%)
25	CLA	e	611	-	46,50,73	1.40	6 (13%)	53,85,113	1.71	6 (11%)
31	DD6	n	621	-	40,45,45	1.34	5 (12%)	51,67,67	1.38	9 (17%)
25	CLA	e	613	-	59,63,73	1.32	7 (11%)	70,101,113	1.69	7 (10%)
31	DD6	e	621	-	40,45,45	1.49	5 (12%)	51,67,67	2.04	13 (25%)
25	CLA	A	793	-	46,50,73	1.40	6 (13%)	53,85,113	1.87	5 (9%)
25	CLA	g	613	-	59,63,73	1.32	7 (11%)	70,101,113	1.75	8 (11%)
25	CLA	i	615	-	54,58,73	1.37	7 (12%)	64,95,113	1.79	6 (9%)
25	CLA	B	779	-	69,73,73	1.24	8 (11%)	82,113,113	1.70	12 (14%)
25	CLA	j	615	-	47,51,73	1.37	7 (14%)	55,86,113	1.83	5 (9%)
25	CLA	o	609	-	49,53,73	1.40	6 (12%)	58,89,113	1.83	7 (12%)
31	DD6	A	4008	-	40,45,45	1.42	4 (10%)	51,67,67	2.25	19 (37%)
25	CLA	d	601	-	54,58,73	1.36	7 (12%)	64,95,113	1.87	9 (14%)
25	CLA	h	612	-	62,66,73	1.29	7 (11%)	73,104,113	1.69	8 (10%)
25	CLA	A	807	-	52,56,73	1.37	6 (11%)	61,92,113	1.91	7 (11%)
25	CLA	h	603	-	47,51,73	1.37	7 (14%)	55,86,113	1.90	6 (10%)
25	CLA	p	601	-	46,50,73	1.39	7 (15%)	53,85,113	1.68	6 (11%)
25	CLA	B	746	-	68,72,73	1.25	7 (10%)	80,111,113	1.67	9 (11%)
25	CLA	m	603	-	58,62,73	1.33	7 (12%)	68,99,113	1.71	9 (13%)
31	DD6	c	623	-	40,45,45	1.36	4 (10%)	51,67,67	2.20	16 (31%)
25	CLA	A	775	-	62,66,73	1.28	6 (9%)	73,104,113	1.69	9 (12%)
25	CLA	m	601	-	46,50,73	1.42	6 (13%)	53,85,113	1.66	8 (15%)
25	CLA	o	601	-	45,49,73	1.47	10 (22%)	54,84,113	1.71	9 (16%)
25	CLA	f	603	-	47,51,73	1.42	6 (12%)	55,86,113	1.81	6 (10%)
25	CLA	o	613	-	46,50,73	1.40	6 (13%)	53,85,113	1.84	6 (11%)
25	CLA	h	614	-	47,51,73	1.38	6 (12%)	55,86,113	1.71	5 (9%)
25	CLA	B	752	-	69,73,73	1.22	6 (8%)	82,113,113	1.60	8 (9%)
25	CLA	n	610	-	45,49,73	1.45	7 (15%)	54,84,113	1.74	7 (12%)
25	CLA	o	610	-	45,49,73	1.44	9 (20%)	54,84,113	1.74	7 (12%)
25	CLA	o	614	-	47,51,73	1.41	7 (14%)	55,86,113	1.78	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	BCR	B	765	-	41,41,41	1.45	4 (9%)	56,56,56	1.32	10 (17%)
25	CLA	e	610	-	59,63,73	1.29	6 (10%)	70,101,113	1.70	9 (12%)
29	BCR	A	787	-	41,41,41	0.82	1 (2%)	56,56,56	1.10	4 (7%)
25	CLA	f	611	-	46,50,73	1.41	7 (15%)	53,85,113	1.91	6 (11%)
25	CLA	e	612	-	47,51,73	1.39	7 (14%)	55,86,113	1.86	5 (9%)
25	CLA	l	601	-	46,50,73	1.40	6 (13%)	53,85,113	1.73	6 (11%)
25	CLA	A	784	-	69,73,73	1.20	6 (8%)	82,113,113	1.51	10 (12%)
25	CLA	p	608	-	46,50,73	1.40	6 (13%)	53,85,113	1.83	5 (9%)
25	CLA	A	772	-	68,72,73	1.23	7 (10%)	80,111,113	1.62	10 (12%)
25	CLA	g	618	-	49,53,73	1.40	7 (14%)	58,89,113	1.76	6 (10%)
25	CLA	i	604	-	47,51,73	1.38	7 (14%)	55,86,113	1.75	5 (9%)
30	SQD	c	245	-	37,39,54	1.76	8 (21%)	47,50,65	1.47	7 (14%)
25	CLA	A	770	-	69,73,73	1.21	7 (10%)	82,113,113	1.56	11 (13%)
25	CLA	o	612	-	46,50,73	1.57	9 (19%)	55,84,113	1.91	5 (9%)
27	LHG	h	189	-	29,29,48	1.78	2 (6%)	32,35,54	1.12	2 (6%)
25	CLA	g	604	-	47,51,73	1.38	7 (14%)	55,86,113	1.68	4 (7%)
25	CLA	i	601	-	57,61,73	1.34	7 (12%)	67,98,113	1.73	8 (11%)
28	PQN	B	761	-	34,34,34	1.13	3 (8%)	43,45,45	1.81	10 (23%)
25	CLA	c	619	-	45,49,73	1.44	8 (17%)	54,84,113	1.98	8 (14%)
25	CLA	B	750	-	64,68,73	1.25	6 (9%)	76,107,113	1.72	11 (14%)
35	CHL	d	608	-	40,54,74	2.20	12 (30%)	34,90,114	3.02	16 (47%)
25	CLA	k	608	-	54,58,73	1.37	7 (12%)	64,95,113	1.82	8 (12%)
25	CLA	p	604	-	47,51,73	1.41	7 (14%)	55,86,113	1.83	6 (10%)
25	CLA	c	603	-	57,61,73	1.33	7 (12%)	67,98,113	1.74	9 (13%)
31	DD6	A	4002	-	40,45,45	1.54	4 (10%)	51,67,67	2.14	15 (29%)
34	DGD	B	787	-	55,55,67	1.09	1 (1%)	69,69,81	1.03	1 (1%)
25	CLA	B	775	-	54,58,73	1.38	6 (11%)	64,95,113	1.62	9 (14%)
31	DD6	h	620	-	40,45,45	1.47	5 (12%)	51,67,67	2.03	12 (23%)
25	CLA	B	777	-	57,61,73	1.34	7 (12%)	67,98,113	1.64	8 (11%)
25	CLA	i	614	-	46,50,73	1.39	6 (13%)	53,85,113	1.74	6 (11%)
25	CLA	i	608	-	69,73,73	1.22	7 (10%)	82,113,113	1.66	8 (9%)
30	SQD	j	200	-	34,36,54	1.77	7 (20%)	44,47,65	1.69	10 (22%)
29	BCR	B	762	-	41,41,41	0.80	2 (4%)	56,56,56	1.19	5 (8%)
25	CLA	c	611	-	47,51,73	1.39	6 (12%)	55,86,113	1.76	5 (9%)
25	CLA	A	782	-	52,56,73	1.38	7 (13%)	61,92,113	1.78	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	a	603	-	57,61,73	1.34	7 (12%)	67,98,113	1.74	8 (11%)
25	CLA	A	794	-	61,65,73	1.28	7 (11%)	72,103,113	1.68	7 (9%)
25	CLA	B	759	-	47,51,73	1.37	7 (14%)	55,86,113	1.63	4 (7%)
25	CLA	c	614	-	46,50,73	1.40	7 (15%)	53,85,113	1.76	6 (11%)
33	LMG	a	182	-	43,43,55	0.88	2 (4%)	51,51,63	1.17	2 (3%)
27	LHG	b	181	-	30,30,48	1.81	2 (6%)	33,36,54	1.33	4 (12%)
25	CLA	B	741	-	69,73,73	1.21	6 (8%)	82,113,113	1.64	8 (9%)
25	CLA	B	743	-	46,50,73	1.39	6 (13%)	53,85,113	1.84	4 (7%)
25	CLA	l	604	-	47,51,73	1.39	6 (12%)	55,86,113	1.71	5 (9%)
25	CLA	B	784	-	69,73,73	1.20	7 (10%)	82,113,113	1.68	8 (9%)
25	CLA	m	610	-	46,50,73	1.38	6 (13%)	53,85,113	1.73	5 (9%)
25	CLA	j	602	-	59,63,73	1.28	5 (8%)	70,101,113	1.75	8 (11%)
31	DD6	b	620	-	40,45,45	1.39	4 (10%)	51,67,67	2.13	12 (23%)
25	CLA	c	616	-	51,55,73	1.36	6 (11%)	60,91,113	1.73	6 (10%)
31	DD6	k	621	-	40,45,45	1.41	4 (10%)	51,67,67	2.02	13 (25%)
29	BCR	B	764	-	41,41,41	0.79	2 (4%)	56,56,56	1.02	4 (7%)
25	CLA	A	768	-	60,64,73	1.30	8 (13%)	71,102,113	1.68	6 (8%)
25	CLA	A	755	-	64,68,73	1.28	8 (12%)	76,107,113	1.73	10 (13%)
31	DD6	d	620	-	40,45,45	1.48	5 (12%)	51,67,67	2.03	13 (25%)
25	CLA	j	604	-	61,65,73	1.31	7 (11%)	72,103,113	1.74	10 (13%)
29	BCR	A	790	-	41,41,41	0.76	1 (2%)	56,56,56	1.04	5 (8%)
25	CLA	A	765	-	63,67,73	1.28	7 (11%)	74,105,113	1.73	10 (13%)
25	CLA	g	614	-	46,50,73	1.39	6 (13%)	53,85,113	1.86	7 (13%)
25	CLA	B	749	-	53,57,73	1.36	6 (11%)	61,93,113	1.71	7 (11%)
25	CLA	d	614	-	46,50,73	1.37	6 (13%)	53,85,113	1.76	5 (9%)
25	CLA	a	601	-	54,58,73	1.38	6 (11%)	64,95,113	1.67	8 (12%)
25	CLA	b	613	-	46,50,73	1.40	6 (13%)	53,85,113	1.82	6 (11%)
25	CLA	a	619	-	67,71,73	1.24	6 (8%)	79,110,113	1.69	10 (12%)
25	CLA	A	778	-	47,51,73	1.38	7 (14%)	55,86,113	1.82	6 (10%)
25	CLA	B	748	-	63,67,73	1.28	7 (11%)	74,105,113	1.71	9 (12%)
25	CLA	B	751	-	54,58,73	1.38	7 (12%)	64,95,113	1.70	7 (10%)
25	CLA	f	602	-	63,67,73	1.28	6 (9%)	74,105,113	1.66	10 (13%)
25	CLA	A	771	-	61,65,73	1.29	7 (11%)	72,103,113	1.76	11 (15%)
25	CLA	l	603	-	47,51,73	1.39	7 (14%)	55,86,113	1.86	5 (9%)
25	CLA	m	612	-	47,51,73	1.39	6 (12%)	55,86,113	1.81	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	B	740	-	46,50,73	1.39	7 (15%)	53,85,113	1.81	7 (13%)
25	CLA	a	608	-	57,61,73	1.33	6 (10%)	67,98,113	1.72	8 (11%)
27	LHG	g	189	-	34,34,48	1.63	2 (5%)	37,40,54	1.32	5 (13%)
25	CLA	j	608	-	51,55,73	1.39	8 (15%)	60,91,113	1.86	5 (8%)
31	DD6	c	621	-	40,45,45	1.51	6 (15%)	51,67,67	2.02	16 (31%)
25	CLA	l	611	-	47,51,73	1.39	6 (12%)	55,86,113	1.82	6 (10%)
27	LHG	i	194	-	35,35,48	1.58	2 (5%)	38,41,54	1.30	5 (13%)
25	CLA	g	603	-	46,50,73	1.43	7 (15%)	53,85,113	1.73	5 (9%)
25	CLA	o	604	-	46,50,73	1.41	7 (15%)	53,85,113	1.81	6 (11%)
25	CLA	m	602	-	64,68,73	1.27	6 (9%)	76,107,113	1.51	9 (11%)
25	CLA	A	783	-	69,73,73	1.22	6 (8%)	82,113,113	1.56	10 (12%)
25	CLA	k	609	-	54,58,73	1.37	7 (12%)	64,95,113	1.74	8 (12%)
31	DD6	i	620	-	40,45,45	1.50	6 (15%)	51,67,67	2.05	12 (23%)
31	DD6	h	621	-	40,45,45	1.46	4 (10%)	51,67,67	2.01	13 (25%)
25	CLA	c	602	-	63,67,73	1.27	7 (11%)	74,105,113	1.66	11 (14%)
25	CLA	k	612	-	47,51,73	1.39	7 (14%)	55,86,113	1.80	6 (10%)
25	CLA	e	614	-	46,50,73	1.38	6 (13%)	53,85,113	1.81	3 (5%)
26	LMT	A	754	-	36,36,36	0.55	0	47,47,47	0.66	0
25	CLA	n	606	-	46,50,73	1.39	6 (13%)	53,85,113	1.81	3 (5%)
25	CLA	B	737	-	59,63,73	1.30	5 (8%)	70,101,113	1.89	11 (15%)
31	DD6	l	620	-	40,45,45	1.44	5 (12%)	51,67,67	2.03	14 (27%)
31	DD6	d	621	-	40,45,45	1.54	5 (12%)	51,67,67	2.05	13 (25%)
25	CLA	k	611	-	46,50,73	1.40	6 (13%)	53,85,113	1.80	4 (7%)
25	CLA	b	601	-	46,50,73	1.41	7 (15%)	53,85,113	1.84	6 (11%)
25	CLA	c	604	-	52,56,73	1.37	6 (11%)	61,92,113	1.77	7 (11%)
25	CLA	i	602	-	68,72,73	1.24	7 (10%)	80,111,113	1.64	9 (11%)
29	BCR	B	767	-	41,41,41	0.81	1 (2%)	56,56,56	1.13	4 (7%)
25	CLA	p	612	-	47,51,73	1.39	6 (12%)	55,86,113	1.66	5 (9%)
25	CLA	b	603	-	47,51,73	1.38	7 (14%)	55,86,113	1.83	4 (7%)
25	CLA	A	800	-	52,56,73	1.36	7 (13%)	61,92,113	1.74	7 (11%)
25	CLA	A	752	-	69,73,73	1.20	7 (10%)	82,113,113	1.73	12 (14%)
25	CLA	j	603	-	46,50,73	1.41	7 (15%)	53,85,113	1.84	5 (9%)
25	CLA	e	603	-	49,53,73	1.40	8 (16%)	58,89,113	1.80	6 (10%)
25	CLA	b	608	-	45,49,73	1.44	8 (17%)	54,84,113	1.85	7 (12%)
25	CLA	A	798	-	56,60,73	1.36	6 (10%)	65,97,113	1.85	9 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	j	601	-	54,58,73	1.37	7 (12%)	64,95,113	1.70	9 (14%)
31	DD6	a	620	-	40,45,45	1.41	4 (10%)	51,67,67	2.10	13 (25%)
25	CLA	A	758	-	69,73,73	1.20	7 (10%)	82,113,113	1.64	8 (9%)
31	DD6	i	625	-	40,45,45	1.35	4 (10%)	51,67,67	2.04	13 (25%)
25	CLA	B	744	-	47,51,73	1.38	7 (14%)	55,86,113	1.78	5 (9%)
25	CLA	j	614	-	46,50,73	1.39	6 (13%)	53,85,113	1.83	6 (11%)
25	CLA	g	615	-	46,50,73	1.40	6 (13%)	53,85,113	1.85	5 (9%)
31	DD6	c	624	-	40,45,45	1.36	6 (15%)	51,67,67	1.43	8 (15%)
29	BCR	A	796	-	41,41,41	0.73	0	56,56,56	1.24	6 (10%)
25	CLA	A	764	-	62,66,73	1.28	6 (9%)	73,104,113	1.67	8 (10%)
25	CLA	c	609	-	64,68,73	1.27	6 (9%)	76,107,113	1.72	8 (10%)
31	DD6	a	621	-	40,45,45	1.51	6 (15%)	51,67,67	1.99	12 (23%)
35	CHL	c	607	-	43,57,74	2.16	11 (25%)	37,93,114	3.07	17 (45%)
31	DD6	m	620	-	40,45,45	1.36	4 (10%)	51,67,67	2.02	12 (23%)
31	DD6	F	4002	-	40,45,45	1.36	4 (10%)	51,67,67	1.37	8 (15%)
25	CLA	A	776	-	69,73,73	1.23	7 (10%)	82,113,113	1.59	10 (12%)
25	CLA	n	608	-	45,49,73	1.44	8 (17%)	54,84,113	1.85	9 (16%)
25	CLA	c	601	-	46,50,73	1.38	7 (15%)	53,85,113	1.73	5 (9%)
25	CLA	l	608	-	47,51,73	1.38	7 (14%)	55,86,113	1.79	6 (10%)
25	CLA	j	612	-	59,63,73	1.32	7 (11%)	70,101,113	1.71	8 (11%)
35	CHL	d	605	-	45,59,74	2.16	12 (26%)	40,96,114	3.06	19 (47%)
25	CLA	p	603	-	46,50,73	1.45	7 (15%)	53,85,113	1.61	4 (7%)
25	CLA	d	611	-	49,53,73	1.41	7 (14%)	58,89,113	1.79	6 (10%)

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	h	618	-	1/1/10/20	2/13/89/115	-
25	CLA	m	604	-	1/1/10/20	3/13/89/115	-
25	CLA	e	602	-	1/1/15/20	20/39/115/115	-
25	CLA	d	609	-	1/1/11/20	5/20/96/115	-
25	CLA	B	742	-	1/1/10/20	3/13/89/115	-
25	CLA	A	760	-	1/1/15/20	22/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	CHL	e	606	-	3/3/16/26	8/15/113/137	-
25	CLA	l	617	-	1/1/10/20	6/12/88/115	-
25	CLA	A	797	-	1/1/11/20	9/20/96/115	-
25	CLA	k	613	-	1/1/12/20	8/24/100/115	-
25	CLA	B	778	-	1/1/14/20	14/37/113/115	-
25	CLA	B	757	-	1/1/14/20	9/33/109/115	-
25	CLA	B	782	-	1/1/12/20	5/21/97/115	-
25	CLA	g	602	-	1/1/12/20	14/25/101/115	-
25	CLA	d	613	-	1/1/10/20	4/12/88/115	-
31	DD6	g	620	-	-	4/26/80/80	0/3/3/3
25	CLA	o	602	-	1/1/11/20	8/18/94/115	-
25	CLA	l	609	-	1/1/14/20	12/33/109/115	-
25	CLA	c	613	-	1/1/12/20	8/25/101/115	-
25	CLA	B	736	-	1/1/15/20	9/39/115/115	-
25	CLA	B	783	-	1/1/12/20	3/21/97/115	-
25	CLA	B	738	-	1/1/15/20	17/39/115/115	-
32	SF4	C	83	-	-	-	0/6/5/5
28	PQN	A	785	-	-	7/23/43/43	0/2/2/2
32	SF4	B	735	-	-	-	0/6/5/5
30	SQD	A	795	-	-	9/21/41/69	0/1/1/1
25	CLA	A	803	-	1/1/12/20	8/23/99/115	-
25	CLA	k	615	-	1/1/10/20	5/12/88/115	-
25	CLA	c	612	-	1/1/10/20	3/13/89/115	-
25	CLA	A	781	-	1/1/12/20	8/24/100/115	-
31	DD6	l	621	-	-	3/26/80/80	0/3/3/3
25	CLA	A	753	-	1/1/14/20	10/37/113/115	-
25	CLA	d	602	-	1/1/13/20	5/30/106/115	-
25	CLA	d	610	-	1/1/13/20	14/32/108/115	-
27	LHG	a	181	-	-	8/30/30/53	-
30	SQD	g	190	-	-	13/27/47/69	0/1/1/1
25	CLA	o	603	-	1/1/10/20	5/13/89/115	-
25	CLA	a	611	-	1/1/11/20	5/15/91/115	-
25	CLA	A	774	-	1/1/14/20	14/38/114/115	-
25	CLA	a	613	-	1/1/13/20	13/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	n	602	-	1/1/13/20	14/32/108/115	-
25	CLA	a	610	-	1/1/12/20	9/26/102/115	-
31	DD6	j	620	-	-	4/26/80/80	0/3/3/3
25	CLA	e	608	-	1/1/11/20	6/19/95/115	-
27	LHG	m	182	-	-	19/36/36/53	-
25	CLA	i	609	-	1/1/10/20	4/13/89/115	-
25	CLA	d	612	-	1/1/10/20	2/12/88/115	-
25	CLA	A	804	-	1/1/12/20	8/21/97/115	-
29	BCR	A	792	-	-	17/29/63/63	0/2/2/2
25	CLA	b	602	-	1/1/12/20	9/25/101/115	-
25	CLA	m	613	-	1/1/10/20	5/12/88/115	-
25	CLA	e	604	-	1/1/12/20	4/21/97/115	-
25	CLA	k	602	-	1/1/12/20	10/25/101/115	-
25	CLA	k	610	-	1/1/13/20	15/30/106/115	-
25	CLA	B	781	-	1/1/15/20	9/39/115/115	-
25	CLA	A	801	-	1/1/15/20	20/39/115/115	-
25	CLA	B	753	-	1/1/15/20	14/39/115/115	-
31	DD6	o	620	-	-	5/26/80/80	0/3/3/3
25	CLA	A	762	-	1/1/12/20	2/21/97/115	-
25	CLA	A	808	-	1/1/12/20	12/25/101/115	-
25	CLA	B	756	-	1/1/14/20	18/33/109/115	-
25	CLA	a	612	-	1/1/10/20	4/13/89/115	-
25	CLA	g	601	-	1/1/10/20	5/12/88/115	-
25	CLA	o	608	-	1/1/10/20	5/13/89/115	-
25	CLA	i	610	-	1/1/13/20	11/27/103/115	-
35	CHL	d	607	-	3/3/15/26	4/12/110/137	-
31	DD6	f	620	-	-	5/26/80/80	0/3/3/3
25	CLA	l	612	-	1/1/10/20	6/13/89/115	-
25	CLA	g	611	-	1/1/10/20	3/12/88/115	-
31	DD6	n	623	-	-	8/26/80/80	0/3/3/3
25	CLA	B	774	-	1/1/14/20	13/33/109/115	-
25	CLA	f	614	-	1/1/10/20	5/12/88/115	-
25	CLA	B	776	-	1/1/13/20	9/32/108/115	-
25	CLA	h	609	-	1/1/12/20	7/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	g	608	-	1/1/11/20	6/15/91/115	-
25	CLA	J	101	-	1/1/12/20	11/21/97/115	-
31	DD6	e	623	-	-	15/26/80/80	0/3/3/3
25	CLA	k	614	-	1/1/10/20	4/12/88/115	-
28	PQN	B	769	-	-	5/16/36/43	0/2/2/2
25	CLA	d	604	-	1/1/12/20	7/24/100/115	-
25	CLA	i	612	-	1/1/10/20	4/13/89/115	-
25	CLA	h	602	-	1/1/13/20	16/27/103/115	-
25	CLA	B	760	-	1/1/10/20	4/13/89/115	-
25	CLA	j	609	-	1/1/12/20	5/21/97/115	-
25	CLA	A	761	-	1/1/15/20	14/39/115/115	-
25	CLA	k	618	-	1/1/12/20	3/21/97/115	-
29	BCR	A	789	-	-	5/29/63/63	0/2/2/2
25	CLA	f	609	-	1/1/10/20	4/12/88/115	-
25	CLA	A	805	-	1/1/13/20	7/27/103/115	-
25	CLA	h	615	-	1/1/10/20	6/12/88/115	-
25	CLA	f	610	-	1/1/13/20	15/27/103/115	-
25	CLA	B	758	-	1/1/15/20	21/39/115/115	-
25	CLA	B	754	-	1/1/10/20	6/13/89/115	-
31	DD6	m	621	-	-	6/26/80/80	0/3/3/3
25	CLA	j	611	-	1/1/12/20	8/21/97/115	-
25	CLA	A	767	-	1/1/10/20	5/13/89/115	-
25	CLA	B	745	-	1/1/14/20	17/37/113/115	-
25	CLA	A	779	-	1/1/10/20	6/13/89/115	-
25	CLA	c	608	-	1/1/12/20	10/21/97/115	-
25	CLA	j	613	-	1/1/14/20	9/36/112/115	-
25	CLA	A	769	-	1/1/15/20	12/39/115/115	-
31	DD6	j	621	-	-	3/26/80/80	0/3/3/3
25	CLA	f	615	-	1/1/10/20	8/13/89/115	-
25	CLA	j	610	-	1/1/14/20	20/38/114/115	-
25	CLA	A	757	-	1/1/11/20	6/15/91/115	-
33	LMG	i	195	-	-	11/39/59/70	0/1/1/1
31	DD6	f	621	-	-	7/26/80/80	0/3/3/3
29	BCR	B	766	-	-	13/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	c	606	-	1/1/10/20	3/13/89/115	-
25	CLA	A	791	-	1/1/14/20	12/37/113/115	-
25	CLA	h	611	-	1/1/10/20	4/13/89/115	-
25	CLA	g	612	-	1/1/10/20	4/12/88/115	-
25	CLA	a	604	-	1/1/11/20	4/15/91/115	-
25	CLA	h	613	-	1/1/12/20	8/25/101/115	-
28	PQN	d	223	-	-	6/15/35/43	0/2/2/2
29	BCR	A	788	-	-	11/29/63/63	0/2/2/2
25	CLA	h	610	-	1/1/12/20	8/26/102/115	-
25	CLA	n	613	-	1/1/10/20	4/12/88/115	-
25	CLA	A	802	-	1/1/10/20	6/13/89/115	-
25	CLA	A	763	-	1/1/15/20	15/39/115/115	-
25	CLA	f	613	-	1/1/13/20	13/32/108/115	-
31	DD6	i	621	-	-	3/26/80/80	0/3/3/3
25	CLA	n	609	-	1/1/11/20	7/15/91/115	-
25	CLA	k	601	-	1/1/10/20	3/13/89/115	-
25	CLA	n	607	-	1/1/10/20	3/12/88/115	-
35	CHL	d	606	-	3/3/16/26	8/15/113/137	-
25	CLA	A	759	-	1/1/14/20	11/33/109/115	-
31	DD6	g	621	-	-	4/26/80/80	0/3/3/3
25	CLA	n	612	-	1/1/10/20	4/12/88/115	-
25	CLA	n	603	-	1/1/13/20	13/27/103/115	-
27	LHG	d	237	-	-	13/33/33/53	-
25	CLA	j	618	-	1/1/12/20	6/21/97/115	-
25	CLA	A	806	-	1/1/11/20	1/15/91/115	-
25	CLA	i	603	-	1/1/10/20	7/13/89/115	-
25	CLA	f	612	-	1/1/10/20	4/12/88/115	-
25	CLA	i	611	-	1/1/10/20	4/13/89/115	-
25	CLA	c	610	-	1/1/13/20	13/27/103/115	-
25	CLA	b	609	-	1/1/11/20	2/15/91/115	-
25	CLA	h	608	-	1/1/11/20	7/19/95/115	-
31	DD6	p	621	-	-	3/26/80/80	0/3/3/3
25	CLA	A	766	-	1/1/13/20	17/31/107/115	-
27	LHG	c	243	-	-	11/34/34/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	m	611	-	1/1/10/20	2/13/89/115	-
25	CLA	B	771	-	1/1/12/20	10/25/101/115	-
27	LHG	h	190	-	-	11/35/35/53	-
25	CLA	h	604	-	1/1/14/20	9/33/109/115	-
25	CLA	B	747	-	1/1/11/20	5/19/95/115	-
25	CLA	B	770	-	1/1/12/20	7/25/101/115	-
27	LHG	A	786	-	-	22/53/53/53	-
25	CLA	b	610	-	1/1/10/20	4/12/88/115	-
29	BCR	M	201	-	-	6/29/63/63	0/2/2/2
25	CLA	m	609	-	1/1/12/20	3/21/97/115	-
25	CLA	p	610	-	1/1/11/20	11/15/91/115	-
27	LHG	j	198	-	-	24/41/41/53	-
25	CLA	n	604	-	1/1/11/20	7/19/95/115	-
31	DD6	e	620	-	-	10/26/80/80	0/3/3/3
34	DGD	e	205	-	-	6/24/64/95	0/2/2/2
25	CLA	A	780	-	1/1/13/20	13/31/107/115	-
25	CLA	b	604	-	1/1/11/20	5/15/91/115	-
25	CLA	g	609	-	1/1/12/20	2/21/97/115	-
31	DD6	o	621	-	-	3/26/80/80	0/3/3/3
34	DGD	b	182	-	-	19/37/77/95	0/2/2/2
25	CLA	A	777	-	1/1/15/20	13/39/115/115	-
25	CLA	A	773	-	1/1/12/20	8/25/101/115	-
25	CLA	l	614	-	1/1/10/20	4/12/88/115	-
25	CLA	b	612	-	1/1/12/20	9/24/100/115	-
25	CLA	l	602	-	1/1/13/20	12/32/108/115	-
31	DD6	n	620	-	-	5/26/80/80	0/3/3/3
25	CLA	p	609	-	1/1/12/20	10/21/97/115	-
25	CLA	B	739	-	1/1/15/20	13/39/115/115	-
25	CLA	l	610	-	1/1/12/20	14/26/102/115	-
31	DD6	J	4002	-	-	2/26/80/80	0/3/3/3
33	LMG	k	179	-	-	16/31/51/70	0/1/1/1
25	CLA	B	785	-	1/1/11/20	7/15/91/115	-
25	CLA	h	601	-	1/1/12/20	7/21/97/115	-
25	CLA	p	602	-	1/1/10/20	8/13/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	f	604	-	1/1/10/20	3/12/88/115	-
29	BCR	B	763	-	-	2/29/63/63	0/2/2/2
25	CLA	k	604	-	1/1/15/20	18/39/115/115	-
25	CLA	B	755	-	1/1/14/20	17/33/109/115	-
25	CLA	b	605	-	1/1/11/20	6/15/91/115	-
25	CLA	p	613	-	1/1/10/20	5/13/89/115	-
31	DD6	c	620	-	-	4/26/80/80	0/3/3/3
25	CLA	i	613	-	1/1/13/20	10/32/108/115	-
25	CLA	n	605	-	1/1/10/20	4/12/88/115	-
25	CLA	B	768	-	1/1/13/20	6/27/103/115	-
25	CLA	A	799	-	1/1/14/20	16/33/109/115	-
31	DD6	d	623	-	-	4/26/80/80	0/3/3/3
31	DD6	k	620	-	-	2/26/80/80	0/3/3/3
25	CLA	e	605	-	1/1/10/20	2/12/88/115	-
25	CLA	f	608	-	1/1/10/20	2/12/88/115	-
27	LHG	A	756	-	-	17/42/42/53	-
25	CLA	B	780	-	1/1/12/20	5/25/101/115	-
25	CLA	k	603	-	1/1/10/20	4/12/88/115	-
25	CLA	e	607	-	1/1/10/20	6/13/89/115	-
25	CLA	e	609	-	1/1/12/20	8/24/100/115	-
25	CLA	d	603	-	1/1/10/20	4/12/88/115	-
25	CLA	B	773	-	1/1/14/20	6/35/111/115	-
25	CLA	B	772	-	1/1/12/20	11/21/97/115	-
25	CLA	l	613	-	1/1/11/20	7/19/95/115	-
33	LMG	B	786	-	-	19/47/67/70	0/1/1/1
32	SF4	C	82	-	-	-	0/6/5/5
25	CLA	g	610	-	1/1/13/20	11/27/103/115	-
25	CLA	f	601	-	1/1/10/20	6/12/88/115	-
25	CLA	a	609	-	1/1/12/20	5/21/97/115	-
25	CLA	e	601	-	1/1/10/20	5/10/86/115	-
25	CLA	b	611	-	1/1/10/20	4/12/88/115	-
25	CLA	m	608	-	1/1/10/20	2/12/88/115	-
31	DD6	b	621	-	-	1/26/80/80	0/3/3/3
25	CLA	a	602	-	1/1/14/20	17/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	e	611	-	1/1/10/20	3/12/88/115	-
31	DD6	n	621	-	-	13/26/80/80	0/3/3/3
25	CLA	e	613	-	1/1/13/20	4/27/103/115	-
31	DD6	e	621	-	-	5/26/80/80	0/3/3/3
25	CLA	A	793	-	1/1/10/20	0/12/88/115	-
25	CLA	g	613	-	1/1/13/20	12/27/103/115	-
25	CLA	i	615	-	1/1/12/20	2/21/97/115	-
25	CLA	B	779	-	1/1/15/20	14/39/115/115	-
25	CLA	j	615	-	1/1/10/20	5/13/89/115	-
25	CLA	o	609	-	1/1/11/20	5/15/91/115	-
31	DD6	A	4008	-	-	9/26/80/80	0/3/3/3
25	CLA	d	601	-	1/1/12/20	6/21/97/115	-
25	CLA	h	612	-	1/1/13/20	8/31/107/115	-
25	CLA	A	807	-	1/1/11/20	3/19/95/115	-
25	CLA	h	603	-	1/1/10/20	5/13/89/115	-
25	CLA	p	601	-	1/1/10/20	3/12/88/115	-
25	CLA	B	746	-	1/1/14/20	12/38/114/115	-
25	CLA	m	603	-	1/1/12/20	9/26/102/115	-
31	DD6	c	623	-	-	8/26/80/80	0/3/3/3
25	CLA	A	775	-	1/1/13/20	13/31/107/115	-
25	CLA	m	601	-	1/1/10/20	4/12/88/115	-
25	CLA	o	601	-	1/1/10/20	2/10/86/115	-
25	CLA	f	603	-	1/1/10/20	1/13/89/115	-
25	CLA	o	613	-	1/1/10/20	6/12/88/115	-
25	CLA	h	614	-	1/1/10/20	5/13/89/115	-
25	CLA	B	752	-	1/1/15/20	13/39/115/115	-
25	CLA	n	610	-	1/1/10/20	2/10/86/115	-
25	CLA	o	610	-	1/1/10/20	2/10/86/115	-
25	CLA	o	614	-	1/1/10/20	7/13/89/115	-
29	BCR	B	765	-	-	12/29/63/63	0/2/2/2
25	CLA	e	610	-	1/1/13/20	8/27/103/115	-
29	BCR	A	787	-	-	5/29/63/63	0/2/2/2
25	CLA	f	611	-	1/1/10/20	2/12/88/115	-
25	CLA	e	612	-	1/1/10/20	1/13/89/115	-
25	CLA	l	601	-	1/1/10/20	3/12/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	A	784	-	1/1/15/20	14/39/115/115	-
25	CLA	p	608	-	1/1/10/20	6/12/88/115	-
25	CLA	A	772	-	1/1/14/20	15/37/113/115	-
25	CLA	g	618	-	1/1/11/20	4/15/91/115	-
25	CLA	i	604	-	1/1/10/20	3/13/89/115	-
30	SQD	c	245	-	-	21/34/54/69	0/1/1/1
25	CLA	A	770	-	1/1/15/20	12/39/115/115	-
25	CLA	o	612	-	1/1/9/20	4/13/85/115	-
27	LHG	h	189	-	-	13/33/33/53	-
25	CLA	g	604	-	1/1/10/20	3/13/89/115	-
25	CLA	i	601	-	1/1/12/20	13/25/101/115	-
28	PQN	B	761	-	-	8/23/43/43	0/2/2/2
25	CLA	c	619	-	1/1/10/20	4/10/86/115	-
25	CLA	B	750	-	1/1/14/20	9/33/109/115	-
35	CHL	d	608	-	3/3/16/26	5/15/113/137	-
25	CLA	k	608	-	1/1/12/20	2/21/97/115	-
25	CLA	p	604	-	1/1/10/20	5/13/89/115	-
25	CLA	c	603	-	1/1/12/20	6/25/101/115	-
31	DD6	A	4002	-	-	3/26/80/80	0/3/3/3
34	DGD	B	787	-	-	19/43/83/95	0/2/2/2
25	CLA	B	775	-	1/1/12/20	8/21/97/115	-
31	DD6	h	620	-	-	3/26/80/80	0/3/3/3
25	CLA	B	777	-	1/1/12/20	12/25/101/115	-
25	CLA	i	614	-	1/1/10/20	2/12/88/115	-
25	CLA	i	608	-	1/1/15/20	13/39/115/115	-
30	SQD	j	200	-	-	12/31/51/69	0/1/1/1
29	BCR	B	762	-	-	7/29/63/63	0/2/2/2
25	CLA	c	611	-	1/1/10/20	1/13/89/115	-
25	CLA	A	782	-	1/1/11/20	3/19/95/115	-
25	CLA	a	603	-	1/1/12/20	6/25/101/115	-
25	CLA	A	794	-	1/1/13/20	7/30/106/115	-
25	CLA	B	759	-	1/1/10/20	4/13/89/115	-
25	CLA	c	614	-	1/1/10/20	6/12/88/115	-
33	LMG	a	182	-	-	17/38/58/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LHG	b	181	-	-	23/35/35/53	-
25	CLA	B	741	-	1/1/15/20	15/39/115/115	-
25	CLA	B	743	-	1/1/10/20	4/12/88/115	-
25	CLA	l	604	-	1/1/10/20	2/13/89/115	-
25	CLA	B	784	-	1/1/15/20	18/39/115/115	-
25	CLA	m	610	-	1/1/10/20	6/12/88/115	-
25	CLA	j	602	-	1/1/13/20	4/27/103/115	-
31	DD6	b	620	-	-	5/26/80/80	0/3/3/3
25	CLA	c	616	-	1/1/11/20	3/18/94/115	-
31	DD6	k	621	-	-	3/26/80/80	0/3/3/3
29	BCR	B	764	-	-	6/29/63/63	0/2/2/2
25	CLA	A	768	-	1/1/13/20	10/29/105/115	-
25	CLA	A	755	-	1/1/14/20	8/33/109/115	-
31	DD6	d	620	-	-	2/26/80/80	0/3/3/3
25	CLA	j	604	-	1/1/13/20	10/30/106/115	-
29	BCR	A	790	-	-	10/29/63/63	0/2/2/2
25	CLA	A	765	-	1/1/13/20	10/32/108/115	-
25	CLA	g	614	-	1/1/10/20	3/12/88/115	-
25	CLA	B	749	-	1/1/11/20	8/20/96/115	-
25	CLA	d	614	-	1/1/10/20	4/12/88/115	-
25	CLA	a	601	-	1/1/12/20	5/21/97/115	-
25	CLA	b	613	-	1/1/10/20	4/12/88/115	-
25	CLA	a	619	-	1/1/14/20	9/37/113/115	-
25	CLA	A	778	-	1/1/10/20	3/13/89/115	-
25	CLA	B	748	-	1/1/13/20	10/32/108/115	-
25	CLA	B	751	-	1/1/12/20	9/21/97/115	-
25	CLA	f	602	-	1/1/13/20	14/32/108/115	-
25	CLA	A	771	-	1/1/13/20	9/30/106/115	-
25	CLA	l	603	-	1/1/10/20	1/13/89/115	-
25	CLA	m	612	-	1/1/10/20	3/13/89/115	-
25	CLA	B	740	-	1/1/10/20	2/12/88/115	-
25	CLA	a	608	-	1/1/12/20	12/25/101/115	-
27	LHG	g	189	-	-	25/39/39/53	-
25	CLA	j	608	-	1/1/11/20	5/18/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	DD6	c	621	-	-	0/26/80/80	0/3/3/3
25	CLA	l	611	-	1/1/10/20	3/13/89/115	-
27	LHG	i	194	-	-	20/40/40/53	-
25	CLA	g	603	-	1/1/10/20	2/12/88/115	-
25	CLA	o	604	-	1/1/10/20	3/12/88/115	-
25	CLA	m	602	-	1/1/14/20	16/33/109/115	-
25	CLA	A	783	-	1/1/15/20	12/39/115/115	-
25	CLA	k	609	-	1/1/12/20	2/21/97/115	-
31	DD6	i	620	-	-	2/26/80/80	0/3/3/3
31	DD6	h	621	-	-	0/26/80/80	0/3/3/3
25	CLA	c	602	-	1/1/13/20	14/32/108/115	-
25	CLA	k	612	-	1/1/10/20	1/13/89/115	-
25	CLA	e	614	-	1/1/10/20	4/12/88/115	-
26	LMT	A	754	-	-	7/21/61/61	0/2/2/2
25	CLA	n	606	-	1/1/10/20	6/12/88/115	-
25	CLA	B	737	-	1/1/13/20	10/27/103/115	-
31	DD6	l	620	-	-	2/26/80/80	0/3/3/3
31	DD6	d	621	-	-	3/26/80/80	0/3/3/3
25	CLA	k	611	-	1/1/10/20	2/12/88/115	-
25	CLA	b	601	-	1/1/10/20	4/12/88/115	-
25	CLA	c	604	-	1/1/11/20	5/19/95/115	-
25	CLA	i	602	-	1/1/14/20	13/38/114/115	-
29	BCR	B	767	-	-	4/29/63/63	0/2/2/2
25	CLA	p	612	-	1/1/10/20	3/13/89/115	-
25	CLA	b	603	-	1/1/10/20	5/13/89/115	-
25	CLA	A	800	-	1/1/11/20	5/19/95/115	-
25	CLA	A	752	-	1/1/15/20	16/39/115/115	-
25	CLA	j	603	-	1/1/10/20	1/12/88/115	-
25	CLA	e	603	-	1/1/11/20	5/15/91/115	-
25	CLA	b	608	-	1/1/10/20	2/10/86/115	-
25	CLA	A	798	-	1/1/12/20	11/24/100/115	-
25	CLA	j	601	-	1/1/12/20	7/21/97/115	-
31	DD6	a	620	-	-	5/26/80/80	0/3/3/3
25	CLA	A	758	-	1/1/15/20	10/39/115/115	-
31	DD6	i	625	-	-	1/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B	744	-	1/1/10/20	3/13/89/115	-
25	CLA	j	614	-	1/1/10/20	2/12/88/115	-
25	CLA	g	615	-	1/1/10/20	0/12/88/115	-
31	DD6	c	624	-	-	15/26/80/80	0/3/3/3
29	BCR	A	796	-	-	8/29/63/63	0/2/2/2
25	CLA	A	764	-	1/1/13/20	11/31/107/115	-
25	CLA	c	609	-	1/1/14/20	13/33/109/115	-
31	DD6	a	621	-	-	0/26/80/80	0/3/3/3
35	CHL	c	607	-	3/3/16/26	7/19/117/137	-
31	DD6	m	620	-	-	6/26/80/80	0/3/3/3
31	DD6	F	4002	-	-	18/26/80/80	0/3/3/3
25	CLA	A	776	-	1/1/15/20	8/39/115/115	-
25	CLA	n	608	-	1/1/10/20	2/10/86/115	-
25	CLA	c	601	-	1/1/10/20	5/12/88/115	-
25	CLA	l	608	-	1/1/10/20	5/13/89/115	-
25	CLA	j	612	-	1/1/13/20	9/27/103/115	-
35	CHL	d	605	-	3/3/17/26	7/21/119/137	-
25	CLA	p	603	-	1/1/10/20	4/12/88/115	-
25	CLA	d	611	-	1/1/11/20	5/15/91/115	-

All (2211) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	b	181	LHG	P-O3	6.57	1.85	1.59
27	m	182	LHG	P-O3	6.52	1.84	1.59
27	c	243	LHG	P-O3	6.46	1.84	1.59
27	d	237	LHG	P-O3	6.40	1.84	1.59
27	h	189	LHG	P-O3	6.38	1.84	1.59
27	a	181	LHG	P-O3	6.34	1.84	1.59
27	h	190	LHG	P-O3	6.28	1.84	1.59
27	g	189	LHG	P-O3	6.20	1.83	1.59
27	A	786	LHG	P-O3	6.20	1.83	1.59
31	A	4002	DD6	C28-C27	-6.13	1.46	1.50
27	i	194	LHG	P-O3	6.11	1.83	1.59
27	j	198	LHG	P-O3	6.07	1.83	1.59
27	A	756	LHG	P-O3	5.86	1.82	1.59
35	d	605	CHL	C3B-C4B	5.67	1.46	1.41
35	e	606	CHL	CMC-C2C	5.64	1.56	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	d	608	CHL	CMC-C2C	5.61	1.56	1.44
35	d	606	CHL	CMC-C2C	5.60	1.56	1.44
35	d	607	CHL	C3B-C4B	5.56	1.46	1.41
25	p	603	CLA	MG-NA	5.49	2.19	2.06
35	d	605	CHL	CMC-C2C	5.48	1.56	1.44
35	c	607	CHL	CMC-C2C	5.47	1.56	1.44
27	b	181	LHG	P-O6	5.46	1.80	1.59
27	m	182	LHG	P-O6	5.45	1.80	1.59
35	d	607	CHL	CMC-C2C	5.42	1.56	1.44
27	h	189	LHG	P-O6	5.35	1.80	1.59
25	f	612	CLA	MG-NA	5.34	2.19	2.06
25	g	603	CLA	MG-NA	5.34	2.19	2.06
35	c	607	CHL	C3B-C4B	5.32	1.46	1.41
27	a	181	LHG	P-O6	5.29	1.80	1.59
27	j	198	LHG	P-O6	5.27	1.80	1.59
27	c	243	LHG	P-O6	5.25	1.79	1.59
35	d	606	CHL	C3B-C4B	5.24	1.46	1.41
25	o	603	CLA	MG-NA	5.23	2.18	2.06
27	A	786	LHG	P-O6	5.23	1.79	1.59
35	e	606	CHL	C3B-C4B	5.21	1.46	1.41
25	f	603	CLA	MG-NA	5.21	2.18	2.06
27	g	189	LHG	P-O6	5.20	1.79	1.59
25	p	613	CLA	MG-NA	5.19	2.18	2.06
27	A	756	LHG	P-O6	5.18	1.79	1.59
27	d	237	LHG	P-O6	5.17	1.79	1.59
25	m	603	CLA	MG-NA	5.15	2.18	2.06
25	j	603	CLA	MG-NA	5.14	2.18	2.06
25	l	603	CLA	MG-NA	5.14	2.18	2.06
25	i	603	CLA	MG-NA	5.14	2.18	2.06
25	l	614	CLA	MG-NA	5.14	2.18	2.06
25	m	601	CLA	MG-NA	5.13	2.18	2.06
27	i	194	LHG	P-O6	5.11	1.79	1.59
35	d	608	CHL	C3B-C4B	5.11	1.46	1.41
25	p	610	CLA	MG-NA	5.11	2.18	2.06
25	d	603	CLA	MG-NA	5.09	2.18	2.06
25	n	604	CLA	MG-NA	5.08	2.18	2.06
25	a	612	CLA	MG-NA	5.08	2.18	2.06
27	h	190	LHG	P-O6	5.07	1.79	1.59
25	g	612	CLA	MG-NA	5.07	2.18	2.06
25	b	612	CLA	MG-NA	5.07	2.18	2.06
25	g	608	CLA	MG-NA	5.06	2.18	2.06
25	j	612	CLA	MG-NA	5.06	2.18	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	f	615	CLA	MG-NA	5.06	2.18	2.06
25	o	614	CLA	MG-NA	5.06	2.18	2.06
25	A	793	CLA	MG-NA	5.05	2.18	2.06
25	n	612	CLA	MG-NA	5.03	2.18	2.06
25	n	603	CLA	MG-NA	5.03	2.18	2.06
25	c	612	CLA	MG-NA	5.03	2.18	2.06
25	m	612	CLA	MG-NA	5.03	2.18	2.06
25	k	612	CLA	MG-NA	5.02	2.18	2.06
25	a	603	CLA	MG-NA	5.02	2.18	2.06
25	p	609	CLA	MG-NA	5.02	2.18	2.06
25	j	608	CLA	MG-NA	5.02	2.18	2.06
25	e	612	CLA	MG-NA	5.02	2.18	2.06
25	i	612	CLA	MG-NA	5.02	2.18	2.06
25	d	612	CLA	MG-NA	5.02	2.18	2.06
25	l	612	CLA	MG-NA	5.01	2.18	2.06
25	o	601	CLA	MG-NA	5.01	2.18	2.06
25	h	612	CLA	MG-NA	5.01	2.18	2.06
25	n	609	CLA	MG-NA	5.01	2.18	2.06
25	b	603	CLA	MG-NA	5.01	2.18	2.06
25	e	603	CLA	MG-NA	5.00	2.18	2.06
25	b	601	CLA	MG-NA	5.00	2.18	2.06
25	A	782	CLA	MG-NA	4.99	2.18	2.06
25	n	607	CLA	MG-NA	4.99	2.18	2.06
25	A	772	CLA	MG-NA	4.99	2.18	2.06
25	n	608	CLA	MG-NA	4.99	2.18	2.06
25	d	604	CLA	MG-NA	4.99	2.18	2.06
25	d	614	CLA	MG-NA	4.99	2.18	2.06
25	f	601	CLA	MG-NA	4.98	2.18	2.06
25	n	613	CLA	MG-NA	4.98	2.18	2.06
25	l	617	CLA	MG-NA	4.98	2.18	2.06
25	n	606	CLA	MG-NA	4.98	2.18	2.06
25	o	612	CLA	MG-NA	4.97	2.18	2.06
25	B	747	CLA	MG-NA	4.97	2.18	2.06
25	B	779	CLA	MG-NA	4.97	2.18	2.06
25	n	605	CLA	MG-NA	4.97	2.18	2.06
25	e	604	CLA	MG-NA	4.97	2.18	2.06
25	A	765	CLA	MG-NA	4.97	2.18	2.06
25	o	602	CLA	MG-NA	4.97	2.18	2.06
25	c	603	CLA	MG-NA	4.97	2.18	2.06
25	A	762	CLA	MG-NA	4.96	2.18	2.06
25	p	608	CLA	MG-NA	4.96	2.18	2.06
25	c	604	CLA	MG-NA	4.96	2.18	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	g	601	CLA	MG-NA	4.96	2.18	2.06
25	a	611	CLA	MG-NA	4.96	2.18	2.06
25	f	608	CLA	MG-NA	4.96	2.18	2.06
25	A	776	CLA	MG-NA	4.96	2.18	2.06
25	o	613	CLA	MG-NA	4.96	2.18	2.06
25	o	604	CLA	MG-NA	4.96	2.18	2.06
25	A	777	CLA	MG-NA	4.96	2.18	2.06
25	B	776	CLA	MG-NA	4.96	2.18	2.06
25	B	742	CLA	MG-NA	4.95	2.18	2.06
25	f	609	CLA	MG-NA	4.95	2.18	2.06
25	A	778	CLA	MG-NA	4.95	2.18	2.06
25	p	604	CLA	MG-NA	4.95	2.18	2.06
25	j	614	CLA	MG-NA	4.95	2.18	2.06
25	e	614	CLA	MG-NA	4.95	2.18	2.06
25	k	603	CLA	MG-NA	4.95	2.18	2.06
25	d	611	CLA	MG-NA	4.95	2.18	2.06
25	a	619	CLA	MG-NA	4.94	2.18	2.06
25	f	604	CLA	MG-NA	4.94	2.18	2.06
25	b	605	CLA	MG-NA	4.94	2.18	2.06
25	a	601	CLA	MG-NA	4.94	2.18	2.06
25	g	613	CLA	MG-NA	4.94	2.18	2.06
25	c	611	CLA	MG-NA	4.94	2.18	2.06
25	k	615	CLA	MG-NA	4.94	2.18	2.06
31	J	4002	DD6	C28-C27	-4.94	1.47	1.50
25	c	619	CLA	MG-NA	4.94	2.18	2.06
25	p	602	CLA	MG-NA	4.94	2.18	2.06
25	l	601	CLA	MG-NA	4.94	2.18	2.06
25	f	611	CLA	MG-NA	4.93	2.18	2.06
25	B	741	CLA	MG-NA	4.93	2.18	2.06
25	g	618	CLA	MG-NA	4.93	2.18	2.06
25	e	609	CLA	MG-NA	4.93	2.18	2.06
25	B	768	CLA	MG-NA	4.93	2.18	2.06
25	m	604	CLA	MG-NA	4.93	2.18	2.06
25	J	101	CLA	MG-NA	4.93	2.18	2.06
25	g	614	CLA	MG-NA	4.93	2.18	2.06
25	c	606	CLA	MG-NA	4.93	2.18	2.06
25	B	743	CLA	MG-NA	4.93	2.18	2.06
25	g	615	CLA	MG-NA	4.93	2.18	2.06
25	e	601	CLA	MG-NA	4.93	2.18	2.06
25	p	601	CLA	MG-NA	4.93	2.18	2.06
25	h	618	CLA	MG-NA	4.93	2.18	2.06
25	h	601	CLA	MG-NA	4.92	2.18	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	l	604	CLA	MG-NA	4.92	2.18	2.06
25	e	605	CLA	MG-NA	4.92	2.18	2.06
25	h	602	CLA	MG-NA	4.92	2.18	2.06
25	f	610	CLA	MG-NA	4.92	2.18	2.06
25	k	614	CLA	MG-NA	4.92	2.18	2.06
25	l	611	CLA	MG-NA	4.92	2.18	2.06
25	A	807	CLA	MG-NA	4.92	2.18	2.06
25	a	604	CLA	MG-NA	4.92	2.18	2.06
31	j	620	DD6	C28-C27	-4.92	1.47	1.50
25	B	746	CLA	MG-NA	4.92	2.18	2.06
25	e	611	CLA	MG-NA	4.92	2.18	2.06
25	h	608	CLA	MG-NA	4.92	2.17	2.06
25	b	611	CLA	MG-NA	4.92	2.17	2.06
25	m	608	CLA	MG-NA	4.92	2.17	2.06
25	A	767	CLA	MG-NA	4.92	2.17	2.06
25	B	780	CLA	MG-NA	4.92	2.17	2.06
25	B	771	CLA	MG-NA	4.91	2.17	2.06
25	B	782	CLA	MG-NA	4.91	2.17	2.06
25	A	779	CLA	MG-NA	4.91	2.17	2.06
25	m	611	CLA	MG-NA	4.91	2.17	2.06
25	A	764	CLA	MG-NA	4.91	2.17	2.06
25	B	785	CLA	MG-NA	4.91	2.17	2.06
25	m	613	CLA	MG-NA	4.91	2.17	2.06
25	h	604	CLA	MG-NA	4.91	2.17	2.06
25	f	614	CLA	MG-NA	4.91	2.17	2.06
25	j	604	CLA	MG-NA	4.91	2.17	2.06
25	A	755	CLA	MG-NA	4.90	2.17	2.06
25	A	774	CLA	MG-NA	4.90	2.17	2.06
25	c	614	CLA	MG-NA	4.90	2.17	2.06
25	B	772	CLA	MG-NA	4.90	2.17	2.06
25	c	616	CLA	MG-NA	4.90	2.17	2.06
25	l	608	CLA	MG-NA	4.90	2.17	2.06
25	e	613	CLA	MG-NA	4.90	2.17	2.06
25	c	609	CLA	MG-NA	4.90	2.17	2.06
25	j	618	CLA	MG-NA	4.90	2.17	2.06
25	A	769	CLA	MG-NA	4.89	2.17	2.06
25	k	601	CLA	MG-NA	4.89	2.17	2.06
25	B	754	CLA	MG-NA	4.89	2.17	2.06
25	i	611	CLA	MG-NA	4.89	2.17	2.06
25	B	770	CLA	MG-NA	4.89	2.17	2.06
25	i	614	CLA	MG-NA	4.89	2.17	2.06
25	A	808	CLA	MG-NA	4.89	2.17	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d	601	CLA	MG-NA	4.89	2.17	2.06
25	B	760	CLA	MG-NA	4.89	2.17	2.06
25	h	603	CLA	MG-NA	4.89	2.17	2.06
25	g	611	CLA	MG-NA	4.89	2.17	2.06
25	B	774	CLA	MG-NA	4.89	2.17	2.06
25	d	609	CLA	MG-NA	4.89	2.17	2.06
25	o	608	CLA	MG-NA	4.88	2.17	2.06
25	k	608	CLA	MG-NA	4.88	2.17	2.06
25	i	608	CLA	MG-NA	4.88	2.17	2.06
25	o	609	CLA	MG-NA	4.88	2.17	2.06
25	d	610	CLA	MG-NA	4.88	2.17	2.06
25	i	601	CLA	MG-NA	4.88	2.17	2.06
25	A	780	CLA	MG-NA	4.88	2.17	2.06
25	c	613	CLA	MG-NA	4.88	2.17	2.06
25	b	613	CLA	MG-NA	4.88	2.17	2.06
25	B	738	CLA	MG-NA	4.88	2.17	2.06
25	f	613	CLA	MG-NA	4.88	2.17	2.06
25	n	610	CLA	MG-NA	4.87	2.17	2.06
25	B	781	CLA	MG-NA	4.87	2.17	2.06
25	h	615	CLA	MG-NA	4.87	2.17	2.06
25	B	755	CLA	MG-NA	4.87	2.17	2.06
25	i	615	CLA	MG-NA	4.87	2.17	2.06
25	B	748	CLA	MG-NA	4.87	2.17	2.06
25	h	609	CLA	MG-NA	4.87	2.17	2.06
25	A	761	CLA	MG-NA	4.87	2.17	2.06
25	b	608	CLA	MG-NA	4.87	2.17	2.06
25	a	609	CLA	MG-NA	4.86	2.17	2.06
25	e	607	CLA	MG-NA	4.86	2.17	2.06
25	l	609	CLA	MG-NA	4.86	2.17	2.06
25	h	614	CLA	MG-NA	4.86	2.17	2.06
25	k	604	CLA	MG-NA	4.86	2.17	2.06
25	A	800	CLA	MG-NA	4.86	2.17	2.06
25	f	602	CLA	MG-NA	4.86	2.17	2.06
25	A	804	CLA	MG-NA	4.86	2.17	2.06
25	h	611	CLA	MG-NA	4.85	2.17	2.06
25	A	798	CLA	MG-NA	4.85	2.17	2.06
25	B	749	CLA	MG-NA	4.85	2.17	2.06
25	b	602	CLA	MG-NA	4.85	2.17	2.06
25	j	615	CLA	MG-NA	4.85	2.17	2.06
25	p	612	CLA	MG-NA	4.85	2.17	2.06
25	k	611	CLA	MG-NA	4.85	2.17	2.06
25	g	604	CLA	MG-NA	4.85	2.17	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	604	CLA	MG-NA	4.85	2.17	2.06
25	B	783	CLA	MG-NA	4.84	2.17	2.06
25	j	609	CLA	MG-NA	4.84	2.17	2.06
25	B	752	CLA	MG-NA	4.84	2.17	2.06
25	B	744	CLA	MG-NA	4.84	2.17	2.06
25	B	740	CLA	MG-NA	4.84	2.17	2.06
25	j	601	CLA	MG-NA	4.84	2.17	2.06
25	B	777	CLA	MG-NA	4.84	2.17	2.06
25	A	803	CLA	MG-NA	4.84	2.17	2.06
35	d	605	CHL	C1D-C2D	4.84	1.45	1.39
25	j	611	CLA	MG-NA	4.84	2.17	2.06
25	c	601	CLA	MG-NA	4.83	2.17	2.06
25	l	613	CLA	MG-NA	4.83	2.17	2.06
25	b	609	CLA	MG-NA	4.83	2.17	2.06
25	B	784	CLA	MG-NA	4.83	2.17	2.06
25	A	802	CLA	MG-NA	4.83	2.17	2.06
25	k	618	CLA	MG-NA	4.83	2.17	2.06
25	A	801	CLA	MG-NA	4.83	2.17	2.06
25	l	602	CLA	MG-NA	4.83	2.17	2.06
25	B	759	CLA	MG-NA	4.82	2.17	2.06
25	b	610	CLA	MG-NA	4.82	2.17	2.06
25	m	609	CLA	MG-NA	4.82	2.17	2.06
25	A	773	CLA	MG-NA	4.82	2.17	2.06
25	i	609	CLA	MG-NA	4.82	2.17	2.06
25	A	794	CLA	MG-NA	4.82	2.17	2.06
25	d	613	CLA	MG-NA	4.82	2.17	2.06
35	c	607	CHL	C1D-C2D	4.81	1.45	1.39
25	A	771	CLA	MG-NA	4.81	2.17	2.06
25	B	745	CLA	MG-NA	4.81	2.17	2.06
25	A	766	CLA	MG-NA	4.81	2.17	2.06
25	A	760	CLA	MG-NA	4.81	2.17	2.06
25	A	757	CLA	MG-NA	4.81	2.17	2.06
25	A	806	CLA	MG-NA	4.81	2.17	2.06
25	A	768	CLA	MG-NA	4.81	2.17	2.06
25	i	604	CLA	MG-NA	4.81	2.17	2.06
25	m	610	CLA	MG-NA	4.81	2.17	2.06
25	B	778	CLA	MG-NA	4.81	2.17	2.06
25	A	799	CLA	MG-NA	4.81	2.17	2.06
25	B	758	CLA	MG-NA	4.81	2.17	2.06
25	c	608	CLA	MG-NA	4.80	2.17	2.06
25	k	602	CLA	MG-NA	4.80	2.17	2.06
25	e	602	CLA	MG-NA	4.80	2.17	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	739	CLA	MG-NA	4.80	2.17	2.06
25	a	613	CLA	MG-NA	4.80	2.17	2.06
25	a	608	CLA	MG-NA	4.80	2.17	2.06
25	B	753	CLA	MG-NA	4.80	2.17	2.06
25	e	610	CLA	MG-NA	4.80	2.17	2.06
25	B	775	CLA	MG-NA	4.80	2.17	2.06
25	c	602	CLA	MG-NA	4.79	2.17	2.06
25	g	609	CLA	MG-NA	4.79	2.17	2.06
25	B	773	CLA	MG-NA	4.79	2.17	2.06
25	A	759	CLA	MG-NA	4.78	2.17	2.06
25	k	609	CLA	MG-NA	4.78	2.17	2.06
25	A	781	CLA	MG-NA	4.77	2.17	2.06
31	d	620	DD6	C28-C27	-4.77	1.47	1.50
25	k	613	CLA	MG-NA	4.77	2.17	2.06
35	d	607	CHL	C1D-C2D	4.77	1.45	1.39
25	A	770	CLA	MG-NA	4.77	2.17	2.06
25	A	797	CLA	MG-NA	4.77	2.17	2.06
25	d	602	CLA	MG-NA	4.77	2.17	2.06
25	e	608	CLA	MG-NA	4.77	2.17	2.06
25	A	752	CLA	MG-NA	4.77	2.17	2.06
25	A	775	CLA	MG-NA	4.76	2.17	2.06
25	c	610	CLA	MG-NA	4.76	2.17	2.06
25	B	757	CLA	MG-NA	4.75	2.17	2.06
25	i	602	CLA	MG-NA	4.75	2.17	2.06
25	B	751	CLA	MG-NA	4.74	2.17	2.06
25	A	763	CLA	MG-NA	4.74	2.17	2.06
25	a	602	CLA	MG-NA	4.74	2.17	2.06
25	A	784	CLA	MG-NA	4.74	2.17	2.06
25	g	602	CLA	MG-NA	4.73	2.17	2.06
25	B	756	CLA	MG-NA	4.73	2.17	2.06
25	k	610	CLA	MG-NA	4.73	2.17	2.06
25	m	602	CLA	MG-NA	4.73	2.17	2.06
25	o	610	CLA	MG-NA	4.73	2.17	2.06
25	i	613	CLA	MG-NA	4.73	2.17	2.06
30	g	190	SQD	O48-C23	4.72	1.47	1.33
25	a	610	CLA	MG-NA	4.71	2.17	2.06
25	B	736	CLA	MG-NA	4.71	2.17	2.06
25	B	750	CLA	MG-NA	4.71	2.17	2.06
25	i	610	CLA	MG-NA	4.71	2.17	2.06
25	n	602	CLA	MG-NA	4.71	2.17	2.06
25	j	613	CLA	MG-NA	4.70	2.17	2.06
35	d	608	CHL	C1D-C2D	4.70	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	l	610	CLA	MG-NA	4.69	2.17	2.06
30	j	200	SQD	O48-C23	4.68	1.47	1.33
25	h	613	CLA	MG-NA	4.68	2.17	2.06
25	A	791	CLA	MG-NA	4.67	2.17	2.06
25	A	753	CLA	MG-NA	4.66	2.17	2.06
25	j	610	CLA	MG-NA	4.66	2.17	2.06
35	c	607	CHL	C1B-C2B	4.66	1.44	1.39
25	A	783	CLA	MG-NA	4.65	2.17	2.06
31	a	621	DD6	C28-C27	-4.65	1.47	1.50
25	g	610	CLA	MG-NA	4.65	2.17	2.06
30	c	245	SQD	O48-C23	4.64	1.46	1.33
25	j	602	CLA	MG-NA	4.64	2.17	2.06
31	c	623	DD6	C28-C27	-4.64	1.47	1.50
31	c	621	DD6	C28-C27	-4.63	1.47	1.50
31	A	4008	DD6	C28-C27	-4.62	1.47	1.50
25	h	610	CLA	MG-NA	4.60	2.17	2.06
25	B	737	CLA	MG-NA	4.60	2.17	2.06
31	h	621	DD6	C28-C27	-4.60	1.47	1.50
35	d	606	CHL	C1D-C2D	4.60	1.44	1.39
35	d	606	CHL	C1B-C2B	4.59	1.44	1.39
31	e	621	DD6	C28-C27	-4.58	1.47	1.50
35	e	606	CHL	C1D-C2D	4.58	1.44	1.39
25	A	758	CLA	MG-NA	4.57	2.17	2.06
25	A	805	CLA	MG-NA	4.57	2.17	2.06
31	b	620	DD6	C28-C27	-4.57	1.47	1.50
31	k	620	DD6	C28-C27	-4.54	1.47	1.50
31	j	621	DD6	C28-C27	-4.52	1.47	1.50
35	d	607	CHL	C1B-C2B	4.50	1.44	1.39
31	b	621	DD6	C28-C27	-4.48	1.47	1.50
31	l	620	DD6	C28-C27	-4.48	1.47	1.50
35	d	605	CHL	C1B-C2B	4.47	1.44	1.39
31	d	621	DD6	C28-C27	-4.47	1.48	1.50
31	h	620	DD6	C28-C27	-4.47	1.48	1.50
35	e	606	CHL	C1B-C2B	4.42	1.44	1.39
31	m	621	DD6	C28-C27	-4.42	1.48	1.50
31	g	621	DD6	C28-C27	-4.41	1.48	1.50
31	d	623	DD6	C28-C27	-4.40	1.48	1.50
31	a	620	DD6	C28-C27	-4.36	1.48	1.50
31	i	621	DD6	C28-C27	-4.36	1.48	1.50
31	c	620	DD6	C28-C27	-4.32	1.48	1.50
31	i	620	DD6	C28-C27	-4.31	1.48	1.50
31	k	621	DD6	C28-C27	-4.30	1.48	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	i	625	DD6	C28-C27	-4.30	1.48	1.50
31	f	620	DD6	C28-C27	-4.30	1.48	1.50
35	d	608	CHL	C1B-C2B	4.28	1.44	1.39
31	l	621	DD6	C28-C27	-4.26	1.48	1.50
31	o	621	DD6	C28-C27	-4.23	1.48	1.50
31	m	620	DD6	C28-C27	-4.21	1.48	1.50
31	p	621	DD6	C30-C31	-4.19	1.34	1.42
31	n	620	DD6	C28-C27	-4.18	1.48	1.50
31	c	620	DD6	C30-C31	-4.14	1.34	1.42
31	g	621	DD6	C30-C31	-4.14	1.34	1.42
31	c	623	DD6	C30-C31	-4.13	1.34	1.42
31	A	4002	DD6	C30-C31	-4.13	1.34	1.42
31	i	625	DD6	C30-C31	-4.13	1.34	1.42
31	i	621	DD6	C30-C31	-4.12	1.34	1.42
31	o	620	DD6	C28-C27	-4.12	1.48	1.50
31	m	620	DD6	C30-C31	-4.12	1.34	1.42
31	d	621	DD6	C30-C31	-4.11	1.34	1.42
31	o	621	DD6	C30-C31	-4.11	1.34	1.42
31	o	620	DD6	C30-C31	-4.11	1.34	1.42
31	e	621	DD6	C30-C31	-4.10	1.34	1.42
31	n	620	DD6	C30-C31	-4.10	1.34	1.42
31	d	623	DD6	C30-C31	-4.10	1.34	1.42
31	f	621	DD6	C30-C31	-4.09	1.34	1.42
31	b	621	DD6	C30-C31	-4.07	1.34	1.42
31	d	620	DD6	C30-C31	-4.06	1.34	1.42
25	o	612	CLA	CAD-C3D	-4.06	1.44	1.50
31	j	620	DD6	C30-C31	-4.06	1.34	1.42
31	J	4002	DD6	C30-C31	-4.06	1.34	1.42
31	b	620	DD6	C30-C31	-4.05	1.34	1.42
31	f	621	DD6	C28-C27	-4.05	1.48	1.50
31	h	621	DD6	C30-C31	-4.05	1.34	1.42
31	k	621	DD6	C30-C31	-4.05	1.34	1.42
31	c	621	DD6	C30-C31	-4.05	1.34	1.42
31	f	620	DD6	C30-C31	-4.04	1.34	1.42
31	a	620	DD6	C30-C31	-4.04	1.34	1.42
31	h	620	DD6	C30-C31	-4.03	1.34	1.42
31	j	621	DD6	C30-C31	-4.03	1.34	1.42
31	i	620	DD6	C30-C31	-4.02	1.34	1.42
31	a	621	DD6	C30-C31	-4.02	1.34	1.42
31	l	621	DD6	C30-C31	-4.02	1.34	1.42
31	A	4008	DD6	C30-C31	-4.01	1.34	1.42
31	l	620	DD6	C30-C31	-4.01	1.34	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	d	621	DD6	O1-C20	-4.00	1.41	1.46
31	m	621	DD6	C30-C31	-4.00	1.34	1.42
31	k	620	DD6	C30-C31	-3.98	1.34	1.42
31	g	620	DD6	C30-C31	-3.95	1.34	1.42
31	g	620	DD6	C28-C27	-3.93	1.48	1.50
31	p	621	DD6	C28-C27	-3.91	1.48	1.50
31	c	620	DD6	O1-C20	-3.85	1.41	1.46
29	B	766	BCR	C23-C22	-3.80	1.37	1.46
31	e	621	DD6	O1-C20	-3.79	1.41	1.46
31	J	4002	DD6	O1-C20	-3.78	1.41	1.46
30	j	200	SQD	O47-C45	-3.78	1.37	1.46
31	j	620	DD6	O1-C20	-3.72	1.41	1.46
31	a	621	DD6	O1-C20	-3.72	1.41	1.46
30	g	190	SQD	O47-C45	-3.70	1.37	1.46
31	i	620	DD6	O1-C20	-3.68	1.41	1.46
30	A	795	SQD	O47-C45	-3.68	1.37	1.46
31	m	621	DD6	O1-C20	-3.67	1.41	1.46
30	c	245	SQD	O47-C45	-3.66	1.38	1.46
31	k	620	DD6	O1-C20	-3.66	1.41	1.46
31	j	621	DD6	O1-C20	-3.65	1.41	1.46
31	c	621	DD6	O1-C20	-3.62	1.41	1.46
29	A	788	BCR	C23-C22	-3.62	1.38	1.46
35	d	605	CHL	C3B-C2B	-3.59	1.35	1.40
31	l	621	DD6	O1-C20	-3.58	1.41	1.46
31	h	620	DD6	O1-C20	-3.56	1.41	1.46
31	g	620	DD6	O1-C20	-3.55	1.41	1.46
31	i	621	DD6	O1-C20	-3.54	1.41	1.46
31	d	620	DD6	O1-C20	-3.53	1.41	1.46
35	d	607	CHL	C3B-C2B	-3.52	1.35	1.40
31	l	620	DD6	O1-C20	-3.50	1.41	1.46
35	c	607	CHL	C3B-C2B	-3.50	1.35	1.40
31	h	621	DD6	O1-C20	-3.47	1.41	1.46
29	B	766	BCR	C8-C9	-3.44	1.38	1.46
35	d	608	CHL	C3B-C2B	-3.44	1.35	1.40
35	d	605	CHL	CHA-CBD	3.39	1.55	1.51
35	e	606	CHL	O2D-CGD	3.38	1.41	1.33
31	b	621	DD6	O1-C20	-3.38	1.41	1.46
31	a	620	DD6	O1-C20	-3.37	1.41	1.46
29	B	765	BCR	C23-C22	-3.37	1.38	1.46
30	g	190	SQD	O5-C1	3.37	1.50	1.41
35	d	608	CHL	O2A-CGA	3.36	1.41	1.30
35	e	606	CHL	CHA-CBD	3.36	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	e	606	CHL	O2A-CGA	3.35	1.41	1.30
35	c	607	CHL	O2D-CGD	3.35	1.41	1.33
35	c	607	CHL	CHA-CBD	3.35	1.55	1.51
31	g	621	DD6	O1-C20	-3.35	1.41	1.46
30	A	795	SQD	O5-C1	3.34	1.50	1.41
35	d	605	CHL	O2D-CGD	3.34	1.41	1.33
35	d	606	CHL	CHA-CBD	3.33	1.55	1.51
30	c	245	SQD	O47-C7	3.33	1.43	1.34
29	A	788	BCR	C8-C9	-3.33	1.38	1.46
35	d	607	CHL	O2D-CGD	3.33	1.41	1.33
35	d	606	CHL	O2A-CGA	3.32	1.41	1.30
31	k	621	DD6	O1-C20	-3.32	1.41	1.46
35	d	606	CHL	O2D-CGD	3.32	1.41	1.33
31	o	621	DD6	O1-C20	-3.31	1.41	1.46
30	A	795	SQD	O47-C7	3.31	1.43	1.34
29	B	765	BCR	C8-C9	-3.30	1.38	1.46
35	d	607	CHL	CHA-CBD	3.29	1.55	1.51
35	d	608	CHL	O2D-CGD	3.28	1.41	1.33
35	d	606	CHL	C3B-C2B	-3.25	1.36	1.40
35	e	606	CHL	C3B-C2B	-3.25	1.36	1.40
30	g	190	SQD	O47-C7	3.24	1.43	1.34
35	d	608	CHL	CHA-CBD	3.20	1.55	1.51
29	A	792	BCR	C8-C9	-3.20	1.39	1.46
31	A	4008	DD6	O1-C20	-3.20	1.42	1.46
28	B	761	PQN	C2M-C2	-3.19	1.44	1.50
30	c	245	SQD	O5-C1	3.19	1.50	1.41
30	j	200	SQD	O47-C7	3.17	1.43	1.34
31	F	4002	DD6	C24-C1	-3.10	1.39	1.46
29	A	792	BCR	C23-C22	-3.08	1.39	1.46
31	m	620	DD6	O1-C20	-3.07	1.42	1.46
28	B	761	PQN	C10-C5	-3.06	1.35	1.40
30	A	795	SQD	C24-C23	3.05	1.59	1.49
30	j	200	SQD	C24-C23	3.05	1.59	1.50
30	c	245	SQD	C24-C23	3.04	1.59	1.50
31	e	620	DD6	C24-C1	-3.03	1.39	1.46
30	g	190	SQD	C24-C23	3.02	1.59	1.50
28	A	785	PQN	C10-C5	-3.01	1.35	1.40
31	e	620	DD6	C13-C11	-2.99	1.39	1.46
25	A	753	CLA	C1D-ND	-2.98	1.33	1.37
31	i	625	DD6	O1-C20	-2.97	1.42	1.46
29	B	765	BCR	C19-C18	-2.97	1.39	1.46
31	o	620	DD6	O1-C20	-2.96	1.42	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	788	BCR	C19-C18	-2.96	1.39	1.46
35	c	607	CHL	O2A-CGA	2.96	1.42	1.33
29	B	766	BCR	C19-C18	-2.96	1.39	1.46
31	F	4002	DD6	C25-C26	-2.95	1.34	1.43
31	b	620	DD6	O1-C20	-2.95	1.42	1.46
31	A	4002	DD6	O1-C20	-2.95	1.42	1.46
25	A	780	CLA	C1D-ND	-2.93	1.34	1.37
25	B	737	CLA	C1D-ND	-2.93	1.34	1.37
31	e	620	DD6	C8-C6	-2.93	1.39	1.46
31	d	621	DD6	C19-C20	-2.93	1.48	1.52
25	A	798	CLA	C1D-ND	-2.91	1.34	1.37
35	d	605	CHL	O2A-CGA	2.89	1.41	1.33
31	c	624	DD6	C24-C1	-2.89	1.39	1.46
31	n	621	DD6	C24-C1	-2.88	1.39	1.46
25	A	791	CLA	C1D-ND	-2.88	1.34	1.37
29	B	766	BCR	C12-C13	-2.88	1.39	1.46
31	F	4002	DD6	C13-C11	-2.87	1.39	1.46
31	p	621	DD6	O1-C20	-2.87	1.42	1.46
31	e	623	DD6	C26-C27	2.86	1.43	1.37
30	j	200	SQD	O5-C1	2.86	1.49	1.41
29	A	788	BCR	C12-C13	-2.86	1.39	1.46
30	A	795	SQD	O48-C23	2.85	1.47	1.33
31	n	621	DD6	C8-C6	-2.85	1.39	1.46
25	j	610	CLA	C1D-ND	-2.84	1.34	1.37
35	d	606	CHL	C1A-CHA	2.83	1.43	1.40
25	A	783	CLA	C1D-ND	-2.82	1.34	1.37
25	A	758	CLA	C1D-ND	-2.82	1.34	1.37
31	j	620	DD6	C35-C36	-2.82	1.46	1.51
25	h	610	CLA	C1D-ND	-2.81	1.34	1.37
35	c	607	CHL	C1A-CHA	2.81	1.43	1.40
31	n	621	DD6	C13-C11	-2.81	1.39	1.46
25	B	756	CLA	C1D-ND	-2.81	1.34	1.37
31	c	620	DD6	C15-C14	-2.81	1.45	1.50
31	F	4002	DD6	C8-C6	-2.80	1.40	1.46
25	A	773	CLA	C1D-ND	-2.79	1.34	1.37
25	A	804	CLA	C1D-ND	-2.79	1.34	1.37
25	k	609	CLA	C1D-ND	-2.79	1.34	1.37
25	B	773	CLA	C1D-ND	-2.79	1.34	1.37
25	i	602	CLA	C1D-ND	-2.78	1.34	1.37
28	B	769	PQN	C10-C5	-2.78	1.36	1.40
25	a	609	CLA	C1D-ND	-2.78	1.34	1.37
25	A	801	CLA	C1D-ND	-2.78	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	e	613	CLA	C1D-ND	-2.77	1.34	1.37
29	A	789	BCR	C1-C6	-2.77	1.50	1.53
25	h	602	CLA	C1D-ND	-2.77	1.34	1.37
25	A	797	CLA	C1D-ND	-2.77	1.34	1.37
25	p	603	CLA	MG-NB	2.76	2.11	2.05
35	e	606	CHL	C1A-CHA	2.76	1.43	1.40
25	A	805	CLA	C1D-ND	-2.76	1.34	1.37
29	B	765	BCR	C12-C13	-2.75	1.40	1.46
25	B	775	CLA	C1D-ND	-2.75	1.34	1.37
25	j	611	CLA	C1D-ND	-2.74	1.34	1.37
25	a	610	CLA	C1D-ND	-2.74	1.34	1.37
25	j	604	CLA	C1D-ND	-2.74	1.34	1.37
25	g	610	CLA	C1D-ND	-2.73	1.34	1.37
25	B	752	CLA	C1D-ND	-2.73	1.34	1.37
25	k	602	CLA	C1D-ND	-2.73	1.34	1.37
25	m	602	CLA	C1D-ND	-2.73	1.34	1.37
25	B	748	CLA	C1D-ND	-2.72	1.34	1.37
25	i	610	CLA	C1D-ND	-2.72	1.34	1.37
25	B	778	CLA	C1D-ND	-2.72	1.34	1.37
25	A	800	CLA	C1D-ND	-2.72	1.34	1.37
25	B	740	CLA	C1D-ND	-2.72	1.34	1.37
25	i	609	CLA	C1D-ND	-2.71	1.34	1.37
25	B	759	CLA	C1D-ND	-2.71	1.34	1.37
25	A	760	CLA	C1D-ND	-2.71	1.34	1.37
25	B	746	CLA	C1D-ND	-2.71	1.34	1.37
25	B	736	CLA	C1D-ND	-2.71	1.34	1.37
25	b	602	CLA	C1D-ND	-2.71	1.34	1.37
25	B	771	CLA	C1D-ND	-2.70	1.34	1.37
25	j	609	CLA	C1D-ND	-2.70	1.34	1.37
25	B	772	CLA	C1D-ND	-2.70	1.34	1.37
25	A	776	CLA	C1D-ND	-2.70	1.34	1.37
35	d	605	CHL	C1A-CHA	2.70	1.43	1.40
28	d	223	PQN	C10-C5	-2.70	1.36	1.40
25	A	799	CLA	C1D-ND	-2.70	1.34	1.37
31	d	623	DD6	O1-C20	-2.70	1.42	1.46
25	B	753	CLA	C1D-ND	-2.69	1.34	1.37
25	A	781	CLA	C1D-ND	-2.69	1.34	1.37
25	B	744	CLA	C1D-ND	-2.69	1.34	1.37
25	B	774	CLA	C1D-ND	-2.69	1.34	1.37
25	o	612	CLA	C4D-C3D	-2.69	1.40	1.45
25	B	770	CLA	C1D-ND	-2.69	1.34	1.37
25	B	758	CLA	C1D-ND	-2.69	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	610	CLA	C1D-ND	-2.69	1.34	1.37
25	d	613	CLA	C1D-ND	-2.69	1.34	1.37
25	A	777	CLA	C1D-ND	-2.69	1.34	1.37
25	A	762	CLA	C1D-ND	-2.69	1.34	1.37
25	B	777	CLA	C1D-ND	-2.69	1.34	1.37
25	a	613	CLA	C1D-ND	-2.69	1.34	1.37
25	B	760	CLA	C1D-ND	-2.68	1.34	1.37
25	d	610	CLA	C1D-ND	-2.68	1.34	1.37
25	A	768	CLA	C1D-ND	-2.68	1.34	1.37
25	B	754	CLA	C1D-ND	-2.68	1.34	1.37
25	o	608	CLA	C1D-ND	-2.68	1.34	1.37
25	k	610	CLA	C1D-ND	-2.68	1.34	1.37
25	j	601	CLA	C1D-ND	-2.68	1.34	1.37
25	k	618	CLA	C1D-ND	-2.68	1.34	1.37
25	e	602	CLA	C1D-ND	-2.68	1.34	1.37
25	g	601	CLA	C1D-ND	-2.68	1.34	1.37
25	n	609	CLA	C1D-ND	-2.68	1.34	1.37
25	i	601	CLA	C1D-ND	-2.67	1.34	1.37
25	d	602	CLA	C1D-ND	-2.67	1.34	1.37
25	A	757	CLA	C1D-ND	-2.67	1.34	1.37
25	B	755	CLA	C1D-ND	-2.67	1.34	1.37
25	B	747	CLA	C1D-ND	-2.67	1.34	1.37
25	A	763	CLA	C1D-ND	-2.67	1.34	1.37
25	B	779	CLA	C1D-ND	-2.67	1.34	1.37
25	b	608	CLA	C1D-ND	-2.67	1.34	1.37
25	m	601	CLA	MG-NB	2.67	2.11	2.05
25	j	602	CLA	C1D-ND	-2.67	1.34	1.37
25	b	604	CLA	C1D-ND	-2.66	1.34	1.37
25	A	802	CLA	C1D-ND	-2.66	1.34	1.37
25	B	738	CLA	C1D-ND	-2.66	1.34	1.37
31	c	624	DD6	C8-C6	-2.66	1.40	1.46
25	A	770	CLA	C1D-ND	-2.66	1.34	1.37
25	A	794	CLA	C1D-ND	-2.66	1.34	1.37
25	i	611	CLA	C1D-ND	-2.66	1.34	1.37
29	A	792	BCR	C12-C13	-2.66	1.40	1.46
25	A	761	CLA	C1D-ND	-2.65	1.34	1.37
31	f	621	DD6	O1-C20	-2.65	1.42	1.46
25	B	776	CLA	C1D-ND	-2.65	1.34	1.37
25	e	610	CLA	C1D-ND	-2.65	1.34	1.37
25	j	618	CLA	C1D-ND	-2.65	1.34	1.37
25	B	768	CLA	C1D-ND	-2.65	1.34	1.37
25	l	602	CLA	C1D-ND	-2.65	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	o	610	CLA	C1D-ND	-2.65	1.34	1.37
25	d	604	CLA	C1D-ND	-2.65	1.34	1.37
25	B	751	CLA	C1D-ND	-2.65	1.34	1.37
25	h	613	CLA	C1D-ND	-2.65	1.34	1.37
25	i	608	CLA	C1D-ND	-2.65	1.34	1.37
31	A	4002	DD6	C35-C36	-2.64	1.46	1.51
25	A	775	CLA	C1D-ND	-2.64	1.34	1.37
25	m	608	CLA	C1D-ND	-2.64	1.34	1.37
31	e	623	DD6	C28-C27	-2.64	1.49	1.50
25	a	602	CLA	C1D-ND	-2.64	1.34	1.37
25	o	602	CLA	C1D-ND	-2.64	1.34	1.37
25	h	609	CLA	C1D-ND	-2.64	1.34	1.37
25	b	610	CLA	C1D-ND	-2.64	1.34	1.37
31	J	4002	DD6	C35-C36	-2.64	1.46	1.51
31	i	620	DD6	C15-C14	-2.64	1.46	1.50
25	B	741	CLA	C1D-ND	-2.64	1.34	1.37
25	B	742	CLA	C1D-ND	-2.64	1.34	1.37
25	B	780	CLA	C1D-ND	-2.64	1.34	1.37
25	A	765	CLA	C1D-ND	-2.63	1.34	1.37
25	d	609	CLA	C1D-ND	-2.63	1.34	1.37
25	k	604	CLA	C1D-ND	-2.63	1.34	1.37
25	l	608	CLA	C1D-ND	-2.63	1.34	1.37
25	k	614	CLA	C1D-ND	-2.63	1.34	1.37
25	n	602	CLA	CHC-C1C	2.63	1.43	1.38
28	A	785	PQN	C2M-C2	-2.63	1.45	1.50
25	A	784	CLA	C1D-ND	-2.63	1.34	1.37
25	h	604	CLA	C1D-ND	-2.63	1.34	1.37
25	l	609	CLA	C1D-ND	-2.63	1.34	1.37
25	j	614	CLA	C1D-ND	-2.63	1.34	1.37
25	A	755	CLA	C1D-ND	-2.63	1.34	1.37
31	f	620	DD6	O1-C20	-2.63	1.42	1.46
25	b	609	CLA	C1D-ND	-2.63	1.34	1.37
25	m	609	CLA	C1D-ND	-2.63	1.34	1.37
31	c	623	DD6	C35-C36	-2.62	1.46	1.51
25	l	610	CLA	C1D-ND	-2.62	1.34	1.37
25	A	778	CLA	C1D-ND	-2.62	1.34	1.37
25	g	604	CLA	C1D-ND	-2.62	1.34	1.37
25	A	767	CLA	C1D-ND	-2.62	1.34	1.37
25	k	611	CLA	C1D-ND	-2.62	1.34	1.37
25	a	604	CLA	C1D-ND	-2.62	1.34	1.37
25	i	613	CLA	C1D-ND	-2.62	1.34	1.37
25	n	608	CLA	CHC-C1C	2.62	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	o	614	CLA	C1D-ND	-2.62	1.34	1.37
25	B	781	CLA	C1D-ND	-2.62	1.34	1.37
25	A	779	CLA	C1D-ND	-2.62	1.34	1.37
25	g	602	CLA	C1D-ND	-2.62	1.34	1.37
25	f	611	CLA	C1D-ND	-2.62	1.34	1.37
25	o	614	CLA	CHC-C1C	2.61	1.43	1.38
25	c	611	CLA	C1D-ND	-2.61	1.34	1.37
25	c	602	CLA	C1D-ND	-2.61	1.34	1.37
25	c	608	CLA	C1D-ND	-2.61	1.34	1.37
25	A	764	CLA	C1D-ND	-2.61	1.34	1.37
25	h	601	CLA	C1D-ND	-2.61	1.34	1.37
25	p	612	CLA	CHC-C1C	2.61	1.43	1.38
25	d	611	CLA	C1D-ND	-2.61	1.34	1.37
31	i	621	DD6	C35-C36	-2.61	1.47	1.51
25	h	618	CLA	C1D-ND	-2.61	1.34	1.37
25	g	613	CLA	C1D-ND	-2.61	1.34	1.37
25	k	613	CLA	C1D-ND	-2.61	1.34	1.37
25	B	781	CLA	CHC-C1C	2.60	1.43	1.38
25	B	749	CLA	C1D-ND	-2.60	1.34	1.37
25	h	611	CLA	C1D-ND	-2.60	1.34	1.37
25	l	617	CLA	C1D-ND	-2.60	1.34	1.37
25	c	613	CLA	C1D-ND	-2.60	1.34	1.37
25	A	752	CLA	C1D-ND	-2.60	1.34	1.37
25	c	604	CLA	C1D-ND	-2.60	1.34	1.37
35	d	607	CHL	C1A-CHA	2.60	1.43	1.40
25	A	793	CLA	C1D-ND	-2.60	1.34	1.37
25	c	601	CLA	C1D-ND	-2.60	1.34	1.37
25	j	608	CLA	C1D-ND	-2.60	1.34	1.37
25	f	602	CLA	C1D-ND	-2.60	1.34	1.37
25	A	806	CLA	C1D-ND	-2.59	1.34	1.37
25	e	609	CLA	C1D-ND	-2.59	1.34	1.37
25	i	604	CLA	C1D-ND	-2.59	1.34	1.37
25	o	603	CLA	MG-NB	2.59	2.10	2.05
31	a	620	DD6	C35-C36	-2.59	1.47	1.51
25	a	611	CLA	C1D-ND	-2.59	1.34	1.37
25	e	608	CLA	C1D-ND	-2.59	1.34	1.37
25	p	604	CLA	CHC-C1C	2.59	1.43	1.38
25	k	608	CLA	C1D-ND	-2.59	1.34	1.37
25	o	609	CLA	C1D-ND	-2.59	1.34	1.37
31	i	620	DD6	C35-C36	-2.59	1.47	1.51
25	f	612	CLA	MG-NB	2.58	2.10	2.05
25	j	613	CLA	C1D-ND	-2.58	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	c	620	DD6	C35-C36	-2.58	1.47	1.51
25	m	610	CLA	C1D-ND	-2.57	1.34	1.37
31	e	623	DD6	C24-C1	-2.57	1.40	1.46
25	A	808	CLA	C1D-ND	-2.57	1.34	1.37
25	B	757	CLA	C1D-ND	-2.57	1.34	1.37
25	i	614	CLA	C1D-ND	-2.57	1.34	1.37
25	c	619	CLA	C1D-ND	-2.57	1.34	1.37
25	m	601	CLA	MG-NC	2.57	2.12	2.06
25	l	613	CLA	C1D-ND	-2.57	1.34	1.37
25	J	101	CLA	C1D-ND	-2.56	1.34	1.37
25	h	614	CLA	C1D-ND	-2.56	1.34	1.37
25	i	615	CLA	C1D-ND	-2.56	1.34	1.37
25	g	614	CLA	C1D-ND	-2.56	1.34	1.37
25	A	782	CLA	C1D-ND	-2.56	1.34	1.37
25	l	604	CLA	C1D-ND	-2.56	1.34	1.37
25	m	613	CLA	C1D-ND	-2.56	1.34	1.37
25	m	604	CLA	C1D-ND	-2.56	1.34	1.37
25	n	607	CLA	C1D-ND	-2.56	1.34	1.37
25	e	605	CLA	C1D-ND	-2.56	1.34	1.37
25	g	615	CLA	C1D-ND	-2.56	1.34	1.37
25	e	603	CLA	C1D-ND	-2.55	1.34	1.37
31	n	621	DD6	C26-C27	2.55	1.42	1.37
25	B	783	CLA	C1D-ND	-2.55	1.34	1.37
25	j	615	CLA	C1D-ND	-2.55	1.34	1.37
31	n	623	DD6	C25-C26	-2.55	1.35	1.43
25	a	608	CLA	C1D-ND	-2.55	1.34	1.37
25	o	604	CLA	C1D-ND	-2.54	1.34	1.37
31	c	624	DD6	C13-C11	-2.54	1.40	1.46
25	p	602	CLA	CHB-C1B	-2.54	1.33	1.39
25	g	611	CLA	C1D-ND	-2.54	1.34	1.37
25	B	750	CLA	C1D-ND	-2.54	1.34	1.37
35	d	606	CHL	C2C-C3C	2.54	1.38	1.36
25	f	604	CLA	C1D-ND	-2.54	1.34	1.37
25	i	602	CLA	CHC-C1C	2.54	1.43	1.38
25	c	614	CLA	C1D-ND	-2.54	1.34	1.37
25	A	807	CLA	C1D-ND	-2.54	1.34	1.37
25	k	615	CLA	C1D-ND	-2.54	1.34	1.37
25	A	769	CLA	C1D-ND	-2.54	1.34	1.37
29	B	762	BCR	C30-C25	-2.53	1.50	1.53
25	A	803	CLA	C1D-ND	-2.53	1.34	1.37
25	A	771	CLA	C1D-ND	-2.53	1.34	1.37
31	l	621	DD6	C19-C20	-2.53	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	g	609	CLA	C1D-ND	-2.53	1.34	1.37
25	A	769	CLA	CHB-C1B	-2.53	1.33	1.39
25	c	606	CLA	C1D-ND	-2.52	1.34	1.37
25	B	743	CLA	CHC-C1C	2.52	1.43	1.38
31	a	621	DD6	C19-C20	-2.52	1.48	1.52
31	b	621	DD6	C35-C36	-2.52	1.47	1.51
25	o	603	CLA	C1D-ND	-2.52	1.34	1.37
25	B	745	CLA	C1D-ND	-2.52	1.34	1.37
25	h	608	CLA	C1D-ND	-2.52	1.34	1.37
25	k	601	CLA	C1D-ND	-2.52	1.34	1.37
25	g	603	CLA	MG-NC	2.52	2.12	2.06
31	h	620	DD6	C35-C36	-2.51	1.47	1.51
31	b	620	DD6	C35-C36	-2.51	1.47	1.51
25	n	610	CLA	CHC-C1C	2.51	1.43	1.38
25	g	602	CLA	CHC-C1C	2.51	1.43	1.38
25	A	766	CLA	C1D-ND	-2.51	1.34	1.37
25	B	757	CLA	CHC-C1C	2.51	1.43	1.38
25	b	605	CLA	C1D-ND	-2.51	1.34	1.37
25	e	604	CLA	C1D-ND	-2.51	1.34	1.37
25	e	611	CLA	C1D-ND	-2.51	1.34	1.37
25	p	603	CLA	MG-NC	2.51	2.12	2.06
25	c	609	CLA	C1D-ND	-2.51	1.34	1.37
25	g	618	CLA	C1D-ND	-2.51	1.34	1.37
25	p	610	CLA	C1D-ND	-2.51	1.34	1.37
25	e	607	CLA	C1D-ND	-2.51	1.34	1.37
31	e	620	DD6	C28-C27	-2.50	1.49	1.50
31	d	620	DD6	C35-C36	-2.50	1.47	1.51
31	c	621	DD6	C19-C20	-2.50	1.48	1.52
31	d	623	DD6	C35-C36	-2.50	1.47	1.51
25	e	614	CLA	CHC-C1C	2.50	1.43	1.38
25	f	610	CLA	CHC-C1C	2.50	1.43	1.38
25	p	610	CLA	MG-NB	2.50	2.10	2.05
25	a	601	CLA	C1D-ND	-2.50	1.34	1.37
25	h	615	CLA	C1D-ND	-2.50	1.34	1.37
25	p	601	CLA	CHC-C1C	2.50	1.43	1.38
25	c	612	CLA	C1D-ND	-2.49	1.34	1.37
25	f	610	CLA	C1D-ND	-2.49	1.34	1.37
25	m	602	CLA	CHC-C1C	2.49	1.43	1.38
25	p	609	CLA	C1D-ND	-2.49	1.34	1.37
25	p	604	CLA	C1D-ND	-2.49	1.34	1.37
25	m	611	CLA	C1D-ND	-2.49	1.34	1.37
25	f	602	CLA	CHC-C1C	2.49	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	774	CLA	C1D-ND	-2.49	1.34	1.37
25	f	604	CLA	CHC-C1C	2.49	1.43	1.38
31	n	623	DD6	C13-C11	-2.49	1.40	1.46
25	f	601	CLA	C1D-ND	-2.49	1.34	1.37
25	B	746	CLA	CHC-C1C	2.49	1.43	1.38
25	b	611	CLA	C1D-ND	-2.48	1.34	1.37
25	g	603	CLA	MG-NB	2.48	2.10	2.05
25	n	613	CLA	CHC-C1C	2.48	1.43	1.38
25	i	612	CLA	C1D-ND	-2.48	1.34	1.37
25	B	773	CLA	CHC-C1C	2.48	1.43	1.38
25	n	602	CLA	C1D-ND	-2.48	1.34	1.37
31	c	624	DD6	C26-C27	2.48	1.42	1.37
31	g	621	DD6	C35-C36	-2.48	1.47	1.51
25	b	613	CLA	C1D-ND	-2.48	1.34	1.37
25	B	775	CLA	CHC-C1C	2.48	1.43	1.38
25	A	759	CLA	C1D-ND	-2.48	1.34	1.37
25	n	604	CLA	C1D-ND	-2.47	1.34	1.37
25	g	603	CLA	CHB-C1B	-2.47	1.33	1.39
25	A	755	CLA	CHC-C1C	2.47	1.43	1.38
25	B	785	CLA	C1D-ND	-2.47	1.34	1.37
25	f	612	CLA	MG-NC	2.47	2.12	2.06
29	B	764	BCR	C1-C6	-2.47	1.50	1.53
25	B	739	CLA	C1D-ND	-2.47	1.34	1.37
25	B	744	CLA	CHC-C1C	2.47	1.43	1.38
31	e	621	DD6	C35-C36	-2.47	1.47	1.51
28	d	223	PQN	C2M-C2	-2.47	1.45	1.50
25	f	603	CLA	MG-NB	2.47	2.10	2.05
25	l	611	CLA	C1D-ND	-2.47	1.34	1.37
25	f	608	CLA	CHC-C1C	2.47	1.43	1.38
25	j	612	CLA	CHB-C1B	-2.47	1.33	1.39
25	d	601	CLA	C1D-ND	-2.46	1.34	1.37
25	l	601	CLA	C1D-ND	-2.46	1.34	1.37
25	n	610	CLA	C1D-ND	-2.46	1.34	1.37
25	d	612	CLA	C1D-ND	-2.46	1.34	1.37
31	d	621	DD6	C35-C36	-2.46	1.47	1.51
25	A	753	CLA	CHC-C1C	2.46	1.43	1.38
25	l	614	CLA	C1D-ND	-2.46	1.34	1.37
25	c	619	CLA	CHC-C1C	2.46	1.43	1.38
25	A	781	CLA	CHC-C1C	2.46	1.43	1.38
25	a	619	CLA	C1D-ND	-2.46	1.34	1.37
25	A	807	CLA	CHC-C1C	2.46	1.43	1.38
25	o	601	CLA	MG-NB	2.45	2.10	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	n	603	CLA	CHC-C1C	2.45	1.43	1.38
25	l	602	CLA	CHC-C1C	2.45	1.43	1.38
25	p	613	CLA	C1D-ND	-2.45	1.34	1.37
25	e	608	CLA	CHC-C1C	2.45	1.43	1.38
25	f	614	CLA	C1D-ND	-2.45	1.34	1.37
25	A	791	CLA	CHC-C1C	2.45	1.43	1.38
25	o	610	CLA	CHC-C1C	2.45	1.43	1.38
25	o	603	CLA	MG-NC	2.45	2.12	2.06
25	l	617	CLA	CHC-C1C	2.45	1.43	1.38
25	A	799	CLA	CHC-C1C	2.45	1.43	1.38
25	n	612	CLA	CHC-C1C	2.45	1.43	1.38
25	B	782	CLA	C1D-ND	-2.45	1.34	1.37
25	o	604	CLA	CHC-C1C	2.45	1.43	1.38
25	B	779	CLA	CHC-C1C	2.44	1.43	1.38
25	B	743	CLA	C1D-ND	-2.44	1.34	1.37
25	B	784	CLA	CHC-C1C	2.44	1.43	1.38
31	h	621	DD6	C35-C36	-2.44	1.47	1.51
25	g	608	CLA	C1D-ND	-2.44	1.34	1.37
25	a	603	CLA	C1D-ND	-2.44	1.34	1.37
25	h	610	CLA	CHC-C1C	2.44	1.43	1.38
25	A	772	CLA	C1D-ND	-2.44	1.34	1.37
25	o	613	CLA	C1D-ND	-2.44	1.34	1.37
25	h	603	CLA	CHC-C1C	2.44	1.43	1.38
25	l	610	CLA	CHC-C1C	2.44	1.43	1.38
25	g	608	CLA	CHC-C1C	2.44	1.43	1.38
25	h	612	CLA	C1D-ND	-2.44	1.34	1.37
25	o	612	CLA	CHC-C1C	2.43	1.43	1.38
25	f	603	CLA	MG-NC	2.43	2.12	2.06
25	f	609	CLA	CHC-C1C	2.43	1.43	1.38
31	e	623	DD6	C13-C11	-2.43	1.40	1.46
25	l	611	CLA	CHC-C1C	2.43	1.43	1.38
25	n	605	CLA	C1D-ND	-2.43	1.34	1.37
25	b	604	CLA	CHC-C1C	2.43	1.43	1.38
25	h	608	CLA	CHC-C1C	2.43	1.43	1.38
25	p	602	CLA	CHC-C1C	2.43	1.43	1.38
25	A	802	CLA	CHC-C1C	2.43	1.43	1.38
31	j	621	DD6	C35-C36	-2.43	1.47	1.51
35	d	605	CHL	MG-NB	2.43	2.10	2.05
25	B	739	CLA	CHC-C1C	2.43	1.43	1.38
25	j	603	CLA	CHB-C1B	-2.43	1.34	1.39
25	k	612	CLA	CHB-C1B	-2.43	1.34	1.39
31	a	621	DD6	C35-C36	-2.43	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	f	613	CLA	C1D-ND	-2.43	1.34	1.37
25	l	604	CLA	CHC-C1C	2.43	1.43	1.38
25	A	776	CLA	CHB-C1B	-2.42	1.34	1.39
25	p	608	CLA	C1D-ND	-2.42	1.34	1.37
25	p	602	CLA	MG-NB	2.42	2.10	2.05
25	A	797	CLA	CHC-C1C	2.42	1.43	1.38
31	k	621	DD6	C35-C36	-2.42	1.47	1.51
25	b	601	CLA	C1D-ND	-2.42	1.34	1.37
25	k	612	CLA	C1D-ND	-2.42	1.34	1.37
25	A	798	CLA	CHC-C1C	2.42	1.43	1.38
25	B	784	CLA	C1D-ND	-2.42	1.34	1.37
25	B	748	CLA	CHB-C1B	-2.42	1.34	1.39
25	o	601	CLA	C1D-ND	-2.42	1.34	1.37
25	B	773	CLA	CHB-C1B	-2.42	1.34	1.39
25	o	601	CLA	CHB-C1B	-2.42	1.34	1.39
31	n	623	DD6	C24-C1	-2.42	1.40	1.46
25	j	602	CLA	CHC-C1C	2.41	1.43	1.38
25	f	612	CLA	CHB-C1B	-2.41	1.34	1.39
25	f	614	CLA	CHC-C1C	2.41	1.43	1.38
25	g	609	CLA	CHC-C1C	2.41	1.43	1.38
25	A	807	CLA	CHB-C1B	-2.41	1.34	1.39
25	j	612	CLA	C1D-ND	-2.41	1.34	1.37
25	l	612	CLA	C1D-ND	-2.41	1.34	1.37
25	i	610	CLA	CHC-C1C	2.41	1.43	1.38
25	d	601	CLA	CHC-C1C	2.41	1.43	1.38
25	k	602	CLA	CHC-C1C	2.41	1.43	1.38
25	n	606	CLA	MG-NB	2.41	2.10	2.05
35	c	607	CHL	MG-NB	2.41	2.10	2.05
35	d	608	CHL	C1A-CHA	2.41	1.42	1.40
25	n	606	CLA	MG-NC	2.41	2.12	2.06
25	a	613	CLA	CHC-C1C	2.41	1.43	1.38
25	i	603	CLA	CHB-C1B	-2.40	1.34	1.39
25	A	759	CLA	CHC-C1C	2.40	1.43	1.38
25	j	613	CLA	CHC-C1C	2.40	1.43	1.38
25	A	765	CLA	CHB-C1B	-2.40	1.34	1.39
25	e	612	CLA	CHB-C1B	-2.40	1.34	1.39
35	d	606	CHL	MG-NB	2.40	2.10	2.05
35	d	607	CHL	MG-NB	2.40	2.10	2.05
25	a	612	CLA	C1D-ND	-2.40	1.34	1.37
25	B	777	CLA	CHC-C1C	2.40	1.43	1.38
25	B	780	CLA	CHC-C1C	2.40	1.43	1.38
31	p	621	DD6	C35-C36	-2.40	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	610	CLA	CHC-C1C	2.40	1.43	1.38
25	m	604	CLA	CHC-C1C	2.40	1.43	1.38
25	l	603	CLA	CHB-C1B	-2.40	1.34	1.39
25	d	612	CLA	CHC-C1C	2.40	1.43	1.38
25	f	609	CLA	MG-NB	2.40	2.10	2.05
25	A	805	CLA	CHC-C1C	2.40	1.43	1.38
25	p	603	CLA	CHC-C1C	2.40	1.43	1.38
25	B	753	CLA	CHC-C1C	2.40	1.43	1.38
31	A	4008	DD6	C35-C36	-2.40	1.47	1.51
25	p	612	CLA	C1D-ND	-2.40	1.34	1.37
25	m	609	CLA	CHB-C1B	-2.39	1.34	1.39
25	e	601	CLA	MG-NB	2.39	2.10	2.05
31	k	620	DD6	C35-C36	-2.39	1.47	1.51
25	n	604	CLA	CHC-C1C	2.39	1.43	1.38
25	J	101	CLA	CHB-C1B	-2.39	1.34	1.39
31	e	620	DD6	C26-C27	2.39	1.42	1.37
25	j	608	CLA	CHC-C1C	2.39	1.43	1.38
25	c	612	CLA	CHC-C1C	2.39	1.43	1.38
25	f	615	CLA	MG-NB	2.39	2.10	2.05
25	B	737	CLA	CHC-C1C	2.39	1.43	1.38
25	g	610	CLA	CHC-C1C	2.39	1.43	1.38
25	A	782	CLA	CHC-C1C	2.39	1.43	1.38
25	p	609	CLA	CHC-C1C	2.39	1.43	1.38
35	d	606	CHL	CBA-CGA	2.39	1.56	1.50
25	A	753	CLA	C1B-NB	-2.39	1.34	1.37
25	A	760	CLA	CHC-C1C	2.39	1.43	1.38
25	b	612	CLA	CHC-C1C	2.39	1.43	1.38
25	e	602	CLA	CHC-C1C	2.39	1.43	1.38
25	a	602	CLA	CHC-C1C	2.38	1.43	1.38
25	m	601	CLA	CHB-C1B	-2.38	1.34	1.39
25	m	603	CLA	CHB-C1B	-2.38	1.34	1.39
25	B	779	CLA	CHB-C1B	-2.38	1.34	1.39
25	l	613	CLA	CHC-C1C	2.38	1.43	1.38
25	A	782	CLA	CHB-C1B	-2.38	1.34	1.39
25	a	609	CLA	CHB-C1B	-2.38	1.34	1.39
25	B	739	CLA	CHB-C1B	-2.38	1.34	1.39
25	e	605	CLA	CHC-C1C	2.38	1.43	1.38
25	b	601	CLA	MG-NB	2.38	2.10	2.05
25	A	797	CLA	CHB-C1B	-2.38	1.34	1.39
25	o	601	CLA	CHC-C1C	2.38	1.43	1.38
25	e	601	CLA	C1D-ND	-2.38	1.34	1.37
25	h	612	CLA	CHC-C1C	2.38	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	f	601	CLA	CHC-C1C	2.38	1.43	1.38
25	g	612	CLA	CHC-C1C	2.38	1.43	1.38
25	b	613	CLA	CHC-C1C	2.38	1.43	1.38
25	l	601	CLA	CHC-C1C	2.38	1.43	1.38
25	b	612	CLA	CHB-C1B	-2.38	1.34	1.39
25	k	601	CLA	CHC-C1C	2.38	1.43	1.38
25	g	618	CLA	CHC-C1C	2.37	1.43	1.38
25	h	603	CLA	C1D-ND	-2.37	1.34	1.37
25	a	619	CLA	CHC-C1C	2.37	1.43	1.38
25	h	604	CLA	CHC-C1C	2.37	1.43	1.38
25	A	794	CLA	CHC-C1C	2.37	1.43	1.38
25	g	612	CLA	C1D-ND	-2.37	1.34	1.37
25	B	785	CLA	MG-NB	2.37	2.10	2.05
35	e	606	CHL	CBA-CGA	2.37	1.56	1.50
31	n	623	DD6	C8-C6	-2.37	1.40	1.46
25	o	603	CLA	CHB-C1B	-2.37	1.34	1.39
25	A	762	CLA	CHB-C1B	-2.37	1.34	1.39
25	n	607	CLA	CHC-C1C	2.37	1.43	1.38
25	n	603	CLA	C1D-ND	-2.37	1.34	1.37
25	n	613	CLA	C1D-ND	-2.37	1.34	1.37
25	k	612	CLA	CHC-C1C	2.37	1.43	1.38
25	B	751	CLA	CHB-C1B	-2.37	1.34	1.39
25	g	601	CLA	CHB-C1B	-2.37	1.34	1.39
25	A	773	CLA	CHC-C1C	2.37	1.43	1.38
25	i	613	CLA	CHC-C1C	2.37	1.43	1.38
25	o	609	CLA	CHC-C1C	2.37	1.43	1.38
25	b	612	CLA	C1D-ND	-2.37	1.34	1.37
25	j	609	CLA	CHB-C1B	-2.37	1.34	1.39
25	m	610	CLA	CHC-C1C	2.37	1.43	1.38
25	c	609	CLA	CHC-C1C	2.37	1.43	1.38
31	l	621	DD6	C35-C36	-2.37	1.47	1.51
25	A	777	CLA	CHB-C1B	-2.36	1.34	1.39
25	b	602	CLA	CHC-C1C	2.36	1.43	1.38
25	g	604	CLA	CHC-C1C	2.36	1.43	1.38
25	A	798	CLA	C1B-NB	-2.36	1.34	1.37
25	l	614	CLA	MG-NB	2.36	2.10	2.05
25	B	783	CLA	CHB-C1B	-2.36	1.34	1.39
25	g	612	CLA	CHB-C1B	-2.36	1.34	1.39
25	n	606	CLA	C1D-ND	-2.36	1.34	1.37
25	c	606	CLA	CHC-C1C	2.36	1.43	1.38
25	a	611	CLA	CHC-C1C	2.36	1.43	1.38
25	A	793	CLA	CHB-C1B	-2.36	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	e	612	CLA	CHC-C1C	2.36	1.43	1.38
25	k	608	CLA	CHB-C1B	-2.36	1.34	1.39
25	e	603	CLA	CHB-C1B	-2.36	1.34	1.39
25	A	783	CLA	CHC-C1C	2.36	1.43	1.38
25	o	602	CLA	CHC-C1C	2.36	1.43	1.38
25	g	611	CLA	CHC-C1C	2.36	1.43	1.38
25	m	612	CLA	CHB-C1B	-2.36	1.34	1.39
25	d	612	CLA	CHB-C1B	-2.36	1.34	1.39
25	b	610	CLA	CHC-C1C	2.35	1.43	1.38
25	d	614	CLA	CHC-C1C	2.35	1.43	1.38
25	A	784	CLA	CHB-C1B	-2.35	1.34	1.39
29	A	792	BCR	C19-C18	-2.35	1.40	1.46
25	h	613	CLA	CHC-C1C	2.35	1.43	1.38
25	h	612	CLA	CHB-C1B	-2.35	1.34	1.39
25	g	615	CLA	CHC-C1C	2.35	1.43	1.38
25	c	616	CLA	C1D-ND	-2.35	1.34	1.37
25	B	774	CLA	CHB-C1B	-2.35	1.34	1.39
25	e	612	CLA	C1D-ND	-2.35	1.34	1.37
25	A	806	CLA	CHC-C1C	2.35	1.43	1.38
25	m	613	CLA	CHC-C1C	2.35	1.43	1.38
25	g	613	CLA	CHC-C1C	2.35	1.43	1.38
25	A	768	CLA	CHB-C1B	-2.35	1.34	1.39
25	a	603	CLA	CHB-C1B	-2.35	1.34	1.39
25	i	612	CLA	CHC-C1C	2.35	1.43	1.38
25	c	603	CLA	C1D-ND	-2.35	1.34	1.37
25	B	751	CLA	CHC-C1C	2.35	1.43	1.38
25	a	601	CLA	CHC-C1C	2.35	1.43	1.38
25	p	613	CLA	CHC-C1C	2.35	1.43	1.38
25	f	608	CLA	C1D-ND	-2.35	1.34	1.37
25	f	609	CLA	C1D-ND	-2.35	1.34	1.37
25	e	611	CLA	CHC-C1C	2.35	1.43	1.38
25	p	610	CLA	CHB-C1B	-2.35	1.34	1.39
25	A	799	CLA	CHB-C1B	-2.35	1.34	1.39
25	c	613	CLA	CHB-C1B	-2.35	1.34	1.39
25	i	611	CLA	CHC-C1C	2.35	1.43	1.38
25	B	776	CLA	CHC-C1C	2.35	1.43	1.38
25	d	609	CLA	CHC-C1C	2.35	1.43	1.38
25	f	613	CLA	CHC-C1C	2.35	1.43	1.38
25	A	752	CLA	CHB-C1B	-2.35	1.34	1.39
25	B	776	CLA	CHB-C1B	-2.35	1.34	1.39
25	f	612	CLA	C1D-ND	-2.35	1.34	1.37
25	A	801	CLA	CHC-C1C	2.35	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	780	CLA	CHB-C1B	-2.35	1.34	1.39
25	h	604	CLA	CHB-C1B	-2.35	1.34	1.39
25	k	604	CLA	CHB-C1B	-2.35	1.34	1.39
25	n	608	CLA	C1D-ND	-2.35	1.34	1.37
25	l	612	CLA	CHC-C1C	2.35	1.43	1.38
31	n	620	DD6	O1-C20	-2.35	1.43	1.46
25	e	607	CLA	CHB-C1B	-2.35	1.34	1.39
25	m	612	CLA	CHC-C1C	2.35	1.43	1.38
25	g	613	CLA	CHB-C1B	-2.35	1.34	1.39
25	f	615	CLA	C1D-ND	-2.34	1.34	1.37
28	B	769	PQN	C2M-C2	-2.34	1.46	1.50
25	A	761	CLA	CHC-C1C	2.34	1.43	1.38
25	b	601	CLA	CHC-C1C	2.34	1.43	1.38
25	j	604	CLA	CHC-C1C	2.34	1.43	1.38
25	n	610	CLA	MG-NB	2.34	2.10	2.05
25	p	609	CLA	CHB-C1B	-2.34	1.34	1.39
25	f	601	CLA	MG-NB	2.34	2.10	2.05
35	d	608	CHL	CBA-CGA	2.34	1.56	1.50
25	f	611	CLA	CHC-C1C	2.34	1.43	1.38
25	i	603	CLA	MG-NB	2.34	2.10	2.05
25	B	741	CLA	CHB-C1B	-2.34	1.34	1.39
25	d	609	CLA	CHB-C1B	-2.34	1.34	1.39
29	B	767	BCR	C30-C25	-2.34	1.50	1.53
25	B	768	CLA	CHB-C1B	-2.34	1.34	1.39
31	e	623	DD6	C8-C6	-2.34	1.40	1.46
25	B	760	CLA	CHB-C1B	-2.34	1.34	1.39
25	j	601	CLA	CHB-C1B	-2.34	1.34	1.39
25	B	738	CLA	CHC-C1C	2.34	1.43	1.38
25	k	610	CLA	CHC-C1C	2.34	1.43	1.38
25	d	603	CLA	CHB-C1B	-2.34	1.34	1.39
25	g	608	CLA	MG-NB	2.34	2.10	2.05
35	d	608	CHL	MG-NB	2.34	2.10	2.05
25	B	750	CLA	CHC-C1C	2.34	1.43	1.38
25	A	808	CLA	CHB-C1B	-2.34	1.34	1.39
25	h	601	CLA	CHC-C1C	2.34	1.43	1.38
25	b	603	CLA	C1D-ND	-2.34	1.34	1.37
25	d	603	CLA	C1D-ND	-2.34	1.34	1.37
25	A	767	CLA	MG-NB	2.34	2.10	2.05
31	n	623	DD6	C5-C6	2.34	1.41	1.35
25	k	611	CLA	CHC-C1C	2.34	1.43	1.38
25	o	613	CLA	CHC-C1C	2.34	1.43	1.38
25	B	785	CLA	CHB-C1B	-2.34	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	i	601	CLA	CHB-C1B	-2.34	1.34	1.39
25	j	603	CLA	MG-NB	2.34	2.10	2.05
25	n	603	CLA	MG-NB	2.34	2.10	2.05
25	e	611	CLA	MG-NB	2.34	2.10	2.05
25	l	609	CLA	CHB-C1B	-2.34	1.34	1.39
25	i	608	CLA	CHC-C1C	2.33	1.43	1.38
25	l	608	CLA	CHC-C1C	2.33	1.43	1.38
25	e	614	CLA	C1D-ND	-2.33	1.34	1.37
25	B	771	CLA	CHB-C1B	-2.33	1.34	1.39
25	d	604	CLA	CHB-C1B	-2.33	1.34	1.39
25	g	608	CLA	CHB-C1B	-2.33	1.34	1.39
25	B	749	CLA	CHC-C1C	2.33	1.43	1.38
25	B	746	CLA	CHB-C1B	-2.33	1.34	1.39
25	b	611	CLA	MG-NB	2.33	2.10	2.05
25	l	614	CLA	CHB-C1B	-2.33	1.34	1.39
25	n	604	CLA	CHB-C1B	-2.33	1.34	1.39
25	c	611	CLA	CHC-C1C	2.33	1.43	1.38
25	p	602	CLA	MG-NC	2.33	2.11	2.06
25	A	762	CLA	CHC-C1C	2.33	1.43	1.38
25	j	614	CLA	CHB-C1B	-2.33	1.34	1.39
25	e	604	CLA	CHB-C1B	-2.33	1.34	1.39
25	e	607	CLA	CHC-C1C	2.33	1.43	1.38
25	k	603	CLA	C1D-ND	-2.33	1.34	1.37
25	B	742	CLA	CHB-C1B	-2.33	1.34	1.39
25	i	612	CLA	CHB-C1B	-2.33	1.34	1.39
25	A	776	CLA	CHC-C1C	2.33	1.43	1.38
25	o	604	CLA	CHB-C1B	-2.33	1.34	1.39
31	e	620	DD6	C25-C26	-2.33	1.36	1.43
25	b	611	CLA	CHC-C1C	2.33	1.43	1.38
25	c	616	CLA	CHC-C1C	2.33	1.43	1.38
25	A	775	CLA	CHB-C1B	-2.33	1.34	1.39
25	l	601	CLA	MG-NB	2.33	2.10	2.05
25	i	603	CLA	MG-NC	2.33	2.11	2.06
25	j	601	CLA	CHC-C1C	2.33	1.43	1.38
25	c	612	CLA	CHB-C1B	-2.33	1.34	1.39
25	A	781	CLA	CHB-C1B	-2.33	1.34	1.39
25	A	760	CLA	C1B-NB	-2.32	1.34	1.37
25	a	601	CLA	CHB-C1B	-2.32	1.34	1.39
25	A	763	CLA	CHB-C1B	-2.32	1.34	1.39
25	d	611	CLA	CHC-C1C	2.32	1.43	1.38
25	n	612	CLA	C1D-ND	-2.32	1.34	1.37
25	h	612	CLA	MG-NB	2.32	2.10	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	m	611	CLA	CHC-C1C	2.32	1.43	1.38
25	B	749	CLA	CHB-C1B	-2.32	1.34	1.39
25	b	603	CLA	CHC-C1C	2.32	1.43	1.38
25	A	763	CLA	CHC-C1C	2.32	1.43	1.38
25	h	601	CLA	CHB-C1B	-2.32	1.34	1.39
25	B	752	CLA	CHB-C1B	-2.32	1.34	1.39
25	B	770	CLA	CHB-C1B	-2.32	1.34	1.39
25	B	747	CLA	CHB-C1B	-2.32	1.34	1.39
25	c	609	CLA	CHB-C1B	-2.32	1.34	1.39
25	c	614	CLA	CHC-C1C	2.32	1.43	1.38
25	o	610	CLA	MG-NB	2.32	2.10	2.05
25	g	612	CLA	MG-NC	2.32	2.11	2.06
25	j	608	CLA	CHB-C1B	-2.32	1.34	1.39
25	d	610	CLA	CHC-C1C	2.32	1.43	1.38
25	m	608	CLA	CHB-C1B	-2.32	1.34	1.39
25	B	778	CLA	CHB-C1B	-2.32	1.34	1.39
25	b	603	CLA	CHB-C1B	-2.32	1.34	1.39
25	B	758	CLA	CHB-C1B	-2.32	1.34	1.39
25	k	615	CLA	CHC-C1C	2.32	1.43	1.38
25	l	603	CLA	MG-NB	2.32	2.10	2.05
25	g	611	CLA	CHB-C1B	-2.32	1.34	1.39
25	a	612	CLA	CHC-C1C	2.32	1.43	1.38
25	f	603	CLA	C1D-ND	-2.32	1.34	1.37
25	c	606	CLA	CHB-C1B	-2.31	1.34	1.39
25	B	741	CLA	MG-NB	2.31	2.10	2.05
25	g	614	CLA	MG-NB	2.31	2.10	2.05
25	i	608	CLA	CHB-C1B	-2.31	1.34	1.39
25	m	611	CLA	MG-NB	2.31	2.10	2.05
25	B	783	CLA	CHC-C1C	2.31	1.43	1.38
31	c	623	DD6	O1-C20	-2.31	1.43	1.46
25	m	603	CLA	C1D-ND	-2.31	1.34	1.37
25	e	613	CLA	CHC-C1C	2.31	1.43	1.38
25	p	609	CLA	MG-NB	2.31	2.10	2.05
25	B	736	CLA	CHB-C1B	-2.31	1.34	1.39
25	A	803	CLA	CHC-C1C	2.31	1.43	1.38
25	d	602	CLA	CHC-C1C	2.31	1.43	1.38
25	B	781	CLA	CHB-C1B	-2.31	1.34	1.39
25	c	603	CLA	CHB-C1B	-2.31	1.34	1.39
25	A	778	CLA	CHB-C1B	-2.31	1.34	1.39
25	B	745	CLA	CHB-C1B	-2.31	1.34	1.39
25	c	608	CLA	CHC-C1C	2.31	1.43	1.38
25	h	611	CLA	CHC-C1C	2.31	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	f	615	CLA	CHC-C1C	2.31	1.43	1.38
25	c	601	CLA	CHC-C1C	2.31	1.43	1.38
25	i	604	CLA	CHC-C1C	2.31	1.43	1.38
31	i	621	DD6	C19-C20	-2.31	1.48	1.52
25	B	774	CLA	CHC-C1C	2.31	1.43	1.38
25	n	603	CLA	CHB-C1B	-2.31	1.34	1.39
25	B	779	CLA	MG-NB	2.31	2.10	2.05
25	n	605	CLA	MG-NB	2.31	2.10	2.05
25	l	610	CLA	CHB-C1B	-2.31	1.34	1.39
25	h	615	CLA	CHB-C1B	-2.31	1.34	1.39
25	n	610	CLA	CHB-C1B	-2.31	1.34	1.39
25	k	604	CLA	CHC-C1C	2.31	1.43	1.38
31	o	621	DD6	C35-C36	-2.31	1.47	1.51
25	b	609	CLA	CHB-C1B	-2.31	1.34	1.39
25	h	609	CLA	CHB-C1B	-2.31	1.34	1.39
25	A	791	CLA	CHB-C1B	-2.31	1.34	1.39
25	e	609	CLA	CHB-C1B	-2.31	1.34	1.39
31	f	620	DD6	C35-C36	-2.31	1.47	1.51
25	B	772	CLA	CHC-C1C	2.31	1.43	1.38
25	p	601	CLA	C1D-ND	-2.31	1.34	1.37
25	p	610	CLA	CHC-C1C	2.30	1.43	1.38
25	a	603	CLA	CHC-C1C	2.30	1.43	1.38
31	c	624	DD6	C25-C26	-2.30	1.36	1.43
25	h	618	CLA	CHC-C1C	2.30	1.43	1.38
25	A	807	CLA	C1B-NB	-2.30	1.34	1.37
25	n	609	CLA	CHC-C1C	2.30	1.43	1.38
25	A	779	CLA	CHB-C1B	-2.30	1.34	1.39
31	c	621	DD6	C15-C14	-2.30	1.46	1.50
25	n	605	CLA	CHC-C1C	2.30	1.43	1.38
25	l	603	CLA	C1D-ND	-2.30	1.34	1.37
25	f	603	CLA	CHB-C1B	-2.30	1.34	1.39
25	j	603	CLA	MG-NC	2.30	2.11	2.06
25	B	745	CLA	CHC-C1C	2.30	1.43	1.38
25	A	772	CLA	CHC-C1C	2.30	1.43	1.38
25	e	603	CLA	CHC-C1C	2.30	1.43	1.38
25	p	608	CLA	MG-NB	2.30	2.10	2.05
25	l	608	CLA	CHB-C1B	-2.30	1.34	1.39
31	n	623	DD6	C2-C1	2.30	1.41	1.35
25	B	759	CLA	CHB-C1B	-2.30	1.34	1.39
25	k	614	CLA	MG-NB	2.30	2.10	2.05
25	A	765	CLA	MG-NB	2.30	2.10	2.05
25	c	604	CLA	CHB-C1B	-2.30	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	i	614	CLA	CHB-C1B	-2.30	1.34	1.39
25	d	611	CLA	CHB-C1B	-2.30	1.34	1.39
25	B	768	CLA	CHC-C1C	2.30	1.43	1.38
25	A	761	CLA	CHB-C1B	-2.30	1.34	1.39
25	B	755	CLA	CHC-C1C	2.30	1.43	1.38
25	a	604	CLA	CHC-C1C	2.30	1.43	1.38
25	l	614	CLA	CHC-C1C	2.30	1.43	1.38
25	n	607	CLA	MG-NB	2.30	2.10	2.05
25	g	609	CLA	CHB-C1B	-2.29	1.34	1.39
25	p	602	CLA	CHD-C1D	2.29	1.42	1.38
25	o	603	CLA	CHC-C1C	2.29	1.43	1.38
25	f	611	CLA	MG-NB	2.29	2.10	2.05
25	a	604	CLA	CHB-C1B	-2.29	1.34	1.39
25	c	610	CLA	CHB-C1B	-2.29	1.34	1.39
25	A	777	CLA	C1B-NB	-2.29	1.34	1.37
25	d	614	CLA	C1D-ND	-2.29	1.34	1.37
25	A	793	CLA	CHC-C1C	2.29	1.43	1.38
25	b	605	CLA	CHB-C1B	-2.29	1.34	1.39
25	b	605	CLA	MG-NB	2.29	2.10	2.05
25	A	771	CLA	CHB-C1B	-2.29	1.34	1.39
25	a	611	CLA	CHB-C1B	-2.29	1.34	1.39
25	A	777	CLA	CHC-C1C	2.29	1.43	1.38
25	f	614	CLA	MG-NB	2.29	2.10	2.05
25	c	614	CLA	CHB-C1B	-2.29	1.34	1.39
25	b	608	CLA	CHC-C1C	2.29	1.43	1.38
25	A	766	CLA	C1B-NB	-2.29	1.34	1.37
25	j	614	CLA	MG-NB	2.29	2.10	2.05
25	e	612	CLA	MG-NB	2.29	2.10	2.05
25	a	612	CLA	CHB-C1B	-2.29	1.34	1.39
25	j	618	CLA	CHC-C1C	2.29	1.43	1.38
25	h	608	CLA	CHB-C1B	-2.29	1.34	1.39
25	k	609	CLA	CHC-C1C	2.29	1.43	1.38
25	h	618	CLA	CHB-C1B	-2.29	1.34	1.39
25	d	610	CLA	CHB-C1B	-2.29	1.34	1.39
25	A	778	CLA	MG-NB	2.29	2.10	2.05
25	m	608	CLA	CHC-C1C	2.28	1.43	1.38
25	l	612	CLA	CHB-C1B	-2.28	1.34	1.39
25	g	609	CLA	MG-NB	2.28	2.10	2.05
31	n	620	DD6	C35-C36	-2.28	1.47	1.51
25	f	604	CLA	MG-NB	2.28	2.10	2.05
25	B	770	CLA	CHC-C1C	2.28	1.43	1.38
25	A	767	CLA	CHB-C1B	-2.28	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	755	CLA	CHB-C1B	-2.28	1.34	1.39
25	i	601	CLA	CHC-C1C	2.28	1.43	1.38
25	k	608	CLA	CHC-C1C	2.28	1.43	1.38
25	k	601	CLA	MG-NB	2.28	2.10	2.05
35	e	606	CHL	MG-NB	2.28	2.10	2.05
25	B	743	CLA	CHB-C1B	-2.28	1.34	1.39
25	b	601	CLA	CHB-C1B	-2.28	1.34	1.39
25	B	740	CLA	CHC-C1C	2.28	1.43	1.38
25	e	604	CLA	CHC-C1C	2.28	1.43	1.38
25	J	101	CLA	MG-NB	2.28	2.10	2.05
25	B	772	CLA	CHB-C1B	-2.28	1.34	1.39
25	n	607	CLA	CHB-C1B	-2.28	1.34	1.39
25	b	604	CLA	CHB-C1B	-2.28	1.34	1.39
25	e	601	CLA	CHB-C1B	-2.28	1.34	1.39
25	e	608	CLA	CHB-C1B	-2.28	1.34	1.39
25	B	736	CLA	MG-NB	2.28	2.10	2.05
25	A	764	CLA	CHB-C1B	-2.28	1.34	1.39
25	g	615	CLA	CHB-C1B	-2.28	1.34	1.39
25	a	609	CLA	CHC-C1C	2.28	1.43	1.38
25	B	750	CLA	CHB-C1B	-2.28	1.34	1.39
25	k	618	CLA	CHB-C1B	-2.28	1.34	1.39
25	A	760	CLA	CHB-C1B	-2.28	1.34	1.39
25	h	613	CLA	CHB-C1B	-2.28	1.34	1.39
25	b	611	CLA	CHB-C1B	-2.28	1.34	1.39
25	j	615	CLA	CHB-C1B	-2.28	1.34	1.39
25	l	601	CLA	CHB-C1B	-2.28	1.34	1.39
25	e	601	CLA	CHC-C1C	2.28	1.43	1.38
25	c	608	CLA	CHB-C1B	-2.28	1.34	1.39
25	A	757	CLA	CHC-C1C	2.28	1.43	1.38
25	c	610	CLA	CHC-C1C	2.28	1.43	1.38
31	n	621	DD6	C25-C26	-2.28	1.36	1.43
25	f	608	CLA	MG-NB	2.28	2.10	2.05
25	n	606	CLA	CHB-C1B	-2.27	1.34	1.39
25	j	612	CLA	MG-NC	2.27	2.11	2.06
25	j	611	CLA	CHB-C1B	-2.27	1.34	1.39
25	A	768	CLA	CHC-C1C	2.27	1.43	1.38
25	B	748	CLA	CHC-C1C	2.27	1.43	1.38
25	n	604	CLA	MG-NB	2.27	2.10	2.05
25	A	753	CLA	CHB-C1B	-2.27	1.34	1.39
25	m	609	CLA	CHC-C1C	2.27	1.43	1.38
25	o	608	CLA	CHC-C1C	2.27	1.43	1.38
25	e	602	CLA	CHB-C1B	-2.27	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	i	602	CLA	CHB-C1B	-2.27	1.34	1.39
25	A	769	CLA	MG-NB	2.27	2.10	2.05
25	A	808	CLA	MG-NB	2.27	2.10	2.05
25	A	772	CLA	CHB-C1B	-2.27	1.34	1.39
25	d	601	CLA	CHB-C1B	-2.27	1.34	1.39
25	B	752	CLA	MG-NB	2.27	2.10	2.05
33	a	182	LMG	O8-C28	2.27	1.40	1.33
25	c	602	CLA	CHC-C1C	2.27	1.43	1.38
25	c	602	CLA	CHB-C1B	-2.27	1.34	1.39
25	i	615	CLA	CHB-C1B	-2.27	1.34	1.39
25	B	737	CLA	C1B-NB	-2.27	1.34	1.37
25	b	608	CLA	CHB-C1B	-2.27	1.34	1.39
25	k	603	CLA	CHB-C1B	-2.27	1.34	1.39
25	f	609	CLA	MG-NC	2.27	2.11	2.06
25	o	613	CLA	CHB-C1B	-2.27	1.34	1.39
25	B	752	CLA	CHC-C1C	2.27	1.43	1.38
25	h	614	CLA	CHC-C1C	2.27	1.43	1.38
25	A	769	CLA	CHC-C1C	2.27	1.43	1.38
25	j	611	CLA	CHC-C1C	2.27	1.43	1.38
25	f	610	CLA	CHB-C1B	-2.27	1.34	1.39
25	c	616	CLA	MG-NB	2.27	2.10	2.05
25	o	612	CLA	C1D-ND	-2.27	1.34	1.37
25	B	744	CLA	CHB-C1B	-2.27	1.34	1.39
25	e	613	CLA	CHB-C1B	-2.27	1.34	1.39
33	B	786	LMG	O8-C28	2.27	1.40	1.33
25	l	602	CLA	CHB-C1B	-2.27	1.34	1.39
25	a	608	CLA	CHC-C1C	2.27	1.43	1.38
25	A	784	CLA	CHC-C1C	2.27	1.43	1.38
25	a	619	CLA	CHB-C1B	-2.27	1.34	1.39
25	A	764	CLA	CHC-C1C	2.27	1.43	1.38
25	h	614	CLA	CHB-C1B	-2.27	1.34	1.39
25	i	609	CLA	CHC-C1C	2.27	1.43	1.38
25	f	603	CLA	CHC-C1C	2.27	1.43	1.38
25	m	610	CLA	CHB-C1B	-2.27	1.34	1.39
25	A	803	CLA	MG-NB	2.27	2.10	2.05
25	k	613	CLA	CHC-C1C	2.26	1.43	1.38
25	c	616	CLA	CHB-C1B	-2.26	1.34	1.39
25	k	614	CLA	CHB-C1B	-2.26	1.34	1.39
25	m	612	CLA	C1D-ND	-2.26	1.34	1.37
25	m	603	CLA	MG-NB	2.26	2.10	2.05
25	A	794	CLA	CHB-C1B	-2.26	1.34	1.39
25	f	614	CLA	CHB-C1B	-2.26	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	f	613	CLA	CHB-C1B	-2.26	1.34	1.39
25	h	602	CLA	CHB-C1B	-2.26	1.34	1.39
25	j	604	CLA	CHB-C1B	-2.26	1.34	1.39
25	n	613	CLA	CHB-C1B	-2.26	1.34	1.39
30	A	795	SQD	O9-S	2.26	1.51	1.45
25	k	609	CLA	CHB-C1B	-2.26	1.34	1.39
31	m	620	DD6	C35-C36	-2.26	1.47	1.51
25	B	768	CLA	MG-NB	2.26	2.10	2.05
25	j	618	CLA	CHB-C1B	-2.26	1.34	1.39
25	i	614	CLA	CHC-C1C	2.26	1.43	1.38
25	k	614	CLA	CHC-C1C	2.26	1.43	1.38
25	n	605	CLA	CHB-C1B	-2.26	1.34	1.39
25	d	613	CLA	CHC-C1C	2.26	1.43	1.38
25	h	615	CLA	CHC-C1C	2.26	1.43	1.38
25	A	758	CLA	CHC-C1C	2.26	1.43	1.38
25	l	604	CLA	CHB-C1B	-2.26	1.34	1.39
25	o	613	CLA	MG-NB	2.26	2.10	2.05
25	h	602	CLA	CHC-C1C	2.26	1.43	1.38
25	A	766	CLA	CHB-C1B	-2.26	1.34	1.39
25	c	611	CLA	CHB-C1B	-2.26	1.34	1.39
25	e	610	CLA	CHC-C1C	2.26	1.43	1.38
25	A	779	CLA	CHC-C1C	2.26	1.43	1.38
25	f	615	CLA	MG-NC	2.26	2.11	2.06
25	o	610	CLA	CHB-C1B	-2.26	1.34	1.39
25	g	614	CLA	CHC-C1C	2.26	1.43	1.38
25	l	603	CLA	MG-NC	2.26	2.11	2.06
25	A	755	CLA	CHB-C1B	-2.26	1.34	1.39
25	p	602	CLA	CAA-C2A	2.26	1.58	1.54
25	k	603	CLA	CHC-C1C	2.26	1.43	1.38
25	i	604	CLA	CHB-C1B	-2.26	1.34	1.39
25	e	603	CLA	MG-NB	2.26	2.10	2.05
25	B	747	CLA	CHC-C1C	2.26	1.43	1.38
25	B	756	CLA	CHC-C1C	2.26	1.43	1.38
25	A	803	CLA	CHB-C1B	-2.26	1.34	1.39
25	m	612	CLA	MG-NC	2.26	2.11	2.06
25	c	619	CLA	CHB-C1B	-2.25	1.34	1.39
25	k	615	CLA	CHB-C1B	-2.25	1.34	1.39
25	b	605	CLA	CHC-C1C	2.25	1.43	1.38
25	k	613	CLA	CHB-C1B	-2.25	1.34	1.39
34	b	182	DGD	C1E-C2E	2.25	1.59	1.52
25	p	604	CLA	CHB-C1B	-2.25	1.34	1.39
25	g	612	CLA	MG-NB	2.25	2.10	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	604	CLA	MG-NB	2.25	2.10	2.05
25	a	603	CLA	MG-NB	2.25	2.10	2.05
35	e	606	CHL	C2C-C3C	2.25	1.38	1.36
31	l	620	DD6	C35-C36	-2.25	1.47	1.51
25	e	610	CLA	CHB-C1B	-2.25	1.34	1.39
25	k	618	CLA	CHC-C1C	2.25	1.43	1.38
25	m	603	CLA	MG-NC	2.25	2.11	2.06
25	A	759	CLA	CHB-C1B	-2.25	1.34	1.39
28	B	761	PQN	C11-C12	-2.25	1.47	1.50
25	B	740	CLA	CHB-C1B	-2.25	1.34	1.39
25	h	603	CLA	CHB-C1B	-2.25	1.34	1.39
25	m	612	CLA	MG-NB	2.25	2.10	2.05
31	i	621	DD6	C15-C14	-2.25	1.46	1.50
25	g	608	CLA	MG-NC	2.25	2.11	2.06
25	e	605	CLA	CHB-C1B	-2.25	1.34	1.39
25	A	775	CLA	MG-NB	2.25	2.10	2.05
25	a	613	CLA	CHB-C1B	-2.25	1.34	1.39
25	a	612	CLA	MG-NB	2.25	2.10	2.05
25	n	609	CLA	CHB-C1B	-2.25	1.34	1.39
25	l	613	CLA	MG-NB	2.25	2.10	2.05
25	A	765	CLA	CHC-C1C	2.25	1.43	1.38
25	B	759	CLA	CHC-C1C	2.25	1.43	1.38
25	d	602	CLA	CHB-C1B	-2.25	1.34	1.39
25	B	782	CLA	CHC-C1C	2.25	1.43	1.38
25	A	802	CLA	CHB-C1B	-2.25	1.34	1.39
25	b	602	CLA	CHB-C1B	-2.25	1.34	1.39
25	c	603	CLA	MG-NB	2.25	2.10	2.05
25	B	771	CLA	CHC-C1C	2.25	1.43	1.38
31	e	623	DD6	C10-C11	2.25	1.41	1.35
25	i	610	CLA	CHB-C1B	-2.25	1.34	1.39
29	A	792	BCR	C21-C22	2.25	1.41	1.35
25	c	601	CLA	CHB-C1B	-2.25	1.34	1.39
25	f	609	CLA	CHB-C1B	-2.25	1.34	1.39
25	l	611	CLA	MG-NB	2.25	2.10	2.05
31	n	623	DD6	C10-C11	2.25	1.41	1.35
25	l	614	CLA	MG-NC	2.24	2.11	2.06
25	B	782	CLA	C1B-NB	-2.24	1.34	1.37
25	B	775	CLA	CHB-C1B	-2.24	1.34	1.39
25	k	611	CLA	CHB-C1B	-2.24	1.34	1.39
25	B	783	CLA	MG-NB	2.24	2.10	2.05
25	B	756	CLA	CHB-C1B	-2.24	1.34	1.39
25	g	614	CLA	CHB-C1B	-2.24	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	782	CLA	MG-NB	2.24	2.10	2.05
25	a	601	CLA	MG-NB	2.24	2.10	2.05
29	A	787	BCR	C1-C6	-2.24	1.50	1.53
25	A	757	CLA	CHB-C1B	-2.24	1.34	1.39
25	o	604	CLA	MG-NB	2.24	2.10	2.05
25	B	750	CLA	C1B-NB	-2.24	1.34	1.37
25	A	806	CLA	CHB-C1B	-2.24	1.34	1.39
25	g	618	CLA	CHB-C1B	-2.24	1.34	1.39
25	p	608	CLA	CHC-C1C	2.24	1.43	1.38
31	g	621	DD6	C19-C20	-2.24	1.48	1.52
25	A	764	CLA	MG-NB	2.24	2.10	2.05
25	o	609	CLA	CHB-C1B	-2.24	1.34	1.39
30	c	245	SQD	O9-S	2.24	1.51	1.45
25	e	611	CLA	CHB-C1B	-2.24	1.34	1.39
25	A	774	CLA	CHC-C1C	2.24	1.43	1.38
25	b	609	CLA	CHC-C1C	2.24	1.43	1.38
25	n	612	CLA	CHB-C1B	-2.24	1.34	1.39
31	o	620	DD6	C35-C36	-2.24	1.47	1.51
25	m	613	CLA	MG-NB	2.24	2.10	2.05
25	A	780	CLA	CHB-C1B	-2.24	1.34	1.39
25	c	613	CLA	CHC-C1C	2.24	1.43	1.38
25	j	603	CLA	C1D-ND	-2.24	1.34	1.37
25	p	610	CLA	MG-NC	2.24	2.11	2.06
31	e	621	DD6	C19-C20	-2.24	1.49	1.52
25	i	603	CLA	C1D-ND	-2.24	1.34	1.37
25	p	609	CLA	MG-NC	2.24	2.11	2.06
25	A	752	CLA	CHC-C1C	2.24	1.43	1.38
25	A	783	CLA	CHB-C1B	-2.24	1.34	1.39
25	j	609	CLA	CHC-C1C	2.24	1.43	1.38
25	n	612	CLA	MG-NC	2.24	2.11	2.06
25	A	776	CLA	MG-NB	2.24	2.10	2.05
25	A	805	CLA	CHB-C1B	-2.24	1.34	1.39
25	f	610	CLA	MG-NB	2.24	2.10	2.05
25	c	614	CLA	MG-NB	2.23	2.10	2.05
25	o	614	CLA	MG-NB	2.23	2.10	2.05
30	g	190	SQD	O9-S	2.23	1.51	1.45
25	j	610	CLA	CHC-C1C	2.23	1.43	1.38
25	l	604	CLA	MG-NB	2.23	2.10	2.05
25	B	784	CLA	CHB-C1B	-2.23	1.34	1.39
25	m	611	CLA	CHB-C1B	-2.23	1.34	1.39
25	i	609	CLA	CHB-C1B	-2.23	1.34	1.39
31	i	625	DD6	C35-C36	-2.23	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d	609	CLA	MG-NB	2.23	2.10	2.05
25	i	614	CLA	MG-NB	2.23	2.10	2.05
25	B	754	CLA	CHB-C1B	-2.23	1.34	1.39
25	k	611	CLA	MG-NB	2.23	2.10	2.05
25	n	609	CLA	MG-NB	2.23	2.10	2.05
25	B	781	CLA	C1B-NB	-2.23	1.34	1.37
25	B	758	CLA	CHC-C1C	2.23	1.43	1.38
25	c	606	CLA	MG-NB	2.23	2.10	2.05
25	B	753	CLA	CHB-C1B	-2.23	1.34	1.39
25	o	602	CLA	CHB-C1B	-2.23	1.34	1.39
25	B	747	CLA	MG-NB	2.23	2.10	2.05
25	f	615	CLA	CHB-C1B	-2.23	1.34	1.39
25	o	612	CLA	CHB-C1B	-2.23	1.34	1.39
25	f	602	CLA	MG-NB	2.23	2.10	2.05
25	n	612	CLA	MG-NB	2.23	2.10	2.05
25	i	611	CLA	CHB-C1B	-2.23	1.34	1.39
25	n	604	CLA	MG-NC	2.23	2.11	2.06
25	A	801	CLA	CHB-C1B	-2.23	1.34	1.39
25	j	613	CLA	CHB-C1B	-2.23	1.34	1.39
25	A	782	CLA	MG-NC	2.23	2.11	2.06
25	m	603	CLA	CHC-C1C	2.23	1.42	1.38
25	e	607	CLA	MG-NB	2.23	2.10	2.05
25	A	762	CLA	MG-NB	2.23	2.10	2.05
31	c	624	DD6	C28-C27	-2.23	1.49	1.50
25	p	608	CLA	CHB-C1B	-2.22	1.34	1.39
25	l	609	CLA	CHC-C1C	2.22	1.42	1.38
25	l	611	CLA	CHB-C1B	-2.22	1.34	1.39
30	A	795	SQD	O7-S	2.22	1.51	1.45
25	n	608	CLA	CHB-C1B	-2.22	1.34	1.39
25	a	609	CLA	C1B-NB	-2.22	1.34	1.37
25	A	791	CLA	MG-NB	2.22	2.10	2.05
25	d	611	CLA	MG-NB	2.22	2.10	2.05
25	g	618	CLA	MG-NB	2.22	2.10	2.05
25	j	611	CLA	C1B-NB	-2.22	1.34	1.37
25	A	770	CLA	CHC-C1C	2.22	1.42	1.38
25	a	619	CLA	MG-NB	2.22	2.10	2.05
25	n	603	CLA	MG-NC	2.22	2.11	2.06
25	l	612	CLA	MG-NB	2.22	2.10	2.05
25	k	615	CLA	MG-NB	2.22	2.10	2.05
25	p	613	CLA	MG-NC	2.22	2.11	2.06
25	B	782	CLA	CHB-C1B	-2.22	1.34	1.39
25	f	604	CLA	CHB-C1B	-2.22	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	g	604	CLA	CHB-C1B	-2.22	1.34	1.39
25	m	604	CLA	CHB-C1B	-2.22	1.34	1.39
25	c	609	CLA	MG-NB	2.22	2.10	2.05
25	k	612	CLA	MG-NC	2.22	2.11	2.06
25	d	604	CLA	CHC-C1C	2.22	1.42	1.38
25	j	615	CLA	CHC-C1C	2.22	1.42	1.38
25	A	780	CLA	C1B-NB	-2.22	1.34	1.37
25	B	757	CLA	CHB-C1B	-2.22	1.34	1.39
25	B	780	CLA	MG-NB	2.22	2.10	2.05
25	c	604	CLA	CHC-C1C	2.22	1.42	1.38
25	b	613	CLA	CHB-C1B	-2.22	1.34	1.39
25	h	601	CLA	MG-NB	2.22	2.10	2.05
25	l	603	CLA	CHC-C1C	2.21	1.42	1.38
25	n	606	CLA	CHC-C1C	2.21	1.42	1.38
25	n	609	CLA	MG-NC	2.21	2.11	2.06
25	b	612	CLA	MG-NB	2.21	2.10	2.05
25	h	608	CLA	MG-NB	2.21	2.10	2.05
25	n	613	CLA	MG-NB	2.21	2.10	2.05
25	m	604	CLA	MG-NB	2.21	2.10	2.05
25	A	804	CLA	CHB-C1B	-2.21	1.34	1.39
25	f	611	CLA	CHB-C1B	-2.21	1.34	1.39
25	A	778	CLA	CHC-C1C	2.21	1.42	1.38
25	A	757	CLA	MG-NB	2.21	2.10	2.05
25	i	612	CLA	MG-NB	2.21	2.10	2.05
25	a	612	CLA	MG-NC	2.21	2.11	2.06
25	d	603	CLA	MG-NC	2.21	2.11	2.06
25	A	798	CLA	CHB-C1B	-2.21	1.34	1.39
25	o	609	CLA	MG-NB	2.21	2.10	2.05
25	p	601	CLA	MG-NC	2.21	2.11	2.06
25	i	615	CLA	CHC-C1C	2.21	1.42	1.38
25	e	614	CLA	CHB-C1B	-2.21	1.34	1.39
25	B	747	CLA	MG-NC	2.21	2.11	2.06
25	k	603	CLA	MG-NB	2.21	2.10	2.05
25	k	613	CLA	MG-NB	2.21	2.10	2.05
29	B	764	BCR	C30-C25	-2.21	1.51	1.53
25	d	612	CLA	MG-NB	2.21	2.10	2.05
25	h	615	CLA	MG-NB	2.21	2.10	2.05
25	e	605	CLA	MG-NB	2.21	2.10	2.05
25	j	608	CLA	MG-NC	2.21	2.11	2.06
25	j	614	CLA	CHC-C1C	2.21	1.42	1.38
31	j	621	DD6	C19-C20	-2.20	1.49	1.52
25	h	602	CLA	C1B-NB	-2.20	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	751	CLA	MG-NB	2.20	2.10	2.05
25	p	604	CLA	MG-NB	2.20	2.10	2.05
25	A	780	CLA	CHC-C1C	2.20	1.42	1.38
25	m	613	CLA	CHB-C1B	-2.20	1.34	1.39
25	j	609	CLA	C1B-NB	-2.20	1.35	1.37
25	l	617	CLA	CHB-C1B	-2.20	1.34	1.39
25	m	602	CLA	CHB-C1B	-2.20	1.34	1.39
25	l	612	CLA	MG-NC	2.20	2.11	2.06
25	B	785	CLA	MG-NC	2.20	2.11	2.06
31	j	620	DD6	C15-C14	-2.20	1.46	1.50
34	e	205	DGD	O2G-C2G	-2.20	1.41	1.46
25	k	612	CLA	MG-NB	2.20	2.10	2.05
25	d	614	CLA	MG-NC	2.20	2.11	2.06
25	o	608	CLA	CHB-C1B	-2.20	1.34	1.39
25	l	617	CLA	MG-NB	2.20	2.10	2.05
25	b	610	CLA	CHB-C1B	-2.20	1.34	1.39
25	f	602	CLA	CHB-C1B	-2.20	1.34	1.39
25	j	603	CLA	CHC-C1C	2.20	1.42	1.38
30	j	200	SQD	O9-S	2.20	1.51	1.45
25	a	608	CLA	MG-NB	2.20	2.10	2.05
33	i	195	LMG	O8-C28	2.20	1.39	1.33
25	m	610	CLA	MG-NB	2.20	2.10	2.05
25	j	615	CLA	MG-NB	2.20	2.10	2.05
25	e	609	CLA	CHC-C1C	2.20	1.42	1.38
25	B	760	CLA	MG-NC	2.20	2.11	2.06
25	e	611	CLA	MG-NC	2.20	2.11	2.06
25	h	612	CLA	MG-NC	2.20	2.11	2.06
25	A	774	CLA	CHB-C1B	-2.20	1.34	1.39
25	B	772	CLA	MG-NB	2.20	2.10	2.05
25	n	608	CLA	MG-NC	2.19	2.11	2.06
31	l	621	DD6	C15-C14	-2.19	1.46	1.50
33	B	786	LMG	O7-C8	-2.19	1.41	1.46
25	g	615	CLA	MG-NB	2.19	2.10	2.05
25	A	775	CLA	CHC-C1C	2.19	1.42	1.38
25	A	800	CLA	CHB-C1B	-2.19	1.34	1.39
25	A	772	CLA	MG-NC	2.19	2.11	2.06
25	c	611	CLA	MG-NC	2.19	2.11	2.06
25	b	612	CLA	MG-NC	2.19	2.11	2.06
25	d	612	CLA	MG-NC	2.19	2.11	2.06
25	B	736	CLA	CHC-C1C	2.19	1.42	1.38
25	o	614	CLA	MG-NC	2.19	2.11	2.06
25	j	610	CLA	CHB-C1B	-2.19	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	742	CLA	CHC-C1C	2.19	1.42	1.38
25	a	608	CLA	CHB-C1B	-2.19	1.34	1.39
25	k	602	CLA	CHB-C1B	-2.19	1.34	1.39
25	A	808	CLA	CHC-C1C	2.19	1.42	1.38
25	c	602	CLA	C1B-NB	-2.19	1.35	1.37
31	c	621	DD6	C35-C36	-2.19	1.47	1.51
25	A	770	CLA	CHB-C1B	-2.19	1.34	1.39
25	i	613	CLA	CHB-C1B	-2.19	1.34	1.39
25	e	601	CLA	MG-NC	2.19	2.11	2.06
25	l	601	CLA	MG-NC	2.19	2.11	2.06
25	h	609	CLA	CHC-C1C	2.19	1.42	1.38
25	A	779	CLA	MG-NB	2.19	2.10	2.05
25	d	612	CLA	C1B-NB	-2.19	1.35	1.37
25	A	774	CLA	MG-NC	2.19	2.11	2.06
25	h	611	CLA	CHB-C1B	-2.19	1.34	1.39
25	o	608	CLA	MG-NB	2.19	2.10	2.05
25	B	778	CLA	CHC-C1C	2.19	1.42	1.38
25	d	604	CLA	MG-NC	2.19	2.11	2.06
25	A	755	CLA	MG-NB	2.19	2.10	2.05
25	A	793	CLA	MG-NB	2.19	2.10	2.05
25	i	615	CLA	MG-NB	2.19	2.10	2.05
25	d	603	CLA	CHC-C1C	2.19	1.42	1.38
25	c	611	CLA	MG-NB	2.19	2.10	2.05
25	p	613	CLA	MG-NB	2.19	2.10	2.05
25	B	738	CLA	C1B-NB	-2.19	1.35	1.37
25	a	611	CLA	MG-NB	2.19	2.10	2.05
31	m	621	DD6	C35-C36	-2.18	1.47	1.51
25	A	758	CLA	CHB-C1B	-2.18	1.34	1.39
31	j	620	DD6	C19-C20	-2.18	1.49	1.52
25	m	602	CLA	MG-NB	2.18	2.10	2.05
25	f	608	CLA	CHB-C1B	-2.18	1.34	1.39
25	j	612	CLA	CHC-C1C	2.18	1.42	1.38
25	B	746	CLA	MG-NB	2.18	2.10	2.05
25	b	613	CLA	MG-NB	2.18	2.10	2.05
25	o	612	CLA	MG-NB	2.18	2.10	2.05
31	i	620	DD6	C19-C20	-2.18	1.49	1.52
25	A	767	CLA	MG-NC	2.18	2.11	2.06
25	B	754	CLA	CHC-C1C	2.18	1.42	1.38
25	i	612	CLA	MG-NC	2.18	2.11	2.06
25	e	609	CLA	MG-NC	2.18	2.11	2.06
25	n	605	CLA	MG-NC	2.18	2.11	2.06
25	A	762	CLA	MG-NC	2.18	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	603	CLA	MG-NB	2.18	2.10	2.05
25	A	804	CLA	C1B-NB	-2.18	1.35	1.37
25	f	601	CLA	CHB-C1B	-2.18	1.34	1.39
25	d	614	CLA	CHB-C1B	-2.18	1.34	1.39
25	A	773	CLA	CHB-C1B	-2.18	1.34	1.39
25	a	601	CLA	MG-NC	2.18	2.11	2.06
25	c	616	CLA	MG-NC	2.18	2.11	2.06
25	B	738	CLA	CHB-C1B	-2.18	1.34	1.39
25	n	607	CLA	MG-NC	2.18	2.11	2.06
25	A	766	CLA	CHC-C1C	2.18	1.42	1.38
25	d	604	CLA	MG-NB	2.18	2.10	2.05
25	A	774	CLA	C1B-NB	-2.18	1.35	1.37
25	h	610	CLA	C1B-NB	-2.18	1.35	1.37
25	b	601	CLA	MG-NC	2.18	2.11	2.06
25	h	603	CLA	C1B-NB	-2.18	1.35	1.37
25	c	604	CLA	MG-NC	2.18	2.11	2.06
25	e	603	CLA	MG-NC	2.18	2.11	2.06
25	B	777	CLA	CHB-C1B	-2.18	1.34	1.39
25	e	608	CLA	MG-NB	2.18	2.10	2.05
25	j	602	CLA	C1B-NB	-2.18	1.35	1.37
25	p	608	CLA	MG-NC	2.18	2.11	2.06
25	k	610	CLA	CHB-C1B	-2.18	1.34	1.39
25	B	756	CLA	C1B-NB	-2.18	1.35	1.37
25	f	601	CLA	MG-NC	2.17	2.11	2.06
25	g	604	CLA	MG-NB	2.17	2.10	2.05
25	c	603	CLA	MG-NC	2.17	2.11	2.06
25	k	601	CLA	CHB-C1B	-2.17	1.34	1.39
25	A	775	CLA	MG-NC	2.17	2.11	2.06
25	j	608	CLA	MG-NB	2.17	2.10	2.05
25	l	603	CLA	C1B-NB	-2.17	1.35	1.37
25	A	804	CLA	MG-NC	2.17	2.11	2.06
25	l	613	CLA	CHB-C1B	-2.17	1.34	1.39
25	f	610	CLA	MG-NC	2.17	2.11	2.06
25	c	612	CLA	MG-NC	2.17	2.11	2.06
25	j	601	CLA	MG-NB	2.17	2.10	2.05
25	m	604	CLA	MG-NC	2.17	2.11	2.06
25	h	608	CLA	MG-NC	2.17	2.11	2.06
25	g	601	CLA	MG-NC	2.17	2.11	2.06
25	A	764	CLA	MG-NC	2.17	2.11	2.06
25	B	754	CLA	MG-NC	2.17	2.11	2.06
25	B	778	CLA	MG-NB	2.17	2.10	2.05
25	p	613	CLA	CHB-C1B	-2.17	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	611	CLA	MG-NC	2.17	2.11	2.06
25	a	610	CLA	CHB-C1B	-2.17	1.34	1.39
31	e	623	DD6	C5-C6	2.17	1.40	1.35
25	A	761	CLA	C1B-NB	-2.17	1.35	1.37
25	e	612	CLA	MG-NC	2.17	2.11	2.06
25	B	768	CLA	MG-NC	2.16	2.11	2.06
25	B	782	CLA	MG-NC	2.16	2.11	2.06
25	a	603	CLA	MG-NC	2.16	2.11	2.06
25	o	601	CLA	MG-NC	2.16	2.11	2.06
25	A	776	CLA	MG-NC	2.16	2.11	2.06
25	j	604	CLA	MG-NC	2.16	2.11	2.06
25	B	748	CLA	C1B-NB	-2.16	1.35	1.37
25	B	776	CLA	MG-NB	2.16	2.10	2.05
25	c	612	CLA	MG-NB	2.16	2.10	2.05
25	A	807	CLA	MG-NC	2.16	2.11	2.06
25	j	612	CLA	C1B-NB	-2.16	1.35	1.37
25	d	614	CLA	MG-NB	2.16	2.10	2.05
25	j	612	CLA	MG-NB	2.16	2.10	2.05
25	p	601	CLA	MG-NB	2.16	2.10	2.05
31	e	623	DD6	C25-C26	-2.16	1.36	1.43
25	a	604	CLA	MG-NB	2.16	2.10	2.05
25	f	613	CLA	MG-NB	2.16	2.10	2.05
25	b	605	CLA	MG-NC	2.16	2.11	2.06
25	e	609	CLA	MG-NB	2.16	2.10	2.05
25	c	610	CLA	MG-NB	2.16	2.10	2.05
25	g	602	CLA	MG-NB	2.16	2.10	2.05
25	f	611	CLA	MG-NC	2.16	2.11	2.06
25	c	608	CLA	MG-NB	2.16	2.10	2.05
25	m	609	CLA	MG-NB	2.16	2.10	2.05
25	a	611	CLA	MG-NC	2.16	2.11	2.06
25	B	741	CLA	CHC-C1C	2.16	1.42	1.38
25	A	793	CLA	MG-NC	2.16	2.11	2.06
25	B	741	CLA	MG-NC	2.16	2.11	2.06
25	k	608	CLA	MG-NC	2.16	2.11	2.06
25	o	602	CLA	MG-NC	2.16	2.11	2.06
25	h	614	CLA	MG-NB	2.16	2.10	2.05
25	m	611	CLA	MG-NC	2.16	2.11	2.06
25	f	613	CLA	MG-NC	2.16	2.11	2.06
25	A	770	CLA	C1B-NB	-2.16	1.35	1.37
25	a	602	CLA	CHB-C1B	-2.15	1.34	1.39
25	c	619	CLA	MG-NC	2.15	2.11	2.06
25	e	613	CLA	MG-NC	2.15	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	l	617	CLA	MG-NC	2.15	2.11	2.06
25	o	612	CLA	MG-NC	2.15	2.11	2.06
25	B	754	CLA	C1B-NB	-2.15	1.35	1.37
25	A	752	CLA	MG-NB	2.15	2.10	2.05
25	n	613	CLA	MG-NC	2.15	2.11	2.06
25	n	610	CLA	C3B-C4B	2.15	1.49	1.42
25	b	602	CLA	C1B-NB	-2.15	1.35	1.37
25	c	614	CLA	MG-NC	2.15	2.11	2.06
25	B	774	CLA	C1B-NB	-2.15	1.35	1.37
25	B	760	CLA	MG-NB	2.15	2.10	2.05
25	p	610	CLA	CAA-C2A	2.15	1.58	1.54
25	f	612	CLA	CHC-C1C	2.15	1.42	1.38
25	k	611	CLA	MG-NC	2.15	2.11	2.06
30	j	200	SQD	O7-S	2.15	1.51	1.45
25	B	771	CLA	MG-NC	2.15	2.11	2.06
25	k	608	CLA	MG-NB	2.15	2.10	2.05
25	B	740	CLA	C1B-NB	-2.15	1.35	1.37
35	d	608	CHL	C2C-C3C	2.15	1.38	1.36
25	B	785	CLA	CHC-C1C	2.15	1.42	1.38
25	f	610	CLA	C3B-C4B	2.15	1.49	1.42
25	b	609	CLA	MG-NB	2.15	2.10	2.05
25	p	601	CLA	CHB-C1B	-2.15	1.34	1.39
30	g	190	SQD	O7-S	2.15	1.51	1.45
25	j	614	CLA	MG-NC	2.15	2.11	2.06
31	J	4002	DD6	C15-C14	-2.15	1.46	1.50
25	l	610	CLA	MG-NB	2.15	2.10	2.05
25	b	604	CLA	C1B-NB	-2.15	1.35	1.37
25	d	610	CLA	C1B-NB	-2.15	1.35	1.37
25	c	603	CLA	CHC-C1C	2.14	1.42	1.38
25	B	770	CLA	MG-NB	2.14	2.10	2.05
25	f	608	CLA	MG-NC	2.14	2.11	2.06
25	g	601	CLA	MG-NB	2.14	2.10	2.05
25	g	610	CLA	CHB-C1B	-2.14	1.34	1.39
25	k	601	CLA	MG-NC	2.14	2.11	2.06
25	J	101	CLA	MG-NC	2.14	2.11	2.06
31	c	620	DD6	C19-C20	-2.14	1.49	1.52
25	e	614	CLA	MG-NC	2.14	2.11	2.06
31	g	620	DD6	C35-C36	-2.14	1.47	1.51
25	A	752	CLA	C1B-NB	-2.14	1.35	1.37
25	f	604	CLA	MG-NC	2.14	2.11	2.06
25	f	614	CLA	MG-NC	2.14	2.11	2.06
25	o	609	CLA	MG-NC	2.14	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	o	602	CLA	MG-NB	2.14	2.10	2.05
25	g	601	CLA	CHC-C1C	2.14	1.42	1.38
25	h	604	CLA	MG-NC	2.14	2.11	2.06
25	A	765	CLA	MG-NC	2.14	2.11	2.06
25	l	608	CLA	MG-NC	2.14	2.11	2.06
25	m	613	CLA	MG-NC	2.14	2.11	2.06
34	b	182	DGD	O2G-C1B	2.14	1.40	1.34
25	A	757	CLA	C1B-NB	-2.14	1.35	1.37
25	b	610	CLA	MG-NB	2.14	2.10	2.05
25	B	778	CLA	MG-NC	2.14	2.11	2.06
25	p	604	CLA	MG-NC	2.14	2.11	2.06
25	d	613	CLA	CHB-C1B	-2.14	1.34	1.39
25	B	772	CLA	MG-NC	2.14	2.11	2.06
25	l	602	CLA	MG-NB	2.14	2.10	2.05
25	j	602	CLA	CHB-C1B	-2.14	1.34	1.39
25	k	614	CLA	MG-NC	2.14	2.11	2.06
34	b	182	DGD	C3D-C2D	2.13	1.57	1.52
25	B	770	CLA	MG-NC	2.13	2.11	2.06
25	B	737	CLA	CHB-C1B	-2.13	1.34	1.39
25	p	612	CLA	CHB-C1B	-2.13	1.34	1.39
25	J	101	CLA	CHC-C1C	2.13	1.42	1.38
25	k	618	CLA	MG-NB	2.13	2.10	2.05
25	i	604	CLA	C1B-NB	-2.13	1.35	1.37
25	k	604	CLA	MG-NB	2.13	2.10	2.05
25	c	619	CLA	MG-NB	2.13	2.10	2.05
25	d	603	CLA	MG-NB	2.13	2.10	2.05
25	m	608	CLA	MG-NC	2.13	2.11	2.06
35	c	607	CHL	C2C-C3C	2.13	1.38	1.36
25	B	777	CLA	MG-NC	2.13	2.11	2.06
25	i	601	CLA	MG-NB	2.13	2.10	2.05
25	b	603	CLA	MG-NC	2.13	2.11	2.06
25	l	613	CLA	MG-NC	2.13	2.11	2.06
25	d	611	CLA	MG-NC	2.13	2.11	2.06
25	l	604	CLA	MG-NC	2.13	2.11	2.06
25	g	603	CLA	C1D-ND	-2.13	1.35	1.37
25	e	604	CLA	MG-NB	2.13	2.10	2.05
25	l	611	CLA	MG-NC	2.13	2.11	2.06
25	l	609	CLA	MG-NB	2.13	2.10	2.05
25	B	745	CLA	MG-NB	2.13	2.10	2.05
25	i	611	CLA	MG-NB	2.13	2.10	2.05
25	A	778	CLA	MG-NC	2.13	2.11	2.06
25	A	780	CLA	MG-NC	2.13	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	608	CLA	MG-NC	2.13	2.11	2.06
35	d	605	CHL	C2-C3	2.13	1.38	1.32
25	b	613	CLA	MG-NC	2.13	2.11	2.06
25	g	602	CLA	CHB-C1B	-2.13	1.34	1.39
25	o	614	CLA	CHB-C1B	-2.13	1.34	1.39
25	A	784	CLA	MG-NB	2.13	2.10	2.05
25	i	615	CLA	MG-NC	2.13	2.11	2.06
25	o	604	CLA	MG-NC	2.13	2.11	2.06
25	e	612	CLA	C1B-NB	-2.13	1.35	1.37
25	a	604	CLA	MG-NC	2.13	2.11	2.06
25	g	615	CLA	MG-NC	2.12	2.11	2.06
31	d	620	DD6	C15-C14	-2.12	1.47	1.50
25	j	615	CLA	C1B-NB	-2.12	1.35	1.37
25	A	800	CLA	C1B-NB	-2.12	1.35	1.37
25	k	615	CLA	MG-NC	2.12	2.11	2.06
25	e	614	CLA	MG-NB	2.12	2.10	2.05
25	B	742	CLA	MG-NC	2.12	2.11	2.06
25	B	771	CLA	MG-NB	2.12	2.10	2.05
25	B	757	CLA	MG-NB	2.12	2.10	2.05
25	a	619	CLA	MG-NC	2.12	2.11	2.06
25	j	603	CLA	C1B-NB	-2.12	1.35	1.37
25	B	771	CLA	C1B-NB	-2.12	1.35	1.37
25	h	613	CLA	C1B-NB	-2.12	1.35	1.37
25	A	804	CLA	CHC-C1C	2.12	1.42	1.38
25	c	606	CLA	MG-NC	2.12	2.11	2.06
25	b	610	CLA	MG-NC	2.12	2.11	2.06
25	B	742	CLA	C1B-NB	-2.12	1.35	1.37
25	g	611	CLA	MG-NB	2.12	2.10	2.05
25	g	614	CLA	MG-NC	2.12	2.11	2.06
25	B	748	CLA	MG-NB	2.12	2.10	2.05
25	A	800	CLA	MG-NC	2.12	2.11	2.06
25	o	613	CLA	MG-NC	2.12	2.11	2.06
25	A	769	CLA	C1B-NB	-2.12	1.35	1.37
25	b	609	CLA	MG-NC	2.12	2.11	2.06
25	B	758	CLA	MG-NB	2.12	2.10	2.05
25	A	800	CLA	CHC-C1C	2.11	1.42	1.38
25	B	755	CLA	C1B-NB	-2.11	1.35	1.37
25	g	618	CLA	MG-NC	2.11	2.11	2.06
25	p	603	CLA	CHB-C1B	-2.11	1.34	1.39
25	B	776	CLA	MG-NC	2.11	2.11	2.06
25	B	749	CLA	MG-NB	2.11	2.10	2.05
25	b	608	CLA	C1B-NB	-2.11	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	j	604	CLA	C1B-NB	-2.11	1.35	1.37
25	h	615	CLA	MG-NC	2.11	2.11	2.06
25	B	736	CLA	MG-NC	2.11	2.11	2.06
25	h	603	CLA	MG-NB	2.11	2.10	2.05
25	k	609	CLA	C1B-NB	-2.11	1.35	1.37
25	m	602	CLA	C3B-C4B	2.11	1.48	1.42
25	i	614	CLA	MG-NC	2.11	2.11	2.06
25	B	743	CLA	MG-NC	2.11	2.11	2.06
25	A	776	CLA	C1B-NB	-2.11	1.35	1.37
25	B	773	CLA	C1B-NB	-2.11	1.35	1.37
25	h	618	CLA	MG-NB	2.11	2.10	2.05
25	k	603	CLA	MG-NC	2.11	2.11	2.06
25	c	610	CLA	C1B-NB	-2.11	1.35	1.37
25	m	610	CLA	MG-NC	2.11	2.11	2.06
25	c	601	CLA	MG-NB	2.11	2.10	2.05
25	A	767	CLA	CHC-C1C	2.11	1.42	1.38
25	B	779	CLA	MG-NC	2.11	2.11	2.06
25	h	610	CLA	CHB-C1B	-2.11	1.34	1.39
25	B	783	CLA	MG-NC	2.11	2.11	2.06
25	B	742	CLA	MG-NB	2.11	2.10	2.05
25	B	758	CLA	C1B-NB	-2.11	1.35	1.37
25	A	757	CLA	MG-NC	2.11	2.11	2.06
25	h	604	CLA	MG-NB	2.11	2.10	2.05
25	A	777	CLA	MG-NC	2.11	2.11	2.06
25	B	745	CLA	C1B-NB	-2.11	1.35	1.37
25	i	610	CLA	C1B-NB	-2.11	1.35	1.37
25	n	610	CLA	MG-NC	2.11	2.11	2.06
25	e	604	CLA	MG-NC	2.10	2.11	2.06
25	k	612	CLA	C1B-NB	-2.10	1.35	1.37
25	B	755	CLA	MG-NB	2.10	2.10	2.05
29	A	792	BCR	C17-C18	2.10	1.40	1.35
25	A	772	CLA	C1B-NB	-2.10	1.35	1.37
25	g	613	CLA	MG-NC	2.10	2.11	2.06
25	A	797	CLA	MG-NB	2.10	2.10	2.05
25	h	611	CLA	MG-NC	2.10	2.11	2.06
25	i	608	CLA	MG-NB	2.10	2.10	2.05
25	A	797	CLA	C1B-NB	-2.10	1.35	1.37
33	k	179	LMG	O8-C28	2.10	1.39	1.33
25	A	808	CLA	MG-NC	2.10	2.11	2.06
25	B	746	CLA	C1B-NB	-2.10	1.35	1.37
25	h	615	CLA	C1B-NB	-2.10	1.35	1.37
25	c	609	CLA	MG-NC	2.10	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d	601	CLA	MG-NC	2.10	2.11	2.06
25	B	746	CLA	MG-NC	2.10	2.11	2.06
25	e	605	CLA	MG-NC	2.10	2.11	2.06
25	i	604	CLA	MG-NC	2.10	2.11	2.06
25	A	773	CLA	MG-NB	2.10	2.09	2.05
25	B	759	CLA	MG-NC	2.10	2.11	2.06
25	A	783	CLA	MG-NB	2.10	2.09	2.05
30	c	245	SQD	C8-C7	2.10	1.56	1.50
25	A	779	CLA	MG-NC	2.10	2.11	2.06
29	B	763	BCR	C30-C25	-2.10	1.51	1.53
25	c	613	CLA	C1B-NB	-2.10	1.35	1.37
25	p	602	CLA	C1B-NB	-2.10	1.35	1.37
25	o	608	CLA	MG-NC	2.10	2.11	2.06
25	e	613	CLA	C1B-NB	-2.10	1.35	1.37
25	p	604	CLA	C3B-C4B	2.10	1.48	1.42
25	A	771	CLA	CHC-C1C	2.10	1.42	1.38
25	j	604	CLA	MG-NB	2.10	2.09	2.05
31	f	621	DD6	C35-C36	-2.10	1.47	1.51
25	c	603	CLA	C1B-NB	-2.10	1.35	1.37
25	i	603	CLA	CHC-C1C	2.10	1.42	1.38
25	d	613	CLA	MG-NC	2.09	2.11	2.06
25	k	613	CLA	MG-NC	2.09	2.11	2.06
25	g	604	CLA	MG-NC	2.09	2.11	2.06
25	b	602	CLA	MG-NB	2.09	2.09	2.05
25	d	604	CLA	C1B-NB	-2.09	1.35	1.37
25	i	601	CLA	MG-NC	2.09	2.11	2.06
25	B	749	CLA	MG-NC	2.09	2.11	2.06
25	a	608	CLA	MG-NC	2.09	2.11	2.06
25	A	791	CLA	C1B-NB	-2.09	1.35	1.37
25	d	601	CLA	C1B-NB	-2.09	1.35	1.37
30	c	245	SQD	O7-S	2.09	1.51	1.45
25	j	613	CLA	MG-NB	2.09	2.09	2.05
25	g	613	CLA	MG-NB	2.09	2.09	2.05
25	i	609	CLA	MG-NC	2.09	2.11	2.06
25	l	608	CLA	C1B-NB	-2.09	1.35	1.37
25	c	613	CLA	MG-NB	2.09	2.09	2.05
25	h	611	CLA	MG-NB	2.09	2.09	2.05
25	A	752	CLA	MG-NC	2.09	2.11	2.06
25	B	751	CLA	C1B-NB	-2.09	1.35	1.37
25	h	609	CLA	C1B-NB	-2.09	1.35	1.37
25	m	609	CLA	C1B-NB	-2.09	1.35	1.37
25	A	755	CLA	MG-NC	2.09	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	B	787	DGD	O3G-C3G	-2.09	1.40	1.43
25	k	602	CLA	MG-NB	2.09	2.09	2.05
25	b	602	CLA	MG-NC	2.09	2.11	2.06
25	h	609	CLA	MG-NB	2.09	2.09	2.05
25	B	754	CLA	MG-NB	2.09	2.09	2.05
25	k	618	CLA	MG-NC	2.09	2.11	2.06
25	m	608	CLA	C1B-NB	-2.09	1.35	1.37
35	d	605	CHL	C2C-C3C	2.09	1.38	1.36
25	d	610	CLA	MG-NC	2.09	2.11	2.06
25	i	611	CLA	MG-NC	2.09	2.11	2.06
25	i	609	CLA	MG-NB	2.09	2.09	2.05
25	A	771	CLA	C1B-NB	-2.09	1.35	1.37
25	h	603	CLA	MG-NC	2.08	2.11	2.06
25	k	604	CLA	MG-NC	2.08	2.11	2.06
25	p	613	CLA	C3B-C4B	2.08	1.48	1.42
25	j	615	CLA	MG-NC	2.08	2.11	2.06
25	j	618	CLA	MG-NC	2.08	2.11	2.06
25	a	612	CLA	C1B-NB	-2.08	1.35	1.37
25	h	608	CLA	C1B-NB	-2.08	1.35	1.37
25	A	781	CLA	MG-NB	2.08	2.09	2.05
25	k	610	CLA	MG-NB	2.08	2.09	2.05
25	i	602	CLA	MG-NB	2.08	2.09	2.05
34	b	182	DGD	C3E-C2E	2.08	1.57	1.52
25	b	609	CLA	C1B-NB	-2.08	1.35	1.37
25	o	610	CLA	MG-NC	2.08	2.11	2.06
25	c	601	CLA	MG-NC	2.08	2.11	2.06
25	g	603	CLA	C1B-NB	-2.08	1.35	1.37
25	B	748	CLA	MG-NC	2.08	2.11	2.06
25	i	613	CLA	MG-NB	2.08	2.09	2.05
25	d	603	CLA	C1B-NB	-2.08	1.35	1.37
33	k	179	LMG	O7-C8	-2.08	1.41	1.46
25	n	613	CLA	C1B-NB	-2.08	1.35	1.37
25	f	604	CLA	C3B-C4B	2.08	1.48	1.42
25	B	739	CLA	C1B-NB	-2.08	1.35	1.37
25	B	776	CLA	C1B-NB	-2.08	1.35	1.37
29	M	201	BCR	C30-C25	-2.08	1.51	1.53
25	A	763	CLA	C1B-NB	-2.08	1.35	1.37
25	m	601	CLA	C1D-ND	-2.08	1.35	1.37
25	B	752	CLA	MG-NC	2.08	2.11	2.06
25	B	753	CLA	MG-NC	2.08	2.11	2.06
25	A	808	CLA	C1B-NB	-2.08	1.35	1.37
25	B	760	CLA	C1B-NB	-2.08	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	798	CLA	MG-NC	2.08	2.11	2.06
25	d	601	CLA	MG-NB	2.08	2.09	2.05
25	j	611	CLA	MG-NB	2.08	2.09	2.05
25	d	602	CLA	C1B-NB	-2.08	1.35	1.37
25	g	610	CLA	MG-NB	2.08	2.09	2.05
25	p	612	CLA	MG-NC	2.08	2.11	2.06
31	m	621	DD6	C19-C20	-2.08	1.49	1.52
25	h	609	CLA	MG-NC	2.08	2.11	2.06
25	B	744	CLA	C1B-NB	-2.08	1.35	1.37
25	B	738	CLA	MG-NC	2.08	2.11	2.06
25	i	608	CLA	MG-NC	2.08	2.11	2.06
25	B	774	CLA	MG-NB	2.07	2.09	2.05
31	h	620	DD6	C15-C14	-2.07	1.47	1.50
25	h	602	CLA	MG-NC	2.07	2.11	2.06
25	A	771	CLA	MG-NB	2.07	2.09	2.05
25	A	758	CLA	C1B-NB	-2.07	1.35	1.37
25	A	762	CLA	C1B-NB	-2.07	1.35	1.37
25	A	770	CLA	MG-NB	2.07	2.09	2.05
25	g	608	CLA	C3B-C4B	2.07	1.48	1.42
25	n	608	CLA	C3B-C4B	2.07	1.48	1.42
25	b	605	CLA	C1B-NB	-2.07	1.35	1.37
25	j	601	CLA	C1B-NB	-2.07	1.35	1.37
25	j	601	CLA	MG-NC	2.07	2.11	2.06
25	B	751	CLA	C3B-C4B	2.07	1.48	1.42
25	B	774	CLA	MG-NC	2.07	2.11	2.06
25	c	613	CLA	MG-NC	2.07	2.11	2.06
25	B	744	CLA	MG-NC	2.07	2.11	2.06
25	n	603	CLA	C3B-C4B	2.07	1.48	1.42
25	B	740	CLA	MG-NC	2.07	2.11	2.06
31	l	620	DD6	C15-C14	-2.07	1.47	1.50
25	A	763	CLA	MG-NB	2.07	2.09	2.05
25	A	799	CLA	MG-NB	2.07	2.09	2.05
25	b	608	CLA	MG-NB	2.07	2.09	2.05
25	l	602	CLA	C1B-NB	-2.07	1.35	1.37
25	o	612	CLA	C1B-NB	-2.07	1.35	1.37
25	a	610	CLA	MG-NB	2.07	2.09	2.05
25	A	782	CLA	C1B-NB	-2.07	1.35	1.37
25	n	602	CLA	C1B-NB	-2.07	1.35	1.37
25	A	803	CLA	MG-NC	2.07	2.11	2.06
25	m	609	CLA	MG-NC	2.07	2.11	2.06
25	l	608	CLA	MG-NB	2.07	2.09	2.05
25	B	753	CLA	C1B-NB	-2.07	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	e	603	CLA	C1B-NB	-2.07	1.35	1.37
25	A	761	CLA	MG-NC	2.07	2.11	2.06
25	b	604	CLA	MG-NC	2.07	2.11	2.06
25	n	602	CLA	CHB-C1B	-2.07	1.34	1.39
25	m	601	CLA	CHC-C1C	2.07	1.42	1.38
25	j	610	CLA	C1B-NB	-2.07	1.35	1.37
25	A	759	CLA	MG-NC	2.07	2.11	2.06
25	B	756	CLA	MG-NB	2.06	2.09	2.05
25	A	755	CLA	C1B-NB	-2.06	1.35	1.37
25	B	773	CLA	MG-NB	2.06	2.09	2.05
25	A	805	CLA	C1B-NB	-2.06	1.35	1.37
25	i	603	CLA	C1B-NB	-2.06	1.35	1.37
31	b	621	DD6	C26-C27	-2.06	1.32	1.37
25	o	603	CLA	C3B-C4B	2.06	1.48	1.42
25	o	610	CLA	C3B-C4B	2.06	1.48	1.42
25	f	608	CLA	C3B-C4B	2.06	1.48	1.42
25	a	604	CLA	C1B-NB	-2.06	1.35	1.37
25	i	601	CLA	C1B-NB	-2.06	1.35	1.37
25	d	609	CLA	MG-NC	2.06	2.11	2.06
25	b	604	CLA	MG-NB	2.06	2.09	2.05
25	A	766	CLA	MG-NC	2.06	2.11	2.06
25	p	603	CLA	CMD-C2D	2.06	1.55	1.50
25	g	601	CLA	C1B-NB	-2.06	1.35	1.37
25	i	613	CLA	C1B-NB	-2.06	1.35	1.37
25	a	609	CLA	MG-NB	2.06	2.09	2.05
25	j	609	CLA	MG-NC	2.06	2.11	2.06
25	h	604	CLA	C1B-NB	-2.06	1.35	1.37
25	i	602	CLA	C3B-C4B	2.06	1.48	1.42
25	B	780	CLA	MG-NC	2.06	2.11	2.06
29	A	792	BCR	C14-C13	2.06	1.40	1.35
25	k	608	CLA	C1B-NB	-2.06	1.35	1.37
25	n	613	CLA	C3B-C4B	2.06	1.48	1.42
25	A	773	CLA	MG-NC	2.06	2.11	2.06
25	i	608	CLA	C1B-NB	-2.06	1.35	1.37
25	n	608	CLA	MG-NB	2.06	2.09	2.05
25	A	791	CLA	MG-NC	2.06	2.11	2.06
25	g	609	CLA	MG-NC	2.06	2.11	2.06
25	k	609	CLA	MG-NB	2.06	2.09	2.05
25	e	602	CLA	MG-NC	2.06	2.11	2.06
25	l	602	CLA	MG-NC	2.06	2.11	2.06
25	h	618	CLA	MG-NC	2.06	2.11	2.06
25	o	610	CLA	C3A-C2A	-2.05	1.52	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	801	CLA	MG-NB	2.05	2.09	2.05
25	e	610	CLA	MG-NB	2.05	2.09	2.05
25	o	604	CLA	C3B-C4B	2.05	1.48	1.42
25	k	609	CLA	MG-NC	2.05	2.11	2.06
25	A	767	CLA	C1B-NB	-2.05	1.35	1.37
25	e	610	CLA	MG-NC	2.05	2.11	2.06
25	A	801	CLA	C1B-NB	-2.05	1.35	1.37
25	A	806	CLA	C1B-NB	-2.05	1.35	1.37
25	A	759	CLA	MG-NB	2.05	2.09	2.05
25	B	745	CLA	MG-NC	2.05	2.11	2.06
25	e	602	CLA	C1B-NB	-2.05	1.35	1.37
25	B	755	CLA	MG-NC	2.05	2.11	2.06
25	e	607	CLA	MG-NC	2.05	2.11	2.06
25	B	780	CLA	C1B-NB	-2.05	1.35	1.37
25	a	603	CLA	C1B-NB	-2.05	1.35	1.37
25	a	609	CLA	MG-NC	2.05	2.11	2.06
31	i	621	DD6	C26-C27	-2.05	1.32	1.37
25	e	608	CLA	MG-NC	2.05	2.11	2.06
25	B	743	CLA	C1B-NB	-2.05	1.35	1.37
25	c	602	CLA	C3D-C4D	-2.05	1.39	1.44
25	g	602	CLA	C3B-C4B	2.05	1.48	1.42
25	B	777	CLA	MG-NB	2.05	2.09	2.05
31	a	621	DD6	C15-C14	-2.05	1.47	1.50
25	n	608	CLA	CAA-C2A	2.05	1.57	1.53
25	k	610	CLA	MG-NC	2.05	2.11	2.06
25	c	610	CLA	C3B-C4B	2.05	1.48	1.42
34	b	182	DGD	C4E-C3E	2.04	1.57	1.52
25	A	781	CLA	C1B-NB	-2.04	1.35	1.37
25	e	603	CLA	C3B-C4B	2.04	1.48	1.42
25	o	601	CLA	CAA-C2A	2.04	1.57	1.53
25	h	610	CLA	MG-NB	2.04	2.09	2.05
25	c	608	CLA	MG-NC	2.04	2.11	2.06
25	c	608	CLA	C1B-NB	-2.04	1.35	1.37
25	A	772	CLA	MG-NB	2.04	2.09	2.05
25	j	609	CLA	MG-NB	2.04	2.09	2.05
25	A	769	CLA	MG-NC	2.04	2.11	2.06
25	g	610	CLA	MG-NC	2.04	2.11	2.06
25	j	618	CLA	C1B-NB	-2.04	1.35	1.37
25	m	608	CLA	MG-NB	2.04	2.09	2.05
25	A	768	CLA	C3D-C4D	-2.04	1.39	1.44
25	B	783	CLA	C1B-NB	-2.04	1.35	1.37
25	d	613	CLA	MG-NB	2.04	2.09	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	775	CLA	MG-NC	2.04	2.11	2.06
25	B	781	CLA	MG-NC	2.04	2.11	2.06
25	h	614	CLA	MG-NC	2.04	2.11	2.06
25	p	609	CLA	C3B-C4B	2.04	1.48	1.42
25	A	794	CLA	C1B-NB	-2.04	1.35	1.37
25	A	802	CLA	C1B-NB	-2.04	1.35	1.37
25	B	775	CLA	C1B-NB	-2.04	1.35	1.37
25	A	773	CLA	C1B-NB	-2.04	1.35	1.37
25	a	613	CLA	C1B-NB	-2.04	1.35	1.37
25	p	603	CLA	C3B-C4B	2.04	1.48	1.42
25	A	771	CLA	MG-NC	2.04	2.11	2.06
25	h	612	CLA	C1B-NB	-2.04	1.35	1.37
31	c	620	DD6	C26-C27	-2.04	1.32	1.37
25	j	611	CLA	MG-NC	2.04	2.11	2.06
25	n	602	CLA	C3B-C4B	2.04	1.48	1.42
25	B	758	CLA	MG-NC	2.04	2.11	2.06
25	c	619	CLA	CAA-C2A	2.04	1.57	1.53
25	p	609	CLA	CAA-C2A	2.04	1.57	1.54
25	A	770	CLA	MG-NC	2.03	2.11	2.06
25	g	611	CLA	MG-NC	2.03	2.11	2.06
25	A	800	CLA	MG-NB	2.03	2.09	2.05
25	b	612	CLA	C3B-C4B	2.03	1.48	1.42
25	g	618	CLA	C3B-C4B	2.03	1.48	1.42
25	A	778	CLA	C1B-NB	-2.03	1.35	1.37
25	k	613	CLA	C1B-NB	-2.03	1.35	1.37
25	l	609	CLA	MG-NC	2.03	2.11	2.06
25	J	101	CLA	C1B-NB	-2.03	1.35	1.37
25	k	603	CLA	C1B-NB	-2.03	1.35	1.37
25	g	613	CLA	C1B-NB	-2.03	1.35	1.37
25	A	758	CLA	C3D-C4D	-2.03	1.39	1.44
25	c	610	CLA	MG-NC	2.03	2.11	2.06
25	o	610	CLA	CAA-C2A	2.03	1.57	1.53
25	h	613	CLA	MG-NB	2.03	2.09	2.05
25	A	768	CLA	MG-NC	2.03	2.11	2.06
25	B	777	CLA	C1B-NB	-2.03	1.35	1.37
25	b	612	CLA	C1B-NB	-2.03	1.35	1.37
25	e	613	CLA	MG-NB	2.03	2.09	2.05
25	g	612	CLA	C1B-NB	-2.03	1.35	1.37
25	l	602	CLA	C3B-C4B	2.03	1.48	1.42
25	B	739	CLA	MG-NC	2.03	2.11	2.06
25	A	784	CLA	MG-NC	2.03	2.11	2.06
25	c	601	CLA	C1B-NB	-2.03	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	p	601	CLA	C3B-C4B	2.03	1.48	1.42
33	a	182	LMG	O7-C8	-2.03	1.41	1.46
25	A	768	CLA	MG-NB	2.03	2.09	2.05
25	j	608	CLA	C1B-NB	-2.03	1.35	1.37
25	k	615	CLA	C1B-NB	-2.03	1.35	1.37
25	e	608	CLA	C3B-C4B	2.03	1.48	1.42
25	f	609	CLA	C3B-C4B	2.03	1.48	1.42
25	k	602	CLA	MG-NC	2.03	2.11	2.06
25	n	612	CLA	C3B-C4B	2.02	1.48	1.42
25	e	604	CLA	C1B-NB	-2.02	1.35	1.37
25	A	755	CLA	C3B-C4B	2.02	1.48	1.42
25	p	612	CLA	C3B-C4B	2.02	1.48	1.42
25	g	604	CLA	C1B-NB	-2.02	1.35	1.37
25	A	760	CLA	C3D-C4D	-2.02	1.39	1.44
25	h	618	CLA	C1B-NB	-2.02	1.35	1.37
25	o	614	CLA	C3B-C4B	2.02	1.48	1.42
25	m	603	CLA	C1B-NB	-2.02	1.35	1.37
25	g	609	CLA	C3B-C4B	2.02	1.48	1.42
25	B	744	CLA	MG-NB	2.02	2.09	2.05
25	i	615	CLA	C1B-NB	-2.02	1.35	1.37
25	c	602	CLA	MG-NC	2.02	2.11	2.06
35	d	607	CHL	C2C-C3C	2.02	1.38	1.36
25	d	602	CLA	MG-NB	2.02	2.09	2.05
25	A	801	CLA	MG-NC	2.02	2.11	2.06
25	B	740	CLA	MG-NB	2.02	2.09	2.05
25	B	784	CLA	MG-NC	2.02	2.11	2.06
25	B	779	CLA	C1B-NB	-2.02	1.35	1.37
25	B	756	CLA	MG-NC	2.02	2.11	2.06
25	A	777	CLA	MG-NB	2.02	2.09	2.05
25	j	608	CLA	CAA-C2A	2.02	1.57	1.54
25	d	609	CLA	CAA-C2A	2.02	1.57	1.54
25	A	783	CLA	MG-NC	2.02	2.11	2.06
25	i	613	CLA	MG-NC	2.02	2.11	2.06
25	f	602	CLA	MG-NC	2.02	2.11	2.06
25	m	611	CLA	C3B-C4B	2.02	1.48	1.42
25	A	765	CLA	C1B-NB	-2.02	1.35	1.37
25	n	604	CLA	C3B-C4B	2.02	1.48	1.42
25	A	799	CLA	MG-NC	2.02	2.11	2.06
25	g	602	CLA	MG-NC	2.02	2.11	2.06
25	B	759	CLA	C1B-NB	-2.02	1.35	1.37
25	k	601	CLA	C3B-C4B	2.02	1.48	1.42
25	B	772	CLA	C1B-NB	-2.02	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	k	620	DD6	C15-C14	-2.02	1.47	1.50
25	B	784	CLA	MG-NB	2.02	2.09	2.05
25	i	602	CLA	C3D-C4D	-2.02	1.39	1.44
25	B	759	CLA	MG-NB	2.02	2.09	2.05
25	g	603	CLA	CHC-C1C	2.02	1.42	1.38
31	J	4002	DD6	C37-C36	-2.01	1.47	1.50
25	A	768	CLA	C1B-NB	-2.01	1.35	1.37
25	B	784	CLA	C1B-NB	-2.01	1.35	1.37
25	A	794	CLA	MG-NB	2.01	2.09	2.05
25	A	806	CLA	MG-NB	2.01	2.09	2.05
25	c	612	CLA	C1B-NB	-2.01	1.35	1.37
25	l	617	CLA	C3B-C4B	2.01	1.48	1.42
25	B	770	CLA	C1B-NB	-2.01	1.35	1.37
25	o	601	CLA	C3B-C4B	2.01	1.48	1.42
25	B	747	CLA	C1B-NB	-2.01	1.35	1.37
25	A	806	CLA	MG-NC	2.01	2.11	2.06
25	B	773	CLA	C3B-C4B	2.01	1.48	1.42
25	A	794	CLA	MG-NC	2.01	2.11	2.06
25	A	799	CLA	C3B-C4B	2.01	1.48	1.42
25	A	805	CLA	MG-NB	2.01	2.09	2.05
25	h	602	CLA	MG-NB	2.01	2.09	2.05
25	f	615	CLA	C3B-C4B	2.01	1.48	1.42
25	i	612	CLA	C1B-NB	-2.01	1.35	1.37
25	B	753	CLA	MG-NB	2.01	2.09	2.05
25	b	608	CLA	CAA-C2A	2.01	1.57	1.53
25	o	601	CLA	C3A-C2A	-2.01	1.52	1.54
25	B	750	CLA	MG-NB	2.01	2.09	2.05
25	d	613	CLA	C1B-NB	-2.01	1.35	1.37
25	n	609	CLA	C1B-NB	-2.01	1.35	1.37
25	d	611	CLA	C1B-NB	-2.01	1.35	1.37
25	B	779	CLA	C3B-C4B	2.01	1.48	1.42
29	B	762	BCR	C1-C6	-2.01	1.51	1.53
25	c	619	CLA	C3B-C4B	2.01	1.48	1.42
25	b	603	CLA	C1B-NB	-2.01	1.35	1.37
25	b	601	CLA	C3B-C4B	2.01	1.48	1.42
25	a	613	CLA	CAA-C2A	2.01	1.57	1.54
25	c	614	CLA	C1B-NB	-2.01	1.35	1.37
25	B	773	CLA	MG-NC	2.01	2.11	2.06
25	A	758	CLA	MG-NB	2.01	2.09	2.05
25	k	602	CLA	CAA-C2A	2.01	1.57	1.54
25	h	601	CLA	MG-NC	2.01	2.11	2.06
25	l	609	CLA	C1B-NB	-2.01	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	n	607	CLA	C3B-C4B	2.00	1.48	1.42
25	o	608	CLA	C1B-NB	-2.00	1.35	1.37
29	A	790	BCR	C30-C25	-2.00	1.51	1.53
25	i	604	CLA	MG-NB	2.00	2.09	2.05
25	p	602	CLA	CMD-C2D	2.00	1.54	1.50
25	f	611	CLA	C3B-C4B	2.00	1.48	1.42
25	B	754	CLA	C3D-C4D	-2.00	1.39	1.44
25	o	601	CLA	C1B-NB	-2.00	1.35	1.37
25	a	602	CLA	C1B-NB	-2.00	1.35	1.37
25	e	602	CLA	MG-NB	2.00	2.09	2.05
34	b	182	DGD	O1G-C1A	2.00	1.39	1.33
25	j	618	CLA	MG-NB	2.00	2.09	2.05

All (2802) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	e	606	CHL	C1B-CHB-C4A	12.30	129.23	121.32
35	d	606	CHL	C1B-CHB-C4A	12.13	129.12	121.32
35	d	605	CHL	C1B-CHB-C4A	11.88	128.96	121.32
25	A	774	CLA	C4A-NA-C1A	11.45	111.90	106.68
25	k	603	CLA	C4A-NA-C1A	11.39	111.88	106.68
35	d	607	CHL	C1B-CHB-C4A	11.38	128.65	121.32
35	c	607	CHL	C1B-CHB-C4A	11.29	128.58	121.32
25	B	737	CLA	C4A-NA-C1A	11.10	111.74	106.68
25	o	612	CLA	C4A-NA-C1A	11.06	111.73	106.68
25	A	777	CLA	C4A-NA-C1A	11.00	111.70	106.68
25	l	617	CLA	C4A-NA-C1A	10.91	111.66	106.68
25	A	766	CLA	C4A-NA-C1A	10.87	111.64	106.68
25	B	782	CLA	C4A-NA-C1A	10.85	111.63	106.68
25	p	602	CLA	C4A-NA-C1A	10.73	111.58	106.68
25	A	761	CLA	C4A-NA-C1A	10.69	111.56	106.68
25	B	745	CLA	C4A-NA-C1A	10.68	111.55	106.68
25	c	619	CLA	C4A-NA-C1A	10.65	111.54	106.68
25	A	807	CLA	C4A-NA-C1A	10.62	111.52	106.68
25	h	603	CLA	C4A-NA-C1A	10.58	111.51	106.68
25	A	808	CLA	C4A-NA-C1A	10.56	111.50	106.68
25	d	601	CLA	C4A-NA-C1A	10.56	111.50	106.68
25	n	612	CLA	C4A-NA-C1A	10.55	111.49	106.68
25	B	738	CLA	C4A-NA-C1A	10.49	111.47	106.68
25	f	608	CLA	C4A-NA-C1A	10.49	111.47	106.68
25	d	603	CLA	C4A-NA-C1A	10.48	111.46	106.68
25	m	604	CLA	C4A-NA-C1A	10.47	111.45	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	f	611	CLA	C4A-NA-C1A	10.44	111.44	106.68
25	B	741	CLA	C4A-NA-C1A	10.43	111.44	106.68
25	e	612	CLA	C4A-NA-C1A	10.40	111.42	106.68
25	A	798	CLA	C4A-NA-C1A	10.39	111.42	106.68
25	h	615	CLA	C4A-NA-C1A	10.35	111.40	106.68
25	A	757	CLA	C4A-NA-C1A	10.34	111.40	106.68
25	A	801	CLA	C4A-NA-C1A	10.32	111.39	106.68
25	A	771	CLA	C4A-NA-C1A	10.29	111.37	106.68
25	j	608	CLA	C4A-NA-C1A	10.29	111.37	106.68
25	n	609	CLA	C4A-NA-C1A	10.29	111.37	106.68
25	k	608	CLA	C4A-NA-C1A	10.26	111.36	106.68
25	a	612	CLA	C4A-NA-C1A	10.25	111.36	106.68
25	i	608	CLA	C4A-NA-C1A	10.25	111.35	106.68
25	A	793	CLA	C4A-NA-C1A	10.24	111.35	106.68
25	B	781	CLA	C4A-NA-C1A	10.23	111.34	106.68
25	B	772	CLA	C4A-NA-C1A	10.22	111.34	106.68
25	B	784	CLA	C4A-NA-C1A	10.21	111.34	106.68
35	d	608	CHL	C1B-CHB-C4A	10.21	127.89	121.32
25	l	614	CLA	C4A-NA-C1A	10.21	111.34	106.68
25	j	604	CLA	C4A-NA-C1A	10.21	111.34	106.68
25	d	612	CLA	C4A-NA-C1A	10.20	111.33	106.68
25	j	618	CLA	C4A-NA-C1A	10.20	111.33	106.68
25	B	774	CLA	C4A-NA-C1A	10.19	111.33	106.68
25	j	615	CLA	C4A-NA-C1A	10.17	111.32	106.68
25	k	615	CLA	C4A-NA-C1A	10.17	111.32	106.68
25	l	603	CLA	C4A-NA-C1A	10.17	111.32	106.68
25	A	759	CLA	C4A-NA-C1A	10.16	111.31	106.68
25	n	602	CLA	C4A-NA-C1A	10.14	111.31	106.68
25	B	780	CLA	C4A-NA-C1A	10.14	111.30	106.68
25	B	779	CLA	C4A-NA-C1A	10.13	111.30	106.68
25	c	612	CLA	C4A-NA-C1A	10.12	111.30	106.68
25	i	609	CLA	C4A-NA-C1A	10.12	111.29	106.68
25	g	612	CLA	C4A-NA-C1A	10.11	111.29	106.68
25	d	609	CLA	C4A-NA-C1A	10.09	111.28	106.68
25	k	613	CLA	C4A-NA-C1A	10.08	111.28	106.68
25	i	615	CLA	C4A-NA-C1A	10.07	111.28	106.68
25	B	756	CLA	C4A-NA-C1A	10.06	111.27	106.68
25	g	613	CLA	C4A-NA-C1A	10.06	111.27	106.68
25	f	603	CLA	C4A-NA-C1A	10.06	111.27	106.68
25	l	609	CLA	C4A-NA-C1A	10.06	111.27	106.68
25	b	603	CLA	C4A-NA-C1A	10.05	111.26	106.68
25	f	615	CLA	C4A-NA-C1A	10.04	111.26	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	g	608	CLA	C4A-NA-C1A	10.03	111.26	106.68
25	m	612	CLA	C4A-NA-C1A	10.03	111.25	106.68
25	e	605	CLA	C4A-NA-C1A	10.02	111.25	106.68
25	i	611	CLA	C4A-NA-C1A	10.02	111.25	106.68
25	B	783	CLA	C4A-NA-C1A	10.02	111.25	106.68
25	i	612	CLA	C4A-NA-C1A	10.01	111.25	106.68
25	B	760	CLA	C4A-NA-C1A	10.00	111.24	106.68
25	g	615	CLA	C4A-NA-C1A	10.00	111.24	106.68
25	b	605	CLA	C4A-NA-C1A	9.99	111.24	106.68
25	h	608	CLA	C4A-NA-C1A	9.99	111.24	106.68
25	A	767	CLA	C4A-NA-C1A	9.99	111.24	106.68
25	B	746	CLA	C4A-NA-C1A	9.99	111.23	106.68
25	A	803	CLA	C4A-NA-C1A	9.98	111.23	106.68
25	J	101	CLA	C4A-NA-C1A	9.98	111.23	106.68
25	A	778	CLA	C4A-NA-C1A	9.98	111.23	106.68
25	A	760	CLA	C4A-NA-C1A	9.97	111.23	106.68
25	h	604	CLA	C4A-NA-C1A	9.96	111.22	106.68
25	n	603	CLA	C4A-NA-C1A	9.96	111.22	106.68
25	o	609	CLA	C4A-NA-C1A	9.96	111.22	106.68
25	l	612	CLA	C4A-NA-C1A	9.95	111.22	106.68
25	A	779	CLA	C4A-NA-C1A	9.94	111.22	106.68
25	A	762	CLA	C4A-NA-C1A	9.93	111.21	106.68
25	e	607	CLA	C4A-NA-C1A	9.92	111.21	106.68
25	b	612	CLA	C4A-NA-C1A	9.92	111.21	106.68
25	o	613	CLA	C4A-NA-C1A	9.92	111.20	106.68
25	g	614	CLA	C4A-NA-C1A	9.91	111.20	106.68
25	B	739	CLA	C4A-NA-C1A	9.91	111.20	106.68
25	c	609	CLA	C4A-NA-C1A	9.90	111.19	106.68
25	o	608	CLA	C4A-NA-C1A	9.89	111.19	106.68
25	B	776	CLA	C4A-NA-C1A	9.89	111.19	106.68
25	a	610	CLA	C4A-NA-C1A	9.89	111.19	106.68
25	A	758	CLA	C4A-NA-C1A	9.88	111.19	106.68
25	B	750	CLA	C4A-NA-C1A	9.87	111.18	106.68
25	p	608	CLA	C4A-NA-C1A	9.87	111.18	106.68
25	j	603	CLA	C4A-NA-C1A	9.86	111.18	106.68
25	d	613	CLA	C4A-NA-C1A	9.85	111.17	106.68
25	e	601	CLA	C4A-NA-C1A	9.85	111.17	106.68
25	l	611	CLA	C4A-NA-C1A	9.85	111.17	106.68
25	A	755	CLA	C4A-NA-C1A	9.84	111.17	106.68
25	d	602	CLA	C4A-NA-C1A	9.84	111.17	106.68
25	A	765	CLA	C4A-NA-C1A	9.84	111.17	106.68
25	a	611	CLA	C4A-NA-C1A	9.83	111.16	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	604	CLA	C4A-NA-C1A	9.83	111.16	106.68
25	B	754	CLA	C4A-NA-C1A	9.82	111.16	106.68
25	k	612	CLA	C4A-NA-C1A	9.82	111.16	106.68
25	o	603	CLA	C4A-NA-C1A	9.82	111.16	106.68
25	j	614	CLA	C4A-NA-C1A	9.80	111.15	106.68
25	k	618	CLA	C4A-NA-C1A	9.80	111.15	106.68
25	B	752	CLA	C4A-NA-C1A	9.80	111.15	106.68
25	e	609	CLA	C4A-NA-C1A	9.80	111.15	106.68
25	h	601	CLA	C4A-NA-C1A	9.79	111.15	106.68
25	B	768	CLA	C4A-NA-C1A	9.79	111.15	106.68
25	j	609	CLA	C4A-NA-C1A	9.78	111.14	106.68
25	n	606	CLA	C4A-NA-C1A	9.78	111.14	106.68
25	m	608	CLA	C4A-NA-C1A	9.77	111.14	106.68
25	A	782	CLA	C4A-NA-C1A	9.77	111.14	106.68
25	e	603	CLA	C4A-NA-C1A	9.76	111.13	106.68
25	b	601	CLA	C4A-NA-C1A	9.76	111.13	106.68
25	a	619	CLA	C4A-NA-C1A	9.76	111.13	106.68
25	h	612	CLA	C4A-NA-C1A	9.75	111.13	106.68
25	b	611	CLA	C4A-NA-C1A	9.75	111.13	106.68
25	j	611	CLA	C4A-NA-C1A	9.75	111.13	106.68
25	a	603	CLA	C4A-NA-C1A	9.74	111.12	106.68
25	A	797	CLA	C4A-NA-C1A	9.73	111.12	106.68
25	B	773	CLA	C4A-NA-C1A	9.72	111.11	106.68
25	n	604	CLA	C4A-NA-C1A	9.72	111.11	106.68
25	j	602	CLA	C4A-NA-C1A	9.71	111.11	106.68
25	B	755	CLA	C4A-NA-C1A	9.71	111.11	106.68
25	o	602	CLA	C4A-NA-C1A	9.70	111.10	106.68
25	n	605	CLA	C4A-NA-C1A	9.69	111.10	106.68
25	d	610	CLA	C4A-NA-C1A	9.69	111.10	106.68
25	B	743	CLA	C4A-NA-C1A	9.69	111.10	106.68
25	p	604	CLA	C4A-NA-C1A	9.69	111.10	106.68
25	g	611	CLA	C4A-NA-C1A	9.68	111.10	106.68
25	i	601	CLA	C4A-NA-C1A	9.68	111.10	106.68
25	b	613	CLA	C4A-NA-C1A	9.64	111.08	106.68
25	l	608	CLA	C4A-NA-C1A	9.64	111.08	106.68
25	B	742	CLA	C4A-NA-C1A	9.64	111.08	106.68
25	m	609	CLA	C4A-NA-C1A	9.64	111.08	106.68
25	c	603	CLA	C4A-NA-C1A	9.63	111.07	106.68
25	d	611	CLA	C4A-NA-C1A	9.62	111.07	106.68
25	f	610	CLA	C4A-NA-C1A	9.58	111.05	106.68
25	c	606	CLA	C4A-NA-C1A	9.58	111.05	106.68
25	e	604	CLA	C4A-NA-C1A	9.58	111.05	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	604	CLA	C4A-NA-C1A	9.57	111.05	106.68
25	a	609	CLA	C4A-NA-C1A	9.56	111.04	106.68
25	A	764	CLA	C4A-NA-C1A	9.55	111.04	106.68
25	A	773	CLA	C4A-NA-C1A	9.55	111.03	106.68
25	a	613	CLA	C4A-NA-C1A	9.53	111.03	106.68
25	h	609	CLA	C4A-NA-C1A	9.53	111.03	106.68
25	k	614	CLA	C4A-NA-C1A	9.52	111.02	106.68
25	c	611	CLA	C4A-NA-C1A	9.51	111.02	106.68
25	A	799	CLA	C4A-NA-C1A	9.51	111.02	106.68
25	A	806	CLA	C4A-NA-C1A	9.49	111.01	106.68
25	p	609	CLA	C4A-NA-C1A	9.49	111.01	106.68
25	h	611	CLA	C4A-NA-C1A	9.49	111.01	106.68
25	g	618	CLA	C4A-NA-C1A	9.48	111.00	106.68
25	p	613	CLA	C4A-NA-C1A	9.48	111.00	106.68
25	B	748	CLA	C4A-NA-C1A	9.47	111.00	106.68
25	B	771	CLA	C4A-NA-C1A	9.46	111.00	106.68
25	b	609	CLA	C4A-NA-C1A	9.46	110.99	106.68
25	n	607	CLA	C4A-NA-C1A	9.44	110.98	106.68
25	g	601	CLA	C4A-NA-C1A	9.43	110.98	106.68
25	A	763	CLA	C4A-NA-C1A	9.42	110.98	106.68
25	B	770	CLA	C4A-NA-C1A	9.42	110.98	106.68
25	A	804	CLA	C4A-NA-C1A	9.41	110.97	106.68
25	j	612	CLA	C4A-NA-C1A	9.41	110.97	106.68
25	e	610	CLA	C4A-NA-C1A	9.41	110.97	106.68
25	b	608	CLA	C4A-NA-C1A	9.41	110.97	106.68
25	B	740	CLA	C4A-NA-C1A	9.40	110.97	106.68
25	e	613	CLA	C4A-NA-C1A	9.37	110.95	106.68
25	h	618	CLA	C4A-NA-C1A	9.37	110.95	106.68
25	b	602	CLA	C4A-NA-C1A	9.36	110.95	106.68
25	k	604	CLA	C4A-NA-C1A	9.36	110.95	106.68
25	e	614	CLA	C4A-NA-C1A	9.35	110.95	106.68
25	B	744	CLA	C4A-NA-C1A	9.35	110.94	106.68
25	l	613	CLA	C4A-NA-C1A	9.34	110.94	106.68
25	A	780	CLA	C4A-NA-C1A	9.33	110.94	106.68
25	B	747	CLA	C4A-NA-C1A	9.32	110.93	106.68
25	A	768	CLA	C4A-NA-C1A	9.32	110.93	106.68
25	d	604	CLA	C4A-NA-C1A	9.32	110.93	106.68
25	f	604	CLA	C4A-NA-C1A	9.31	110.93	106.68
25	m	613	CLA	C4A-NA-C1A	9.31	110.92	106.68
25	c	616	CLA	C4A-NA-C1A	9.29	110.92	106.68
25	g	609	CLA	C4A-NA-C1A	9.28	110.91	106.68
25	A	775	CLA	C4A-NA-C1A	9.28	110.91	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	k	611	CLA	C4A-NA-C1A	9.27	110.91	106.68
25	h	602	CLA	C4A-NA-C1A	9.27	110.91	106.68
25	k	609	CLA	C4A-NA-C1A	9.25	110.90	106.68
25	o	604	CLA	C4A-NA-C1A	9.23	110.89	106.68
25	b	610	CLA	C4A-NA-C1A	9.23	110.89	106.68
25	c	613	CLA	C4A-NA-C1A	9.22	110.89	106.68
25	A	772	CLA	C4A-NA-C1A	9.21	110.88	106.68
25	c	610	CLA	C4A-NA-C1A	9.21	110.88	106.68
25	i	602	CLA	C4A-NA-C1A	9.20	110.87	106.68
25	k	601	CLA	C4A-NA-C1A	9.19	110.87	106.68
25	f	609	CLA	C4A-NA-C1A	9.19	110.87	106.68
25	k	602	CLA	C4A-NA-C1A	9.18	110.87	106.68
25	i	604	CLA	C4A-NA-C1A	9.17	110.86	106.68
25	i	613	CLA	C4A-NA-C1A	9.15	110.85	106.68
25	a	608	CLA	C4A-NA-C1A	9.14	110.85	106.68
25	A	800	CLA	C4A-NA-C1A	9.14	110.85	106.68
25	a	604	CLA	C4A-NA-C1A	9.14	110.85	106.68
25	o	614	CLA	C4A-NA-C1A	9.14	110.85	106.68
25	h	613	CLA	C4A-NA-C1A	9.13	110.85	106.68
25	B	749	CLA	C4A-NA-C1A	9.13	110.84	106.68
25	A	776	CLA	C4A-NA-C1A	9.13	110.84	106.68
25	n	608	CLA	C4A-NA-C1A	9.13	110.84	106.68
25	c	614	CLA	C4A-NA-C1A	9.12	110.84	106.68
25	A	794	CLA	C4A-NA-C1A	9.11	110.84	106.68
25	B	785	CLA	C4A-NA-C1A	9.11	110.83	106.68
25	B	758	CLA	C4A-NA-C1A	9.10	110.83	106.68
25	i	603	CLA	C4A-NA-C1A	9.08	110.82	106.68
25	f	613	CLA	C4A-NA-C1A	9.07	110.81	106.68
25	A	752	CLA	C4A-NA-C1A	9.03	110.80	106.68
25	g	603	CLA	C4A-NA-C1A	9.03	110.80	106.68
25	e	602	CLA	C4A-NA-C1A	9.02	110.79	106.68
25	j	613	CLA	C4A-NA-C1A	8.99	110.78	106.68
25	h	614	CLA	C4A-NA-C1A	8.99	110.78	106.68
25	g	610	CLA	C4A-NA-C1A	8.98	110.78	106.68
25	l	601	CLA	C4A-NA-C1A	8.98	110.77	106.68
25	c	601	CLA	C4A-NA-C1A	8.97	110.77	106.68
25	m	603	CLA	C4A-NA-C1A	8.95	110.76	106.68
25	c	608	CLA	C4A-NA-C1A	8.94	110.76	106.68
25	f	614	CLA	C4A-NA-C1A	8.93	110.75	106.68
25	j	601	CLA	C4A-NA-C1A	8.92	110.75	106.68
25	l	602	CLA	C4A-NA-C1A	8.91	110.74	106.68
25	A	770	CLA	C4A-NA-C1A	8.91	110.74	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	d	614	CLA	C4A-NA-C1A	8.90	110.74	106.68
25	A	753	CLA	C4A-NA-C1A	8.90	110.74	106.68
25	B	778	CLA	C4A-NA-C1A	8.90	110.74	106.68
25	m	611	CLA	C4A-NA-C1A	8.89	110.74	106.68
25	e	608	CLA	C4A-NA-C1A	8.89	110.73	106.68
25	i	614	CLA	C4A-NA-C1A	8.87	110.72	106.68
25	k	610	CLA	C4A-NA-C1A	8.86	110.72	106.68
25	l	604	CLA	C4A-NA-C1A	8.83	110.71	106.68
25	A	769	CLA	C4A-NA-C1A	8.81	110.70	106.68
25	f	601	CLA	C4A-NA-C1A	8.81	110.70	106.68
25	B	736	CLA	C4A-NA-C1A	8.79	110.69	106.68
25	g	604	CLA	C4A-NA-C1A	8.77	110.68	106.68
31	J	4002	DD6	C14-C13-C11	8.76	139.13	125.53
25	p	610	CLA	C4A-NA-C1A	8.74	110.67	106.68
25	A	791	CLA	C4A-NA-C1A	8.73	110.66	106.68
25	f	602	CLA	C4A-NA-C1A	8.71	110.65	106.68
25	B	751	CLA	C4A-NA-C1A	8.70	110.65	106.68
25	c	602	CLA	C4A-NA-C1A	8.70	110.65	106.68
25	a	601	CLA	C4A-NA-C1A	8.70	110.65	106.68
25	m	610	CLA	C4A-NA-C1A	8.70	110.65	106.68
25	n	613	CLA	C4A-NA-C1A	8.66	110.63	106.68
31	j	620	DD6	C14-C13-C11	8.63	138.92	125.53
25	e	611	CLA	C4A-NA-C1A	8.57	110.59	106.68
25	g	602	CLA	C4A-NA-C1A	8.57	110.59	106.68
31	g	621	DD6	C14-C13-C11	8.56	138.81	125.53
25	A	802	CLA	C4A-NA-C1A	8.54	110.58	106.68
25	i	610	CLA	C4A-NA-C1A	8.54	110.57	106.68
31	k	620	DD6	C14-C13-C11	8.46	138.66	125.53
25	l	610	CLA	C4A-NA-C1A	8.43	110.53	106.68
25	B	777	CLA	C4A-NA-C1A	8.43	110.53	106.68
31	i	620	DD6	C14-C13-C11	8.43	138.61	125.53
25	j	610	CLA	C4A-NA-C1A	8.38	110.50	106.68
31	A	4008	DD6	C14-C13-C11	8.36	138.50	125.53
31	g	620	DD6	C14-C13-C11	8.34	138.47	125.53
25	o	601	CLA	C4A-NA-C1A	8.33	110.48	106.68
25	B	753	CLA	C4A-NA-C1A	8.33	110.48	106.68
25	m	601	CLA	C4A-NA-C1A	8.31	110.47	106.68
31	h	620	DD6	C14-C13-C11	8.23	138.30	125.53
25	B	759	CLA	C4A-NA-C1A	8.18	110.41	106.68
31	m	621	DD6	C14-C13-C11	8.17	138.21	125.53
25	n	610	CLA	C4A-NA-C1A	8.16	110.40	106.68
25	p	603	CLA	C4A-NA-C1A	8.16	110.40	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	620	DD6	C15-C14-C13	8.12	143.17	125.99
25	h	610	CLA	C4A-NA-C1A	8.11	110.38	106.68
25	p	601	CLA	C4A-NA-C1A	8.10	110.38	106.68
31	c	620	DD6	C14-C13-C11	8.09	138.09	125.53
25	A	781	CLA	C4A-NA-C1A	8.07	110.36	106.68
25	A	784	CLA	C4A-NA-C1A	8.06	110.36	106.68
25	B	775	CLA	C4A-NA-C1A	8.06	110.36	106.68
25	f	612	CLA	C4A-NA-C1A	8.04	110.35	106.68
31	l	620	DD6	C14-C13-C11	8.04	138.00	125.53
31	e	621	DD6	C14-C13-C11	8.03	137.98	125.53
25	A	783	CLA	C4A-NA-C1A	8.01	110.33	106.68
25	o	610	CLA	C4A-NA-C1A	7.98	110.32	106.68
31	j	621	DD6	C14-C13-C11	7.97	137.89	125.53
31	d	620	DD6	C14-C13-C11	7.93	137.83	125.53
31	a	621	DD6	C14-C13-C11	7.93	137.83	125.53
25	p	612	CLA	C4A-NA-C1A	7.87	110.27	106.68
31	d	621	DD6	C14-C13-C11	7.84	137.70	125.53
31	b	621	DD6	C14-C13-C11	7.81	137.65	125.53
31	l	621	DD6	C14-C13-C11	7.69	137.46	125.53
25	a	602	CLA	C4A-NA-C1A	7.68	110.18	106.68
31	o	621	DD6	C14-C13-C11	7.63	137.37	125.53
31	b	620	DD6	C15-C14-C13	7.63	142.12	125.99
31	p	621	DD6	C14-C13-C11	7.62	137.35	125.53
31	h	621	DD6	C14-C13-C11	7.60	137.32	125.53
25	m	602	CLA	C4A-NA-C1A	7.55	110.12	106.68
25	A	805	CLA	C4A-NA-C1A	7.52	110.11	106.68
31	i	621	DD6	C14-C13-C11	7.50	137.17	125.53
31	n	620	DD6	C15-C14-C13	7.49	141.83	125.99
31	c	621	DD6	C14-C13-C11	7.43	137.06	125.53
31	n	620	DD6	C14-C13-C11	7.39	137.00	125.53
31	o	620	DD6	C14-C13-C11	7.33	136.90	125.53
31	k	621	DD6	C14-C13-C11	7.30	136.85	125.53
31	m	620	DD6	C14-C13-C11	7.30	136.85	125.53
25	B	757	CLA	C4A-NA-C1A	7.26	109.99	106.68
31	c	623	DD6	C15-C14-C13	7.19	141.20	125.99
31	f	621	DD6	C15-C14-C13	7.09	140.98	125.99
31	d	623	DD6	C14-C13-C11	6.80	136.08	125.53
31	n	620	DD6	O1-C20-C19	6.59	119.67	113.49
31	A	4002	DD6	C15-C14-C13	6.54	139.82	125.99
35	e	606	CHL	O2D-CGD-CBD	6.54	118.13	110.95
35	d	606	CHL	O2D-CGD-CBD	6.47	118.05	110.95
35	d	608	CHL	O2D-CGD-CBD	6.45	118.03	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	d	607	CHL	O2D-CGD-CBD	6.44	118.02	110.95
35	d	605	CHL	O2D-CGD-CBD	6.40	117.98	110.95
28	B	769	PQN	C14-C13-C15	6.38	126.30	115.23
31	i	625	DD6	C14-C13-C11	6.36	135.40	125.53
35	c	607	CHL	O2D-CGD-CBD	6.35	117.92	110.95
31	f	620	DD6	C14-C13-C11	6.32	135.33	125.53
28	A	785	PQN	C14-C13-C15	6.25	126.08	115.23
28	d	223	PQN	C14-C13-C15	6.23	126.04	115.23
28	B	761	PQN	C14-C13-C15	6.23	126.03	115.23
31	f	620	DD6	C15-C14-C13	6.22	139.14	125.99
31	i	625	DD6	C15-C14-C13	5.97	138.62	125.99
31	f	621	DD6	C14-C13-C11	5.95	134.76	125.53
31	f	621	DD6	O1-C20-C19	5.93	119.05	113.49
31	c	623	DD6	O1-C20-C19	5.89	119.01	113.49
25	A	752	CLA	O2D-CGD-CBD	5.87	121.49	111.23
31	d	623	DD6	C15-C14-C13	5.85	138.36	125.99
31	f	620	DD6	O1-C20-C19	5.81	118.93	113.49
31	A	4002	DD6	C25-C26-C27	-5.58	111.01	126.61
31	d	623	DD6	O1-C20-C19	5.42	118.57	113.49
31	A	4002	DD6	C14-C13-C11	5.40	133.90	125.53
31	b	620	DD6	C14-C13-C11	5.19	133.58	125.53
31	o	620	DD6	C15-C14-C13	5.18	136.95	125.99
31	m	620	DD6	C15-C14-C13	5.13	136.84	125.99
31	c	623	DD6	C14-C13-C11	5.09	133.43	125.53
31	p	621	DD6	C15-C14-C13	5.07	136.71	125.99
31	a	620	DD6	C14-C13-C11	5.05	133.36	125.53
31	k	621	DD6	C15-C14-C13	5.01	136.59	125.99
31	A	4002	DD6	O1-C20-C19	4.97	118.15	113.49
31	A	4008	DD6	C15-C14-C13	4.90	136.35	125.99
31	g	620	DD6	C25-C26-C27	-4.82	113.13	126.61
31	h	621	DD6	C15-C14-C13	4.82	136.18	125.99
31	c	621	DD6	C15-C14-C13	4.80	136.15	125.99
31	o	621	DD6	C15-C14-C13	4.78	136.10	125.99
31	i	621	DD6	C15-C14-C13	4.77	136.09	125.99
31	d	621	DD6	C15-C14-C13	4.76	136.05	125.99
35	c	607	CHL	C3D-C4D-CHA	4.75	115.76	108.54
35	c	607	CHL	C4D-CHA-CBD	-4.68	104.25	108.97
35	e	606	CHL	C3D-C4D-CHA	4.68	115.65	108.54
31	p	621	DD6	C25-C26-C27	-4.67	113.55	126.61
35	d	606	CHL	C3D-C4D-CHA	4.66	115.62	108.54
35	d	605	CHL	C3D-C4D-CHA	4.64	115.59	108.54
31	b	620	DD6	O1-C20-C19	4.61	117.81	113.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	b	621	DD6	C15-C14-C13	4.60	135.72	125.99
35	d	607	CHL	C3D-C4D-CHA	4.58	115.50	108.54
35	d	606	CHL	C4D-CHA-CBD	-4.57	104.36	108.97
31	j	621	DD6	C15-C14-C13	4.56	135.63	125.99
31	p	621	DD6	O1-C20-C19	4.54	117.75	113.49
35	d	608	CHL	C3D-C4D-CHA	4.53	115.43	108.54
31	d	623	DD6	C25-C26-C27	-4.53	113.94	126.61
25	A	759	CLA	O2D-CGD-CBD	4.50	119.09	111.23
31	g	621	DD6	C25-C26-C27	-4.49	114.04	126.61
35	e	606	CHL	C4D-CHA-CBD	-4.47	104.47	108.97
25	p	613	CLA	O2D-CGD-CBD	4.46	119.03	111.23
25	m	611	CLA	O2D-CGD-CBD	4.46	119.03	111.23
25	c	610	CLA	O2D-CGD-CBD	4.45	119.01	111.23
25	d	609	CLA	O2D-CGD-CBD	4.44	118.99	111.23
25	A	755	CLA	O2D-CGD-CBD	4.44	118.99	111.23
31	e	623	DD6	C4-C3-C2	4.43	132.59	123.52
31	n	620	DD6	C25-C26-C27	-4.43	114.22	126.61
35	d	605	CHL	C4D-CHA-CBD	-4.42	104.51	108.97
25	i	609	CLA	O2D-CGD-CBD	4.40	118.92	111.23
25	a	610	CLA	O2D-CGD-CBD	4.39	118.90	111.23
25	l	603	CLA	O2D-CGD-CBD	4.38	118.89	111.23
25	h	610	CLA	O2D-CGD-CBD	4.38	118.88	111.23
35	d	607	CHL	C4D-CHA-CBD	-4.38	104.56	108.97
30	c	245	SQD	O47-C7-C8	4.37	120.94	111.48
27	j	198	LHG	C25-C24-C23	4.37	129.71	113.69
25	j	613	CLA	O2D-CGD-CBD	4.37	118.87	111.23
31	f	621	DD6	C25-C26-C27	-4.37	114.40	126.61
31	g	620	DD6	C15-C14-C13	4.37	135.22	125.99
25	e	605	CLA	O2D-CGD-CBD	4.36	118.84	111.23
31	e	621	DD6	C15-C14-C13	4.35	135.20	125.99
25	B	779	CLA	O2D-CGD-CBD	4.35	118.83	111.23
31	e	621	DD6	C25-C26-C27	-4.35	114.45	126.61
25	j	602	CLA	O2D-CGD-CBD	4.35	118.83	111.23
31	J	4002	DD6	C25-C26-C27	-4.34	114.47	126.61
25	c	609	CLA	O2D-CGD-CBD	4.34	118.81	111.23
25	A	776	CLA	O2D-CGD-CBD	4.34	118.81	111.23
25	m	608	CLA	O2D-CGD-CBD	4.33	118.79	111.23
25	l	610	CLA	O2D-CGD-CBD	4.32	118.79	111.23
25	n	602	CLA	O2D-CGD-CBD	4.31	118.76	111.23
27	i	194	LHG	C25-C24-C23	4.31	129.47	113.69
31	l	621	DD6	C15-C14-C13	4.31	135.10	125.99
27	h	190	LHG	C25-C24-C23	4.30	129.45	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	608	CLA	O2D-CGD-CBD	4.30	118.74	111.23
25	B	784	CLA	O2D-CGD-CBD	4.30	118.74	111.23
25	h	612	CLA	O2D-CGD-CBD	4.29	118.74	111.23
25	p	609	CLA	O2D-CGD-CBD	4.29	118.73	111.23
25	j	608	CLA	O2D-CGD-CBD	4.29	118.73	111.23
25	A	774	CLA	O2D-CGD-CBD	4.29	118.73	111.23
25	h	615	CLA	O2D-CGD-CBD	4.29	118.72	111.23
25	m	610	CLA	O2D-CGD-CBD	4.28	118.72	111.23
25	B	744	CLA	O2D-CGD-CBD	4.28	118.72	111.23
25	g	610	CLA	O2D-CGD-CBD	4.28	118.72	111.23
31	d	620	DD6	C15-C14-C13	4.28	135.04	125.99
25	B	781	CLA	O2D-CGD-CBD	4.27	118.69	111.23
25	B	783	CLA	O2D-CGD-CBD	4.26	118.68	111.23
25	A	781	CLA	O2D-CGD-CBD	4.26	118.68	111.23
25	i	610	CLA	O2D-CGD-CBD	4.25	118.67	111.23
25	n	610	CLA	O2D-CGD-CBD	4.25	118.66	111.23
31	n	623	DD6	C3-C4-C5	4.25	132.21	123.52
25	i	613	CLA	O2D-CGD-CBD	4.25	118.66	111.23
35	d	608	CHL	C4D-CHA-CBD	-4.25	104.69	108.97
25	h	609	CLA	O2D-CGD-CBD	4.25	118.65	111.23
25	i	604	CLA	O2D-CGD-CBD	4.25	118.65	111.23
25	f	608	CLA	O2D-CGD-CBD	4.25	118.65	111.23
31	i	625	DD6	O1-C20-C19	4.24	117.47	113.49
31	l	620	DD6	C15-C14-C13	4.24	134.96	125.99
25	f	609	CLA	O2D-CGD-CBD	4.22	118.61	111.23
27	m	182	LHG	C25-C24-C23	4.22	129.17	113.69
25	m	609	CLA	O2D-CGD-CBD	4.22	118.61	111.23
27	g	189	LHG	C25-C24-C23	4.22	129.15	113.69
25	k	611	CLA	O2D-CGD-CBD	4.22	118.60	111.23
31	c	623	DD6	C25-C26-C27	-4.22	114.81	126.61
25	b	601	CLA	O2D-CGD-CBD	4.22	118.60	111.23
25	l	608	CLA	O2D-CGD-CBD	4.22	118.60	111.23
25	n	609	CLA	O2D-CGD-CBD	4.22	118.60	111.23
27	b	181	LHG	C25-C24-C23	4.21	129.13	113.69
25	b	611	CLA	O2D-CGD-CBD	4.21	118.58	111.23
25	B	773	CLA	O2D-CGD-CBD	4.21	118.58	111.23
27	A	786	LHG	C25-C24-C23	4.20	129.09	113.69
25	g	611	CLA	O2D-CGD-CBD	4.20	118.57	111.23
25	g	612	CLA	O2D-CGD-CBD	4.20	118.57	111.23
25	B	743	CLA	O2D-CGD-CBD	4.20	118.56	111.23
25	o	613	CLA	O2D-CGD-CBD	4.19	118.56	111.23
31	d	621	DD6	C25-C26-C27	-4.19	114.89	126.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	k	609	CLA	O2D-CGD-CBD	4.18	118.53	111.23
31	g	621	DD6	C15-C14-C13	4.17	134.81	125.99
25	h	613	CLA	O2D-CGD-CBD	4.17	118.52	111.23
25	B	742	CLA	O2D-CGD-CBD	4.17	118.51	111.23
25	B	746	CLA	O2D-CGD-CBD	4.17	118.51	111.23
25	A	800	CLA	O2D-CGD-CBD	4.16	118.51	111.23
25	B	753	CLA	O2D-CGD-CBD	4.15	118.49	111.23
25	g	603	CLA	O2D-CGD-CBD	4.15	118.49	111.23
25	l	611	CLA	O2D-CGD-CBD	4.15	118.49	111.23
25	B	738	CLA	O2D-CGD-CBD	4.15	118.48	111.23
27	a	181	LHG	C25-C24-C23	4.15	128.89	113.69
31	a	621	DD6	C15-C14-C13	4.14	134.75	125.99
25	f	610	CLA	O2D-CGD-CBD	4.14	118.47	111.23
27	c	243	LHG	C25-C24-C23	4.14	128.87	113.69
25	b	604	CLA	O2D-CGD-CBD	4.14	118.47	111.23
25	d	613	CLA	O2D-CGD-CBD	4.14	118.47	111.23
25	n	602	CLA	C3B-C4B-NB	-4.14	106.84	110.53
25	i	608	CLA	O2D-CGD-CBD	4.14	118.46	111.23
25	A	793	CLA	O2D-CGD-CBD	4.13	118.46	111.23
25	o	614	CLA	O2D-CGD-CBD	4.13	118.46	111.23
25	e	610	CLA	O2D-CGD-CBD	4.13	118.45	111.23
25	j	610	CLA	O2D-CGD-CBD	4.12	118.43	111.23
25	n	606	CLA	O2D-CGD-CBD	4.12	118.43	111.23
25	B	737	CLA	O2D-CGD-CBD	4.12	118.43	111.23
30	g	190	SQD	O47-C7-C8	4.12	120.39	111.48
25	A	805	CLA	O2A-CGA-CBA	4.12	124.39	111.83
25	h	610	CLA	O2A-CGA-CBA	4.12	124.39	111.83
25	k	603	CLA	O2D-CGD-CBD	4.12	118.43	111.23
25	j	609	CLA	O2D-CGD-CBD	4.12	118.42	111.23
25	b	610	CLA	O2D-CGD-CBD	4.11	118.42	111.23
31	m	621	DD6	C15-C14-C13	4.11	134.67	125.99
28	B	761	PQN	C15-C13-C12	-4.10	111.95	121.17
25	A	783	CLA	O2D-CGD-CBD	4.10	118.40	111.23
25	e	607	CLA	O2D-CGD-CBD	4.10	118.40	111.23
31	h	620	DD6	C15-C14-C13	4.10	134.66	125.99
25	A	767	CLA	O2D-CGD-CBD	4.10	118.40	111.23
27	A	756	LHG	C25-C24-C23	4.10	128.71	113.69
25	g	608	CLA	O2D-CGD-CBD	4.10	118.39	111.23
25	A	797	CLA	O2D-CGD-CBD	4.10	118.39	111.23
25	j	615	CLA	O2D-CGD-CBD	4.10	118.39	111.23
25	g	604	CLA	O2D-CGD-CBD	4.10	118.39	111.23
28	B	769	PQN	C15-C13-C12	-4.09	111.98	121.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	n	604	CLA	O2D-CGD-CBD	4.09	118.38	111.23
25	f	613	CLA	O2D-CGD-CBD	4.09	118.38	111.23
25	g	615	CLA	O2D-CGD-CBD	4.09	118.38	111.23
25	B	751	CLA	O2D-CGD-CBD	4.09	118.37	111.23
25	B	760	CLA	O2D-CGD-CBD	4.08	118.37	111.23
25	o	610	CLA	O2D-CGD-CBD	4.08	118.37	111.23
25	g	618	CLA	O2D-CGD-CBD	4.08	118.37	111.23
25	A	805	CLA	O2D-CGD-CBD	4.08	118.37	111.23
25	B	741	CLA	O2D-CGD-CBD	4.08	118.36	111.23
25	B	755	CLA	O2D-CGD-CBD	4.08	118.36	111.23
25	B	776	CLA	O2D-CGD-CBD	4.07	118.35	111.23
25	A	773	CLA	O2D-CGD-CBD	4.07	118.35	111.23
25	o	601	CLA	O2D-CGD-CBD	4.07	118.35	111.23
25	B	759	CLA	O2D-CGD-CBD	4.07	118.34	111.23
25	b	603	CLA	O2D-CGD-CBD	4.06	118.33	111.23
30	A	795	SQD	O9-S-O7	-4.06	100.62	113.82
25	A	772	CLA	O2D-CGD-CBD	4.06	118.32	111.23
25	a	603	CLA	O2D-CGD-CBD	4.06	118.32	111.23
25	n	613	CLA	O2D-CGD-CBD	4.05	118.31	111.23
25	j	613	CLA	O2A-CGA-CBA	4.05	124.17	111.83
25	j	602	CLA	C3B-C4B-NB	-4.04	106.92	110.53
25	d	610	CLA	O2D-CGD-CBD	4.04	118.30	111.23
25	i	611	CLA	O2D-CGD-CBD	4.04	118.30	111.23
31	l	620	DD6	C25-C26-C27	-4.04	115.31	126.61
25	n	612	CLA	O2D-CGD-CBD	4.04	118.29	111.23
25	n	607	CLA	O2D-CGD-CBD	4.03	118.28	111.23
25	p	612	CLA	C3B-C4B-NB	-4.03	106.93	110.53
25	l	609	CLA	O2D-CGD-CBD	4.03	118.28	111.23
25	b	605	CLA	O2D-CGD-CBD	4.03	118.28	111.23
25	p	612	CLA	O2D-CGD-CBD	4.03	118.28	111.23
25	B	772	CLA	O2D-CGD-CBD	4.03	118.27	111.23
25	A	762	CLA	O2D-CGD-CBD	4.03	118.27	111.23
25	A	764	CLA	O2D-CGD-CBD	4.03	118.27	111.23
25	A	763	CLA	O2D-CGD-CBD	4.02	118.27	111.23
25	g	613	CLA	O2D-CGD-CBD	4.02	118.26	111.23
25	k	615	CLA	O2D-CGD-CBD	4.02	118.26	111.23
25	p	608	CLA	O2D-CGD-CBD	4.02	118.25	111.23
25	g	614	CLA	O2D-CGD-CBD	4.01	118.25	111.23
31	n	623	DD6	C24-C1-C2	4.01	125.32	119.01
25	p	603	CLA	O2D-CGD-CBD	4.01	118.24	111.23
25	B	785	CLA	O2D-CGD-CBD	4.01	118.24	111.23
25	a	608	CLA	O2D-CGD-CBD	4.01	118.24	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	o	608	CLA	O2D-CGD-CBD	4.00	118.23	111.23
25	h	604	CLA	O2D-CGD-CBD	4.00	118.23	111.23
31	m	620	DD6	O1-C20-C19	4.00	117.24	113.49
28	A	785	PQN	C15-C13-C12	-4.00	112.19	121.17
25	p	610	CLA	O2D-CGD-CBD	4.00	118.22	111.23
25	e	609	CLA	O2D-CGD-CBD	3.99	118.21	111.23
25	d	601	CLA	O2D-CGD-CBD	3.99	118.21	111.23
28	d	223	PQN	C15-C13-C12	-3.99	112.20	121.17
25	k	618	CLA	O2D-CGD-CBD	3.99	118.20	111.23
25	A	780	CLA	O2D-CGD-CBD	3.99	118.20	111.23
30	g	190	SQD	O9-S-O7	-3.98	100.87	113.82
25	a	609	CLA	O2D-CGD-CBD	3.98	118.19	111.23
25	B	758	CLA	O2D-CGD-CBD	3.98	118.19	111.23
25	i	615	CLA	O2D-CGD-CBD	3.98	118.19	111.23
25	c	604	CLA	O2D-CGD-CBD	3.98	118.19	111.23
25	k	610	CLA	O2D-CGD-CBD	3.98	118.19	111.23
31	i	625	DD6	C25-C26-C27	-3.98	115.47	126.61
25	B	768	CLA	O2D-CGD-CBD	3.98	118.19	111.23
25	a	613	CLA	O2D-CGD-CBD	3.98	118.18	111.23
25	J	101	CLA	O2D-CGD-CBD	3.97	118.18	111.23
25	d	611	CLA	O2D-CGD-CBD	3.97	118.17	111.23
25	B	747	CLA	O2D-CGD-CBD	3.97	118.17	111.23
25	A	777	CLA	O2D-CGD-CBD	3.97	118.17	111.23
25	B	781	CLA	C3B-C4B-NB	-3.97	106.99	110.53
25	B	750	CLA	O2D-CGD-CBD	3.97	118.17	111.23
25	b	613	CLA	O2D-CGD-CBD	3.97	118.17	111.23
30	c	245	SQD	O9-S-O7	-3.97	100.92	113.82
29	A	792	BCR	C16-C15-C14	3.97	131.63	123.52
31	b	620	DD6	C25-C26-C27	-3.96	115.52	126.61
25	e	614	CLA	O2D-CGD-CBD	3.96	118.16	111.23
25	p	601	CLA	O2D-CGD-CBD	3.96	118.15	111.23
25	e	613	CLA	O2D-CGD-CBD	3.96	118.15	111.23
31	a	620	DD6	C25-C26-C27	-3.96	115.54	126.61
25	A	768	CLA	O2D-CGD-CBD	3.96	118.15	111.23
25	o	603	CLA	O2D-CGD-CBD	3.96	118.14	111.23
31	h	621	DD6	C25-C26-C27	-3.95	115.55	126.61
25	k	614	CLA	O2D-CGD-CBD	3.95	118.14	111.23
31	k	620	DD6	C15-C14-C13	3.95	134.34	125.99
31	f	620	DD6	C25-C26-C27	-3.95	115.57	126.61
25	d	604	CLA	O2D-CGD-CBD	3.95	118.13	111.23
25	f	601	CLA	O2D-CGD-CBD	3.95	118.13	111.23
25	h	608	CLA	O2D-CGD-CBD	3.94	118.12	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	j	618	CLA	O2D-CGD-CBD	3.94	118.12	111.23
25	d	603	CLA	O2D-CGD-CBD	3.94	118.12	111.23
25	e	601	CLA	O2D-CGD-CBD	3.94	118.12	111.23
25	c	611	CLA	O2D-CGD-CBD	3.94	118.11	111.23
31	A	4008	DD6	O1-C20-C19	3.94	117.18	113.49
25	i	602	CLA	O2D-CGD-CBD	3.94	118.11	111.23
31	c	620	DD6	C25-C26-C27	-3.94	115.60	126.61
25	B	770	CLA	O2D-CGD-CBD	3.93	118.11	111.23
25	n	605	CLA	O2D-CGD-CBD	3.93	118.10	111.23
25	i	613	CLA	O2A-CGA-CBA	3.93	123.82	111.83
25	c	608	CLA	O2D-CGD-CBD	3.93	118.10	111.23
25	B	752	CLA	O2D-CGD-CBD	3.93	118.09	111.23
31	o	620	DD6	C25-C26-C27	-3.93	115.63	126.61
25	f	602	CLA	O2D-CGD-CBD	3.93	118.09	111.23
25	k	604	CLA	O2D-CGD-CBD	3.93	118.09	111.23
25	j	603	CLA	O2D-CGD-CBD	3.92	118.09	111.23
25	b	609	CLA	O2D-CGD-CBD	3.92	118.08	111.23
25	o	604	CLA	O2D-CGD-CBD	3.92	118.08	111.23
25	h	618	CLA	O2D-CGD-CBD	3.92	118.08	111.23
25	n	603	CLA	O2D-CGD-CBD	3.92	118.08	111.23
25	A	807	CLA	C3B-C4B-NB	-3.92	107.03	110.53
25	a	612	CLA	O2D-CGD-CBD	3.92	118.08	111.23
25	e	603	CLA	O2D-CGD-CBD	3.91	118.07	111.23
31	a	621	DD6	C25-C26-C27	-3.91	115.67	126.61
25	A	804	CLA	O2D-CGD-CBD	3.91	118.06	111.23
25	A	808	CLA	O2D-CGD-CBD	3.91	118.06	111.23
25	m	601	CLA	O2D-CGD-CBD	3.91	118.06	111.23
31	n	623	DD6	C4-C3-C2	3.91	131.51	123.52
25	c	616	CLA	O2D-CGD-CBD	3.90	118.05	111.23
25	A	758	CLA	O2D-CGD-CBD	3.90	118.05	111.23
25	B	775	CLA	C3B-C4B-NB	-3.89	107.05	110.53
35	c	607	CHL	CAA-C2A-C3A	-3.89	102.47	113.00
25	l	617	CLA	O2D-CGD-CBD	3.89	118.03	111.23
25	p	604	CLA	O2D-CGD-CBD	3.89	118.03	111.23
25	j	611	CLA	O2D-CGD-CBD	3.89	118.03	111.23
25	A	784	CLA	O2D-CGD-CBD	3.89	118.03	111.23
31	d	620	DD6	C25-C26-C27	-3.88	115.74	126.61
25	k	602	CLA	O2D-CGD-CBD	3.88	118.02	111.23
25	l	614	CLA	O2D-CGD-CBD	3.88	118.01	111.23
30	j	200	SQD	O47-C7-C8	3.88	119.87	111.48
31	A	4008	DD6	C25-C26-C27	-3.88	115.76	126.61
25	j	614	CLA	O2D-CGD-CBD	3.88	118.01	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	d	612	CLA	O2D-CGD-CBD	3.87	118.00	111.23
25	n	608	CLA	C3B-C4B-NB	-3.87	107.07	110.53
25	A	794	CLA	O2D-CGD-CBD	3.86	117.97	111.23
30	j	200	SQD	O9-S-O7	-3.86	101.28	113.82
25	A	797	CLA	C3B-C4B-NB	-3.86	107.09	110.53
25	B	773	CLA	C3B-C4B-NB	-3.85	107.09	110.53
25	B	740	CLA	O2D-CGD-CBD	3.84	117.95	111.23
25	g	609	CLA	O2D-CGD-CBD	3.84	117.94	111.23
31	i	620	DD6	C25-C26-C27	-3.84	115.88	126.61
25	B	778	CLA	O2D-CGD-CBD	3.83	117.92	111.23
25	f	611	CLA	O2D-CGD-CBD	3.82	117.92	111.23
25	m	604	CLA	O2D-CGD-CBD	3.82	117.91	111.23
25	A	760	CLA	O2D-CGD-CBD	3.82	117.91	111.23
31	e	623	DD6	C24-C1-C2	3.81	125.00	119.01
25	f	603	CLA	O2D-CGD-CBD	3.80	117.88	111.23
25	d	602	CLA	O2D-CGD-CBD	3.80	117.88	111.23
25	p	613	CLA	C3B-C4B-NB	-3.80	107.14	110.53
25	A	803	CLA	O2D-CGD-CBD	3.80	117.88	111.23
25	c	606	CLA	O2D-CGD-CBD	3.80	117.87	111.23
35	c	607	CHL	CBC-CAC-C3C	-3.80	107.43	112.87
25	A	806	CLA	O2D-CGD-CBD	3.80	117.87	111.23
25	o	609	CLA	O2D-CGD-CBD	3.80	117.87	111.23
25	h	614	CLA	O2D-CGD-CBD	3.79	117.85	111.23
25	A	798	CLA	O2D-CGD-CBD	3.79	117.85	111.23
25	a	619	CLA	O2D-CGD-CBD	3.79	117.85	111.23
31	c	620	DD6	C15-C14-C13	3.79	134.00	125.99
25	A	753	CLA	O2D-CGD-CBD	3.78	117.84	111.23
25	A	778	CLA	O2D-CGD-CBD	3.78	117.84	111.23
28	B	761	PQN	C9-C10-C5	3.78	123.51	119.26
25	l	610	CLA	C3B-C4B-NB	-3.78	107.16	110.53
25	d	614	CLA	O2D-CGD-CBD	3.78	117.83	111.23
25	g	602	CLA	C3B-C4B-NB	-3.78	107.16	110.53
25	A	753	CLA	C3B-C4B-NB	-3.78	107.16	110.53
25	e	608	CLA	O2D-CGD-CBD	3.77	117.83	111.23
25	m	602	CLA	C3B-C4B-NB	-3.77	107.16	110.53
25	l	612	CLA	O2D-CGD-CBD	3.76	117.80	111.23
25	A	760	CLA	C3B-C4B-NB	-3.76	107.17	110.53
25	A	799	CLA	C3B-C4B-NB	-3.76	107.17	110.53
25	B	744	CLA	C3B-C4B-NB	-3.76	107.17	110.53
25	e	612	CLA	O2D-CGD-CBD	3.76	117.80	111.23
25	A	765	CLA	O2D-CGD-CBD	3.76	117.80	111.23
25	k	608	CLA	O2D-CGD-CBD	3.75	117.79	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	c	607	CHL	CMA-C3A-C4A	-3.75	106.53	114.61
25	b	612	CLA	O2D-CGD-CBD	3.74	117.77	111.23
25	c	619	CLA	O2D-CGD-CBD	3.74	117.77	111.23
25	h	602	CLA	O2A-CGA-CBA	3.74	123.24	111.83
25	h	613	CLA	O2A-CGA-CBA	3.74	123.24	111.83
25	i	614	CLA	O2D-CGD-CBD	3.74	117.77	111.23
25	A	779	CLA	O2D-CGD-CBD	3.74	117.77	111.23
25	A	755	CLA	C3B-C4B-NB	-3.74	107.19	110.53
25	k	601	CLA	O2D-CGD-CBD	3.74	117.76	111.23
31	m	620	DD6	C25-C26-C27	-3.73	116.17	126.61
25	A	799	CLA	O2D-CGD-CBD	3.73	117.75	111.23
25	B	757	CLA	O2D-CGD-CBD	3.73	117.75	111.23
25	i	602	CLA	C3B-C4B-NB	-3.73	107.20	110.53
31	j	620	DD6	C15-C14-C13	3.73	133.88	125.99
25	A	791	CLA	C3B-C4B-NB	-3.73	107.20	110.53
25	e	614	CLA	C3B-C4B-NB	-3.73	107.20	110.53
31	k	620	DD6	C25-C26-C27	-3.72	116.19	126.61
25	B	737	CLA	C3B-C4B-NB	-3.72	107.20	110.53
25	A	802	CLA	C3B-C4B-NB	-3.72	107.21	110.53
25	A	761	CLA	O2D-CGD-CBD	3.72	117.73	111.23
25	f	615	CLA	O2D-CGD-CBD	3.72	117.73	111.23
25	c	614	CLA	O2D-CGD-CBD	3.72	117.72	111.23
25	B	746	CLA	C3B-C4B-NB	-3.71	107.22	110.53
31	k	621	DD6	C25-C26-C27	-3.71	116.24	126.61
31	l	621	DD6	C25-C26-C27	-3.71	116.24	126.61
31	i	620	DD6	C15-C14-C13	3.71	133.83	125.99
31	o	621	DD6	C25-C26-C27	-3.70	116.25	126.61
25	a	602	CLA	O2A-CGA-CBA	3.70	123.13	111.83
25	p	604	CLA	C3B-C4B-NB	-3.70	107.22	110.53
25	p	602	CLA	C3B-C4B-NB	-3.70	107.23	110.53
25	c	613	CLA	O2D-CGD-CBD	3.70	117.70	111.23
25	h	611	CLA	O2D-CGD-CBD	3.70	117.70	111.23
25	A	781	CLA	C3B-C4B-NB	-3.70	107.23	110.53
25	B	748	CLA	O2D-CGD-CBD	3.69	117.69	111.23
25	h	613	CLA	C3B-C4B-NB	-3.69	107.23	110.53
25	j	613	CLA	C3B-C4B-NB	-3.69	107.24	110.53
25	B	782	CLA	O2D-CGD-CBD	3.69	117.68	111.23
25	c	619	CLA	C3B-C4B-NB	-3.69	107.24	110.53
25	A	783	CLA	C3B-C4B-NB	-3.68	107.24	110.53
25	l	601	CLA	O2D-CGD-CBD	3.68	117.67	111.23
25	j	608	CLA	C3B-C4B-NB	-3.68	107.24	110.53
25	B	784	CLA	C3B-C4B-NB	-3.68	107.25	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	757	CLA	O2D-CGD-CBD	3.68	117.66	111.23
25	p	602	CLA	O2D-CGD-CBD	3.68	117.66	111.23
25	f	604	CLA	O2D-CGD-CBD	3.68	117.66	111.23
25	B	743	CLA	C3B-C4B-NB	-3.68	107.25	110.53
25	e	604	CLA	O2D-CGD-CBD	3.67	117.65	111.23
25	m	603	CLA	O2D-CGD-CBD	3.67	117.64	111.23
25	k	612	CLA	O2D-CGD-CBD	3.67	117.64	111.23
25	i	613	CLA	C3B-C4B-NB	-3.67	107.26	110.53
25	i	603	CLA	O2D-CGD-CBD	3.67	117.64	111.23
27	d	237	LHG	C25-C24-C23	3.66	129.15	114.36
25	a	602	CLA	C3B-C4B-NB	-3.66	107.26	110.53
25	e	608	CLA	C3B-C4B-NB	-3.66	107.26	110.53
35	e	606	CHL	CMA-C3A-C4A	-3.66	106.72	114.61
25	a	613	CLA	C3B-C4B-NB	-3.66	107.26	110.53
25	A	768	CLA	C3B-C4B-NB	-3.66	107.27	110.53
25	B	739	CLA	C3B-C4B-NB	-3.66	107.27	110.53
31	J	4002	DD6	C15-C14-C13	3.65	133.72	125.99
25	g	610	CLA	C3B-C4B-NB	-3.65	107.27	110.53
25	A	775	CLA	O2D-CGD-CBD	3.65	117.61	111.23
25	j	601	CLA	O2D-CGD-CBD	3.65	117.61	111.23
35	d	608	CHL	CBC-CAC-C3C	-3.65	107.65	112.87
25	h	608	CLA	C3B-C4B-NB	-3.65	107.27	110.53
25	o	610	CLA	C3B-C4B-NB	-3.65	107.27	110.53
25	h	602	CLA	O2D-CGD-CBD	3.65	117.60	111.23
25	j	612	CLA	O2D-CGD-CBD	3.65	117.60	111.23
25	A	752	CLA	O1D-CGD-CBD	-3.64	117.34	124.52
25	B	738	CLA	C3B-C4B-NB	-3.64	107.28	110.53
25	A	794	CLA	C3B-C4B-NB	-3.64	107.28	110.53
25	f	614	CLA	O2D-CGD-CBD	3.63	117.58	111.23
25	n	608	CLA	O2D-CGD-CBD	3.63	117.58	111.23
31	e	623	DD6	C12-C11-C10	-3.63	116.94	122.82
25	b	602	CLA	O2D-CGD-CBD	3.62	117.56	111.23
25	A	791	CLA	O2D-CGD-CBD	3.62	117.56	111.23
25	A	802	CLA	O2D-CGD-CBD	3.62	117.56	111.23
25	A	807	CLA	O2D-CGD-CBD	3.62	117.56	111.23
25	k	613	CLA	O2D-CGD-CBD	3.61	117.55	111.23
25	A	806	CLA	C3B-C4B-NB	-3.61	107.31	110.53
28	d	223	PQN	C9-C10-C5	3.61	123.31	119.26
25	B	753	CLA	C3B-C4B-NB	-3.60	107.31	110.53
25	d	601	CLA	C3B-C4B-NB	-3.60	107.31	110.53
25	l	604	CLA	O2D-CGD-CBD	3.60	117.53	111.23
25	B	757	CLA	C3B-C4B-NB	-3.60	107.32	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	739	CLA	O2D-CGD-CBD	3.60	117.52	111.23
25	A	759	CLA	C3B-C4B-NB	-3.60	107.32	110.53
25	j	604	CLA	O2D-CGD-CBD	3.60	117.52	111.23
28	B	769	PQN	C9-C10-C5	3.59	123.30	119.26
25	c	601	CLA	O2D-CGD-CBD	3.59	117.51	111.23
25	e	607	CLA	C3B-C4B-NB	-3.59	107.32	110.53
25	f	610	CLA	C3B-C4B-NB	-3.59	107.33	110.53
25	B	771	CLA	O2D-CGD-CBD	3.59	117.50	111.23
35	d	605	CHL	CBC-CAC-C3C	-3.59	107.74	112.87
25	m	612	CLA	O2D-CGD-CBD	3.58	117.49	111.23
28	A	785	PQN	C9-C10-C5	3.58	123.28	119.26
31	h	620	DD6	C25-C26-C27	-3.58	116.60	126.61
25	i	601	CLA	O2D-CGD-CBD	3.58	117.49	111.23
25	l	617	CLA	C3B-C4B-NB	-3.58	107.33	110.53
25	B	777	CLA	C3B-C4B-NB	-3.57	107.34	110.53
25	e	613	CLA	C3B-C4B-NB	-3.57	107.34	110.53
25	c	603	CLA	O2D-CGD-CBD	3.57	117.48	111.23
25	B	774	CLA	C3B-C4B-NB	-3.57	107.34	110.53
25	a	610	CLA	C3B-C4B-NB	-3.57	107.34	110.53
25	d	609	CLA	C3B-C4B-NB	-3.57	107.34	110.53
25	B	745	CLA	O2D-CGD-CBD	3.57	117.47	111.23
25	a	611	CLA	O2D-CGD-CBD	3.57	117.47	111.23
35	d	606	CHL	CAA-C2A-C3A	-3.56	103.37	113.00
25	B	756	CLA	O2D-CGD-CBD	3.56	117.45	111.23
25	e	611	CLA	O2D-CGD-CBD	3.55	117.44	111.23
25	B	754	CLA	O2D-CGD-CBD	3.55	117.44	111.23
25	B	736	CLA	O2D-CGD-CBD	3.55	117.44	111.23
25	B	780	CLA	O2D-CGD-CBD	3.55	117.44	111.23
25	A	777	CLA	C3B-C4B-NB	-3.55	107.36	110.53
25	A	766	CLA	O2D-CGD-CBD	3.55	117.44	111.23
25	B	774	CLA	O2D-CGD-CBD	3.55	117.43	111.23
25	l	602	CLA	C3B-C4B-NB	-3.55	107.36	110.53
31	c	624	DD6	C12-C11-C10	-3.54	117.08	122.82
25	B	780	CLA	C3B-C4B-NB	-3.54	107.37	110.53
25	o	614	CLA	C3B-C4B-NB	-3.54	107.37	110.53
25	j	618	CLA	C3B-C4B-NB	-3.53	107.38	110.53
25	f	604	CLA	C3B-C4B-NB	-3.53	107.38	110.53
25	i	612	CLA	O2D-CGD-CBD	3.53	117.41	111.23
25	A	770	CLA	O2D-CGD-CBD	3.53	117.40	111.23
25	m	613	CLA	O2D-CGD-CBD	3.53	117.40	111.23
25	o	604	CLA	C3B-C4B-NB	-3.53	107.38	110.53
25	B	749	CLA	O2D-CGD-CBD	3.53	117.40	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	o	602	CLA	O2D-CGD-CBD	3.53	117.39	111.23
25	A	780	CLA	C3B-C4B-NB	-3.53	107.38	110.53
31	c	624	DD6	C3-C4-C5	3.52	130.73	123.52
25	e	610	CLA	C3B-C4B-NB	-3.52	107.39	110.53
31	n	621	DD6	C12-C11-C10	-3.52	117.11	122.82
25	A	761	CLA	C3B-C4B-NB	-3.52	107.39	110.53
25	a	604	CLA	O2D-CGD-CBD	3.52	117.39	111.23
25	A	782	CLA	O2D-CGD-CBD	3.52	117.38	111.23
25	g	602	CLA	O2D-CGD-CBD	3.52	117.38	111.23
25	j	610	CLA	C3B-C4B-NB	-3.52	107.39	110.53
25	k	604	CLA	C3B-C4B-NB	-3.52	107.39	110.53
29	A	788	BCR	C16-C15-C14	3.51	130.71	123.52
25	h	610	CLA	CMB-C2B-C1B	-3.51	120.07	125.42
25	i	604	CLA	C3B-C4B-NB	-3.51	107.40	110.53
25	i	611	CLA	C3B-C4B-NB	-3.50	107.40	110.53
25	B	779	CLA	C3B-C4B-NB	-3.50	107.40	110.53
25	e	602	CLA	C3B-C4B-NB	-3.50	107.41	110.53
25	a	601	CLA	O2D-CGD-CBD	3.50	117.34	111.23
25	A	766	CLA	C3B-C4B-NB	-3.49	107.41	110.53
25	n	610	CLA	C3B-C4B-NB	-3.49	107.41	110.53
31	i	621	DD6	C28-C27-C26	3.49	130.97	124.18
31	e	620	DD6	C12-C11-C10	-3.49	117.16	122.82
35	d	605	CHL	CAA-C2A-C3A	-3.49	103.58	113.00
35	d	607	CHL	CMA-C3A-C4A	-3.48	107.11	114.61
25	k	602	CLA	C3B-C4B-NB	-3.48	107.42	110.53
25	g	611	CLA	C3B-C4B-NB	-3.48	107.42	110.53
25	p	601	CLA	C3B-C4B-NB	-3.48	107.42	110.53
31	j	620	DD6	C25-C26-C27	-3.48	116.88	126.61
25	B	759	CLA	C3B-C4B-NB	-3.48	107.42	110.53
31	j	621	DD6	C25-C26-C27	-3.48	116.88	126.61
25	A	758	CLA	C3B-C4B-NB	-3.48	107.42	110.53
31	b	621	DD6	C28-C27-C26	3.47	130.94	124.18
25	B	777	CLA	O2D-CGD-CBD	3.47	117.30	111.23
25	A	777	CLA	O2A-CGA-CBA	3.47	122.42	111.83
25	B	776	CLA	C3B-C4B-NB	-3.47	107.44	110.53
25	h	604	CLA	C3B-C4B-NB	-3.47	107.44	110.53
35	d	608	CHL	OBD-CAD-CBD	-3.47	120.74	125.82
30	g	190	SQD	O7-S-C6	3.47	111.93	106.76
25	g	602	CLA	O2A-CGA-CBA	3.47	122.40	111.83
25	h	603	CLA	C3B-C4B-NB	-3.46	107.44	110.53
25	A	762	CLA	C3B-C4B-NB	-3.46	107.44	110.53
25	k	608	CLA	C3B-C4B-NB	-3.46	107.44	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	801	CLA	O2D-CGD-CBD	3.46	117.28	111.23
29	A	792	BCR	C34-C9-C10	-3.45	117.22	122.82
35	d	605	CHL	CMA-C3A-C4A	-3.45	107.17	114.61
25	A	798	CLA	C3B-C4B-NB	-3.45	107.45	110.53
25	A	801	CLA	C3B-C4B-NB	-3.45	107.45	110.53
25	A	782	CLA	C3B-C4B-NB	-3.45	107.45	110.53
25	f	608	CLA	C3B-C4B-NB	-3.44	107.46	110.53
25	k	611	CLA	C3B-C4B-NB	-3.44	107.46	110.53
25	B	749	CLA	C3B-C4B-NB	-3.44	107.46	110.53
25	m	610	CLA	C3B-C4B-NB	-3.44	107.46	110.53
25	g	613	CLA	C3B-C4B-NB	-3.44	107.46	110.53
31	m	621	DD6	C25-C26-C27	-3.44	116.99	126.61
25	A	773	CLA	C3B-C4B-NB	-3.44	107.46	110.53
25	l	604	CLA	C3B-C4B-NB	-3.44	107.46	110.53
35	e	606	CHL	CAA-C2A-C3A	-3.44	103.72	113.00
29	A	792	BCR	C37-C22-C21	-3.43	117.25	122.82
25	B	751	CLA	C3B-C4B-NB	-3.43	107.47	110.53
25	e	604	CLA	C3B-C4B-NB	-3.43	107.47	110.53
25	g	608	CLA	C3B-C4B-NB	-3.43	107.47	110.53
25	a	613	CLA	O2A-CGA-CBA	3.43	122.29	111.83
25	b	613	CLA	C3B-C4B-NB	-3.43	107.47	110.53
35	d	606	CHL	OBD-CAD-CBD	-3.43	120.80	125.82
25	j	604	CLA	C3B-C4B-NB	-3.43	107.47	110.53
25	f	602	CLA	C3B-C4B-NB	-3.43	107.47	110.53
25	h	603	CLA	O2D-CGD-CBD	3.42	117.22	111.23
25	a	604	CLA	C3B-C4B-NB	-3.42	107.47	110.53
25	a	609	CLA	C3B-C4B-NB	-3.42	107.47	110.53
31	m	621	DD6	C21-C20-C15	-3.42	116.67	122.30
25	B	748	CLA	C3B-C4B-NB	-3.42	107.48	110.53
25	l	608	CLA	C3B-C4B-NB	-3.42	107.48	110.53
25	B	768	CLA	O2A-CGA-CBA	3.42	122.25	111.83
25	B	750	CLA	C3B-C4B-NB	-3.42	107.48	110.53
31	n	623	DD6	C12-C11-C10	-3.41	117.28	122.82
25	c	601	CLA	C3B-C4B-NB	-3.41	107.48	110.53
31	F	4002	DD6	C12-C11-C10	-3.41	117.29	122.82
25	B	737	CLA	O2A-CGA-CBA	3.41	122.24	111.83
25	c	608	CLA	C3B-C4B-NB	-3.41	107.48	110.53
25	f	613	CLA	C3B-C4B-NB	-3.41	107.49	110.53
25	d	610	CLA	O2A-CGA-CBA	3.41	122.23	111.83
25	B	771	CLA	C3B-C4B-NB	-3.41	107.49	110.53
35	d	608	CHL	CAA-C2A-C3A	-3.41	103.79	113.00
25	A	763	CLA	C3B-C4B-NB	-3.41	107.49	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	m	613	CLA	C3B-C4B-NB	-3.41	107.49	110.53
25	A	775	CLA	C3B-C4B-NB	-3.40	107.49	110.53
25	a	611	CLA	C3B-C4B-NB	-3.40	107.49	110.53
25	e	605	CLA	C3B-C4B-NB	-3.40	107.50	110.53
25	c	606	CLA	C3B-C4B-NB	-3.40	107.50	110.53
29	B	766	BCR	C34-C9-C10	-3.40	117.31	122.82
25	d	609	CLA	O2A-CGA-CBA	3.40	122.19	111.83
35	d	606	CHL	CBC-CAC-C3C	-3.39	108.01	112.87
25	B	745	CLA	C3B-C4B-NB	-3.39	107.50	110.53
25	o	610	CLA	CMA-C3A-C2A	-3.39	108.45	116.23
25	B	775	CLA	O2D-CGD-CBD	3.39	117.16	111.23
25	A	784	CLA	C3B-C4B-NB	-3.39	107.50	110.53
25	A	752	CLA	O2D-CGD-O1D	-3.39	117.25	123.85
25	a	602	CLA	O2D-CGD-CBD	3.39	117.15	111.23
25	k	604	CLA	O2A-CGA-CBA	3.38	122.16	111.83
25	g	604	CLA	C3B-C4B-NB	-3.38	107.51	110.53
25	n	604	CLA	C3B-C4B-NB	-3.38	107.51	110.53
29	B	765	BCR	C34-C9-C10	-3.38	117.34	122.82
25	A	766	CLA	C1-C2-C3	3.38	131.74	126.20
25	A	776	CLA	C3B-C4B-NB	-3.38	107.51	110.53
25	k	609	CLA	C3B-C4B-NB	-3.38	107.51	110.53
25	j	611	CLA	C3B-C4B-NB	-3.38	107.51	110.53
25	B	740	CLA	C3B-C4B-NB	-3.38	107.52	110.53
29	A	788	BCR	C37-C22-C21	-3.38	117.34	122.82
25	c	609	CLA	O2A-CGA-CBA	3.38	122.13	111.83
31	c	621	DD6	C28-C27-C26	3.38	130.74	124.18
25	i	610	CLA	C3B-C4B-NB	-3.38	107.52	110.53
25	A	752	CLA	C3B-C4B-NB	-3.37	107.52	110.53
25	g	615	CLA	C3B-C4B-NB	-3.37	107.52	110.53
29	B	765	BCR	C37-C22-C21	-3.37	117.36	122.82
25	A	805	CLA	C3B-C4B-NB	-3.37	107.52	110.53
25	h	602	CLA	C3B-C4B-NB	-3.37	107.52	110.53
25	c	612	CLA	O2D-CGD-CBD	3.37	117.12	111.23
25	p	609	CLA	O2A-CGA-CBA	3.37	122.10	111.83
31	k	621	DD6	O1-C20-C19	3.37	116.65	113.49
25	a	601	CLA	C3B-C4B-NB	-3.37	107.53	110.53
25	m	604	CLA	C3B-C4B-NB	-3.37	107.53	110.53
25	l	613	CLA	O2D-CGD-CBD	3.36	117.11	111.23
25	o	602	CLA	C3B-C4B-NB	-3.36	107.53	110.53
25	c	602	CLA	C3B-C4B-NB	-3.36	107.53	110.53
25	n	612	CLA	C3B-C4B-NB	-3.36	107.53	110.53
25	a	619	CLA	C3B-C4B-NB	-3.36	107.53	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	m	608	CLA	C3B-C4B-NB	-3.36	107.53	110.53
25	j	608	CLA	O2A-CGA-CBA	3.36	122.07	111.83
25	d	612	CLA	C3B-C4B-NB	-3.36	107.53	110.53
25	b	608	CLA	C3B-C4B-NB	-3.35	107.54	110.53
25	n	604	CLA	O2A-CGA-CBA	3.35	122.06	111.83
25	b	610	CLA	C3B-C4B-NB	-3.35	107.54	110.53
25	j	618	CLA	O2A-CGA-CBA	3.35	122.06	111.83
31	n	620	DD6	O1-C20-C21	-3.35	111.31	115.05
25	B	783	CLA	C3B-C4B-NB	-3.35	107.54	110.53
25	d	613	CLA	C3B-C4B-NB	-3.34	107.55	110.53
25	i	608	CLA	C3B-C4B-NB	-3.34	107.55	110.53
31	i	621	DD6	C25-C26-C27	-3.34	117.27	126.61
25	j	609	CLA	C3B-C4B-NB	-3.34	107.55	110.53
35	d	606	CHL	CMA-C3A-C4A	-3.34	107.42	114.61
25	l	610	CLA	O2A-CGA-CBA	3.34	122.02	111.83
25	e	610	CLA	O2A-CGA-CBA	3.34	122.01	111.83
25	l	611	CLA	C3B-C4B-NB	-3.33	107.55	110.53
25	B	774	CLA	O2A-CGA-CBA	3.33	122.00	111.83
25	g	609	CLA	O2A-CGA-CBA	3.33	122.00	111.83
25	B	751	CLA	O2A-CGA-CBA	3.33	121.99	111.83
25	h	611	CLA	C3B-C4B-NB	-3.33	107.56	110.53
25	n	613	CLA	C3B-C4B-NB	-3.33	107.56	110.53
31	c	624	DD6	C24-C1-C2	3.33	124.25	119.01
25	k	618	CLA	C3B-C4B-NB	-3.33	107.56	110.53
25	b	602	CLA	O2A-CGA-CBA	3.33	121.99	111.83
25	o	602	CLA	O2A-CGA-CBA	3.33	121.98	111.83
25	d	610	CLA	C3B-C4B-NB	-3.33	107.56	110.53
25	g	614	CLA	C3B-C4B-NB	-3.33	107.56	110.53
25	c	611	CLA	C3B-C4B-NB	-3.33	107.56	110.53
25	c	609	CLA	C3B-C4B-NB	-3.33	107.56	110.53
25	B	770	CLA	C3B-C4B-NB	-3.32	107.56	110.53
25	e	603	CLA	C3B-C4B-NB	-3.32	107.56	110.53
25	c	602	CLA	O2D-CGD-CBD	3.32	117.04	111.23
25	h	609	CLA	C3B-C4B-NB	-3.32	107.57	110.53
25	A	771	CLA	O2A-CGA-CBA	3.32	121.96	111.83
25	A	765	CLA	C3B-C4B-NB	-3.32	107.57	110.53
25	i	601	CLA	O2A-CGA-CBA	3.32	121.95	111.83
25	A	772	CLA	C3B-C4B-NB	-3.32	107.57	110.53
25	l	613	CLA	C3B-C4B-NB	-3.31	107.57	110.53
31	a	620	DD6	O1-C20-C19	3.31	116.60	113.49
25	o	612	CLA	C3B-C4B-NB	-3.31	107.57	110.53
25	f	611	CLA	C3B-C4B-NB	-3.31	107.57	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	n	607	CLA	C3B-C4B-NB	-3.31	107.57	110.53
25	A	771	CLA	O2D-CGD-CBD	3.31	117.02	111.23
25	d	602	CLA	C3B-C4B-NB	-3.31	107.57	110.53
25	k	601	CLA	C3B-C4B-NB	-3.31	107.57	110.53
29	B	766	BCR	C37-C22-C21	-3.31	117.45	122.82
29	A	788	BCR	C34-C9-C10	-3.31	117.46	122.82
25	a	619	CLA	O2A-CGA-CBA	3.31	121.92	111.83
31	e	623	DD6	C-C1-C2	-3.31	117.46	122.82
25	h	618	CLA	C3B-C4B-NB	-3.31	107.58	110.53
25	A	774	CLA	C3B-C4B-NB	-3.31	107.58	110.53
25	c	612	CLA	C3B-C4B-NB	-3.31	107.58	110.53
25	B	773	CLA	C1-C2-C3	3.31	131.61	126.20
25	g	610	CLA	O2A-CGA-CBA	3.30	121.90	111.83
31	n	620	DD6	C41-C32-C31	3.29	116.43	110.52
25	B	742	CLA	C3B-C4B-NB	-3.29	107.59	110.53
25	i	612	CLA	C3B-C4B-NB	-3.29	107.59	110.53
25	i	609	CLA	C3B-C4B-NB	-3.29	107.59	110.53
25	o	609	CLA	C3B-C4B-NB	-3.29	107.59	110.53
25	B	781	CLA	O2A-CGA-CBA	3.29	121.87	111.83
25	f	609	CLA	C3B-C4B-NB	-3.29	107.59	110.53
25	p	609	CLA	C3B-C4B-NB	-3.29	107.59	110.53
31	c	621	DD6	C25-C26-C27	-3.29	117.41	126.61
25	A	784	CLA	O2A-CGA-CBA	3.29	121.87	111.83
25	e	602	CLA	O2D-CGD-CBD	3.29	116.98	111.23
25	b	602	CLA	C3B-C4B-NB	-3.29	107.59	110.53
30	j	200	SQD	O6-C1-C2	3.29	113.27	108.27
25	A	758	CLA	O2A-CGA-CBA	3.29	121.85	111.83
25	m	611	CLA	C3B-C4B-NB	-3.28	107.60	110.53
25	m	609	CLA	C3B-C4B-NB	-3.28	107.60	110.53
25	k	613	CLA	C3B-C4B-NB	-3.28	107.60	110.53
31	f	621	DD6	C21-C20-C15	-3.28	116.90	122.30
25	h	604	CLA	O2A-CGA-CBA	3.28	121.84	111.83
25	c	608	CLA	O2A-CGA-CBA	3.28	121.84	111.83
25	g	609	CLA	C3B-C4B-NB	-3.28	107.60	110.53
25	h	614	CLA	C3B-C4B-NB	-3.28	107.60	110.53
25	o	613	CLA	C3B-C4B-NB	-3.28	107.60	110.53
29	A	796	BCR	C29-C30-C25	3.28	115.20	110.44
30	c	245	SQD	O7-S-C6	3.28	111.65	106.76
25	f	602	CLA	O2A-CGA-CBA	3.28	121.83	111.83
31	F	4002	DD6	C4-C3-C2	3.27	130.22	123.52
31	J	4002	DD6	C37-C36-C35	3.27	120.44	114.42
35	c	607	CHL	OBD-CAD-CBD	-3.27	121.02	125.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	756	CLA	C3B-C4B-NB	-3.27	107.61	110.53
25	m	602	CLA	O2D-CGD-CBD	3.27	116.94	111.23
25	A	764	CLA	C3B-C4B-NB	-3.26	107.62	110.53
25	b	611	CLA	C3B-C4B-NB	-3.26	107.62	110.53
25	l	609	CLA	C3B-C4B-NB	-3.26	107.62	110.53
35	d	605	CHL	O1D-CGD-CBD	-3.26	119.77	124.72
31	n	623	DD6	C-C1-C2	-3.26	117.53	122.82
25	c	616	CLA	O2A-CGA-CBA	3.26	121.79	111.83
25	B	758	CLA	C3B-C4B-NB	-3.26	107.62	110.53
25	d	611	CLA	C3B-C4B-NB	-3.26	107.62	110.53
25	l	613	CLA	O2A-CGA-CBA	3.26	121.78	111.83
25	d	614	CLA	C3B-C4B-NB	-3.26	107.62	110.53
31	e	620	DD6	C24-C1-C2	3.26	124.14	119.01
31	n	621	DD6	C4-C3-C2	3.26	130.19	123.52
25	a	608	CLA	C3B-C4B-NB	-3.26	107.62	110.53
31	d	623	DD6	C21-C20-C15	-3.26	116.94	122.30
25	B	778	CLA	C3B-C4B-NB	-3.26	107.62	110.53
25	A	799	CLA	O2A-CGA-CBA	3.26	121.76	111.83
25	A	781	CLA	O2A-CGA-CBA	3.25	121.75	111.83
25	o	612	CLA	O2D-CGD-CBD	3.25	117.75	111.61
25	B	778	CLA	O2A-CGA-CBA	3.25	121.75	111.83
25	d	604	CLA	C3B-C4B-NB	-3.25	107.63	110.53
25	B	772	CLA	C3B-C4B-NB	-3.25	107.63	110.53
25	i	615	CLA	C3B-C4B-NB	-3.25	107.63	110.53
25	A	803	CLA	O2A-CGA-CBA	3.25	121.73	111.83
31	A	4002	DD6	C21-C20-C15	-3.25	116.96	122.30
25	f	612	CLA	O2D-CGD-CBD	3.24	116.90	111.23
31	p	621	DD6	C37-C36-C35	3.24	120.38	114.42
25	b	612	CLA	C3B-C4B-NB	-3.24	107.64	110.53
25	h	608	CLA	O2A-CGA-CBA	3.24	121.71	111.83
25	A	803	CLA	C4-C3-C5	-3.24	112.32	116.13
25	h	612	CLA	C3B-C4B-NB	-3.24	107.64	110.53
25	A	774	CLA	O2A-CGA-CBA	3.24	121.71	111.83
25	c	604	CLA	C3B-C4B-NB	-3.24	107.64	110.53
25	B	757	CLA	O2A-CGA-CBA	3.24	121.70	111.83
25	k	618	CLA	O2A-CGA-CBA	3.24	121.70	111.83
25	f	614	CLA	C3B-C4B-NB	-3.23	107.64	110.53
25	A	753	CLA	O2A-CGA-CBA	3.23	121.69	111.83
31	c	621	DD6	C41-C32-C31	3.23	116.32	110.52
25	i	610	CLA	O2A-CGA-CBA	3.23	121.69	111.83
25	n	603	CLA	C3B-C4B-NB	-3.23	107.64	110.53
31	e	623	DD6	C3-C4-C5	3.23	130.13	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	780	CLA	O2A-CGA-CBA	3.23	121.68	111.83
25	f	613	CLA	O2A-CGA-CBA	3.23	121.68	111.83
25	B	768	CLA	C3B-C4B-NB	-3.23	107.65	110.53
25	c	613	CLA	C3B-C4B-NB	-3.22	107.65	110.53
25	e	611	CLA	C3B-C4B-NB	-3.22	107.65	110.53
31	f	621	DD6	C41-C32-C31	3.22	116.30	110.52
25	b	603	CLA	C3B-C4B-NB	-3.22	107.65	110.53
25	c	616	CLA	C3B-C4B-NB	-3.22	107.65	110.53
25	h	601	CLA	C3B-C4B-NB	-3.22	107.65	110.53
35	d	608	CHL	CMA-C3A-C4A	-3.22	107.67	114.61
25	l	612	CLA	C3B-C4B-NB	-3.22	107.66	110.53
25	g	612	CLA	C3B-C4B-NB	-3.22	107.66	110.53
31	o	621	DD6	C28-C27-C26	3.22	130.44	124.18
25	a	609	CLA	O2A-CGA-CBA	3.22	121.65	111.83
25	A	791	CLA	O2A-CGA-CBA	3.21	121.62	111.83
25	i	602	CLA	O2D-CGD-O1D	-3.21	117.60	123.85
25	k	610	CLA	O2A-CGA-CBA	3.21	121.62	111.83
31	n	623	DD6	C8-C6-C5	3.21	124.06	119.01
31	J	4002	DD6	C21-C20-C15	-3.21	117.03	122.30
31	f	620	DD6	C41-C32-C31	3.21	116.27	110.52
25	g	613	CLA	O2A-CGA-CBA	3.20	121.61	111.83
25	B	756	CLA	O2A-CGA-CBA	3.20	121.61	111.83
31	h	620	DD6	C21-C20-C15	-3.20	117.03	122.30
25	b	609	CLA	C3B-C4B-NB	-3.20	107.67	110.53
25	l	601	CLA	C3B-C4B-NB	-3.20	107.67	110.53
31	i	621	DD6	O1-C20-C19	3.20	116.49	113.49
31	g	621	DD6	C37-C36-C35	3.20	120.31	114.42
25	B	754	CLA	C3B-C4B-NB	-3.20	107.67	110.53
25	k	612	CLA	C3B-C4B-NB	-3.20	107.67	110.53
31	d	623	DD6	C41-C32-C31	3.20	116.25	110.52
25	e	613	CLA	O2A-CGA-CBA	3.20	121.58	111.83
31	o	620	DD6	O1-C20-C19	3.20	116.49	113.49
25	e	612	CLA	C3B-C4B-NB	-3.20	107.68	110.53
25	i	601	CLA	C3B-C4B-NB	-3.20	107.68	110.53
31	l	620	DD6	C21-C20-C15	-3.19	117.04	122.30
31	g	620	DD6	C21-C20-C15	-3.19	117.05	122.30
25	B	752	CLA	C3B-C4B-NB	-3.19	107.68	110.53
31	J	4002	DD6	C41-C32-C31	3.19	116.24	110.52
31	o	620	DD6	C41-C32-C31	3.19	116.24	110.52
31	m	620	DD6	C37-C36-C35	3.19	120.28	114.42
25	k	608	CLA	O2A-CGA-CBA	3.19	121.55	111.83
31	o	620	DD6	C37-C36-C35	3.18	120.28	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	604	CLA	C3B-C4B-NB	-3.18	107.69	110.53
25	j	602	CLA	O2A-CGA-CBA	3.18	121.54	111.83
31	k	621	DD6	C28-C27-C26	3.18	130.37	124.18
25	n	609	CLA	C3B-C4B-NB	-3.18	107.69	110.53
25	h	601	CLA	O2A-CGA-CBA	3.18	121.53	111.83
31	j	621	DD6	C41-C32-C31	3.18	116.22	110.52
25	j	610	CLA	O2A-CGA-CBA	3.18	121.53	111.83
31	p	621	DD6	C41-C32-C31	3.18	116.22	110.52
25	i	614	CLA	C3B-C4B-NB	-3.18	107.69	110.53
25	b	601	CLA	C3B-C4B-NB	-3.18	107.69	110.53
31	f	621	DD6	C37-C36-C35	3.18	120.26	114.42
31	j	620	DD6	C28-C27-C26	3.18	130.36	124.18
31	m	620	DD6	C28-C27-C26	3.18	130.35	124.18
25	A	769	CLA	O2D-CGD-CBD	3.17	116.78	111.23
25	J	101	CLA	C3B-C4B-NB	-3.17	107.70	110.53
25	a	612	CLA	C3B-C4B-NB	-3.17	107.70	110.53
25	k	610	CLA	C3B-C4B-NB	-3.17	107.70	110.53
25	m	603	CLA	O2A-CGA-CBA	3.17	121.50	111.83
31	d	621	DD6	C41-C32-C31	3.17	116.20	110.52
31	m	621	DD6	C28-C27-C26	3.17	130.34	124.18
25	a	619	CLA	C1-C2-C3	3.17	131.39	126.20
25	A	793	CLA	C3B-C4B-NB	-3.17	107.70	110.53
25	g	601	CLA	O2D-CGD-CBD	3.17	116.77	111.23
25	A	800	CLA	C3B-C4B-NB	-3.17	107.70	110.53
30	j	200	SQD	C3-C4-C5	3.17	115.97	110.23
25	A	803	CLA	C3B-C4B-NB	-3.17	107.70	110.53
29	B	762	BCR	C15-C14-C13	-3.17	122.84	127.28
25	e	604	CLA	O2A-CGA-CBA	3.16	121.48	111.83
25	B	755	CLA	C3B-C4B-NB	-3.16	107.71	110.53
31	A	4002	DD6	C41-C32-C31	3.16	116.19	110.52
35	e	606	CHL	CBC-CAC-C3C	-3.16	108.35	112.87
31	e	621	DD6	C41-C32-C31	3.16	116.19	110.52
31	A	4008	DD6	C37-C36-C35	3.16	120.23	114.42
25	A	769	CLA	C3B-C4B-NB	-3.16	107.71	110.53
31	m	621	DD6	C41-C32-C31	3.16	116.18	110.52
25	n	605	CLA	C3B-C4B-NB	-3.16	107.71	110.53
31	k	620	DD6	C41-C32-C31	3.16	116.18	110.52
31	o	620	DD6	C28-C27-C26	3.16	130.32	124.18
31	f	620	DD6	C37-C36-C35	3.16	120.23	114.42
25	a	603	CLA	C3B-C4B-NB	-3.15	107.71	110.53
25	A	780	CLA	O2A-CGA-CBA	3.15	121.45	111.83
25	j	609	CLA	O2A-CGA-CBA	3.15	121.45	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	779	CLA	C3B-C4B-NB	-3.15	107.72	110.53
31	l	621	DD6	C28-C27-C26	3.15	130.30	124.18
25	d	601	CLA	O2A-CGA-CBA	3.15	121.43	111.83
25	n	603	CLA	O2A-CGA-CBA	3.15	121.43	111.83
31	n	620	DD6	C37-C36-C35	3.14	120.20	114.42
31	i	620	DD6	C21-C20-C15	-3.14	117.13	122.30
31	p	621	DD6	C21-C20-C15	-3.14	117.13	122.30
31	j	620	DD6	C37-C36-C35	3.14	120.20	114.42
25	k	603	CLA	C3B-C4B-NB	-3.14	107.73	110.53
31	k	620	DD6	C21-C20-C15	-3.14	117.13	122.30
25	A	782	CLA	O2A-CGA-CBA	3.14	121.41	111.83
31	j	621	DD6	C28-C27-C26	3.14	130.28	124.18
31	h	620	DD6	C41-C32-C31	3.14	116.15	110.52
31	c	623	DD6	O1-C20-C21	-3.14	111.54	115.05
25	h	609	CLA	O2A-CGA-CBA	3.14	121.40	111.83
25	c	610	CLA	C3B-C4B-NB	-3.14	107.73	110.53
31	g	620	DD6	C41-C32-C31	3.14	116.14	110.52
31	i	621	DD6	C37-C36-C35	3.14	120.19	114.42
31	A	4008	DD6	C41-C32-C31	3.14	116.14	110.52
25	e	602	CLA	O2A-CGA-CBA	3.13	121.39	111.83
25	B	772	CLA	O2A-CGA-CBA	3.13	121.39	111.83
31	l	620	DD6	C41-C32-C31	3.13	116.14	110.52
29	B	765	BCR	C16-C15-C14	3.13	129.93	123.52
25	c	604	CLA	O2A-CGA-CBA	3.13	121.38	111.83
25	g	618	CLA	C3B-C4B-NB	-3.13	107.74	110.53
25	l	602	CLA	C1-C2-C3	3.13	131.32	126.20
25	j	601	CLA	C3B-C4B-NB	-3.13	107.74	110.53
25	a	608	CLA	O2A-CGA-CBA	3.13	121.37	111.83
25	l	614	CLA	C3B-C4B-NB	-3.13	107.74	110.53
25	l	609	CLA	O2A-CGA-CBA	3.13	121.36	111.83
25	k	615	CLA	C3B-C4B-NB	-3.13	107.74	110.53
31	b	620	DD6	C37-C36-C35	3.12	120.16	114.42
25	B	776	CLA	O2A-CGA-CBA	3.12	121.36	111.83
25	B	777	CLA	O2A-CGA-CBA	3.12	121.36	111.83
31	e	621	DD6	C37-C36-C35	3.12	120.16	114.42
31	o	621	DD6	C41-C32-C31	3.12	116.12	110.52
25	A	776	CLA	O2A-CGA-CBA	3.12	121.35	111.83
31	b	621	DD6	C25-C26-C27	-3.12	117.88	126.61
31	o	621	DD6	C37-C36-C35	3.12	120.15	114.42
25	l	602	CLA	O2D-CGD-CBD	3.12	116.68	111.23
25	B	736	CLA	C3B-C4B-NB	-3.12	107.75	110.53
25	A	798	CLA	O2A-CGA-CBA	3.11	121.33	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	4008	DD6	C21-C20-C15	-3.11	117.18	122.30
25	j	611	CLA	O2A-CGA-CBA	3.11	121.33	111.83
25	c	614	CLA	C3B-C4B-NB	-3.11	107.75	110.53
31	a	620	DD6	C41-C32-C31	3.11	116.09	110.52
25	A	778	CLA	C3B-C4B-NB	-3.11	107.76	110.53
35	d	607	CHL	CBC-CAC-C3C	-3.11	108.42	112.87
25	B	748	CLA	O2A-CGA-CBA	3.11	121.31	111.83
31	c	620	DD6	C41-C32-C31	3.11	116.09	110.52
31	h	621	DD6	C37-C36-C35	3.10	120.13	114.42
25	m	612	CLA	C3B-C4B-NB	-3.10	107.76	110.53
31	g	620	DD6	C37-C36-C35	3.10	120.12	114.42
31	k	621	DD6	C41-C32-C31	3.10	116.08	110.52
25	e	609	CLA	C3B-C4B-NB	-3.10	107.76	110.53
25	o	608	CLA	C3B-C4B-NB	-3.10	107.76	110.53
31	l	621	DD6	C41-C32-C31	3.10	116.08	110.52
25	B	746	CLA	O2A-CGA-CBA	3.10	121.28	111.83
25	f	601	CLA	C3B-C4B-NB	-3.10	107.76	110.53
25	B	752	CLA	O2A-CGA-CBA	3.10	121.28	111.83
30	j	200	SQD	O9-S-C6	3.10	111.38	106.76
25	d	603	CLA	C3B-C4B-NB	-3.10	107.77	110.53
31	n	621	DD6	C24-C1-C2	3.10	123.88	119.01
31	i	625	DD6	C28-C27-C26	3.10	130.20	124.18
25	h	601	CLA	O1D-CGD-CBD	-3.10	118.41	124.52
31	k	621	DD6	C37-C36-C35	3.09	120.11	114.42
25	A	804	CLA	C3B-C4B-NB	-3.09	107.77	110.53
31	i	625	DD6	C37-C36-C35	3.09	120.10	114.42
31	i	621	DD6	C41-C32-C31	3.09	116.06	110.52
25	o	602	CLA	O1D-CGD-CBD	-3.09	118.43	124.52
25	A	752	CLA	O2A-CGA-CBA	3.09	121.25	111.83
31	i	625	DD6	C41-C32-C31	3.08	116.05	110.52
31	h	620	DD6	C28-C27-C26	3.08	130.18	124.18
25	B	741	CLA	C3B-C4B-NB	-3.08	107.78	110.53
31	o	620	DD6	C21-C20-C15	-3.08	117.23	122.30
25	m	609	CLA	O2A-CGA-CBA	3.08	121.23	111.83
25	A	761	CLA	O2A-CGA-CBA	3.08	121.23	111.83
25	B	753	CLA	O2A-CGA-CBA	3.08	121.23	111.83
25	c	603	CLA	O2A-CGA-CBA	3.08	121.22	111.83
31	j	620	DD6	C41-C32-C31	3.08	116.04	110.52
31	h	621	DD6	C28-C27-C26	3.07	130.16	124.18
25	l	602	CLA	O2A-CGA-CBA	3.07	121.21	111.83
31	m	620	DD6	C41-C32-C31	3.07	116.03	110.52
31	c	623	DD6	C37-C36-C35	3.07	120.07	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	c	621	DD6	C40-C32-C31	-3.07	105.01	110.52
25	e	601	CLA	C3B-C4B-NB	-3.07	107.79	110.53
31	n	620	DD6	C21-C20-C15	-3.07	117.25	122.30
25	B	747	CLA	C3B-C4B-NB	-3.07	107.79	110.53
31	d	620	DD6	C41-C32-C31	3.07	116.02	110.52
25	d	602	CLA	O2A-CGA-CBA	3.07	121.19	111.83
25	A	765	CLA	O2A-CGA-CBA	3.07	121.18	111.83
31	g	621	DD6	C41-C32-C31	3.06	116.02	110.52
31	a	621	DD6	C37-C36-C35	3.06	120.05	114.42
35	d	608	CHL	C1A-CHA-C4D	3.06	124.09	118.98
31	b	620	DD6	O1-C20-C21	-3.06	111.63	115.05
25	A	763	CLA	O2A-CGA-CBA	3.06	121.16	111.83
31	a	620	DD6	C28-C27-C26	3.06	130.12	124.18
25	B	773	CLA	O2A-CGA-CBA	3.05	121.15	111.83
31	c	620	DD6	C28-C27-C26	3.05	130.12	124.18
25	B	739	CLA	C1-C2-C3	3.05	131.20	126.20
25	g	601	CLA	C3B-C4B-NB	-3.05	107.81	110.53
31	j	620	DD6	C21-C20-C15	-3.05	117.28	122.30
31	a	621	DD6	C41-C32-C31	3.05	115.99	110.52
25	A	797	CLA	O2A-CGA-CBA	3.05	121.14	111.83
25	i	615	CLA	O2A-CGA-CBA	3.05	121.14	111.83
25	A	770	CLA	C3B-C4B-NB	-3.05	107.81	110.53
31	e	620	DD6	C4-C3-C2	3.05	129.76	123.52
31	i	620	DD6	C41-C32-C31	3.05	115.99	110.52
25	b	605	CLA	C3B-C4B-NB	-3.05	107.81	110.53
30	j	200	SQD	O7-S-C6	3.05	111.31	106.76
31	d	621	DD6	C21-C20-C15	-3.05	117.29	122.30
25	A	794	CLA	O2A-CGA-CBA	3.04	121.12	111.83
25	c	602	CLA	O2A-CGA-CBA	3.04	121.11	111.83
31	c	620	DD6	C37-C36-C35	3.04	120.01	114.42
31	n	623	DD6	C13-C11-C10	3.04	123.79	119.01
29	B	766	BCR	C15-C16-C17	3.04	129.74	123.52
31	i	620	DD6	C28-C27-C26	3.04	130.09	124.18
31	i	620	DD6	C37-C36-C35	3.04	120.01	114.42
25	k	613	CLA	O2A-CGA-CBA	3.04	121.10	111.83
25	B	749	CLA	O2A-CGA-CBA	3.04	121.10	111.83
25	n	610	CLA	CMA-C3A-C2A	-3.04	109.27	116.23
25	B	775	CLA	O2A-CGA-CBA	3.04	121.09	111.83
25	b	602	CLA	O1D-CGD-CBD	-3.04	118.53	124.52
25	m	603	CLA	C3B-C4B-NB	-3.04	107.82	110.53
25	A	807	CLA	O2A-CGA-CBA	3.03	121.09	111.83
25	l	603	CLA	C3B-C4B-NB	-3.03	107.82	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	f	615	CLA	C3B-C4B-NB	-3.03	107.82	110.53
25	j	612	CLA	O2A-CGA-CBA	3.03	121.08	111.83
31	o	621	DD6	C21-C20-C15	-3.03	117.31	122.30
31	h	621	DD6	C21-C20-C15	-3.03	117.31	122.30
25	j	604	CLA	O2A-CGA-CBA	3.03	121.08	111.83
31	b	621	DD6	C21-C20-C15	-3.03	117.32	122.30
25	c	610	CLA	O2A-CGA-CBA	3.03	121.07	111.83
25	k	609	CLA	O2A-CGA-CBA	3.03	121.07	111.83
25	A	799	CLA	O2D-CGD-O1D	-3.03	117.96	123.85
31	h	620	DD6	C37-C36-C35	3.03	119.98	114.42
31	f	621	DD6	O1-C20-C21	-3.03	111.67	115.05
31	h	621	DD6	C41-C32-C31	3.03	115.94	110.52
25	j	612	CLA	C1-C2-C3	3.02	131.15	126.20
31	a	620	DD6	C37-C36-C35	3.02	119.98	114.42
31	d	620	DD6	C21-C20-C15	-3.02	117.33	122.30
25	c	603	CLA	C1-C2-C3	3.02	131.14	126.20
31	j	621	DD6	O1-C20-C19	3.02	116.32	113.49
25	B	782	CLA	O2A-CGA-CBA	3.02	121.03	111.83
31	l	621	DD6	C21-C20-C15	-3.01	117.34	122.30
31	e	620	DD6	C-C1-C2	-3.01	117.93	122.82
31	f	620	DD6	C28-C27-C26	3.01	130.04	124.18
25	A	804	CLA	O2A-CGA-CBA	3.01	121.02	111.83
25	e	608	CLA	O2A-CGA-CBA	3.01	121.02	111.83
25	c	602	CLA	C12-C11-C10	-3.01	102.27	113.62
31	j	621	DD6	C21-C20-C15	-3.01	117.34	122.30
25	h	615	CLA	C3B-C4B-NB	-3.01	107.84	110.53
35	d	606	CHL	C1A-CHA-C4D	3.01	124.00	118.98
25	B	783	CLA	O2A-CGA-CBA	3.01	121.00	111.83
31	k	620	DD6	C28-C27-C26	3.01	130.03	124.18
25	a	610	CLA	O2A-CGA-CBA	3.01	121.00	111.83
25	A	762	CLA	O2A-CGA-CBA	3.00	121.00	111.83
31	c	623	DD6	C41-C32-C31	3.00	115.90	110.52
25	A	768	CLA	O2A-CGA-CBA	3.00	120.98	111.83
35	d	605	CHL	C1-C2-C3	3.00	131.62	126.76
31	d	620	DD6	C28-C27-C26	3.00	130.01	124.18
25	B	785	CLA	C3B-C4B-NB	-3.00	107.85	110.53
31	k	620	DD6	C37-C36-C35	3.00	119.93	114.42
25	B	755	CLA	O2A-CGA-CBA	3.00	120.98	111.83
25	m	602	CLA	O2A-CGA-CBA	2.99	120.97	111.83
25	A	775	CLA	O2A-CGA-CBA	2.99	120.97	111.83
31	g	620	DD6	C3-C2-C1	-2.99	123.08	127.28
25	g	601	CLA	O1D-CGD-CBD	-2.99	118.62	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	f	610	CLA	O2A-CGA-CBA	2.99	120.96	111.83
31	g	621	DD6	C21-C20-C15	-2.99	117.38	122.30
31	b	621	DD6	C37-C36-C35	2.99	119.92	114.42
31	d	620	DD6	C37-C36-C35	2.99	119.92	114.42
25	j	603	CLA	C3B-C4B-NB	-2.99	107.86	110.53
25	o	601	CLA	C3B-C4B-NB	-2.99	107.86	110.53
25	c	613	CLA	O2A-CGA-CBA	2.99	120.95	111.83
31	b	620	DD6	C28-C27-C26	2.99	129.99	124.18
29	B	762	BCR	C2-C1-C6	2.99	114.78	110.44
25	b	612	CLA	O2A-CGA-CBA	2.99	120.94	111.83
25	i	602	CLA	O2A-CGA-CBA	2.98	120.94	111.83
31	a	621	DD6	C28-C27-C26	2.98	129.98	124.18
25	h	610	CLA	O2A-CGA-O1A	-2.98	116.17	123.63
25	B	758	CLA	O2A-CGA-CBA	2.98	120.93	111.83
25	A	757	CLA	C3B-C4B-NB	-2.98	107.87	110.53
25	A	771	CLA	C3B-C4B-NB	-2.98	107.87	110.53
31	l	621	DD6	C37-C36-C35	2.98	119.90	114.42
30	A	795	SQD	O9-S-C6	2.98	111.20	106.76
31	a	620	DD6	C21-C20-C15	-2.98	117.40	122.30
25	A	770	CLA	O2A-CGA-CBA	2.98	120.92	111.83
25	f	613	CLA	C12-C11-C10	-2.98	102.40	113.62
25	J	101	CLA	O2A-CGA-CBA	2.98	120.91	111.83
31	n	620	DD6	C28-C27-C26	2.98	129.97	124.18
25	A	808	CLA	O2A-CGA-CBA	2.98	120.91	111.83
25	d	604	CLA	O2A-CGA-CBA	2.98	120.91	111.83
25	B	741	CLA	O2A-CGA-CBA	2.97	120.90	111.83
30	A	795	SQD	O7-S-C6	2.97	111.19	106.76
25	b	608	CLA	CMA-C3A-C2A	-2.97	109.43	116.23
31	g	621	DD6	C28-C27-C26	2.96	129.94	124.18
31	f	620	DD6	C21-C20-C15	-2.96	117.42	122.30
31	j	620	DD6	C40-C32-C31	-2.96	105.21	110.52
31	e	621	DD6	C28-C27-C26	2.96	129.93	124.18
31	b	620	DD6	C41-C32-C31	2.96	115.82	110.52
31	c	624	DD6	C-C1-C2	-2.96	118.03	122.82
25	A	765	CLA	C1-C2-C3	2.96	131.04	126.20
25	j	615	CLA	C3B-C4B-NB	-2.96	107.89	110.53
25	A	759	CLA	O2A-CGA-CBA	2.96	120.84	111.83
25	B	776	CLA	C12-C11-C10	-2.95	102.49	113.62
31	c	623	DD6	C28-C27-C26	2.95	129.92	124.18
31	n	623	DD6	C7-C6-C5	-2.95	118.03	122.82
25	p	610	CLA	C3B-C4B-NB	-2.95	107.89	110.53
35	d	607	CHL	C1A-CHA-C4D	2.95	123.91	118.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	799	CLA	O1D-CGD-CBD	-2.95	118.70	124.52
25	B	739	CLA	O2A-CGA-CBA	2.95	120.83	111.83
35	d	605	CHL	O2A-CGA-CBA	2.95	120.83	111.83
25	c	603	CLA	C3B-C4B-NB	-2.95	107.90	110.53
31	h	621	DD6	C40-C32-C31	-2.95	105.24	110.52
25	h	601	CLA	O2D-CGD-CBD	2.95	116.38	111.23
25	n	602	CLA	C12-C11-C10	-2.95	102.51	113.62
31	c	620	DD6	C21-C20-C15	-2.95	117.45	122.30
27	h	189	LHG	O7-C7-C8	2.95	117.86	111.48
29	A	796	BCR	C2-C1-C6	2.95	114.72	110.44
28	B	761	PQN	C2M-C2-C1	-2.95	111.25	116.68
31	e	623	DD6	C8-C6-C5	2.95	123.64	119.01
31	l	620	DD6	C28-C27-C26	2.95	129.91	124.18
31	d	623	DD6	C37-C36-C35	2.95	119.84	114.42
25	f	602	CLA	C12-C11-C10	-2.95	102.52	113.62
31	p	621	DD6	C28-C27-C26	2.94	129.90	124.18
25	B	782	CLA	C3B-C4B-NB	-2.94	107.90	110.53
25	a	601	CLA	O2A-CGA-CBA	2.94	120.81	111.83
25	j	614	CLA	C3B-C4B-NB	-2.94	107.90	110.53
30	j	200	SQD	C1-O5-C5	-2.94	107.98	113.72
35	d	607	CHL	O1D-CGD-CBD	-2.94	120.26	124.72
31	d	621	DD6	C28-C27-C26	2.94	129.90	124.18
31	A	4008	DD6	C28-C27-C26	2.94	129.89	124.18
31	d	623	DD6	O1-C20-C21	-2.94	111.77	115.05
30	A	795	SQD	O6-C1-C2	2.94	112.73	108.27
25	k	614	CLA	C3B-C4B-NB	-2.93	107.91	110.53
25	h	610	CLA	C3B-C4B-NB	-2.93	107.91	110.53
31	f	620	DD6	O1-C20-C21	-2.93	111.77	115.05
25	h	612	CLA	O2A-CGA-CBA	2.93	120.77	111.83
25	B	770	CLA	O2A-CGA-CBA	2.93	120.77	111.83
25	j	601	CLA	O2A-CGA-CBA	2.93	120.76	111.83
25	B	771	CLA	O2A-CGA-CBA	2.93	120.76	111.83
25	p	608	CLA	C3B-C4B-NB	-2.93	107.92	110.53
31	J	4002	DD6	C40-C32-C31	-2.93	105.27	110.52
31	m	620	DD6	C21-C20-C15	-2.93	117.49	122.30
31	J	4002	DD6	C28-C27-C26	2.93	129.87	124.18
25	d	610	CLA	C12-C11-C10	-2.92	102.60	113.62
25	e	609	CLA	O2A-CGA-CBA	2.92	120.75	111.83
25	p	603	CLA	C3B-C4B-NB	-2.92	107.92	110.53
35	c	607	CHL	O1D-CGD-CBD	-2.92	120.29	124.72
25	B	779	CLA	O2A-CGA-CBA	2.92	120.74	111.83
25	A	755	CLA	O2A-CGA-CBA	2.92	120.74	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	f	603	CLA	C3B-C4B-NB	-2.92	107.92	110.53
31	n	621	DD6	C-C1-C2	-2.92	118.09	122.82
25	A	755	CLA	C1-C2-C3	2.92	130.98	126.20
31	l	620	DD6	C37-C36-C35	2.92	119.78	114.42
31	i	620	DD6	C40-C32-C31	-2.92	105.29	110.52
25	l	609	CLA	C1-C2-C3	2.91	130.97	126.20
35	d	607	CHL	C1C-CHC-C4B	2.91	126.49	116.07
35	d	605	CHL	CHA-C1A-C2A	-2.91	126.47	133.31
25	c	613	CLA	C1-C2-C3	2.91	130.96	126.20
30	j	200	SQD	O48-C23-C24	2.91	120.69	111.83
35	d	607	CHL	OBD-CAD-CBD	-2.90	121.56	125.82
25	A	801	CLA	O2A-CGA-CBA	2.90	120.68	111.83
31	e	623	DD6	C7-C6-C5	-2.90	118.11	122.82
31	e	620	DD6	C3-C4-C5	2.90	129.45	123.52
25	A	783	CLA	O2A-CGA-CBA	2.90	120.68	111.83
25	c	602	CLA	O1D-CGD-CBD	-2.89	118.81	124.52
28	B	761	PQN	C6-C5-C4	-2.89	115.87	120.10
25	l	602	CLA	C12-C11-C10	-2.89	102.72	113.62
25	B	750	CLA	O2A-CGA-CBA	2.89	120.63	111.83
27	g	189	LHG	O7-C7-C8	2.88	117.72	111.48
25	d	604	CLA	C1-C2-C3	2.88	130.92	126.20
29	A	788	BCR	C1-C6-C5	-2.88	118.70	122.64
29	A	792	BCR	C15-C16-C17	2.88	129.41	123.52
31	m	621	DD6	C37-C36-C35	2.88	119.71	114.42
31	f	621	DD6	C28-C27-C26	2.88	129.78	124.18
25	B	748	CLA	C12-C11-C10	-2.88	102.78	113.62
29	A	792	BCR	C36-C18-C17	-2.88	118.16	122.82
35	d	605	CHL	C1A-CHA-C4D	2.87	123.77	118.98
31	e	623	DD6	C13-C11-C10	2.87	123.53	119.01
34	e	205	DGD	O6D-C1D-O3G	-2.87	103.27	110.04
29	A	792	BCR	C12-C13-C14	2.86	123.51	119.01
31	b	620	DD6	C40-C32-C31	-2.86	105.39	110.52
30	c	245	SQD	O9-S-C6	2.86	111.03	106.76
25	A	808	CLA	C3B-C4B-NB	-2.86	107.98	110.53
25	j	612	CLA	C3B-C4B-NB	-2.86	107.98	110.53
31	o	621	DD6	C40-C32-C31	-2.86	105.40	110.52
31	c	620	DD6	C40-C32-C31	-2.86	105.40	110.52
25	i	602	CLA	O1D-CGD-CBD	-2.86	118.88	124.52
27	m	182	LHG	O7-C7-C8	2.86	117.66	111.48
31	g	621	DD6	C40-C32-C31	-2.86	105.40	110.52
31	c	621	DD6	C37-C36-C35	2.85	119.67	114.42
31	m	620	DD6	C40-C32-C31	-2.85	105.41	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	766	CLA	O2A-CGA-CBA	2.85	120.53	111.83
31	e	621	DD6	C21-C20-C15	-2.85	117.61	122.30
25	i	608	CLA	O2A-CGA-CBA	2.85	120.52	111.83
25	A	808	CLA	C1-C2-C3	2.85	130.86	126.20
25	A	760	CLA	O2A-CGA-CBA	2.85	120.52	111.83
30	g	190	SQD	O48-C23-C24	2.85	120.51	111.83
31	d	623	DD6	C28-C27-C26	2.85	129.71	124.18
31	g	620	DD6	C32-C33-C34	-2.84	107.36	113.59
31	c	624	DD6	C8-C6-C5	2.84	123.48	119.01
35	d	605	CHL	OMC-CMC-C2C	-2.84	120.18	125.12
31	j	621	DD6	C40-C32-C31	-2.84	105.43	110.52
35	d	608	CHL	C3C-C4C-NC	-2.84	107.71	114.65
29	A	792	BCR	C29-C30-C25	2.84	114.56	110.44
31	c	624	DD6	C7-C6-C5	-2.84	118.22	122.82
31	j	621	DD6	C37-C36-C35	2.84	119.64	114.42
27	h	190	LHG	O7-C7-C8	2.83	117.61	111.48
25	n	606	CLA	C3B-C4B-NB	-2.83	108.00	110.53
31	g	621	DD6	O1-C20-C19	2.83	116.14	113.49
31	d	621	DD6	C37-C36-C35	2.82	119.61	114.42
31	a	621	DD6	C21-C20-C15	-2.82	117.66	122.30
31	l	621	DD6	C40-C32-C31	-2.82	105.46	110.52
28	d	223	PQN	C6-C5-C4	-2.82	115.98	120.10
29	A	792	BCR	C35-C13-C14	-2.82	118.25	122.82
25	f	611	CLA	O1D-CGD-CBD	-2.82	118.95	124.52
35	d	608	CHL	C1C-CHC-C4B	2.82	126.16	116.07
29	B	762	BCR	C29-C30-C25	2.82	114.53	110.44
25	A	764	CLA	O2A-CGA-CBA	2.82	120.42	111.83
25	n	602	CLA	O2A-CGA-CBA	2.82	120.42	111.83
25	B	738	CLA	O2A-CGA-CBA	2.82	120.42	111.83
31	A	4008	DD6	C9-C8-C6	2.81	134.08	126.36
27	A	786	LHG	O7-C7-C8	2.81	117.56	111.48
27	i	194	LHG	O7-C7-C8	2.81	117.56	111.48
35	d	606	CHL	O1D-CGD-CBD	-2.81	120.46	124.72
31	b	621	DD6	C40-C32-C31	-2.81	105.49	110.52
25	A	805	CLA	C2A-C1A-CHA	2.81	128.74	123.87
31	i	621	DD6	C40-C32-C31	-2.81	105.49	110.52
25	B	745	CLA	O2A-CGA-CBA	2.81	120.39	111.83
25	a	603	CLA	O2A-CGA-CBA	2.80	120.39	111.83
25	k	602	CLA	O2A-CGA-CBA	2.80	120.38	111.83
31	h	620	DD6	C40-C32-C31	-2.80	105.50	110.52
25	e	613	CLA	C1-C2-C3	2.80	130.78	126.20
35	e	606	CHL	C1A-CHA-C4D	2.80	123.65	118.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	d	237	LHG	O7-C7-C8	2.80	117.54	111.48
31	k	620	DD6	C40-C32-C31	-2.80	105.50	110.52
31	f	620	DD6	C40-C32-C31	-2.79	105.51	110.52
25	B	771	CLA	C1-C2-C3	2.79	130.78	126.20
25	m	603	CLA	O1D-CGD-CBD	-2.79	119.01	124.52
29	B	765	BCR	C15-C16-C17	2.79	129.23	123.52
25	n	608	CLA	CMA-C3A-C2A	-2.79	109.83	116.23
25	B	760	CLA	C3B-C4B-NB	-2.79	108.04	110.53
25	b	612	CLA	C1-C2-C3	2.79	130.76	126.20
25	h	603	CLA	O1D-CGD-CBD	-2.79	119.02	124.52
35	c	607	CHL	O2A-CGA-CBA	2.78	120.33	111.83
31	i	620	DD6	C32-C33-C34	-2.78	107.49	113.59
28	B	761	PQN	C9-C10-C1	-2.78	116.03	120.10
25	e	609	CLA	C1-C2-C3	2.78	130.76	126.20
31	b	621	DD6	C41-C32-C31	2.78	115.51	110.52
25	A	775	CLA	C1-C2-C3	2.78	130.75	126.20
25	B	784	CLA	O2A-CGA-CBA	2.78	120.31	111.83
31	b	621	DD6	O1-C20-C19	2.78	116.10	113.49
25	B	771	CLA	O1D-CGD-CBD	-2.78	119.04	124.52
27	c	243	LHG	O7-C7-C8	2.78	117.49	111.48
31	k	621	DD6	C21-C20-C15	-2.78	117.73	122.30
31	m	621	DD6	C40-C32-C31	-2.78	105.54	110.52
25	l	602	CLA	O1D-CGD-CBD	-2.78	119.04	124.52
29	A	788	BCR	C35-C13-C14	-2.78	118.32	122.82
25	A	783	CLA	C1-C2-C3	2.77	130.74	126.20
35	d	605	CHL	C1C-CHC-C4B	2.77	125.99	116.07
35	d	605	CHL	OBD-CAD-CBD	-2.77	121.76	125.82
25	B	771	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
29	B	765	BCR	C35-C13-C14	-2.77	118.33	122.82
28	A	785	PQN	C6-C5-C4	-2.77	116.06	120.10
31	c	623	DD6	C40-C32-C31	-2.76	105.56	110.52
31	c	621	DD6	C21-C20-C15	-2.76	117.75	122.30
29	A	792	BCR	C19-C18-C17	2.76	123.36	119.01
29	A	787	BCR	C2-C1-C6	2.76	114.45	110.44
30	c	245	SQD	O48-C23-C24	2.76	120.26	111.83
31	i	625	DD6	C21-C20-C15	-2.76	117.76	122.30
27	A	756	LHG	O7-C7-C8	2.76	117.45	111.48
29	A	788	BCR	C12-C13-C14	2.76	123.35	119.01
25	B	756	CLA	O1D-CGD-CBD	-2.76	119.08	124.52
29	A	790	BCR	C2-C1-C6	2.76	114.45	110.44
25	c	619	CLA	CMA-C3A-C2A	-2.75	109.92	116.23
31	e	620	DD6	C7-C6-C5	-2.75	118.36	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	621	DD6	O1-C20-C15	-2.75	56.75	58.93
31	e	621	DD6	C32-C33-C34	-2.74	107.58	113.59
25	A	800	CLA	O2A-CGA-CBA	2.74	120.20	111.83
31	a	621	DD6	C40-C32-C31	-2.74	105.60	110.52
31	A	4002	DD6	C37-C36-C35	2.74	119.46	114.42
28	B	761	PQN	C11-C3-C4	-2.74	115.69	118.58
25	o	603	CLA	C3B-C4B-NB	-2.74	108.08	110.53
31	n	623	DD6	C28-C27-C26	-2.74	118.86	124.18
31	g	620	DD6	O1-C20-C19	2.74	116.06	113.49
29	B	765	BCR	C12-C13-C14	2.74	123.31	119.01
31	A	4008	DD6	C40-C32-C31	-2.74	105.62	110.52
27	j	198	LHG	O7-C7-C8	2.73	117.40	111.48
29	B	766	BCR	C35-C13-C14	-2.73	118.39	122.82
35	c	607	CHL	OMC-CMC-C2C	-2.73	120.37	125.12
28	d	223	PQN	C10-C5-C4	2.73	123.65	120.71
28	B	769	PQN	C6-C5-C4	-2.73	116.11	120.10
25	h	602	CLA	C1-C2-C3	2.73	130.67	126.20
31	o	620	DD6	C40-C32-C31	-2.73	105.63	110.52
25	e	602	CLA	O1D-CGD-CBD	-2.72	119.14	124.52
25	f	612	CLA	C3B-C4B-NB	-2.72	108.10	110.53
25	B	757	CLA	C1-C2-C3	2.72	130.65	126.20
29	B	766	BCR	C29-C30-C25	2.72	114.39	110.44
25	k	601	CLA	O1D-CGD-CBD	-2.72	119.16	124.52
25	p	604	CLA	CHD-C1D-ND	-2.72	120.98	124.80
31	d	623	DD6	C40-C32-C31	-2.72	105.65	110.52
25	A	760	CLA	C1-C2-C3	2.72	130.65	126.20
25	g	602	CLA	O1D-CGD-CBD	-2.71	119.16	124.52
31	F	4002	DD6	C3-C4-C5	2.71	129.07	123.52
31	e	621	DD6	C40-C32-C31	-2.71	105.66	110.52
25	A	769	CLA	O1D-CGD-CBD	-2.71	119.17	124.52
31	k	621	DD6	C40-C32-C31	-2.71	105.67	110.52
31	F	4002	DD6	C7-C6-C5	-2.71	118.43	122.82
31	A	4008	DD6	C4-C5-C6	-2.71	123.48	127.28
35	d	606	CHL	C1C-CHC-C4B	2.71	125.75	116.07
27	a	181	LHG	O7-C7-C8	2.70	117.33	111.48
25	A	791	CLA	O1D-CGD-CBD	-2.70	119.19	124.52
25	i	610	CLA	CMB-C2B-C1B	-2.70	121.31	125.42
25	d	610	CLA	C1-C2-C3	2.69	130.61	126.20
25	e	602	CLA	C1-C2-C3	2.69	130.61	126.20
35	d	605	CHL	C4C-CHD-C1D	2.69	125.69	116.07
31	i	621	DD6	C21-C20-C15	-2.69	117.88	122.30
31	o	621	DD6	O1-C20-C19	2.68	116.01	113.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	j	620	DD6	C32-C33-C34	-2.68	107.71	113.59
35	e	606	CHL	OBD-CAD-CBD	-2.68	121.89	125.82
31	a	620	DD6	C32-C33-C34	-2.68	107.71	113.59
25	g	610	CLA	C1-C2-C3	2.68	130.59	126.20
25	B	736	CLA	O1D-CGD-CBD	-2.68	119.23	124.52
25	f	614	CLA	O1D-CGD-CBD	-2.68	119.23	124.52
25	m	602	CLA	O1D-CGD-CBD	-2.68	119.23	124.52
33	i	195	LMG	O6-C1-O1	-2.68	103.72	110.04
31	d	621	DD6	C21-C20-C19	2.68	117.25	114.24
25	A	768	CLA	C1-C2-C3	2.68	130.58	126.20
31	d	620	DD6	C40-C32-C31	-2.68	105.72	110.52
31	A	4008	DD6	C32-C33-C34	-2.68	107.73	113.59
33	a	182	LMG	O1-C7-C8	-2.67	104.31	110.82
35	c	607	CHL	C1C-CHC-C4B	2.67	125.64	116.07
31	a	620	DD6	C40-C32-C31	-2.66	105.74	110.52
25	m	613	CLA	O1D-CGD-CBD	-2.66	119.26	124.52
25	A	767	CLA	C3B-C4B-NB	-2.66	108.15	110.53
31	o	620	DD6	C32-C33-C34	-2.66	107.75	113.59
25	a	601	CLA	O1D-CGD-CBD	-2.66	119.27	124.52
29	B	764	BCR	C2-C1-C6	2.66	114.30	110.44
35	e	606	CHL	C4C-CHD-C1D	2.66	125.57	116.07
35	e	606	CHL	C1C-CHC-C4B	2.66	125.57	116.07
31	n	621	DD6	C7-C6-C5	-2.65	118.52	122.82
31	l	620	DD6	C40-C32-C31	-2.65	105.76	110.52
31	k	620	DD6	C32-C33-C34	-2.65	107.77	113.59
31	A	4002	DD6	C40-C32-C31	-2.65	105.77	110.52
25	A	765	CLA	C12-C11-C10	-2.65	103.63	113.62
31	c	623	DD6	C21-C20-C15	-2.65	117.94	122.30
27	A	786	LHG	O8-C23-C24	2.65	119.91	111.83
25	A	783	CLA	C12-C11-C10	-2.65	101.41	113.28
29	B	762	BCR	C11-C10-C9	-2.65	123.56	127.28
25	o	601	CLA	CMA-C3A-C2A	-2.65	110.16	116.23
25	n	603	CLA	C1-C2-C3	2.65	130.53	126.20
31	b	621	DD6	C26-C25-C24	-2.64	115.54	123.20
31	d	621	DD6	C32-C33-C34	-2.64	107.80	113.59
35	d	606	CHL	CHA-C1A-C2A	-2.64	127.10	133.31
31	p	621	DD6	C40-C32-C31	-2.64	105.79	110.52
28	B	769	PQN	C11-C3-C4	-2.64	115.80	118.58
31	h	621	DD6	C32-C33-C34	-2.64	107.81	113.59
35	d	607	CHL	C4C-CHD-C1D	2.64	125.51	116.07
28	A	785	PQN	C11-C3-C4	-2.64	115.80	118.58
25	A	772	CLA	O1D-CGD-CBD	-2.64	119.32	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	602	CLA	O1D-CGD-CBD	-2.64	119.32	124.52
25	A	752	CLA	C4D-C3D-CAD	-2.63	105.25	108.11
25	i	614	CLA	O1D-CGD-CBD	-2.63	119.32	124.52
31	f	621	DD6	C40-C32-C31	-2.63	105.80	110.52
25	B	754	CLA	O1D-CGD-CBD	-2.63	119.33	124.52
27	d	237	LHG	O8-C23-C24	2.63	119.86	111.83
25	p	613	CLA	O1D-CGD-CBD	-2.63	119.33	124.52
25	p	613	CLA	CHD-C1D-ND	-2.63	121.10	124.80
31	g	620	DD6	C40-C32-C31	-2.63	105.81	110.52
25	e	610	CLA	C1-C2-C3	2.63	130.50	126.20
29	A	788	BCR	C36-C18-C17	-2.63	118.56	122.82
27	b	181	LHG	O8-C23-C24	2.63	119.84	111.83
31	A	4002	DD6	O1-C20-C21	-2.63	112.11	115.05
31	g	621	DD6	C32-C33-C34	-2.63	107.83	113.59
25	e	611	CLA	O1D-CGD-CBD	-2.63	119.34	124.52
25	A	794	CLA	C1-C2-C3	2.62	130.50	126.20
25	i	608	CLA	O2A-CGA-O1A	-2.62	117.07	123.63
35	d	608	CHL	C4C-CHD-C1D	2.62	125.45	116.07
25	i	613	CLA	C12-C11-C10	-2.62	103.74	113.62
28	B	761	PQN	C10-C5-C4	2.62	123.53	120.71
27	h	190	LHG	O8-C23-C24	2.62	119.83	111.83
25	B	747	CLA	O1D-CGD-CBD	-2.62	119.35	124.52
28	B	769	PQN	C2M-C2-C1	-2.62	111.85	116.68
27	g	189	LHG	O8-C23-C24	2.62	119.82	111.83
28	d	223	PQN	C9-C10-C1	-2.62	116.28	120.10
25	A	769	CLA	O2A-CGA-CBA	2.62	119.81	111.83
25	A	760	CLA	C12-C11-C10	-2.62	101.56	113.28
31	c	621	DD6	C32-C33-C34	-2.61	107.87	113.59
31	n	621	DD6	C3-C4-C5	2.61	128.86	123.52
28	B	769	PQN	C9-C10-C1	-2.61	116.29	120.10
25	A	770	CLA	O1D-CGD-CBD	-2.61	119.37	124.52
31	a	621	DD6	C32-C33-C34	-2.60	107.88	113.59
31	d	621	DD6	C40-C32-C31	-2.60	105.86	110.52
25	A	774	CLA	C1-C2-C3	2.60	130.46	126.20
35	d	605	CHL	C3C-C4C-NC	-2.60	108.30	114.65
28	B	769	PQN	C10-C5-C4	2.60	123.50	120.71
29	A	789	BCR	C29-C30-C25	2.60	114.21	110.44
31	A	4002	DD6	C32-C33-C34	-2.60	107.89	113.59
25	B	779	CLA	CHD-C1D-ND	-2.60	121.15	124.80
31	i	620	DD6	C21-C20-C19	2.60	117.16	114.24
25	A	804	CLA	O1D-CGD-CBD	-2.60	119.39	124.52
31	m	621	DD6	O1-C20-C15	-2.60	56.87	58.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	761	CLA	C12-C11-C10	-2.60	101.65	113.28
25	m	602	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
31	e	621	DD6	O1-C20-C15	-2.59	56.87	58.93
25	B	738	CLA	C12-C11-C10	-2.59	101.66	113.28
25	B	758	CLA	C4-C3-C5	-2.59	110.73	115.23
27	c	243	LHG	O8-C23-C24	2.59	119.74	111.83
25	B	755	CLA	C1-C2-C3	2.59	130.44	126.20
35	d	606	CHL	C4C-CHD-C1D	2.59	125.34	116.07
35	c	607	CHL	C3C-C4C-NC	-2.59	108.32	114.65
31	i	625	DD6	C40-C32-C31	-2.59	105.88	110.52
25	A	772	CLA	C1-C2-C3	2.59	130.44	126.20
29	B	763	BCR	C2-C1-C6	2.59	114.20	110.44
31	n	620	DD6	C40-C32-C31	-2.59	105.88	110.52
25	c	610	CLA	CMB-C2B-C1B	-2.59	121.48	125.42
31	p	621	DD6	C32-C33-C34	-2.59	107.92	113.59
25	A	773	CLA	O2A-CGA-CBA	2.59	119.72	111.83
31	h	620	DD6	C32-C33-C34	-2.58	107.93	113.59
31	f	621	DD6	C32-C33-C34	-2.58	107.93	113.59
25	m	601	CLA	C3B-C4B-NB	-2.58	108.23	110.53
31	m	620	DD6	C32-C33-C34	-2.58	107.94	113.59
25	d	611	CLA	O1D-CGD-CBD	-2.58	119.43	124.52
35	c	607	CHL	C4C-CHD-C1D	2.58	125.29	116.07
31	k	621	DD6	C32-C33-C34	-2.58	107.94	113.59
31	l	620	DD6	C21-C20-C19	2.58	117.14	114.24
25	B	776	CLA	C1-C2-C3	2.58	130.42	126.20
28	A	785	PQN	C9-C10-C1	-2.58	116.34	120.10
25	B	736	CLA	O2A-CGA-CBA	2.57	119.69	111.83
25	B	768	CLA	C1-C2-C3	2.57	130.41	126.20
31	g	620	DD6	O1-C20-C15	-2.57	56.89	58.93
25	A	759	CLA	O1D-CGD-CBD	-2.57	119.45	124.52
25	l	611	CLA	O1D-CGD-CBD	-2.57	119.45	124.52
25	B	780	CLA	C1-C2-C3	2.57	130.41	126.20
25	m	609	CLA	C1-C2-C3	2.57	130.92	126.76
25	f	610	CLA	C1-C2-C3	2.57	130.41	126.20
25	b	602	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
31	d	621	DD6	C37-C36-C31	-2.56	119.36	124.16
31	l	621	DD6	C21-C20-C19	2.56	117.12	114.24
27	j	198	LHG	O8-C23-C24	2.56	119.65	111.83
25	B	777	CLA	C1-C2-C3	2.56	130.40	126.20
31	g	620	DD6	C28-C27-C26	2.56	129.16	124.18
31	n	620	DD6	C32-C33-C34	-2.56	107.98	113.59
31	e	620	DD6	C8-C6-C5	2.56	123.03	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	776	CLA	C4-C3-C5	-2.56	110.79	115.23
25	j	613	CLA	O2A-CGA-O1A	-2.55	117.24	123.63
25	h	601	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
25	B	740	CLA	O1D-CGD-CBD	-2.55	119.48	124.52
27	i	194	LHG	O8-C23-C24	2.55	119.62	111.83
29	A	789	BCR	C20-C21-C22	-2.55	123.70	127.28
25	k	604	CLA	C1-C2-C3	2.55	130.38	126.20
25	p	602	CLA	O1D-CGD-CBD	-2.55	119.48	124.52
28	d	223	PQN	C2M-C2-C1	-2.55	111.98	116.68
25	B	748	CLA	O1D-CGD-CBD	-2.55	119.49	124.52
25	e	607	CLA	CMD-C2D-C1D	2.55	129.22	124.73
29	B	765	BCR	C36-C18-C17	-2.55	118.69	122.82
35	d	607	CHL	OMC-CMC-C2C	-2.55	120.70	125.12
25	k	613	CLA	C1-C2-C3	2.55	130.37	126.20
31	p	621	DD6	O1-C20-C21	-2.55	112.20	115.05
31	d	620	DD6	O1-C20-C19	2.55	115.88	113.49
25	A	758	CLA	CHD-C1D-ND	-2.54	121.22	124.80
28	A	785	PQN	C10-C5-C4	2.54	123.44	120.71
25	i	603	CLA	O1D-CGD-CBD	-2.54	119.50	124.52
25	A	783	CLA	C2A-C1A-CHA	2.54	128.28	123.87
25	l	610	CLA	O1D-CGD-CBD	-2.54	119.50	124.52
31	f	621	DD6	C9-C10-C11	-2.54	123.71	127.28
31	c	624	DD6	C4-C3-C2	2.54	128.72	123.52
25	j	613	CLA	C2A-C1A-CHA	2.54	128.27	123.87
25	g	608	CLA	O2A-CGA-CBA	2.54	122.02	114.00
28	A	785	PQN	C2M-C2-C1	-2.54	112.00	116.68
31	A	4008	DD6	O1-C20-C21	-2.54	112.21	115.05
31	A	4002	DD6	C3-C2-C1	-2.54	123.72	127.28
31	l	621	DD6	C32-C33-C34	-2.54	108.03	113.59
25	j	601	CLA	C1-C2-C3	2.53	130.86	126.76
31	j	621	DD6	C32-C33-C34	-2.53	108.04	113.59
25	A	801	CLA	O1D-CGD-CBD	-2.53	119.52	124.52
25	h	611	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
25	j	601	CLA	O1D-CGD-CBD	-2.53	119.52	124.52
25	A	770	CLA	C1-C2-C3	2.53	130.34	126.20
25	A	780	CLA	C1-C2-C3	2.53	130.34	126.20
25	B	756	CLA	C12-C11-C10	-2.53	101.94	113.28
31	c	623	DD6	C4-C5-C6	-2.53	123.73	127.28
25	B	748	CLA	O2D-CGD-O1D	-2.53	118.93	123.85
25	A	762	CLA	C1-C2-C3	2.53	130.85	126.76
25	A	799	CLA	CHD-C1D-ND	-2.53	121.25	124.80
25	a	611	CLA	O2A-CGA-CBA	2.52	121.98	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	d	601	CLA	C1-C2-C3	2.52	130.84	126.76
25	g	603	CLA	C3B-C4B-NB	-2.52	108.28	110.53
31	h	620	DD6	C21-C20-C19	2.52	117.07	114.24
25	k	610	CLA	CMB-C2B-C1B	-2.51	121.59	125.42
31	d	620	DD6	C32-C33-C34	-2.51	108.09	113.59
25	A	805	CLA	CAA-C2A-C3A	-2.51	106.22	113.00
25	B	774	CLA	C1-C2-C3	2.51	130.31	126.20
25	i	611	CLA	O1D-CGD-CBD	-2.51	119.57	124.52
29	B	763	BCR	C29-C30-C25	2.51	114.08	110.44
25	l	610	CLA	C1-C2-C3	2.51	130.31	126.20
31	n	621	DD6	C8-C6-C5	2.51	122.95	119.01
31	l	620	DD6	C32-C33-C34	-2.51	108.09	113.59
25	i	603	CLA	C3B-C4B-NB	-2.51	108.29	110.53
25	f	602	CLA	O1D-CGD-CBD	-2.51	119.58	124.52
31	b	620	DD6	C32-C33-C34	-2.50	108.11	113.59
25	B	750	CLA	O1D-CGD-CBD	-2.50	119.58	124.52
31	d	621	DD6	O1-C20-C15	-2.50	56.95	58.93
25	l	610	CLA	CHD-C1D-ND	-2.50	121.28	124.80
31	i	621	DD6	C32-C33-C34	-2.50	108.11	113.59
25	A	752	CLA	CHD-C1D-ND	-2.50	121.28	124.80
31	m	621	DD6	C21-C20-C19	2.50	117.05	114.24
25	A	800	CLA	O1D-CGD-CBD	-2.50	119.59	124.52
31	F	4002	DD6	C8-C6-C5	2.50	122.94	119.01
25	B	755	CLA	C12-C11-C10	-2.50	102.08	113.28
25	f	602	CLA	O2D-CGD-O1D	-2.50	118.98	123.85
35	d	606	CHL	C3C-C4C-NC	-2.50	108.55	114.65
31	d	620	DD6	O1-C20-C15	-2.50	56.95	58.93
25	a	602	CLA	C12-C11-C10	-2.50	102.09	113.28
25	a	613	CLA	C1-C2-C3	2.50	130.29	126.20
35	d	608	CHL	CHA-C1A-C2A	-2.50	127.44	133.31
31	c	620	DD6	C32-C33-C34	-2.50	108.12	113.59
25	A	798	CLA	CMB-C2B-C1B	-2.49	121.62	125.42
25	A	800	CLA	O2D-CGD-O1D	-2.49	118.99	123.85
25	B	773	CLA	C12-C11-C10	-2.49	102.11	113.28
29	B	766	BCR	C12-C13-C14	2.49	122.93	119.01
30	A	795	SQD	O47-C7-C8	2.49	120.08	110.93
25	a	604	CLA	O1D-CGD-CBD	-2.49	119.61	124.52
25	h	612	CLA	C1-C2-C3	2.49	130.27	126.20
31	A	4008	DD6	C10-C9-C8	-2.48	116.00	123.20
25	B	782	CLA	C1-C2-C3	2.48	130.78	126.76
25	k	602	CLA	O1D-CGD-CBD	-2.48	119.62	124.52
25	A	798	CLA	C1-C2-C3	2.48	130.26	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	614	CLA	O1D-CGD-CBD	-2.48	119.62	124.52
25	l	604	CLA	O1D-CGD-CBD	-2.48	119.62	124.52
25	B	775	CLA	O1D-CGD-CBD	-2.48	119.62	124.52
25	B	736	CLA	O2A-CGA-O1A	-2.48	117.42	123.63
25	l	609	CLA	C12-C11-C10	-2.48	102.16	113.28
25	c	619	CLA	CHD-C1D-ND	-2.48	121.31	124.80
25	i	610	CLA	O1D-CGD-CBD	-2.48	119.63	124.52
25	d	613	CLA	CBA-CAA-C2A	2.48	118.67	113.41
25	m	604	CLA	CHD-C1D-ND	-2.48	121.31	124.80
25	A	782	CLA	O1D-CGD-CBD	-2.48	119.63	124.52
25	B	779	CLA	C1-C2-C3	2.48	130.26	126.20
25	g	618	CLA	O2A-CGA-CBA	2.48	121.83	114.00
25	A	799	CLA	C4-C3-C5	-2.47	110.93	115.23
25	B	778	CLA	C1-C2-C3	2.47	130.25	126.20
29	A	788	BCR	C19-C18-C17	2.47	122.90	119.01
25	b	608	CLA	CAA-C2A-C3A	-2.47	110.56	116.23
25	A	772	CLA	O2D-CGD-O1D	-2.47	119.03	123.85
31	b	620	DD6	C21-C20-C15	-2.47	118.23	122.30
25	l	617	CLA	CHD-C1D-ND	-2.47	121.32	124.80
25	c	613	CLA	O1D-CGD-CBD	-2.47	119.64	124.52
35	e	606	CHL	O1D-CGD-CBD	-2.47	120.97	124.72
31	m	621	DD6	C32-C33-C34	-2.47	108.17	113.59
31	o	621	DD6	C32-C33-C34	-2.47	108.17	113.59
25	A	801	CLA	C12-C11-C10	-2.47	102.21	113.28
31	f	621	DD6	C13-C11-C10	2.47	122.89	119.01
25	B	737	CLA	CHD-C1D-ND	-2.47	121.33	124.80
25	h	604	CLA	C12-C11-C10	-2.47	102.21	113.28
35	d	608	CHL	OMC-CMC-C2C	-2.47	120.83	125.12
29	M	201	BCR	C2-C1-C6	2.47	114.03	110.44
25	A	771	CLA	O1D-CGD-CBD	-2.47	119.65	124.52
31	A	4002	DD6	C37-C36-C31	-2.47	119.55	124.16
25	j	614	CLA	O1D-CGD-CBD	-2.47	119.65	124.52
25	f	612	CLA	O1D-CGD-CBD	-2.47	119.65	124.52
25	o	601	CLA	CAA-C2A-C3A	-2.47	110.57	116.23
35	d	605	CHL	O2A-CGA-O1A	-2.47	117.46	123.63
25	A	791	CLA	CHD-C1D-ND	-2.47	121.33	124.80
25	k	604	CLA	C12-C11-C10	-2.47	102.23	113.28
25	i	601	CLA	O1D-CGD-CBD	-2.46	119.66	124.52
25	A	765	CLA	O2A-CGA-O1A	-2.46	117.47	123.63
25	c	602	CLA	O2D-CGD-O1D	-2.46	119.05	123.85
25	e	603	CLA	O2A-CGA-CBA	2.46	121.78	114.00
25	o	602	CLA	O2D-CGD-O1D	-2.46	119.06	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	767	BCR	C2-C1-C6	2.46	114.01	110.44
27	m	182	LHG	O8-C23-C24	2.46	119.33	111.83
25	f	615	CLA	O1D-CGD-CBD	-2.46	119.67	124.52
25	A	801	CLA	O2D-CGD-O1D	-2.46	119.07	123.85
25	B	778	CLA	C12-C11-C10	-2.45	102.28	113.28
29	A	787	BCR	C29-C30-C25	2.45	114.00	110.44
25	a	603	CLA	C2A-C1A-CHA	2.45	128.12	123.87
31	g	621	DD6	O1-C20-C15	-2.45	56.99	58.93
25	j	612	CLA	O1D-CGD-CBD	-2.45	119.69	124.52
29	A	787	BCR	C37-C22-C23	2.45	121.83	118.09
25	l	602	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
31	c	620	DD6	C21-C20-C19	2.45	116.99	114.24
25	c	612	CLA	O1D-CGD-CBD	-2.45	119.69	124.52
25	b	610	CLA	O1D-CGD-CBD	-2.45	119.69	124.52
25	B	746	CLA	C1-C2-C3	2.44	130.20	126.20
25	B	779	CLA	O2A-CGA-O1A	-2.44	117.52	123.63
25	A	763	CLA	C12-C11-C10	-2.44	102.33	113.28
25	c	601	CLA	O1D-CGD-CBD	-2.44	119.70	124.52
25	A	757	CLA	O2A-CGA-CBA	2.44	121.72	114.00
27	A	756	LHG	O8-C23-C24	2.44	119.28	111.83
30	A	795	SQD	O8-S-C6	2.44	110.69	105.97
29	B	766	BCR	C36-C18-C17	-2.44	118.86	122.82
25	B	757	CLA	CHD-C1D-ND	-2.44	121.37	124.80
25	B	774	CLA	C12-C11-C10	-2.44	102.34	113.28
25	a	609	CLA	C1-C2-C3	2.44	130.71	126.76
31	k	621	DD6	O1-C20-C21	-2.44	112.32	115.05
25	m	603	CLA	C1-C2-C3	2.44	130.19	126.20
25	a	602	CLA	O2D-CGD-O1D	-2.44	119.10	123.85
25	m	604	CLA	O1D-CGD-CBD	-2.44	119.71	124.52
25	a	608	CLA	C1-C2-C3	2.44	130.19	126.20
25	i	601	CLA	C1-C2-C3	2.43	130.19	126.20
31	i	625	DD6	C32-C33-C34	-2.43	108.25	113.59
25	A	755	CLA	C12-C11-C10	-2.43	102.37	113.28
25	k	602	CLA	O2A-CGA-O1A	-2.43	117.54	123.63
35	e	606	CHL	C3C-C4C-NC	-2.43	108.71	114.65
25	B	756	CLA	C1-C2-C3	2.43	130.18	126.20
25	i	602	CLA	C1-C2-C3	2.43	130.18	126.20
35	d	607	CHL	C3C-C4C-NC	-2.43	108.71	114.65
25	o	614	CLA	CHD-C1D-ND	-2.43	121.38	124.80
25	f	614	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
25	j	602	CLA	C1-C2-C3	2.43	130.18	126.20
25	d	602	CLA	C1-C2-C3	2.43	130.18	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	749	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
25	A	806	CLA	O1D-CGD-CBD	-2.43	119.73	124.52
33	k	179	LMG	O1-C7-C8	-2.43	104.91	110.82
25	j	610	CLA	C1-C2-C3	2.43	130.17	126.20
25	k	609	CLA	C1-C2-C3	2.43	130.69	126.76
25	a	611	CLA	O1D-CGD-CBD	-2.43	119.73	124.52
25	h	610	CLA	CMB-C2B-C3B	2.43	132.25	126.55
27	a	181	LHG	O8-C23-C24	2.42	119.23	111.83
25	B	741	CLA	C12-C11-C10	-2.42	102.42	113.28
25	A	781	CLA	O2A-CGA-O1A	-2.42	117.57	123.63
25	B	755	CLA	C4-C3-C5	-2.42	111.02	115.23
25	A	791	CLA	C12-C11-C10	-2.42	102.43	113.28
25	g	609	CLA	C1-C2-C3	2.42	130.68	126.76
25	c	611	CLA	O1D-CGD-CBD	-2.42	119.75	124.52
25	B	782	CLA	CMB-C2B-C1B	-2.42	121.74	125.42
31	p	621	DD6	C3-C2-C1	-2.42	123.89	127.28
25	e	611	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
33	B	786	LMG	C1-C2-C3	-2.42	104.92	110.01
25	B	738	CLA	O2A-CGA-O1A	-2.42	117.58	123.63
25	A	771	CLA	C1-C2-C3	2.42	130.16	126.20
25	i	610	CLA	CHD-C1D-ND	-2.42	121.40	124.80
25	B	784	CLA	O1D-CGD-CBD	-2.42	119.75	124.52
25	e	602	CLA	O2D-CGD-O1D	-2.42	119.15	123.85
35	e	606	CHL	CHA-C1A-C2A	-2.41	127.64	133.31
25	A	759	CLA	C12-C11-C10	-2.41	102.47	113.28
25	h	604	CLA	C4-C3-C5	-2.41	111.05	115.23
25	e	608	CLA	O1D-CGD-CBD	-2.41	119.77	124.52
30	c	245	SQD	O8-S-C6	2.41	110.62	105.97
30	g	190	SQD	O9-S-C6	2.41	110.35	106.76
25	A	805	CLA	O2A-CGA-O1A	-2.41	117.61	123.63
25	A	803	CLA	O1D-CGD-CBD	-2.41	119.77	124.52
31	h	621	DD6	C21-C20-C19	2.41	116.94	114.24
25	A	755	CLA	C4-C3-C5	-2.41	111.05	115.23
31	A	4008	DD6	C8-C6-C5	2.41	122.79	119.01
31	d	623	DD6	C32-C33-C34	-2.40	108.32	113.59
25	i	610	CLA	C1-C2-C3	2.40	130.13	126.20
25	m	603	CLA	O2A-CGA-O1A	-2.40	117.62	123.63
25	A	764	CLA	O1D-CGD-CBD	-2.40	119.78	124.52
25	a	610	CLA	CHD-C1D-ND	-2.40	121.43	124.80
25	j	618	CLA	C1-C2-C3	2.40	130.65	126.76
25	B	748	CLA	CHD-C1D-ND	-2.40	121.43	124.80
31	b	621	DD6	C32-C33-C34	-2.40	108.34	113.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	g	601	CLA	O2D-CGD-O1D	-2.39	119.19	123.85
25	j	618	CLA	O1D-CGD-CBD	-2.39	119.80	124.52
31	c	621	DD6	O1-C20-C19	2.39	115.73	113.49
25	A	807	CLA	O1D-CGD-CBD	-2.39	119.80	124.52
25	o	604	CLA	CHD-C1D-ND	-2.39	121.44	124.80
35	d	607	CHL	CHA-C1A-C2A	-2.39	127.70	133.31
25	B	753	CLA	C12-C11-C10	-2.39	102.58	113.28
31	j	620	DD6	C21-C20-C19	2.39	116.92	114.24
25	k	608	CLA	C1-C2-C3	2.39	130.62	126.76
25	J	101	CLA	O1D-CGD-CBD	-2.39	119.81	124.52
31	h	621	DD6	O1-C20-C19	2.39	115.73	113.49
25	A	766	CLA	O1D-CGD-CBD	-2.38	119.82	124.52
35	d	608	CHL	O1D-CGD-CBD	-2.38	121.11	124.72
27	i	194	LHG	O8-C23-O10	-2.38	117.67	123.63
25	A	776	CLA	C1-C2-C3	2.38	130.10	126.20
31	f	620	DD6	C32-C33-C34	-2.38	108.37	113.59
31	k	620	DD6	C21-C20-C19	2.38	116.91	114.24
25	B	745	CLA	C12-C11-C10	-2.38	102.62	113.28
25	A	780	CLA	C4-C3-C5	-2.38	111.10	115.23
31	j	620	DD6	O1-C20-C15	-2.38	57.04	58.93
25	A	801	CLA	C4-C3-C5	-2.38	111.10	115.23
25	f	602	CLA	CHD-C1D-ND	-2.38	121.46	124.80
25	B	755	CLA	O2A-CGA-O1A	-2.38	117.68	123.63
31	F	4002	DD6	C26-C25-C24	2.38	130.09	123.20
25	a	619	CLA	C4-C3-C5	-2.38	111.10	115.23
25	B	749	CLA	O1D-CGD-CBD	-2.38	119.83	124.52
25	i	608	CLA	C12-C11-C10	-2.38	102.63	113.28
29	B	763	BCR	C37-C22-C23	2.37	121.72	118.09
25	b	608	CLA	O1D-CGD-CBD	-2.37	119.83	124.52
31	o	621	DD6	O1-C20-C15	-2.37	57.05	58.93
25	m	613	CLA	CHD-C1D-ND	-2.37	121.46	124.80
25	d	601	CLA	O1D-CGD-CBD	-2.37	119.84	124.52
25	A	758	CLA	C1-C2-C3	2.37	130.08	126.20
25	A	803	CLA	C1-C2-C3	2.37	130.08	126.20
25	B	780	CLA	CHD-C1D-ND	-2.37	121.47	124.80
25	f	604	CLA	CHD-C1D-ND	-2.37	121.47	124.80
25	e	604	CLA	O1D-CGD-CBD	-2.37	119.84	124.52
25	k	613	CLA	O1D-CGD-CBD	-2.37	119.84	124.52
25	g	614	CLA	O1D-CGD-CBD	-2.37	119.84	124.52
25	j	604	CLA	C1-C2-C3	2.37	130.08	126.20
25	k	610	CLA	C1-C2-C3	2.37	130.08	126.20
25	o	610	CLA	CHD-C1D-ND	-2.37	121.47	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	745	CLA	O2A-CGA-O1A	-2.37	117.70	123.63
25	B	774	CLA	O1D-CGD-CBD	-2.37	119.85	124.52
25	k	615	CLA	O1D-CGD-CBD	-2.37	119.85	124.52
25	A	759	CLA	O2D-CGD-O1D	-2.37	119.24	123.85
25	e	607	CLA	CHD-C1D-ND	-2.37	121.47	124.80
25	g	602	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
33	a	182	LMG	C1-C2-C3	-2.36	105.04	110.01
25	B	736	CLA	CHD-C1D-ND	-2.36	121.48	124.80
29	M	201	BCR	C24-C23-C22	-2.36	122.74	126.23
25	B	740	CLA	CHD-C1D-ND	-2.36	121.48	124.80
25	A	808	CLA	O1D-CGD-CBD	-2.36	119.86	124.52
25	b	609	CLA	O1D-CGD-CBD	-2.36	119.86	124.52
30	g	190	SQD	O8-S-C6	2.36	110.53	105.97
25	c	610	CLA	CHD-C1D-ND	-2.36	121.48	124.80
28	A	785	PQN	C17-C16-C15	-2.36	106.97	113.26
25	b	602	CLA	C4-C3-C5	-2.36	111.13	115.23
33	i	195	LMG	C1-C2-C3	-2.36	105.05	110.01
31	c	623	DD6	C32-C33-C34	-2.36	108.42	113.59
25	k	602	CLA	O2D-CGD-O1D	-2.36	119.26	123.85
31	c	621	DD6	C21-C20-C19	2.36	116.89	114.24
31	l	621	DD6	O1-C20-C15	-2.36	57.06	58.93
25	A	752	CLA	C1-C2-C3	2.36	130.06	126.20
29	B	764	BCR	C29-C30-C25	2.36	113.86	110.44
25	B	751	CLA	CHD-C1D-ND	-2.36	121.49	124.80
25	B	752	CLA	O1D-CGD-CBD	-2.35	119.87	124.52
25	i	612	CLA	O1D-CGD-CBD	-2.35	119.88	124.52
31	J	4002	DD6	C21-C20-C19	2.35	116.89	114.24
25	i	614	CLA	O2D-CGD-O1D	-2.35	119.27	123.85
25	B	756	CLA	O2D-CGD-O1D	-2.35	119.27	123.85
25	g	613	CLA	O1D-CGD-CBD	-2.35	119.88	124.52
25	A	776	CLA	C12-C11-C10	-2.35	102.75	113.28
29	M	201	BCR	C29-C30-C25	2.35	113.85	110.44
25	A	799	CLA	C12-C11-C10	-2.35	102.76	113.28
29	A	788	BCR	C15-C16-C17	2.35	128.32	123.52
31	J	4002	DD6	C32-C33-C34	-2.35	108.45	113.59
25	m	603	CLA	O2D-CGD-O1D	-2.35	119.28	123.85
25	A	763	CLA	CHD-C1D-ND	-2.35	121.50	124.80
25	B	779	CLA	C12-C11-C10	-2.34	102.77	113.28
25	B	754	CLA	O2D-CGD-O1D	-2.34	119.28	123.85
25	A	762	CLA	O1D-CGD-CBD	-2.34	119.89	124.52
25	A	765	CLA	CHD-C1D-ND	-2.34	121.50	124.80
27	g	189	LHG	O4-P-O5	2.34	123.35	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	J	4002	DD6	O1-C20-C19	2.34	115.69	113.49
25	h	613	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
25	a	619	CLA	CHD-C1D-ND	-2.34	121.51	124.80
28	B	761	PQN	C17-C16-C15	-2.34	107.02	113.26
25	B	746	CLA	C12-C11-C10	-2.34	102.79	113.28
31	c	620	DD6	O1-C20-C15	-2.34	57.07	58.93
25	B	760	CLA	O1D-CGD-CBD	-2.34	119.90	124.52
25	A	763	CLA	C1-C2-C3	2.34	130.03	126.20
27	b	181	LHG	O8-C23-O10	-2.34	117.78	123.63
31	i	620	DD6	O1-C20-C15	-2.34	57.08	58.93
25	m	602	CLA	C12-C11-C10	-2.34	102.80	113.28
25	k	601	CLA	CHD-C1D-ND	-2.34	121.51	124.80
27	A	756	LHG	O4-P-O5	2.34	123.31	112.44
25	n	602	CLA	O1D-CGD-CBD	-2.34	119.91	124.52
31	F	4002	DD6	C24-C1-C2	2.34	122.68	119.01
25	c	604	CLA	O1D-CGD-CBD	-2.33	119.91	124.52
27	i	194	LHG	O4-P-O5	2.33	123.31	112.44
31	k	621	DD6	O1-C20-C15	-2.33	57.08	58.93
25	i	608	CLA	C1-C2-C3	2.33	130.02	126.20
25	A	806	CLA	CHD-C1D-ND	-2.33	121.52	124.80
25	B	768	CLA	O1D-CGD-CBD	-2.33	119.92	124.52
25	l	601	CLA	O1D-CGD-CBD	-2.33	119.92	124.52
29	B	767	BCR	C29-C30-C25	2.33	113.83	110.44
25	f	610	CLA	CHD-C1D-ND	-2.33	121.52	124.80
25	A	775	CLA	O1D-CGD-CBD	-2.33	119.92	124.52
33	k	179	LMG	C1-C2-C3	-2.33	105.11	110.01
25	f	610	CLA	O1D-CGD-CBD	-2.33	119.92	124.52
25	b	601	CLA	CHD-C1D-ND	-2.33	121.53	124.80
25	A	794	CLA	CHD-C1D-ND	-2.33	121.53	124.80
25	a	613	CLA	O1D-CGD-CBD	-2.33	119.93	124.52
25	j	610	CLA	O1D-CGD-CBD	-2.33	119.93	124.52
25	l	611	CLA	CHD-C1D-ND	-2.33	121.53	124.80
35	d	606	CHL	OMC-CMC-C2C	-2.33	121.08	125.12
35	c	607	CHL	O2A-CGA-O1A	-2.33	117.81	123.63
25	o	612	CLA	O1D-CGD-CBD	-2.33	119.94	124.50
25	o	604	CLA	O1D-CGD-CBD	-2.32	119.94	124.52
25	B	750	CLA	O2A-CGA-O1A	-2.32	117.82	123.63
27	c	243	LHG	O4-P-O5	2.32	123.24	112.44
25	n	610	CLA	CAA-C2A-C3A	-2.32	110.91	116.23
25	a	619	CLA	O1D-CGD-CBD	-2.32	119.94	124.52
25	i	608	CLA	O1D-CGD-CBD	-2.32	119.94	124.52
25	p	613	CLA	CED-O2D-CGD	2.32	121.18	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	613	CLA	CHD-C1D-ND	-2.32	121.54	124.80
25	g	614	CLA	CHD-C1D-ND	-2.32	121.54	124.80
25	A	797	CLA	CHD-C1D-ND	-2.32	121.54	124.80
25	f	609	CLA	CHD-C1D-ND	-2.32	121.54	124.80
25	j	609	CLA	C1-C2-C3	2.32	130.51	126.76
25	j	613	CLA	C12-C11-C10	-2.32	102.90	113.28
25	e	612	CLA	O1D-CGD-CBD	-2.31	119.95	124.52
29	B	765	BCR	C19-C18-C17	2.31	122.65	119.01
25	g	611	CLA	CHD-C1D-ND	-2.31	121.55	124.80
25	j	604	CLA	O1D-CGD-CBD	-2.31	119.95	124.52
29	A	790	BCR	C29-C30-C25	2.31	113.80	110.44
25	A	757	CLA	O1D-CGD-CBD	-2.31	119.96	124.52
25	B	757	CLA	C12-C11-C10	-2.31	102.93	113.28
25	g	611	CLA	O1D-CGD-CBD	-2.31	119.96	124.52
34	b	182	DGD	O6D-C1D-O3G	-2.31	104.59	110.04
25	B	777	CLA	O1D-CGD-CBD	-2.31	119.97	124.52
25	f	601	CLA	O1D-CGD-CBD	-2.31	119.97	124.52
25	a	602	CLA	O2A-CGA-O1A	-2.31	117.85	123.63
25	A	779	CLA	O1D-CGD-CBD	-2.31	119.97	124.52
25	o	609	CLA	O2A-CGA-CBA	2.31	121.29	114.00
25	B	750	CLA	C1-C2-C3	2.31	129.98	126.20
27	d	237	LHG	O8-C23-O10	-2.31	117.86	123.63
25	h	608	CLA	O1D-CGD-CBD	-2.31	119.97	124.52
25	c	606	CLA	O1D-CGD-CBD	-2.30	119.97	124.52
25	k	618	CLA	O1D-CGD-CBD	-2.30	119.97	124.52
27	j	198	LHG	O8-C23-O10	-2.30	117.87	123.63
25	A	773	CLA	O1D-CGD-CBD	-2.30	119.98	124.52
31	h	620	DD6	O1-C20-C15	-2.30	57.11	58.93
25	e	601	CLA	O1D-CGD-CBD	-2.30	119.98	124.52
31	i	621	DD6	O1-C20-C15	-2.30	57.11	58.93
25	c	619	CLA	CAA-C2A-C3A	-2.30	110.95	116.23
25	B	784	CLA	C4-C3-C5	-2.30	111.23	115.23
25	i	602	CLA	C12-C11-C10	-2.30	102.97	113.28
25	k	608	CLA	O1D-CGD-CBD	-2.30	119.98	124.52
27	g	189	LHG	O8-C23-O10	-2.30	117.88	123.63
27	j	198	LHG	O4-P-O5	2.30	123.14	112.44
25	g	609	CLA	CHD-C1D-ND	-2.30	121.57	124.80
25	p	609	CLA	C1-C2-C3	2.30	130.48	126.76
25	a	608	CLA	O1D-CGD-CBD	-2.30	119.99	124.52
25	b	610	CLA	CBA-CAA-C2A	2.30	118.28	113.41
27	b	181	LHG	O4-P-O5	2.30	123.13	112.44
30	j	200	SQD	O8-S-C6	2.30	110.41	105.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	766	BCR	C23-C22-C21	2.30	122.62	119.01
31	b	620	DD6	O1-C20-C15	-2.30	57.11	58.93
25	B	739	CLA	C12-C11-C10	-2.29	103.00	113.28
29	A	796	BCR	C20-C21-C22	-2.29	124.06	127.28
25	p	610	CLA	O2A-CGA-CBA	2.29	121.25	114.00
25	c	609	CLA	C12-C11-C10	-2.29	103.00	113.28
25	A	801	CLA	C1-C2-C3	2.29	129.95	126.20
31	o	620	DD6	O1-C20-C15	-2.29	57.11	58.93
25	A	770	CLA	C12-C11-C10	-2.29	103.01	113.28
25	A	777	CLA	C1-C2-C3	2.29	129.95	126.20
25	a	604	CLA	O2A-CGA-CBA	2.29	121.24	114.00
27	a	181	LHG	O4-P-O5	2.29	123.10	112.44
25	A	753	CLA	CMB-C2B-C1B	-2.29	121.93	125.42
25	A	777	CLA	C12-C11-C10	-2.29	103.02	113.28
25	A	778	CLA	O1D-CGD-CBD	-2.29	120.00	124.52
25	A	783	CLA	C4-C3-C5	-2.29	111.26	115.23
25	h	603	CLA	O2D-CGD-O1D	-2.29	119.39	123.85
31	j	621	DD6	C37-C36-C31	-2.29	119.89	124.16
25	B	759	CLA	O1D-CGD-CBD	-2.29	120.01	124.52
25	d	614	CLA	O1D-CGD-CBD	-2.29	120.01	124.52
25	B	781	CLA	C12-C11-C10	-2.28	103.04	113.28
25	j	611	CLA	C1-C2-C3	2.28	130.46	126.76
27	h	189	LHG	O4-P-O5	2.28	123.07	112.44
25	A	784	CLA	C1-C2-C3	2.28	129.94	126.20
25	A	773	CLA	O2A-CGA-O1A	-2.28	117.92	123.63
25	e	613	CLA	O1D-CGD-CBD	-2.28	120.02	124.52
25	f	613	CLA	C1-C2-C3	2.28	129.94	126.20
27	h	190	LHG	O4-P-O5	2.28	123.06	112.44
31	i	625	DD6	O1-C20-C21	-2.28	112.50	115.05
25	A	753	CLA	CHD-C1D-ND	-2.28	121.59	124.80
25	a	610	CLA	O2A-CGA-O1A	-2.28	117.92	123.63
25	m	611	CLA	O1D-CGD-CBD	-2.28	120.02	124.52
25	j	610	CLA	C12-C11-C10	-2.28	103.06	113.28
25	A	776	CLA	O1D-CGD-CBD	-2.28	120.02	124.52
25	d	611	CLA	O2A-CGA-CBA	2.28	121.20	114.00
27	d	237	LHG	O4-P-O5	2.28	123.04	112.44
25	c	602	CLA	C1-C2-C3	2.28	129.93	126.20
29	A	788	BCR	C8-C9-C10	2.28	122.59	119.01
25	k	613	CLA	CHD-C1D-ND	-2.28	121.60	124.80
25	A	760	CLA	O2A-CGA-O1A	-2.28	117.94	123.63
25	B	745	CLA	O1D-CGD-CBD	-2.27	120.03	124.52
25	A	774	CLA	C12-C11-C10	-2.27	103.09	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	n	608	CLA	O1D-CGD-CBD	-2.27	120.03	124.52
25	n	609	CLA	O2A-CGA-CBA	2.27	121.18	114.00
25	h	604	CLA	C1-C2-C3	2.27	129.92	126.20
25	f	602	CLA	C1-C2-C3	2.27	129.92	126.20
25	B	780	CLA	O1D-CGD-CBD	-2.27	120.03	124.52
25	j	603	CLA	O1D-CGD-CBD	-2.27	120.03	124.52
25	m	611	CLA	CHD-C1D-ND	-2.27	121.60	124.80
27	m	182	LHG	O4-P-O5	2.27	123.02	112.44
25	o	601	CLA	CHD-C1D-ND	-2.27	121.61	124.80
31	b	621	DD6	C21-C20-C19	2.27	116.79	114.24
31	i	621	DD6	O1-C20-C21	-2.27	112.51	115.05
25	B	737	CLA	C1-C2-C3	2.27	129.92	126.20
25	a	602	CLA	CHD-C1D-ND	-2.27	121.61	124.80
29	A	790	BCR	C15-C16-C17	-2.27	118.87	123.52
25	b	612	CLA	O1D-CGD-CBD	-2.27	120.04	124.52
25	B	745	CLA	O2D-CGD-O1D	-2.27	119.43	123.85
25	A	781	CLA	C2A-C1A-CHA	2.27	127.80	123.87
25	l	613	CLA	O1D-CGD-CBD	-2.27	120.05	124.52
25	n	607	CLA	CHD-C1D-ND	-2.26	121.62	124.80
27	m	182	LHG	O8-C23-O10	-2.26	117.97	123.63
25	A	773	CLA	CHD-C1D-ND	-2.26	121.62	124.80
31	e	621	DD6	C21-C20-C19	2.26	116.78	114.24
25	p	609	CLA	O1D-CGD-CBD	-2.26	120.06	124.52
25	b	605	CLA	O2A-CGA-CBA	2.26	121.14	114.00
31	c	620	DD6	C4-C3-C2	-2.26	118.89	123.52
31	k	620	DD6	O1-C20-C15	-2.26	57.14	58.93
25	i	615	CLA	O2A-CGA-O1A	-2.26	117.98	123.63
31	e	620	DD6	C33-C32-C31	2.26	113.94	109.49
25	B	782	CLA	O1D-CGD-CBD	-2.26	120.06	124.52
25	f	604	CLA	O1D-CGD-CBD	-2.26	120.06	124.52
25	d	609	CLA	CHD-C1D-ND	-2.26	121.63	124.80
27	A	756	LHG	O8-C23-O10	-2.26	117.98	123.63
25	B	758	CLA	C12-C11-C10	-2.26	103.17	113.28
25	A	781	CLA	O1D-CGD-CBD	-2.26	120.07	124.52
31	h	621	DD6	O1-C20-C15	-2.26	57.14	58.93
25	i	613	CLA	O2A-CGA-O1A	-2.25	117.99	123.63
25	p	603	CLA	CMD-C2D-C1D	2.25	128.70	124.73
25	n	608	CLA	CHD-C1D-ND	-2.25	121.63	124.80
25	f	611	CLA	CHD-C1D-ND	-2.25	121.63	124.80
25	p	613	CLA	CMD-C2D-C1D	2.25	128.69	124.73
31	F	4002	DD6	C-C1-C2	-2.25	119.17	122.82
25	A	798	CLA	C4-C3-C5	-2.25	111.32	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	e	605	CLA	CHD-C1D-ND	-2.25	121.64	124.80
25	A	782	CLA	O2D-CGD-O1D	-2.25	119.47	123.85
25	a	612	CLA	O1D-CGD-CBD	-2.25	120.08	124.52
25	d	611	CLA	O2D-CGD-O1D	-2.25	119.47	123.85
31	c	621	DD6	O1-C20-C15	-2.25	57.15	58.93
25	b	613	CLA	O1D-CGD-CBD	-2.25	120.08	124.52
25	h	618	CLA	O1D-CGD-CBD	-2.25	120.09	124.52
25	h	602	CLA	O2A-CGA-O1A	-2.25	118.01	123.63
31	A	4008	DD6	C7-C6-C5	-2.25	119.18	122.82
27	h	190	LHG	O8-C23-O10	-2.24	118.01	123.63
31	l	621	DD6	C19-C18-C17	-2.24	106.59	110.79
31	a	620	DD6	O1-C20-C21	-2.24	112.54	115.05
25	j	614	CLA	O2D-CGD-O1D	-2.24	119.48	123.85
25	A	772	CLA	C12-C11-C10	-2.24	103.22	113.28
25	A	804	CLA	O2D-CGD-O1D	-2.24	119.48	123.85
25	l	614	CLA	O1D-CGD-CBD	-2.24	120.09	124.52
25	p	602	CLA	CHD-C1D-ND	-2.24	121.65	124.80
25	o	613	CLA	CBA-CAA-C2A	2.24	118.17	113.41
25	a	601	CLA	C1-C2-C3	2.24	130.39	126.76
25	B	746	CLA	CHD-C1D-ND	-2.24	121.65	124.80
25	k	611	CLA	CHD-C1D-ND	-2.24	121.65	124.80
25	c	609	CLA	CHD-C1D-ND	-2.24	121.65	124.80
25	d	610	CLA	CHD-C1D-ND	-2.24	121.65	124.80
25	e	611	CLA	CHD-C1D-ND	-2.24	121.65	124.80
25	i	602	CLA	CHD-C1D-ND	-2.24	121.65	124.80
25	f	601	CLA	CHD-C1D-ND	-2.24	121.65	124.80
25	k	614	CLA	O1D-CGD-CBD	-2.24	120.10	124.52
25	h	610	CLA	CHD-C1D-ND	-2.24	121.65	124.80
25	m	601	CLA	C4B-CHC-C1C	-2.24	120.98	126.25
25	f	611	CLA	O2D-CGD-O1D	-2.24	119.49	123.85
25	h	609	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
25	b	610	CLA	CHD-C1D-ND	-2.24	121.65	124.80
25	B	771	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
31	A	4008	DD6	C25-C24-C1	-2.24	120.22	126.36
25	B	776	CLA	O1D-CGD-CBD	-2.24	120.10	124.52
31	A	4002	DD6	C28-C27-C26	2.24	128.53	124.18
25	A	761	CLA	C1-C2-C3	2.24	129.87	126.20
31	m	620	DD6	O1-C20-C21	-2.24	112.55	115.05
25	B	751	CLA	C1-C2-C3	2.24	130.38	126.76
34	b	182	DGD	O2D-C2D-C1D	-2.24	104.75	110.08
25	d	610	CLA	O1D-CGD-CBD	-2.24	120.11	124.52
25	A	775	CLA	C2A-C1A-CHA	2.24	127.75	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	786	LHG	O4-P-O5	2.24	122.84	112.44
25	h	612	CLA	O2A-CGA-O1A	-2.24	118.04	123.63
25	A	769	CLA	O2D-CGD-O1D	-2.23	119.50	123.85
25	n	602	CLA	O2A-CGA-O1A	-2.23	118.04	123.63
25	c	609	CLA	C4-C3-C5	-2.23	111.35	115.23
25	A	752	CLA	C2A-C1A-CHA	2.23	127.74	123.87
25	b	611	CLA	CHD-C1D-ND	-2.23	121.66	124.80
31	c	624	DD6	C13-C11-C10	2.23	122.52	119.01
25	d	602	CLA	C12-C11-C10	-2.23	102.41	113.23
25	i	603	CLA	O2D-CGD-O1D	-2.23	119.50	123.85
25	B	750	CLA	C12-C11-C10	-2.23	103.28	113.28
25	A	779	CLA	CHD-C1D-ND	-2.23	121.66	124.80
25	A	766	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
25	B	752	CLA	C12-C11-C10	-2.23	103.29	113.28
25	l	613	CLA	O2D-CGD-O1D	-2.23	119.51	123.85
25	B	784	CLA	C12-C11-C10	-2.23	103.29	113.28
29	B	765	BCR	C23-C22-C21	2.23	122.51	119.01
31	d	623	DD6	C37-C36-C31	-2.23	120.00	124.16
25	l	613	CLA	CHD-C1D-ND	-2.23	121.67	124.80
25	A	772	CLA	C4-C3-C5	-2.23	111.36	115.23
25	A	802	CLA	CHD-C1D-ND	-2.23	121.67	124.80
25	a	603	CLA	O1D-CGD-CBD	-2.22	120.13	124.52
25	n	605	CLA	O1D-CGD-CBD	-2.22	120.13	124.52
25	b	609	CLA	O2D-CGD-O1D	-2.22	119.52	123.85
25	c	616	CLA	O1D-CGD-CBD	-2.22	120.14	124.52
25	j	609	CLA	CHD-C1D-ND	-2.22	121.68	124.80
25	h	601	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
25	A	808	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
25	B	773	CLA	O1D-CGD-CBD	-2.22	120.14	124.52
25	c	619	CLA	O1D-CGD-CBD	-2.22	120.14	124.52
25	c	611	CLA	O2D-CGD-O1D	-2.22	119.53	123.85
29	A	788	BCR	C24-C23-C22	-2.22	122.95	126.23
25	g	603	CLA	C2D-C1D-ND	2.22	112.32	110.13
31	n	621	DD6	C28-C27-C26	-2.22	119.88	124.18
35	e	606	CHL	O2A-CGA-CBA	2.22	121.01	114.00
25	k	612	CLA	O1D-CGD-CBD	-2.22	120.14	124.52
25	f	609	CLA	CMD-C2D-C1D	2.22	128.63	124.73
25	A	784	CLA	C12-C11-C10	-2.22	103.35	113.28
25	c	610	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
25	A	804	CLA	C1-C2-C3	2.22	130.35	126.76
25	B	740	CLA	O2D-CGD-O1D	-2.22	119.54	123.85
31	m	620	DD6	O1-C20-C15	-2.21	57.17	58.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	758	CLA	C1-C2-C3	2.21	129.83	126.20
25	B	747	CLA	C1-C2-C3	2.21	130.35	126.76
25	B	770	CLA	O1D-CGD-CBD	-2.21	120.15	124.52
25	k	604	CLA	CHD-C1D-ND	-2.21	121.69	124.80
25	o	609	CLA	O1D-CGD-CBD	-2.21	120.15	124.52
27	c	243	LHG	O8-C23-O10	-2.21	118.09	123.63
25	l	604	CLA	CHD-C1D-ND	-2.21	121.69	124.80
25	b	612	CLA	CHD-C1D-ND	-2.21	121.69	124.80
25	A	771	CLA	CHD-C1D-ND	-2.21	121.69	124.80
25	b	608	CLA	C2A-C3A-C4A	2.21	104.18	101.59
25	B	772	CLA	CHD-C1D-ND	-2.21	121.69	124.80
25	A	806	CLA	O2D-CGD-O1D	-2.21	119.55	123.85
34	B	787	DGD	O6D-C1D-O3G	-2.21	104.82	110.04
31	j	621	DD6	O1-C20-C15	-2.21	57.18	58.93
25	B	757	CLA	CMD-C2D-C1D	2.21	128.62	124.73
25	j	609	CLA	O1D-CGD-CBD	-2.21	120.16	124.52
35	d	608	CHL	O2A-CGA-CBA	2.21	120.98	114.00
25	B	739	CLA	CMD-C2D-C1D	2.21	128.62	124.73
25	k	610	CLA	CHD-C1D-ND	-2.21	121.69	124.80
25	A	784	CLA	C2A-C1A-CHA	2.21	127.70	123.87
25	A	753	CLA	C1-C2-C3	2.21	129.81	126.20
25	A	769	CLA	CHB-C1B-NB	2.21	127.36	124.05
25	A	763	CLA	O1D-CGD-CBD	-2.21	120.17	124.52
25	o	609	CLA	CHD-C1D-ND	-2.21	121.70	124.80
25	p	613	CLA	O2D-CGD-O1D	-2.20	119.56	123.85
25	p	610	CLA	CHD-C1D-ND	-2.20	121.70	124.80
31	i	625	DD6	O1-C20-C15	-2.20	57.18	58.93
25	b	613	CLA	CHD-C1D-ND	-2.20	121.70	124.80
31	a	621	DD6	C19-C18-C17	-2.20	106.67	110.79
25	B	747	CLA	O2D-CGD-O1D	-2.20	119.56	123.85
25	B	779	CLA	O1D-CGD-CBD	-2.20	120.17	124.52
25	p	604	CLA	O1D-CGD-CBD	-2.20	120.18	124.52
35	d	605	CHL	O2D-CGD-O1D	-2.20	119.56	123.85
29	A	789	BCR	C2-C1-C6	2.20	113.64	110.44
25	B	739	CLA	C4-C3-C5	-2.20	111.41	115.23
25	j	602	CLA	O1D-CGD-CBD	-2.20	120.18	124.52
25	A	784	CLA	O2A-CGA-O1A	-2.20	118.13	123.63
25	A	758	CLA	C12-C11-C10	-2.20	103.43	113.28
25	B	737	CLA	C4D-CHA-C1A	2.20	123.87	121.24
25	h	611	CLA	O1D-CGD-CBD	-2.20	120.18	124.52
25	B	746	CLA	CMD-C2D-C1D	2.20	128.60	124.73
25	a	610	CLA	O1D-CGD-CBD	-2.20	120.19	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	762	CLA	O2A-CGA-O1A	-2.20	118.13	123.63
25	j	612	CLA	O2D-CGD-O1D	-2.20	119.58	123.85
25	i	613	CLA	C4-C3-C5	-2.19	111.42	115.23
25	m	603	CLA	CMD-C2D-C1D	2.19	128.59	124.73
25	A	799	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
29	A	788	BCR	C23-C22-C21	2.19	122.46	119.01
29	B	766	BCR	C19-C18-C17	2.19	122.46	119.01
25	a	611	CLA	O2D-CGD-O1D	-2.19	119.58	123.85
29	B	763	BCR	C21-C20-C19	-2.19	116.85	123.20
25	B	785	CLA	CMD-C2D-C1D	2.19	128.59	124.73
31	e	620	DD6	C15-C14-C13	-2.19	121.36	125.99
25	A	761	CLA	O1D-CGD-CBD	-2.19	120.20	124.52
25	B	775	CLA	O2D-CGD-O1D	-2.19	119.59	123.85
25	A	801	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
25	A	759	CLA	C1-C2-C3	2.19	129.78	126.20
25	A	769	CLA	C12-C11-C10	-2.19	103.47	113.28
25	j	613	CLA	CAA-C2A-C3A	-2.19	107.09	113.00
25	h	613	CLA	CHD-C1D-ND	-2.19	121.72	124.80
25	o	610	CLA	O1D-CGD-CBD	-2.19	120.20	124.52
35	d	606	CHL	O2A-CGA-CBA	2.19	120.91	114.00
25	A	769	CLA	CHD-C1D-ND	-2.19	121.73	124.80
25	c	619	CLA	C2A-C3A-C4A	2.19	104.15	101.59
25	h	614	CLA	O1D-CGD-CBD	-2.19	120.21	124.52
35	e	606	CHL	OMC-CMC-C2C	-2.19	121.33	125.12
25	A	791	CLA	O2D-CGD-O1D	-2.18	119.60	123.85
25	B	752	CLA	O2A-CGA-O1A	-2.18	118.16	123.63
25	B	744	CLA	O1D-CGD-CBD	-2.18	120.21	124.52
25	c	603	CLA	O1D-CGD-CBD	-2.18	120.21	124.52
25	h	613	CLA	C1-C2-C3	2.18	129.77	126.20
25	f	613	CLA	CHD-C1D-ND	-2.18	121.73	124.80
25	B	736	CLA	O2D-CGD-O1D	-2.18	119.60	123.85
27	A	786	LHG	O8-C23-O10	-2.18	118.17	123.63
25	B	779	CLA	C4-C3-C5	-2.18	111.44	115.23
31	b	621	DD6	O1-C20-C15	-2.18	57.20	58.93
25	a	604	CLA	O2D-CGD-O1D	-2.18	119.60	123.85
25	i	611	CLA	CHD-C1D-ND	-2.18	121.73	124.80
25	B	785	CLA	O1D-CGD-CBD	-2.18	120.22	124.52
25	m	602	CLA	CHD-C1D-ND	-2.18	121.73	124.80
25	m	609	CLA	CHD-C1D-ND	-2.18	121.73	124.80
25	A	800	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
31	a	621	DD6	C21-C20-C19	2.18	116.69	114.24
25	i	609	CLA	CHD-C1D-ND	-2.18	121.74	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	755	CLA	O1D-CGD-CBD	-2.18	120.22	124.52
25	J	101	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
25	B	779	CLA	C4D-CHA-C1A	2.18	123.84	121.24
25	A	778	CLA	CHD-C1D-ND	-2.18	121.74	124.80
25	p	602	CLA	CMD-C2D-C1D	2.18	128.56	124.73
25	A	753	CLA	C12-C11-C10	-2.18	103.53	113.28
25	A	807	CLA	O2D-CGD-O1D	-2.17	119.62	123.85
25	B	741	CLA	O1D-CGD-CBD	-2.17	120.23	124.52
25	b	609	CLA	O2A-CGA-CBA	2.17	120.87	114.00
25	A	779	CLA	O2D-CGD-O1D	-2.17	119.62	123.85
25	k	610	CLA	C12-C11-C10	-2.17	102.69	113.23
25	n	602	CLA	C1-C2-C3	2.17	129.76	126.20
29	B	767	BCR	C24-C25-C26	2.17	126.56	121.56
30	j	200	SQD	O5-C5-C4	2.17	113.61	109.70
25	f	609	CLA	O1D-CGD-CBD	-2.17	120.23	124.52
25	A	752	CLA	C12-C11-C10	-2.17	103.55	113.28
25	B	785	CLA	O2A-CGA-CBA	2.17	120.86	114.00
28	B	761	PQN	C10-C1-C2	-2.17	115.95	118.97
27	a	181	LHG	O8-C23-O10	-2.17	118.20	123.63
31	d	620	DD6	C21-C20-C19	2.17	116.68	114.24
25	i	613	CLA	C2A-C1A-CHA	2.17	127.63	123.87
25	a	609	CLA	CHD-C1D-ND	-2.17	121.75	124.80
30	c	245	SQD	O5-C5-C4	2.17	113.61	109.70
29	B	764	BCR	C37-C22-C23	2.17	121.40	118.09
25	c	606	CLA	CHD-C1D-ND	-2.17	121.75	124.80
25	e	602	CLA	C12-C11-C10	-2.17	103.58	113.28
25	h	602	CLA	O1D-CGD-CBD	-2.16	120.25	124.52
25	A	764	CLA	CHD-C1D-ND	-2.16	121.76	124.80
25	i	615	CLA	O1D-CGD-CBD	-2.16	120.25	124.52
28	B	769	PQN	C17-C16-C15	-2.16	107.50	113.26
25	c	602	CLA	CMB-C2B-C1B	-2.16	122.13	125.42
31	J	4002	DD6	O1-C20-C15	-2.16	57.22	58.93
25	A	799	CLA	CMD-C2D-C1D	2.16	128.53	124.73
25	a	619	CLA	C12-C11-C10	-2.16	103.59	113.28
29	A	792	BCR	C23-C22-C21	2.16	122.41	119.01
25	B	750	CLA	CHD-C1D-ND	-2.16	121.76	124.80
25	o	613	CLA	CHD-C1D-ND	-2.16	121.76	124.80
25	B	748	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
25	p	608	CLA	O1D-CGD-CBD	-2.16	120.26	124.52
29	B	767	BCR	C37-C22-C23	2.16	121.39	118.09
25	B	750	CLA	O2D-CGD-O1D	-2.16	119.65	123.85
25	A	775	CLA	CHD-C1D-ND	-2.16	121.77	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	j	601	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
31	c	623	DD6	O1-C20-C15	-2.16	57.22	58.93
25	e	604	CLA	C1-C2-C3	2.16	130.25	126.76
28	d	223	PQN	C10-C1-C2	-2.16	115.98	118.97
25	B	739	CLA	CHD-C1D-ND	-2.15	121.77	124.80
25	a	601	CLA	CHD-C1D-ND	-2.15	121.77	124.80
25	c	610	CLA	C1-C2-C3	2.15	129.72	126.20
31	l	620	DD6	O1-C20-C15	-2.15	57.22	58.93
25	A	765	CLA	O1D-CGD-CBD	-2.15	120.27	124.52
31	A	4008	DD6	O1-C20-C15	-2.15	57.22	58.93
25	b	604	CLA	O2A-CGA-CBA	2.15	120.80	114.00
25	A	778	CLA	O2D-CGD-O1D	-2.15	119.66	123.85
25	j	612	CLA	CMB-C2B-C1B	-2.15	122.15	125.42
25	B	757	CLA	C4-C3-C5	-2.15	111.50	115.23
25	f	608	CLA	CMD-C2D-C1D	2.15	128.51	124.73
31	n	623	DD6	C25-C26-C27	-2.15	120.60	126.61
25	m	613	CLA	O2D-CGD-O1D	-2.15	119.67	123.85
25	l	603	CLA	O1D-CGD-CBD	-2.15	120.28	124.52
25	g	610	CLA	CHD-C1D-ND	-2.15	121.78	124.80
31	k	620	DD6	O1-C20-C19	2.15	115.50	113.49
25	b	613	CLA	CBA-CAA-C2A	2.15	117.97	113.41
25	n	610	CLA	CHD-C1D-ND	-2.15	121.78	124.80
25	p	609	CLA	CHD-C1D-ND	-2.15	121.78	124.80
25	k	610	CLA	C4-C3-C5	-2.15	111.50	115.23
25	J	101	CLA	O2D-CGD-O1D	-2.15	119.67	123.85
25	a	602	CLA	C4-C3-C5	-2.14	111.51	115.23
25	n	610	CLA	O1D-CGD-CBD	-2.14	120.29	124.52
25	A	781	CLA	CHD-C1D-ND	-2.14	121.79	124.80
31	l	620	DD6	O1-C20-C19	2.14	115.50	113.49
25	i	611	CLA	O2D-CGD-O1D	-2.14	119.68	123.85
25	a	613	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
31	j	620	DD6	C19-C18-C17	-2.14	106.78	110.79
31	c	620	DD6	C19-C18-C17	-2.14	106.79	110.79
25	A	762	CLA	CHD-C1D-ND	-2.14	121.79	124.80
25	g	613	CLA	CHD-C1D-ND	-2.14	121.79	124.80
25	l	617	CLA	O1D-CGD-CBD	-2.14	120.30	124.52
25	l	602	CLA	C4-C3-C5	-2.14	111.51	115.23
25	n	608	CLA	CAA-C2A-C3A	-2.14	111.32	116.23
25	B	747	CLA	O2A-CGA-CBA	2.14	121.56	110.32
25	B	785	CLA	CHD-C1D-ND	-2.14	121.79	124.80
25	h	615	CLA	O1D-CGD-CBD	-2.14	120.30	124.52
25	m	601	CLA	O1D-CGD-CBD	-2.14	120.30	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	h	604	CLA	CHD-C1D-ND	-2.14	121.79	124.80
31	f	620	DD6	O1-C20-C15	-2.14	57.24	58.93
25	a	608	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
25	A	803	CLA	CHD-C1D-ND	-2.14	121.80	124.80
25	a	604	CLA	CHD-C1D-ND	-2.14	121.80	124.80
25	m	610	CLA	CHD-C1D-ND	-2.14	121.80	124.80
28	B	769	PQN	C10-C1-C2	-2.14	116.00	118.97
25	B	752	CLA	O2D-CGD-O1D	-2.14	119.69	123.85
25	A	761	CLA	CED-O2D-CGD	2.14	120.76	115.92
25	a	611	CLA	CHD-C1D-ND	-2.14	121.80	124.80
25	A	806	CLA	O2A-CGA-CBA	2.14	120.75	114.00
25	A	772	CLA	O2A-CGA-CBA	2.14	121.53	110.32
25	j	604	CLA	C12-C11-C10	-2.14	102.88	113.23
25	l	614	CLA	CHD-C1D-ND	-2.13	121.80	124.80
25	p	612	CLA	O1D-CGD-CBD	-2.13	120.31	124.52
25	j	603	CLA	CMD-C2D-C1D	2.13	128.49	124.73
25	d	604	CLA	O1D-CGD-CBD	-2.13	120.31	124.52
25	k	609	CLA	CHD-C1D-ND	-2.13	121.80	124.80
25	c	604	CLA	CHD-C1D-ND	-2.13	121.80	124.80
25	e	613	CLA	CHD-C1D-ND	-2.13	121.80	124.80
25	c	613	CLA	O2D-CGD-O1D	-2.13	119.70	123.85
25	c	614	CLA	O2D-CGD-O1D	-2.13	119.70	123.85
25	d	602	CLA	O1D-CGD-CBD	-2.13	120.31	124.52
25	j	610	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
29	A	789	BCR	C28-C27-C26	-2.13	110.26	114.06
25	c	613	CLA	CHD-C1D-ND	-2.13	121.81	124.80
25	m	612	CLA	O1D-CGD-CBD	-2.13	120.32	124.52
29	M	201	BCR	C24-C25-C26	2.13	126.46	121.56
25	A	771	CLA	C12-C11-C10	-2.13	102.91	113.23
29	B	762	BCR	C37-C22-C23	2.13	121.34	118.09
25	h	613	CLA	C2A-C1A-CHA	2.13	127.56	123.87
25	A	784	CLA	O1D-CGD-CBD	-2.13	120.32	124.52
31	h	620	DD6	C19-C18-C17	-2.13	106.81	110.79
25	B	750	CLA	CMD-C2D-C1D	2.12	128.47	124.73
25	k	602	CLA	CHD-C1D-ND	-2.12	121.81	124.80
25	B	778	CLA	O1D-CGD-CBD	-2.12	120.33	124.52
31	d	623	DD6	C7-C6-C5	-2.12	119.38	122.82
25	j	611	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
25	A	779	CLA	CMD-C2D-C1D	2.12	128.46	124.73
25	i	612	CLA	CMD-C2D-C1D	2.12	128.46	124.73
31	c	621	DD6	C37-C36-C31	-2.12	120.20	124.16
25	k	615	CLA	CHD-C1D-ND	-2.12	121.82	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	l	603	CLA	CMD-C2D-C1D	2.12	128.46	124.73
25	A	764	CLA	C1-C2-C3	2.12	129.67	126.20
25	A	769	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
25	A	807	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
25	c	601	CLA	O2D-CGD-O1D	-2.12	119.72	123.85
31	d	623	DD6	C4-C5-C6	-2.12	124.31	127.28
25	d	602	CLA	CHD-C1D-ND	-2.12	121.82	124.80
31	c	623	DD6	O4-C34-C33	-2.12	105.42	109.75
25	c	608	CLA	CMD-C2D-C1D	2.12	128.46	124.73
25	c	602	CLA	CHD-C1D-ND	-2.12	121.83	124.80
25	c	602	CLA	CMD-C2D-C1D	2.12	128.45	124.73
25	c	614	CLA	CHD-C1D-ND	-2.12	121.83	124.80
31	A	4002	DD6	O1-C20-C15	-2.11	57.25	58.93
25	B	768	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
25	g	601	CLA	CHD-C1D-ND	-2.11	121.83	124.80
25	n	604	CLA	O1D-CGD-CBD	-2.11	120.35	124.52
29	M	201	BCR	C30-C25-C24	-2.11	109.92	115.65
25	n	604	CLA	CMD-C2D-C1D	2.11	128.45	124.73
25	A	755	CLA	CHD-C1D-ND	-2.11	121.83	124.80
31	n	620	DD6	O4-C34-C33	-2.11	105.43	109.75
25	p	601	CLA	O1D-CGD-CBD	-2.11	120.35	124.52
25	B	737	CLA	C4-C3-C5	-2.11	111.56	115.23
25	f	602	CLA	C4-C3-C5	-2.11	111.56	115.23
25	f	603	CLA	O1D-CGD-CBD	-2.11	120.36	124.52
25	n	613	CLA	O1D-CGD-CBD	-2.11	120.36	124.52
25	f	615	CLA	CHD-C1D-ND	-2.11	121.83	124.80
25	o	610	CLA	CAA-C2A-C3A	-2.11	111.39	116.23
29	A	796	BCR	C11-C10-C9	-2.11	124.32	127.28
25	A	798	CLA	O1D-CGD-CBD	-2.11	120.36	124.52
25	A	793	CLA	CHD-C1D-ND	-2.11	121.84	124.80
25	j	602	CLA	CHD-C1D-ND	-2.11	121.84	124.80
25	b	605	CLA	CHD-C1D-ND	-2.11	121.84	124.80
25	A	783	CLA	CHD-C1D-ND	-2.11	121.84	124.80
25	B	773	CLA	CHD-C1D-ND	-2.11	121.84	124.80
31	d	623	DD6	O1-C20-C15	-2.11	57.26	58.93
25	A	784	CLA	CHD-C1D-ND	-2.11	121.84	124.80
35	e	606	CHL	CMB-C2B-C3B	2.11	128.89	124.68
25	h	609	CLA	O1D-CGD-CBD	-2.11	120.37	124.52
25	e	605	CLA	O1D-CGD-CBD	-2.10	120.37	124.52
25	B	758	CLA	CHD-C1D-ND	-2.10	121.84	124.80
25	h	618	CLA	CHD-C1D-ND	-2.10	121.84	124.80
25	c	613	CLA	C4-C3-C5	-2.10	111.58	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	787	BCR	C16-C17-C18	-2.10	124.33	127.28
25	g	615	CLA	CMD-C2D-C1D	2.10	128.43	124.73
25	a	610	CLA	C1-C2-C3	2.10	129.64	126.20
25	m	610	CLA	O1D-CGD-CBD	-2.10	120.37	124.52
25	A	791	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
25	l	609	CLA	CHD-C1D-ND	-2.10	121.84	124.80
25	B	758	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
25	h	601	CLA	CHD-C1D-ND	-2.10	121.84	124.80
25	h	602	CLA	C4D-CHA-C1A	2.10	123.75	121.24
25	j	608	CLA	O1D-CGD-CBD	-2.10	120.38	124.52
31	f	621	DD6	C7-C6-C5	-2.10	119.41	122.82
25	j	601	CLA	CHD-C1D-ND	-2.10	121.85	124.80
31	J	4002	DD6	O4-C34-C33	-2.10	105.45	109.75
25	j	604	CLA	O2D-CGD-O1D	-2.10	119.76	123.85
25	A	781	CLA	C1-C2-C3	2.10	129.64	126.20
25	l	609	CLA	O1D-CGD-CBD	-2.10	120.38	124.52
25	A	794	CLA	C12-C11-C10	-2.10	103.05	113.23
25	f	603	CLA	CMD-C2D-C1D	2.10	128.42	124.73
25	a	609	CLA	O1D-CGD-CBD	-2.10	120.38	124.52
25	g	618	CLA	O1D-CGD-CBD	-2.10	120.38	124.52
29	A	790	BCR	C37-C22-C23	2.10	121.29	118.09
25	B	739	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
25	l	612	CLA	O1D-CGD-CBD	-2.10	120.38	124.52
25	A	759	CLA	O2A-CGA-O1A	-2.10	118.39	123.63
25	i	613	CLA	CHD-C1D-ND	-2.10	121.85	124.80
31	c	623	DD6	C7-C6-C5	-2.09	119.42	122.82
31	k	621	DD6	C21-C20-C19	2.09	116.59	114.24
25	B	777	CLA	CED-O2D-CGD	2.09	120.67	115.92
25	B	753	CLA	C2A-C1A-CHA	2.09	127.50	123.87
25	A	764	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
25	B	736	CLA	C1-C2-C3	2.09	129.63	126.20
25	B	746	CLA	O1D-CGD-CBD	-2.09	120.39	124.52
25	e	610	CLA	CMD-C2D-C1D	2.09	128.41	124.73
31	n	621	DD6	C13-C11-C10	2.09	122.30	119.01
29	A	796	BCR	C24-C23-C22	-2.09	123.14	126.23
25	k	603	CLA	CMD-C2D-C1D	2.09	128.41	124.73
25	h	613	CLA	O1D-CGD-CBD	-2.09	120.39	124.52
25	B	782	CLA	CHD-C1D-ND	-2.09	121.86	124.80
25	A	767	CLA	O1D-CGD-CBD	-2.09	120.39	124.52
25	B	757	CLA	O1D-CGD-CBD	-2.09	120.39	124.52
25	j	611	CLA	CHD-C1D-ND	-2.09	121.86	124.80
31	c	620	DD6	O4-C34-C33	-2.09	105.47	109.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	753	CLA	O1D-CGD-CBD	-2.09	120.39	124.52
25	g	613	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
25	B	779	CLA	CMD-C2D-C1D	2.09	128.41	124.73
25	h	603	CLA	CMD-C2D-C1D	2.09	128.41	124.73
25	c	608	CLA	O1D-CGD-CBD	-2.09	120.40	124.52
25	c	610	CLA	O1D-CGD-CBD	-2.09	120.40	124.52
25	a	608	CLA	CHD-C1D-ND	-2.09	121.86	124.80
25	m	601	CLA	C2D-C1D-ND	2.09	112.19	110.13
25	i	601	CLA	O2D-CGD-O1D	-2.09	119.78	123.85
25	c	609	CLA	O1D-CGD-CBD	-2.09	120.40	124.52
31	i	621	DD6	C21-C20-C19	2.09	116.59	114.24
25	A	808	CLA	CHD-C1D-ND	-2.09	121.86	124.80
25	b	601	CLA	O1D-CGD-CBD	-2.09	120.40	124.52
25	A	762	CLA	O2D-CGD-O1D	-2.09	119.79	123.85
25	g	610	CLA	O1D-CGD-CBD	-2.09	120.40	124.52
25	i	604	CLA	CHD-C1D-ND	-2.09	121.87	124.80
25	j	611	CLA	O1D-CGD-CBD	-2.09	120.40	124.52
25	B	768	CLA	CHD-C1D-ND	-2.09	121.87	124.80
31	g	620	DD6	C37-C36-C31	-2.09	120.26	124.16
25	h	611	CLA	CHD-C1D-ND	-2.08	121.87	124.80
25	o	613	CLA	O1D-CGD-CBD	-2.08	120.41	124.52
25	A	771	CLA	CED-O2D-CGD	2.08	120.64	115.92
25	B	772	CLA	C1-C2-C3	2.08	130.13	126.76
25	e	604	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
25	b	609	CLA	CHD-C1D-ND	-2.08	121.87	124.80
25	c	603	CLA	CMD-C2D-C1D	2.08	128.40	124.73
25	B	736	CLA	C12-C11-C10	-2.08	103.95	113.28
25	m	612	CLA	CMD-C2D-C1D	2.08	128.39	124.73
25	A	777	CLA	CHD-C1D-ND	-2.08	121.87	124.80
31	a	620	DD6	O1-C20-C15	-2.08	57.28	58.93
25	B	781	CLA	CMD-C2D-C1D	2.08	128.39	124.73
25	J	101	CLA	CHD-C1D-ND	-2.08	121.88	124.80
25	k	613	CLA	O2D-CGD-O1D	-2.08	119.80	123.85
31	p	621	DD6	O1-C20-C15	-2.08	57.28	58.93
25	a	603	CLA	C1-C2-C3	2.08	129.60	126.20
25	g	615	CLA	CHD-C1D-ND	-2.08	121.88	124.80
28	A	785	PQN	C10-C1-C2	-2.08	116.08	118.97
25	A	765	CLA	C4-C3-C5	-2.08	111.62	115.23
25	a	601	CLA	O2D-CGD-O1D	-2.08	119.81	123.85
25	f	608	CLA	O1D-CGD-CBD	-2.08	120.42	124.52
25	B	774	CLA	CHD-C1D-ND	-2.08	121.88	124.80
25	m	609	CLA	O2A-CGA-O1A	-2.08	118.44	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	773	CLA	C1-C2-C3	2.08	129.60	126.20
25	A	805	CLA	O1D-CGD-CBD	-2.08	120.42	124.52
25	a	602	CLA	C4D-CHA-C1A	2.08	123.72	121.24
25	o	601	CLA	O1D-CGD-CBD	-2.07	120.43	124.52
35	d	606	CHL	O2D-CGD-O1D	-2.07	119.81	123.85
35	c	607	CHL	O2D-CGD-O1D	-2.07	119.81	123.85
25	h	602	CLA	CHD-C1D-ND	-2.07	121.89	124.80
25	c	604	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
25	o	603	CLA	CMD-C2D-C1D	2.07	128.38	124.73
25	A	770	CLA	O2D-CGD-O1D	-2.07	119.81	123.85
25	k	608	CLA	CMD-C2D-C1D	2.07	128.38	124.73
25	B	757	CLA	C3C-C4C-NC	-2.07	107.78	110.43
25	J	101	CLA	CMD-C2D-C1D	2.07	128.38	124.73
25	d	613	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
25	B	741	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
25	k	604	CLA	C4-C3-C5	-2.07	111.64	115.23
25	g	614	CLA	O2D-CGD-O1D	-2.07	119.82	123.85
25	n	607	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
25	i	614	CLA	CBA-CAA-C2A	2.07	117.80	113.41
25	k	602	CLA	C1-C2-C3	2.07	129.59	126.20
25	A	755	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
25	g	604	CLA	CHD-C1D-ND	-2.07	121.89	124.80
25	l	608	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
25	d	601	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
25	o	614	CLA	C3C-C4C-NC	-2.07	107.78	110.43
35	c	607	CHL	C1A-CHA-C4D	2.07	122.43	118.98
25	f	613	CLA	CMD-C2D-C1D	2.07	128.37	124.73
25	A	752	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
25	p	608	CLA	CMD-C2D-C1D	2.07	128.37	124.73
25	b	604	CLA	CHD-C1D-ND	-2.07	121.89	124.80
25	B	743	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
25	h	610	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
31	l	620	DD6	C37-C36-C31	-2.07	120.30	124.16
25	l	608	CLA	CMD-C2D-C1D	2.07	128.37	124.73
25	k	601	CLA	O2D-CGD-O1D	-2.07	119.83	123.85
25	e	601	CLA	CMD-C2D-C1D	2.06	128.36	124.73
31	g	620	DD6	C21-C20-C19	2.06	116.56	114.24
25	e	610	CLA	O2A-CGA-O1A	-2.06	118.46	123.63
25	h	612	CLA	CHD-C1D-ND	-2.06	121.90	124.80
25	B	782	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
25	i	609	CLA	O1D-CGD-CBD	-2.06	120.45	124.52
31	f	621	DD6	C37-C36-C31	-2.06	120.30	124.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	e	609	CLA	CHD-C1D-ND	-2.06	121.90	124.80
25	d	604	CLA	CHB-C1B-NB	2.06	127.14	124.05
25	d	601	CLA	CHD-C1D-ND	-2.06	121.90	124.80
31	c	623	DD6	C37-C36-C31	-2.06	120.31	124.16
25	c	608	CLA	CHD-C1D-ND	-2.06	121.90	124.80
25	B	737	CLA	C2C-C1C-NC	-2.06	107.82	109.98
25	B	775	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
25	p	612	CLA	CBA-CAA-C2A	2.06	118.30	114.05
25	e	602	CLA	CHD-C1D-ND	-2.06	121.91	124.80
25	f	603	CLA	CHD-C1D-ND	-2.06	121.91	124.80
31	l	620	DD6	O4-C34-C33	-2.06	105.54	109.75
31	d	623	DD6	O4-C34-C33	-2.06	105.54	109.75
25	A	753	CLA	O1D-CGD-CBD	-2.06	120.46	124.52
31	g	621	DD6	C37-C36-C31	-2.06	120.32	124.16
29	A	792	BCR	C2-C1-C6	2.06	113.42	110.44
25	A	770	CLA	CED-O2D-CGD	2.06	120.58	115.92
31	e	621	DD6	C37-C36-C31	-2.06	120.32	124.16
25	e	612	CLA	CMD-C2D-C1D	2.05	128.35	124.73
25	h	612	CLA	C2D-C1D-ND	2.05	112.16	110.13
25	l	611	CLA	O2D-CGD-O1D	-2.05	119.85	123.85
33	B	786	LMG	O6-C1-O1	-2.05	105.19	110.04
25	B	749	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
31	A	4002	DD6	O4-C34-C33	-2.05	105.55	109.75
25	f	610	CLA	O2D-CGD-O1D	-2.05	119.85	123.85
25	o	601	CLA	CED-O2D-CGD	2.05	120.57	115.92
25	c	612	CLA	O2D-CGD-O1D	-2.05	119.85	123.85
25	c	608	CLA	C1-C2-C3	2.05	130.08	126.76
25	h	601	CLA	C1-C2-C3	2.05	130.08	126.76
25	l	602	CLA	CHD-C1D-ND	-2.05	121.92	124.80
25	A	805	CLA	C3C-C4C-NC	-2.05	107.80	110.43
25	k	609	CLA	O1D-CGD-CBD	-2.05	120.47	124.52
31	c	621	DD6	O4-C34-C33	-2.05	105.55	109.75
25	n	605	CLA	CBA-CAA-C2A	2.05	117.76	113.41
25	A	793	CLA	O1D-CGD-CBD	-2.05	120.47	124.52
25	g	603	CLA	O1D-CGD-CBD	-2.05	120.47	124.52
25	A	768	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
25	b	602	CLA	CHD-C1D-ND	-2.05	121.92	124.80
25	e	609	CLA	C4-C3-C5	-2.05	111.67	115.23
31	n	620	DD6	O1-C20-C15	-2.05	57.30	58.93
25	A	804	CLA	CHD-C1D-ND	-2.05	121.92	124.80
25	h	609	CLA	CHD-C1D-ND	-2.05	121.92	124.80
25	o	601	CLA	CMD-C2D-C1D	2.05	128.34	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	n	605	CLA	O2D-CGD-O1D	-2.05	119.86	123.85
25	A	770	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
25	B	737	CLA	CHD-C4C-C3C	2.05	127.76	124.77
25	B	770	CLA	CHD-C1D-ND	-2.05	121.92	124.80
25	j	615	CLA	O1D-CGD-CBD	-2.05	120.48	124.52
31	o	621	DD6	O4-C34-C33	-2.05	105.56	109.75
25	B	756	CLA	CHD-C1D-ND	-2.05	121.92	124.80
25	f	614	CLA	CHD-C1D-ND	-2.05	121.92	124.80
25	B	774	CLA	CED-O2D-CGD	2.05	120.56	115.92
25	j	601	CLA	O2D-CGD-O1D	-2.05	119.86	123.85
25	o	604	CLA	CMD-C2D-C1D	2.05	128.33	124.73
25	A	770	CLA	CHD-C1D-ND	-2.05	121.92	124.80
25	A	804	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
31	d	620	DD6	C37-C36-C31	-2.05	120.33	124.16
25	A	776	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
25	A	808	CLA	CMB-C2B-C1B	-2.05	122.30	125.42
25	k	612	CLA	CHD-C1D-ND	-2.05	121.92	124.80
25	g	602	CLA	CHD-C1D-ND	-2.05	121.92	124.80
25	g	611	CLA	C4D-CHA-C1A	2.04	123.68	121.24
25	B	756	CLA	O2A-CGA-O1A	-2.04	118.51	123.63
25	i	601	CLA	CHD-C1D-ND	-2.04	121.93	124.80
25	A	757	CLA	O2D-CGD-O1D	-2.04	119.87	123.85
25	A	801	CLA	CHD-C1D-ND	-2.04	121.93	124.80
25	B	778	CLA	CHD-C1D-ND	-2.04	121.93	124.80
25	e	610	CLA	O1D-CGD-CBD	-2.04	120.49	124.52
25	B	740	CLA	C4D-CHA-C1A	2.04	123.68	121.24
25	b	601	CLA	CMD-C2D-C1D	2.04	128.32	124.73
25	p	602	CLA	CED-O2D-CGD	2.04	120.55	115.92
25	n	604	CLA	CHD-C1D-ND	-2.04	121.93	124.80
25	B	783	CLA	O1D-CGD-CBD	-2.04	120.49	124.52
25	e	610	CLA	CHD-C1D-ND	-2.04	121.93	124.80
25	g	618	CLA	CHD-C1D-ND	-2.04	121.93	124.80
25	m	602	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
25	a	602	CLA	CMD-C2D-C1D	2.04	128.32	124.73
30	A	795	SQD	O5-C5-C4	2.04	113.37	109.70
25	j	614	CLA	CHD-C1D-ND	-2.04	121.94	124.80
25	A	766	CLA	O2D-CGD-O1D	-2.04	119.88	123.85
25	l	614	CLA	CMD-C2D-C1D	2.04	128.32	124.73
25	a	602	CLA	C1-C2-C3	2.04	129.53	126.20
25	B	775	CLA	C1-C2-C3	2.04	130.06	126.76
25	c	603	CLA	O2D-CGD-O1D	-2.04	119.88	123.85
33	k	179	LMG	O6-C1-O1	-2.04	105.23	110.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	j	602	CLA	CMD-C2D-C1D	2.04	128.31	124.73
29	A	789	BCR	C24-C23-C22	-2.04	123.22	126.23
25	B	778	CLA	CED-O2D-CGD	2.04	120.53	115.92
31	o	621	DD6	C21-C20-C19	2.03	116.53	114.24
25	A	798	CLA	CHD-C1D-ND	-2.03	121.94	124.80
31	d	621	DD6	C23-C16-C17	-2.03	105.39	108.97
25	b	612	CLA	O2D-CGD-O1D	-2.03	119.89	123.85
25	p	602	CLA	O2D-CGD-O1D	-2.03	119.89	123.85
25	B	758	CLA	O1D-CGD-CBD	-2.03	120.51	124.52
25	d	602	CLA	CMD-C2D-C1D	2.03	128.31	124.73
25	g	610	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
31	A	4008	DD6	C37-C36-C31	-2.03	120.36	124.16
25	e	603	CLA	CED-O2D-CGD	2.03	120.52	115.92
25	m	613	CLA	CBA-CAA-C2A	2.03	117.72	113.41
25	A	775	CLA	C4-C3-C5	-2.03	111.70	115.23
25	j	604	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
29	B	765	BCR	C8-C9-C10	2.03	122.20	119.01
25	o	608	CLA	CED-O2D-CGD	2.03	120.52	115.92
31	m	621	DD6	C37-C36-C31	-2.03	120.36	124.16
25	k	614	CLA	CHD-C1D-ND	-2.03	121.95	124.80
25	b	603	CLA	CMD-C2D-C1D	2.03	128.30	124.73
25	A	771	CLA	O2D-CGD-O1D	-2.03	119.90	123.85
31	a	620	DD6	C37-C36-C31	-2.03	120.37	124.16
25	B	751	CLA	CMD-C2D-C1D	2.03	128.30	124.73
25	d	614	CLA	CHD-C1D-ND	-2.03	121.95	124.80
25	p	601	CLA	CHD-C1D-ND	-2.03	121.95	124.80
31	h	621	DD6	C19-C18-C17	-2.03	107.00	110.79
25	k	618	CLA	C1-C2-C3	2.03	130.04	126.76
25	A	771	CLA	C3C-C4C-NC	-2.03	107.83	110.43
25	j	613	CLA	CHD-C1D-ND	-2.03	121.95	124.80
25	c	613	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
25	B	737	CLA	C3C-C4C-NC	-2.03	107.83	110.43
25	n	608	CLA	C2A-C3A-C4A	2.03	103.97	101.59
25	k	618	CLA	CHD-C1D-ND	-2.02	121.95	124.80
31	J	4002	DD6	C10-C9-C8	-2.02	117.33	123.20
25	e	604	CLA	CMD-C2D-C1D	2.02	128.29	124.73
25	e	604	CLA	CHB-C1B-NB	2.02	127.08	124.05
31	c	621	DD6	C19-C18-C17	-2.02	107.00	110.79
25	A	755	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
25	g	613	CLA	O2D-CGD-O1D	-2.02	119.91	123.85
25	A	782	CLA	CHD-C1D-ND	-2.02	121.95	124.80
25	B	770	CLA	CED-O2D-CGD	2.02	120.50	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	g	614	CLA	CBA-CAA-C2A	2.02	117.70	113.41
31	f	621	DD6	C8-C6-C5	2.02	122.19	119.01
25	k	608	CLA	CED-O2D-CGD	2.02	120.50	115.92
25	k	615	CLA	CBA-CAA-C2A	2.02	117.70	113.41
25	d	601	CLA	CMD-C2D-C1D	2.02	128.29	124.73
25	A	781	CLA	O2D-CGD-O1D	-2.02	119.91	123.85
25	B	782	CLA	CED-O2D-CGD	2.02	120.50	115.92
25	e	602	CLA	CMD-C2D-C1D	2.02	128.29	124.73
31	i	620	DD6	C19-C18-C17	-2.02	107.01	110.79
31	m	621	DD6	O4-C34-C33	-2.02	105.61	109.75
25	o	612	CLA	CMD-C2D-C1D	2.02	128.29	124.73
25	j	615	CLA	CHD-C1D-ND	-2.02	121.96	124.80
31	e	621	DD6	C19-C18-C17	-2.02	107.01	110.79
25	A	769	CLA	CED-O2D-CGD	2.02	120.50	115.92
25	A	783	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
25	c	606	CLA	CMD-C2D-C1D	2.02	128.28	124.73
25	o	609	CLA	CMD-C2D-C1D	2.02	128.28	124.73
25	e	608	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
31	c	621	DD6	C33-C32-C31	-2.02	105.51	109.49
25	i	610	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
25	e	601	CLA	CBA-CAA-C2A	2.02	117.69	113.41
25	A	777	CLA	O1D-CGD-CBD	-2.02	120.54	124.52
29	B	764	BCR	C21-C20-C19	-2.02	117.36	123.20
25	A	772	CLA	CHD-C1D-ND	-2.02	121.96	124.80
25	f	610	CLA	CMD-C2D-C1D	2.02	128.28	124.73
25	n	608	CLA	CMD-C2D-C1D	2.02	128.28	124.73
31	l	621	DD6	C4-C5-C6	-2.02	124.45	127.28
25	o	602	CLA	CHD-C1D-ND	-2.02	121.97	124.80
25	o	603	CLA	CHD-C1D-ND	-2.02	121.97	124.80
25	B	742	CLA	O1D-CGD-CBD	-2.01	120.54	124.52
25	p	604	CLA	CMD-C2D-C1D	2.01	128.28	124.73
25	i	604	CLA	O1D-CGD-CBD	-2.01	120.55	124.52
25	n	603	CLA	CMD-C2D-C1D	2.01	128.28	124.73
25	b	602	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
25	m	601	CLA	CMD-C2D-C1D	2.01	128.27	124.73
25	p	601	CLA	CMD-C2D-C1D	2.01	128.27	124.73
25	i	613	CLA	O1D-CGD-CBD	-2.01	120.55	124.52
25	c	608	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
25	B	777	CLA	CMD-C2D-C1D	2.01	128.27	124.73
25	B	741	CLA	C1-C2-C3	2.01	129.50	126.20
31	i	625	DD6	O4-C34-C33	-2.01	105.63	109.75
25	A	757	CLA	CHD-C1D-ND	-2.01	121.97	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	b	621	DD6	C37-C36-C31	-2.01	120.40	124.16
25	m	601	CLA	CBA-CAA-C2A	2.01	117.68	113.41
34	b	182	DGD	C4E-C3E-C2E	2.01	114.36	110.83
31	f	621	DD6	O1-C20-C15	-2.01	57.34	58.93
25	c	616	CLA	CMD-C2D-C1D	2.01	128.27	124.73
25	f	614	CLA	CMD-C2D-C1D	2.01	128.27	124.73
25	A	803	CLA	CMD-C2D-C1D	2.01	128.27	124.73
25	e	603	CLA	CHD-C1D-ND	-2.01	121.97	124.80
25	h	614	CLA	CHD-C1D-ND	-2.01	121.97	124.80
25	B	784	CLA	CMD-C2D-C1D	2.01	128.27	124.73
31	p	621	DD6	O4-C34-C33	-2.01	105.64	109.75
25	o	614	CLA	CED-O2D-CGD	2.01	120.47	115.92
29	A	790	BCR	C20-C21-C22	-2.01	124.46	127.28
25	d	603	CLA	CMD-C2D-C1D	2.01	128.26	124.73
29	A	796	BCR	C28-C27-C26	-2.01	110.47	114.06
25	B	745	CLA	CHD-C1D-ND	-2.01	121.98	124.80
25	B	783	CLA	CED-O2D-CGD	2.01	120.47	115.92
25	A	797	CLA	CMD-C2D-C1D	2.01	128.26	124.73
25	k	612	CLA	CMD-C2D-C1D	2.01	128.26	124.73
25	k	609	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
25	f	610	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
25	a	603	CLA	CHD-C1D-ND	-2.01	121.98	124.80
25	B	783	CLA	C1-C2-C3	2.01	130.01	126.76
28	d	223	PQN	C17-C16-C15	-2.01	107.92	113.26
25	c	603	CLA	CHD-C1D-ND	-2.00	121.98	124.80
25	e	601	CLA	CHD-C1D-ND	-2.00	121.98	124.80
25	B	775	CLA	CHD-C1D-ND	-2.00	121.98	124.80
25	A	762	CLA	CED-O2D-CGD	2.00	120.46	115.92
25	l	601	CLA	CBA-CAA-C2A	2.00	117.66	113.41
25	g	602	CLA	C1-C2-C3	2.00	129.48	126.20
25	m	608	CLA	O1D-CGD-CBD	-2.00	120.57	124.52
25	d	604	CLA	CHD-C1D-ND	-2.00	121.98	124.80
25	l	608	CLA	CHD-C1D-ND	-2.00	121.98	124.80
25	f	604	CLA	CED-O2D-CGD	2.00	120.46	115.92
25	A	806	CLA	O2A-CGA-O1A	-2.00	118.18	123.33
25	A	808	CLA	C4-C3-C5	-2.00	111.75	115.23
25	j	604	CLA	CED-O2D-CGD	2.00	120.46	115.92
25	a	619	CLA	CMD-C2D-C1D	2.00	128.25	124.73
25	A	758	CLA	CMD-C2D-C1D	2.00	128.25	124.73
25	e	604	CLA	CHD-C1D-ND	-2.00	121.99	124.80
25	i	603	CLA	CMD-C2D-C1D	2.00	128.25	124.73
31	l	621	DD6	O4-C34-C33	-2.00	105.65	109.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	744	CLA	CHD-C1D-ND	-2.00	121.99	124.80
25	I	601	CLA	CHD-C1D-ND	-2.00	121.99	124.80
25	A	776	CLA	O2D-CGD-O1D	-2.00	119.95	123.85
25	B	757	CLA	CED-O2D-CGD	2.00	120.45	115.92

All (294) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	A	752	CLA	ND
25	A	753	CLA	ND
25	A	755	CLA	ND
25	A	757	CLA	ND
25	A	758	CLA	ND
25	A	759	CLA	ND
25	A	760	CLA	ND
25	A	761	CLA	ND
25	A	762	CLA	ND
25	A	763	CLA	ND
25	A	764	CLA	ND
25	A	765	CLA	ND
25	A	766	CLA	ND
25	A	767	CLA	ND
25	A	768	CLA	ND
25	A	769	CLA	ND
25	A	770	CLA	ND
25	A	771	CLA	ND
25	A	772	CLA	ND
25	A	773	CLA	ND
25	A	774	CLA	ND
25	A	775	CLA	ND
25	A	776	CLA	ND
25	A	777	CLA	ND
25	A	778	CLA	ND
25	A	779	CLA	ND
25	A	780	CLA	ND
25	A	781	CLA	ND
25	A	782	CLA	ND
25	A	783	CLA	ND
25	A	784	CLA	ND
25	A	791	CLA	ND
25	A	793	CLA	ND
25	A	794	CLA	ND

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Mol	Chain	Res	Type	Atom
25	A	797	CLA	ND
25	A	798	CLA	ND
25	A	799	CLA	ND
25	A	800	CLA	ND
25	A	801	CLA	ND
25	A	802	CLA	ND
25	A	803	CLA	ND
25	A	804	CLA	ND
25	A	805	CLA	ND
25	A	806	CLA	ND
25	A	807	CLA	ND
25	A	808	CLA	ND
25	B	736	CLA	ND
25	B	737	CLA	ND
25	B	738	CLA	ND
25	B	739	CLA	ND
25	B	740	CLA	ND
25	B	741	CLA	ND
25	B	742	CLA	ND
25	B	743	CLA	ND
25	B	744	CLA	ND
25	B	745	CLA	ND
25	B	746	CLA	ND
25	B	747	CLA	ND
25	B	748	CLA	ND
25	B	749	CLA	ND
25	B	750	CLA	ND
25	B	751	CLA	ND
25	B	752	CLA	ND
25	B	753	CLA	ND
25	B	754	CLA	ND
25	B	755	CLA	ND
25	B	756	CLA	ND
25	B	757	CLA	ND
25	B	758	CLA	ND
25	B	759	CLA	ND
25	B	760	CLA	ND
25	B	768	CLA	ND
25	B	770	CLA	ND
25	B	771	CLA	ND
25	B	772	CLA	ND
25	B	773	CLA	ND

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Mol	Chain	Res	Type	Atom
25	B	774	CLA	ND
25	B	775	CLA	ND
25	B	776	CLA	ND
25	B	777	CLA	ND
25	B	778	CLA	ND
25	B	779	CLA	ND
25	B	780	CLA	ND
25	B	781	CLA	ND
25	B	782	CLA	ND
25	B	783	CLA	ND
25	B	784	CLA	ND
25	B	785	CLA	ND
25	J	101	CLA	ND
25	a	601	CLA	ND
25	a	602	CLA	ND
25	a	603	CLA	ND
25	a	604	CLA	ND
25	a	608	CLA	ND
25	a	609	CLA	ND
25	a	610	CLA	ND
25	a	611	CLA	ND
25	a	612	CLA	ND
25	a	613	CLA	ND
25	a	619	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	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	c	601	CLA	ND
25	c	602	CLA	ND
25	c	603	CLA	ND
25	c	604	CLA	ND
25	c	606	CLA	ND
25	c	608	CLA	ND
25	c	609	CLA	ND

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Mol	Chain	Res	Type	Atom
25	c	610	CLA	ND
25	c	611	CLA	ND
25	c	612	CLA	ND
25	c	613	CLA	ND
25	c	614	CLA	ND
25	c	616	CLA	ND
25	c	619	CLA	ND
25	d	601	CLA	ND
25	d	602	CLA	ND
25	d	603	CLA	ND
25	d	604	CLA	ND
25	d	609	CLA	ND
25	d	610	CLA	ND
25	d	611	CLA	ND
25	d	612	CLA	ND
25	d	613	CLA	ND
25	d	614	CLA	ND
25	e	601	CLA	ND
25	e	602	CLA	ND
25	e	603	CLA	ND
25	e	604	CLA	ND
25	e	605	CLA	ND
25	e	607	CLA	ND
25	e	608	CLA	ND
25	e	609	CLA	ND
25	e	610	CLA	ND
25	e	611	CLA	ND
25	e	612	CLA	ND
25	e	613	CLA	ND
25	e	614	CLA	ND
25	h	601	CLA	ND
25	h	602	CLA	ND
25	h	603	CLA	ND
25	h	604	CLA	ND
25	h	608	CLA	ND
25	h	609	CLA	ND
25	h	610	CLA	ND
25	h	611	CLA	ND
25	h	612	CLA	ND
25	h	613	CLA	ND
25	h	614	CLA	ND
25	h	615	CLA	ND

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Mol	Chain	Res	Type	Atom
25	h	618	CLA	ND
25	i	601	CLA	ND
25	i	602	CLA	ND
25	i	603	CLA	ND
25	i	604	CLA	ND
25	i	608	CLA	ND
25	i	609	CLA	ND
25	i	610	CLA	ND
25	i	611	CLA	ND
25	i	612	CLA	ND
25	i	613	CLA	ND
25	i	614	CLA	ND
25	i	615	CLA	ND
25	j	601	CLA	ND
25	j	602	CLA	ND
25	j	603	CLA	ND
25	j	604	CLA	ND
25	j	608	CLA	ND
25	j	609	CLA	ND
25	j	610	CLA	ND
25	j	611	CLA	ND
25	j	612	CLA	ND
25	j	613	CLA	ND
25	j	614	CLA	ND
25	j	615	CLA	ND
25	j	618	CLA	ND
25	k	601	CLA	ND
25	k	602	CLA	ND
25	k	603	CLA	ND
25	k	604	CLA	ND
25	k	608	CLA	ND
25	k	609	CLA	ND
25	k	610	CLA	ND
25	k	611	CLA	ND
25	k	612	CLA	ND
25	k	613	CLA	ND
25	k	614	CLA	ND
25	k	615	CLA	ND
25	k	618	CLA	ND
25	l	601	CLA	ND
25	l	602	CLA	ND
25	l	603	CLA	ND

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Mol	Chain	Res	Type	Atom
25	l	604	CLA	ND
25	l	608	CLA	ND
25	l	609	CLA	ND
25	l	610	CLA	ND
25	l	611	CLA	ND
25	l	612	CLA	ND
25	l	613	CLA	ND
25	l	614	CLA	ND
25	l	617	CLA	ND
25	m	601	CLA	ND
25	m	602	CLA	ND
25	m	603	CLA	ND
25	m	604	CLA	ND
25	m	608	CLA	ND
25	m	609	CLA	ND
25	m	610	CLA	ND
25	m	611	CLA	ND
25	m	612	CLA	ND
25	m	613	CLA	ND
25	f	601	CLA	ND
25	f	602	CLA	ND
25	f	603	CLA	ND
25	f	604	CLA	ND
25	f	608	CLA	ND
25	f	609	CLA	ND
25	f	610	CLA	ND
25	f	611	CLA	ND
25	f	612	CLA	ND
25	f	613	CLA	ND
25	f	614	CLA	ND
25	f	615	CLA	ND
25	g	601	CLA	ND
25	g	602	CLA	ND
25	g	603	CLA	ND
25	g	604	CLA	ND
25	g	608	CLA	ND
25	g	609	CLA	ND
25	g	610	CLA	ND
25	g	611	CLA	ND
25	g	612	CLA	ND
25	g	613	CLA	ND
25	g	614	CLA	ND

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Mol	Chain	Res	Type	Atom
25	g	615	CLA	ND
25	g	618	CLA	ND
25	n	602	CLA	ND
25	n	603	CLA	ND
25	n	604	CLA	ND
25	n	605	CLA	ND
25	n	606	CLA	ND
25	n	607	CLA	ND
25	n	608	CLA	ND
25	n	609	CLA	ND
25	n	610	CLA	ND
25	n	612	CLA	ND
25	n	613	CLA	ND
25	o	601	CLA	ND
25	o	602	CLA	ND
25	o	603	CLA	ND
25	o	604	CLA	ND
25	o	608	CLA	ND
25	o	609	CLA	ND
25	o	610	CLA	ND
25	o	612	CLA	ND
25	o	613	CLA	ND
25	o	614	CLA	ND
25	p	601	CLA	ND
25	p	602	CLA	ND
25	p	603	CLA	ND
25	p	604	CLA	ND
25	p	608	CLA	ND
25	p	609	CLA	ND
25	p	610	CLA	ND
25	p	612	CLA	ND
25	p	613	CLA	ND
35	c	607	CHL	ND
35	c	607	CHL	NA
35	c	607	CHL	NC
35	d	605	CHL	ND
35	d	605	CHL	NA
35	d	605	CHL	NC
35	d	606	CHL	ND
35	d	606	CHL	NA
35	d	606	CHL	NC
35	d	607	CHL	ND

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Mol	Chain	Res	Type	Atom
35	d	607	CHL	NA
35	d	607	CHL	NC
35	d	608	CHL	ND
35	d	608	CHL	NA
35	d	608	CHL	NC
35	e	606	CHL	ND
35	e	606	CHL	NA
35	e	606	CHL	NC

All (2782) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	A	752	CLA	CAD-CBD-CGD-O2D
25	A	753	CLA	C1-C2-C3-C4
25	A	753	CLA	C1-C2-C3-C5
25	A	757	CLA	C4B-C3B-CAB-CBB
25	A	759	CLA	CHA-CBD-CGD-O1D
25	A	759	CLA	CHA-CBD-CGD-O2D
25	A	760	CLA	C2B-C3B-CAB-CBB
25	A	760	CLA	C4B-C3B-CAB-CBB
25	A	760	CLA	CAD-CBD-CGD-O1D
25	A	760	CLA	CAD-CBD-CGD-O2D
25	A	760	CLA	C1-C2-C3-C4
25	A	760	CLA	C1-C2-C3-C5
25	A	761	CLA	C2B-C3B-CAB-CBB
25	A	761	CLA	C4B-C3B-CAB-CBB
25	A	761	CLA	C12-C13-C15-C16
25	A	763	CLA	CHA-CBD-CGD-O1D
25	A	763	CLA	CHA-CBD-CGD-O2D
25	A	764	CLA	CBD-CGD-O2D-CED
25	A	765	CLA	C1A-C2A-CAA-CBA
25	A	765	CLA	C1-C2-C3-C5
25	A	766	CLA	C2B-C3B-CAB-CBB
25	A	766	CLA	C4B-C3B-CAB-CBB
25	A	766	CLA	C1-C2-C3-C4
25	A	766	CLA	C1-C2-C3-C5
25	A	767	CLA	C1A-C2A-CAA-CBA
25	A	767	CLA	C2B-C3B-CAB-CBB
25	A	767	CLA	C4B-C3B-CAB-CBB
25	A	768	CLA	C3A-C2A-CAA-CBA
25	A	769	CLA	C4B-C3B-CAB-CBB
25	A	770	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	A	771	CLA	C1A-C2A-CAA-CBA
25	A	772	CLA	CHA-CBD-CGD-O1D
25	A	772	CLA	C1-C2-C3-C5
25	A	773	CLA	C2B-C3B-CAB-CBB
25	A	773	CLA	C4B-C3B-CAB-CBB
25	A	774	CLA	C2B-C3B-CAB-CBB
25	A	774	CLA	C4B-C3B-CAB-CBB
25	A	775	CLA	C2B-C3B-CAB-CBB
25	A	775	CLA	C4B-C3B-CAB-CBB
25	A	775	CLA	C1-C2-C3-C5
25	A	777	CLA	CHA-CBD-CGD-O1D
25	A	777	CLA	CHA-CBD-CGD-O2D
25	A	779	CLA	C1A-C2A-CAA-CBA
25	A	779	CLA	C2B-C3B-CAB-CBB
25	A	779	CLA	C4B-C3B-CAB-CBB
25	A	779	CLA	CBD-CGD-O2D-CED
25	A	780	CLA	C1-C2-C3-C5
25	A	781	CLA	C1-C2-C3-C4
25	A	781	CLA	C1-C2-C3-C5
25	A	782	CLA	CBD-CGD-O2D-CED
25	A	783	CLA	C1-C2-C3-C4
25	A	783	CLA	C1-C2-C3-C5
25	A	784	CLA	C1-C2-C3-C4
25	A	784	CLA	C1-C2-C3-C5
25	A	791	CLA	C2B-C3B-CAB-CBB
25	A	791	CLA	C4B-C3B-CAB-CBB
25	A	797	CLA	C1A-C2A-CAA-CBA
25	A	797	CLA	C3A-C2A-CAA-CBA
25	A	797	CLA	C2B-C3B-CAB-CBB
25	A	797	CLA	C4B-C3B-CAB-CBB
25	A	797	CLA	CHA-CBD-CGD-O1D
25	A	797	CLA	CHA-CBD-CGD-O2D
25	A	798	CLA	C1-C2-C3-C4
25	A	798	CLA	C1-C2-C3-C5
25	A	799	CLA	C1A-C2A-CAA-CBA
25	A	799	CLA	C3A-C2A-CAA-CBA
25	A	799	CLA	C4B-C3B-CAB-CBB
25	A	799	CLA	C1-C2-C3-C5
25	A	800	CLA	C1A-C2A-CAA-CBA
25	A	800	CLA	C3A-C2A-CAA-CBA
25	A	801	CLA	C3A-C2A-CAA-CBA
25	A	801	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
25	A	802	CLA	C1A-C2A-CAA-CBA
25	A	802	CLA	C2B-C3B-CAB-CBB
25	A	802	CLA	C4B-C3B-CAB-CBB
25	A	802	CLA	CHA-CBD-CGD-O1D
25	A	802	CLA	CHA-CBD-CGD-O2D
25	A	803	CLA	C4-C3-C5-C6
25	A	804	CLA	C1A-C2A-CAA-CBA
25	A	804	CLA	C3A-C2A-CAA-CBA
25	A	804	CLA	C4B-C3B-CAB-CBB
25	A	805	CLA	C2B-C3B-CAB-CBB
25	A	805	CLA	C4B-C3B-CAB-CBB
25	B	737	CLA	C4B-C3B-CAB-CBB
25	B	737	CLA	CBD-CGD-O2D-CED
25	B	738	CLA	C2B-C3B-CAB-CBB
25	B	738	CLA	C4B-C3B-CAB-CBB
25	B	738	CLA	CAD-CBD-CGD-O2D
25	B	739	CLA	C11-C10-C8-C9
25	B	740	CLA	C1A-C2A-CAA-CBA
25	B	741	CLA	CHA-CBD-CGD-O1D
25	B	741	CLA	CHA-CBD-CGD-O2D
25	B	742	CLA	C2B-C3B-CAB-CBB
25	B	742	CLA	C4B-C3B-CAB-CBB
25	B	745	CLA	C3A-C2A-CAA-CBA
25	B	747	CLA	C2B-C3B-CAB-CBB
25	B	747	CLA	C4B-C3B-CAB-CBB
25	B	748	CLA	C1A-C2A-CAA-CBA
25	B	748	CLA	C3A-C2A-CAA-CBA
25	B	749	CLA	C1A-C2A-CAA-CBA
25	B	749	CLA	C3A-C2A-CAA-CBA
25	B	750	CLA	C2B-C3B-CAB-CBB
25	B	750	CLA	C4B-C3B-CAB-CBB
25	B	750	CLA	CHA-CBD-CGD-O1D
25	B	750	CLA	CHA-CBD-CGD-O2D
25	B	751	CLA	C2B-C3B-CAB-CBB
25	B	751	CLA	C4B-C3B-CAB-CBB
25	B	751	CLA	CHA-CBD-CGD-O1D
25	B	751	CLA	CHA-CBD-CGD-O2D
25	B	752	CLA	C1-C2-C3-C4
25	B	753	CLA	C2B-C3B-CAB-CBB
25	B	753	CLA	C4B-C3B-CAB-CBB
25	B	754	CLA	C1A-C2A-CAA-CBA
25	B	754	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	B	754	CLA	C2B-C3B-CAB-CBB
25	B	754	CLA	C4B-C3B-CAB-CBB
25	B	755	CLA	C1A-C2A-CAA-CBA
25	B	756	CLA	C2B-C3B-CAB-CBB
25	B	756	CLA	C4B-C3B-CAB-CBB
25	B	756	CLA	CHA-CBD-CGD-O2D
25	B	757	CLA	C1A-C2A-CAA-CBA
25	B	758	CLA	C1A-C2A-CAA-CBA
25	B	758	CLA	C2B-C3B-CAB-CBB
25	B	758	CLA	C4B-C3B-CAB-CBB
25	B	759	CLA	C1A-C2A-CAA-CBA
25	B	759	CLA	C3A-C2A-CAA-CBA
25	B	759	CLA	C2A-CAA-CBA-CGA
25	B	760	CLA	C1A-C2A-CAA-CBA
25	B	760	CLA	C3A-C2A-CAA-CBA
25	B	768	CLA	C1-C2-C3-C4
25	B	771	CLA	C2B-C3B-CAB-CBB
25	B	771	CLA	C4B-C3B-CAB-CBB
25	B	772	CLA	C2B-C3B-CAB-CBB
25	B	772	CLA	C4B-C3B-CAB-CBB
25	B	772	CLA	CHA-CBD-CGD-O1D
25	B	772	CLA	CHA-CBD-CGD-O2D
25	B	774	CLA	C1A-C2A-CAA-CBA
25	B	774	CLA	C3A-C2A-CAA-CBA
25	B	774	CLA	C1-C2-C3-C4
25	B	775	CLA	C1A-C2A-CAA-CBA
25	B	776	CLA	C1A-C2A-CAA-CBA
25	B	777	CLA	C2B-C3B-CAB-CBB
25	B	777	CLA	C4B-C3B-CAB-CBB
25	B	778	CLA	C1A-C2A-CAA-CBA
25	B	778	CLA	C3A-C2A-CAA-CBA
25	B	778	CLA	C2B-C3B-CAB-CBB
25	B	778	CLA	C4B-C3B-CAB-CBB
25	B	781	CLA	C1A-C2A-CAA-CBA
25	B	783	CLA	C1-C2-C3-C4
25	B	783	CLA	C1-C2-C3-C5
25	B	784	CLA	C1A-C2A-CAA-CBA
25	B	785	CLA	C1A-C2A-CAA-CBA
25	B	785	CLA	C3A-C2A-CAA-CBA
25	J	101	CLA	C3A-C2A-CAA-CBA
25	J	101	CLA	C2B-C3B-CAB-CBB
25	J	101	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	J	101	CLA	C1-C2-C3-C4
25	a	601	CLA	C1A-C2A-CAA-CBA
25	a	602	CLA	C1A-C2A-CAA-CBA
25	a	602	CLA	C3A-C2A-CAA-CBA
25	a	602	CLA	C2B-C3B-CAB-CBB
25	a	602	CLA	C4B-C3B-CAB-CBB
25	a	602	CLA	CHA-CBD-CGD-O2D
25	a	602	CLA	C1-C2-C3-C4
25	a	602	CLA	C1-C2-C3-C5
25	a	603	CLA	CBA-CGA-O2A-C1
25	a	603	CLA	O1A-CGA-O2A-C1
25	a	608	CLA	C1A-C2A-CAA-CBA
25	a	608	CLA	C3A-C2A-CAA-CBA
25	a	608	CLA	C2B-C3B-CAB-CBB
25	a	608	CLA	C4B-C3B-CAB-CBB
25	a	608	CLA	CBD-CGD-O2D-CED
25	a	609	CLA	C1A-C2A-CAA-CBA
25	a	609	CLA	C1-C2-C3-C4
25	a	609	CLA	C1-C2-C3-C5
25	a	610	CLA	C1A-C2A-CAA-CBA
25	a	610	CLA	C3A-C2A-CAA-CBA
25	a	611	CLA	C1A-C2A-CAA-CBA
25	a	611	CLA	C3A-C2A-CAA-CBA
25	a	612	CLA	C2A-CAA-CBA-CGA
25	a	613	CLA	C1A-C2A-CAA-CBA
25	a	613	CLA	CBA-CGA-O2A-C1
25	a	613	CLA	O1A-CGA-O2A-C1
25	a	619	CLA	CBA-CGA-O2A-C1
25	a	619	CLA	O1A-CGA-O2A-C1
25	a	619	CLA	CBD-CGD-O2D-CED
25	a	619	CLA	O1D-CGD-O2D-CED
25	a	619	CLA	C1-C2-C3-C4
25	a	619	CLA	C1-C2-C3-C5
25	a	619	CLA	C4-C3-C5-C6
25	b	602	CLA	C1A-C2A-CAA-CBA
25	b	602	CLA	C3A-C2A-CAA-CBA
25	b	602	CLA	C2B-C3B-CAB-CBB
25	b	602	CLA	C4B-C3B-CAB-CBB
25	b	602	CLA	CBD-CGD-O2D-CED
25	b	603	CLA	C1A-C2A-CAA-CBA
25	b	603	CLA	C3A-C2A-CAA-CBA
25	b	605	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	b	605	CLA	C4B-C3B-CAB-CBB
25	b	608	CLA	C2B-C3B-CAB-CBB
25	b	608	CLA	C4B-C3B-CAB-CBB
25	b	610	CLA	C3A-C2A-CAA-CBA
25	b	610	CLA	C2B-C3B-CAB-CBB
25	b	610	CLA	C4B-C3B-CAB-CBB
25	b	611	CLA	CHA-CBD-CGD-O1D
25	b	611	CLA	CHA-CBD-CGD-O2D
25	b	612	CLA	CBA-CGA-O2A-C1
25	b	612	CLA	O1A-CGA-O2A-C1
25	b	612	CLA	CHA-CBD-CGD-O1D
25	b	612	CLA	C1-C2-C3-C4
25	b	612	CLA	C1-C2-C3-C5
25	b	613	CLA	C1A-C2A-CAA-CBA
25	b	613	CLA	C3A-C2A-CAA-CBA
25	c	601	CLA	C1A-C2A-CAA-CBA
25	c	601	CLA	C3A-C2A-CAA-CBA
25	c	602	CLA	C1A-C2A-CAA-CBA
25	c	602	CLA	C3A-C2A-CAA-CBA
25	c	603	CLA	CBA-CGA-O2A-C1
25	c	603	CLA	O1A-CGA-O2A-C1
25	c	603	CLA	C4-C3-C5-C6
25	c	604	CLA	C2B-C3B-CAB-CBB
25	c	604	CLA	C4B-C3B-CAB-CBB
25	c	606	CLA	C1A-C2A-CAA-CBA
25	c	608	CLA	C1-C2-C3-C4
25	c	608	CLA	C1-C2-C3-C5
25	c	609	CLA	C1A-C2A-CAA-CBA
25	c	609	CLA	C3A-C2A-CAA-CBA
25	c	610	CLA	C3A-C2A-CAA-CBA
25	c	612	CLA	CHA-CBD-CGD-O1D
25	c	614	CLA	C1A-C2A-CAA-CBA
25	c	614	CLA	C3A-C2A-CAA-CBA
25	c	616	CLA	CAD-CBD-CGD-O1D
25	c	616	CLA	CAD-CBD-CGD-O2D
25	c	619	CLA	CAD-CBD-CGD-O1D
25	c	619	CLA	CBD-CGD-O2D-CED
25	d	602	CLA	C2B-C3B-CAB-CBB
25	d	602	CLA	C4B-C3B-CAB-CBB
25	d	602	CLA	CHA-CBD-CGD-O1D
25	d	602	CLA	CHA-CBD-CGD-O2D
25	d	609	CLA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
25	d	610	CLA	C1A-C2A-CAA-CBA
25	d	610	CLA	C3A-C2A-CAA-CBA
25	d	611	CLA	C1A-C2A-CAA-CBA
25	d	611	CLA	C3A-C2A-CAA-CBA
25	d	613	CLA	C1A-C2A-CAA-CBA
25	d	613	CLA	C3A-C2A-CAA-CBA
25	d	613	CLA	CBD-CGD-O2D-CED
25	d	614	CLA	C1A-C2A-CAA-CBA
25	d	614	CLA	CBD-CGD-O2D-CED
25	e	601	CLA	C3A-C2A-CAA-CBA
25	e	601	CLA	CHA-CBD-CGD-O1D
25	e	601	CLA	CHA-CBD-CGD-O2D
25	e	602	CLA	C1A-C2A-CAA-CBA
25	e	602	CLA	C3A-C2A-CAA-CBA
25	e	602	CLA	C2B-C3B-CAB-CBB
25	e	602	CLA	C4B-C3B-CAB-CBB
25	e	602	CLA	CBD-CGD-O2D-CED
25	e	602	CLA	C1-C2-C3-C4
25	e	605	CLA	C1A-C2A-CAA-CBA
25	e	609	CLA	C1A-C2A-CAA-CBA
25	e	609	CLA	C3A-C2A-CAA-CBA
25	e	609	CLA	C2B-C3B-CAB-CBB
25	e	609	CLA	C4B-C3B-CAB-CBB
25	e	609	CLA	C1-C2-C3-C5
25	e	610	CLA	C1A-C2A-CAA-CBA
25	e	610	CLA	C3A-C2A-CAA-CBA
25	e	610	CLA	C2B-C3B-CAB-CBB
25	e	610	CLA	C4B-C3B-CAB-CBB
25	e	611	CLA	C1A-C2A-CAA-CBA
25	e	611	CLA	C3A-C2A-CAA-CBA
25	e	614	CLA	C1A-C2A-CAA-CBA
25	h	601	CLA	C1A-C2A-CAA-CBA
25	h	601	CLA	C3A-C2A-CAA-CBA
25	h	602	CLA	C2B-C3B-CAB-CBB
25	h	602	CLA	C4B-C3B-CAB-CBB
25	h	602	CLA	CHA-CBD-CGD-O1D
25	h	602	CLA	CHA-CBD-CGD-O2D
25	h	603	CLA	C1A-C2A-CAA-CBA
25	h	603	CLA	C3A-C2A-CAA-CBA
25	h	604	CLA	C1A-C2A-CAA-CBA
25	h	604	CLA	C3A-C2A-CAA-CBA
25	h	604	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	h	604	CLA	O1A-CGA-O2A-C1
25	h	608	CLA	C1A-C2A-CAA-CBA
25	h	608	CLA	C3A-C2A-CAA-CBA
25	h	609	CLA	C1A-C2A-CAA-CBA
25	h	609	CLA	C3A-C2A-CAA-CBA
25	h	610	CLA	C1A-C2A-CAA-CBA
25	h	611	CLA	C2B-C3B-CAB-CBB
25	h	611	CLA	C4B-C3B-CAB-CBB
25	h	612	CLA	C1-C2-C3-C5
25	h	613	CLA	C1-C2-C3-C5
25	h	614	CLA	C1A-C2A-CAA-CBA
25	h	615	CLA	C1A-C2A-CAA-CBA
25	h	615	CLA	C3A-C2A-CAA-CBA
25	h	615	CLA	C2B-C3B-CAB-CBB
25	h	615	CLA	C4B-C3B-CAB-CBB
25	i	601	CLA	C1A-C2A-CAA-CBA
25	i	601	CLA	C3A-C2A-CAA-CBA
25	i	601	CLA	C2B-C3B-CAB-CBB
25	i	601	CLA	C4B-C3B-CAB-CBB
25	i	601	CLA	CBD-CGD-O2D-CED
25	i	602	CLA	C1A-C2A-CAA-CBA
25	i	602	CLA	C3A-C2A-CAA-CBA
25	i	602	CLA	O1A-CGA-O2A-C1
25	i	603	CLA	CHA-CBD-CGD-O1D
25	i	604	CLA	C2B-C3B-CAB-CBB
25	i	604	CLA	C4B-C3B-CAB-CBB
25	i	608	CLA	C1-C2-C3-C4
25	i	609	CLA	C2B-C3B-CAB-CBB
25	i	609	CLA	C4B-C3B-CAB-CBB
25	i	610	CLA	C3A-C2A-CAA-CBA
25	i	611	CLA	C1A-C2A-CAA-CBA
25	i	611	CLA	C3A-C2A-CAA-CBA
25	i	612	CLA	C1A-C2A-CAA-CBA
25	i	613	CLA	C11-C10-C8-C9
25	i	614	CLA	C1A-C2A-CAA-CBA
25	i	614	CLA	C3A-C2A-CAA-CBA
25	j	601	CLA	C1A-C2A-CAA-CBA
25	j	601	CLA	C2B-C3B-CAB-CBB
25	j	601	CLA	C4B-C3B-CAB-CBB
25	j	601	CLA	CBD-CGD-O2D-CED
25	j	601	CLA	C1-C2-C3-C5
25	j	602	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	j	602	CLA	CHA-CBD-CGD-O1D
25	j	602	CLA	CHA-CBD-CGD-O2D
25	j	604	CLA	CBD-CGD-O2D-CED
25	j	604	CLA	O1D-CGD-O2D-CED
25	j	608	CLA	C1A-C2A-CAA-CBA
25	j	608	CLA	CBA-CGA-O2A-C1
25	j	609	CLA	C1-C2-C3-C4
25	j	609	CLA	C1-C2-C3-C5
25	j	610	CLA	C3A-C2A-CAA-CBA
25	j	610	CLA	C2B-C3B-CAB-CBB
25	j	610	CLA	C4B-C3B-CAB-CBB
25	j	610	CLA	C4-C3-C5-C6
25	j	610	CLA	C11-C10-C8-C9
25	j	611	CLA	C1A-C2A-CAA-CBA
25	j	611	CLA	C2B-C3B-CAB-CBB
25	j	611	CLA	C4B-C3B-CAB-CBB
25	j	611	CLA	C1-C2-C3-C5
25	j	614	CLA	C2B-C3B-CAB-CBB
25	j	614	CLA	C4B-C3B-CAB-CBB
25	j	615	CLA	C1A-C2A-CAA-CBA
25	j	615	CLA	C3A-C2A-CAA-CBA
25	j	615	CLA	C2B-C3B-CAB-CBB
25	j	615	CLA	C4B-C3B-CAB-CBB
25	j	618	CLA	C1A-C2A-CAA-CBA
25	j	618	CLA	C3A-C2A-CAA-CBA
25	j	618	CLA	C1-C2-C3-C5
25	k	601	CLA	C1A-C2A-CAA-CBA
25	k	602	CLA	C1A-C2A-CAA-CBA
25	k	602	CLA	C3A-C2A-CAA-CBA
25	k	602	CLA	C2B-C3B-CAB-CBB
25	k	602	CLA	C4B-C3B-CAB-CBB
25	k	602	CLA	C1-C2-C3-C5
25	k	603	CLA	C1A-C2A-CAA-CBA
25	k	603	CLA	C3A-C2A-CAA-CBA
25	k	604	CLA	C1A-C2A-CAA-CBA
25	k	604	CLA	C1-C2-C3-C5
25	k	604	CLA	C11-C10-C8-C9
25	k	610	CLA	C3A-C2A-CAA-CBA
25	k	611	CLA	C1A-C2A-CAA-CBA
25	k	611	CLA	C3A-C2A-CAA-CBA
25	k	613	CLA	C1-C2-C3-C4
25	k	614	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	k	614	CLA	CBD-CGD-O2D-CED
25	k	614	CLA	O1D-CGD-O2D-CED
25	k	615	CLA	C1A-C2A-CAA-CBA
25	k	615	CLA	C2B-C3B-CAB-CBB
25	k	615	CLA	C4B-C3B-CAB-CBB
25	l	601	CLA	C1A-C2A-CAA-CBA
25	l	602	CLA	C1A-C2A-CAA-CBA
25	l	602	CLA	C3A-C2A-CAA-CBA
25	l	602	CLA	C1-C2-C3-C4
25	l	602	CLA	C1-C2-C3-C5
25	l	608	CLA	C1A-C2A-CAA-CBA
25	l	608	CLA	C2A-CAA-CBA-CGA
25	l	608	CLA	C2B-C3B-CAB-CBB
25	l	608	CLA	C4B-C3B-CAB-CBB
25	l	609	CLA	C1A-C2A-CAA-CBA
25	l	609	CLA	C1-C2-C3-C4
25	l	610	CLA	C3A-C2A-CAA-CBA
25	l	610	CLA	C2B-C3B-CAB-CBB
25	l	610	CLA	C4B-C3B-CAB-CBB
25	l	614	CLA	C3A-C2A-CAA-CBA
25	l	614	CLA	CBD-CGD-O2D-CED
25	l	617	CLA	C1A-C2A-CAA-CBA
25	l	617	CLA	C3A-C2A-CAA-CBA
25	l	617	CLA	CHA-CBD-CGD-O1D
25	l	617	CLA	CHA-CBD-CGD-O2D
25	m	601	CLA	C1A-C2A-CAA-CBA
25	m	601	CLA	C3A-C2A-CAA-CBA
25	m	601	CLA	CBD-CGD-O2D-CED
25	m	602	CLA	C1A-C2A-CAA-CBA
25	m	602	CLA	CHA-CBD-CGD-O2D
25	m	602	CLA	C1-C2-C3-C4
25	m	602	CLA	C1-C2-C3-C5
25	m	602	CLA	C4-C3-C5-C6
25	m	603	CLA	CHA-CBD-CGD-O1D
25	m	608	CLA	C2B-C3B-CAB-CBB
25	m	608	CLA	C4B-C3B-CAB-CBB
25	m	609	CLA	C1-C2-C3-C4
25	m	609	CLA	C1-C2-C3-C5
25	m	610	CLA	C1A-C2A-CAA-CBA
25	m	610	CLA	C2B-C3B-CAB-CBB
25	m	610	CLA	C4B-C3B-CAB-CBB
25	m	611	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	m	611	CLA	C3A-C2A-CAA-CBA
25	m	613	CLA	C3A-C2A-CAA-CBA
25	f	601	CLA	C1A-C2A-CAA-CBA
25	f	601	CLA	C2B-C3B-CAB-CBB
25	f	601	CLA	C4B-C3B-CAB-CBB
25	f	601	CLA	CBD-CGD-O2D-CED
25	f	601	CLA	O1D-CGD-O2D-CED
25	f	602	CLA	C1A-C2A-CAA-CBA
25	f	602	CLA	C3A-C2A-CAA-CBA
25	f	604	CLA	C1A-C2A-CAA-CBA
25	f	604	CLA	C3A-C2A-CAA-CBA
25	f	608	CLA	CBD-CGD-O2D-CED
25	f	608	CLA	O1D-CGD-O2D-CED
25	f	609	CLA	C1A-C2A-CAA-CBA
25	f	609	CLA	C3A-C2A-CAA-CBA
25	f	609	CLA	CBD-CGD-O2D-CED
25	f	610	CLA	CHA-CBD-CGD-O1D
25	f	610	CLA	CHA-CBD-CGD-O2D
25	f	610	CLA	CBD-CGD-O2D-CED
25	f	611	CLA	C3A-C2A-CAA-CBA
25	f	612	CLA	C1A-C2A-CAA-CBA
25	f	612	CLA	C3A-C2A-CAA-CBA
25	f	612	CLA	CBD-CGD-O2D-CED
25	f	614	CLA	C1A-C2A-CAA-CBA
25	f	614	CLA	CBD-CGD-O2D-CED
25	f	615	CLA	C1A-C2A-CAA-CBA
25	f	615	CLA	C3A-C2A-CAA-CBA
25	f	615	CLA	C2B-C3B-CAB-CBB
25	f	615	CLA	C4B-C3B-CAB-CBB
25	f	615	CLA	CAD-CBD-CGD-O1D
25	g	601	CLA	C1A-C2A-CAA-CBA
25	g	601	CLA	C3A-C2A-CAA-CBA
25	g	601	CLA	C2B-C3B-CAB-CBB
25	g	601	CLA	C4B-C3B-CAB-CBB
25	g	602	CLA	C3A-C2A-CAA-CBA
25	g	602	CLA	C2B-C3B-CAB-CBB
25	g	602	CLA	C4B-C3B-CAB-CBB
25	g	602	CLA	CBD-CGD-O2D-CED
25	g	603	CLA	C1A-C2A-CAA-CBA
25	g	603	CLA	C3A-C2A-CAA-CBA
25	g	604	CLA	CBD-CGD-O2D-CED
25	g	608	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	g	608	CLA	C3A-C2A-CAA-CBA
25	g	610	CLA	C3A-C2A-CAA-CBA
25	g	610	CLA	C2B-C3B-CAB-CBB
25	g	610	CLA	C4B-C3B-CAB-CBB
25	g	611	CLA	C3A-C2A-CAA-CBA
25	g	612	CLA	CBD-CGD-O2D-CED
25	g	613	CLA	C1-C2-C3-C4
25	g	613	CLA	C1-C2-C3-C5
25	g	614	CLA	C1A-C2A-CAA-CBA
25	g	618	CLA	C1A-C2A-CAA-CBA
25	g	618	CLA	C2B-C3B-CAB-CBB
25	g	618	CLA	C4B-C3B-CAB-CBB
25	n	602	CLA	C1A-C2A-CAA-CBA
25	n	602	CLA	C3A-C2A-CAA-CBA
25	n	602	CLA	CHA-CBD-CGD-O1D
25	n	602	CLA	CHA-CBD-CGD-O2D
25	n	604	CLA	CHA-CBD-CGD-O1D
25	n	604	CLA	CHA-CBD-CGD-O2D
25	n	605	CLA	C1A-C2A-CAA-CBA
25	n	605	CLA	C3A-C2A-CAA-CBA
25	n	606	CLA	C1A-C2A-CAA-CBA
25	n	606	CLA	C3A-C2A-CAA-CBA
25	n	606	CLA	C2B-C3B-CAB-CBB
25	n	606	CLA	C4B-C3B-CAB-CBB
25	n	607	CLA	C1A-C2A-CAA-CBA
25	n	607	CLA	C3A-C2A-CAA-CBA
25	n	609	CLA	C2B-C3B-CAB-CBB
25	n	609	CLA	C4B-C3B-CAB-CBB
25	n	610	CLA	C2B-C3B-CAB-CBB
25	n	610	CLA	C4B-C3B-CAB-CBB
25	n	612	CLA	C1A-C2A-CAA-CBA
25	n	612	CLA	CBD-CGD-O2D-CED
25	n	613	CLA	C1A-C2A-CAA-CBA
25	n	613	CLA	C3A-C2A-CAA-CBA
25	o	601	CLA	CBD-CGD-O2D-CED
25	o	602	CLA	C1A-C2A-CAA-CBA
25	o	602	CLA	C3A-C2A-CAA-CBA
25	o	602	CLA	C2B-C3B-CAB-CBB
25	o	602	CLA	C4B-C3B-CAB-CBB
25	o	602	CLA	CBD-CGD-O2D-CED
25	o	604	CLA	C1A-C2A-CAA-CBA
25	o	604	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	o	608	CLA	C2A-CAA-CBA-CGA
25	o	608	CLA	C2B-C3B-CAB-CBB
25	o	608	CLA	C4B-C3B-CAB-CBB
25	o	609	CLA	C1A-C2A-CAA-CBA
25	o	609	CLA	C3A-C2A-CAA-CBA
25	o	610	CLA	C2B-C3B-CAB-CBB
25	o	610	CLA	C4B-C3B-CAB-CBB
25	o	613	CLA	C1A-C2A-CAA-CBA
25	o	613	CLA	C3A-C2A-CAA-CBA
25	o	613	CLA	CAD-CBD-CGD-O1D
25	o	613	CLA	CAD-CBD-CGD-O2D
25	o	613	CLA	CBD-CGD-O2D-CED
25	p	602	CLA	C1A-C2A-CAA-CBA
25	p	602	CLA	C3A-C2A-CAA-CBA
25	p	603	CLA	CBD-CGD-O2D-CED
25	p	603	CLA	O1D-CGD-O2D-CED
25	p	608	CLA	C2B-C3B-CAB-CBB
25	p	608	CLA	C4B-C3B-CAB-CBB
25	p	609	CLA	C1A-C2A-CAA-CBA
25	p	609	CLA	C3A-C2A-CAA-CBA
25	p	609	CLA	CBD-CGD-O2D-CED
25	p	609	CLA	O1D-CGD-O2D-CED
25	p	609	CLA	C1-C2-C3-C5
25	p	610	CLA	C1A-C2A-CAA-CBA
25	p	610	CLA	C3A-C2A-CAA-CBA
25	p	610	CLA	C2B-C3B-CAB-CBB
25	p	610	CLA	C4B-C3B-CAB-CBB
25	p	610	CLA	CHA-CBD-CGD-O1D
25	p	610	CLA	CHA-CBD-CGD-O2D
25	p	610	CLA	CBD-CGD-O2D-CED
25	p	613	CLA	C1A-C2A-CAA-CBA
25	p	613	CLA	C3A-C2A-CAA-CBA
25	p	613	CLA	CBD-CGD-O2D-CED
26	A	754	LMT	C2-C1-O1'-C1'
27	A	756	LHG	C4-O6-P-O3
27	a	181	LHG	C4-O6-P-O3
27	a	181	LHG	C4-O6-P-O5
27	b	181	LHG	C3-O3-P-O5
27	b	181	LHG	C3-O3-P-O6
27	b	181	LHG	C4-O6-P-O3
27	b	181	LHG	C4-O6-P-O5
27	b	181	LHG	C8-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
27	c	243	LHG	C1-C2-C3-O3
27	d	237	LHG	C8-C7-O7-C5
27	h	189	LHG	O2-C2-C3-O3
27	h	189	LHG	C3-O3-P-O5
27	h	189	LHG	C3-O3-P-O6
27	h	189	LHG	C4-O6-P-O5
27	h	190	LHG	C1-C2-C3-O3
27	h	190	LHG	C8-C7-O7-C5
27	i	194	LHG	C3-O3-P-O4
27	i	194	LHG	C3-O3-P-O6
27	j	198	LHG	O2-C2-C3-O3
27	j	198	LHG	C4-O6-P-O3
27	j	198	LHG	C4-O6-P-O5
27	m	182	LHG	C3-O3-P-O6
27	m	182	LHG	O9-C7-O7-C5
27	g	189	LHG	C3-O3-P-O5
27	g	189	LHG	C3-O3-P-O6
27	g	189	LHG	C4-O6-P-O3
27	g	189	LHG	C8-C7-O7-C5
28	d	223	PQN	C16-C17-C18-C19
29	A	787	BCR	C17-C18-C19-C20
29	A	788	BCR	C6-C7-C8-C9
29	A	788	BCR	C7-C8-C9-C10
29	A	788	BCR	C12-C13-C14-C15
29	A	788	BCR	C35-C13-C14-C15
29	A	788	BCR	C14-C15-C16-C17
29	A	789	BCR	C23-C24-C25-C26
29	A	790	BCR	C7-C8-C9-C10
29	A	790	BCR	C21-C22-C23-C24
29	A	792	BCR	C7-C8-C9-C34
29	A	792	BCR	C11-C10-C9-C8
29	A	792	BCR	C11-C10-C9-C34
29	A	792	BCR	C11-C12-C13-C35
29	A	792	BCR	C12-C13-C14-C15
29	A	792	BCR	C35-C13-C14-C15
29	A	792	BCR	C16-C17-C18-C19
29	A	792	BCR	C16-C17-C18-C36
29	A	796	BCR	C23-C24-C25-C26
29	B	762	BCR	C7-C8-C9-C10
29	B	762	BCR	C7-C8-C9-C34
29	B	765	BCR	C11-C10-C9-C8
29	B	765	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
29	B	765	BCR	C10-C11-C12-C13
29	B	765	BCR	C36-C18-C19-C20
29	B	765	BCR	C18-C19-C20-C21
29	B	766	BCR	C11-C10-C9-C8
29	B	766	BCR	C11-C10-C9-C34
29	B	766	BCR	C10-C11-C12-C13
29	B	766	BCR	C21-C22-C23-C24
29	B	766	BCR	C37-C22-C23-C24
29	B	766	BCR	C22-C23-C24-C25
29	B	767	BCR	C23-C24-C25-C26
29	M	201	BCR	C21-C22-C23-C24
29	M	201	BCR	C37-C22-C23-C24
29	M	201	BCR	C23-C24-C25-C26
30	A	795	SQD	O5-C5-C6-S
30	A	795	SQD	C5-C6-S-O7
30	A	795	SQD	C5-C6-S-O8
30	A	795	SQD	C5-C6-S-O9
30	c	245	SQD	O6-C44-C45-O47
30	c	245	SQD	C8-C7-O47-C45
30	c	245	SQD	C5-C6-S-O7
30	c	245	SQD	C5-C6-S-O8
30	c	245	SQD	C5-C6-S-O9
30	g	190	SQD	O47-C45-C46-O48
30	g	190	SQD	O5-C5-C6-S
31	A	4002	DD6	C13-C14-C15-O1
31	A	4008	DD6	C13-C14-C15-O1
31	A	4008	DD6	C24-C25-C26-C27
31	A	4008	DD6	C5-C6-C8-C9
31	A	4008	DD6	C7-C6-C8-C9
31	F	4002	DD6	C-C1-C2-C3
31	F	4002	DD6	C24-C1-C2-C3
31	F	4002	DD6	C2-C1-C24-C25
31	F	4002	DD6	C25-C26-C27-C29
31	F	4002	DD6	C2-C3-C4-C5
31	F	4002	DD6	C5-C6-C8-C9
31	J	4002	DD6	C13-C14-C15-O1
31	a	620	DD6	C2-C1-C24-C25
31	a	620	DD6	C10-C11-C13-C14
31	a	620	DD6	C12-C11-C13-C14
31	c	620	DD6	C2-C1-C24-C25
31	c	623	DD6	C-C1-C24-C25
31	c	623	DD6	C2-C1-C24-C25

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Mol	Chain	Res	Type	Atoms
31	c	624	DD6	C10-C11-C13-C14
31	c	624	DD6	C12-C11-C13-C14
31	c	624	DD6	C1-C24-C25-C26
31	c	624	DD6	C25-C26-C27-C29
31	d	620	DD6	C2-C1-C24-C25
31	d	621	DD6	C10-C11-C13-C14
31	d	621	DD6	C12-C11-C13-C14
31	d	623	DD6	C10-C11-C13-C14
31	d	623	DD6	C13-C14-C15-O1
31	e	620	DD6	C9-C10-C11-C12
31	e	620	DD6	C9-C10-C11-C13
31	e	620	DD6	C25-C26-C27-C29
31	e	621	DD6	C2-C1-C24-C25
31	e	621	DD6	C10-C11-C13-C14
31	e	623	DD6	C11-C13-C14-C15
31	e	623	DD6	C24-C25-C26-C27
31	e	623	DD6	C25-C26-C27-C28
31	e	623	DD6	C25-C26-C27-C29
31	h	620	DD6	C2-C1-C24-C25
31	i	620	DD6	C2-C1-C24-C25
31	i	621	DD6	C-C1-C24-C25
31	i	621	DD6	C2-C1-C24-C25
31	j	620	DD6	C2-C1-C24-C25
31	j	621	DD6	C-C1-C24-C25
31	j	621	DD6	C2-C1-C24-C25
31	j	621	DD6	C24-C25-C26-C27
31	k	621	DD6	C2-C1-C24-C25
31	l	620	DD6	C10-C11-C13-C14
31	l	621	DD6	C-C1-C24-C25
31	l	621	DD6	C2-C1-C24-C25
31	m	620	DD6	C10-C11-C13-C14
31	m	621	DD6	C-C1-C24-C25
31	m	621	DD6	C2-C1-C24-C25
31	m	621	DD6	C10-C11-C13-C14
31	m	621	DD6	C12-C11-C13-C14
31	f	620	DD6	C10-C11-C13-C14
31	f	621	DD6	C2-C1-C24-C25
31	f	621	DD6	C10-C11-C13-C14
31	f	621	DD6	C12-C11-C13-C14
31	f	621	DD6	C13-C14-C15-C20
31	f	621	DD6	C13-C14-C15-O1
31	n	620	DD6	C13-C14-C15-O1

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Mol	Chain	Res	Type	Atoms
31	n	621	DD6	C11-C13-C14-C15
31	n	621	DD6	C1-C24-C25-C26
31	n	621	DD6	C25-C26-C27-C28
31	n	621	DD6	C25-C26-C27-C29
31	n	621	DD6	C3-C4-C5-C6
31	n	623	DD6	C1-C24-C25-C26
31	n	623	DD6	C3-C4-C5-C6
31	o	620	DD6	C-C1-C24-C25
31	o	620	DD6	C2-C1-C24-C25
31	o	620	DD6	C10-C11-C13-C14
31	o	621	DD6	C-C1-C24-C25
31	o	621	DD6	C2-C1-C24-C25
31	o	621	DD6	C24-C25-C26-C27
31	p	621	DD6	C2-C1-C24-C25
33	a	182	LMG	O9-C10-O7-C8
33	a	182	LMG	C11-C10-O7-C8
33	i	195	LMG	C2-C1-O1-C7
33	i	195	LMG	O6-C1-O1-C7
34	b	182	DGD	O1B-C1B-O2G-C2G
34	b	182	DGD	O1G-C1G-C2G-O2G
35	c	607	CHL	C3C-C2C-CMC-OMC
35	d	605	CHL	C1A-C2A-CAA-CBA
35	d	605	CHL	C3A-C2A-CAA-CBA
35	d	605	CHL	C1C-C2C-CMC-OMC
35	d	605	CHL	C3C-C2C-CMC-OMC
35	d	607	CHL	C1A-C2A-CAA-CBA
35	d	607	CHL	C3A-C2A-CAA-CBA
35	d	607	CHL	C1C-C2C-CMC-OMC
35	d	607	CHL	C4C-C3C-CAC-CBC
35	d	608	CHL	C1A-C2A-CAA-CBA
25	e	607	CLA	O1D-CGD-O2D-CED
25	o	614	CLA	O1D-CGD-O2D-CED
25	p	610	CLA	O1D-CGD-O2D-CED
25	A	764	CLA	O1D-CGD-O2D-CED
25	b	601	CLA	O1D-CGD-O2D-CED
25	l	614	CLA	O1D-CGD-O2D-CED
25	g	604	CLA	O1D-CGD-O2D-CED
25	n	612	CLA	O1D-CGD-O2D-CED
25	A	771	CLA	CBD-CGD-O2D-CED
25	B	746	CLA	CBD-CGD-O2D-CED
25	B	772	CLA	CBD-CGD-O2D-CED
25	B	775	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	b	601	CLA	CBD-CGD-O2D-CED
25	c	601	CLA	CBD-CGD-O2D-CED
25	c	608	CLA	CBD-CGD-O2D-CED
25	c	614	CLA	CBD-CGD-O2D-CED
25	d	603	CLA	CBD-CGD-O2D-CED
25	e	607	CLA	CBD-CGD-O2D-CED
25	k	615	CLA	CBD-CGD-O2D-CED
25	l	602	CLA	CBD-CGD-O2D-CED
25	l	612	CLA	CBD-CGD-O2D-CED
25	l	613	CLA	CBD-CGD-O2D-CED
25	l	617	CLA	CBD-CGD-O2D-CED
25	m	602	CLA	CBD-CGD-O2D-CED
25	m	604	CLA	CBD-CGD-O2D-CED
25	m	613	CLA	CBD-CGD-O2D-CED
25	n	605	CLA	CBD-CGD-O2D-CED
25	n	608	CLA	CBD-CGD-O2D-CED
25	o	614	CLA	CBD-CGD-O2D-CED
25	p	602	CLA	CBD-CGD-O2D-CED
25	p	608	CLA	CBD-CGD-O2D-CED
25	B	758	CLA	O1A-CGA-O2A-C1
25	B	768	CLA	O1A-CGA-O2A-C1
25	c	602	CLA	O1A-CGA-O2A-C1
25	h	608	CLA	O1A-CGA-O2A-C1
25	j	608	CLA	O1A-CGA-O2A-C1
25	f	602	CLA	O1A-CGA-O2A-C1
25	a	608	CLA	O1D-CGD-O2D-CED
25	l	617	CLA	O1D-CGD-O2D-CED
25	m	601	CLA	O1D-CGD-O2D-CED
25	o	601	CLA	O1D-CGD-O2D-CED
25	p	613	CLA	O1D-CGD-O2D-CED
25	A	761	CLA	CBA-CGA-O2A-C1
25	a	608	CLA	CBA-CGA-O2A-C1
25	i	602	CLA	CBA-CGA-O2A-C1
25	f	602	CLA	CBA-CGA-O2A-C1
35	d	608	CHL	CBD-CGD-O2D-CED
25	A	760	CLA	O1A-CGA-O2A-C1
25	A	761	CLA	O1A-CGA-O2A-C1
25	A	803	CLA	O1A-CGA-O2A-C1
25	A	808	CLA	O1A-CGA-O2A-C1
25	B	738	CLA	O1A-CGA-O2A-C1
25	B	752	CLA	O1A-CGA-O2A-C1
25	B	770	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	a	608	CLA	O1A-CGA-O2A-C1
25	j	618	CLA	O1A-CGA-O2A-C1
25	k	618	CLA	O1A-CGA-O2A-C1
25	f	610	CLA	O1A-CGA-O2A-C1
25	o	602	CLA	O1A-CGA-O2A-C1
27	b	181	LHG	O10-C23-O8-C6
27	c	243	LHG	O10-C23-O8-C6
27	m	182	LHG	O10-C23-O8-C6
27	g	189	LHG	O10-C23-O8-C6
33	a	182	LMG	O10-C28-O8-C9
25	A	801	CLA	C15-C16-C17-C18
25	f	612	CLA	O1D-CGD-O2D-CED
25	g	612	CLA	O1D-CGD-O2D-CED
25	n	608	CLA	O1D-CGD-O2D-CED
25	A	778	CLA	O1D-CGD-O2D-CED
25	h	601	CLA	O1D-CGD-O2D-CED
25	n	605	CLA	O1D-CGD-O2D-CED
25	f	615	CLA	C2A-CAA-CBA-CGA
25	B	777	CLA	CBD-CGD-O2D-CED
25	e	614	CLA	CBD-CGD-O2D-CED
27	d	237	LHG	O9-C7-O7-C5
27	h	189	LHG	O9-C7-O7-C5
27	h	190	LHG	O9-C7-O7-C5
27	g	189	LHG	O9-C7-O7-C5
30	c	245	SQD	O49-C7-O47-C45
34	e	205	DGD	O1B-C1B-O2G-C2G
25	d	610	CLA	C3-C5-C6-C7
25	j	610	CLA	C3-C5-C6-C7
25	k	610	CLA	C3-C5-C6-C7
25	g	610	CLA	C3-C5-C6-C7
28	d	223	PQN	C13-C15-C16-C17
25	c	608	CLA	O1D-CGD-O2D-CED
25	d	613	CLA	O1D-CGD-O2D-CED
25	A	760	CLA	CBA-CGA-O2A-C1
25	A	801	CLA	CBA-CGA-O2A-C1
25	A	803	CLA	CBA-CGA-O2A-C1
25	B	745	CLA	CBA-CGA-O2A-C1
25	B	768	CLA	CBA-CGA-O2A-C1
25	B	770	CLA	CBA-CGA-O2A-C1
25	c	602	CLA	CBA-CGA-O2A-C1
25	j	618	CLA	CBA-CGA-O2A-C1
27	c	243	LHG	C24-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
27	g	189	LHG	C24-C23-O8-C6
33	a	182	LMG	C29-C28-O8-C9
25	A	778	CLA	CBD-CGD-O2D-CED
25	A	783	CLA	CBD-CGD-O2D-CED
25	A	803	CLA	CBD-CGD-O2D-CED
25	B	756	CLA	CBD-CGD-O2D-CED
25	B	771	CLA	CBD-CGD-O2D-CED
25	B	780	CLA	CBD-CGD-O2D-CED
25	a	602	CLA	CBD-CGD-O2D-CED
25	j	613	CLA	CBD-CGD-O2D-CED
25	f	615	CLA	CBD-CGD-O2D-CED
25	n	603	CLA	CBD-CGD-O2D-CED
25	n	606	CLA	CBD-CGD-O2D-CED
25	p	604	CLA	CBD-CGD-O2D-CED
27	h	189	LHG	C8-C7-O7-C5
27	m	182	LHG	C8-C7-O7-C5
34	b	182	DGD	C2B-C1B-O2G-C2G
34	e	205	DGD	C2B-C1B-O2G-C2G
25	m	613	CLA	O1D-CGD-O2D-CED
25	B	780	CLA	O1D-CGD-O2D-CED
25	A	765	CLA	C4-C3-C5-C6
25	A	773	CLA	C4-C3-C5-C6
25	A	784	CLA	C4-C3-C5-C6
25	B	739	CLA	C4-C3-C5-C6
25	B	748	CLA	C4-C3-C5-C6
25	B	774	CLA	C4-C3-C5-C6
25	a	602	CLA	C4-C3-C5-C6
25	a	610	CLA	C4-C3-C5-C6
25	a	613	CLA	C4-C3-C5-C6
25	b	602	CLA	C4-C3-C5-C6
25	h	602	CLA	C4-C3-C5-C6
25	h	613	CLA	C4-C3-C5-C6
25	k	613	CLA	C4-C3-C5-C6
25	f	610	CLA	C4-C3-C5-C6
25	n	603	CLA	C4-C3-C5-C6
28	B	769	PQN	C14-C13-C15-C16
25	A	777	CLA	C2-C3-C5-C6
25	A	798	CLA	C2-C3-C5-C6
25	a	610	CLA	C2-C3-C5-C6
25	b	612	CLA	C2-C3-C5-C6
25	e	602	CLA	C2-C3-C5-C6
25	h	602	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	k	613	CLA	C2-C3-C5-C6
25	l	602	CLA	C2-C3-C5-C6
25	l	610	CLA	C2-C3-C5-C6
25	f	610	CLA	C2-C3-C5-C6
25	g	602	CLA	C2-C3-C5-C6
25	g	613	CLA	C2-C3-C5-C6
28	B	769	PQN	C12-C13-C15-C16
25	A	757	CLA	CBD-CGD-O2D-CED
25	o	613	CLA	O1D-CGD-O2D-CED
25	i	615	CLA	C2A-CAA-CBA-CGA
25	m	603	CLA	C2A-CAA-CBA-CGA
35	e	606	CHL	C2A-CAA-CBA-CGA
25	j	609	CLA	O1A-CGA-O2A-C1
25	A	772	CLA	C3-C5-C6-C7
25	A	808	CLA	C3-C5-C6-C7
25	B	741	CLA	C3-C5-C6-C7
25	k	602	CLA	C3-C5-C6-C7
25	n	603	CLA	C3-C5-C6-C7
28	B	761	PQN	C13-C15-C16-C17
25	A	753	CLA	CBA-CGA-O2A-C1
25	A	808	CLA	CBA-CGA-O2A-C1
25	B	738	CLA	CBA-CGA-O2A-C1
25	B	752	CLA	CBA-CGA-O2A-C1
25	B	758	CLA	CBA-CGA-O2A-C1
25	B	773	CLA	CBA-CGA-O2A-C1
25	d	610	CLA	CBA-CGA-O2A-C1
25	h	608	CLA	CBA-CGA-O2A-C1
25	i	608	CLA	CBA-CGA-O2A-C1
25	j	609	CLA	CBA-CGA-O2A-C1
25	k	604	CLA	CBA-CGA-O2A-C1
25	k	613	CLA	CBA-CGA-O2A-C1
25	f	610	CLA	CBA-CGA-O2A-C1
25	o	602	CLA	CBA-CGA-O2A-C1
25	p	609	CLA	CBA-CGA-O2A-C1
27	b	181	LHG	C24-C23-O8-C6
27	m	182	LHG	C24-C23-O8-C6
33	k	179	LMG	C29-C28-O8-C9
25	c	606	CLA	C2A-CAA-CBA-CGA
25	j	615	CLA	C2A-CAA-CBA-CGA
25	o	614	CLA	C2A-CAA-CBA-CGA
25	p	613	CLA	C2A-CAA-CBA-CGA
31	A	4008	DD6	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
31	n	621	DD6	C1-C2-C3-C4
31	p	621	DD6	C24-C25-C26-C27
25	A	753	CLA	O1A-CGA-O2A-C1
25	A	799	CLA	O1A-CGA-O2A-C1
25	B	745	CLA	O1A-CGA-O2A-C1
25	c	610	CLA	O1A-CGA-O2A-C1
25	d	610	CLA	O1A-CGA-O2A-C1
25	k	602	CLA	O1A-CGA-O2A-C1
25	p	609	CLA	O1A-CGA-O2A-C1
27	b	181	LHG	O9-C7-O7-C5
25	A	780	CLA	C3-C5-C6-C7
25	A	791	CLA	C3-C5-C6-C7
25	c	612	CLA	CBD-CGD-O2D-CED
25	g	614	CLA	CBD-CGD-O2D-CED
25	n	613	CLA	CBD-CGD-O2D-CED
25	p	612	CLA	CBD-CGD-O2D-CED
27	c	243	LHG	O2-C2-C3-O3
27	i	194	LHG	O2-C2-C3-O3
25	B	737	CLA	O1D-CGD-O2D-CED
25	B	772	CLA	O1D-CGD-O2D-CED
25	d	603	CLA	O1D-CGD-O2D-CED
25	l	613	CLA	O1D-CGD-O2D-CED
25	f	609	CLA	O1D-CGD-O2D-CED
35	d	606	CHL	O1D-CGD-O2D-CED
25	B	773	CLA	O1A-CGA-O2A-C1
25	e	610	CLA	O1A-CGA-O2A-C1
25	d	612	CLA	CBD-CGD-O2D-CED
25	f	613	CLA	CBD-CGD-O2D-CED
30	A	795	SQD	C8-C7-O47-C45
25	h	603	CLA	C2A-CAA-CBA-CGA
25	a	610	CLA	O1A-CGA-O2A-C1
25	i	601	CLA	O1A-CGA-O2A-C1
25	i	608	CLA	O1A-CGA-O2A-C1
25	n	602	CLA	O1A-CGA-O2A-C1
25	j	613	CLA	O1D-CGD-O2D-CED
25	A	755	CLA	C3-C5-C6-C7
25	A	766	CLA	C3-C5-C6-C7
25	A	768	CLA	CBD-CGD-O2D-CED
35	d	606	CHL	CBD-CGD-O2D-CED
33	B	786	LMG	O6-C5-C6-O5
25	e	604	CLA	O1D-CGD-O2D-CED
25	k	618	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	A	755	CLA	C4-C3-C5-C6
25	e	602	CLA	C4-C3-C5-C6
25	A	765	CLA	C2-C3-C5-C6
25	A	773	CLA	C2-C3-C5-C6
25	A	775	CLA	C2-C3-C5-C6
25	A	784	CLA	C2-C3-C5-C6
25	B	748	CLA	C2-C3-C5-C6
25	h	613	CLA	C2-C3-C5-C6
25	k	610	CLA	C2-C3-C5-C6
25	J	101	CLA	O1A-CGA-O2A-C1
25	k	604	CLA	O1A-CGA-O2A-C1
25	l	610	CLA	O1A-CGA-O2A-C1
25	g	602	CLA	O1A-CGA-O2A-C1
25	g	610	CLA	O1A-CGA-O2A-C1
33	k	179	LMG	O10-C28-O8-C9
27	g	189	LHG	C5-C4-O6-P
25	g	608	CLA	C2A-CAA-CBA-CGA
34	e	205	DGD	O1A-C1A-O1G-C1G
25	A	768	CLA	O1D-CGD-O2D-CED
25	A	764	CLA	O1A-CGA-O2A-C1
25	B	775	CLA	O1A-CGA-O2A-C1
30	c	245	SQD	O5-C1-O6-C44
30	g	190	SQD	O5-C1-O6-C44
34	b	182	DGD	O6D-C1D-O3G-C3G
25	n	606	CLA	O1D-CGD-O2D-CED
25	h	612	CLA	CBA-CGA-O2A-C1
25	g	613	CLA	CBA-CGA-O2A-C1
25	A	763	CLA	CBD-CGD-O2D-CED
25	A	780	CLA	CBD-CGD-O2D-CED
25	A	784	CLA	CBD-CGD-O2D-CED
25	B	739	CLA	CBD-CGD-O2D-CED
25	B	751	CLA	CBD-CGD-O2D-CED
25	B	753	CLA	CBD-CGD-O2D-CED
25	B	754	CLA	CBD-CGD-O2D-CED
25	b	603	CLA	CBD-CGD-O2D-CED
25	c	602	CLA	CBD-CGD-O2D-CED
25	c	603	CLA	CBD-CGD-O2D-CED
25	e	608	CLA	CBD-CGD-O2D-CED
25	h	601	CLA	CBD-CGD-O2D-CED
25	k	601	CLA	CBD-CGD-O2D-CED
25	k	603	CLA	CBD-CGD-O2D-CED
25	l	601	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	m	612	CLA	CBD-CGD-O2D-CED
25	p	601	CLA	CBD-CGD-O2D-CED
34	B	787	DGD	O6E-C5E-C6E-O5E
25	B	782	CLA	CBD-CGD-O2D-CED
25	j	611	CLA	CBD-CGD-O2D-CED
25	m	603	CLA	CBD-CGD-O2D-CED
25	o	603	CLA	CBD-CGD-O2D-CED
31	c	624	DD6	C3-C4-C5-C6
31	n	621	DD6	C11-C10-C9-C8
31	n	623	DD6	C1-C2-C3-C4
27	A	786	LHG	C1-C2-C3-O3
27	h	189	LHG	C1-C2-C3-O3
27	i	194	LHG	C1-C2-C3-O3
27	g	189	LHG	C1-C2-C3-O3
25	A	752	CLA	CBA-CGA-O2A-C1
25	A	777	CLA	CBA-CGA-O2A-C1
25	A	794	CLA	CBA-CGA-O2A-C1
25	A	799	CLA	CBA-CGA-O2A-C1
25	B	755	CLA	CBA-CGA-O2A-C1
25	B	778	CLA	CBA-CGA-O2A-C1
25	c	610	CLA	CBA-CGA-O2A-C1
25	e	610	CLA	CBA-CGA-O2A-C1
25	i	601	CLA	CBA-CGA-O2A-C1
25	j	612	CLA	CBA-CGA-O2A-C1
25	k	602	CLA	CBA-CGA-O2A-C1
25	l	610	CLA	CBA-CGA-O2A-C1
25	g	602	CLA	CBA-CGA-O2A-C1
25	g	610	CLA	CBA-CGA-O2A-C1
34	B	787	DGD	C2A-C1A-O1G-C1G
34	b	182	DGD	C2A-C1A-O1G-C1G
25	A	775	CLA	CBD-CGD-O2D-CED
25	A	799	CLA	CBD-CGD-O2D-CED
25	b	611	CLA	CBD-CGD-O2D-CED
25	i	602	CLA	CBD-CGD-O2D-CED
27	h	189	LHG	C24-C23-O8-C6
25	B	760	CLA	O1D-CGD-O2D-CED
25	c	613	CLA	O1D-CGD-O2D-CED
25	f	614	CLA	O1D-CGD-O2D-CED
25	B	756	CLA	C5-C6-C7-C8
25	B	778	CLA	O1A-CGA-O2A-C1
25	A	766	CLA	C4-C3-C5-C6
25	A	775	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	B	780	CLA	C4-C3-C5-C6
25	b	612	CLA	C4-C3-C5-C6
25	A	755	CLA	C2-C3-C5-C6
25	A	766	CLA	C2-C3-C5-C6
25	B	739	CLA	C2-C3-C5-C6
25	B	780	CLA	C2-C3-C5-C6
25	i	610	CLA	C2-C3-C5-C6
25	j	610	CLA	C2-C3-C5-C6
25	f	602	CLA	C2-C3-C5-C6
25	i	612	CLA	CBD-CGD-O2D-CED
25	n	609	CLA	CBD-CGD-O2D-CED
25	A	759	CLA	C6-C7-C8-C9
25	A	760	CLA	C11-C10-C8-C9
25	A	764	CLA	C11-C10-C8-C9
25	A	775	CLA	C11-C10-C8-C9
25	A	780	CLA	C11-C10-C8-C9
25	A	784	CLA	C11-C12-C13-C14
25	B	738	CLA	C11-C10-C8-C9
25	B	741	CLA	C11-C12-C13-C14
25	B	752	CLA	C14-C13-C15-C16
25	B	753	CLA	C11-C10-C8-C9
25	B	753	CLA	C11-C12-C13-C14
25	B	755	CLA	C11-C10-C8-C9
25	B	774	CLA	C11-C10-C8-C9
25	B	776	CLA	C11-C10-C8-C9
25	B	778	CLA	C11-C10-C8-C9
25	c	602	CLA	C6-C7-C8-C9
25	c	602	CLA	C11-C10-C8-C9
25	d	610	CLA	C11-C10-C8-C9
25	j	613	CLA	C6-C7-C8-C9
25	f	602	CLA	C6-C7-C8-C9
28	A	785	PQN	C16-C17-C18-C19
34	e	205	DGD	C2A-C1A-O1G-C1G
33	a	182	LMG	O6-C5-C6-O5
34	B	787	DGD	C4E-C5E-C6E-O5E
25	b	613	CLA	O1D-CGD-O2D-CED
25	c	619	CLA	O1D-CGD-O2D-CED
25	g	602	CLA	O1D-CGD-O2D-CED
30	A	795	SQD	C2-C1-O6-C44
30	c	245	SQD	C2-C1-O6-C44
30	g	190	SQD	C2-C1-O6-C44
34	b	182	DGD	C2D-C1D-O3G-C3G

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Mol	Chain	Res	Type	Atoms
27	h	190	LHG	O2-C2-C3-O3
25	d	614	CLA	O1D-CGD-O2D-CED
25	A	781	CLA	O1A-CGA-O2A-C1
33	B	786	LMG	C4-C5-C6-O5
25	d	601	CLA	CBD-CGD-O2D-CED
25	i	601	CLA	O1D-CGD-O2D-CED
29	A	787	BCR	C36-C18-C19-C20
29	A	788	BCR	C7-C8-C9-C34
29	A	790	BCR	C7-C8-C9-C34
29	A	790	BCR	C37-C22-C23-C24
29	A	796	BCR	C11-C12-C13-C35
29	B	766	BCR	C36-C18-C19-C20
29	B	767	BCR	C37-C22-C23-C24
31	A	4002	DD6	C12-C11-C13-C14
31	A	4008	DD6	C-C1-C24-C25
31	F	4002	DD6	C-C1-C24-C25
31	F	4002	DD6	C7-C6-C8-C9
31	a	620	DD6	C-C1-C24-C25
31	c	620	DD6	C-C1-C24-C25
31	c	623	DD6	C7-C6-C8-C9
31	c	624	DD6	C7-C6-C8-C9
31	d	620	DD6	C-C1-C24-C25
31	d	623	DD6	C12-C11-C13-C14
31	e	621	DD6	C-C1-C24-C25
31	e	621	DD6	C12-C11-C13-C14
31	h	620	DD6	C-C1-C24-C25
31	i	620	DD6	C-C1-C24-C25
31	j	620	DD6	C-C1-C24-C25
31	k	620	DD6	C-C1-C24-C25
31	k	621	DD6	C-C1-C24-C25
31	l	620	DD6	C12-C11-C13-C14
31	m	620	DD6	C12-C11-C13-C14
31	f	620	DD6	C-C1-C24-C25
31	f	620	DD6	C12-C11-C13-C14
31	f	621	DD6	C-C1-C24-C25
31	n	621	DD6	C12-C11-C13-C14
31	o	620	DD6	C12-C11-C13-C14
31	p	621	DD6	C-C1-C24-C25
29	A	792	BCR	C7-C8-C9-C10
29	A	792	BCR	C11-C12-C13-C14
29	A	796	BCR	C11-C12-C13-C14
29	B	765	BCR	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
29	B	766	BCR	C17-C18-C19-C20
31	A	4008	DD6	C2-C1-C24-C25
31	A	4008	DD6	C10-C11-C13-C14
31	c	623	DD6	C5-C6-C8-C9
31	c	624	DD6	C5-C6-C8-C9
31	e	623	DD6	C5-C6-C8-C9
31	n	620	DD6	C10-C11-C13-C14
25	B	773	CLA	C2A-CAA-CBA-CGA
25	a	608	CLA	C2A-CAA-CBA-CGA
25	f	610	CLA	O1D-CGD-O2D-CED
25	h	602	CLA	O1A-CGA-O2A-C1
25	i	610	CLA	O1A-CGA-O2A-C1
25	A	784	CLA	C10-C11-C12-C13
25	B	772	CLA	CBA-CGA-O2A-C1
25	J	101	CLA	CBA-CGA-O2A-C1
25	a	610	CLA	CBA-CGA-O2A-C1
25	n	602	CLA	CBA-CGA-O2A-C1
27	d	237	LHG	C24-C23-O8-C6
25	A	752	CLA	C15-C16-C17-C18
25	i	612	CLA	C2A-CAA-CBA-CGA
25	A	782	CLA	O1D-CGD-O2D-CED
25	B	785	CLA	O1D-CGD-O2D-CED
25	j	601	CLA	O1D-CGD-O2D-CED
25	p	608	CLA	O1D-CGD-O2D-CED
35	d	608	CHL	O1D-CGD-O2D-CED
25	A	752	CLA	CBD-CGD-O2D-CED
27	b	181	LHG	C25-C26-C27-C28
25	A	761	CLA	C8-C10-C11-C12
25	B	755	CLA	C5-C6-C7-C8
25	a	613	CLA	C5-C6-C7-C8
25	i	608	CLA	C8-C10-C11-C12
25	n	603	CLA	C5-C6-C7-C8
25	f	613	CLA	O1D-CGD-O2D-CED
25	A	761	CLA	C3-C5-C6-C7
25	A	779	CLA	O1D-CGD-O2D-CED
25	B	746	CLA	O1D-CGD-O2D-CED
25	h	618	CLA	O1D-CGD-O2D-CED
25	B	760	CLA	CBD-CGD-O2D-CED
25	c	609	CLA	CBD-CGD-O2D-CED
25	d	602	CLA	CBD-CGD-O2D-CED
25	g	601	CLA	CBD-CGD-O2D-CED
25	A	752	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
25	A	758	CLA	C11-C10-C8-C7
25	A	769	CLA	C11-C10-C8-C7
25	A	774	CLA	C11-C12-C13-C15
25	B	750	CLA	C11-C10-C8-C7
25	B	756	CLA	C11-C10-C8-C7
25	a	619	CLA	C11-C10-C8-C7
25	h	604	CLA	C11-C10-C8-C7
25	k	604	CLA	C12-C13-C15-C16
25	f	602	CLA	C11-C10-C8-C7
25	A	800	CLA	CBA-CGA-O2A-C1
25	A	777	CLA	C4-C3-C5-C6
27	c	243	LHG	C7-C8-C9-C10
27	h	190	LHG	C7-C8-C9-C10
29	B	766	BCR	C19-C20-C21-C22
31	c	624	DD6	C11-C10-C9-C8
31	e	621	DD6	C24-C25-C26-C27
31	e	623	DD6	C3-C4-C5-C6
30	A	795	SQD	O49-C7-O47-C45
25	B	737	CLA	C3-C5-C6-C7
28	B	769	PQN	C13-C15-C16-C17
25	b	603	CLA	C2A-CAA-CBA-CGA
25	A	763	CLA	C15-C16-C17-C18
25	A	776	CLA	C13-C15-C16-C17
25	B	778	CLA	C8-C10-C11-C12
25	k	604	CLA	C10-C11-C12-C13
33	i	195	LMG	C28-C29-C30-C31
25	A	777	CLA	O1A-CGA-O2A-C1
25	j	612	CLA	O1A-CGA-O2A-C1
34	B	787	DGD	O1A-C1A-O1G-C1G
25	B	743	CLA	CBD-CGD-O2D-CED
25	A	791	CLA	C10-C11-C12-C13
25	B	753	CLA	C5-C6-C7-C8
25	B	758	CLA	C15-C16-C17-C18
28	A	785	PQN	C25-C26-C27-C28
28	B	761	PQN	C25-C26-C27-C28
28	B	769	PQN	C15-C16-C17-C18
25	A	763	CLA	C2A-CAA-CBA-CGA
25	A	776	CLA	C2A-CAA-CBA-CGA
25	B	750	CLA	C2A-CAA-CBA-CGA
25	B	755	CLA	C2A-CAA-CBA-CGA
25	B	770	CLA	C2A-CAA-CBA-CGA
25	c	609	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
25	h	609	CLA	C2A-CAA-CBA-CGA
25	h	610	CLA	C2A-CAA-CBA-CGA
25	j	604	CLA	C2A-CAA-CBA-CGA
25	k	610	CLA	C2A-CAA-CBA-CGA
25	l	610	CLA	C2A-CAA-CBA-CGA
25	f	602	CLA	C2A-CAA-CBA-CGA
31	F	4002	DD6	C6-C8-C9-C10
31	e	620	DD6	C6-C8-C9-C10
31	e	623	DD6	C1-C24-C25-C26
25	B	778	CLA	C10-C11-C12-C13
25	i	602	CLA	C10-C11-C12-C13
27	g	189	LHG	C7-C8-C9-C10
30	c	245	SQD	C23-C24-C25-C26
25	A	801	CLA	O1A-CGA-O2A-C1
25	k	613	CLA	O1A-CGA-O2A-C1
25	A	765	CLA	C3-C5-C6-C7
25	e	604	CLA	CBD-CGD-O2D-CED
33	a	182	LMG	O6-C1-O1-C7
34	B	787	DGD	O6D-C1D-O3G-C3G
34	b	182	DGD	O6E-C1E-O5D-C6D
27	h	189	LHG	C10-C11-C12-C13
25	f	604	CLA	O1D-CGD-O2D-CED
25	A	755	CLA	C10-C11-C12-C13
25	A	761	CLA	C15-C16-C17-C18
25	A	763	CLA	C13-C15-C16-C17
25	A	766	CLA	C8-C10-C11-C12
25	A	769	CLA	C10-C11-C12-C13
25	A	772	CLA	C5-C6-C7-C8
25	B	784	CLA	C13-C15-C16-C17
25	c	610	CLA	C5-C6-C7-C8
25	e	602	CLA	C5-C6-C7-C8
25	k	604	CLA	C15-C16-C17-C18
27	A	786	LHG	O2-C2-C3-O3
27	m	182	LHG	O2-C2-C3-O3
27	g	189	LHG	O2-C2-C3-O3
34	b	182	DGD	O1A-C1A-O1G-C1G
25	A	767	CLA	C2A-CAA-CBA-CGA
25	p	602	CLA	C2A-CAA-CBA-CGA
25	A	752	CLA	C8-C10-C11-C12
25	B	748	CLA	C5-C6-C7-C8
25	B	779	CLA	C15-C16-C17-C18
25	B	784	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
33	a	182	LMG	C29-C30-C31-C32
25	A	780	CLA	O1D-CGD-O2D-CED
25	h	603	CLA	O1D-CGD-O2D-CED
25	h	615	CLA	CBD-CGD-O2D-CED
25	c	610	CLA	C4-C3-C5-C6
25	A	783	CLA	O1A-CGA-O2A-C1
25	k	610	CLA	O1A-CGA-O2A-C1
27	d	237	LHG	O10-C23-O8-C6
25	A	798	CLA	O1D-CGD-O2D-CED
25	e	614	CLA	O1D-CGD-O2D-CED
25	A	777	CLA	C5-C6-C7-C8
25	B	745	CLA	C8-C10-C11-C12
25	j	613	CLA	C5-C6-C7-C8
25	A	765	CLA	CBA-CGA-O2A-C1
25	A	797	CLA	CBA-CGA-O2A-C1
25	B	775	CLA	CBA-CGA-O2A-C1
25	e	602	CLA	CBA-CGA-O2A-C1
25	i	610	CLA	CBA-CGA-O2A-C1
25	A	773	CLA	O1A-CGA-O2A-C1
25	h	614	CLA	O1D-CGD-O2D-CED
25	B	753	CLA	C10-C11-C12-C13
25	B	779	CLA	C3-C5-C6-C7
25	c	613	CLA	C3-C5-C6-C7
25	i	603	CLA	C2A-CAA-CBA-CGA
31	c	624	DD6	C1-C2-C3-C4
31	e	623	DD6	C1-C2-C3-C4
25	B	784	CLA	C8-C10-C11-C12
27	d	237	LHG	C7-C8-C9-C10
27	j	198	LHG	C1-C2-C3-O3
27	m	182	LHG	C1-C2-C3-O3
25	A	761	CLA	C2A-CAA-CBA-CGA
25	A	771	CLA	C2A-CAA-CBA-CGA
25	a	611	CLA	C2A-CAA-CBA-CGA
25	i	610	CLA	C2A-CAA-CBA-CGA
25	j	610	CLA	C2A-CAA-CBA-CGA
25	f	610	CLA	C2A-CAA-CBA-CGA
25	i	603	CLA	O1D-CGD-O2D-CED
25	A	764	CLA	CBA-CGA-O2A-C1
25	B	738	CLA	C10-C11-C12-C13
25	B	741	CLA	C8-C10-C11-C12
25	B	773	CLA	C10-C11-C12-C13
25	B	779	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	B	784	CLA	C5-C6-C7-C8
25	l	609	CLA	C5-C6-C7-C8
25	m	602	CLA	C10-C11-C12-C13
31	e	620	DD6	C25-C26-C27-C28
25	A	804	CLA	CBD-CGD-O2D-CED
25	B	785	CLA	CBD-CGD-O2D-CED
25	e	611	CLA	CBD-CGD-O2D-CED
25	B	757	CLA	O1D-CGD-O2D-CED
25	A	777	CLA	C13-C15-C16-C17
25	B	757	CLA	C8-C10-C11-C12
28	B	761	PQN	C20-C21-C22-C23
33	a	182	LMG	C4-C5-C6-O5
25	B	752	CLA	C8-C10-C11-C12
25	B	758	CLA	C5-C6-C7-C8
25	B	779	CLA	C10-C11-C12-C13
25	i	613	CLA	C8-C10-C11-C12
25	m	602	CLA	C5-C6-C7-C8
25	A	766	CLA	O1D-CGD-O2D-CED
25	A	781	CLA	CBA-CGA-O2A-C1
25	d	609	CLA	CBA-CGA-O2A-C1
25	B	744	CLA	C2A-CAA-CBA-CGA
25	o	603	CLA	C2A-CAA-CBA-CGA
25	p	604	CLA	C2A-CAA-CBA-CGA
25	k	610	CLA	C4-C3-C5-C6
25	g	602	CLA	C4-C3-C5-C6
25	a	613	CLA	C2-C3-C5-C6
25	o	609	CLA	O1D-CGD-O2D-CED
25	B	741	CLA	C10-C11-C12-C13
25	B	772	CLA	C1-C2-C3-C5
25	J	101	CLA	C1-C2-C3-C5
25	h	609	CLA	C1-C2-C3-C5
25	j	611	CLA	C1-C2-C3-C4
25	j	618	CLA	C1-C2-C3-C4
25	p	609	CLA	C1-C2-C3-C4
25	l	609	CLA	C11-C10-C8-C9
25	h	615	CLA	O1D-CGD-O2D-CED
25	o	612	CLA	O1D-CGD-O2D-CED
26	A	754	LMT	C2'-C1'-O1'-C1
33	a	182	LMG	C2-C1-O1-C7
33	k	179	LMG	C2-C1-O1-C7
34	B	787	DGD	C2D-C1D-O3G-C3G
34	b	182	DGD	C2E-C1E-O5D-C6D

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Mol	Chain	Res	Type	Atoms
27	d	237	LHG	C10-C11-C12-C13
27	j	198	LHG	C24-C23-O8-C6
25	A	769	CLA	C16-C17-C18-C19
25	g	613	CLA	O1A-CGA-O2A-C1
29	A	788	BCR	C11-C10-C9-C34
29	B	766	BCR	C35-C13-C14-C15
31	F	4002	DD6	C9-C10-C11-C12
31	e	623	DD6	C4-C5-C6-C7
31	n	621	DD6	C9-C10-C11-C12
31	n	621	DD6	C4-C5-C6-C7
31	n	623	DD6	C4-C5-C6-C7
27	h	189	LHG	O10-C23-O8-C6
29	A	789	BCR	C37-C22-C23-C24
29	A	790	BCR	C36-C18-C19-C20
29	B	762	BCR	C37-C22-C23-C24
31	A	4008	DD6	C12-C11-C13-C14
31	b	620	DD6	C12-C11-C13-C14
31	c	623	DD6	C12-C11-C13-C14
31	c	624	DD6	C-C1-C24-C25
31	e	623	DD6	C7-C6-C8-C9
31	g	620	DD6	C12-C11-C13-C14
31	g	621	DD6	C-C1-C24-C25
31	n	620	DD6	C12-C11-C13-C14
29	A	789	BCR	C21-C22-C23-C24
29	B	767	BCR	C21-C22-C23-C24
31	A	4002	DD6	C10-C11-C13-C14
31	c	623	DD6	C10-C11-C13-C14
31	k	620	DD6	C2-C1-C24-C25
31	f	620	DD6	C2-C1-C24-C25
31	n	621	DD6	C10-C11-C13-C14
25	h	609	CLA	O1A-CGA-O2A-C1
25	j	610	CLA	O1A-CGA-O2A-C1
25	B	774	CLA	C2A-CAA-CBA-CGA
25	e	613	CLA	C2A-CAA-CBA-CGA
25	i	601	CLA	C2A-CAA-CBA-CGA
35	d	605	CHL	C2A-CAA-CBA-CGA
25	l	609	CLA	C10-C11-C12-C13
27	b	181	LHG	O1-C1-C2-C3
27	j	198	LHG	O1-C1-C2-C3
25	k	615	CLA	O1D-CGD-O2D-CED
25	a	601	CLA	CBA-CGA-O2A-C1
31	i	621	DD6	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
25	A	801	CLA	C16-C17-C18-C20
25	A	805	CLA	C6-C7-C8-C9
25	a	613	CLA	C6-C7-C8-C9
25	g	613	CLA	C6-C7-C8-C9
25	g	613	CLA	C6-C7-C8-C10
25	p	602	CLA	O1D-CGD-O2D-CED
25	B	776	CLA	C3-C5-C6-C7
25	B	780	CLA	C3-C5-C6-C7
28	A	785	PQN	C13-C15-C16-C17
29	A	788	BCR	C11-C10-C9-C8
29	B	766	BCR	C12-C13-C14-C15
31	F	4002	DD6	C9-C10-C11-C13
31	e	623	DD6	C4-C5-C6-C8
31	n	621	DD6	C9-C10-C11-C13
31	n	621	DD6	C4-C5-C6-C8
31	n	623	DD6	C4-C5-C6-C8
26	A	754	LMT	O5'-C1'-O1'-C1
33	k	179	LMG	O6-C1-O1-C7
25	m	604	CLA	O1D-CGD-O2D-CED
27	A	756	LHG	C34-C35-C36-C37
25	A	768	CLA	CBA-CGA-O2A-C1
30	j	200	SQD	C24-C23-O48-C46
25	j	604	CLA	C5-C6-C7-C8
25	f	613	CLA	C8-C10-C11-C12
25	h	611	CLA	CBD-CGD-O2D-CED
25	i	604	CLA	C2A-CAA-CBA-CGA
25	g	604	CLA	C2A-CAA-CBA-CGA
25	j	604	CLA	C3-C5-C6-C7
25	B	777	CLA	C2-C1-O2A-CGA
25	e	608	CLA	O2A-C1-C2-C3
25	A	801	CLA	C16-C17-C18-C19
25	B	758	CLA	C16-C17-C18-C20
25	B	779	CLA	C16-C17-C18-C19
25	B	779	CLA	C16-C17-C18-C20
25	B	781	CLA	C16-C17-C18-C20
25	B	777	CLA	O1A-CGA-O2A-C1
25	h	612	CLA	O1A-CGA-O2A-C1
25	f	613	CLA	C10-C11-C12-C13
27	h	190	LHG	C10-C11-C12-C13
25	B	750	CLA	CBD-CGD-O2D-CED
25	i	602	CLA	C15-C16-C17-C18
27	b	181	LHG	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
25	c	609	CLA	O1D-CGD-O2D-CED
25	e	602	CLA	O1D-CGD-O2D-CED
25	l	612	CLA	O1D-CGD-O2D-CED
25	B	745	CLA	C10-C11-C12-C13
25	B	752	CLA	C5-C6-C7-C8
27	i	194	LHG	C26-C27-C28-C29
27	g	189	LHG	C9-C10-C11-C12
25	A	752	CLA	O1A-CGA-O2A-C1
25	e	613	CLA	CBA-CGA-O2A-C1
25	h	602	CLA	CBA-CGA-O2A-C1
27	A	756	LHG	C26-C27-C28-C29
33	B	786	LMG	C31-C32-C33-C34
33	i	195	LMG	C34-C35-C36-C37
25	A	772	CLA	C2-C1-O2A-CGA
27	j	198	LHG	O1-C1-C2-O2
25	h	613	CLA	C3-C5-C6-C7
27	g	189	LHG	C10-C11-C12-C13
25	A	783	CLA	O1D-CGD-O2D-CED
25	A	799	CLA	C10-C11-C12-C13
25	A	753	CLA	C4B-C3B-CAB-CBB
25	A	758	CLA	C4B-C3B-CAB-CBB
25	A	772	CLA	C4B-C3B-CAB-CBB
25	A	777	CLA	C4B-C3B-CAB-CBB
25	A	798	CLA	C4B-C3B-CAB-CBB
25	A	808	CLA	C4B-C3B-CAB-CBB
25	B	755	CLA	C4B-C3B-CAB-CBB
25	a	610	CLA	C4B-C3B-CAB-CBB
25	b	604	CLA	C4B-C3B-CAB-CBB
25	c	602	CLA	C4B-C3B-CAB-CBB
25	d	604	CLA	C4B-C3B-CAB-CBB
25	d	610	CLA	C4B-C3B-CAB-CBB
25	i	603	CLA	C4B-C3B-CAB-CBB
27	j	198	LHG	C28-C29-C30-C31
25	A	760	CLA	C16-C17-C18-C19
25	A	760	CLA	C16-C17-C18-C20
25	A	805	CLA	C6-C7-C8-C10
25	e	602	CLA	C16-C17-C18-C19
25	e	602	CLA	C16-C17-C18-C20
25	k	604	CLA	C16-C17-C18-C19
25	k	604	CLA	C16-C17-C18-C20
25	g	610	CLA	C6-C7-C8-C9
25	g	610	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
25	e	601	CLA	O1D-CGD-O2D-CED
25	k	603	CLA	O1D-CGD-O2D-CED
25	A	794	CLA	O1A-CGA-O2A-C1
25	A	798	CLA	O1A-CGA-O2A-C1
25	A	808	CLA	C2A-CAA-CBA-CGA
25	J	101	CLA	C2A-CAA-CBA-CGA
25	c	610	CLA	C2A-CAA-CBA-CGA
33	i	195	LMG	C12-C13-C14-C15
25	m	612	CLA	C2A-CAA-CBA-CGA
25	j	610	CLA	C10-C11-C12-C13
25	c	609	CLA	C11-C10-C8-C7
30	c	245	SQD	C12-C13-C14-C15
30	j	200	SQD	C24-C25-C26-C27
30	j	200	SQD	C23-C24-C25-C26
30	c	245	SQD	C24-C23-O48-C46
25	a	610	CLA	C5-C6-C7-C8
25	h	610	CLA	C5-C6-C7-C8
33	B	786	LMG	C41-C42-C43-C44
34	b	182	DGD	C3A-C4A-C5A-C6A
25	e	608	CLA	O1A-CGA-O2A-C1
25	B	784	CLA	C3-C5-C6-C7
25	f	602	CLA	C3-C5-C6-C7
25	A	765	CLA	C3A-C2A-CAA-CBA
25	A	794	CLA	C3A-C2A-CAA-CBA
25	A	802	CLA	C3A-C2A-CAA-CBA
25	B	756	CLA	C3A-C2A-CAA-CBA
25	B	758	CLA	C3A-C2A-CAA-CBA
25	B	775	CLA	C3A-C2A-CAA-CBA
25	B	776	CLA	C3A-C2A-CAA-CBA
25	B	781	CLA	C3A-C2A-CAA-CBA
25	a	609	CLA	C3A-C2A-CAA-CBA
25	b	604	CLA	C3A-C2A-CAA-CBA
25	c	606	CLA	C3A-C2A-CAA-CBA
25	i	603	CLA	C3A-C2A-CAA-CBA
25	i	612	CLA	C3A-C2A-CAA-CBA
25	j	601	CLA	C3A-C2A-CAA-CBA
25	j	608	CLA	C3A-C2A-CAA-CBA
25	k	604	CLA	C3A-C2A-CAA-CBA
25	l	604	CLA	C3A-C2A-CAA-CBA
25	l	608	CLA	C3A-C2A-CAA-CBA
25	l	612	CLA	C3A-C2A-CAA-CBA
25	m	603	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	o	603	CLA	C3A-C2A-CAA-CBA
25	o	608	CLA	C3A-C2A-CAA-CBA
25	p	604	CLA	C3A-C2A-CAA-CBA
35	c	607	CHL	C3A-C2A-CAA-CBA
35	e	606	CHL	C3A-C2A-CAA-CBA
25	A	761	CLA	O1D-CGD-O2D-CED
25	b	603	CLA	O1D-CGD-O2D-CED
25	B	741	CLA	C15-C16-C17-C18
25	B	753	CLA	C15-C16-C17-C18
25	B	784	CLA	C10-C11-C12-C13
30	g	190	SQD	C23-C24-C25-C26
25	B	773	CLA	O1D-CGD-O2D-CED
25	o	602	CLA	O1D-CGD-O2D-CED
31	F	4002	DD6	C1-C2-C3-C4
31	c	623	DD6	C24-C25-C26-C27
31	d	623	DD6	C24-C25-C26-C27
31	l	621	DD6	C24-C25-C26-C27
31	m	621	DD6	C24-C25-C26-C27
25	B	758	CLA	C16-C17-C18-C19
25	a	613	CLA	C6-C7-C8-C10
27	j	198	LHG	O10-C23-O8-C6
30	j	200	SQD	C25-C26-C27-C28
25	B	745	CLA	CBD-CGD-O2D-CED
25	j	603	CLA	CBD-CGD-O2D-CED
25	A	776	CLA	CBA-CGA-O2A-C1
25	l	602	CLA	CBA-CGA-O2A-C1
25	f	613	CLA	CBA-CGA-O2A-C1
33	k	179	LMG	O1-C7-C8-C9
25	B	770	CLA	C3-C5-C6-C7
25	c	601	CLA	O1D-CGD-O2D-CED
25	B	776	CLA	C10-C11-C12-C13
25	f	602	CLA	C10-C11-C12-C13
27	j	198	LHG	C9-C10-C11-C12
33	k	179	LMG	C30-C31-C32-C33
25	A	774	CLA	O1A-CGA-O2A-C1
25	c	609	CLA	O1A-CGA-O2A-C1
30	c	245	SQD	C11-C12-C13-C14
25	B	736	CLA	O1D-CGD-O2D-CED
25	B	751	CLA	O1D-CGD-O2D-CED
25	f	613	CLA	O1A-CGA-O2A-C1
25	A	757	CLA	C2B-C3B-CAB-CBB
25	A	769	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	A	770	CLA	C2B-C3B-CAB-CBB
25	A	772	CLA	C2B-C3B-CAB-CBB
25	A	777	CLA	C2B-C3B-CAB-CBB
25	A	799	CLA	C2B-C3B-CAB-CBB
25	A	804	CLA	C2B-C3B-CAB-CBB
25	B	737	CLA	C2B-C3B-CAB-CBB
25	B	755	CLA	C2B-C3B-CAB-CBB
25	d	604	CLA	C2B-C3B-CAB-CBB
25	j	602	CLA	C2B-C3B-CAB-CBB
29	A	788	BCR	C23-C24-C25-C26
29	A	788	BCR	C23-C24-C25-C30
29	A	789	BCR	C23-C24-C25-C30
29	A	792	BCR	C23-C24-C25-C26
29	A	792	BCR	C23-C24-C25-C30
29	A	796	BCR	C5-C6-C7-C8
29	M	201	BCR	C23-C24-C25-C30
25	b	613	CLA	CBD-CGD-O2D-CED
25	A	759	CLA	C5-C6-C7-C8
25	f	613	CLA	C3-C5-C6-C7
25	j	610	CLA	C15-C16-C17-C18
25	A	775	CLA	C2A-CAA-CBA-CGA
25	A	803	CLA	C2A-CAA-CBA-CGA
25	h	601	CLA	C2A-CAA-CBA-CGA
35	c	607	CHL	C2A-CAA-CBA-CGA
27	A	756	LHG	C28-C29-C30-C31
27	h	189	LHG	C9-C10-C11-C12
27	i	194	LHG	C11-C12-C13-C14
34	b	182	DGD	C4B-C5B-C6B-C7B
25	B	749	CLA	O1A-CGA-O2A-C1
25	B	756	CLA	O1A-CGA-O2A-C1
25	B	772	CLA	O1A-CGA-O2A-C1
25	c	604	CLA	O1A-CGA-O2A-C1
30	c	245	SQD	O10-C23-O48-C46
30	j	200	SQD	O10-C23-O48-C46
25	l	612	CLA	C2A-CAA-CBA-CGA
29	B	766	BCR	C18-C19-C20-C21
31	F	4002	DD6	C1-C24-C25-C26
31	e	620	DD6	C1-C24-C25-C26
31	e	623	DD6	C6-C8-C9-C10
25	n	603	CLA	C2-C3-C5-C6
27	i	194	LHG	C9-C10-C11-C12
33	B	786	LMG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
25	b	602	CLA	CBA-CGA-O2A-C1
25	c	613	CLA	CBA-CGA-O2A-C1
27	A	756	LHG	C32-C33-C34-C35
25	j	613	CLA	C10-C11-C12-C13
27	A	756	LHG	C24-C25-C26-C27
25	n	603	CLA	O1D-CGD-O2D-CED
25	B	748	CLA	CBD-CGD-O2D-CED
25	B	741	CLA	C5-C6-C7-C8
25	B	768	CLA	C5-C6-C7-C8
33	k	179	LMG	C28-C29-C30-C31
27	A	756	LHG	C30-C31-C32-C33
27	b	181	LHG	C28-C29-C30-C31
25	n	607	CLA	O1D-CGD-O2D-CED
31	k	621	DD6	C24-C25-C26-C27
31	n	623	DD6	C11-C10-C9-C8
25	a	603	CLA	C5-C6-C7-C8
25	h	602	CLA	C6-C7-C8-C9
27	A	786	LHG	C8-C7-O7-C5
27	j	198	LHG	C8-C7-O7-C5
27	A	786	LHG	O9-C7-O7-C5
25	A	776	CLA	C15-C16-C17-C18
25	A	799	CLA	C8-C10-C11-C12
29	A	796	BCR	C7-C8-C9-C34
31	b	620	DD6	C-C1-C24-C25
25	A	760	CLA	C3-C5-C6-C7
29	A	796	BCR	C7-C8-C9-C10
31	b	620	DD6	C10-C11-C13-C14
25	B	781	CLA	C2A-CAA-CBA-CGA
25	h	602	CLA	C6-C7-C8-C10
27	b	181	LHG	C23-C24-C25-C26
33	B	786	LMG	C32-C33-C34-C35
33	k	179	LMG	C34-C35-C36-C37
25	d	609	CLA	O1A-CGA-O2A-C1
25	B	739	CLA	C3-C5-C6-C7
25	h	602	CLA	C3-C5-C6-C7
25	A	783	CLA	C10-C11-C12-C13
25	A	784	CLA	C5-C6-C7-C8
25	k	610	CLA	CBA-CGA-O2A-C1
33	a	182	LMG	C10-C11-C12-C13
27	j	198	LHG	C10-C11-C12-C13
33	B	786	LMG	C29-C30-C31-C32
30	j	200	SQD	C8-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
30	g	190	SQD	C8-C7-O47-C45
33	B	786	LMG	C11-C10-O7-C8
30	c	245	SQD	C9-C10-C11-C12
33	B	786	LMG	C37-C38-C39-C40
27	A	786	LHG	C23-C24-C25-C26
25	A	774	CLA	C10-C11-C12-C13
28	B	761	PQN	C18-C20-C21-C22
25	B	758	CLA	O1D-CGD-O2D-CED
33	k	179	LMG	C12-C13-C14-C15
33	i	195	LMG	O6-C5-C6-O5
25	c	602	CLA	C3-C5-C6-C7
25	A	774	CLA	C15-C16-C17-C18
27	A	756	LHG	C27-C28-C29-C30
27	g	189	LHG	C24-C25-C26-C27
27	m	182	LHG	C9-C10-C11-C12
34	B	787	DGD	C6A-C7A-C8A-C9A
27	i	194	LHG	C27-C28-C29-C30
33	k	179	LMG	C31-C32-C33-C34
27	A	786	LHG	C10-C11-C12-C13
27	d	237	LHG	C9-C10-C11-C12
25	a	603	CLA	C4-C3-C5-C6
25	l	610	CLA	C4-C3-C5-C6
25	n	602	CLA	C4-C3-C5-C6
27	j	198	LHG	O9-C7-O7-C5
25	h	608	CLA	C2A-CAA-CBA-CGA
25	k	613	CLA	C2A-CAA-CBA-CGA
30	g	190	SQD	C24-C23-O48-C46
30	c	245	SQD	C10-C11-C12-C13
25	m	610	CLA	O1D-CGD-O2D-CED
27	i	194	LHG	C10-C11-C12-C13
25	a	602	CLA	C10-C11-C12-C13
27	A	786	LHG	C11-C12-C13-C14
25	k	612	CLA	C2A-CAA-CBA-CGA
25	B	779	CLA	O1D-CGD-O2D-CED
27	b	181	LHG	O1-C1-C2-O2
25	k	609	CLA	O1A-CGA-O2A-C1
25	A	800	CLA	O2A-C1-C2-C3
25	A	762	CLA	C1A-C2A-CAA-CBA
25	A	764	CLA	C1A-C2A-CAA-CBA
25	A	768	CLA	C1A-C2A-CAA-CBA
25	A	780	CLA	C1A-C2A-CAA-CBA
25	A	794	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	A	801	CLA	C1A-C2A-CAA-CBA
25	B	745	CLA	C1A-C2A-CAA-CBA
25	B	756	CLA	C1A-C2A-CAA-CBA
25	B	779	CLA	C1A-C2A-CAA-CBA
25	J	101	CLA	C1A-C2A-CAA-CBA
25	b	604	CLA	C1A-C2A-CAA-CBA
25	c	608	CLA	C1A-C2A-CAA-CBA
25	c	610	CLA	C1A-C2A-CAA-CBA
25	c	611	CLA	C1A-C2A-CAA-CBA
25	d	604	CLA	C1A-C2A-CAA-CBA
25	d	609	CLA	C1A-C2A-CAA-CBA
25	h	602	CLA	C1A-C2A-CAA-CBA
25	h	611	CLA	C1A-C2A-CAA-CBA
25	i	603	CLA	C1A-C2A-CAA-CBA
25	i	610	CLA	C1A-C2A-CAA-CBA
25	j	610	CLA	C1A-C2A-CAA-CBA
25	k	610	CLA	C1A-C2A-CAA-CBA
25	l	604	CLA	C1A-C2A-CAA-CBA
25	l	610	CLA	C1A-C2A-CAA-CBA
25	l	611	CLA	C1A-C2A-CAA-CBA
25	l	612	CLA	C1A-C2A-CAA-CBA
25	m	603	CLA	C1A-C2A-CAA-CBA
25	g	602	CLA	C1A-C2A-CAA-CBA
25	g	610	CLA	C1A-C2A-CAA-CBA
25	o	603	CLA	C1A-C2A-CAA-CBA
25	o	608	CLA	C1A-C2A-CAA-CBA
25	p	604	CLA	C1A-C2A-CAA-CBA
25	A	784	CLA	C15-C16-C17-C18
25	m	602	CLA	O1A-CGA-O2A-C1
25	B	748	CLA	C10-C11-C12-C13
27	h	189	LHG	C11-C10-C9-C8
27	j	198	LHG	C27-C28-C29-C30
27	g	189	LHG	O6-C4-C5-C6
30	j	200	SQD	O49-C7-O47-C45
25	A	752	CLA	C11-C10-C8-C7
25	A	753	CLA	C11-C10-C8-C7
25	A	764	CLA	C11-C10-C8-C7
25	A	777	CLA	C11-C10-C8-C7
25	A	783	CLA	C11-C10-C8-C7
25	A	799	CLA	C11-C10-C8-C7
25	A	801	CLA	C12-C13-C15-C16
25	B	746	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
25	B	752	CLA	C6-C7-C8-C10
25	B	756	CLA	C6-C7-C8-C10
25	B	757	CLA	C11-C10-C8-C7
25	B	784	CLA	C6-C7-C8-C10
25	h	612	CLA	C6-C7-C8-C10
25	i	613	CLA	C11-C10-C8-C7
25	k	610	CLA	C6-C7-C8-C10
28	A	785	PQN	C16-C17-C18-C20
26	A	754	LMT	C2-C3-C4-C5
27	A	786	LHG	C18-C19-C20-C21
25	A	760	CLA	C10-C11-C12-C13
25	a	602	CLA	C5-C6-C7-C8
25	B	740	CLA	C3A-C2A-CAA-CBA
25	b	601	CLA	C3A-C2A-CAA-CBA
25	d	614	CLA	C3A-C2A-CAA-CBA
25	e	614	CLA	C3A-C2A-CAA-CBA
25	f	601	CLA	C3A-C2A-CAA-CBA
25	f	614	CLA	C3A-C2A-CAA-CBA
25	n	612	CLA	C3A-C2A-CAA-CBA
25	p	601	CLA	C3A-C2A-CAA-CBA
25	k	604	CLA	C4-C3-C5-C6
25	A	770	CLA	C2-C3-C5-C6
26	A	754	LMT	O1'-C1-C2-C3
27	g	189	LHG	C25-C26-C27-C28
25	A	762	CLA	C1-C2-C3-C4
25	d	601	CLA	C1-C2-C3-C4
25	m	610	CLA	CBD-CGD-O2D-CED
25	A	801	CLA	C2A-CAA-CBA-CGA
25	b	612	CLA	C2A-CAA-CBA-CGA
25	c	608	CLA	C2A-CAA-CBA-CGA
25	A	769	CLA	C11-C10-C8-C9
25	B	739	CLA	C6-C7-C8-C9
25	B	745	CLA	C11-C12-C13-C14
25	B	757	CLA	C11-C10-C8-C9
25	B	784	CLA	C6-C7-C8-C9
25	h	612	CLA	C6-C7-C8-C9
27	m	182	LHG	C10-C11-C12-C13
25	A	780	CLA	CBA-CGA-O2A-C1
25	j	604	CLA	CBA-CGA-O2A-C1
35	c	607	CHL	CBA-CGA-O2A-C1
25	b	602	CLA	O1D-CGD-O2D-CED
34	B	787	DGD	C4A-C5A-C6A-C7A

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Mol	Chain	Res	Type	Atoms
25	d	612	CLA	O1D-CGD-O2D-CED
30	c	245	SQD	O6-C44-C45-C46
30	j	200	SQD	C44-C45-C46-O48
30	g	190	SQD	C44-C45-C46-O48
33	a	182	LMG	O1-C7-C8-C9
25	A	791	CLA	C5-C6-C7-C8
25	i	608	CLA	C5-C6-C7-C8
25	B	751	CLA	CBA-CGA-O2A-C1
25	B	777	CLA	CBA-CGA-O2A-C1
25	c	609	CLA	CBA-CGA-O2A-C1
27	i	194	LHG	C24-C23-O8-C6
34	b	182	DGD	O6E-C5E-C6E-O5E
29	B	765	BCR	C20-C21-C22-C37
31	c	624	DD6	C4-C5-C6-C7
31	e	623	DD6	C-C1-C2-C3
31	n	623	DD6	C9-C10-C11-C12
27	A	756	LHG	C33-C34-C35-C36
27	i	194	LHG	C23-C24-C25-C26
25	e	609	CLA	O1A-CGA-O2A-C1
25	A	770	CLA	C4-C3-C5-C6
25	A	764	CLA	C5-C6-C7-C8
31	c	624	DD6	C2-C1-C24-C25
30	g	190	SQD	O10-C23-O48-C46
25	A	780	CLA	C5-C6-C7-C8
25	B	739	CLA	C10-C11-C12-C13
28	B	769	PQN	C18-C20-C21-C22
25	o	612	CLA	CHA-CBD-CGD-O1D
25	A	791	CLA	C2A-CAA-CBA-CGA
25	e	608	CLA	C2A-CAA-CBA-CGA
25	p	610	CLA	C2A-CAA-CBA-CGA
25	f	610	CLA	C3-C5-C6-C7
34	b	182	DGD	C2A-C3A-C4A-C5A
25	h	613	CLA	O1D-CGD-O2D-CED
25	n	603	CLA	CBA-CGA-O2A-C1
25	A	760	CLA	O2A-C1-C2-C3
25	B	750	CLA	O2A-C1-C2-C3
25	B	773	CLA	O2A-C1-C2-C3
35	d	605	CHL	O2A-C1-C2-C3
27	A	786	LHG	C16-C17-C18-C19
29	A	796	BCR	C9-C10-C11-C12
31	J	4002	DD6	C1-C2-C3-C4
35	d	606	CHL	C3C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
35	e	606	CHL	C3C-C2C-CMC-OMC
25	A	759	CLA	C11-C12-C13-C14
25	B	756	CLA	C11-C12-C13-C14
34	B	787	DGD	C3A-C4A-C5A-C6A
25	g	609	CLA	CBD-CGD-O2D-CED
27	h	189	LHG	C12-C13-C14-C15
29	B	765	BCR	C20-C21-C22-C23
27	b	181	LHG	O6-C4-C5-O7
33	k	179	LMG	C33-C34-C35-C36
30	c	245	SQD	C11-C10-C9-C8
25	A	771	CLA	C4-C3-C5-C6
25	a	619	CLA	C15-C16-C17-C18
30	c	245	SQD	C24-C25-C26-C27
25	A	766	CLA	C10-C11-C12-C13
25	A	780	CLA	C10-C11-C12-C13
27	c	243	LHG	C24-C25-C26-C27
30	j	200	SQD	C10-C11-C12-C13
25	A	772	CLA	C2A-CAA-CBA-CGA
27	j	198	LHG	C30-C31-C32-C33
27	i	194	LHG	O8-C23-C24-C25
25	B	745	CLA	C15-C16-C17-C18
27	h	190	LHG	C12-C13-C14-C15
28	B	761	PQN	C15-C16-C17-C18
25	g	602	CLA	C5-C6-C7-C8
30	c	245	SQD	C25-C26-C27-C28
27	i	194	LHG	C11-C10-C9-C8
25	A	774	CLA	CBA-CGA-O2A-C1
25	A	798	CLA	CBA-CGA-O2A-C1
25	a	602	CLA	CBA-CGA-O2A-C1
27	i	194	LHG	C28-C29-C30-C31
35	c	607	CHL	C1C-C2C-CMC-OMC
35	e	606	CHL	C1C-C2C-CMC-OMC
25	A	791	CLA	CBD-CGD-O2D-CED
26	A	754	LMT	C3-C4-C5-C6
34	B	787	DGD	C8A-C9A-CAA-CBA
25	c	609	CLA	C10-C11-C12-C13
25	a	603	CLA	C3-C5-C6-C7
25	p	604	CLA	O1D-CGD-O2D-CED
25	A	770	CLA	C13-C15-C16-C17
25	A	768	CLA	C11-C10-C8-C9
25	A	776	CLA	C4-C3-C5-C6
25	B	755	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	c	609	CLA	C4-C3-C5-C6
25	B	777	CLA	C5-C6-C7-C8
25	A	760	CLA	C15-C16-C17-C18
33	B	786	LMG	C38-C39-C40-C41
25	B	747	CLA	C2-C1-O2A-CGA
25	A	752	CLA	C11-C10-C8-C9
25	A	753	CLA	C11-C10-C8-C9
25	A	791	CLA	C11-C12-C13-C14
25	A	799	CLA	C11-C10-C8-C9
25	B	746	CLA	C11-C10-C8-C9
25	B	752	CLA	C6-C7-C8-C9
25	B	756	CLA	C6-C7-C8-C9
25	B	756	CLA	C11-C10-C8-C9
25	d	610	CLA	C6-C7-C8-C9
25	e	602	CLA	C14-C13-C15-C16
25	i	608	CLA	C6-C7-C8-C9
25	k	604	CLA	C6-C7-C8-C9
28	A	785	PQN	C19-C18-C20-C21
25	A	763	CLA	C8-C10-C11-C12
25	B	737	CLA	C5-C6-C7-C8
25	B	758	CLA	C13-C15-C16-C17
25	f	613	CLA	C5-C6-C7-C8
27	h	190	LHG	C2-C3-O3-P
25	B	782	CLA	C4B-C3B-CAB-CBB
25	c	610	CLA	C4B-C3B-CAB-CBB
25	j	612	CLA	C4B-C3B-CAB-CBB
25	k	610	CLA	C4B-C3B-CAB-CBB
25	A	758	CLA	C2A-CAA-CBA-CGA
25	m	602	CLA	C2A-CAA-CBA-CGA
27	A	786	LHG	C25-C26-C27-C28
34	B	787	DGD	C5A-C6A-C7A-C8A
34	B	787	DGD	C3B-C4B-C5B-C6B
25	A	778	CLA	C2A-CAA-CBA-CGA
25	A	772	CLA	C15-C16-C17-C18
27	c	243	LHG	O6-C4-C5-C6
27	d	237	LHG	O6-C4-C5-C6
25	o	612	CLA	CAD-CBD-CGD-O2D
25	A	755	CLA	C11-C10-C8-C7
25	A	760	CLA	C11-C10-C8-C7
25	A	780	CLA	C11-C10-C8-C7
25	A	801	CLA	C11-C12-C13-C15
25	B	738	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
25	B	739	CLA	C11-C10-C8-C7
25	B	745	CLA	C12-C13-C15-C16
25	B	753	CLA	C11-C10-C8-C7
25	B	755	CLA	C11-C10-C8-C7
25	B	758	CLA	C12-C13-C15-C16
25	d	610	CLA	C6-C7-C8-C10
25	e	602	CLA	C12-C13-C15-C16
25	i	608	CLA	C6-C7-C8-C10
25	j	610	CLA	C11-C10-C8-C7
25	k	604	CLA	C11-C10-C8-C7
25	f	602	CLA	C6-C7-C8-C10
28	A	785	PQN	C17-C18-C20-C21
25	B	750	CLA	C10-C11-C12-C13
25	d	610	CLA	C11-C12-C13-C14
25	A	805	CLA	O1D-CGD-O2D-CED
25	A	791	CLA	C15-C16-C17-C18
34	B	787	DGD	C6B-C7B-C8B-C9B
27	m	182	LHG	C24-C25-C26-C27
25	g	608	CLA	C2C-C3C-CAC-CBC
34	b	182	DGD	C5B-C6B-C7B-C8B
25	n	602	CLA	C10-C11-C12-C13
25	B	739	CLA	O1A-CGA-O2A-C1
27	i	194	LHG	O10-C23-O8-C6
25	A	767	CLA	C3A-C2A-CAA-CBA
25	B	744	CLA	C3A-C2A-CAA-CBA
25	B	771	CLA	C3A-C2A-CAA-CBA
25	B	781	CLA	C4-C3-C5-C6
25	c	608	CLA	C3A-C2A-CAA-CBA
25	d	604	CLA	C3A-C2A-CAA-CBA
25	d	609	CLA	C3A-C2A-CAA-CBA
25	h	610	CLA	C3A-C2A-CAA-CBA
25	j	604	CLA	C4-C3-C5-C6
25	j	611	CLA	C3A-C2A-CAA-CBA
25	l	609	CLA	C3A-C2A-CAA-CBA
25	l	611	CLA	C3A-C2A-CAA-CBA
25	m	602	CLA	C3A-C2A-CAA-CBA
25	g	613	CLA	C3A-C2A-CAA-CBA
25	j	610	CLA	CBA-CGA-O2A-C1
29	A	788	BCR	C15-C16-C17-C18
31	f	621	DD6	C24-C25-C26-C27
27	b	181	LHG	C24-C25-C26-C27
25	A	784	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	g	621	DD6	C2-C1-C24-C25
25	h	608	CLA	O2A-C1-C2-C3
25	l	613	CLA	O2A-C1-C2-C3
25	n	609	CLA	O1D-CGD-O2D-CED
25	A	769	CLA	CBA-CGA-O2A-C1
30	g	190	SQD	O6-C44-C45-C46
34	b	182	DGD	O1G-C1G-C2G-C3G
25	A	759	CLA	C3-C5-C6-C7
25	A	801	CLA	C3-C5-C6-C7
25	B	755	CLA	C8-C10-C11-C12
31	c	624	DD6	C25-C26-C27-C28
25	A	763	CLA	O1A-CGA-O2A-C1
25	B	758	CLA	C1-C2-C3-C4
25	B	777	CLA	C1-C2-C3-C4
25	j	612	CLA	C1-C2-C3-C4
35	c	607	CHL	C1A-C2A-CAA-CBA
35	e	606	CHL	C1A-C2A-CAA-CBA
25	B	777	CLA	C4-C3-C5-C6
25	l	609	CLA	C4-C3-C5-C6
25	B	756	CLA	C2-C3-C5-C6
25	a	613	CLA	O1D-CGD-O2D-CED
27	A	786	LHG	C30-C31-C32-C33
27	h	190	LHG	C24-C25-C26-C27
27	A	786	LHG	C32-C33-C34-C35
30	g	190	SQD	O49-C7-O47-C45
27	A	786	LHG	O6-C4-C5-O7
27	c	243	LHG	O6-C4-C5-O7
25	c	612	CLA	C2A-CAA-CBA-CGA
29	B	763	BCR	C23-C24-C25-C26
25	A	808	CLA	C5-C6-C7-C8
25	l	609	CLA	O1D-CGD-O2D-CED
25	p	612	CLA	O1D-CGD-O2D-CED
25	n	604	CLA	O2A-C1-C2-C3
25	B	746	CLA	C16-C17-C18-C19
25	A	784	CLA	CAA-CBA-CGA-O2A
25	B	749	CLA	C2A-CAA-CBA-CGA
25	k	613	CLA	O1D-CGD-O2D-CED
30	j	200	SQD	O47-C45-C46-O48
30	g	190	SQD	O6-C44-C45-O47
33	a	182	LMG	O1-C7-C8-O7
25	B	776	CLA	O1D-CGD-O2D-CED
33	B	786	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
25	A	801	CLA	C4-C3-C5-C6
25	A	775	CLA	C5-C6-C7-C8
25	A	776	CLA	C2-C3-C5-C6
25	l	610	CLA	C5-C6-C7-C8
33	k	179	LMG	C11-C12-C13-C14
25	A	773	CLA	C1-C2-C3-C5
25	A	794	CLA	C1-C2-C3-C5
25	A	803	CLA	C1-C2-C3-C5
25	B	737	CLA	C1-C2-C3-C5
25	B	739	CLA	C1-C2-C3-C5
25	B	755	CLA	C1-C2-C3-C5
25	B	778	CLA	C1-C2-C3-C5
25	B	784	CLA	C1-C2-C3-C5
25	a	613	CLA	C1-C2-C3-C5
25	c	613	CLA	C1-C2-C3-C5
25	d	604	CLA	C1-C2-C3-C5
25	e	610	CLA	C1-C2-C3-C5
25	h	602	CLA	C1-C2-C3-C5
25	h	610	CLA	C1-C2-C3-C5
25	i	613	CLA	C1-C2-C3-C5
25	j	604	CLA	C1-C2-C3-C5
25	j	612	CLA	C1-C2-C3-C5
25	j	613	CLA	C1-C2-C3-C5
25	k	610	CLA	C1-C2-C3-C5
25	k	613	CLA	C1-C2-C3-C5
25	l	609	CLA	C1-C2-C3-C5
25	f	610	CLA	C1-C2-C3-C5
25	n	602	CLA	C1-C2-C3-C5
25	A	769	CLA	C16-C17-C18-C20
25	l	602	CLA	C10-C11-C12-C13
33	i	195	LMG	C32-C33-C34-C35
34	b	182	DGD	C6A-C7A-C8A-C9A
25	h	610	CLA	C6-C7-C8-C9
25	B	782	CLA	C1-C2-C3-C5
25	a	601	CLA	C1-C2-C3-C4
25	d	601	CLA	C1-C2-C3-C5
25	e	604	CLA	C1-C2-C3-C4
25	k	608	CLA	C1-C2-C3-C5
25	k	609	CLA	C1-C2-C3-C4
25	A	761	CLA	C14-C13-C15-C16
25	A	763	CLA	C11-C10-C8-C9
25	B	745	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	B	753	CLA	C6-C7-C8-C9
27	A	756	LHG	O8-C23-C24-C25
25	A	801	CLA	C8-C10-C11-C12
25	B	781	CLA	C16-C17-C18-C19
25	m	602	CLA	O1D-CGD-O2D-CED
34	B	787	DGD	CAA-CBA-CCA-CDA
25	b	601	CLA	C1A-C2A-CAA-CBA
25	b	610	CLA	C1A-C2A-CAA-CBA
25	e	601	CLA	C1A-C2A-CAA-CBA
25	f	611	CLA	C1A-C2A-CAA-CBA
25	g	611	CLA	C1A-C2A-CAA-CBA
25	p	601	CLA	C1A-C2A-CAA-CBA
25	p	603	CLA	C1A-C2A-CAA-CBA
25	n	613	CLA	O1D-CGD-O2D-CED
27	A	756	LHG	C7-C8-C9-C10
25	e	608	CLA	CBA-CGA-O2A-C1
31	F	4002	DD6	C11-C10-C9-C8
31	c	624	DD6	C24-C25-C26-C27
31	n	620	DD6	C24-C25-C26-C27
25	A	770	CLA	C5-C6-C7-C8
27	d	237	LHG	C1-C2-C3-O3
29	A	792	BCR	C20-C21-C22-C37
31	e	620	DD6	C-C1-C2-C3
25	B	778	CLA	C3-C5-C6-C7
25	i	613	CLA	CAA-CBA-CGA-O2A
25	h	609	CLA	CBA-CGA-O2A-C1
27	A	756	LHG	O6-C4-C5-C6
25	A	759	CLA	C11-C12-C13-C15
25	A	777	CLA	C16-C17-C18-C20
31	e	620	DD6	C12-C11-C13-C14
31	m	620	DD6	C-C1-C24-C25
25	A	752	CLA	C12-C13-C15-C16
25	A	758	CLA	C12-C13-C15-C16
25	A	759	CLA	C6-C7-C8-C10
25	A	763	CLA	C12-C13-C15-C16
25	A	771	CLA	C11-C10-C8-C7
25	A	801	CLA	C11-C10-C8-C7
25	B	739	CLA	C6-C7-C8-C10
25	B	753	CLA	C6-C7-C8-C10
25	B	776	CLA	C11-C10-C8-C7
25	j	613	CLA	C6-C7-C8-C10
25	k	604	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
33	a	182	LMG	C14-C15-C16-C17
25	A	774	CLA	C16-C17-C18-C19
29	B	762	BCR	C21-C22-C23-C24
31	b	620	DD6	C2-C1-C24-C25
31	g	620	DD6	C10-C11-C13-C14
25	A	797	CLA	O1A-CGA-O2A-C1
25	B	755	CLA	O1A-CGA-O2A-C1
25	B	784	CLA	O1A-CGA-O2A-C1
25	d	601	CLA	O1A-CGA-O2A-C1
25	A	755	CLA	C2A-CAA-CBA-CGA
25	A	768	CLA	C2A-CAA-CBA-CGA
25	B	746	CLA	C2A-CAA-CBA-CGA
25	B	772	CLA	C2A-CAA-CBA-CGA
25	l	602	CLA	C2A-CAA-CBA-CGA
25	l	613	CLA	C2A-CAA-CBA-CGA
33	a	182	LMG	C11-C12-C13-C14
25	B	755	CLA	C11-C12-C13-C14
25	B	756	CLA	C11-C12-C13-C15
25	B	746	CLA	C4-C3-C5-C6
25	B	746	CLA	O1A-CGA-O2A-C1
25	e	613	CLA	O1A-CGA-O2A-C1
25	B	748	CLA	C11-C12-C13-C14
25	l	610	CLA	C3-C5-C6-C7
25	h	618	CLA	CBD-CGD-O2D-CED
25	B	776	CLA	O2A-C1-C2-C3
25	j	612	CLA	O2A-C1-C2-C3
25	b	604	CLA	O1D-CGD-O2D-CED
25	i	601	CLA	C5-C6-C7-C8
25	B	746	CLA	C3-C5-C6-C7
31	c	624	DD6	C4-C5-C6-C8
31	e	623	DD6	C24-C1-C2-C3
31	n	623	DD6	C9-C10-C11-C13
25	A	770	CLA	C15-C16-C17-C18
27	d	237	LHG	O6-C4-C5-O7
27	m	182	LHG	O6-C4-C5-O7
27	g	189	LHG	O6-C4-C5-O7
25	B	746	CLA	C15-C16-C17-C18
27	b	181	LHG	C4-C5-C6-O8
34	B	787	DGD	C1G-C2G-C3G-O3G
25	B	742	CLA	C2A-CAA-CBA-CGA
25	i	611	CLA	CBD-CGD-O2D-CED
25	A	781	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	j	609	CLA	O1D-CGD-O2D-CED
27	g	189	LHG	O7-C5-C6-O8
30	A	795	SQD	O6-C44-C45-O47
25	A	801	CLA	C11-C10-C8-C9
25	B	758	CLA	C14-C13-C15-C16
25	B	784	CLA	C11-C12-C13-C14
25	j	613	CLA	C14-C13-C15-C16
34	b	182	DGD	C4A-C5A-C6A-C7A
25	a	602	CLA	O1A-CGA-O2A-C1
25	B	779	CLA	C2-C1-O2A-CGA
29	A	792	BCR	C9-C10-C11-C12
25	l	609	CLA	C11-C12-C13-C14
27	A	756	LHG	C23-C24-C25-C26
25	A	760	CLA	C2-C3-C5-C6
25	A	801	CLA	C5-C6-C7-C8
25	B	753	CLA	C8-C10-C11-C12
25	B	781	CLA	C13-C15-C16-C17
25	f	613	CLA	C2A-CAA-CBA-CGA
25	A	777	CLA	C16-C17-C18-C19
25	B	738	CLA	C16-C17-C18-C19
25	f	610	CLA	C6-C7-C8-C9
31	F	4002	DD6	C25-C26-C27-C28
35	d	606	CHL	C4C-C3C-CAC-CBC
25	A	783	CLA	CBA-CGA-O2A-C1
27	c	243	LHG	C11-C10-C9-C8
25	g	602	CLA	C3-C5-C6-C7
31	c	620	DD6	C12-C11-C13-C14
25	A	764	CLA	C4B-C3B-CAB-CBB
25	A	783	CLA	C4B-C3B-CAB-CBB
25	B	736	CLA	C4B-C3B-CAB-CBB
25	B	744	CLA	C1A-C2A-CAA-CBA
25	B	746	CLA	C4B-C3B-CAB-CBB
25	B	774	CLA	C4B-C3B-CAB-CBB
25	c	614	CLA	C4B-C3B-CAB-CBB
25	e	607	CLA	C4B-C3B-CAB-CBB
25	h	614	CLA	C4B-C3B-CAB-CBB
25	k	604	CLA	C4B-C3B-CAB-CBB
25	n	604	CLA	C4B-C3B-CAB-CBB
25	p	602	CLA	C4B-C3B-CAB-CBB
25	B	783	CLA	CBA-CGA-O2A-C1
25	B	756	CLA	C4-C3-C5-C6
29	A	790	BCR	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
31	c	620	DD6	C10-C11-C13-C14
25	A	798	CLA	C2A-CAA-CBA-CGA
25	j	608	CLA	C2A-CAA-CBA-CGA
27	b	181	LHG	O6-C4-C5-C6
25	A	772	CLA	CBD-CGD-O2D-CED
25	A	803	CLA	C2-C3-C5-C6
33	B	786	LMG	C30-C31-C32-C33
25	A	761	CLA	C11-C12-C13-C15
25	A	766	CLA	C11-C10-C8-C7
25	A	770	CLA	C12-C13-C15-C16
25	B	741	CLA	C11-C12-C13-C15
25	B	748	CLA	C11-C10-C8-C7
25	B	774	CLA	C11-C10-C8-C7
25	c	602	CLA	C6-C7-C8-C10
25	d	610	CLA	C11-C10-C8-C7
25	i	608	CLA	C12-C13-C15-C16
25	i	613	CLA	C6-C7-C8-C10
25	A	799	CLA	C11-C12-C13-C14
25	b	605	CLA	O1D-CGD-O2D-CED
25	c	614	CLA	O1D-CGD-O2D-CED
27	a	181	LHG	O2-C2-C3-O3
25	d	603	CLA	C3A-C2A-CAA-CBA
25	k	614	CLA	C3A-C2A-CAA-CBA
25	m	610	CLA	C3A-C2A-CAA-CBA
25	p	603	CLA	C3A-C2A-CAA-CBA
25	B	756	CLA	CBA-CGA-O2A-C1
25	A	807	CLA	O2A-C1-C2-C3
25	B	777	CLA	O1D-CGD-O2D-CED
25	a	612	CLA	CBD-CGD-O2D-CED
25	e	612	CLA	C2A-CAA-CBA-CGA
25	f	603	CLA	O1D-CGD-O2D-CED
35	d	606	CHL	C3A-C2A-CAA-CBA
25	j	604	CLA	C2-C3-C5-C6
25	B	778	CLA	C15-C16-C17-C18
25	o	603	CLA	O1D-CGD-O2D-CED
25	A	752	CLA	C14-C13-C15-C16
25	A	755	CLA	C11-C10-C8-C9
25	A	758	CLA	C14-C13-C15-C16
25	A	771	CLA	C11-C10-C8-C9
25	A	774	CLA	C11-C12-C13-C14
25	e	602	CLA	O1A-CGA-O2A-C1
29	B	762	BCR	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
31	d	621	DD6	C24-C25-C26-C27
25	B	749	CLA	C1-C2-C3-C4
27	i	194	LHG	C24-C25-C26-C27
25	d	610	CLA	C5-C6-C7-C8
27	j	198	LHG	C25-C26-C27-C28
25	a	601	CLA	O1A-CGA-O2A-C1
33	k	179	LMG	O1-C7-C8-O7
27	a	181	LHG	C1-C2-C3-O3
25	c	604	CLA	O2A-C1-C2-C3
27	c	243	LHG	C4-C5-C6-O8
30	A	795	SQD	O6-C44-C45-C46
34	e	205	DGD	C1G-C2G-C3G-O3G
28	d	223	PQN	C15-C16-C17-C18
25	l	609	CLA	O1A-CGA-O2A-C1
25	e	607	CLA	C2A-CAA-CBA-CGA
25	f	602	CLA	CBD-CGD-O2D-CED
25	A	774	CLA	CAD-CBD-CGD-O2D
25	B	743	CLA	CAD-CBD-CGD-O2D
25	B	784	CLA	CAD-CBD-CGD-O2D
25	c	619	CLA	CAD-CBD-CGD-O2D
25	e	603	CLA	CAD-CBD-CGD-O2D
25	f	615	CLA	CAD-CBD-CGD-O2D
25	g	612	CLA	CAD-CBD-CGD-O2D
25	n	603	CLA	CAD-CBD-CGD-O2D
34	B	787	DGD	C7A-C8A-C9A-CAA
25	A	804	CLA	O1A-CGA-O2A-C1
27	j	198	LHG	C12-C13-C14-C15
25	A	759	CLA	O1A-CGA-O2A-C1
25	A	765	CLA	C10-C11-C12-C13
25	i	602	CLA	C16-C17-C18-C20
25	k	608	CLA	O1D-CGD-O2D-CED
25	A	752	CLA	CAD-CBD-CGD-O1D
25	A	757	CLA	CAD-CBD-CGD-O1D
25	A	766	CLA	CAD-CBD-CGD-O1D
25	A	772	CLA	CHA-CBD-CGD-O2D
25	A	774	CLA	CAD-CBD-CGD-O1D
25	A	801	CLA	CHA-CBD-CGD-O2D
25	A	804	CLA	CAD-CBD-CGD-O1D
25	A	808	CLA	CAD-CBD-CGD-O1D
25	B	738	CLA	CAD-CBD-CGD-O1D
25	B	743	CLA	CAD-CBD-CGD-O1D
25	B	745	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	B	749	CLA	CHA-CBD-CGD-O2D
25	B	771	CLA	CHA-CBD-CGD-O2D
25	B	782	CLA	CAD-CBD-CGD-O1D
25	B	784	CLA	CAD-CBD-CGD-O1D
25	c	601	CLA	CAD-CBD-CGD-O1D
25	c	602	CLA	CHA-CBD-CGD-O2D
25	d	601	CLA	CAD-CBD-CGD-O1D
25	e	603	CLA	CAD-CBD-CGD-O1D
25	e	607	CLA	CAD-CBD-CGD-O1D
25	h	603	CLA	CHA-CBD-CGD-O1D
25	i	608	CLA	CHA-CBD-CGD-O1D
25	l	602	CLA	CHA-CBD-CGD-O2D
25	l	612	CLA	CAD-CBD-CGD-O1D
25	l	613	CLA	CHA-CBD-CGD-O1D
25	f	614	CLA	CAD-CBD-CGD-O1D
25	g	602	CLA	CAD-CBD-CGD-O1D
25	g	612	CLA	CAD-CBD-CGD-O1D
25	n	603	CLA	CAD-CBD-CGD-O1D
25	o	614	CLA	CHA-CBD-CGD-O1D
25	o	614	CLA	CHA-CBD-CGD-O2D
25	p	602	CLA	CAD-CBD-CGD-O1D
25	p	608	CLA	CHA-CBD-CGD-O1D
27	b	181	LHG	C3-O3-P-O4
27	b	181	LHG	C4-O6-P-O4
27	h	190	LHG	C3-O3-P-O6
27	j	198	LHG	C4-O6-P-O4
27	m	182	LHG	C3-O3-P-O5
27	m	182	LHG	C4-O6-P-O3
27	g	189	LHG	C3-O3-P-O4
27	g	189	LHG	C4-O6-P-O5
29	A	787	BCR	C9-C10-C11-C12
29	B	763	BCR	C9-C10-C11-C12
29	M	201	BCR	C13-C14-C15-C16
31	c	623	DD6	C11-C10-C9-C8
31	e	623	DD6	C11-C10-C9-C8
31	g	621	DD6	C3-C4-C5-C6
35	c	607	CHL	CHA-CBD-CGD-O2D
35	d	606	CHL	CHA-CBD-CGD-O2D
25	i	608	CLA	C16-C17-C18-C20
25	A	753	CLA	C2B-C3B-CAB-CBB
25	A	758	CLA	C2B-C3B-CAB-CBB
25	A	763	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	A	783	CLA	C2B-C3B-CAB-CBB
25	A	798	CLA	C2B-C3B-CAB-CBB
25	A	808	CLA	C2B-C3B-CAB-CBB
25	B	746	CLA	C2B-C3B-CAB-CBB
25	a	610	CLA	C2B-C3B-CAB-CBB
25	b	604	CLA	C2B-C3B-CAB-CBB
25	c	602	CLA	C2B-C3B-CAB-CBB
25	d	610	CLA	C2B-C3B-CAB-CBB
25	e	607	CLA	C2B-C3B-CAB-CBB
25	i	603	CLA	C2B-C3B-CAB-CBB
25	j	612	CLA	C2B-C3B-CAB-CBB
25	k	604	CLA	C2B-C3B-CAB-CBB
25	n	604	CLA	C2B-C3B-CAB-CBB
25	p	602	CLA	C2B-C3B-CAB-CBB
29	A	796	BCR	C23-C24-C25-C30
25	A	769	CLA	C2-C3-C5-C6
25	B	781	CLA	C2-C3-C5-C6
27	c	243	LHG	C2-C3-O3-P
27	d	237	LHG	C2-C3-O3-P
25	A	781	CLA	CAA-CBA-CGA-O2A
25	A	800	CLA	O1A-CGA-O2A-C1
25	c	616	CLA	CBD-CGD-O2D-CED
27	j	198	LHG	C26-C27-C28-C29
25	A	794	CLA	C3-C5-C6-C7
25	A	769	CLA	C15-C16-C17-C18
25	B	736	CLA	C13-C15-C16-C17
33	k	179	LMG	O6-C5-C6-O5
29	B	762	BCR	C9-C10-C11-C12
25	B	755	CLA	C11-C12-C13-C15
27	A	786	LHG	O6-C4-C5-C6
27	h	190	LHG	O6-C4-C5-C6
25	A	773	CLA	CBA-CGA-O2A-C1
25	B	774	CLA	C3-C5-C6-C7
25	i	601	CLA	C3-C5-C6-C7
25	A	770	CLA	C14-C13-C15-C16
25	B	748	CLA	C11-C10-C8-C9
25	a	602	CLA	C11-C10-C8-C9
25	i	613	CLA	C6-C7-C8-C9
25	k	610	CLA	C6-C7-C8-C9
25	f	602	CLA	C11-C10-C8-C9
25	B	752	CLA	C12-C13-C15-C16
27	A	756	LHG	O6-C4-C5-O7

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Mol	Chain	Res	Type	Atoms
25	a	604	CLA	CBD-CGD-O2D-CED
25	B	738	CLA	C4-C3-C5-C6
25	i	608	CLA	C4-C3-C5-C6
25	c	609	CLA	C2-C3-C5-C6
25	e	610	CLA	C2-C3-C5-C6
25	i	608	CLA	C16-C17-C18-C19
25	B	747	CLA	CBA-CGA-O2A-C1
33	B	786	LMG	C11-C12-C13-C14
25	d	610	CLA	C8-C10-C11-C12
25	l	602	CLA	O1D-CGD-O2D-CED
33	a	182	LMG	C30-C31-C32-C33
25	a	613	CLA	C2A-CAA-CBA-CGA
25	h	612	CLA	C10-C11-C12-C13
25	h	610	CLA	CAA-CBA-CGA-O2A
25	m	602	CLA	CAA-CBA-CGA-O2A
25	A	776	CLA	C10-C11-C12-C13
25	B	737	CLA	C2C-C3C-CAC-CBC
35	d	606	CHL	C1C-C2C-CMC-OMC
27	m	182	LHG	C26-C27-C28-C29
33	i	195	LMG	C8-C7-O1-C1
25	A	784	CLA	C2A-CAA-CBA-CGA
25	B	771	CLA	C4-C3-C5-C6
25	i	610	CLA	C4-C3-C5-C6
25	B	779	CLA	C2-C3-C5-C6
25	i	613	CLA	C2-C3-C5-C6
27	g	189	LHG	C11-C12-C13-C14
34	B	787	DGD	C4B-C5B-C6B-C7B
25	B	784	CLA	CAA-CBA-CGA-O2A
25	A	766	CLA	C11-C10-C8-C9
25	A	771	CLA	O1D-CGD-O2D-CED
25	B	775	CLA	O1D-CGD-O2D-CED
25	A	763	CLA	C4B-C3B-CAB-CBB
25	i	610	CLA	C4B-C3B-CAB-CBB
27	A	786	LHG	C24-C25-C26-C27
25	B	752	CLA	C10-C11-C12-C13
27	A	786	LHG	C19-C20-C21-C22
25	A	776	CLA	O1A-CGA-O2A-C1
25	B	774	CLA	C11-C12-C13-C15
25	c	604	CLA	CBA-CGA-O2A-C1
25	g	609	CLA	CBA-CGA-O2A-C1
25	B	741	CLA	C4-C3-C5-C6
25	f	613	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	A	774	CLA	C11-C10-C8-C7
25	B	745	CLA	C11-C10-C8-C7
25	c	602	CLA	C11-C10-C8-C7
25	j	610	CLA	C11-C12-C13-C15
25	A	768	CLA	O1A-CGA-O2A-C1
25	n	603	CLA	O1A-CGA-O2A-C1
25	A	770	CLA	C3A-C2A-CAA-CBA
25	A	775	CLA	C3A-C2A-CAA-CBA
25	A	779	CLA	C3A-C2A-CAA-CBA
25	A	781	CLA	C3A-C2A-CAA-CBA
25	B	757	CLA	C3A-C2A-CAA-CBA
25	b	605	CLA	C3A-C2A-CAA-CBA
25	e	608	CLA	C3A-C2A-CAA-CBA
25	i	609	CLA	C3A-C2A-CAA-CBA
25	m	609	CLA	C3A-C2A-CAA-CBA
25	g	618	CLA	C3A-C2A-CAA-CBA
33	B	786	LMG	C36-C37-C38-C39
29	A	790	BCR	C11-C10-C9-C34
29	A	790	BCR	C16-C17-C18-C36
29	B	764	BCR	C11-C10-C9-C34
29	B	764	BCR	C20-C21-C22-C37
31	F	4002	DD6	C4-C5-C6-C7
31	g	620	DD6	C4-C5-C6-C7
33	B	786	LMG	C33-C34-C35-C36
27	i	194	LHG	O10-C23-C24-C25
25	A	774	CLA	C5-C6-C7-C8
25	B	752	CLA	C13-C15-C16-C17
25	B	781	CLA	C5-C6-C7-C8
34	e	205	DGD	C1B-C2B-C3B-C4B
27	a	181	LHG	C24-C25-C26-C27
29	A	787	BCR	C15-C16-C17-C18
31	f	620	DD6	C11-C10-C9-C8
31	o	620	DD6	C24-C25-C26-C27
25	B	736	CLA	C15-C16-C17-C18
27	j	198	LHG	C2-C3-O3-P
25	l	603	CLA	C2A-CAA-CBA-CGA
25	g	608	CLA	CAA-CBA-CGA-O2A
31	m	620	DD6	C2-C1-C24-C25
26	A	754	LMT	C5-C6-C7-C8
25	B	745	CLA	C4-C3-C5-C6
25	B	738	CLA	C2-C3-C5-C6
25	k	604	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	p	610	CLA	CAA-CBA-CGA-O2A
35	e	606	CHL	CAA-CBA-CGA-O2A
25	j	610	CLA	O1D-CGD-O2D-CED
25	m	603	CLA	C6-C7-C8-C9
33	B	786	LMG	C21-C22-C23-C24
25	n	604	CLA	C2C-C3C-CAC-CBC
25	o	609	CLA	CAA-CBA-CGA-O2A
25	A	794	CLA	C8-C10-C11-C12
25	A	783	CLA	C11-C12-C13-C14
25	B	738	CLA	C11-C12-C13-C14
25	B	741	CLA	C14-C13-C15-C16
25	j	610	CLA	C11-C12-C13-C14
25	m	602	CLA	C6-C7-C8-C9
28	A	785	PQN	C21-C22-C23-C24
27	g	189	LHG	O1-C1-C2-C3
25	c	613	CLA	CBD-CGD-O2D-CED
25	a	604	CLA	CAA-CBA-CGA-O2A
27	j	198	LHG	C4-C5-O7-C7
27	j	198	LHG	C6-C5-O7-C7
27	g	189	LHG	C6-C5-O7-C7
25	A	772	CLA	C1-C2-C3-C4
25	A	791	CLA	C1-C2-C3-C4
25	A	799	CLA	C1-C2-C3-C4
25	B	757	CLA	C1-C2-C3-C4
25	B	778	CLA	C1-C2-C3-C4
25	h	602	CLA	C1-C2-C3-C4
25	h	604	CLA	C1-C2-C3-C4
25	h	612	CLA	C1-C2-C3-C4
25	h	613	CLA	C1-C2-C3-C4
25	k	602	CLA	C1-C2-C3-C4
25	B	747	CLA	CBD-CGD-O2D-CED
25	e	603	CLA	CBD-CGD-O2D-CED
33	i	195	LMG	C37-C38-C39-C40
25	p	610	CLA	CAA-CBA-CGA-O1A
25	c	613	CLA	C2A-CAA-CBA-CGA
25	A	758	CLA	C1A-C2A-CAA-CBA
25	A	808	CLA	C1A-C2A-CAA-CBA
25	B	738	CLA	C1A-C2A-CAA-CBA
25	B	771	CLA	C1A-C2A-CAA-CBA
25	a	612	CLA	C1A-C2A-CAA-CBA
25	i	609	CLA	C1A-C2A-CAA-CBA
25	g	613	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	o	614	CLA	C1A-C2A-CAA-CBA
29	A	790	BCR	C11-C10-C9-C8
29	A	790	BCR	C16-C17-C18-C19
29	A	792	BCR	C20-C21-C22-C23
29	B	764	BCR	C11-C10-C9-C8
29	B	764	BCR	C20-C21-C22-C23
31	F	4002	DD6	C4-C5-C6-C8
31	g	620	DD6	C4-C5-C6-C8
33	k	179	LMG	C4-C5-C6-O5
25	c	609	CLA	C11-C12-C13-C14
25	B	785	CLA	CAA-CBA-CGA-O1A
33	i	195	LMG	C30-C31-C32-C33
25	B	784	CLA	CAA-CBA-CGA-O1A
25	A	764	CLA	C2B-C3B-CAB-CBB
25	B	736	CLA	C2B-C3B-CAB-CBB
25	B	774	CLA	C2B-C3B-CAB-CBB
25	c	614	CLA	C2B-C3B-CAB-CBB
25	h	614	CLA	C2B-C3B-CAB-CBB
29	A	787	BCR	C23-C24-C25-C26
29	A	792	BCR	C1-C6-C7-C8
29	B	765	BCR	C23-C24-C25-C30
25	e	603	CLA	CAA-CBA-CGA-O1A
27	j	198	LHG	C5-C4-O6-P
25	B	745	CLA	C3-C5-C6-C7
25	d	611	CLA	CAA-CBA-CGA-O1A
25	e	613	CLA	C4-C3-C5-C6
28	d	223	PQN	C14-C13-C15-C16
25	A	771	CLA	O1A-CGA-O2A-C1
25	B	741	CLA	C2-C3-C5-C6
25	B	755	CLA	C2-C3-C5-C6
25	f	613	CLA	C2-C3-C5-C6
25	e	609	CLA	CBA-CGA-O2A-C1
25	A	797	CLA	O2A-C1-C2-C3
25	e	603	CLA	CAA-CBA-CGA-O2A
25	n	602	CLA	C11-C12-C13-C14
31	F	4002	DD6	C24-C25-C26-C27
25	A	775	CLA	C11-C10-C8-C7
25	A	784	CLA	C11-C12-C13-C15
25	B	739	CLA	C11-C12-C13-C15
25	i	602	CLA	C12-C13-C15-C16
25	n	602	CLA	C11-C10-C8-C7
25	B	738	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
25	B	774	CLA	C11-C12-C13-C14
25	A	769	CLA	C2A-CAA-CBA-CGA
25	d	604	CLA	C2A-CAA-CBA-CGA
25	g	613	CLA	C2A-CAA-CBA-CGA
30	j	200	SQD	O6-C44-C45-O47
25	p	608	CLA	C3A-C2A-CAA-CBA
25	B	749	CLA	CBA-CGA-O2A-C1
25	A	768	CLA	C11-C10-C8-C7
31	j	620	DD6	C12-C11-C13-C14
25	B	770	CLA	C4-C3-C5-C6
25	A	791	CLA	C2-C3-C5-C6
25	A	765	CLA	O1A-CGA-O2A-C1
25	A	791	CLA	C1-C2-C3-C5
25	B	757	CLA	C1-C2-C3-C5
25	B	758	CLA	C1-C2-C3-C5
25	B	768	CLA	C2-C1-O2A-CGA
25	B	774	CLA	C1-C2-C3-C5
25	B	777	CLA	C1-C2-C3-C5
25	h	604	CLA	C1-C2-C3-C5
25	k	602	CLA	C2-C1-O2A-CGA
35	e	606	CHL	CAA-CBA-CGA-O1A
31	e	620	DD6	C10-C11-C13-C14
25	f	610	CLA	C6-C7-C8-C10
25	A	759	CLA	C8-C10-C11-C12
35	d	605	CHL	CBA-CGA-O2A-C1
25	B	775	CLA	C1-C2-C3-C5
25	A	774	CLA	C11-C10-C8-C9
31	a	620	DD6	C11-C10-C9-C8
31	m	620	DD6	C3-C4-C5-C6
25	c	613	CLA	C4-C3-C5-C6
28	B	761	PQN	C14-C13-C15-C16
25	o	609	CLA	CAA-CBA-CGA-O1A
27	m	182	LHG	C2-C3-O3-P
27	A	786	LHG	C33-C34-C35-C36
25	a	608	CLA	C2-C3-C5-C6
25	A	808	CLA	O1D-CGD-O2D-CED
25	B	779	CLA	O1A-CGA-O2A-C1
25	c	610	CLA	C6-C7-C8-C9
27	i	194	LHG	C4-C5-C6-O8
25	d	603	CLA	C1A-C2A-CAA-CBA
25	l	614	CLA	C1A-C2A-CAA-CBA
25	A	766	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	h	613	CLA	C5-C6-C7-C8
25	c	602	CLA	C2A-CAA-CBA-CGA
25	d	611	CLA	C2A-CAA-CBA-CGA
27	A	786	LHG	C9-C10-C11-C12
25	A	783	CLA	CAA-CBA-CGA-O2A
27	d	237	LHG	C11-C10-C9-C8
27	g	189	LHG	O1-C1-C2-O2
25	B	758	CLA	C4-C3-C5-C6
25	g	613	CLA	C4-C3-C5-C6
31	b	621	DD6	C24-C25-C26-C27
25	a	604	CLA	CAA-CBA-CGA-O1A
25	m	602	CLA	C2-C3-C5-C6
25	g	608	CLA	CAA-CBA-CGA-O1A
25	B	743	CLA	O1D-CGD-O2D-CED
25	B	755	CLA	O1D-CGD-O2D-CED
25	m	602	CLA	CAA-CBA-CGA-O1A
25	A	773	CLA	C5-C6-C7-C8
25	A	752	CLA	CAA-CBA-CGA-O2A
25	a	602	CLA	CAA-CBA-CGA-O2A
25	d	611	CLA	CAA-CBA-CGA-O2A
25	p	609	CLA	C2C-C3C-CAC-CBC
33	a	182	LMG	C21-C22-C23-C24
25	B	752	CLA	C16-C17-C18-C20
25	m	613	CLA	C2C-C3C-CAC-CBC
29	B	765	BCR	C35-C13-C14-C15
29	B	766	BCR	C20-C21-C22-C37
25	A	753	CLA	C15-C16-C17-C18
25	j	613	CLA	CAA-CBA-CGA-O2A
33	B	786	LMG	C14-C15-C16-C17
27	j	198	LHG	C24-C25-C26-C27
33	B	786	LMG	O7-C8-C9-O8
25	h	613	CLA	CAA-CBA-CGA-O2A
25	e	602	CLA	C8-C10-C11-C12
25	B	741	CLA	C11-C10-C8-C7
25	B	778	CLA	C11-C10-C8-C7
25	B	754	CLA	C2A-CAA-CBA-CGA
25	b	611	CLA	O1D-CGD-O2D-CED
25	A	752	CLA	C11-C12-C13-C14
25	A	758	CLA	C11-C10-C8-C9
25	A	760	CLA	C6-C7-C8-C9
25	B	758	CLA	C6-C7-C8-C9
25	B	758	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
25	h	604	CLA	C11-C10-C8-C9
25	i	608	CLA	C14-C13-C15-C16
25	l	610	CLA	C6-C7-C8-C9
25	B	785	CLA	CAA-CBA-CGA-O2A
25	A	766	CLA	C2A-CAA-CBA-CGA
25	A	799	CLA	C2A-CAA-CBA-CGA
25	g	610	CLA	C2A-CAA-CBA-CGA
25	A	758	CLA	C2-C1-O2A-CGA
25	A	775	CLA	C2-C1-O2A-CGA
25	J	101	CLA	C2-C1-O2A-CGA
25	b	602	CLA	C2-C1-O2A-CGA
25	c	608	CLA	C2-C1-O2A-CGA
25	i	610	CLA	C2-C1-O2A-CGA
25	j	611	CLA	C2-C1-O2A-CGA
25	k	610	CLA	C2-C1-O2A-CGA
25	k	618	CLA	C2-C1-O2A-CGA
25	A	758	CLA	C3A-C2A-CAA-CBA
25	A	808	CLA	C3A-C2A-CAA-CBA
25	B	738	CLA	C3A-C2A-CAA-CBA
25	B	755	CLA	C3A-C2A-CAA-CBA
25	B	770	CLA	C3A-C2A-CAA-CBA
25	B	772	CLA	C3A-C2A-CAA-CBA
25	a	604	CLA	C3A-C2A-CAA-CBA
25	a	612	CLA	C3A-C2A-CAA-CBA
25	a	613	CLA	C3A-C2A-CAA-CBA
25	m	604	CLA	C3A-C2A-CAA-CBA
25	f	613	CLA	C3A-C2A-CAA-CBA
25	n	609	CLA	C3A-C2A-CAA-CBA
25	o	614	CLA	C3A-C2A-CAA-CBA
35	d	608	CHL	C3A-C2A-CAA-CBA
25	l	613	CLA	CAA-CBA-CGA-O2A
27	i	194	LHG	O1-C1-C2-C3
27	A	756	LHG	O10-C23-C24-C25
25	n	609	CLA	CAA-CBA-CGA-O1A
25	A	775	CLA	C10-C11-C12-C13
25	B	776	CLA	CBA-CGA-O2A-C1
25	A	805	CLA	CAA-CBA-CGA-O2A
25	A	804	CLA	O2A-C1-C2-C3
25	B	771	CLA	O2A-C1-C2-C3
25	m	603	CLA	O2A-C1-C2-C3
25	n	603	CLA	O2A-C1-C2-C3
25	h	610	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
33	B	786	LMG	C40-C41-C42-C43
31	b	620	DD6	C13-C14-C15-O1
31	m	621	DD6	C13-C14-C15-O1
25	a	611	CLA	CAA-CBA-CGA-O1A
25	A	769	CLA	C8-C10-C11-C12
34	b	182	DGD	C1G-C2G-C3G-O3G
27	A	756	LHG	O10-C23-O8-C6
25	l	611	CLA	C2A-CAA-CBA-CGA
25	A	765	CLA	C2A-CAA-CBA-CGA
25	B	757	CLA	CBD-CGD-O2D-CED
31	g	621	DD6	C24-C25-C26-C27
25	b	609	CLA	CAA-CBA-CGA-O1A
25	A	761	CLA	CAA-CBA-CGA-O2A
25	A	806	CLA	CAA-CBA-CGA-O1A
25	A	761	CLA	C11-C12-C13-C14
25	A	784	CLA	C6-C7-C8-C9
25	l	610	CLA	CAA-CBA-CGA-O2A
27	m	182	LHG	O6-C4-C5-C6
25	B	779	CLA	C4-C3-C5-C6
25	A	780	CLA	O1A-CGA-O2A-C1
25	B	738	CLA	CAA-CBA-CGA-O2A
25	a	611	CLA	CAA-CBA-CGA-O2A
25	A	760	CLA	C6-C7-C8-C10
25	B	758	CLA	C6-C7-C8-C10
25	B	758	CLA	C11-C12-C13-C15
25	B	779	CLA	C11-C12-C13-C15
25	e	602	CLA	C11-C10-C8-C7
25	f	613	CLA	C11-C10-C8-C7
28	d	223	PQN	C16-C17-C18-C20
25	n	604	CLA	C4C-C3C-CAC-CBC
25	B	782	CLA	C2B-C3B-CAB-CBB
25	c	610	CLA	C2B-C3B-CAB-CBB
25	i	610	CLA	C2B-C3B-CAB-CBB
25	k	610	CLA	C2B-C3B-CAB-CBB
29	A	789	BCR	C1-C6-C7-C8
29	A	792	BCR	C5-C6-C7-C8
29	B	762	BCR	C5-C6-C7-C8
29	B	765	BCR	C23-C24-C25-C26
29	B	767	BCR	C23-C24-C25-C30
30	c	245	SQD	O48-C23-C24-C25
25	h	601	CLA	C2-C1-O2A-CGA
25	j	612	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
25	g	613	CLA	C2-C1-O2A-CGA
31	n	620	DD6	C11-C13-C14-C15
25	A	768	CLA	CAA-CBA-CGA-O2A
25	c	610	CLA	CAA-CBA-CGA-O2A
27	A	786	LHG	O8-C23-C24-C25
25	h	612	CLA	C2-C3-C5-C6
25	B	771	CLA	C2A-CAA-CBA-CGA
25	i	613	CLA	C2A-CAA-CBA-CGA
25	i	610	CLA	CAA-CBA-CGA-O2A
25	A	770	CLA	C3-C5-C6-C7
25	A	759	CLA	CAA-CBA-CGA-O2A
25	A	798	CLA	CAA-CBA-CGA-O2A
25	B	749	CLA	CAA-CBA-CGA-O2A
25	a	603	CLA	CAA-CBA-CGA-O2A
30	g	190	SQD	C4-C5-C6-S
25	A	780	CLA	C4-C3-C5-C6
25	B	752	CLA	C2-C3-C5-C6
27	m	182	LHG	O8-C23-C24-C25
25	A	772	CLA	C6-C7-C8-C9
25	A	801	CLA	C14-C13-C15-C16
25	B	741	CLA	C11-C10-C8-C9
25	a	602	CLA	C6-C7-C8-C9
29	B	764	BCR	C7-C8-C9-C34
27	b	181	LHG	C30-C31-C32-C33
25	A	760	CLA	CAA-CBA-CGA-O2A
27	g	189	LHG	C4-C5-C6-O8
25	j	610	CLA	C8-C10-C11-C12
25	A	757	CLA	C1A-C2A-CAA-CBA
25	A	770	CLA	C1A-C2A-CAA-CBA
25	B	759	CLA	C4B-C3B-CAB-CBB
25	B	777	CLA	C1A-C2A-CAA-CBA
25	b	605	CLA	C1A-C2A-CAA-CBA
25	i	613	CLA	C4B-C3B-CAB-CBB
25	m	612	CLA	C1A-C2A-CAA-CBA
25	n	609	CLA	C1A-C2A-CAA-CBA
25	o	604	CLA	C4B-C3B-CAB-CBB
25	B	753	CLA	CAA-CBA-CGA-O2A
25	c	609	CLA	CAA-CBA-CGA-O2A
25	f	610	CLA	CAA-CBA-CGA-O2A
25	n	603	CLA	CAA-CBA-CGA-O2A
33	k	179	LMG	O7-C8-C9-O8
29	M	201	BCR	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
31	h	620	DD6	C10-C11-C13-C14
31	i	625	DD6	C10-C11-C13-C14
31	j	620	DD6	C10-C11-C13-C14
27	A	756	LHG	C24-C23-O8-C6
25	A	766	CLA	CAA-CBA-CGA-O2A
25	k	610	CLA	CAA-CBA-CGA-O2A
34	B	787	DGD	O2G-C1B-C2B-C3B
25	l	602	CLA	O1A-CGA-O2A-C1
25	B	745	CLA	C13-C15-C16-C17
25	a	608	CLA	C4-C3-C5-C6
25	B	736	CLA	C2-C1-O2A-CGA
25	B	745	CLA	C2-C1-O2A-CGA
25	B	751	CLA	C2-C1-O2A-CGA
25	a	601	CLA	C2-C1-O2A-CGA
25	a	609	CLA	C2-C1-O2A-CGA
25	j	610	CLA	C2-C1-O2A-CGA
25	n	602	CLA	C2-C1-O2A-CGA
25	i	601	CLA	CAA-CBA-CGA-O2A
25	A	753	CLA	C12-C13-C15-C16
25	a	602	CLA	C6-C7-C8-C10
25	A	807	CLA	CBA-CGA-O2A-C1
25	A	801	CLA	C2-C3-C5-C6
25	h	602	CLA	CAA-CBA-CGA-O2A
27	a	181	LHG	O8-C23-C24-C25
25	e	605	CLA	C3A-C2A-CAA-CBA
25	l	601	CLA	C3A-C2A-CAA-CBA
25	g	614	CLA	C3A-C2A-CAA-CBA
29	B	765	BCR	C13-C14-C15-C16
25	A	781	CLA	C2A-CAA-CBA-CGA
25	B	785	CLA	C2A-CAA-CBA-CGA
25	e	602	CLA	C2A-CAA-CBA-CGA
25	g	602	CLA	C2A-CAA-CBA-CGA
25	i	602	CLA	C5-C6-C7-C8
25	b	605	CLA	CAA-CBA-CGA-O1A
35	d	608	CHL	CAA-CBA-CGA-O2A
25	i	615	CLA	CAA-CBA-CGA-O1A
25	B	741	CLA	CBD-CGD-O2D-CED
25	A	757	CLA	C3A-C2A-CAA-CBA
25	A	763	CLA	C4-C3-C5-C6
25	A	771	CLA	C3A-C2A-CAA-CBA
25	A	805	CLA	C3A-C2A-CAA-CBA
25	B	784	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	B	784	CLA	C4-C3-C5-C6
25	h	602	CLA	C3A-C2A-CAA-CBA
25	h	614	CLA	C3A-C2A-CAA-CBA
25	k	601	CLA	C3A-C2A-CAA-CBA
25	l	613	CLA	C3A-C2A-CAA-CBA
25	p	612	CLA	C3A-C2A-CAA-CBA
25	B	736	CLA	CAA-CBA-CGA-O1A
28	B	761	PQN	C23-C25-C26-C27
25	A	763	CLA	C16-C17-C18-C19
25	l	609	CLA	C11-C12-C13-C15
25	A	764	CLA	C10-C11-C12-C13
25	i	602	CLA	C2-C3-C5-C6
28	d	223	PQN	C12-C13-C15-C16
31	e	620	DD6	C24-C1-C2-C3
25	i	601	CLA	CAA-CBA-CGA-O1A
25	e	604	CLA	C2A-CAA-CBA-CGA
25	e	609	CLA	C2A-CAA-CBA-CGA
25	A	763	CLA	C11-C12-C13-C14
25	i	602	CLA	C14-C13-C15-C16
33	a	182	LMG	O7-C10-C11-C12
25	A	752	CLA	CAA-CBA-CGA-O1A
25	B	739	CLA	CAA-CBA-CGA-O1A
27	m	182	LHG	O10-C23-C24-C25
25	A	752	CLA	C10-C11-C12-C13
25	A	760	CLA	C8-C10-C11-C12
27	b	181	LHG	O2-C2-C3-O3
27	d	237	LHG	O2-C2-C3-O3
25	B	737	CLA	C4-C3-C5-C6
25	b	612	CLA	CAA-CBA-CGA-O1A
25	j	612	CLA	CAA-CBA-CGA-O1A
25	n	603	CLA	CAA-CBA-CGA-O1A
28	B	761	PQN	C12-C13-C15-C16
25	m	613	CLA	C4C-C3C-CAC-CBC
25	c	613	CLA	O1A-CGA-O2A-C1
25	c	608	CLA	CAA-CBA-CGA-O1A
25	h	609	CLA	CAA-CBA-CGA-O1A
25	l	610	CLA	CAA-CBA-CGA-O1A
25	m	603	CLA	CAA-CBA-CGA-O1A
27	a	181	LHG	O10-C23-C24-C25
27	i	194	LHG	O1-C1-C2-O2
25	c	608	CLA	CAA-CBA-CGA-O2A
27	A	786	LHG	O7-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
25	A	798	CLA	CBD-CGD-O2D-CED
25	B	768	CLA	CBD-CGD-O2D-CED
29	B	764	BCR	C7-C8-C9-C10
25	f	610	CLA	CAA-CBA-CGA-O1A
25	f	602	CLA	C11-C12-C13-C14
33	i	195	LMG	C31-C32-C33-C34
30	j	200	SQD	C26-C27-C28-C29
34	b	182	DGD	C5D-C6D-O5D-C1E
25	c	603	CLA	CAA-CBA-CGA-O1A
25	A	799	CLA	C4-C3-C5-C6
27	a	181	LHG	C5-C4-O6-P
27	m	182	LHG	O7-C7-C8-C9
31	m	620	DD6	C24-C25-C26-C27
25	a	608	CLA	CAA-CBA-CGA-O1A
27	A	786	LHG	O10-C23-C24-C25
30	c	245	SQD	O10-C23-C24-C25
25	A	772	CLA	CAD-CBD-CGD-O2D
25	A	808	CLA	CAD-CBD-CGD-O2D
25	B	775	CLA	CAD-CBD-CGD-O2D
25	c	610	CLA	CAD-CBD-CGD-O2D
25	d	601	CLA	CAD-CBD-CGD-O2D
25	e	602	CLA	CAD-CBD-CGD-O2D
25	i	602	CLA	CAD-CBD-CGD-O2D
25	i	611	CLA	CAD-CBD-CGD-O2D
25	g	611	CLA	CAD-CBD-CGD-O2D
35	e	606	CHL	CAD-CBD-CGD-O2D
25	p	609	CLA	C4C-C3C-CAC-CBC
25	B	736	CLA	CAA-CBA-CGA-O2A
27	b	181	LHG	O8-C23-C24-C25
25	A	760	CLA	CAA-CBA-CGA-O1A
25	h	601	CLA	CAA-CBA-CGA-O1A
25	A	766	CLA	C2-C1-O2A-CGA
25	c	610	CLA	C2-C1-O2A-CGA
25	b	609	CLA	CAA-CBA-CGA-O2A
34	B	787	DGD	O1B-C1B-C2B-C3B
25	c	603	CLA	CAA-CBA-CGA-O2A
25	m	603	CLA	CAA-CBA-CGA-O2A
25	n	602	CLA	CAA-CBA-CGA-O2A
25	A	780	CLA	C1-C2-C3-C4
25	A	803	CLA	C1-C2-C3-C4
25	B	736	CLA	C1-C2-C3-C4
25	B	756	CLA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
25	B	770	CLA	C1-C2-C3-C4
25	B	771	CLA	C1-C2-C3-C4
25	B	779	CLA	C1-C2-C3-C4
25	a	613	CLA	C1-C2-C3-C4
25	d	604	CLA	C1-C2-C3-C4
25	n	602	CLA	C1-C2-C3-C4
25	A	782	CLA	O2A-C1-C2-C3
25	o	612	CLA	C2A-CAA-CBA-CGA
25	h	608	CLA	CAA-CBA-CGA-O1A
25	A	772	CLA	C10-C11-C12-C13
25	h	604	CLA	C10-C11-C12-C13
25	g	610	CLA	C5-C6-C7-C8
25	A	755	CLA	CAA-CBA-CGA-O2A
25	B	737	CLA	CAA-CBA-CGA-O2A
25	j	610	CLA	CAA-CBA-CGA-O2A
25	A	807	CLA	C2C-C3C-CAC-CBC
35	d	606	CHL	CAA-CBA-CGA-O1A
25	B	753	CLA	CAA-CBA-CGA-O1A
25	J	101	CLA	CAA-CBA-CGA-O1A
27	A	786	LHG	O9-C7-C8-C9
25	B	751	CLA	O1A-CGA-O2A-C1
25	j	604	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

259 monomers are involved in 540 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	e	602	CLA	4	0
25	B	742	CLA	1	0
25	A	760	CLA	6	0
25	l	617	CLA	1	0
25	A	797	CLA	2	0
25	k	613	CLA	2	0
25	B	778	CLA	7	0
25	B	757	CLA	2	0
25	B	782	CLA	4	0
25	g	602	CLA	3	0
25	d	613	CLA	1	0
25	o	602	CLA	2	0
25	l	609	CLA	3	0
25	c	613	CLA	2	0
25	B	736	CLA	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	783	CLA	3	0
25	B	738	CLA	3	0
28	A	785	PQN	5	0
25	c	612	CLA	3	0
25	A	781	CLA	2	0
25	A	753	CLA	7	0
25	d	602	CLA	1	0
25	d	610	CLA	4	0
27	a	181	LHG	1	0
30	g	190	SQD	2	0
25	a	611	CLA	1	0
25	A	774	CLA	3	0
25	a	613	CLA	2	0
25	n	602	CLA	2	0
25	a	610	CLA	3	0
25	e	608	CLA	3	0
27	m	182	LHG	2	0
25	i	609	CLA	1	0
25	A	804	CLA	2	0
29	A	792	BCR	3	0
25	b	602	CLA	1	0
25	m	613	CLA	1	0
25	e	604	CLA	1	0
25	k	602	CLA	1	0
25	k	610	CLA	4	0
25	B	781	CLA	9	0
25	A	801	CLA	1	0
25	B	753	CLA	6	0
25	A	808	CLA	2	0
25	B	756	CLA	4	0
25	g	601	CLA	2	0
25	o	608	CLA	1	0
25	i	610	CLA	3	0
35	d	607	CHL	2	0
25	B	774	CLA	5	0
25	f	614	CLA	1	0
25	B	776	CLA	4	0
25	h	609	CLA	2	0
25	g	608	CLA	4	0
25	J	101	CLA	2	0
25	d	604	CLA	2	0
25	i	612	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	h	602	CLA	1	0
25	B	760	CLA	3	0
25	j	609	CLA	2	0
25	A	761	CLA	3	0
25	k	618	CLA	2	0
29	A	789	BCR	1	0
25	A	805	CLA	2	0
25	h	615	CLA	2	0
25	f	610	CLA	1	0
25	B	758	CLA	5	0
31	m	621	DD6	1	0
25	j	611	CLA	2	0
25	A	767	CLA	3	0
25	B	745	CLA	3	0
25	c	608	CLA	3	0
25	j	613	CLA	4	0
25	A	769	CLA	5	0
25	f	615	CLA	1	0
25	j	610	CLA	3	0
25	A	757	CLA	1	0
29	B	766	BCR	8	0
25	c	606	CLA	1	0
25	A	791	CLA	6	0
25	h	611	CLA	1	0
25	g	612	CLA	1	0
25	a	604	CLA	1	0
25	h	613	CLA	3	0
29	A	788	BCR	3	0
25	h	610	CLA	9	0
25	A	763	CLA	3	0
25	f	613	CLA	3	0
31	i	621	DD6	1	0
25	n	609	CLA	1	0
25	n	607	CLA	1	0
35	d	606	CHL	2	0
25	n	612	CLA	1	0
25	n	603	CLA	3	0
27	d	237	LHG	3	0
25	j	618	CLA	1	0
25	i	603	CLA	2	0
25	c	610	CLA	3	0
25	b	609	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	h	608	CLA	3	0
25	A	766	CLA	5	0
27	c	243	LHG	3	0
25	B	771	CLA	3	0
27	h	190	LHG	2	0
25	h	604	CLA	2	0
25	B	747	CLA	4	0
25	B	770	CLA	1	0
27	A	786	LHG	5	0
25	b	610	CLA	2	0
29	M	201	BCR	2	0
25	p	610	CLA	1	0
27	j	198	LHG	4	0
25	n	604	CLA	2	0
34	e	205	DGD	2	0
25	A	780	CLA	3	0
25	b	604	CLA	3	0
25	g	609	CLA	3	0
34	b	182	DGD	3	0
25	A	777	CLA	4	0
25	A	773	CLA	3	0
25	l	614	CLA	3	0
25	b	612	CLA	4	0
25	l	602	CLA	4	0
25	p	609	CLA	1	0
25	B	739	CLA	5	0
25	l	610	CLA	4	0
33	k	179	LMG	3	0
25	B	785	CLA	3	0
25	h	601	CLA	3	0
25	p	602	CLA	3	0
25	f	604	CLA	1	0
29	B	763	BCR	2	0
25	k	604	CLA	1	0
25	B	755	CLA	2	0
25	b	605	CLA	1	0
25	p	613	CLA	1	0
25	i	613	CLA	2	0
25	A	799	CLA	5	0
31	d	623	DD6	1	0
25	e	605	CLA	1	0
25	f	608	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	A	756	LHG	2	0
25	B	780	CLA	2	0
25	k	603	CLA	1	0
25	d	603	CLA	2	0
25	B	773	CLA	5	0
25	B	772	CLA	3	0
25	l	613	CLA	1	0
33	B	786	LMG	5	0
25	g	610	CLA	7	0
25	a	609	CLA	1	0
25	m	608	CLA	1	0
25	a	602	CLA	7	0
25	e	611	CLA	1	0
31	n	621	DD6	1	0
25	e	613	CLA	1	0
25	A	793	CLA	3	0
25	g	613	CLA	3	0
25	i	615	CLA	2	0
25	B	779	CLA	2	0
25	o	609	CLA	1	0
25	d	601	CLA	1	0
25	h	612	CLA	2	0
25	h	603	CLA	1	0
25	B	746	CLA	3	0
25	m	603	CLA	1	0
25	A	775	CLA	7	0
25	m	601	CLA	5	0
25	o	601	CLA	1	0
25	B	752	CLA	6	0
25	n	610	CLA	1	0
25	o	610	CLA	3	0
25	o	614	CLA	4	0
29	B	765	BCR	4	0
25	e	610	CLA	4	0
29	A	787	BCR	3	0
25	e	612	CLA	3	0
25	A	784	CLA	7	0
25	p	608	CLA	1	0
25	A	772	CLA	4	0
25	i	604	CLA	1	0
25	A	770	CLA	4	0
25	o	612	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	h	189	LHG	1	0
25	i	601	CLA	2	0
28	B	761	PQN	2	0
25	B	750	CLA	4	0
35	d	608	CHL	2	0
25	k	608	CLA	3	0
25	c	603	CLA	4	0
34	B	787	DGD	2	0
25	B	775	CLA	5	0
25	B	777	CLA	5	0
25	i	614	CLA	1	0
25	i	608	CLA	2	0
29	B	762	BCR	2	0
25	c	611	CLA	3	0
25	A	782	CLA	2	0
25	a	603	CLA	1	0
25	A	794	CLA	3	0
25	B	759	CLA	1	0
25	c	614	CLA	1	0
27	b	181	LHG	3	0
25	B	741	CLA	3	0
25	l	604	CLA	1	0
25	B	784	CLA	2	0
25	m	610	CLA	3	0
29	B	764	BCR	5	0
25	A	768	CLA	3	0
25	A	755	CLA	2	0
25	j	604	CLA	2	0
29	A	790	BCR	2	0
25	A	765	CLA	3	0
25	B	749	CLA	1	0
25	d	614	CLA	1	0
25	a	601	CLA	1	0
25	a	619	CLA	5	0
25	B	748	CLA	1	0
25	B	751	CLA	4	0
25	f	602	CLA	2	0
25	A	771	CLA	2	0
25	l	603	CLA	1	0
25	a	608	CLA	3	0
25	j	608	CLA	1	0
27	i	194	LHG	2	0

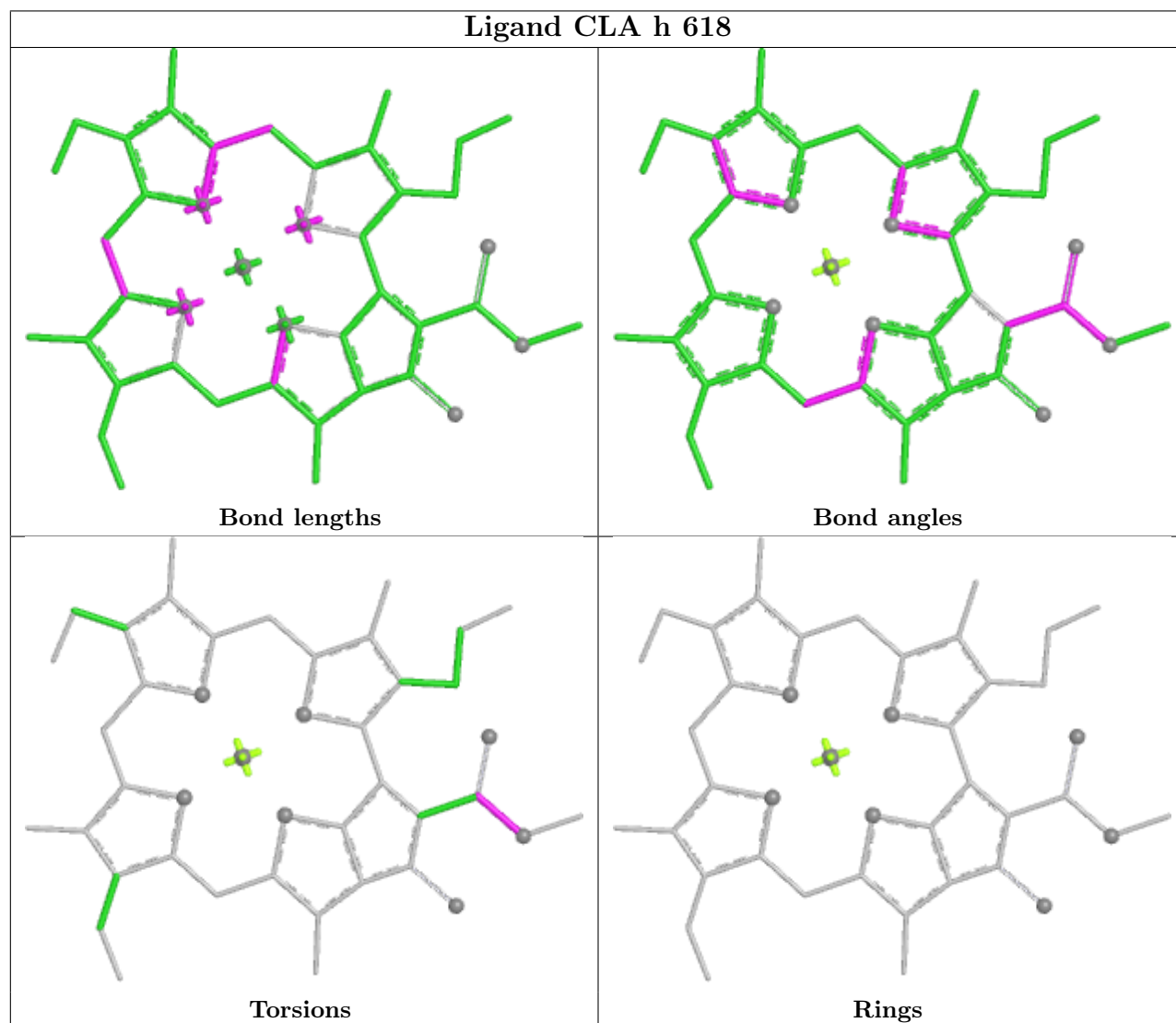
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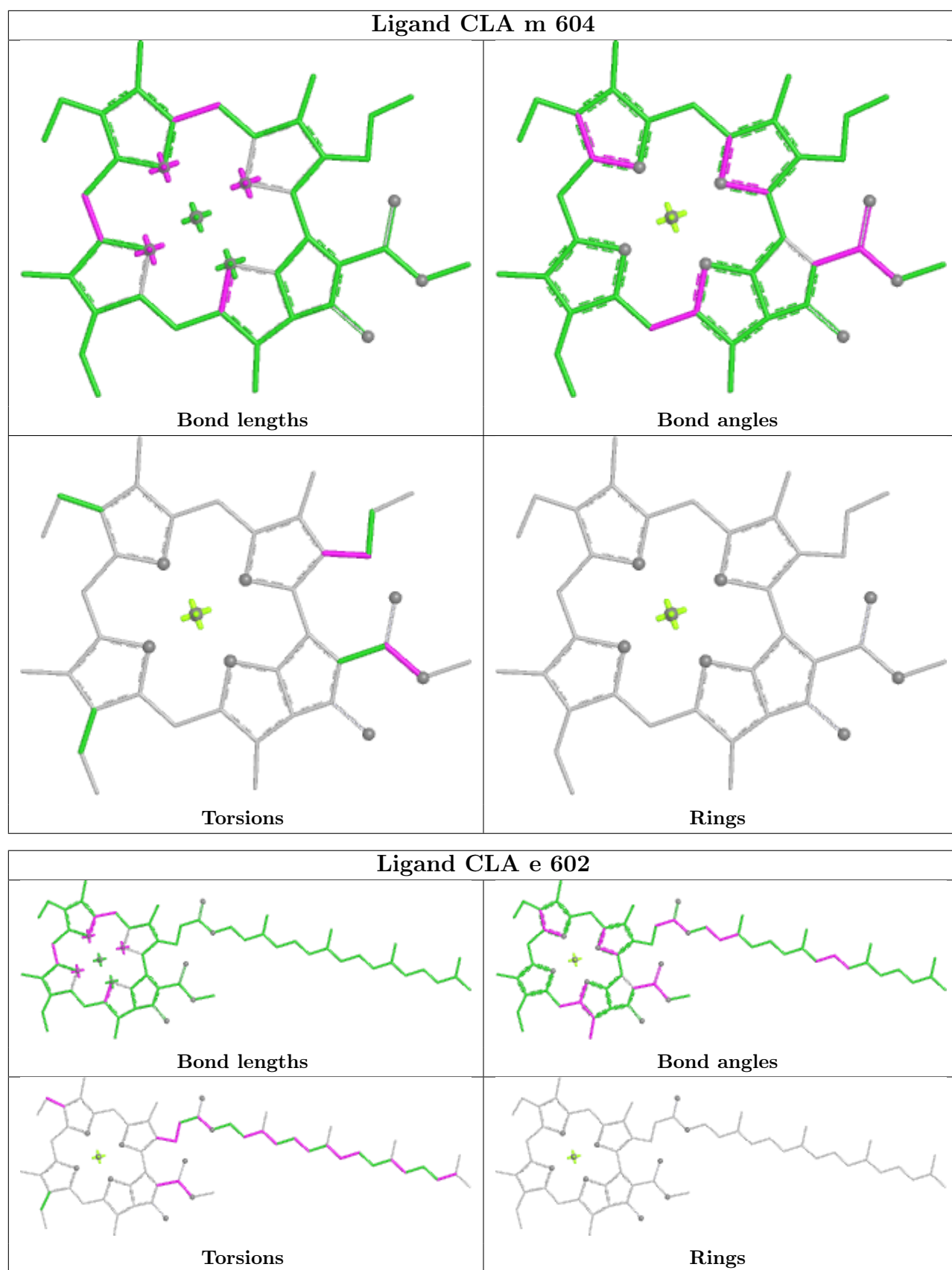
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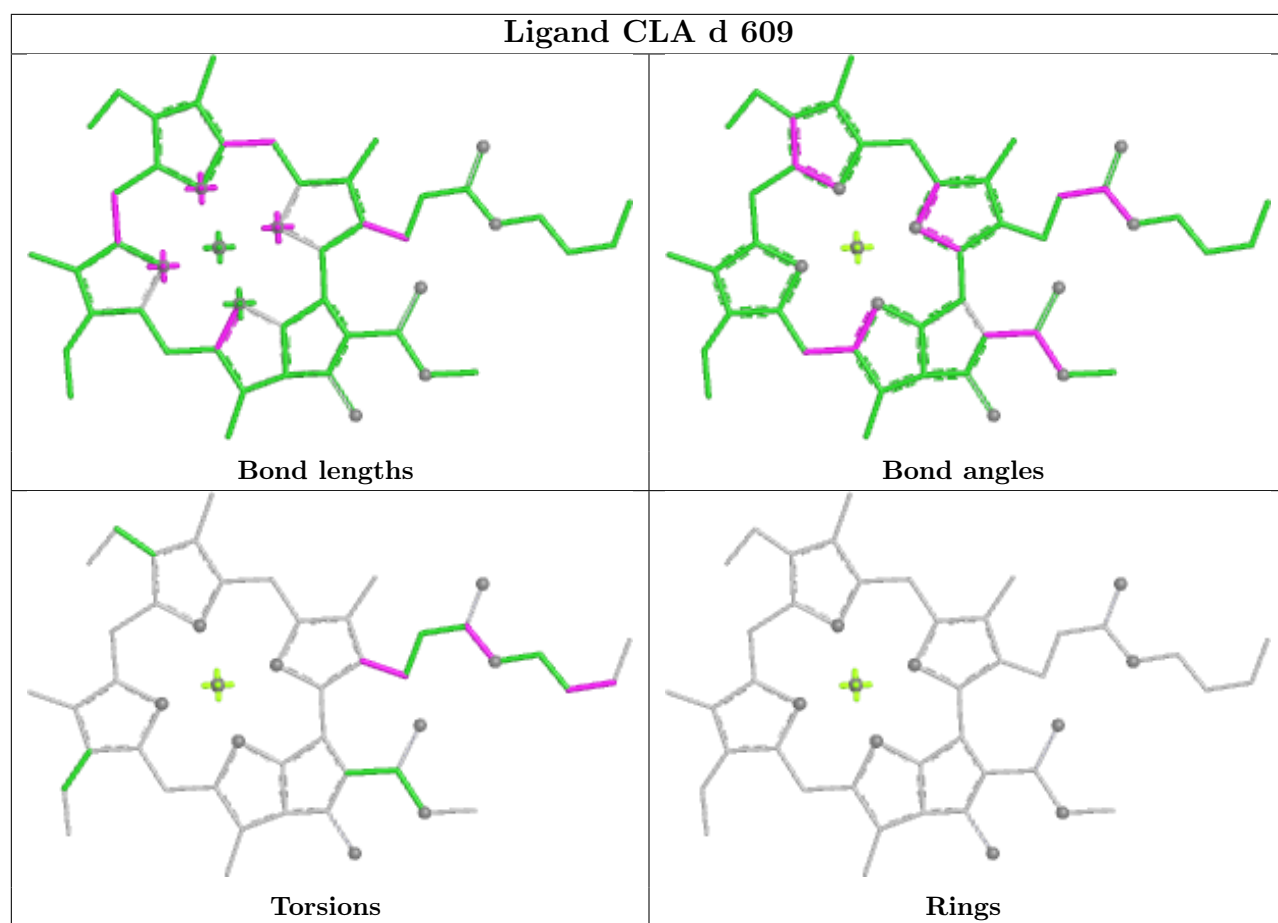
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	g	603	CLA	1	0
25	m	602	CLA	5	0
25	A	783	CLA	5	0
25	k	609	CLA	1	0
25	c	602	CLA	2	0
25	k	612	CLA	1	0
25	n	606	CLA	2	0
25	B	737	CLA	4	0
25	b	601	CLA	1	0
25	i	602	CLA	2	0
29	B	767	BCR	3	0
25	p	612	CLA	1	0
25	A	800	CLA	2	0
25	A	752	CLA	7	0
25	e	603	CLA	1	0
25	b	608	CLA	1	0
25	A	798	CLA	3	0
25	j	601	CLA	4	0
25	A	758	CLA	6	0
25	B	744	CLA	1	0
25	g	615	CLA	1	0
29	A	796	BCR	2	0
25	A	764	CLA	1	0
25	c	609	CLA	2	0
31	a	621	DD6	1	0
35	c	607	CHL	3	0
31	m	620	DD6	1	0
25	A	776	CLA	3	0
25	n	608	CLA	3	0
25	c	601	CLA	1	0
25	l	608	CLA	1	0
35	d	605	CHL	1	0
25	p	603	CLA	4	0
25	d	611	CLA	1	0

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

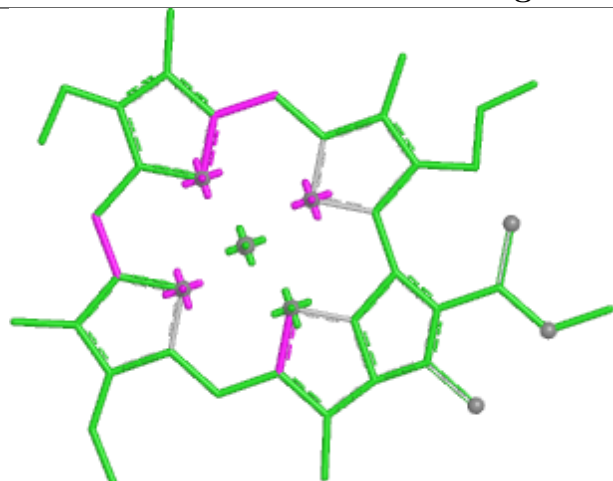
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



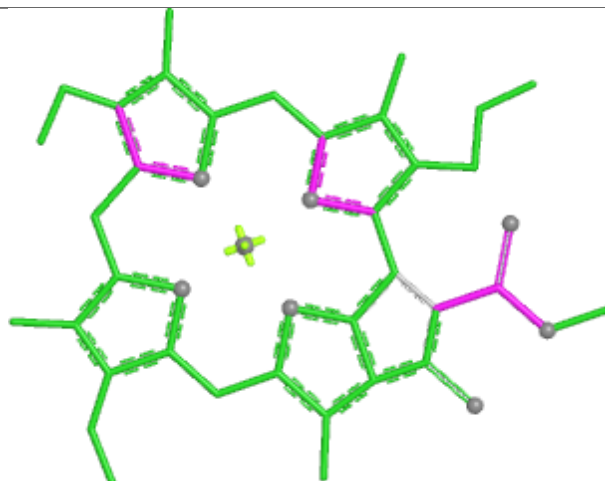




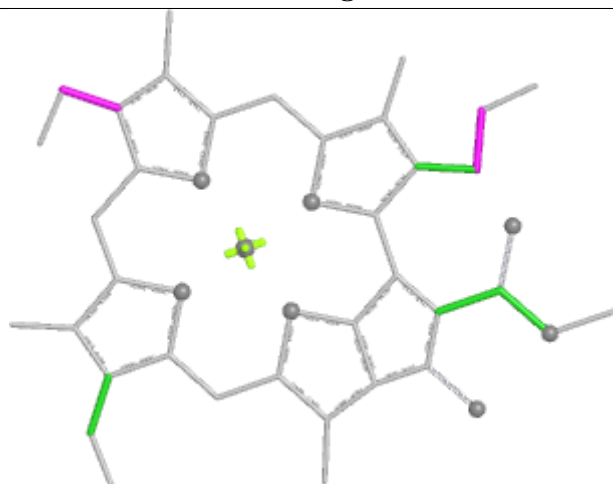
Ligand CLA B 742



Bond lengths



Bond angles

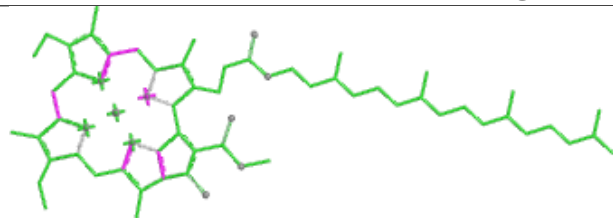


Torsions

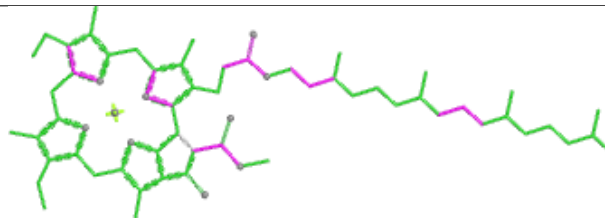


Rings

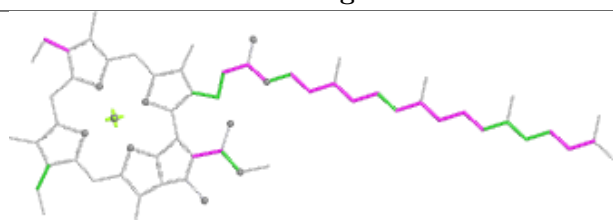
Ligand CLA A 760



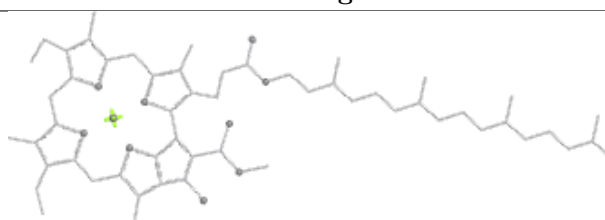
Bond lengths



Bond angles

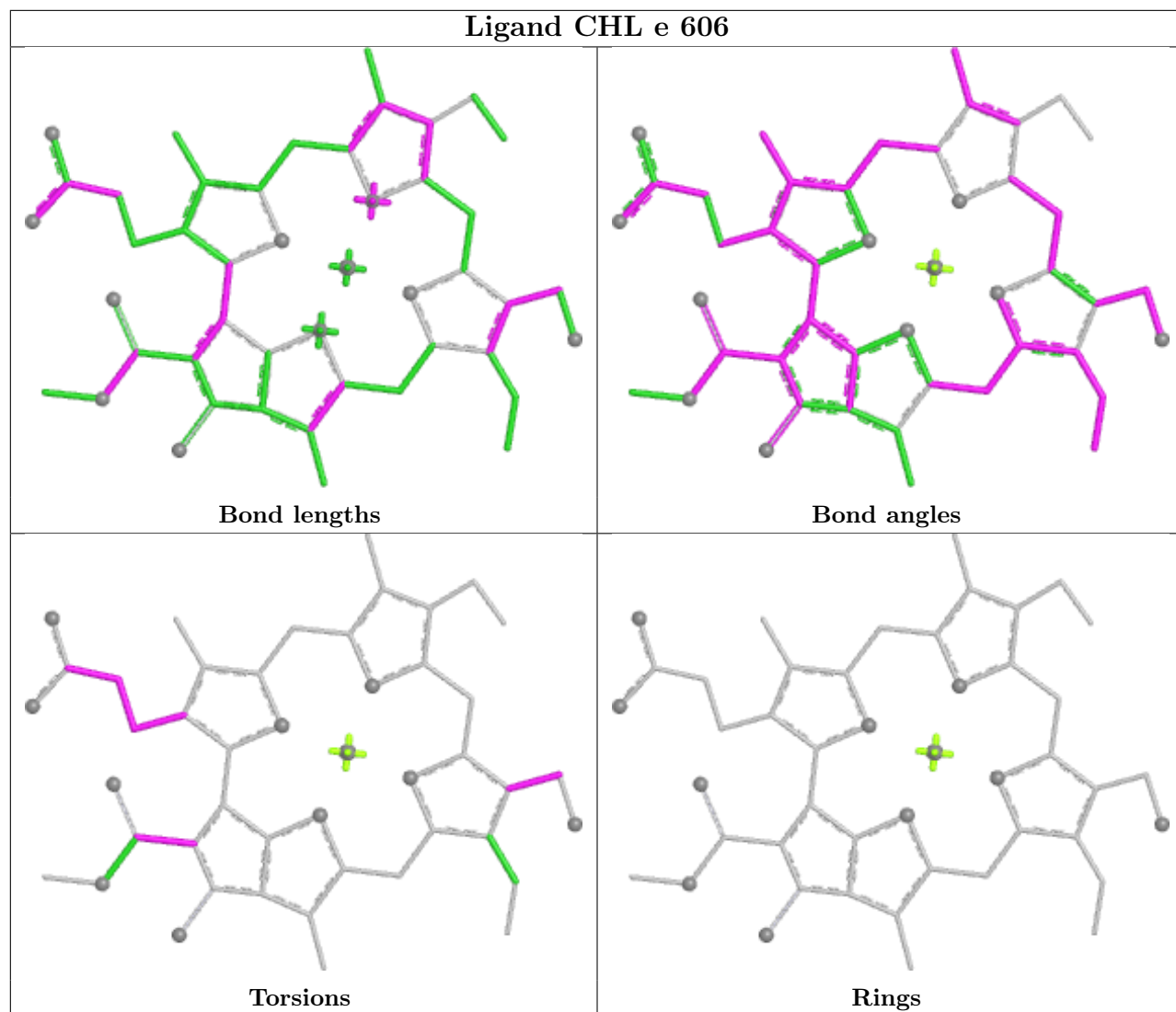


Torsions

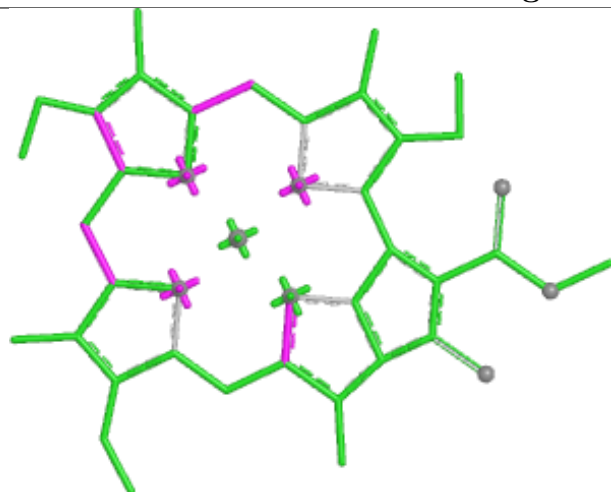


Rings

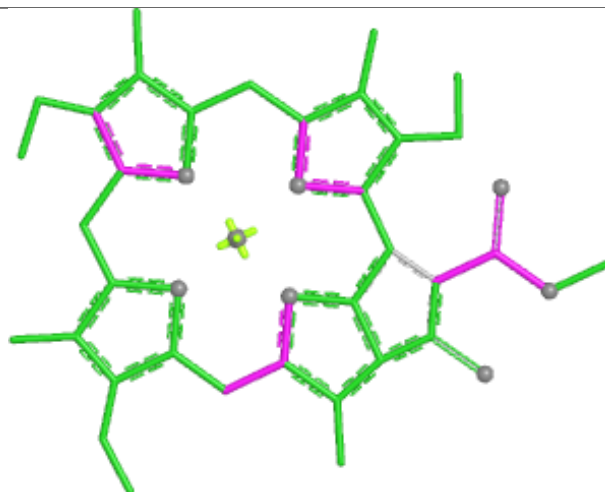
Ligand CHL e 606



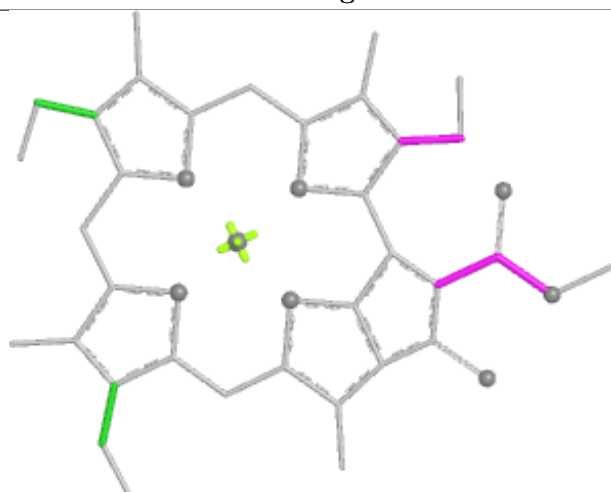
Ligand CLA 1 617



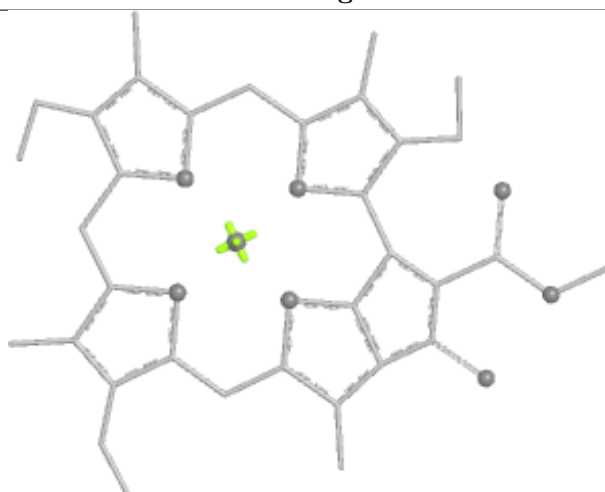
Bond lengths



Bond angles

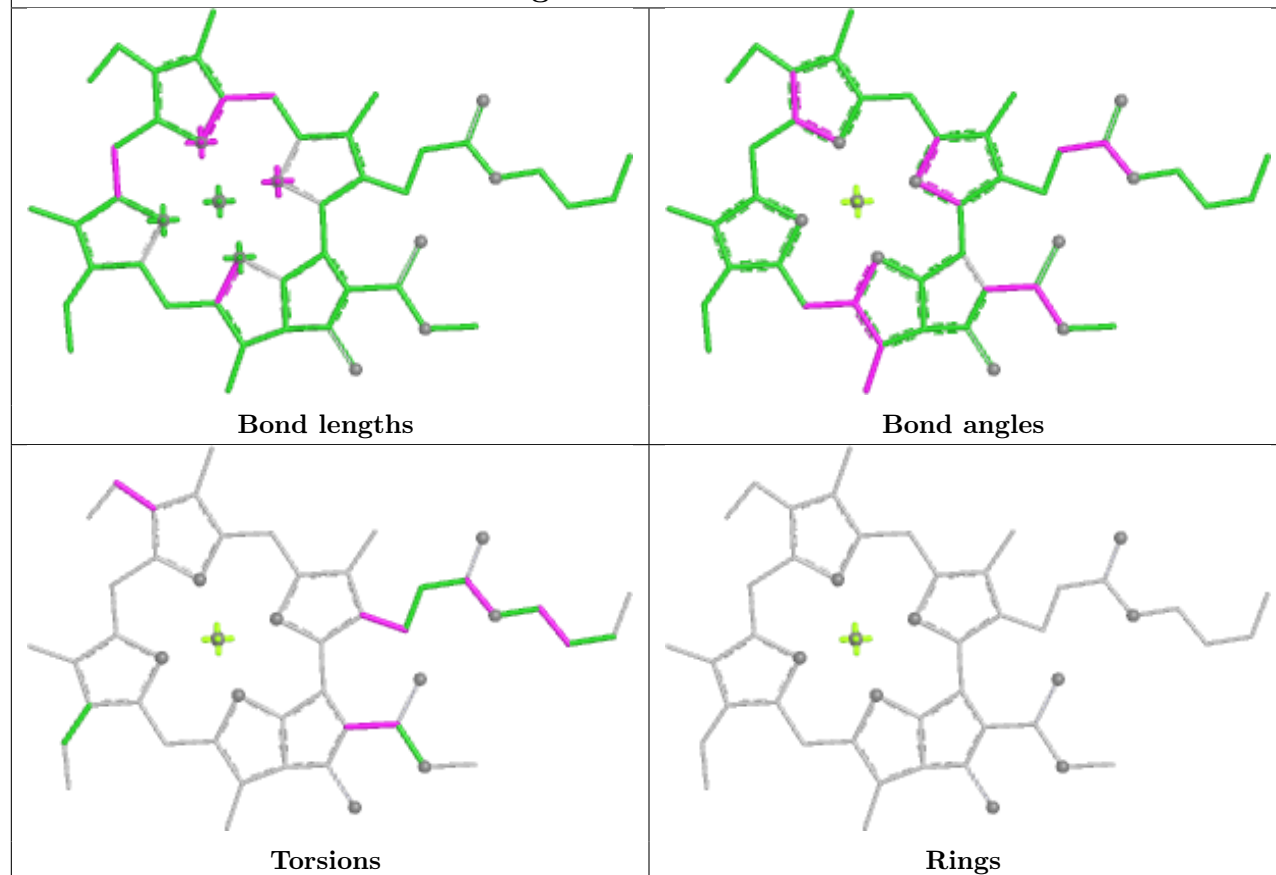


Torsions

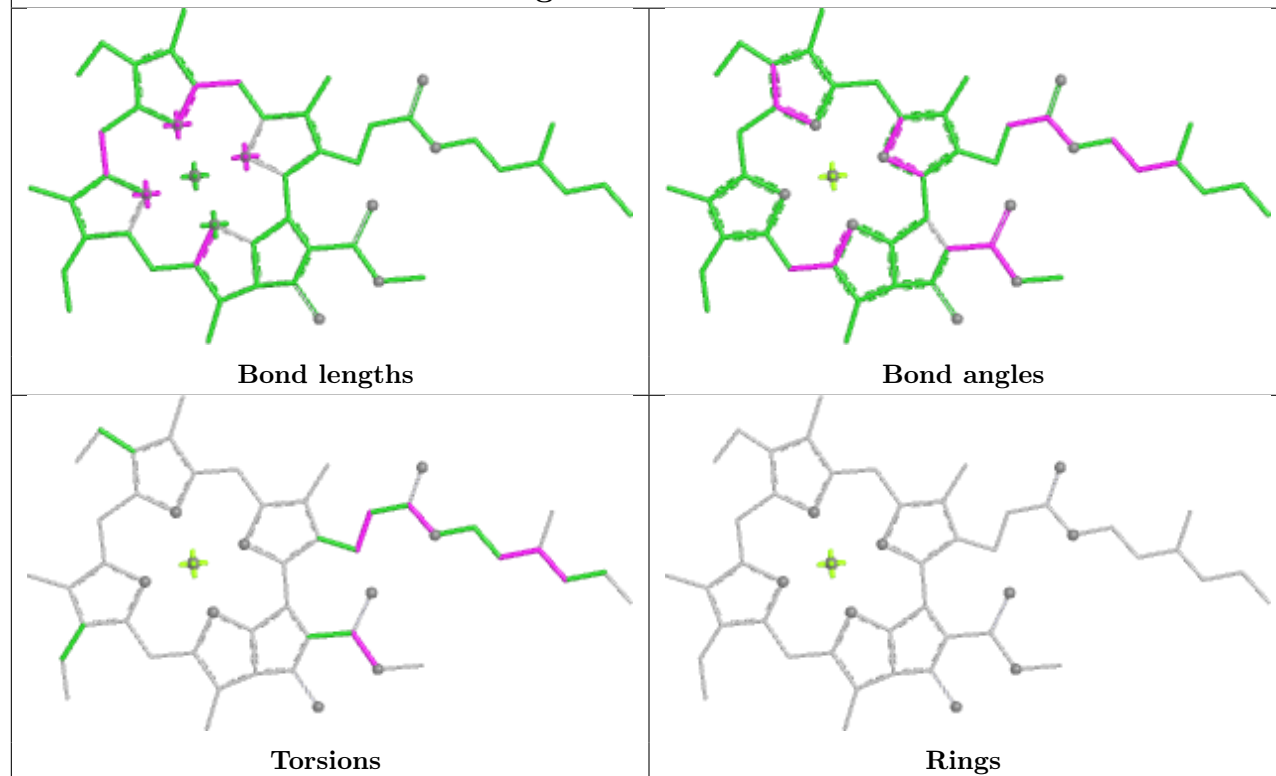


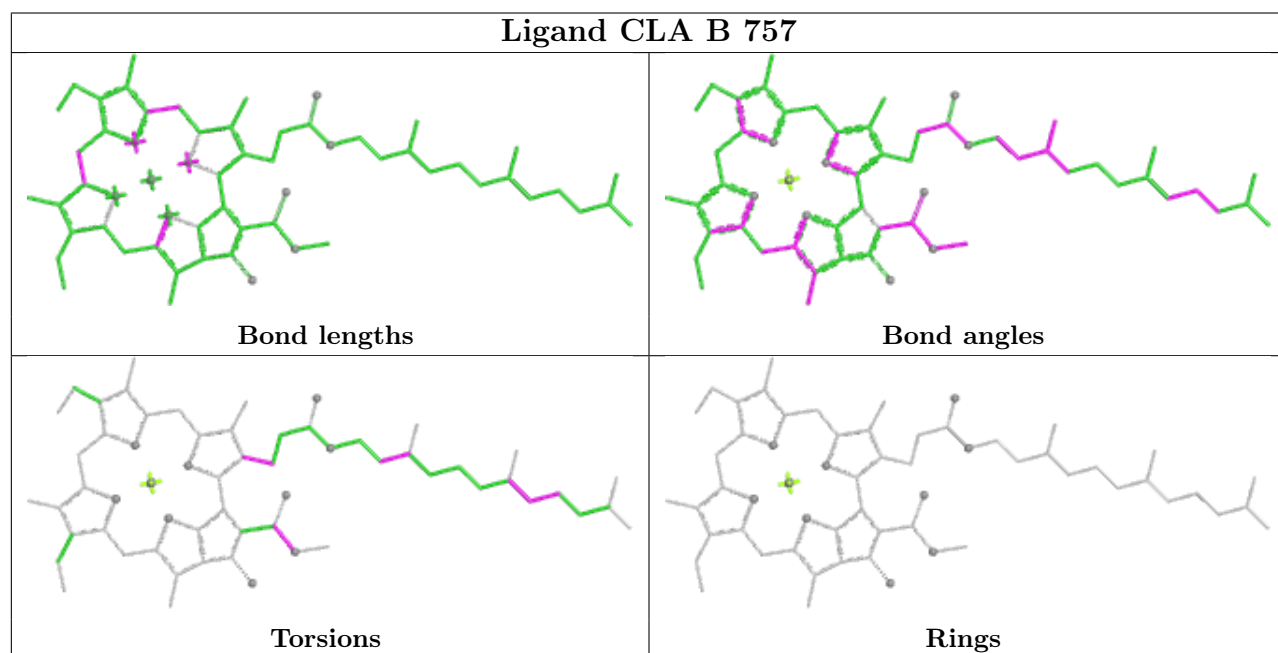
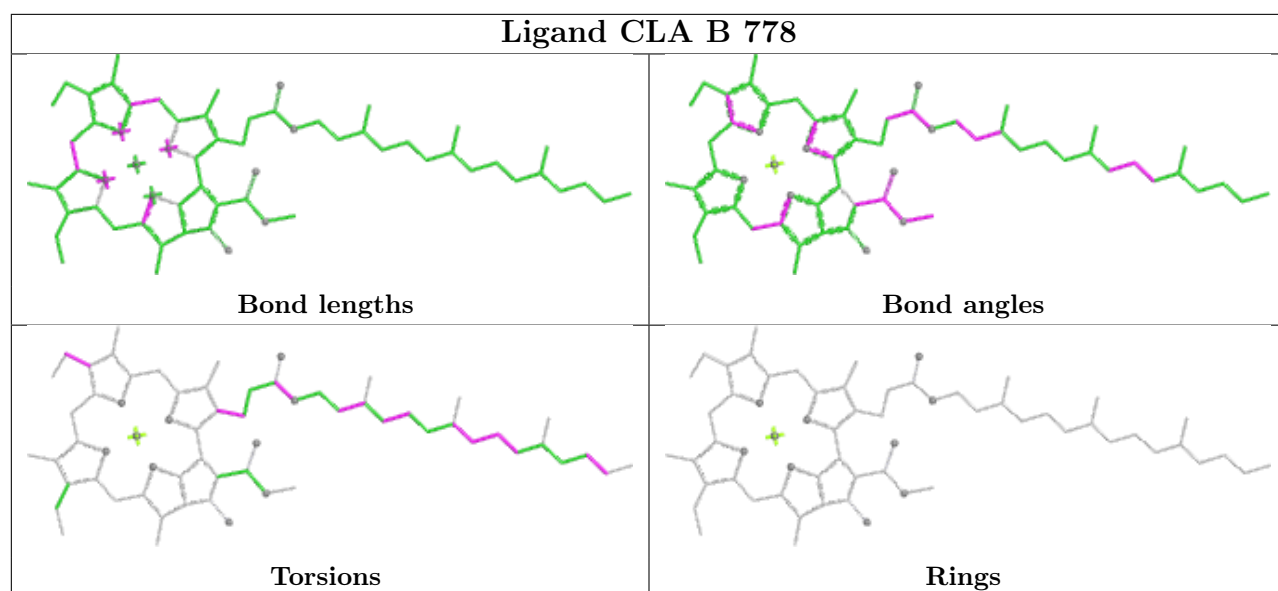
Rings

Ligand CLA A 797

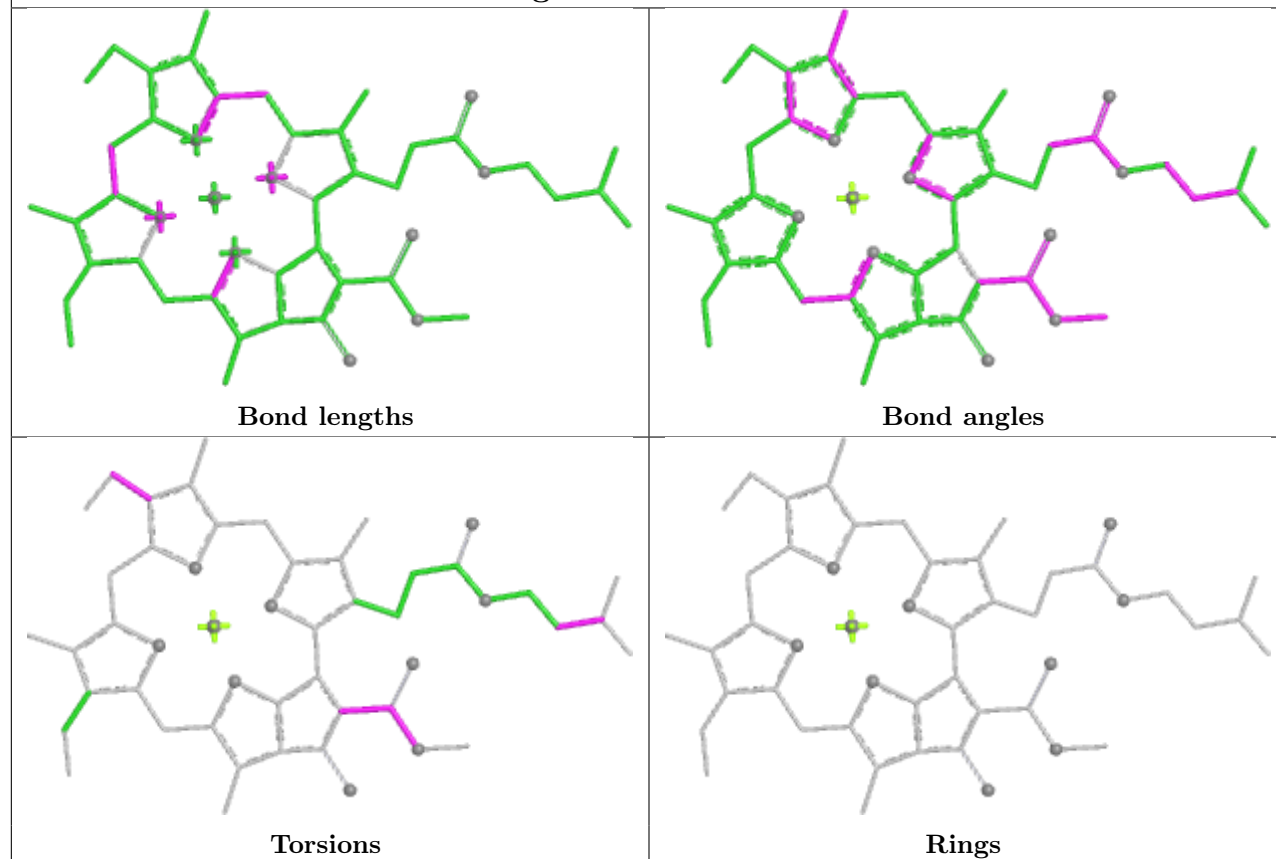


Ligand CLA k 613

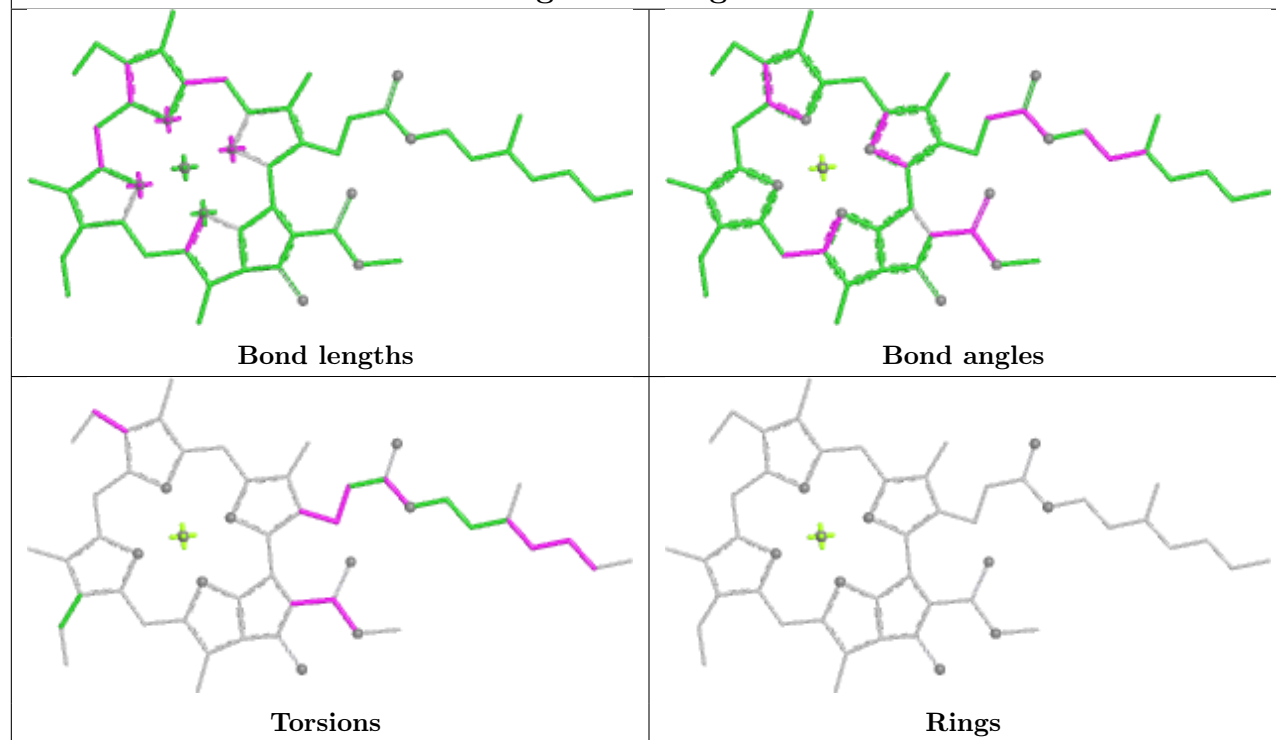




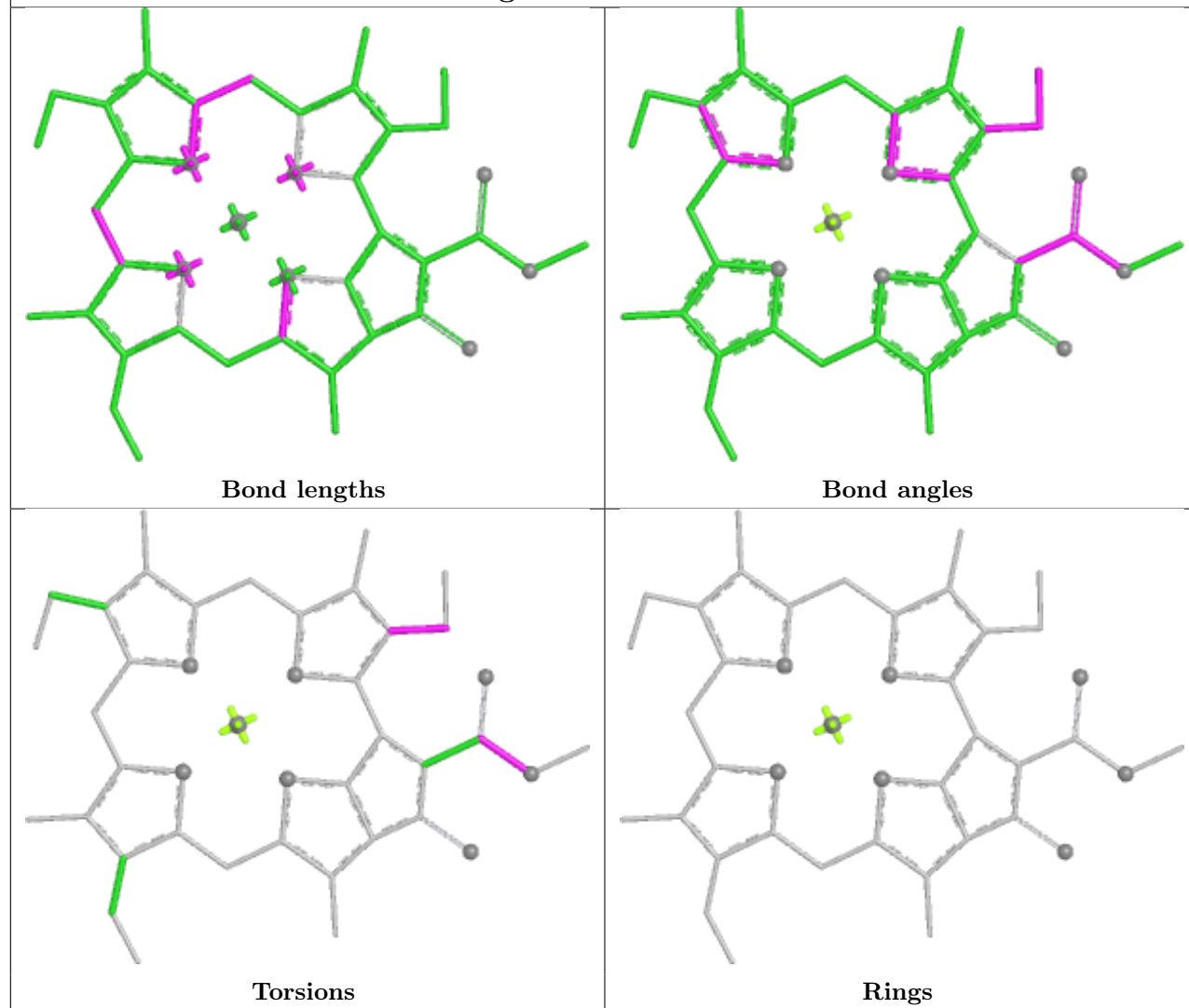
Ligand CLA B 782



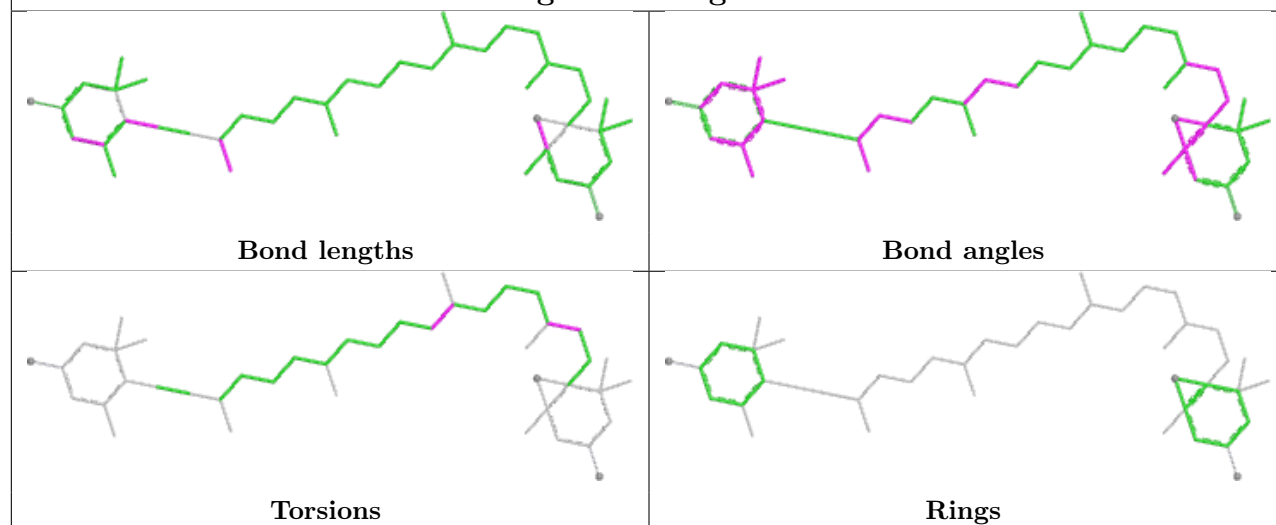
Ligand CLA g 602



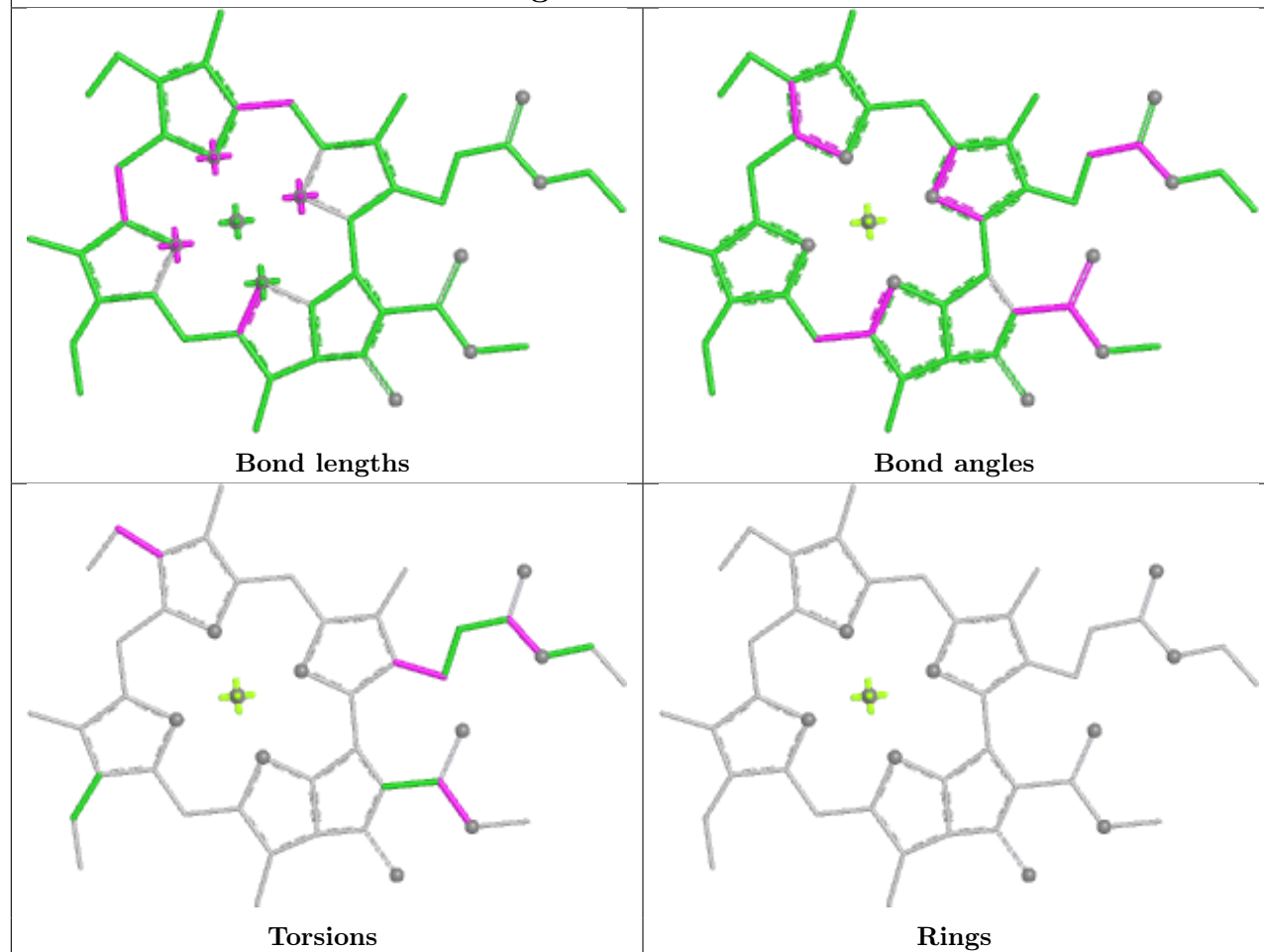
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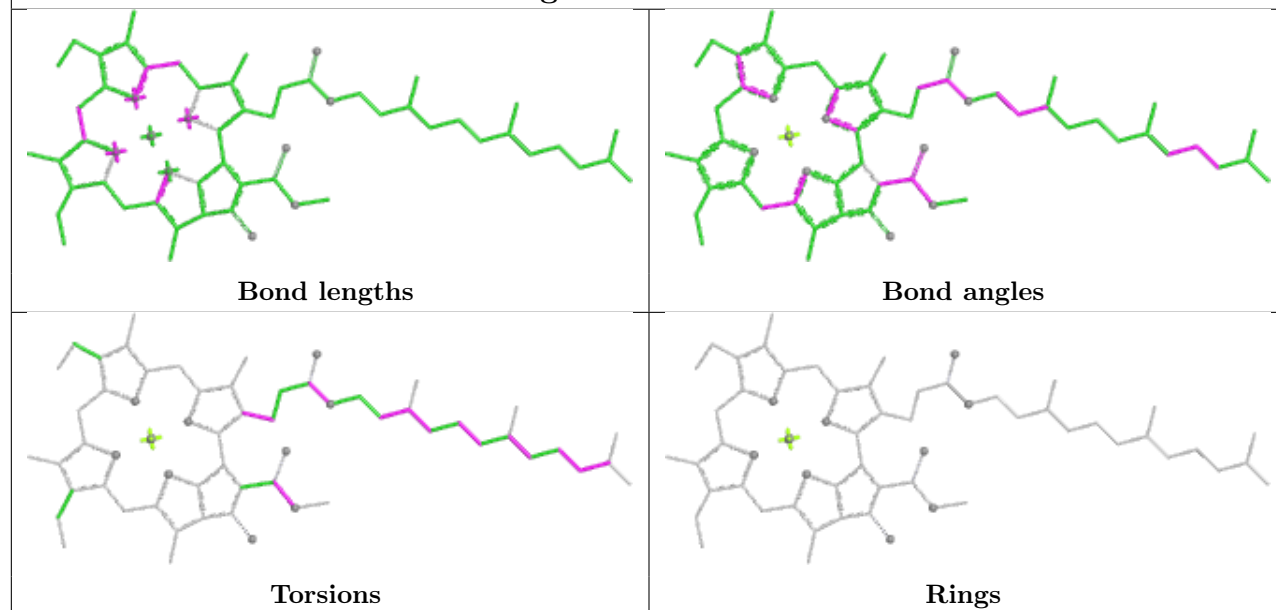
Ligand DD6 g 620

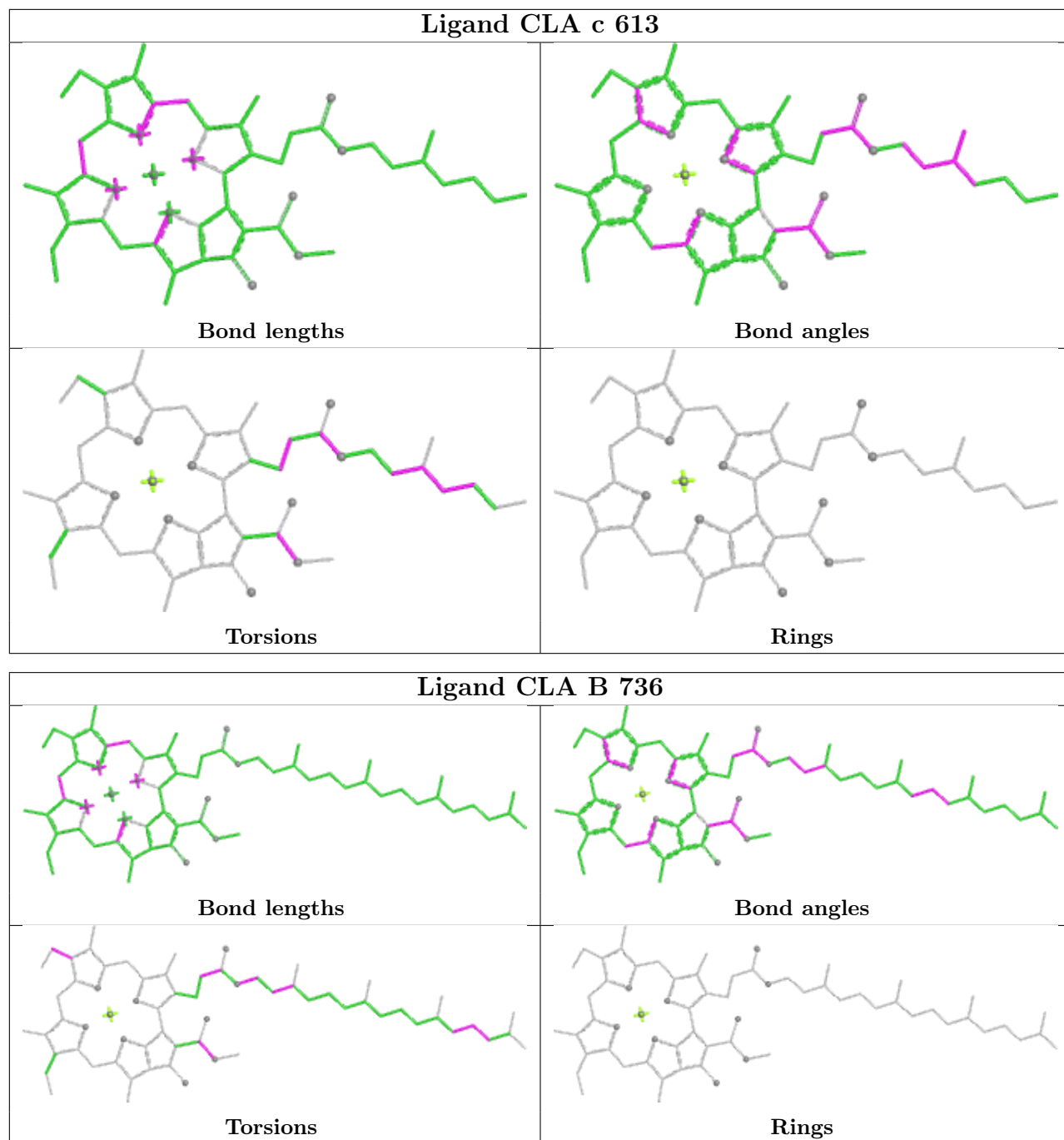


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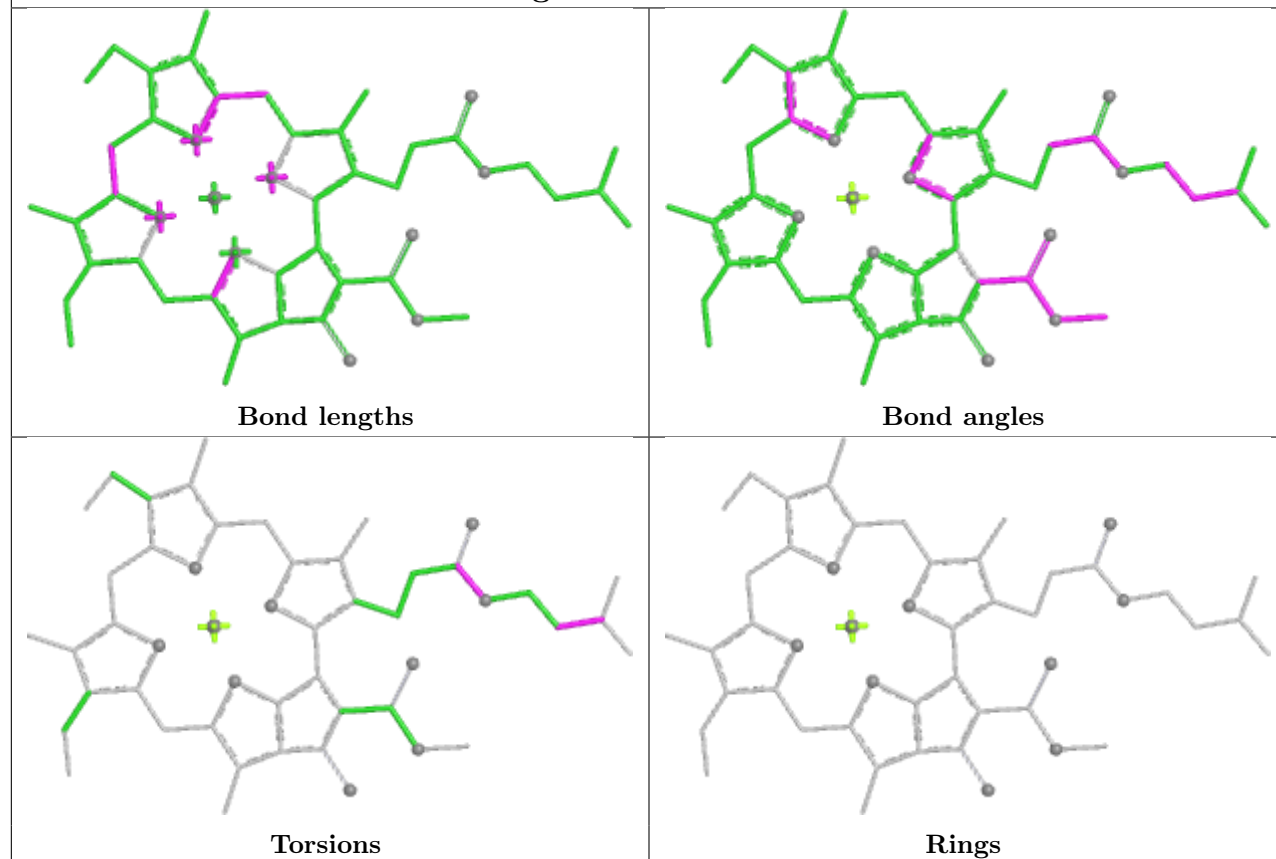


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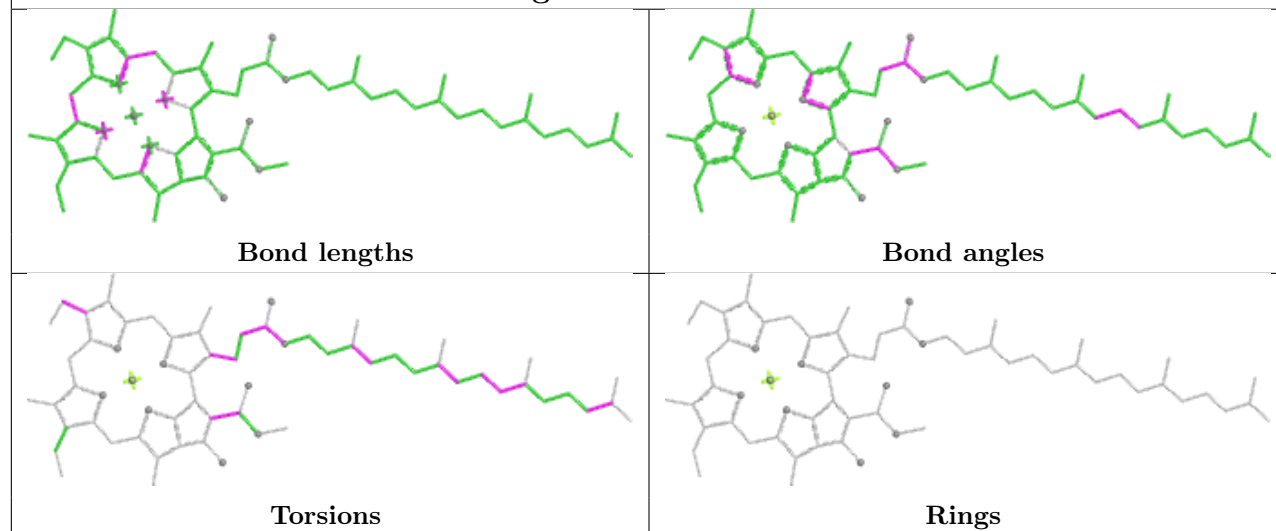


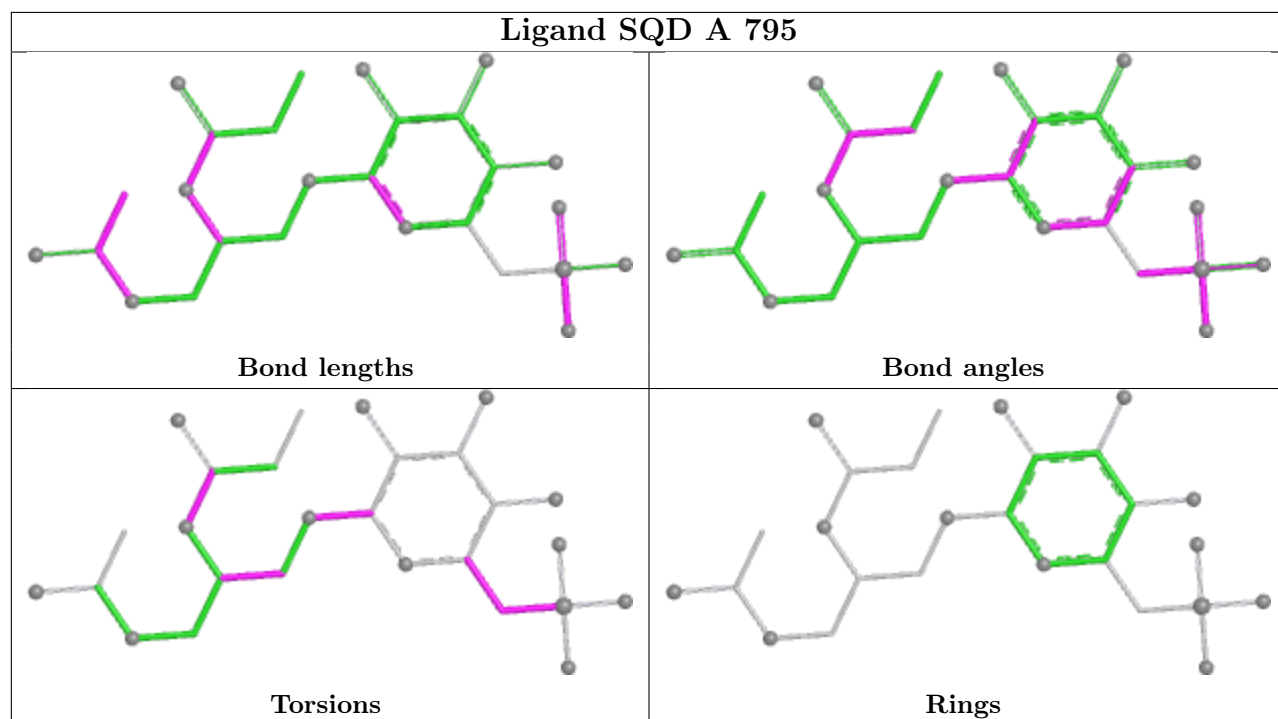
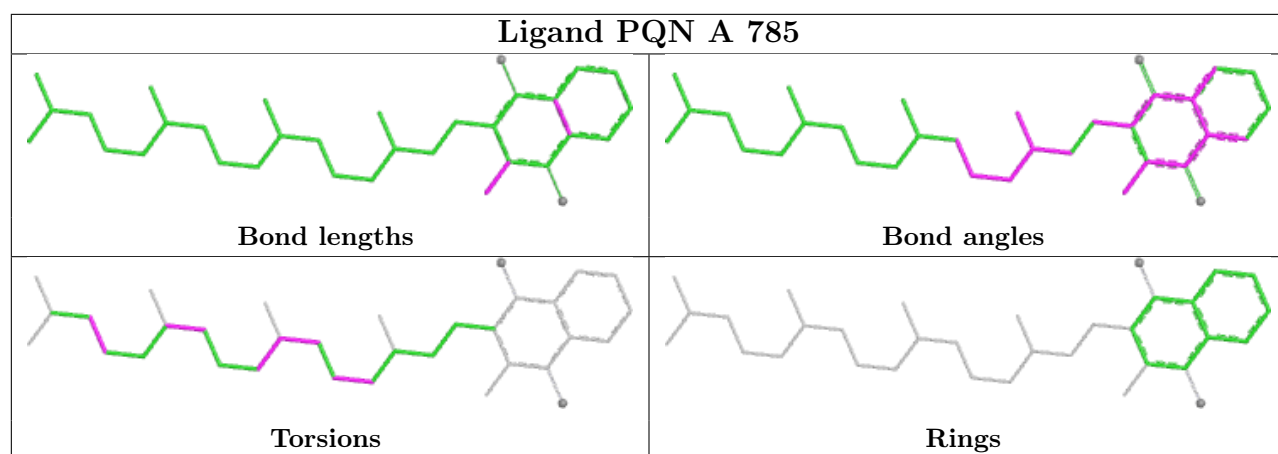


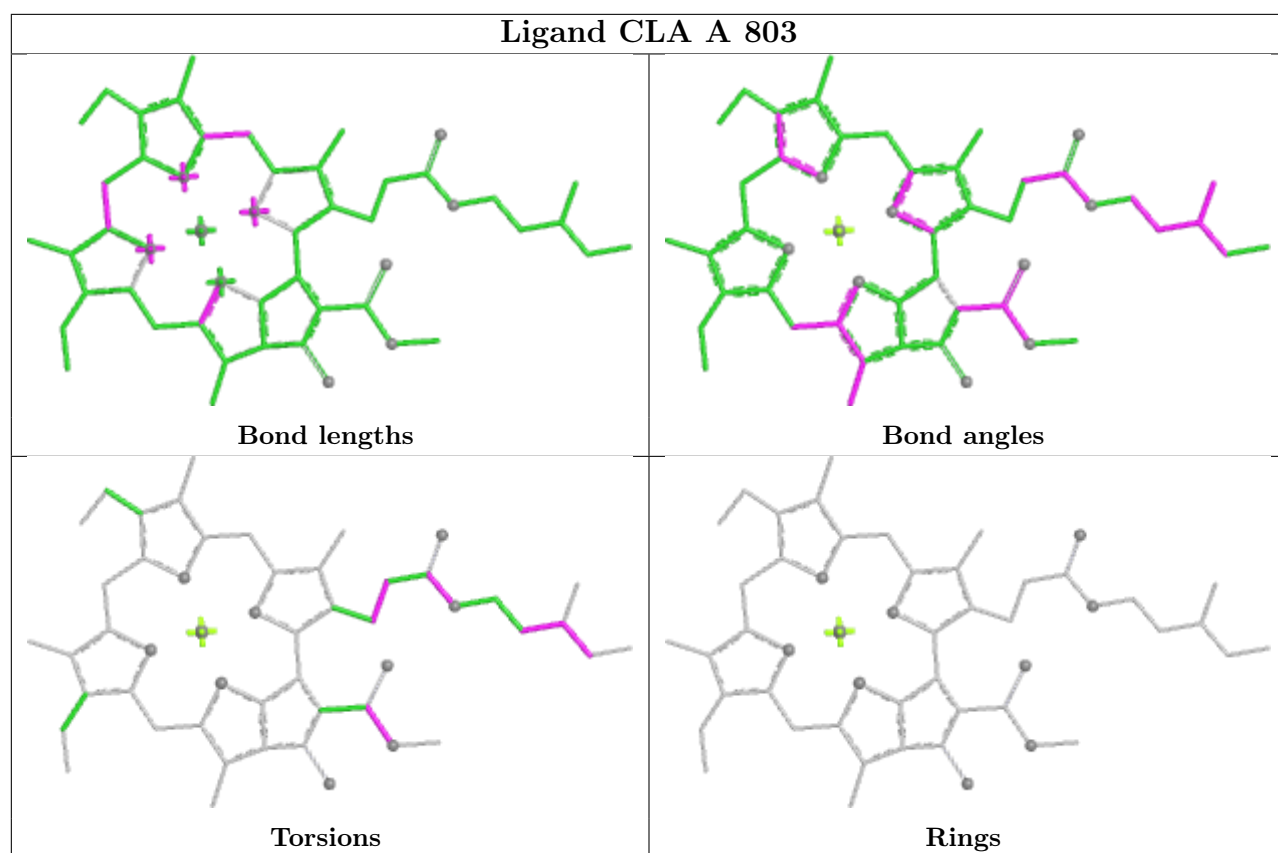
Ligand CLA B 783



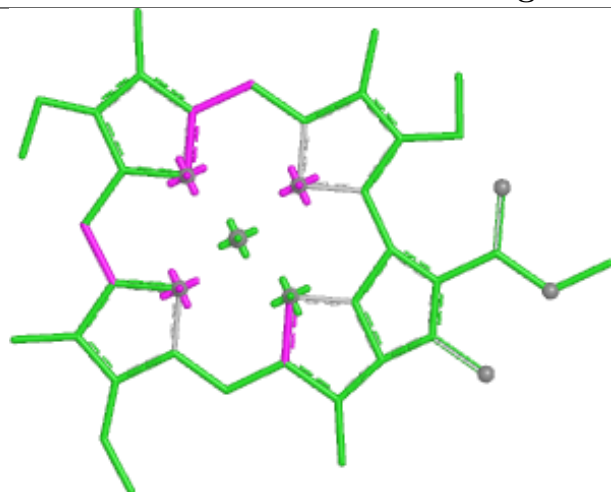
Ligand CLA B 738



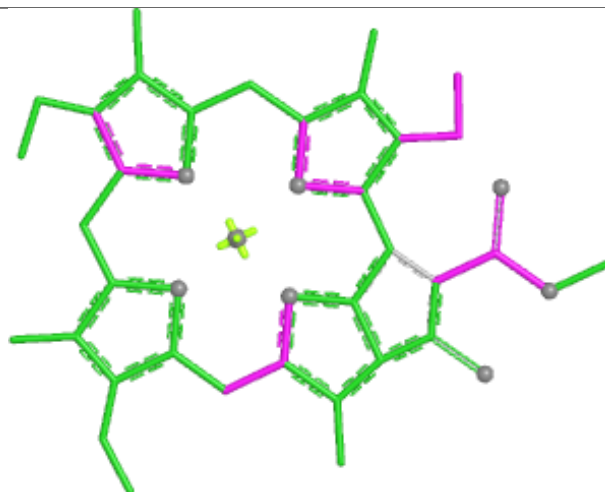




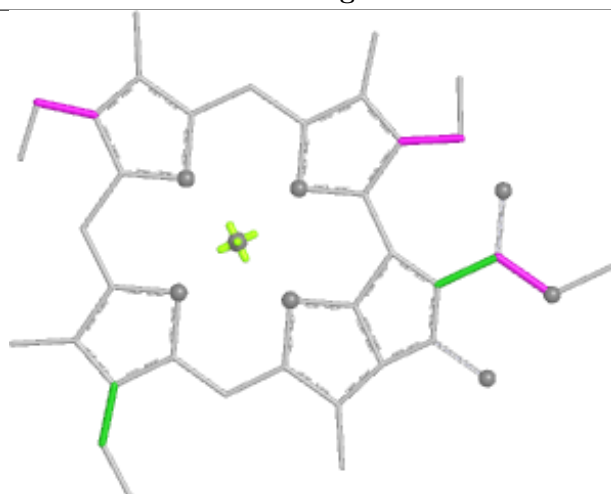
Ligand CLA k 615



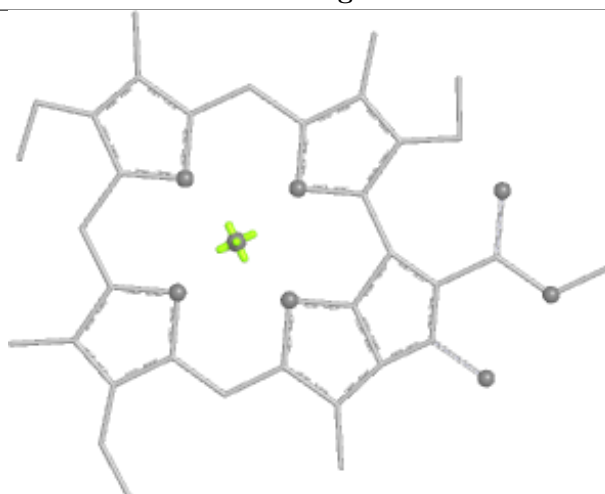
Bond lengths



Bond angles

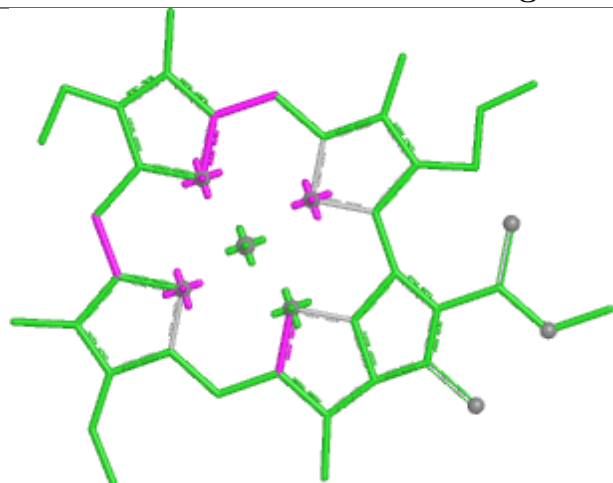


Torsions

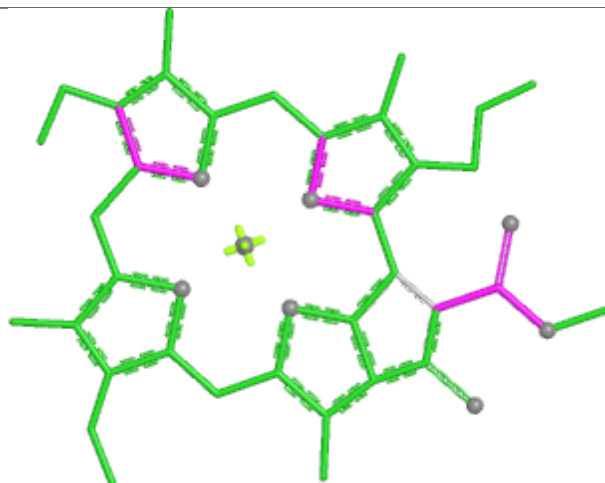


Rings

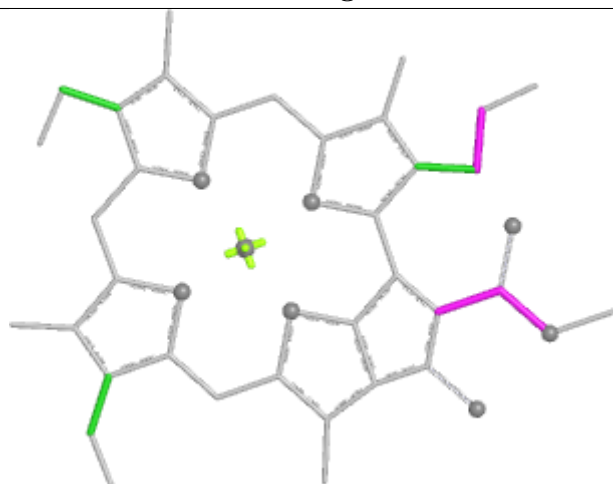
Ligand CLA c 612



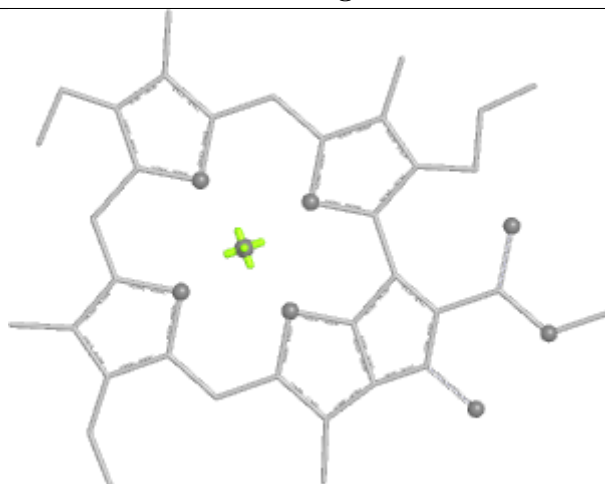
Bond lengths



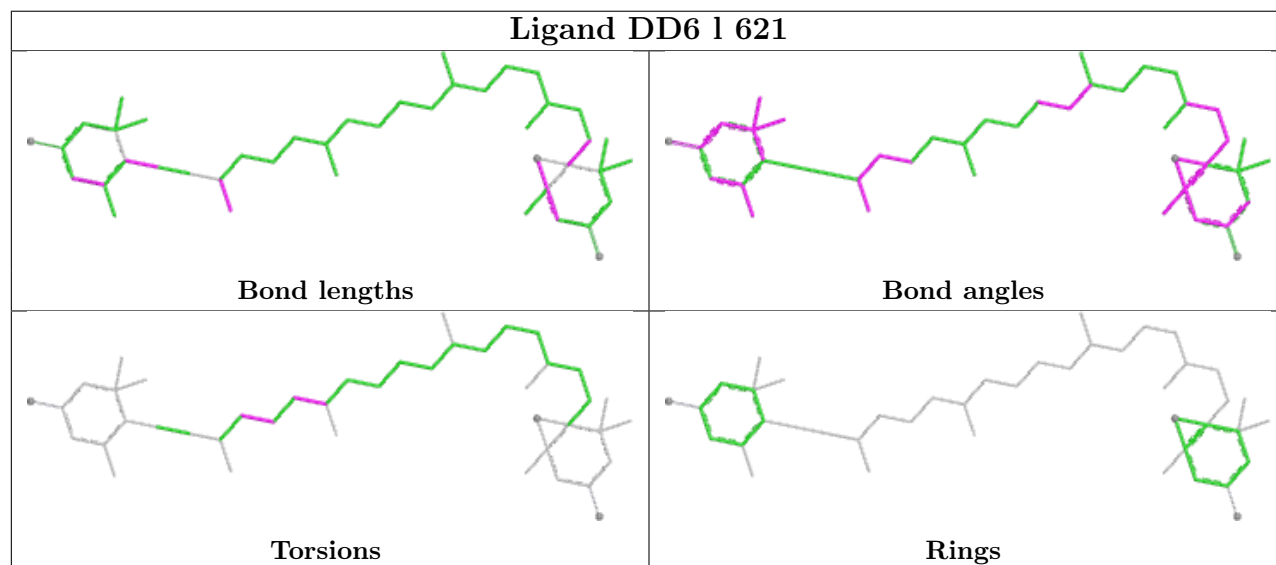
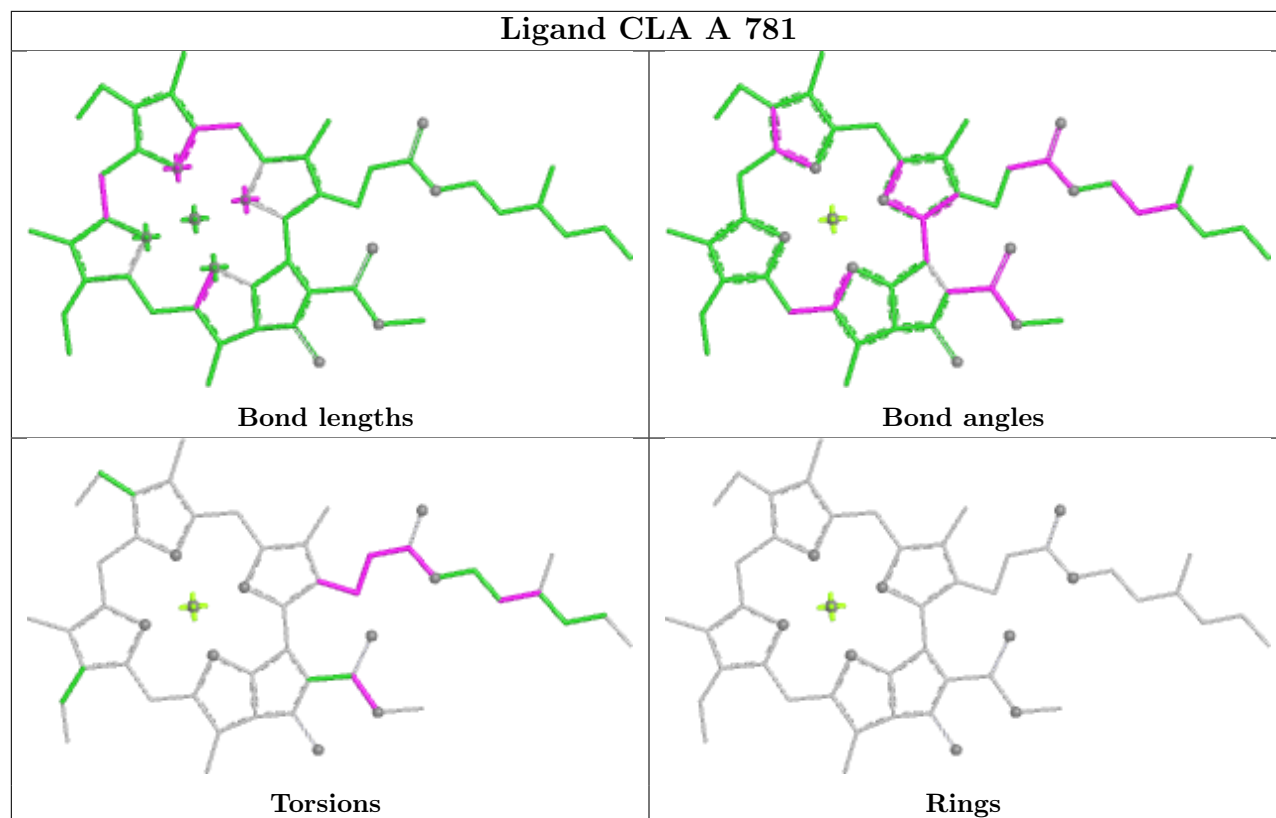
Bond angles

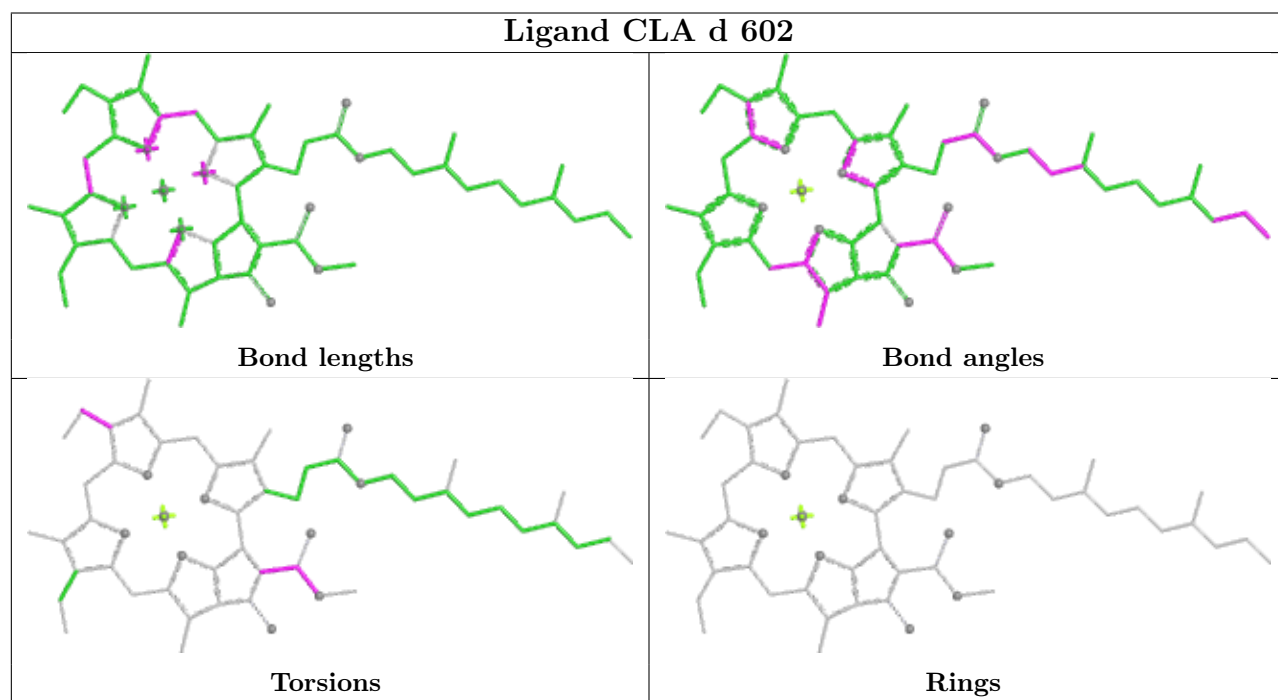
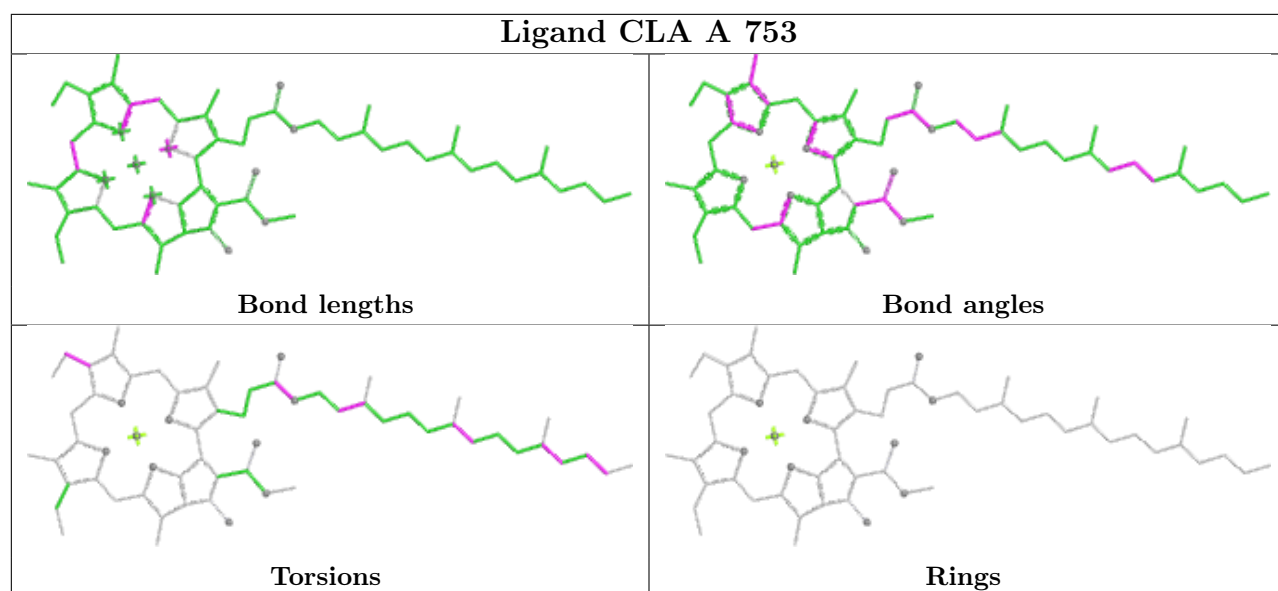


Torsions

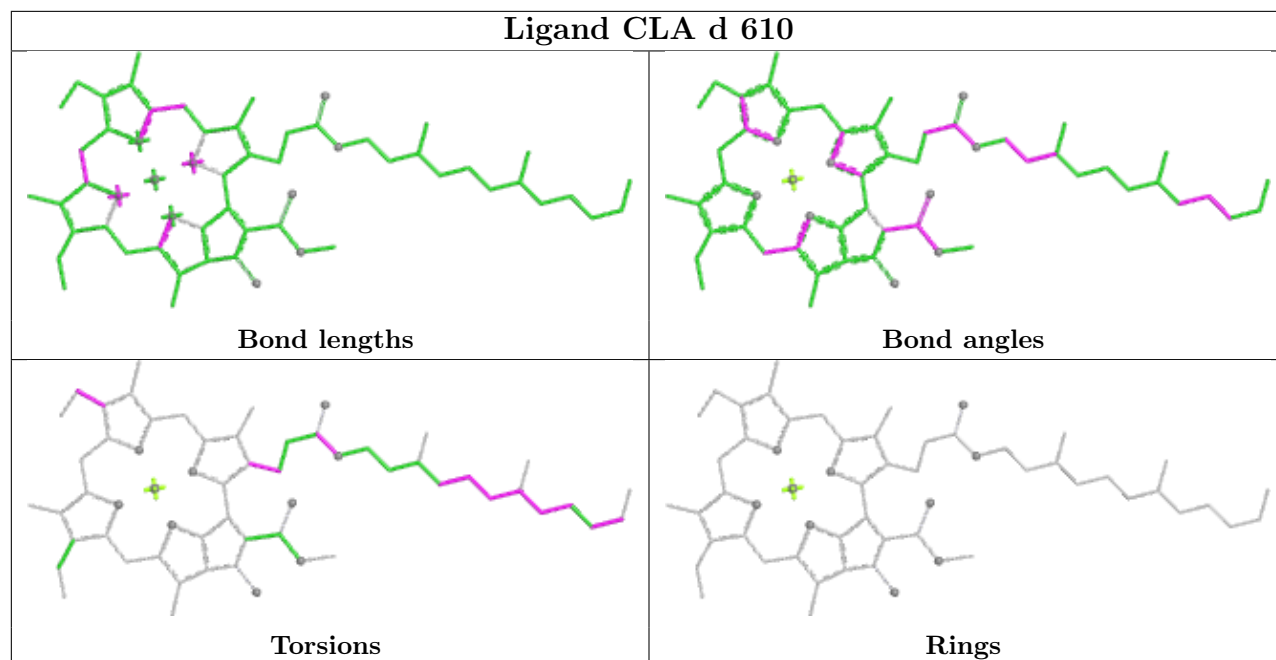


Rings

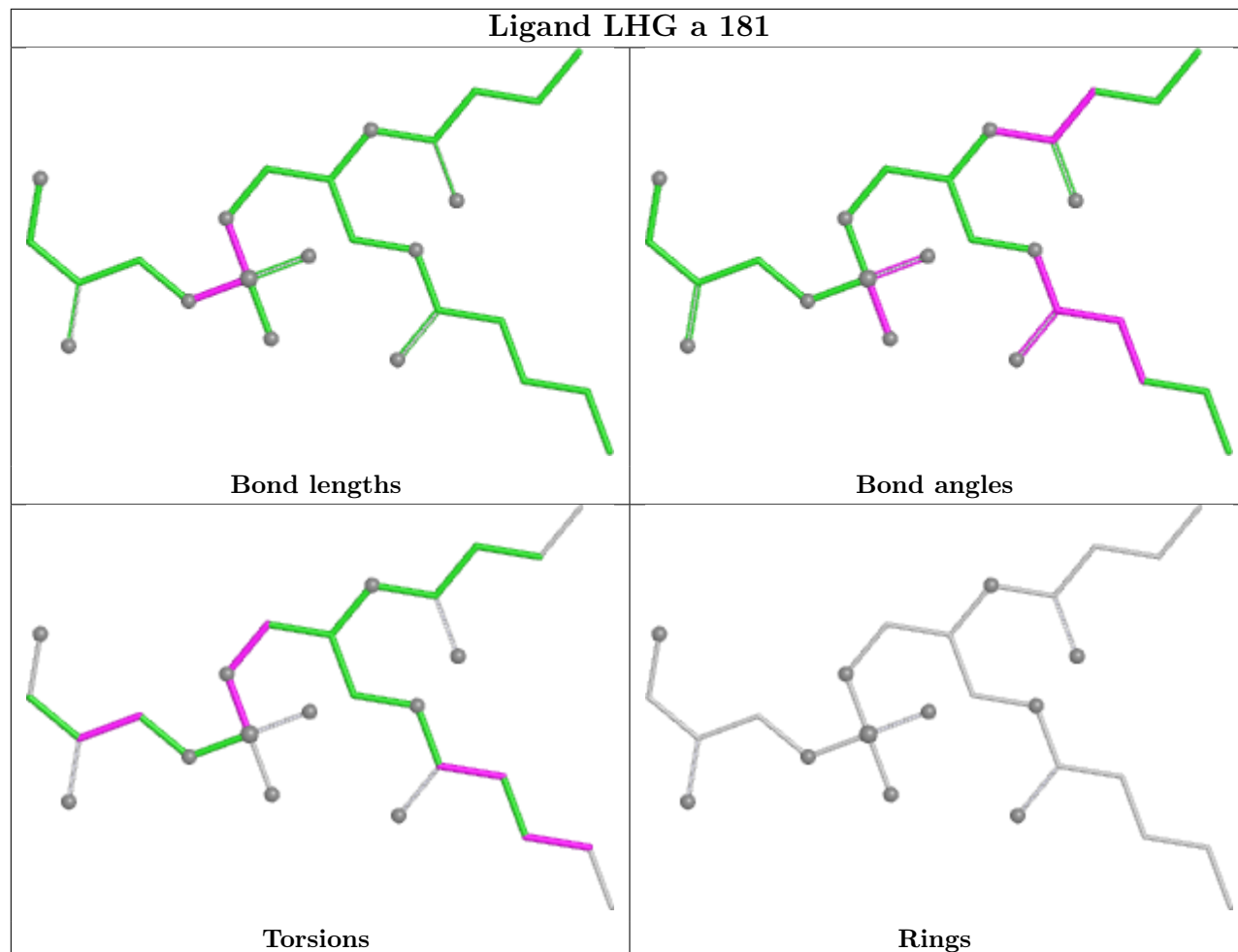


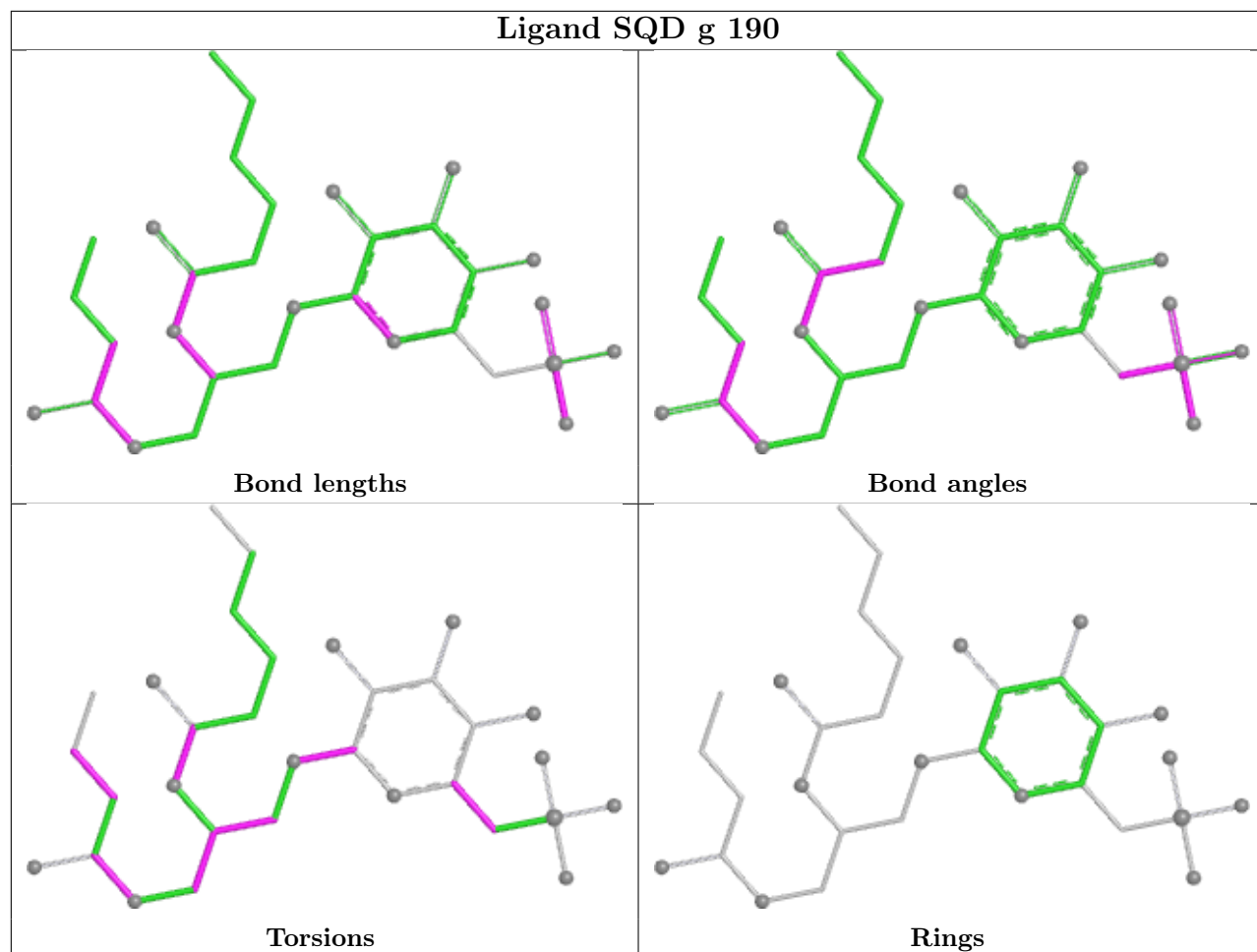


Ligand CLA d 610

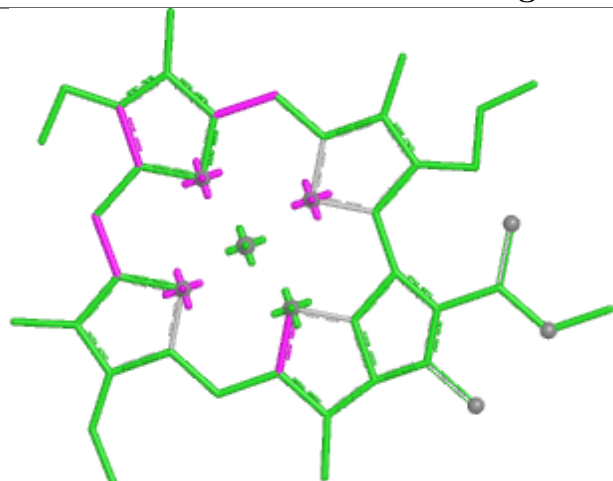


Ligand LHG a 181

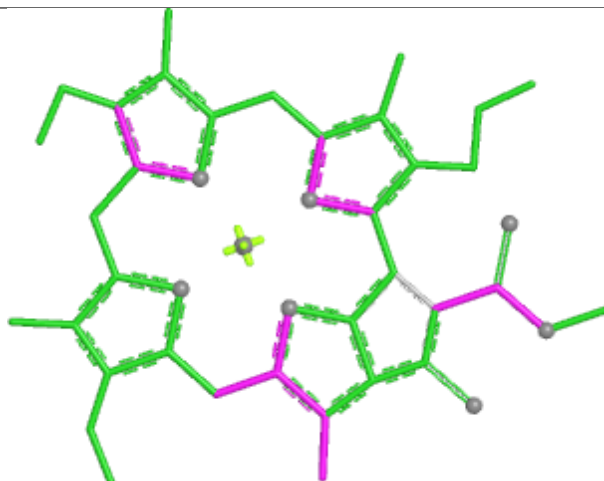




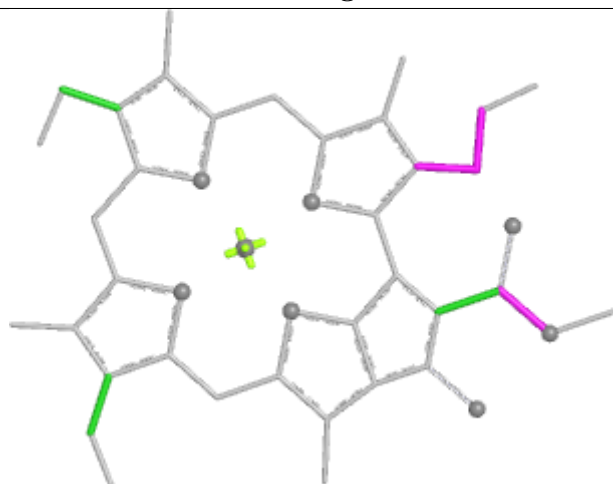
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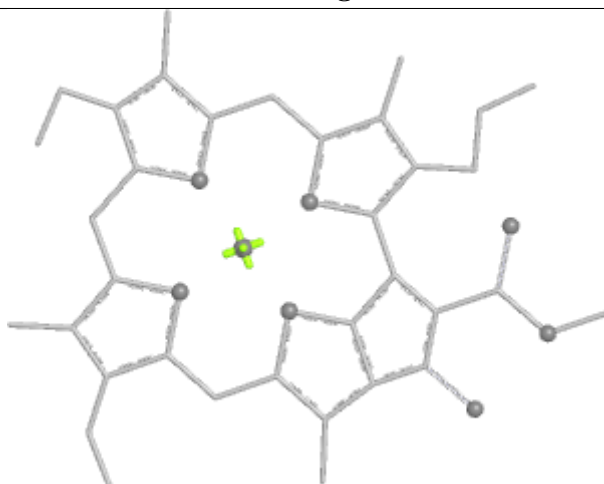
Bond lengths



Bond angles

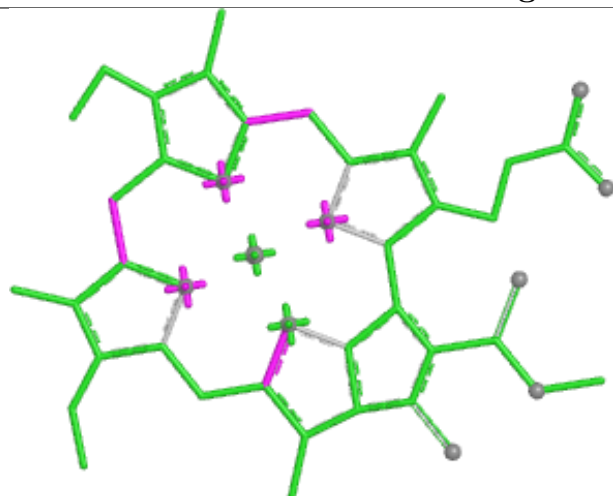


Torsions

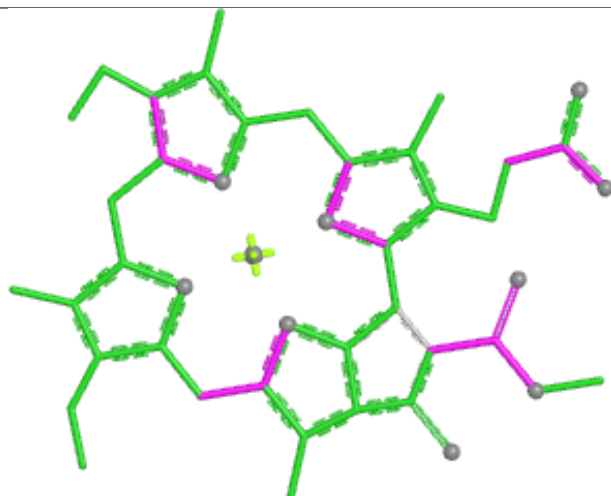


Rings

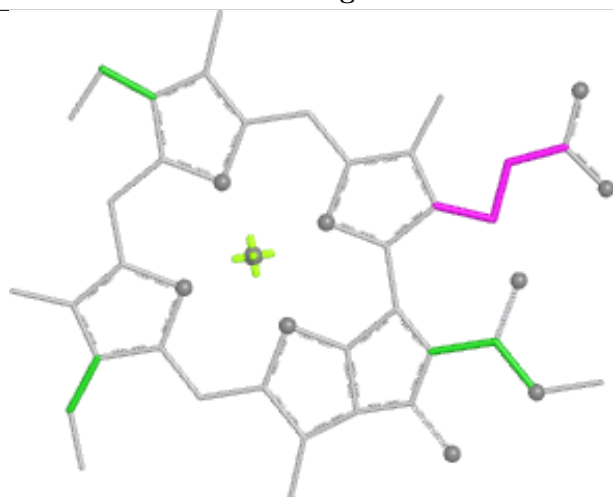
Ligand CLA a 611



Bond lengths



Bond angles

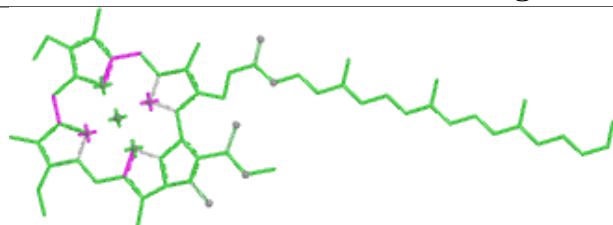


Torsions

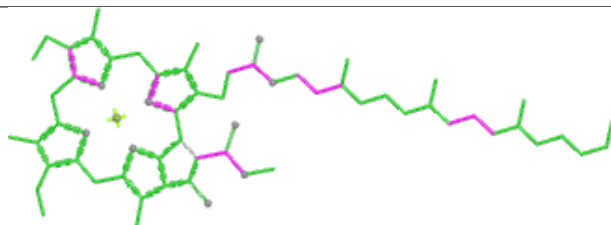


Rings

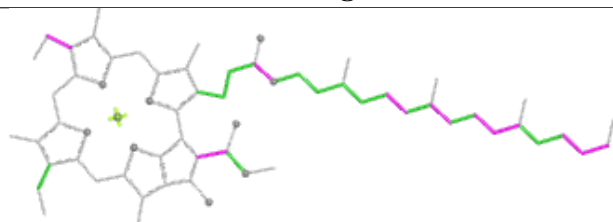
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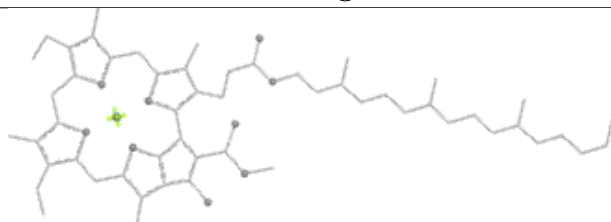
Bond lengths



Bond angles

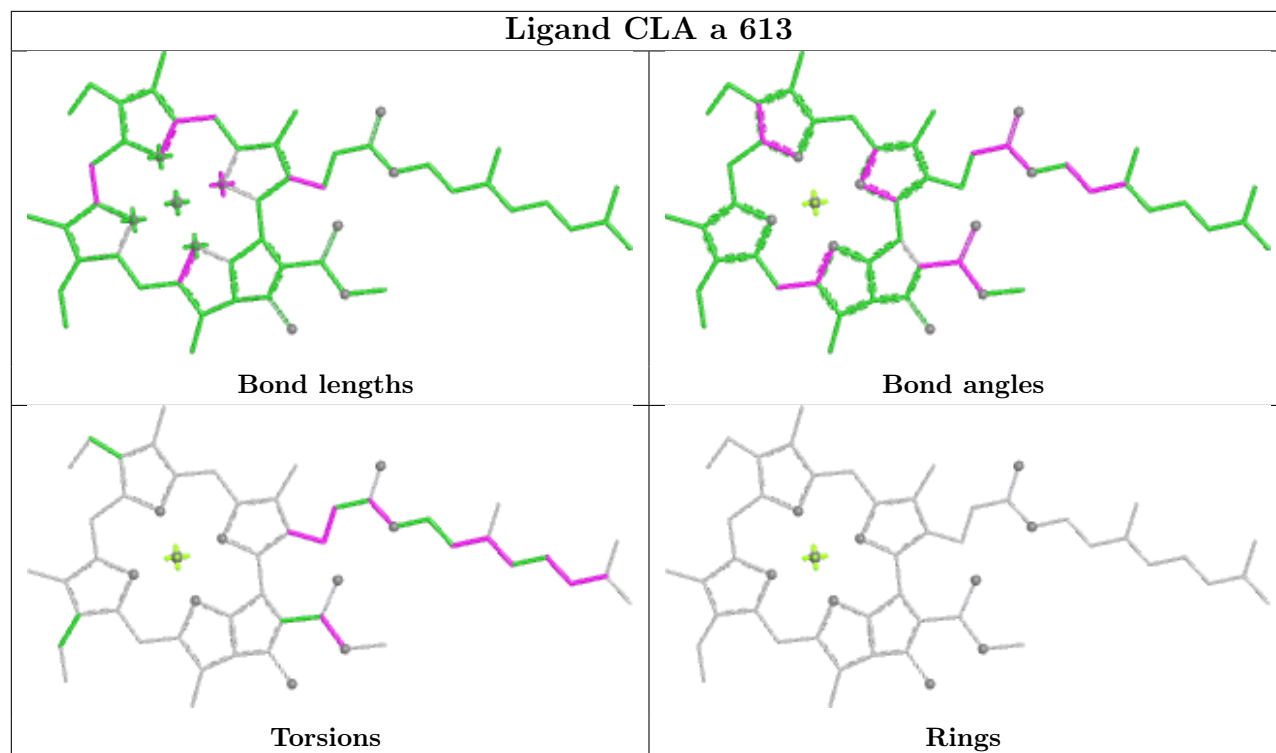


Torsions

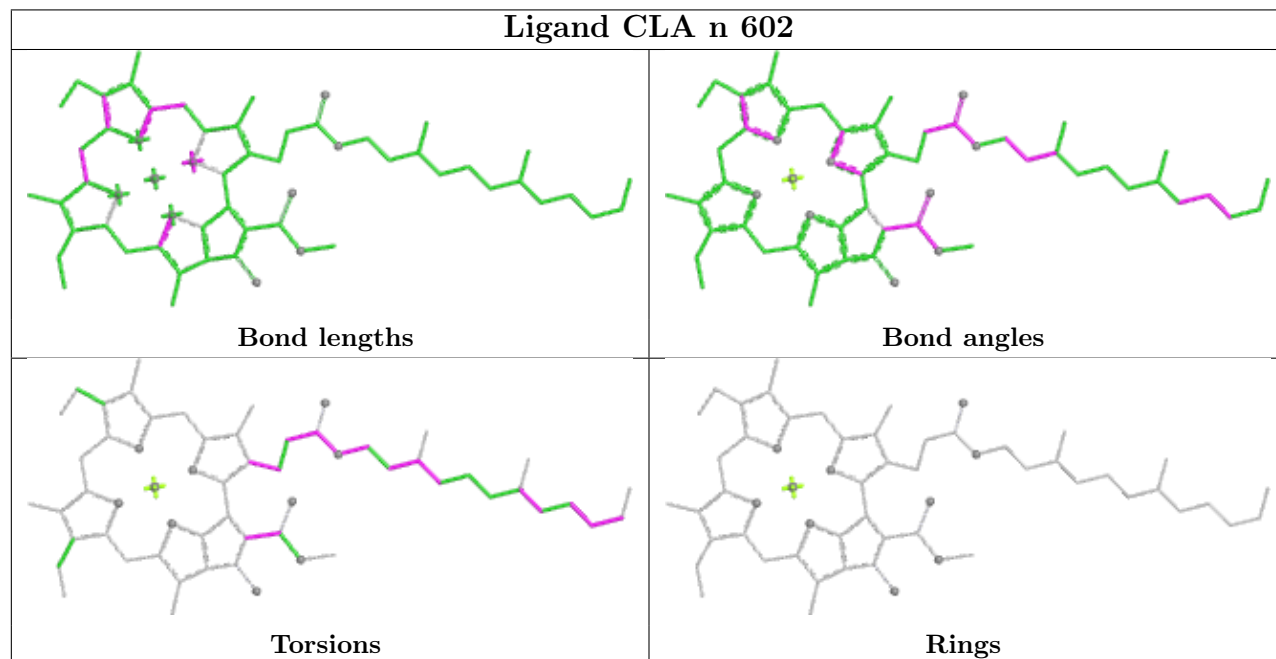


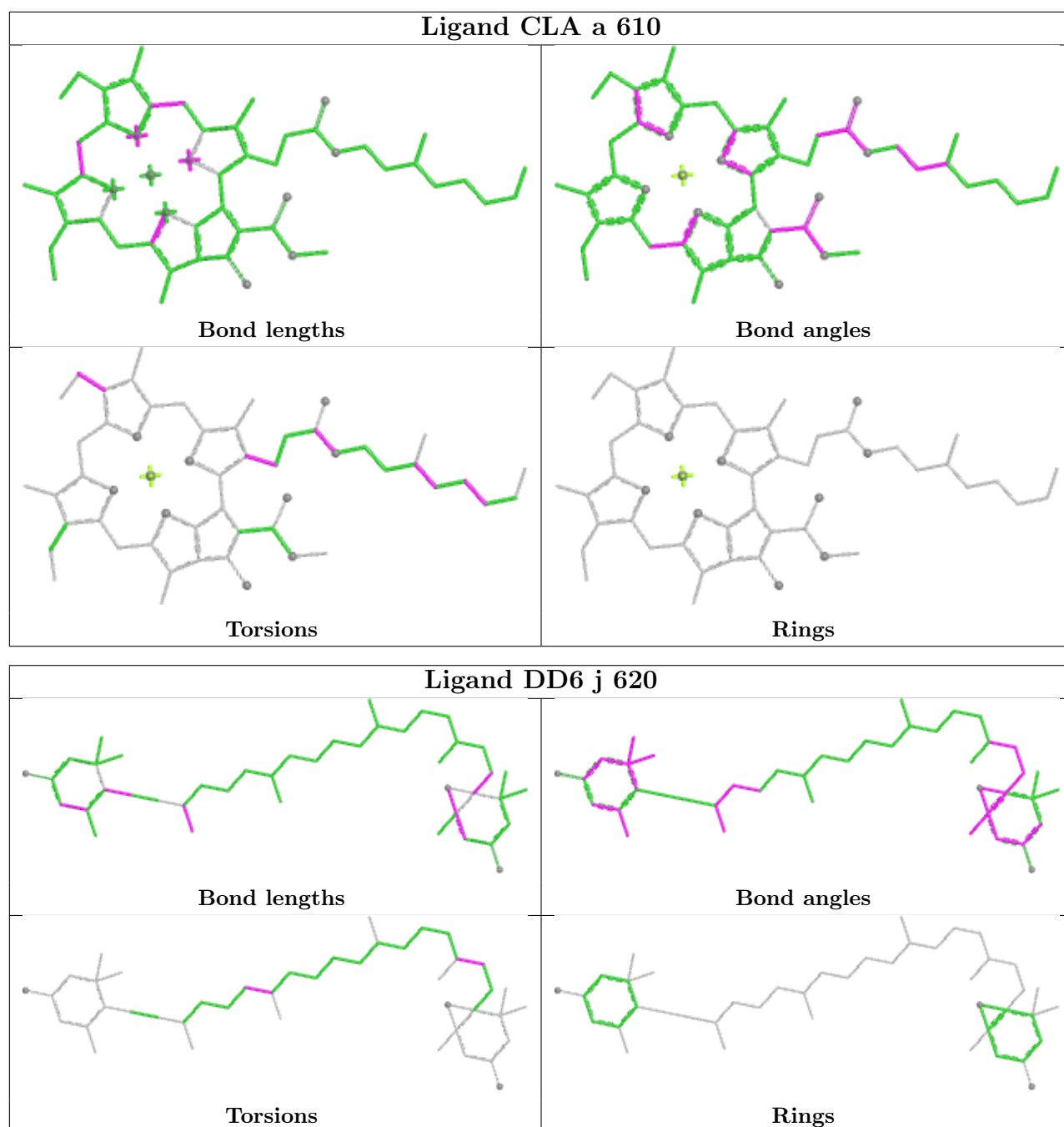
Rings

Ligand CLA a 613

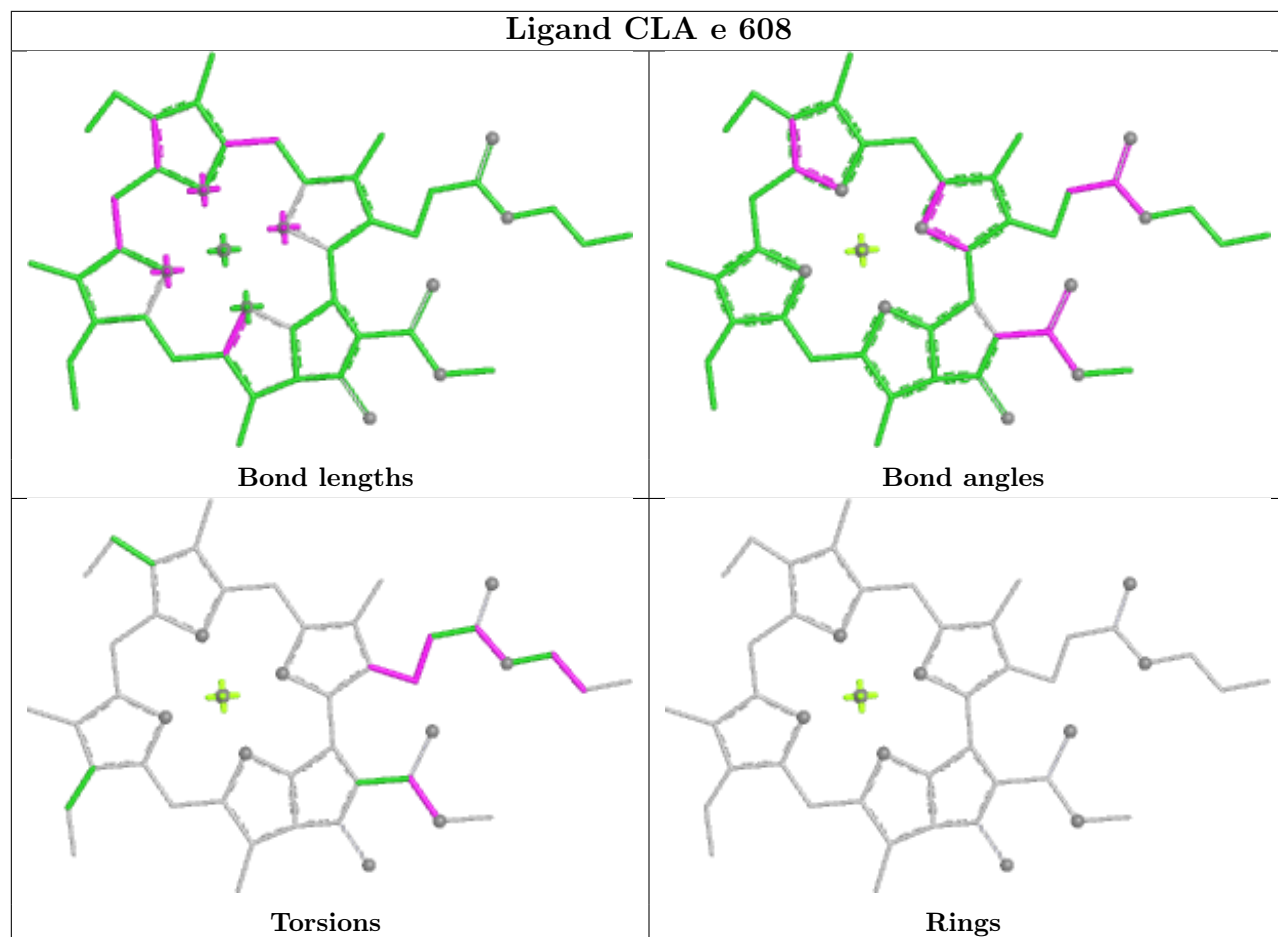


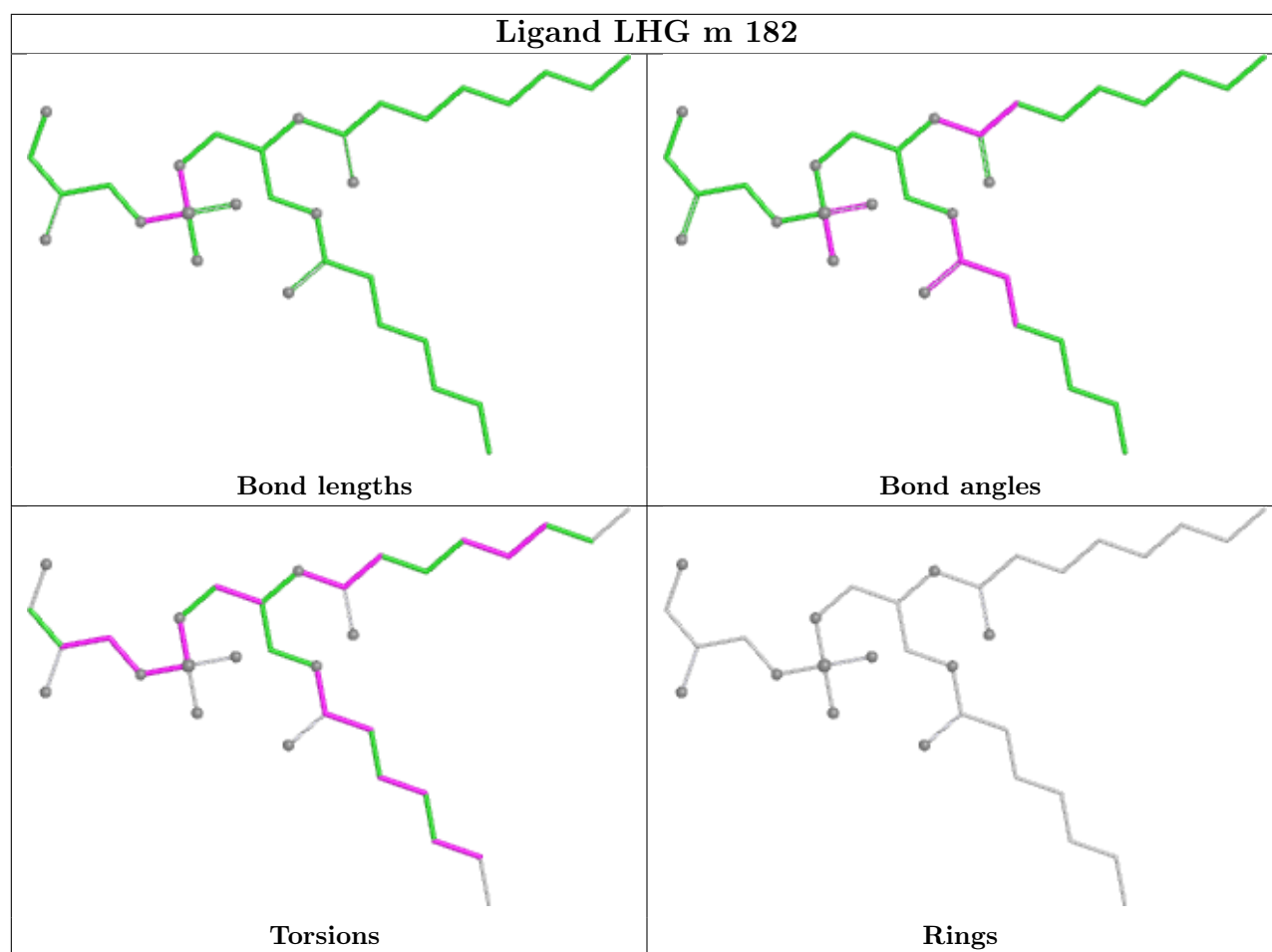
Ligand CLA n 602



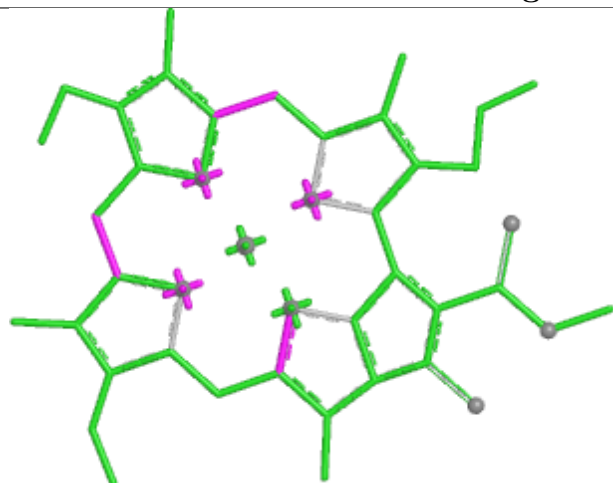


Ligand CLA e 608

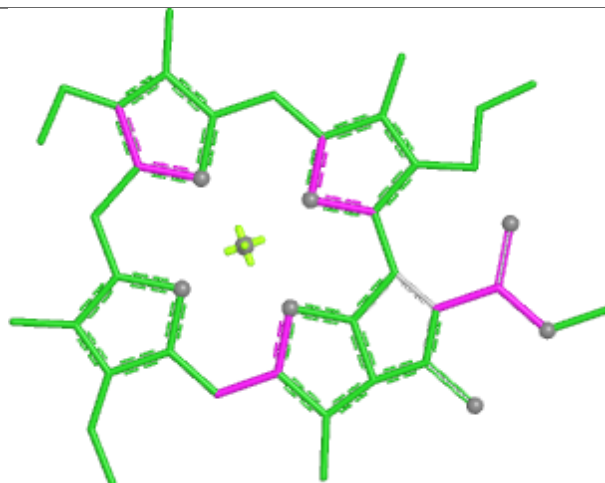




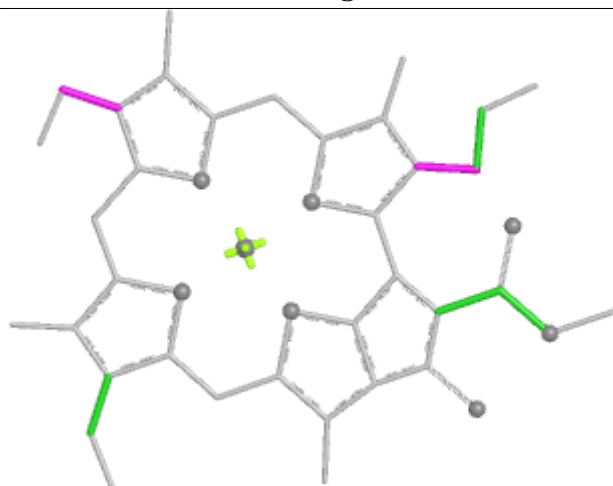
Ligand CLA i 609



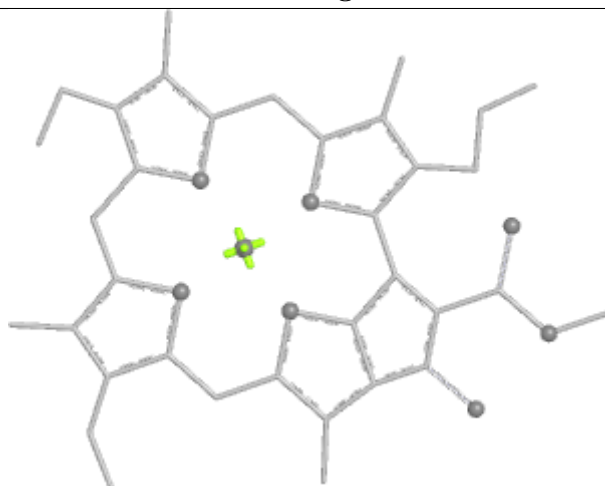
Bond lengths



Bond angles

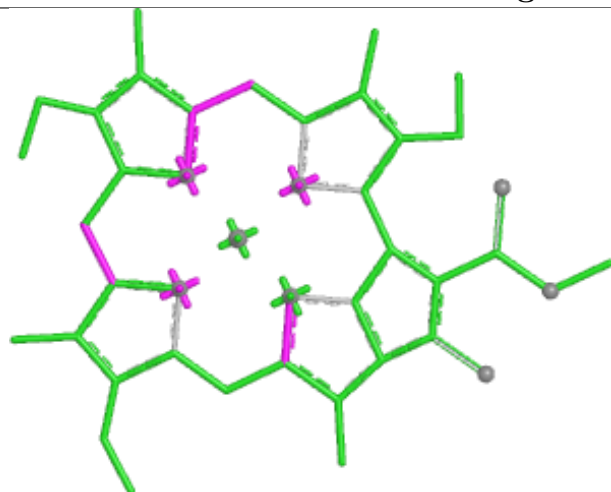


Torsions

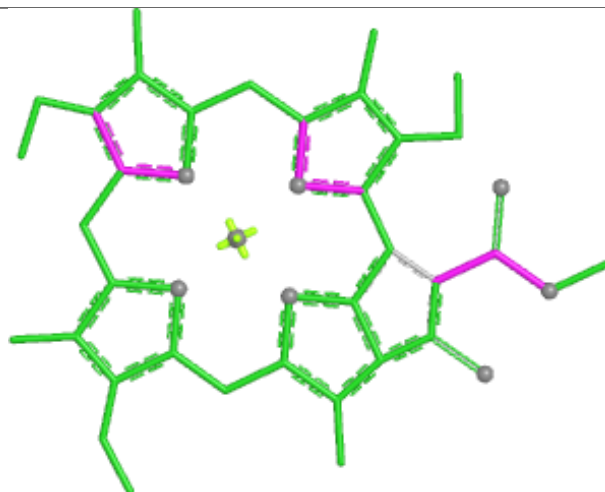


Rings

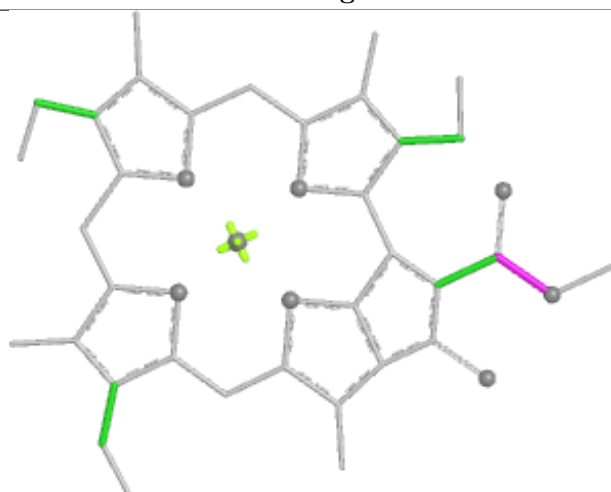
Ligand CLA d 612



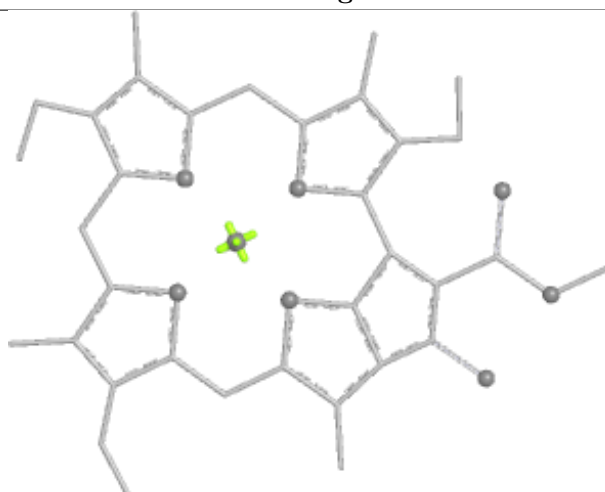
Bond lengths



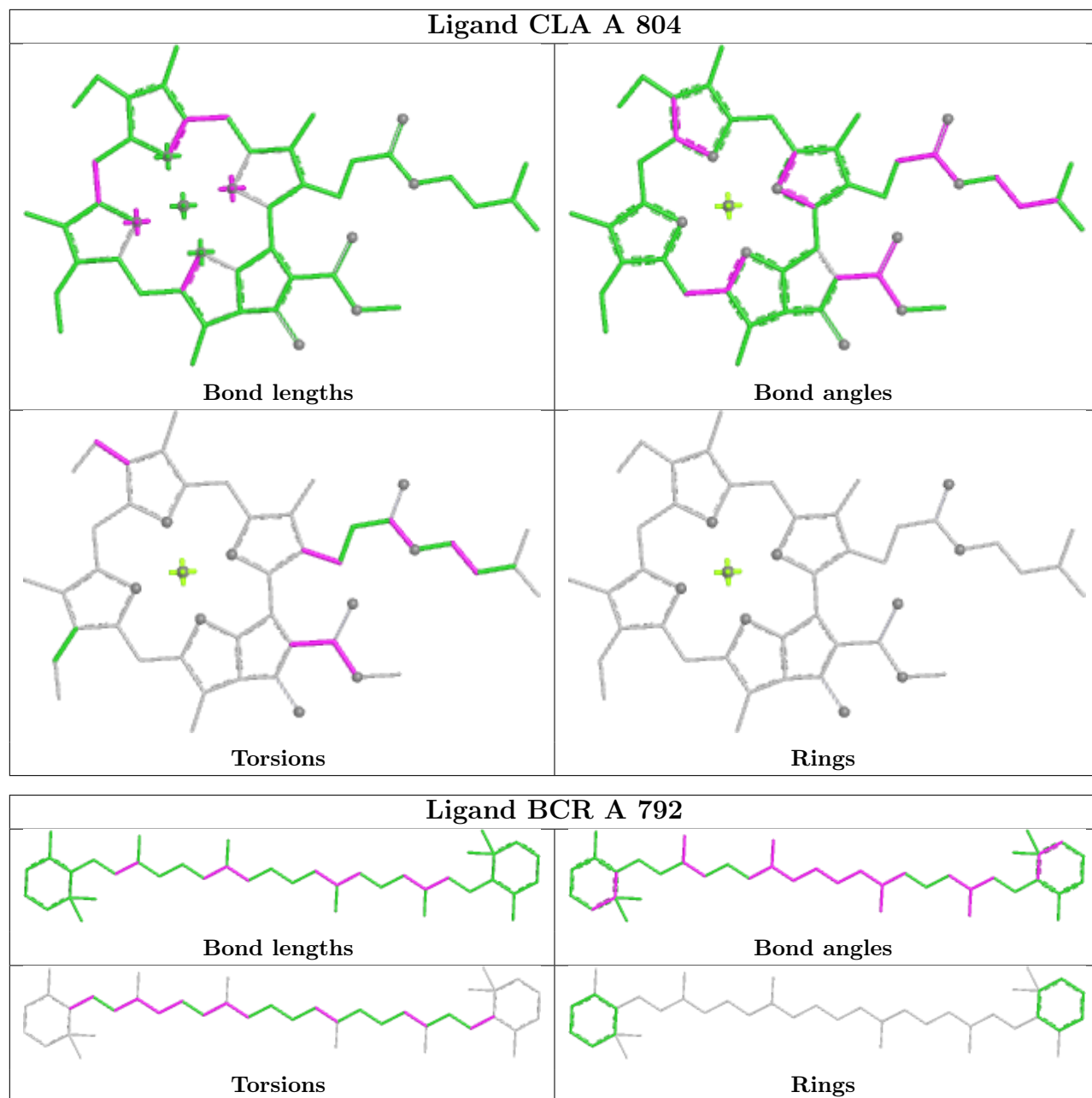
Bond angles

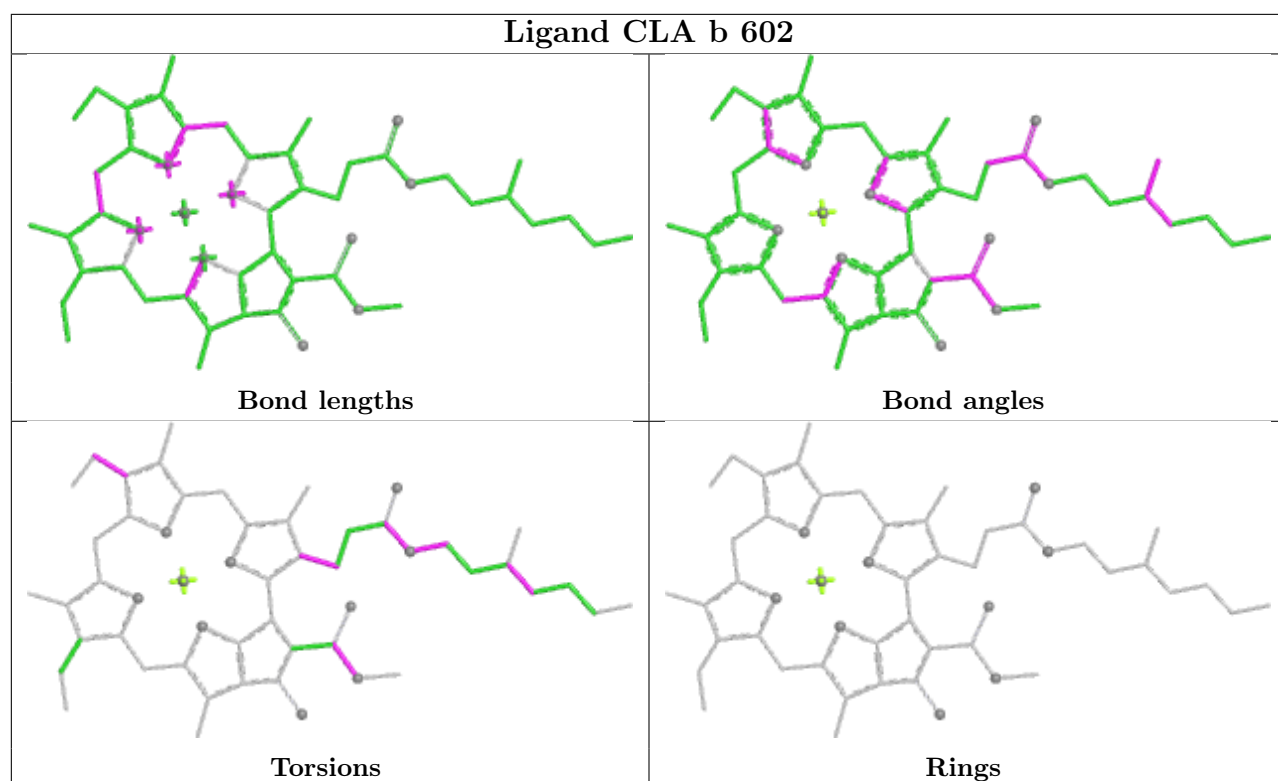


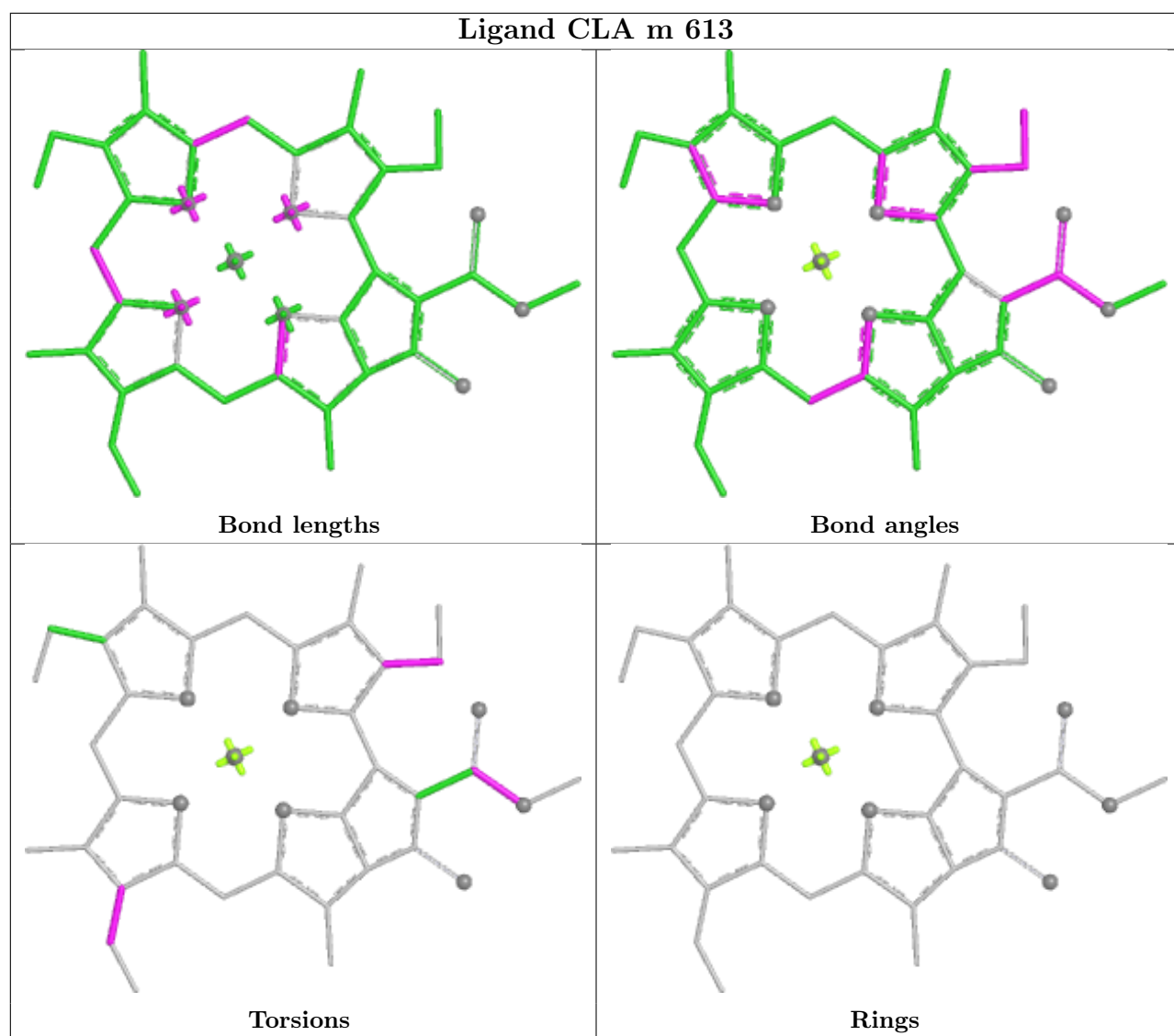
Torsions



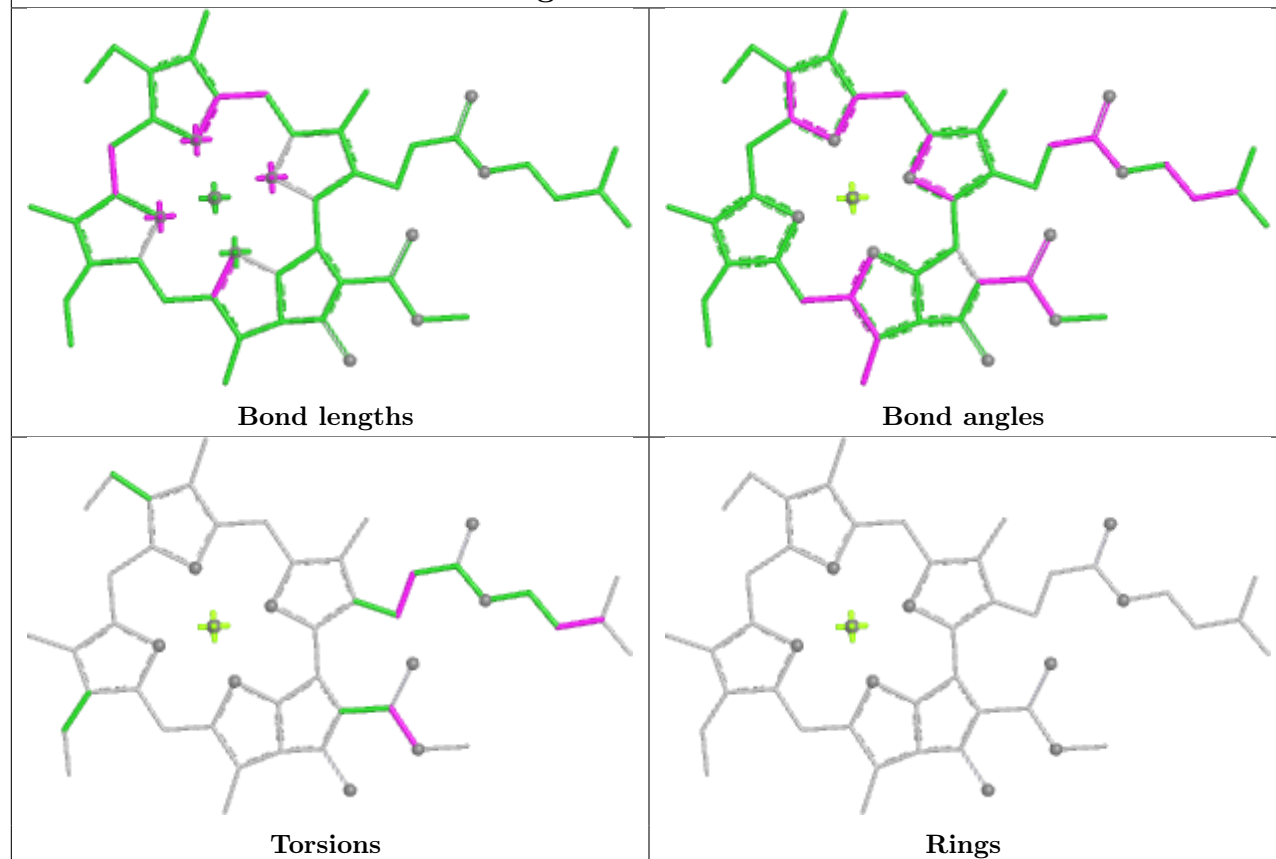
Rings



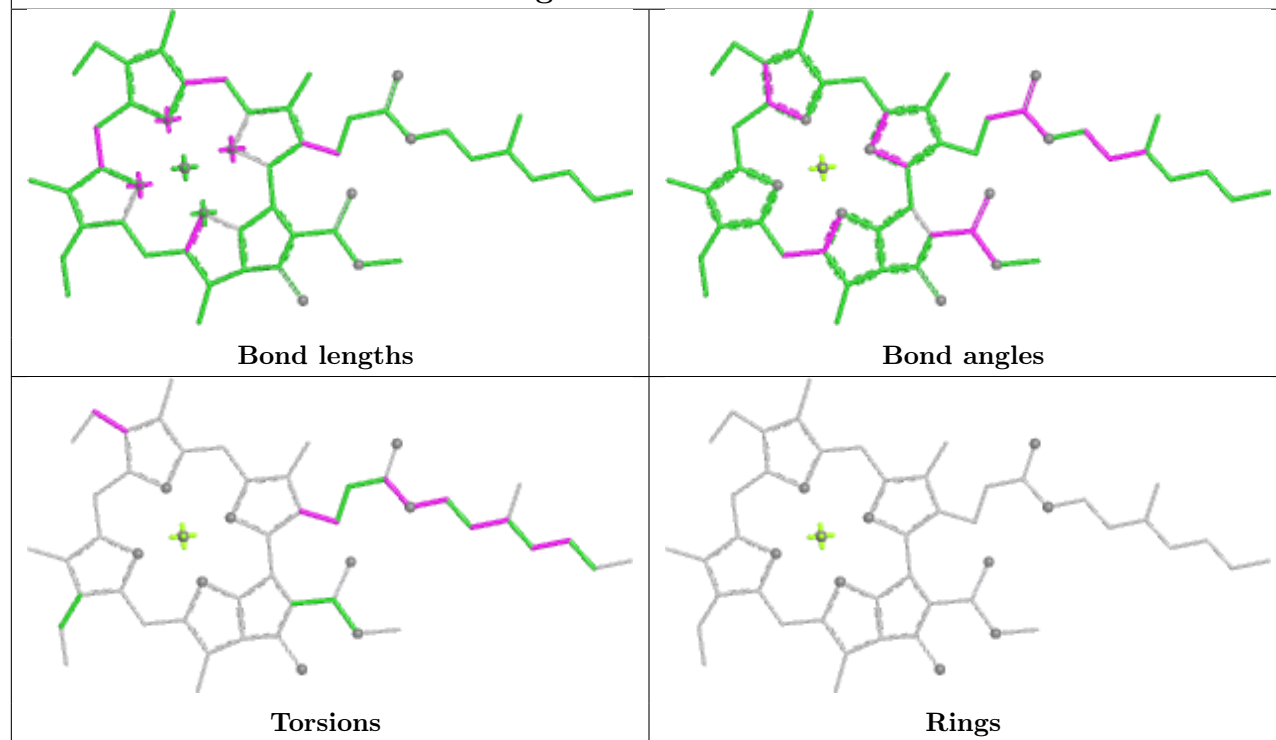


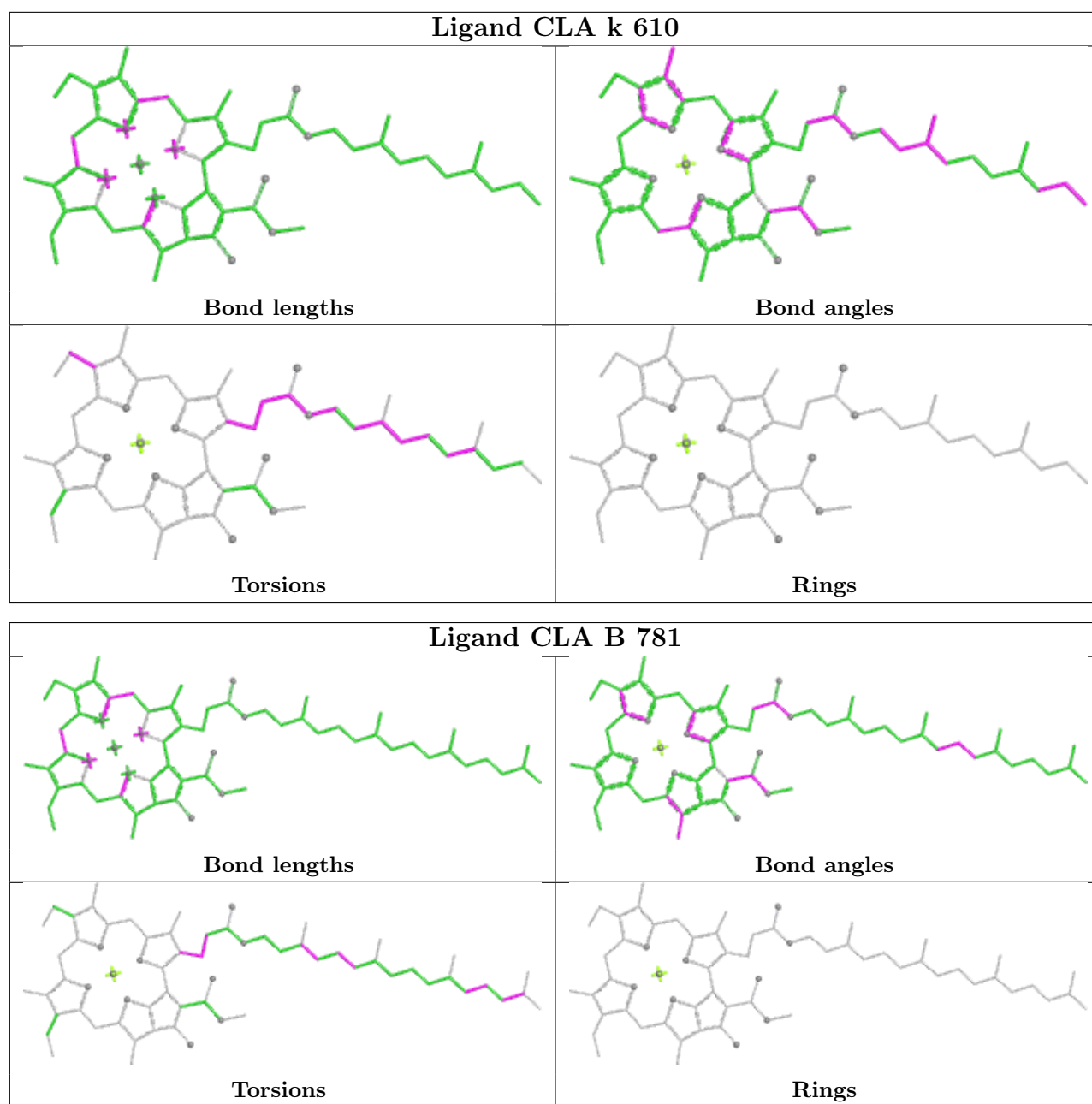


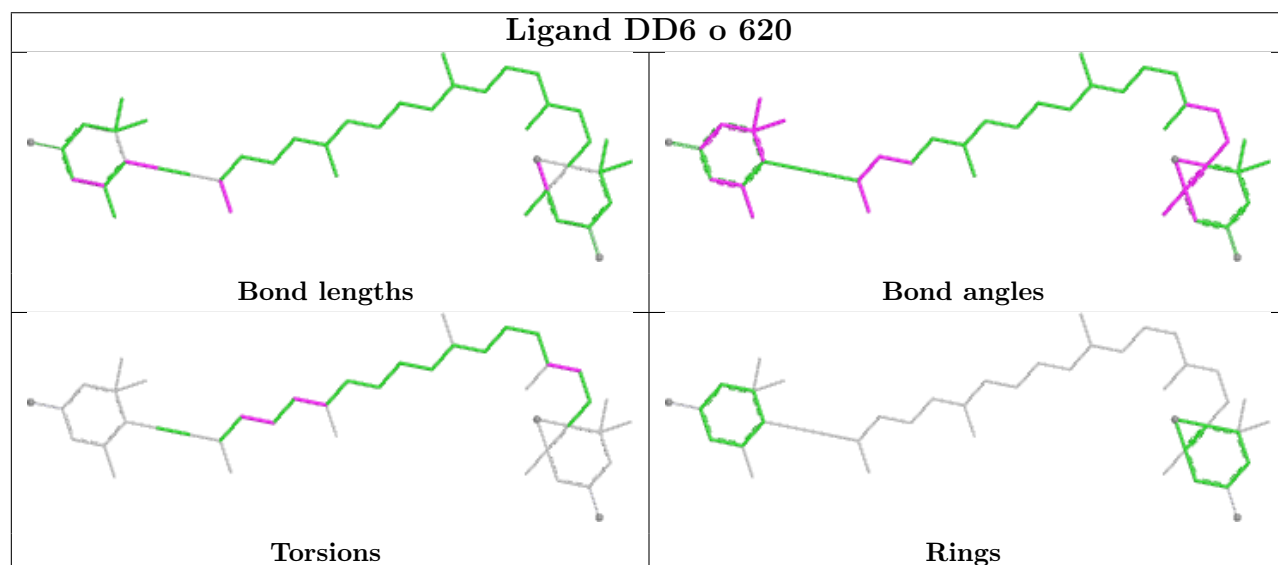
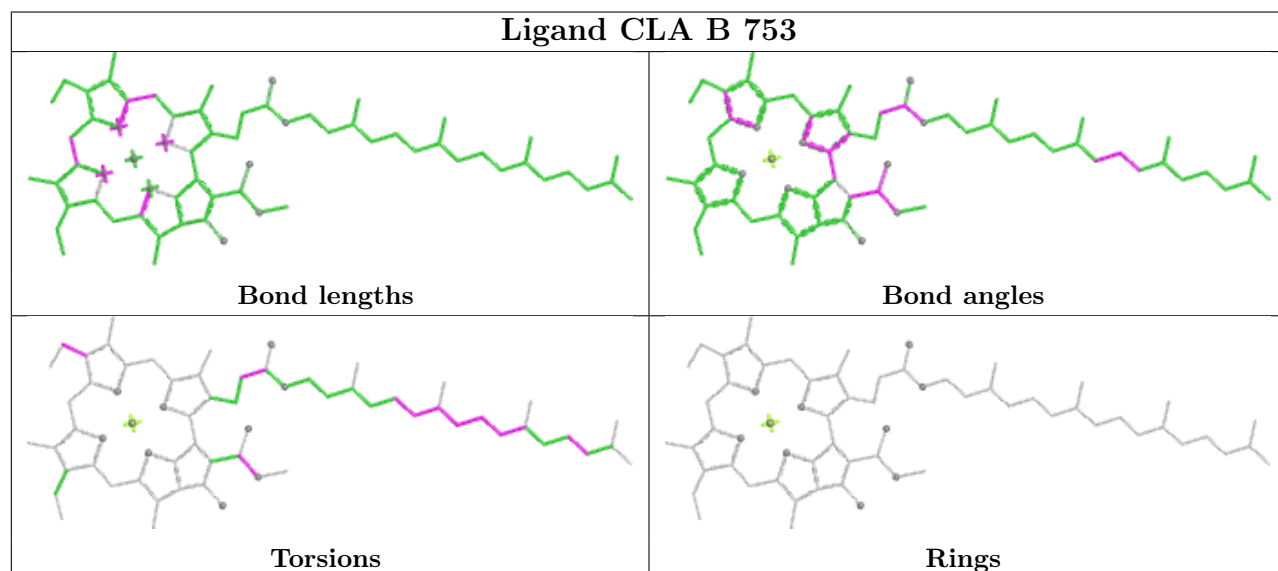
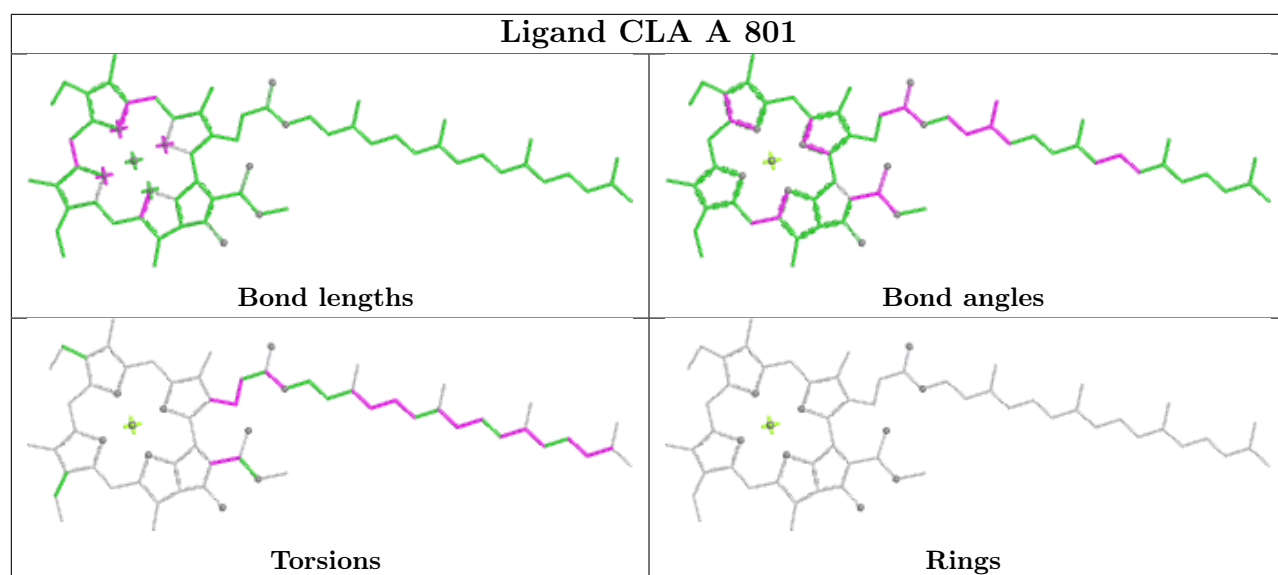
Ligand CLA e 604



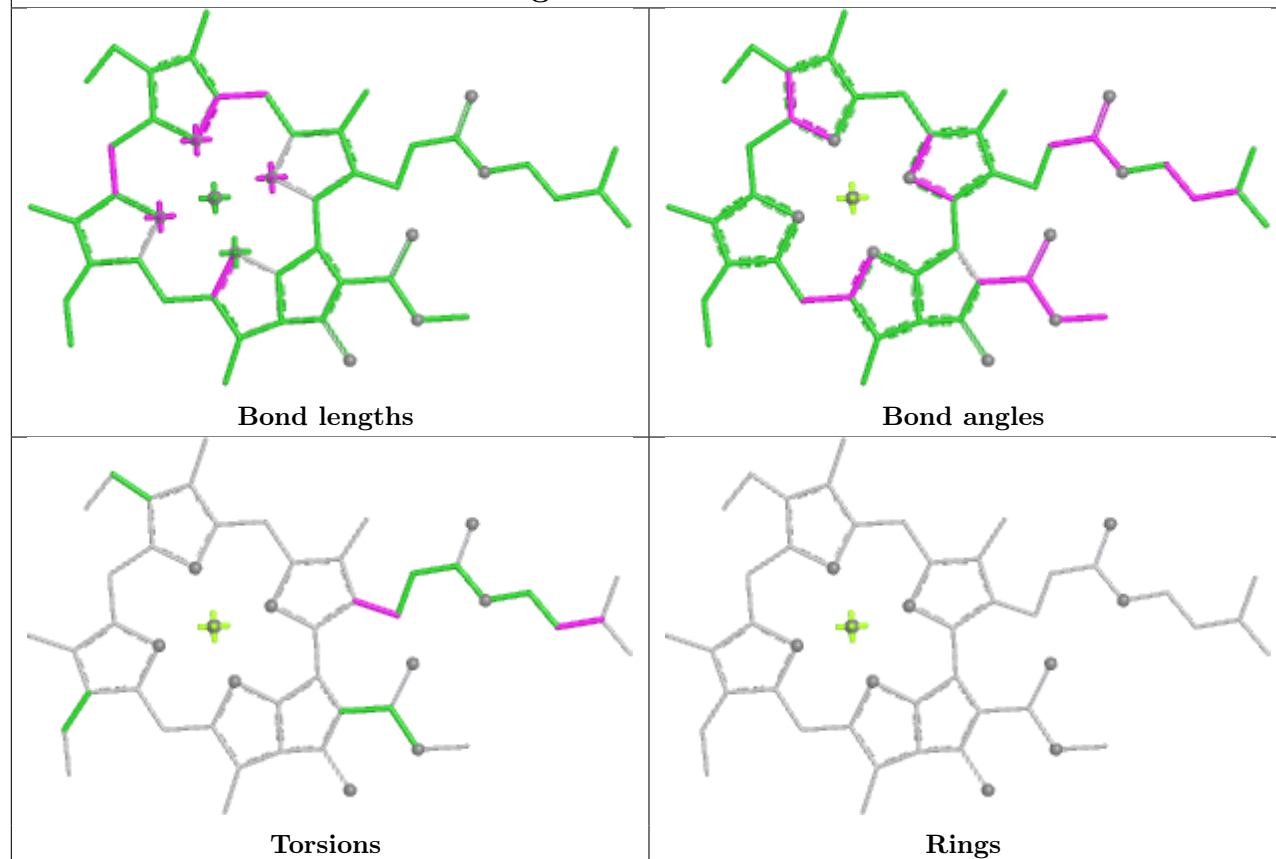
Ligand CLA k 602



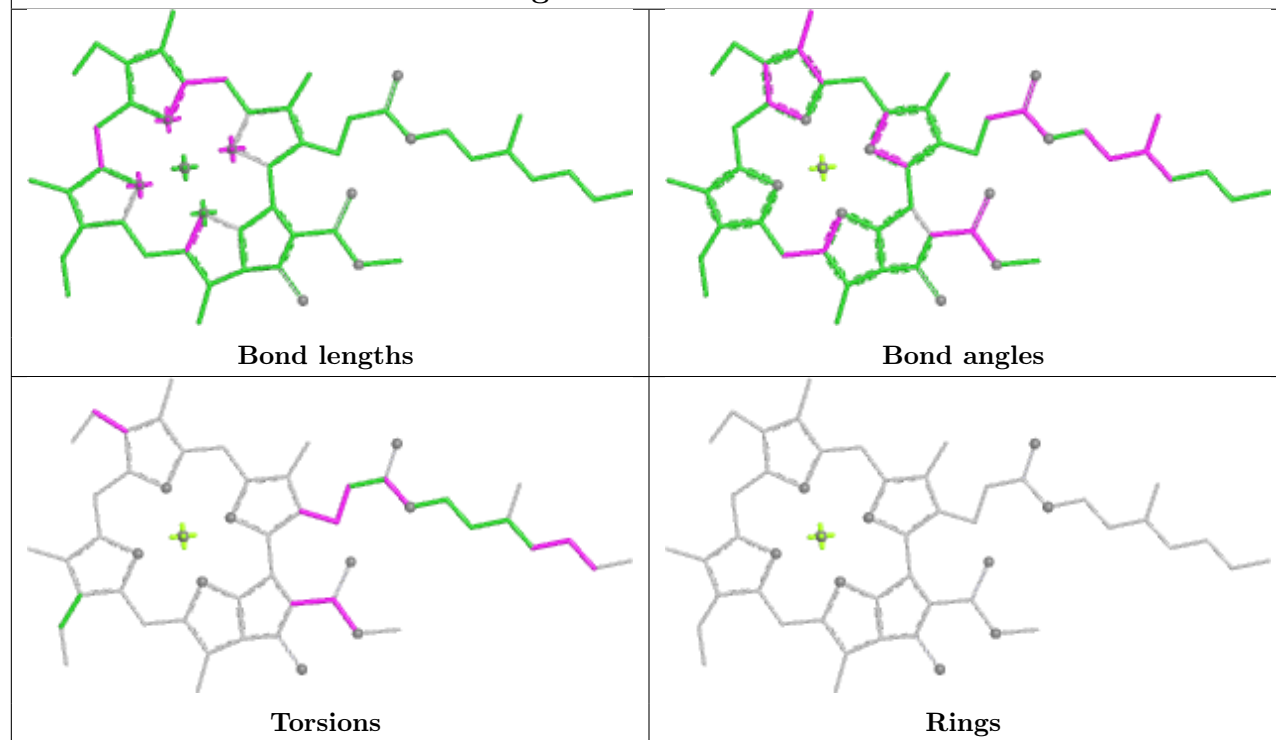




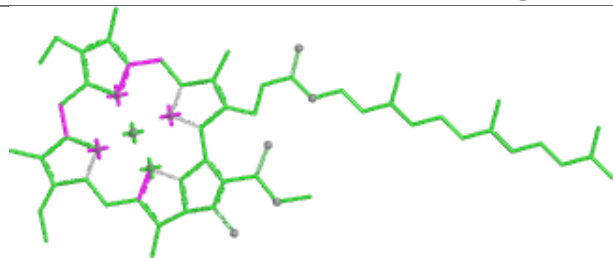
Ligand CLA A 762



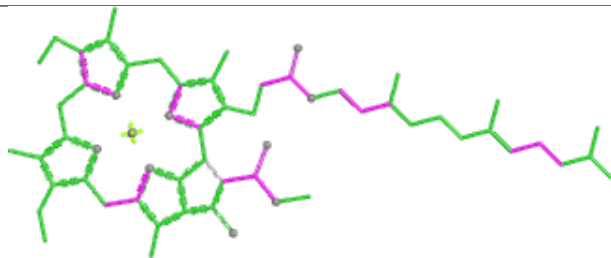
Ligand CLA A 808



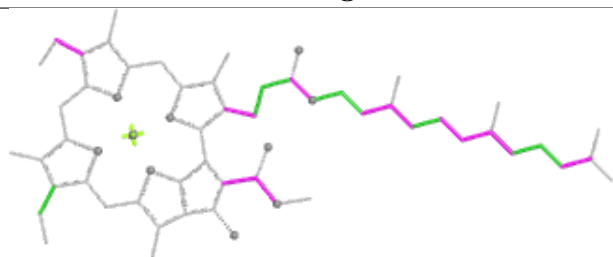
Ligand CLA B 756



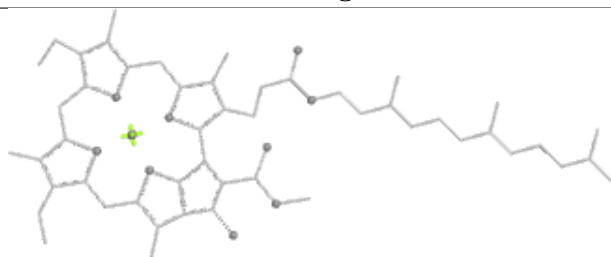
Bond lengths



Bond angles

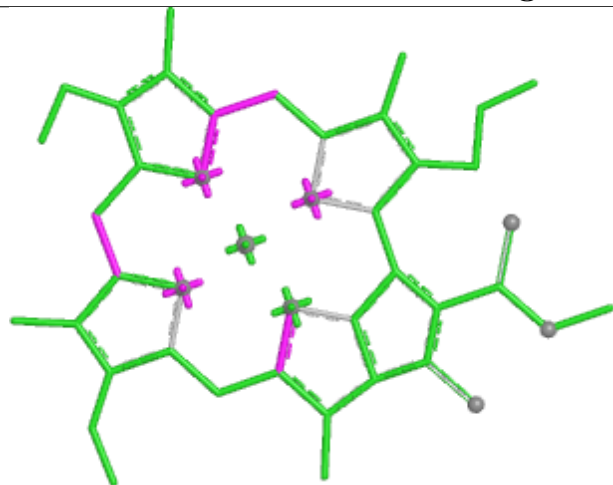


Torsions

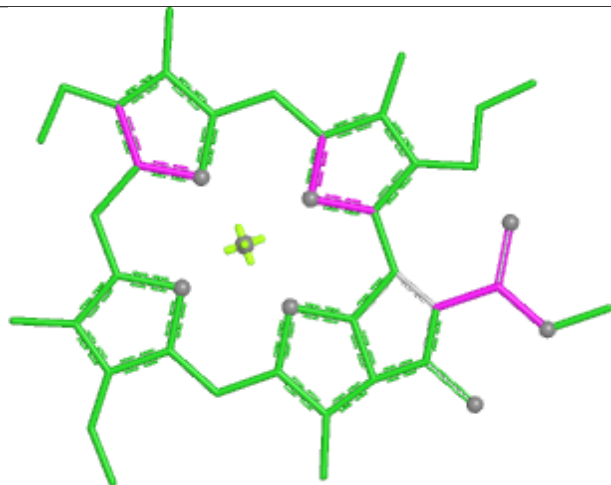


Rings

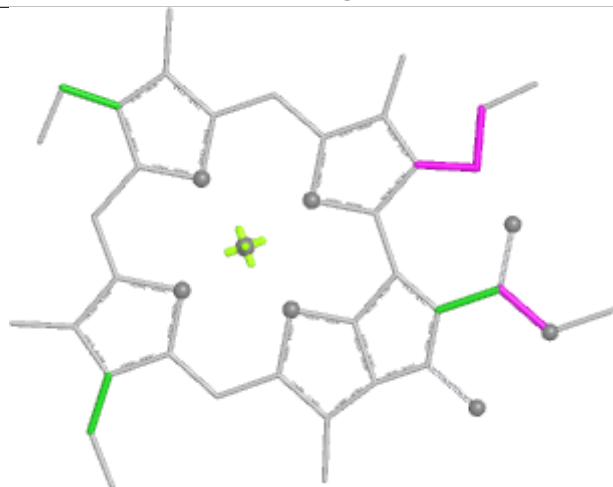
Ligand CLA a 612



Bond lengths



Bond angles

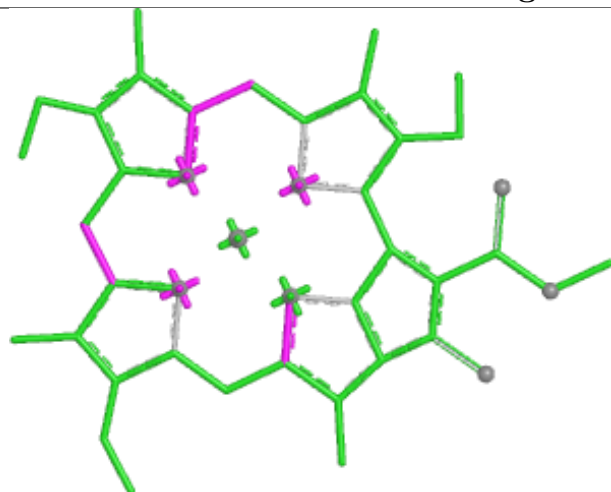


Torsions

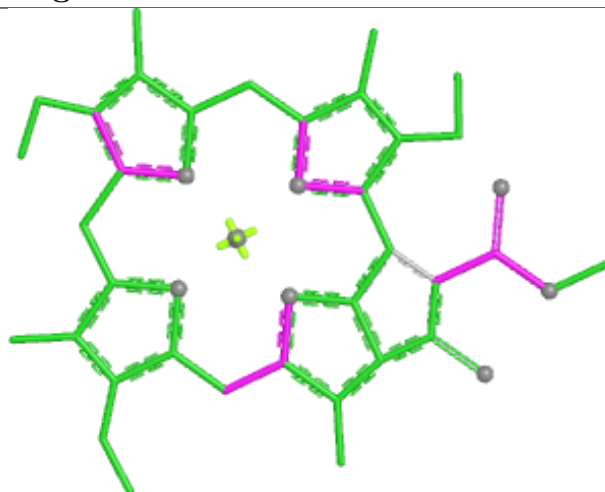


Rings

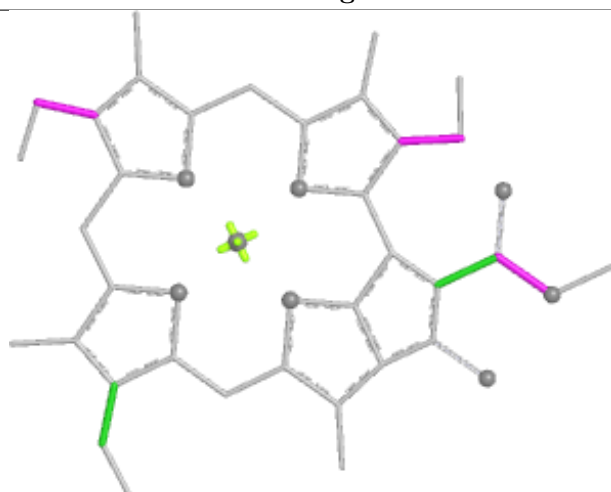
Ligand CLA g 601



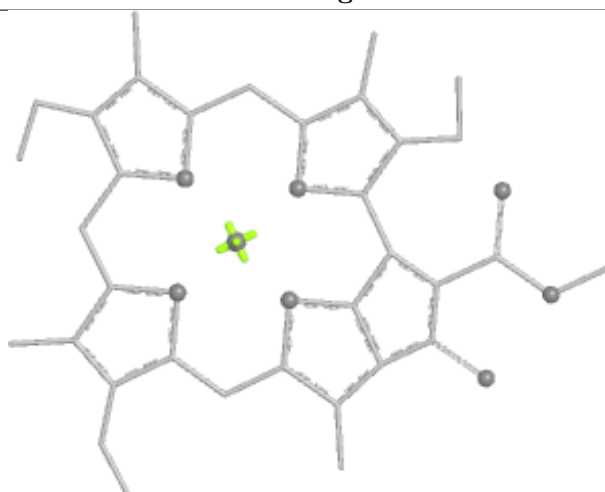
Bond lengths



Bond angles

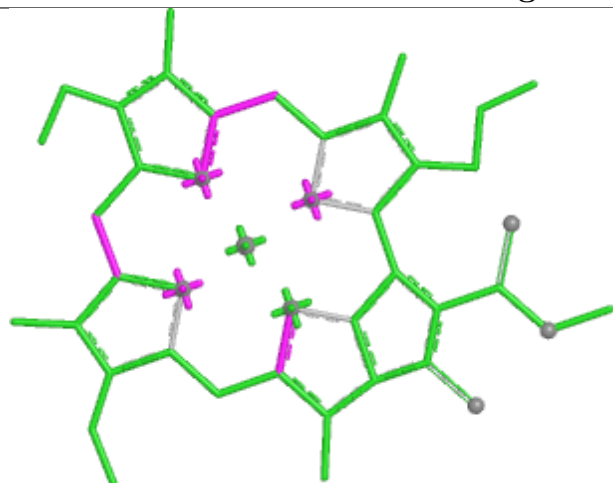


Torsions

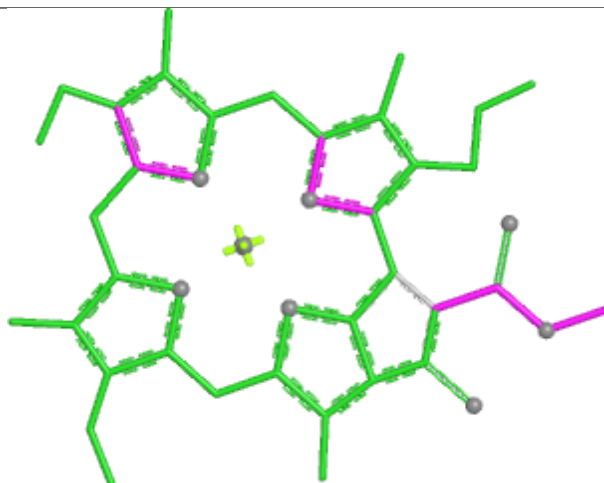


Rings

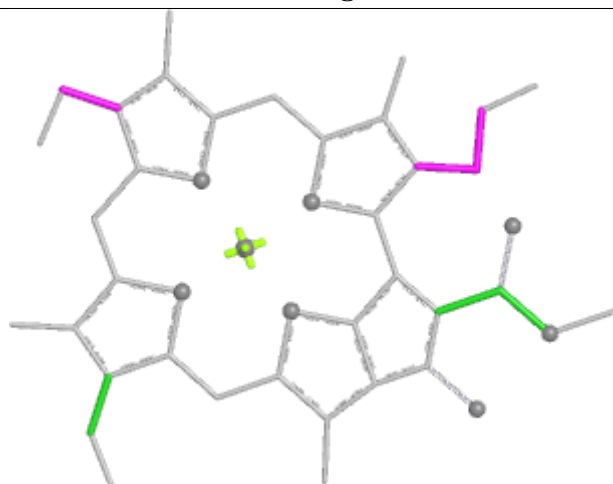
Ligand CLA o 608



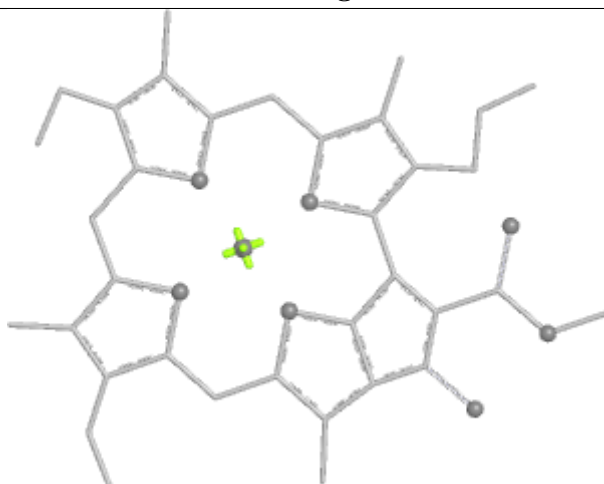
Bond lengths



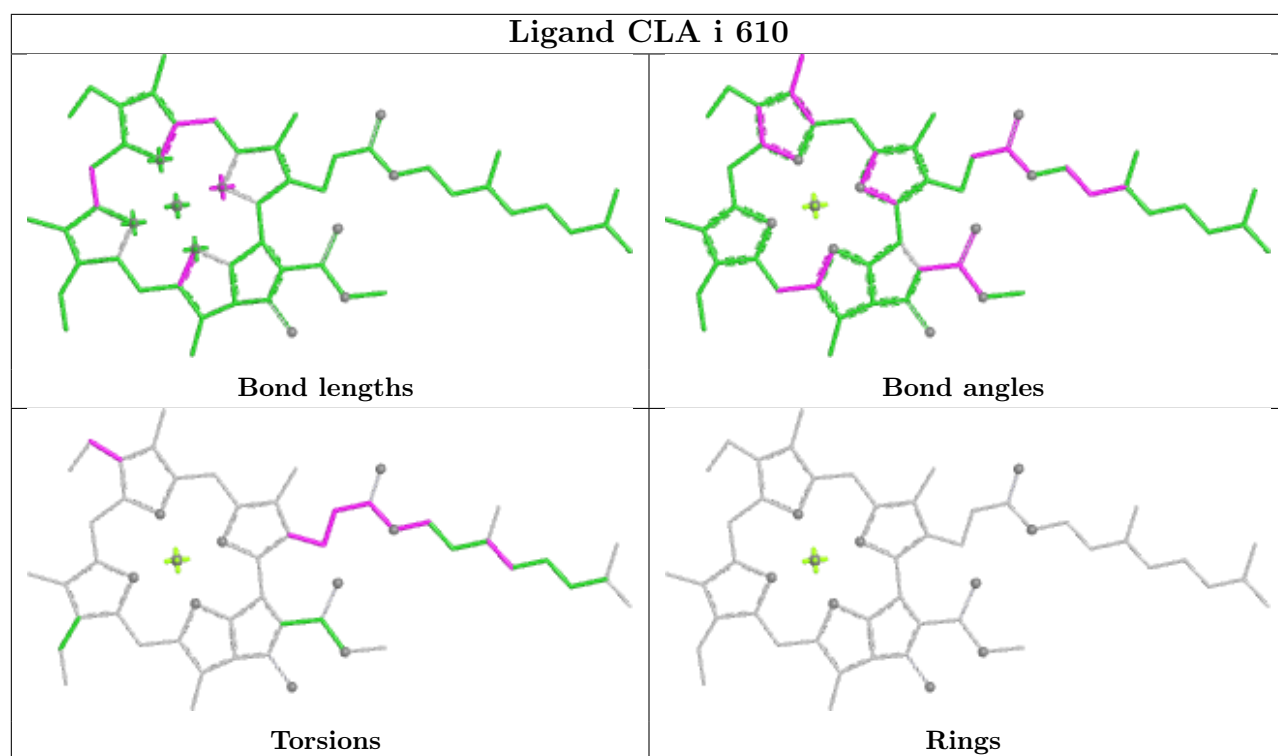
Bond angles



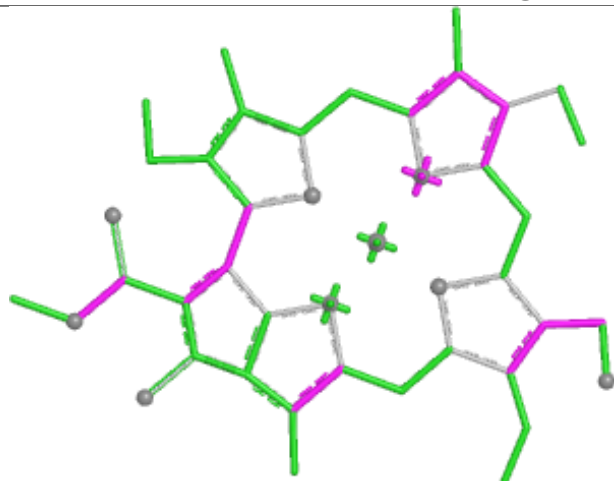
Torsions



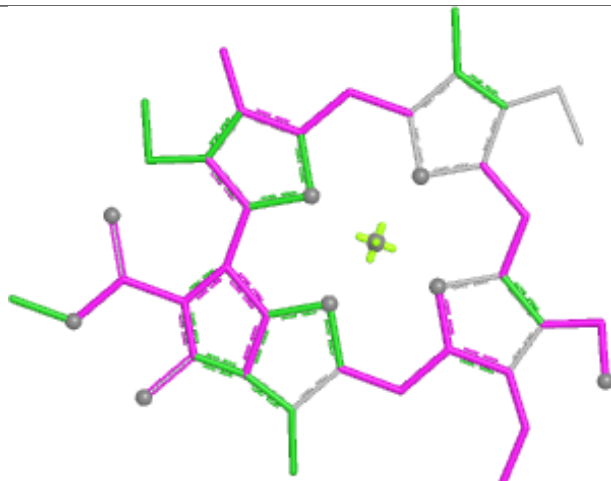
Rings



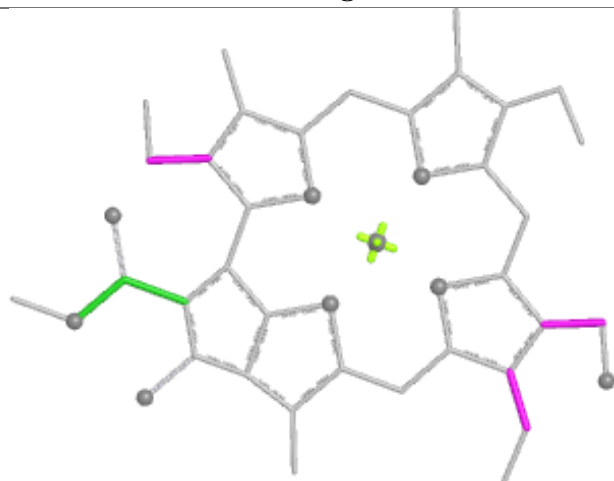
Ligand CHL d 607



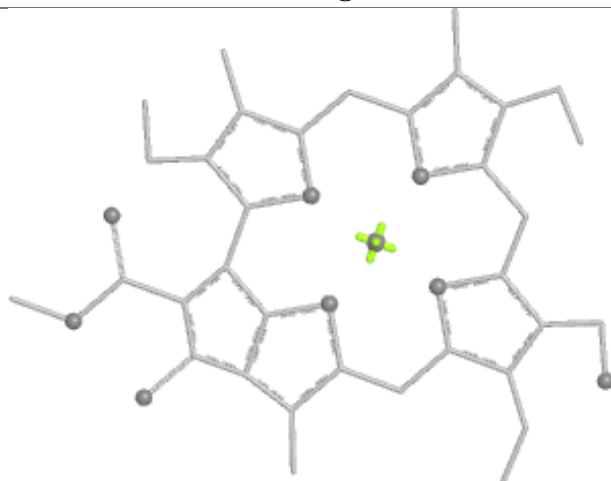
Bond lengths



Bond angles

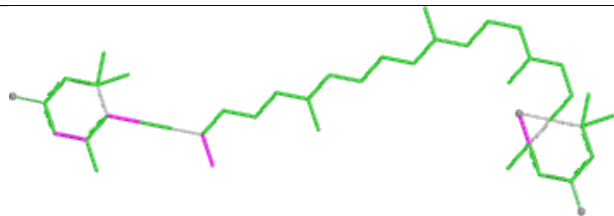


Torsions

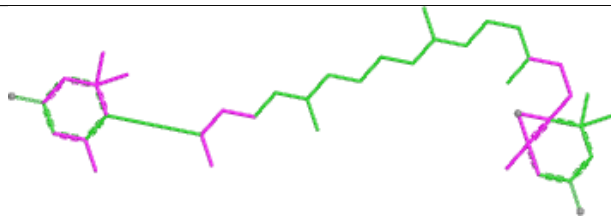


Rings

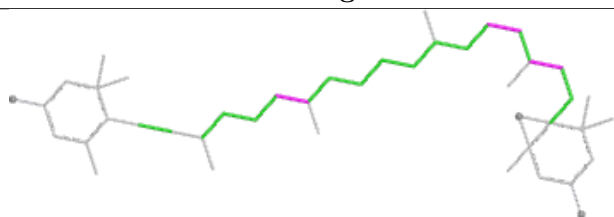
Ligand DD6 f 620



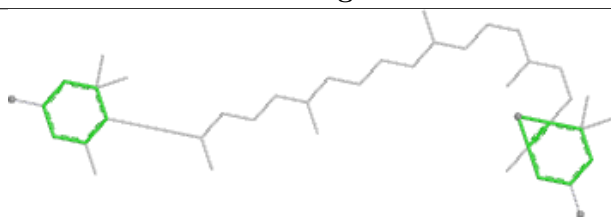
Bond lengths



Bond angles

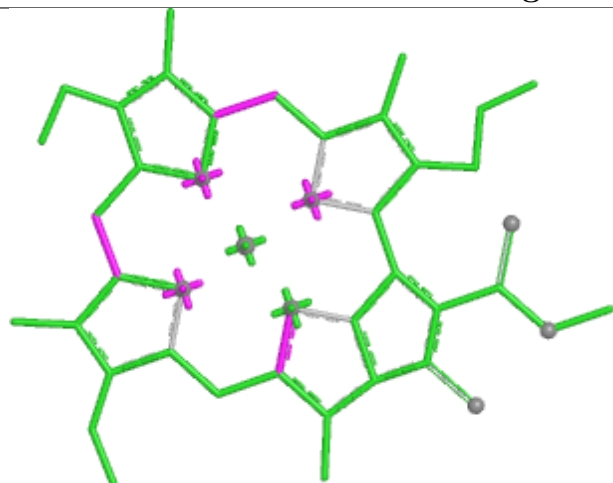


Torsions

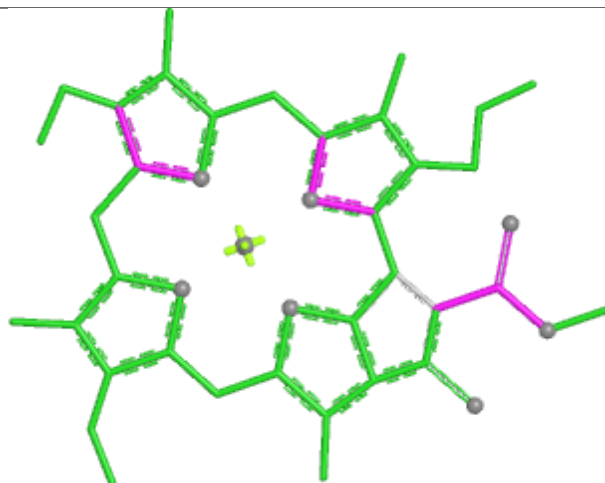


Rings

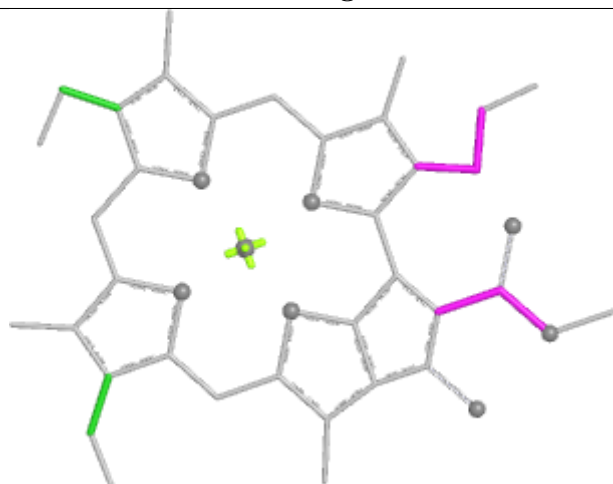
Ligand CLA 1 612



Bond lengths



Bond angles

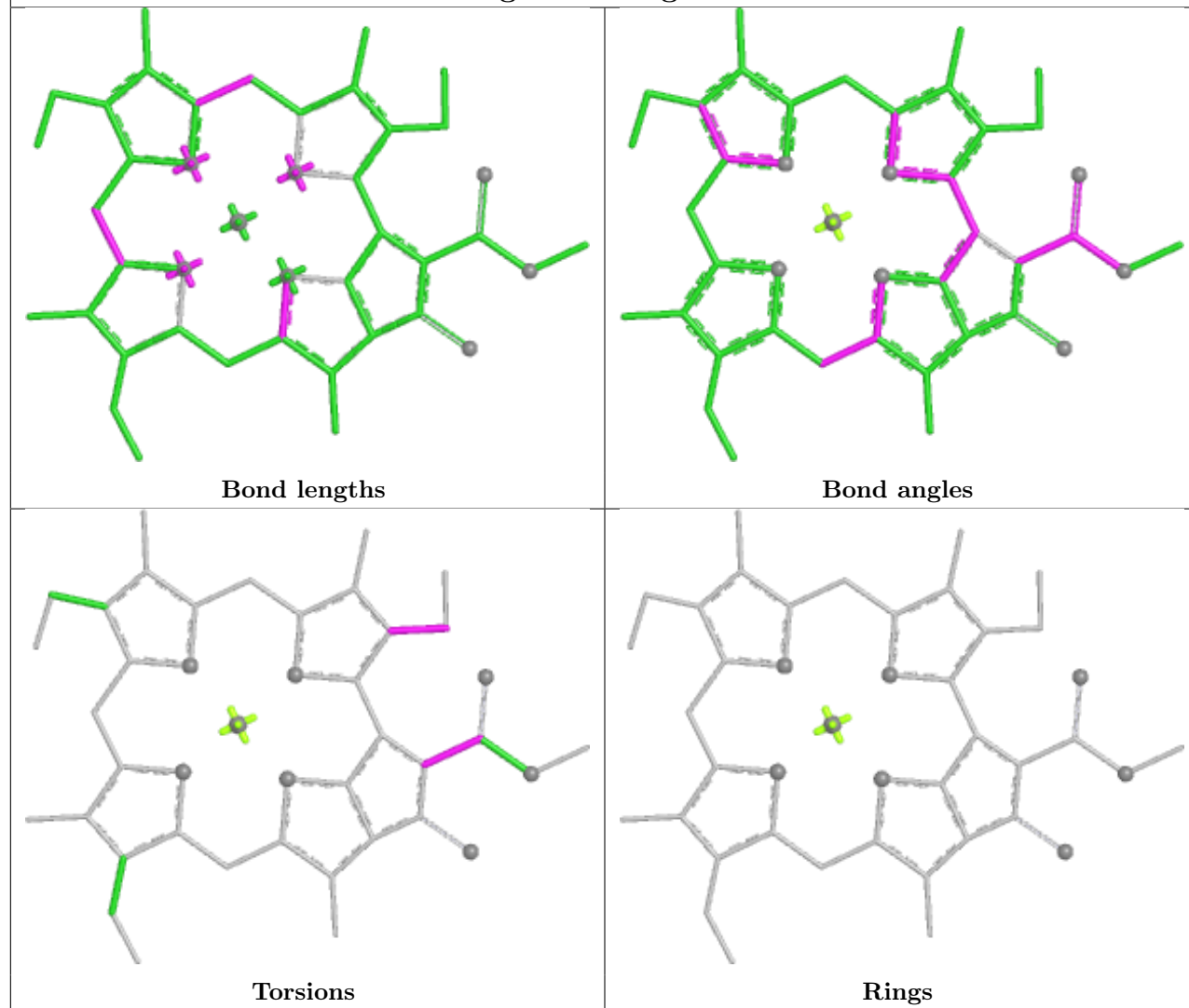


Torsions

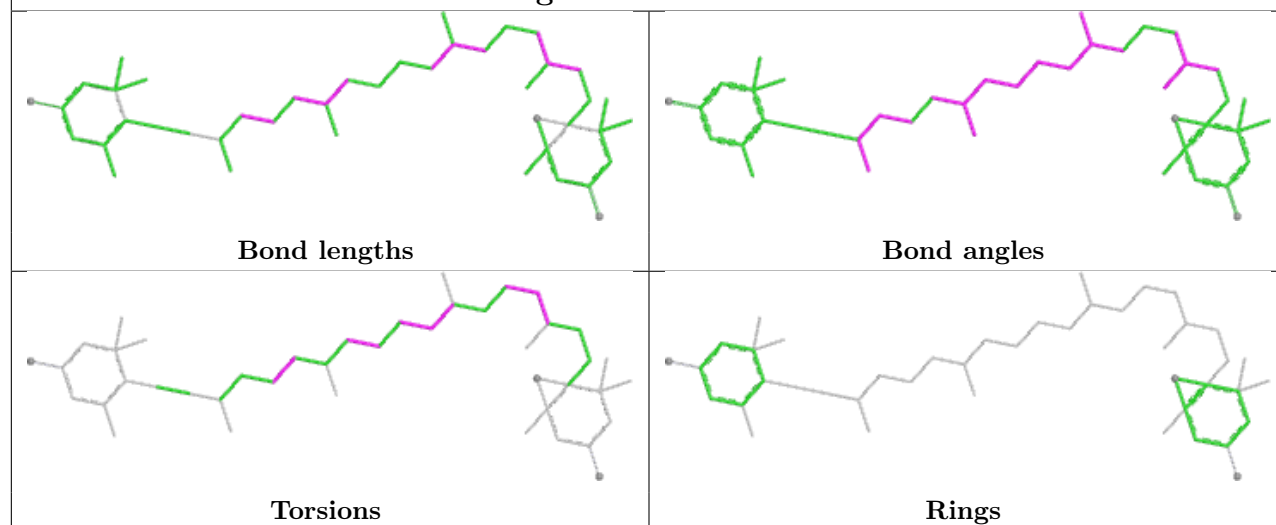


Rings

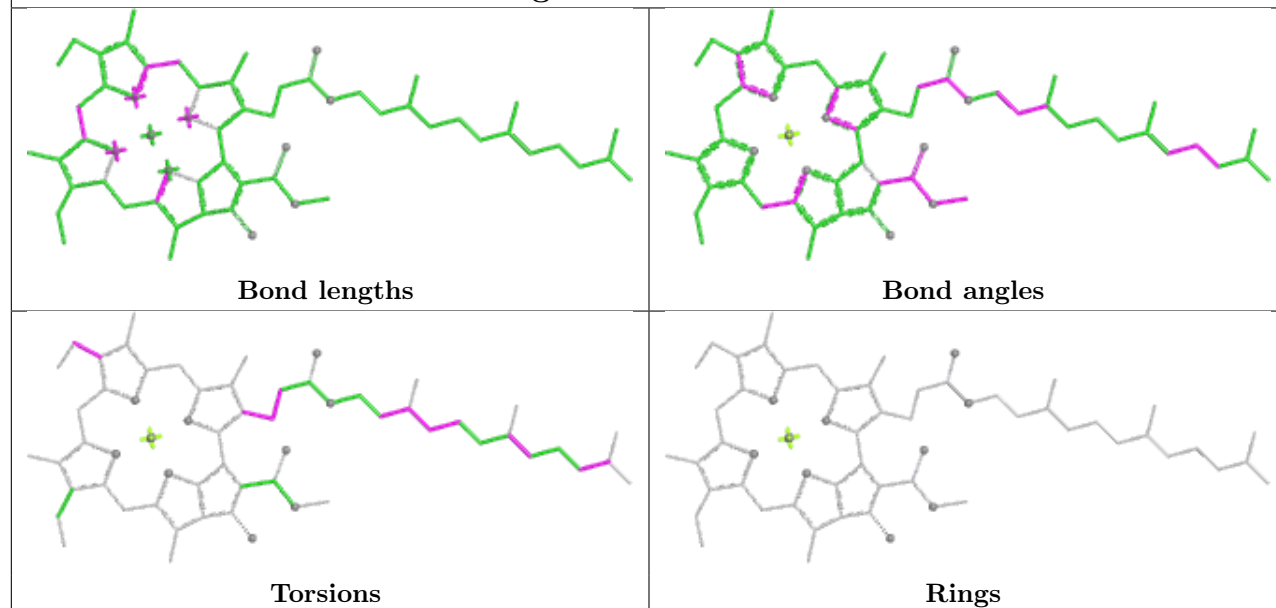
Ligand CLA g 611



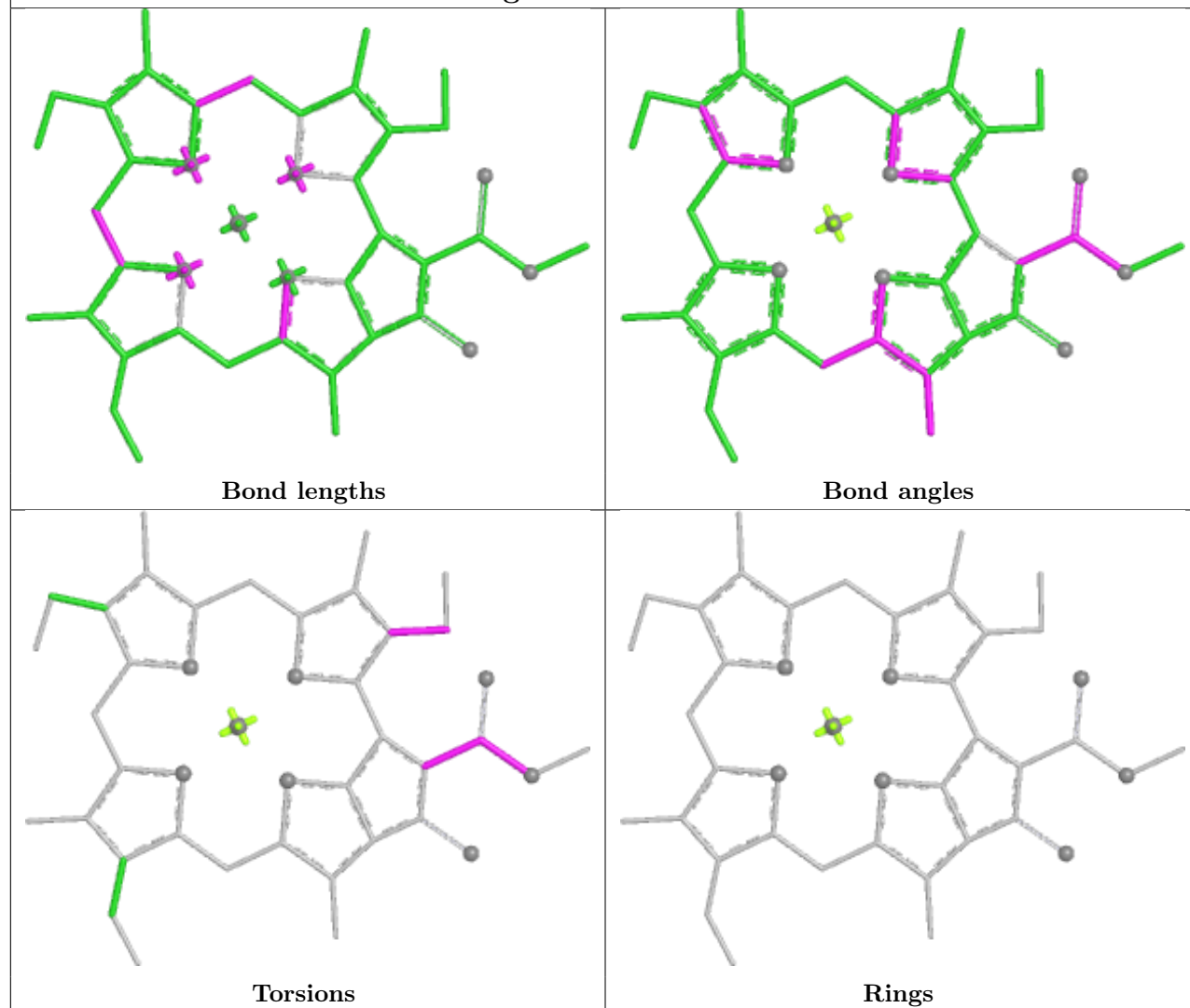
Ligand DD6 n 623



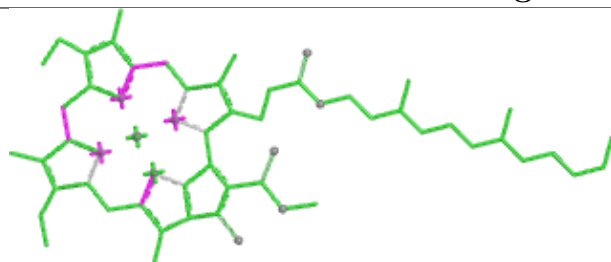
Ligand CLA B 774



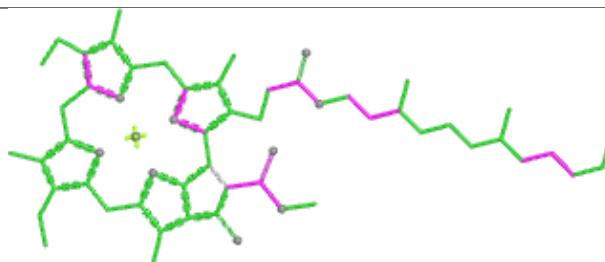
Ligand CLA f 614



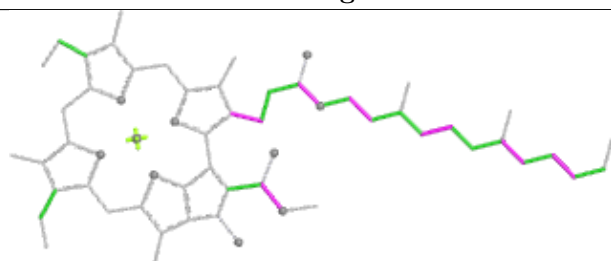
Ligand CLA B 776



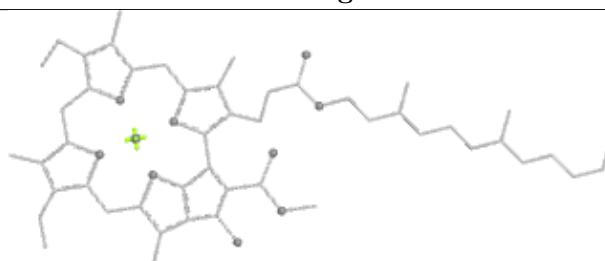
Bond lengths



Bond angles

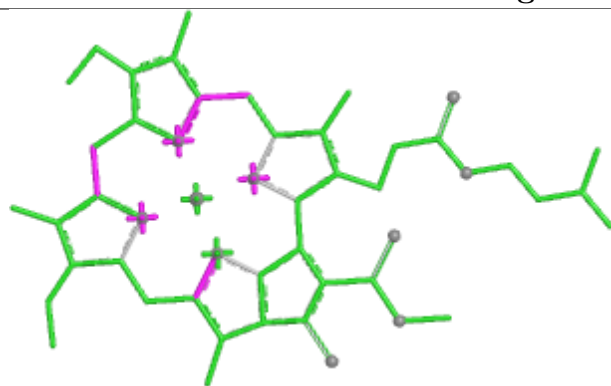


Torsions

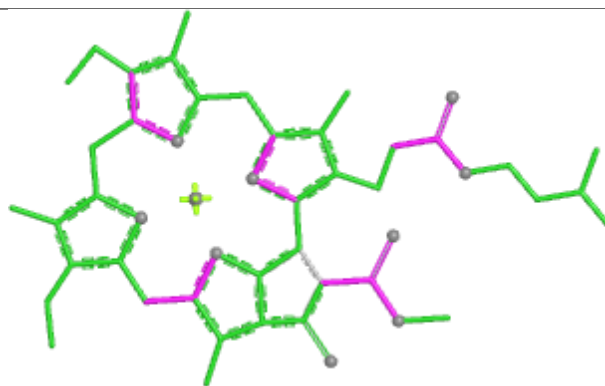


Rings

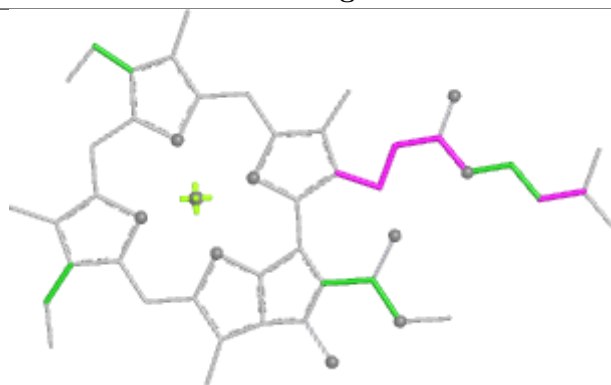
Ligand CLA h 609



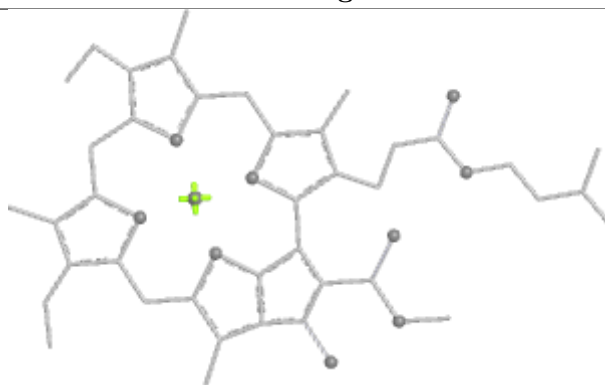
Bond lengths



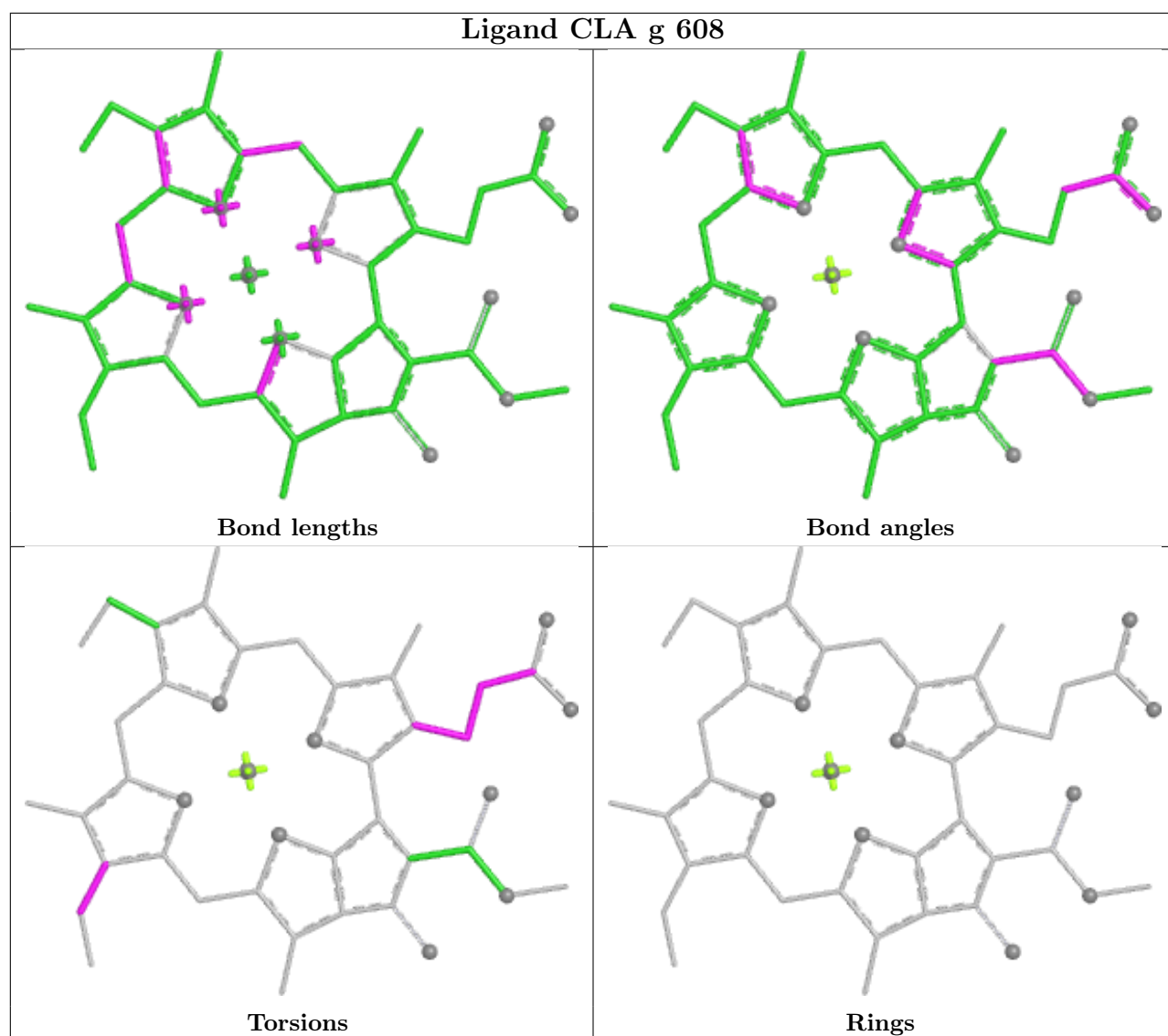
Bond angles



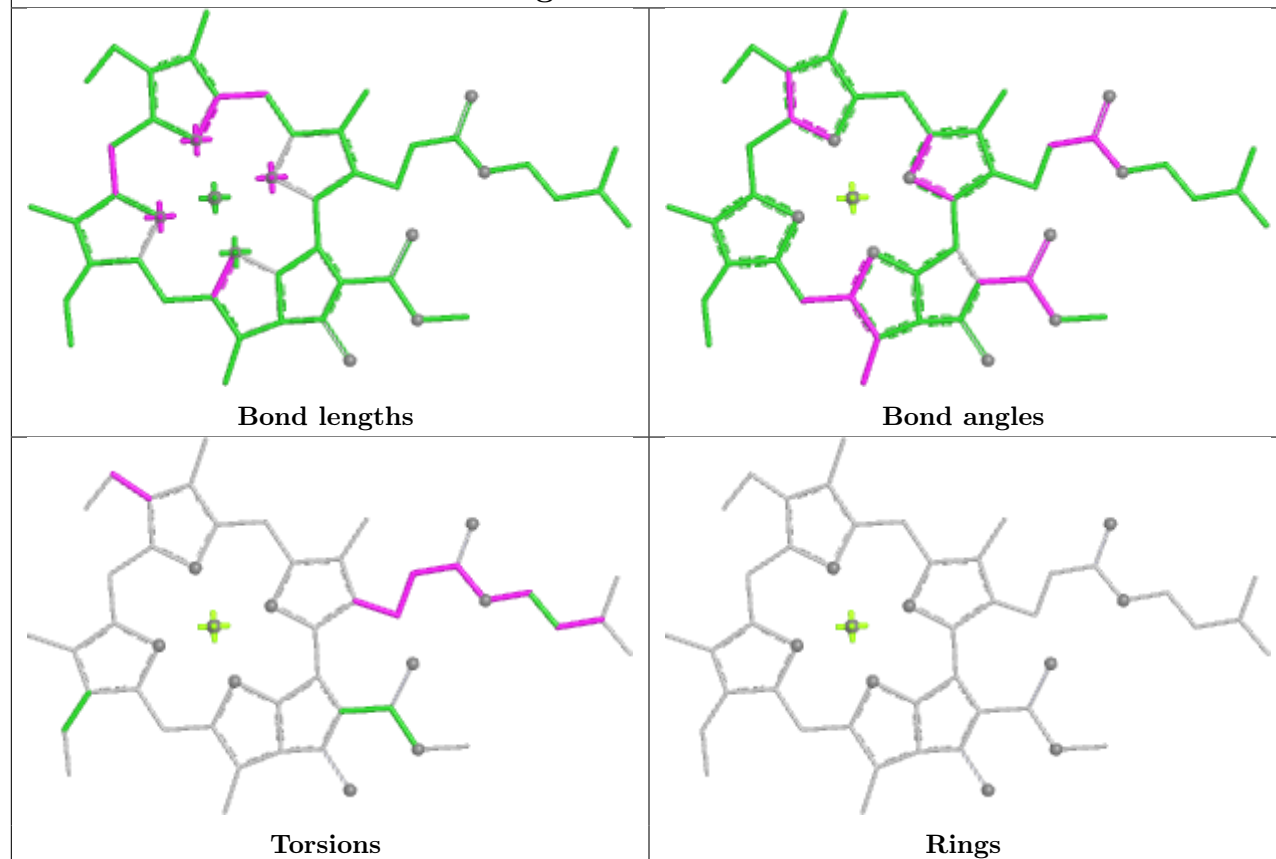
Torsions



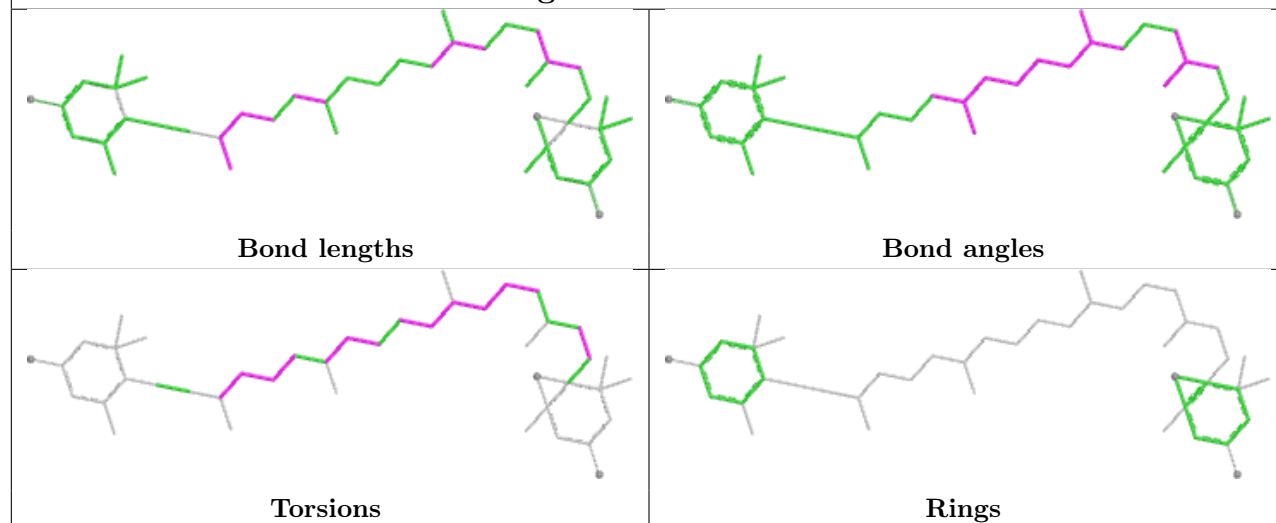
Rings



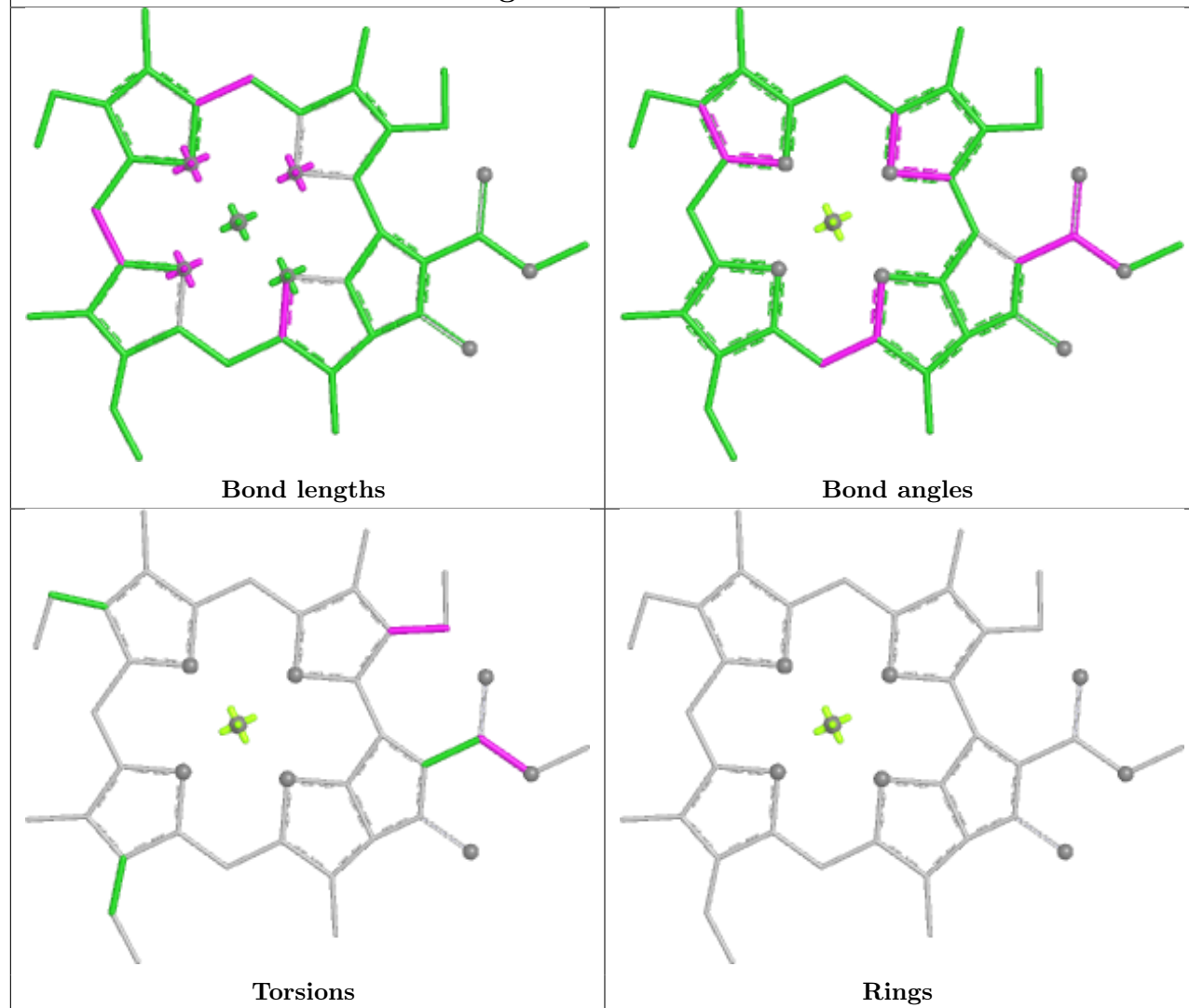
Ligand CLA J 101



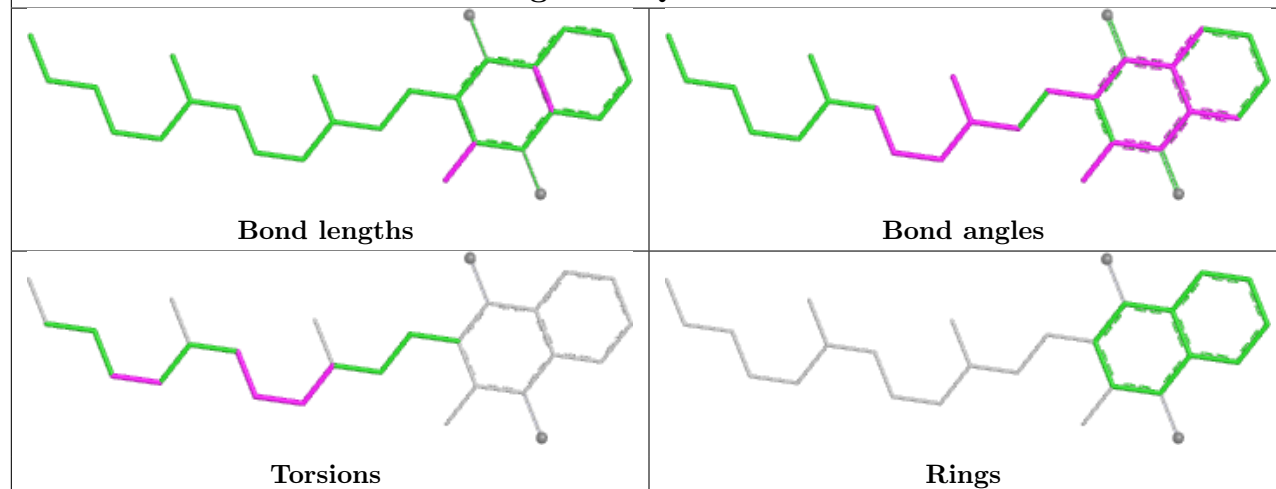
Ligand DD6 e 623

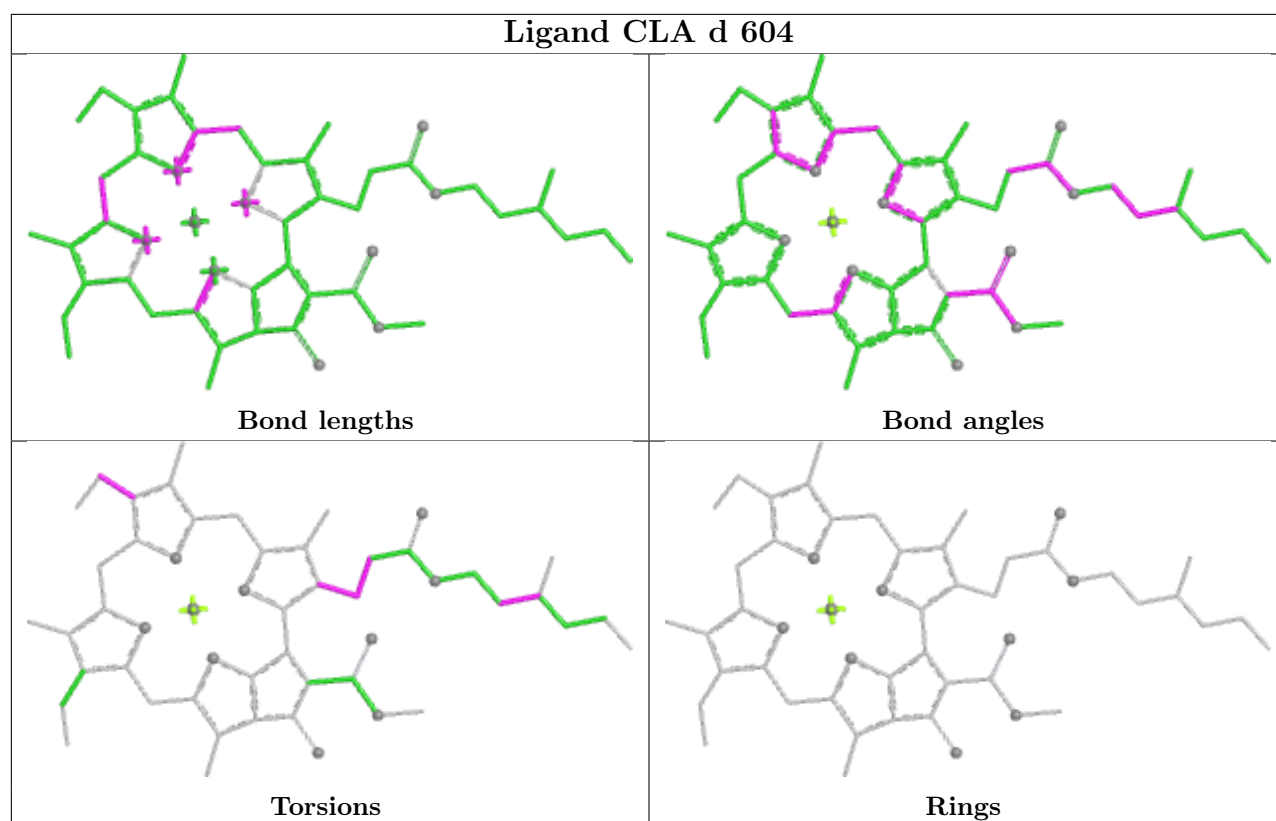


Ligand CLA k 614

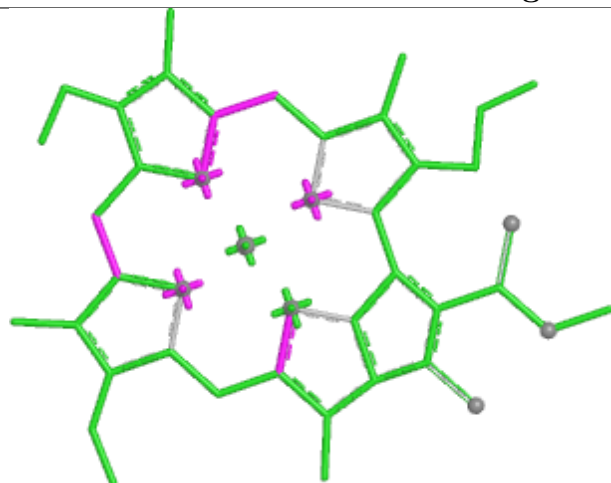


Ligand PQN B 769

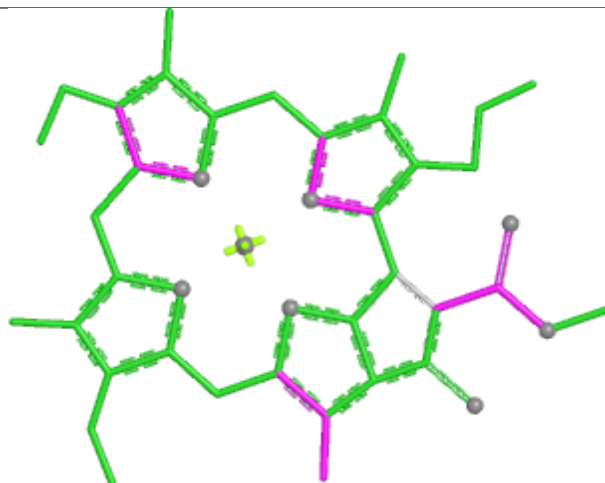




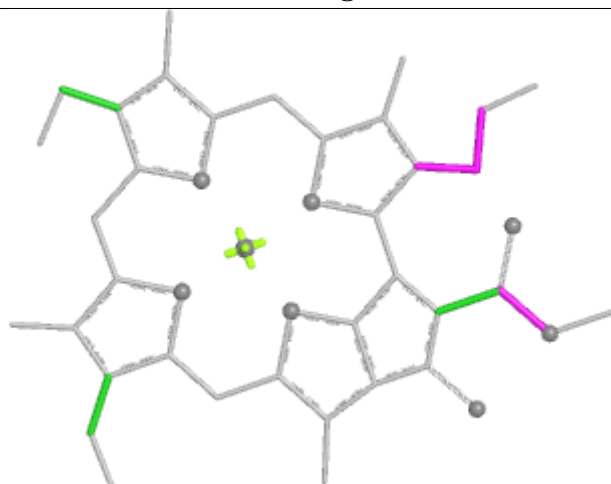
Ligand CLA i 612



Bond lengths



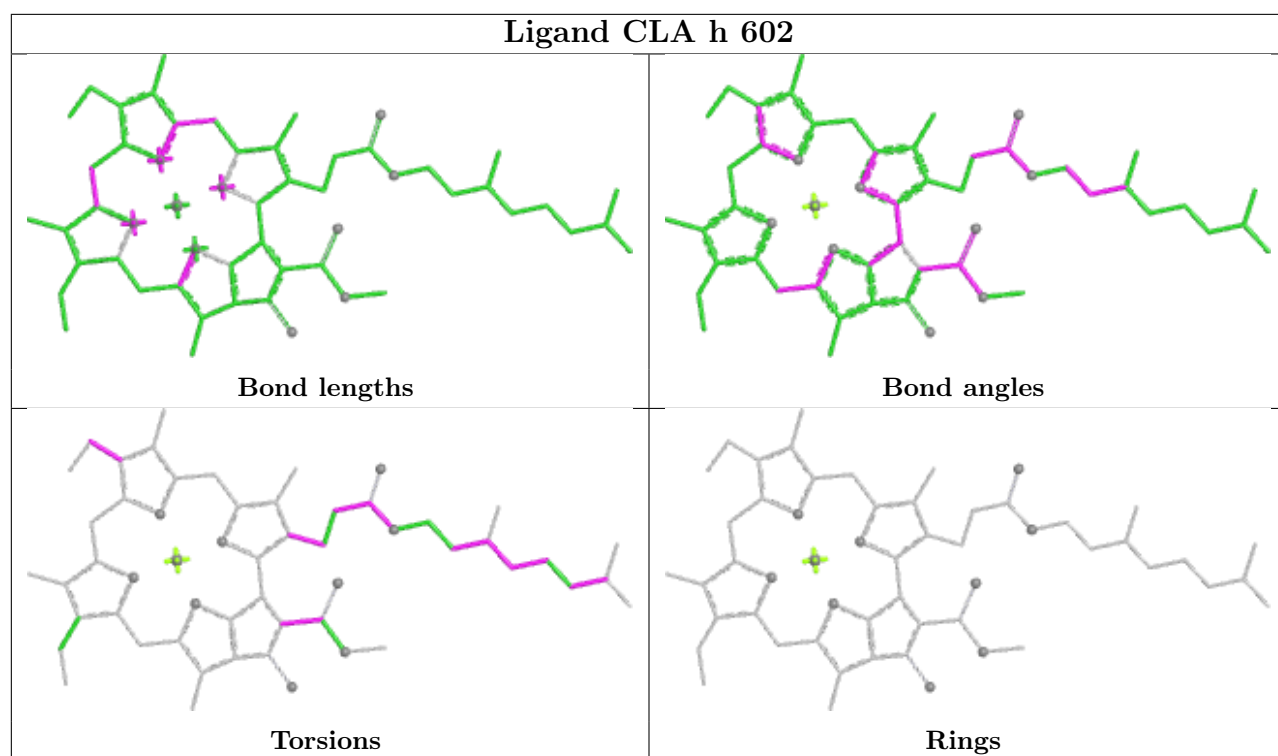
Bond angles

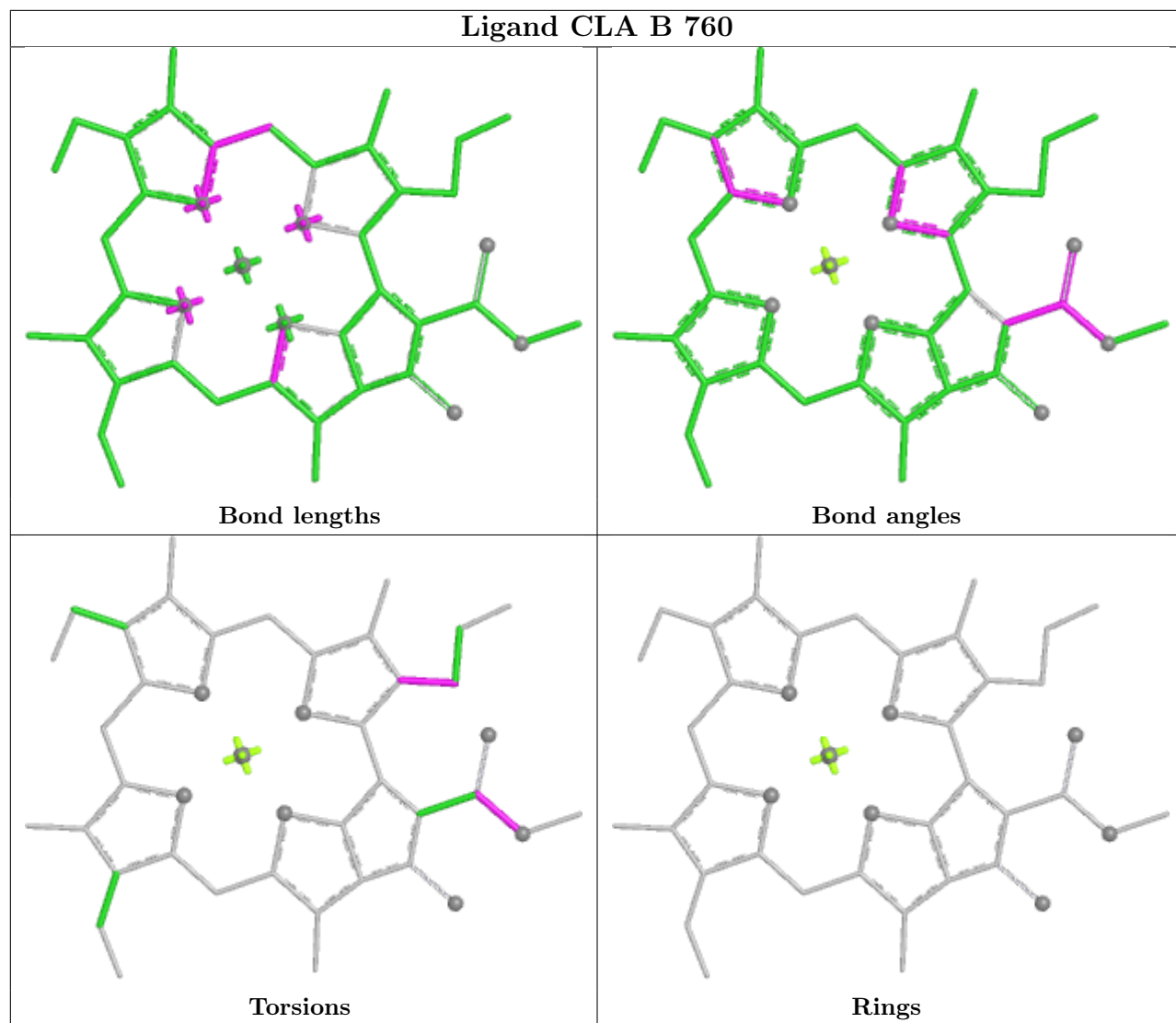


Torsions

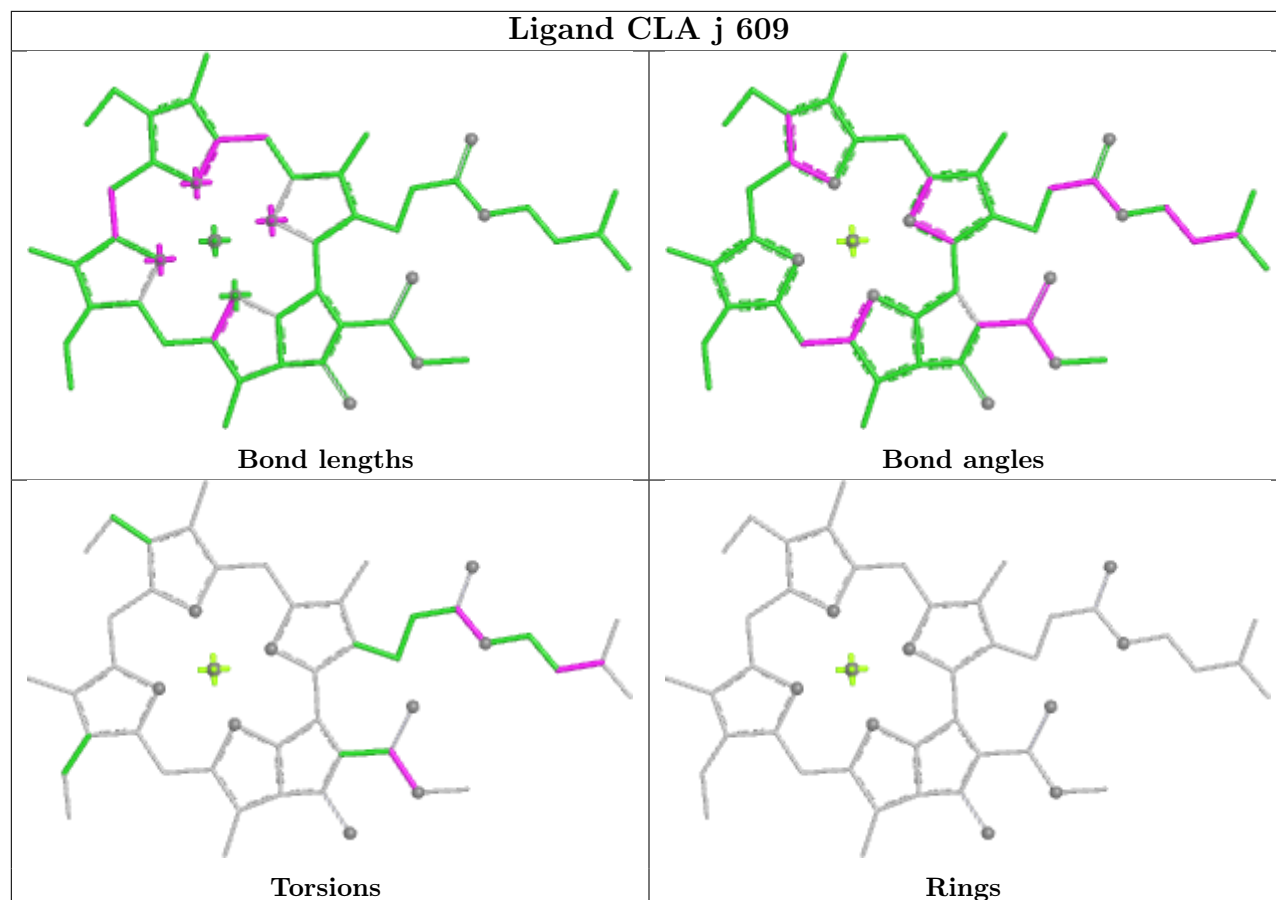


Rings

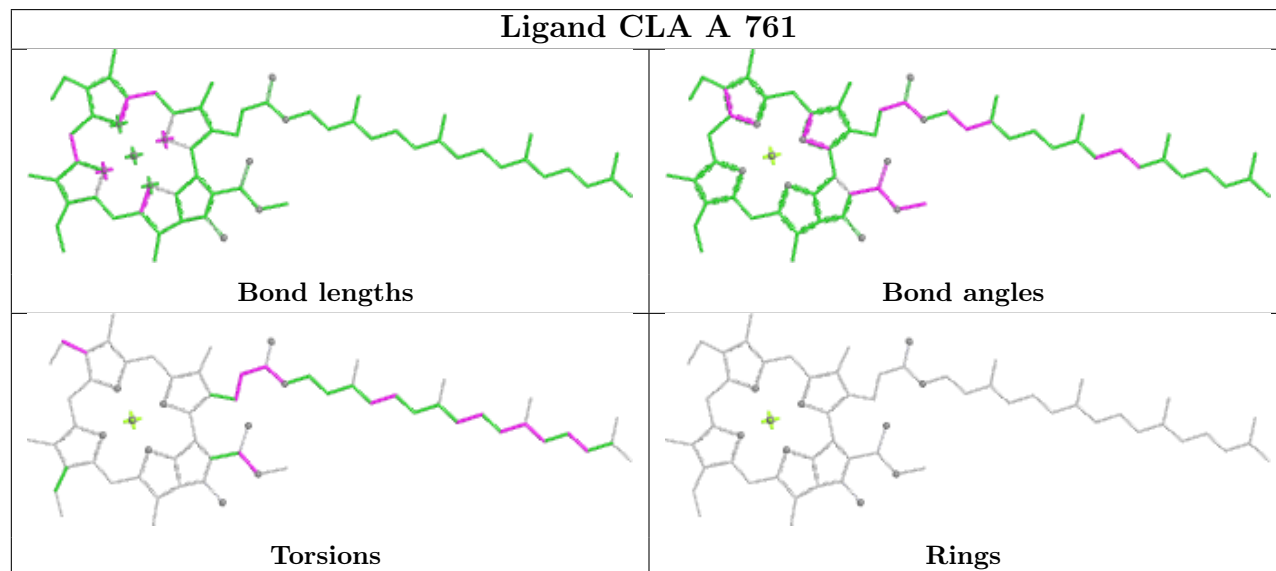


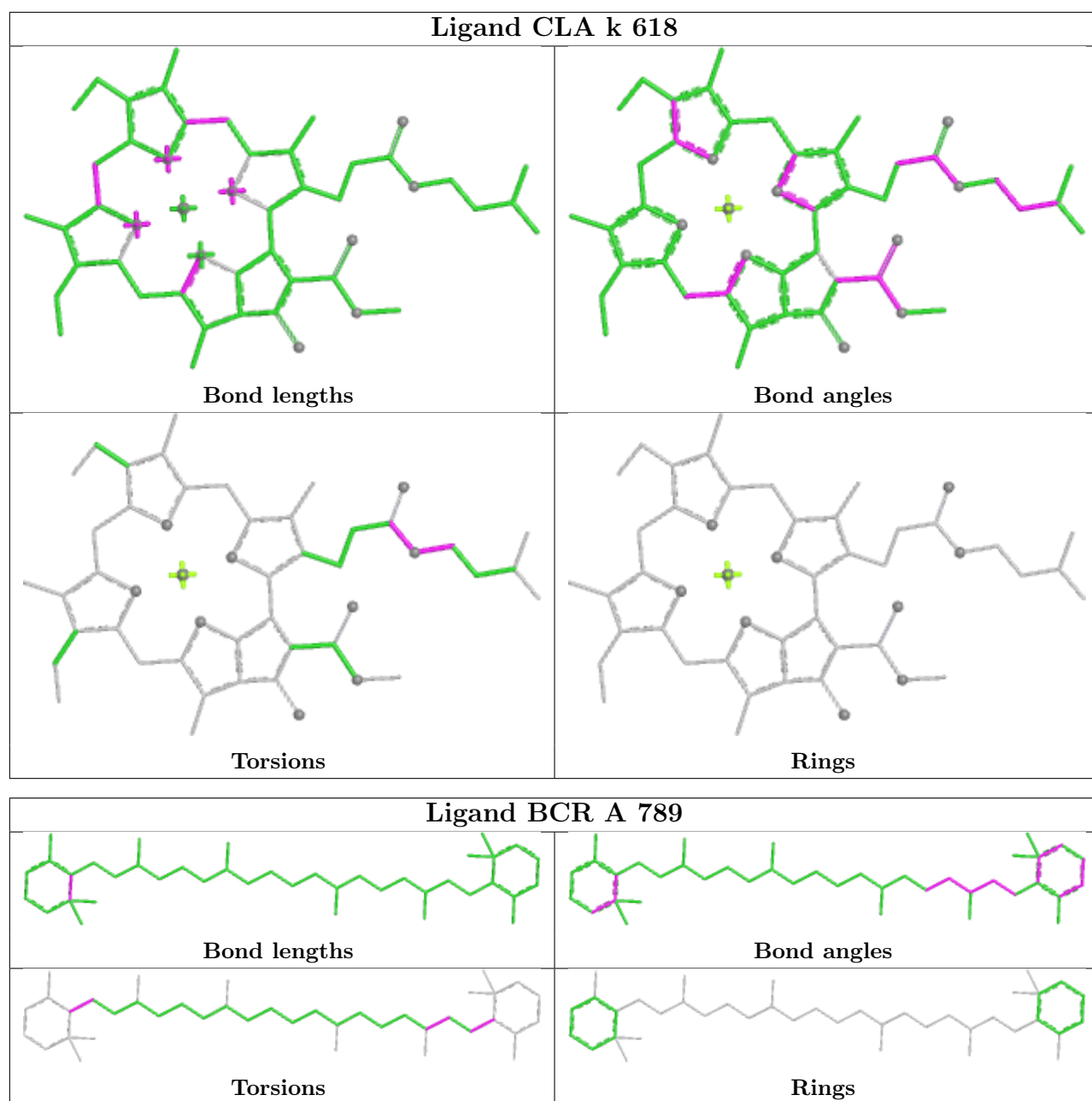


Ligand CLA j 609

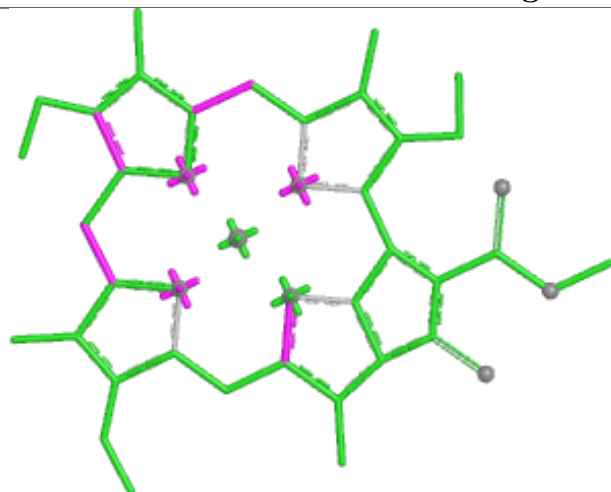


Ligand CLA A 761

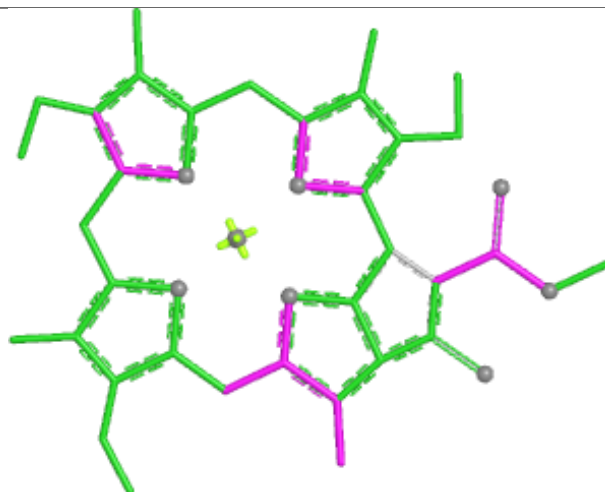




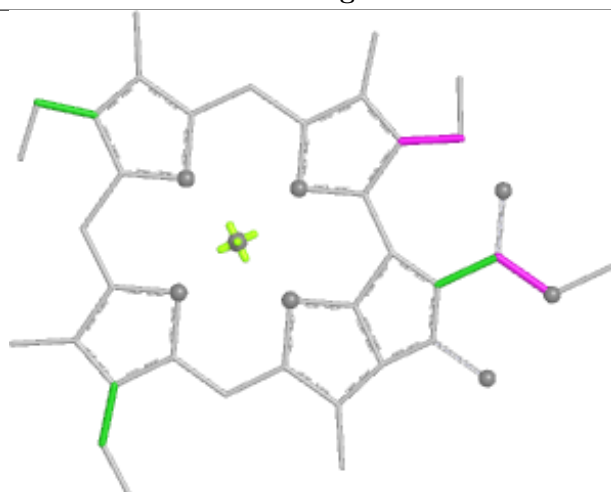
Ligand CLA f 609



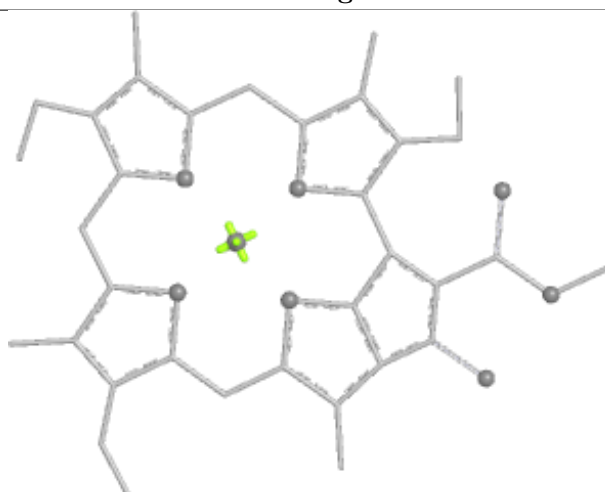
Bond lengths



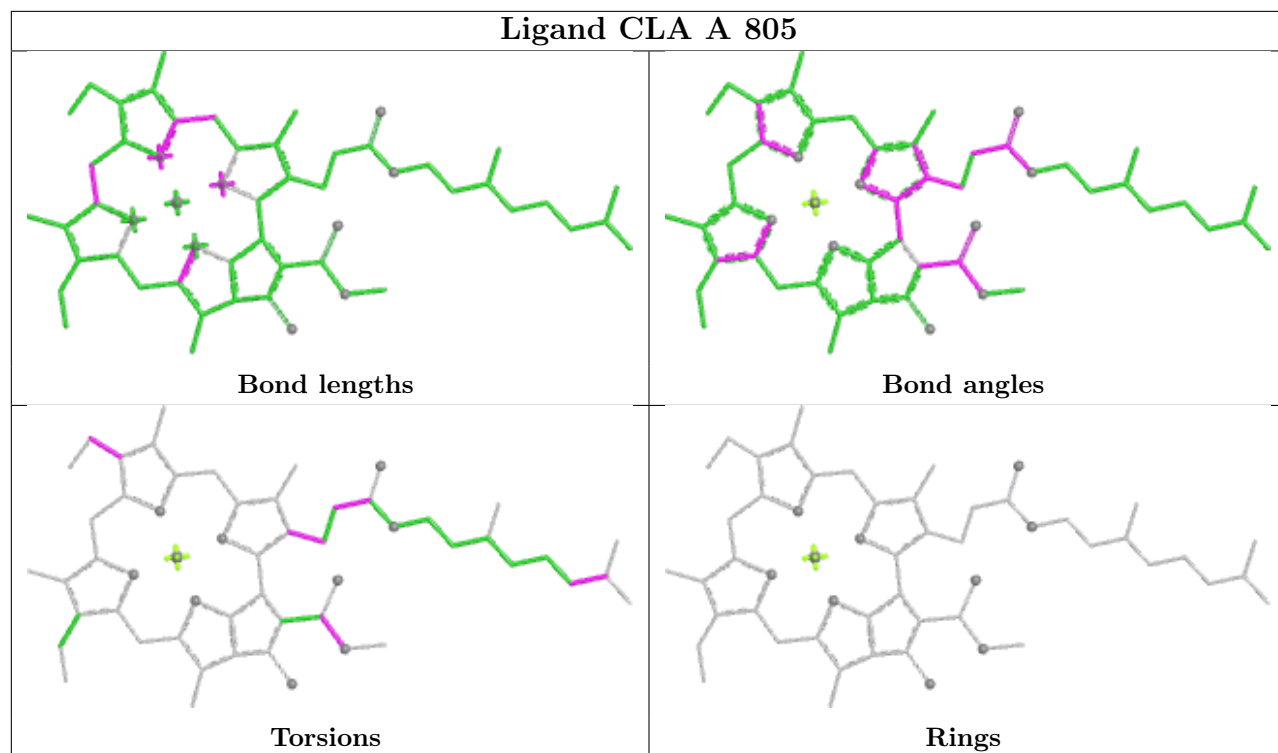
Bond angles



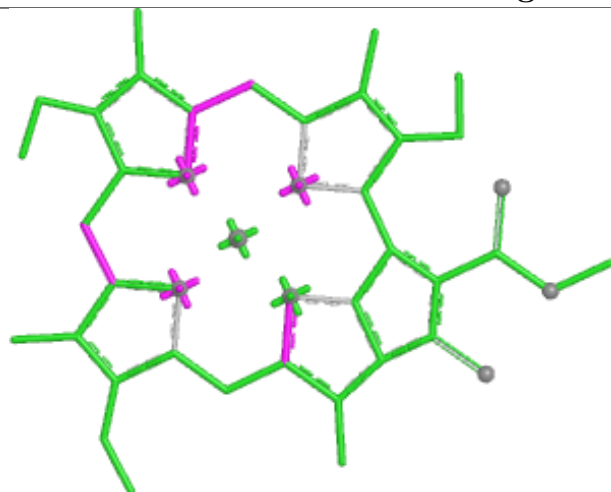
Torsions



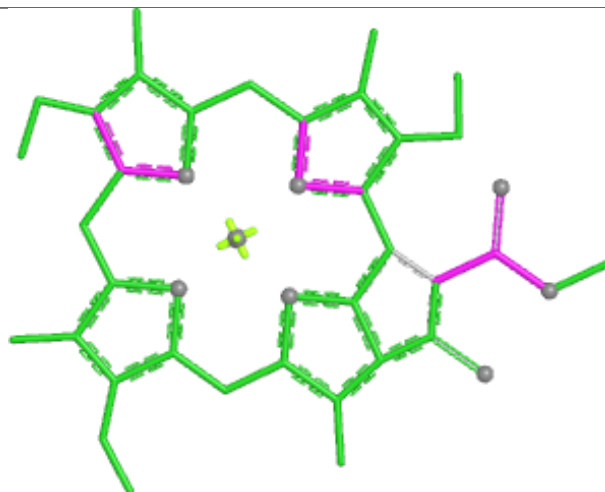
Rings



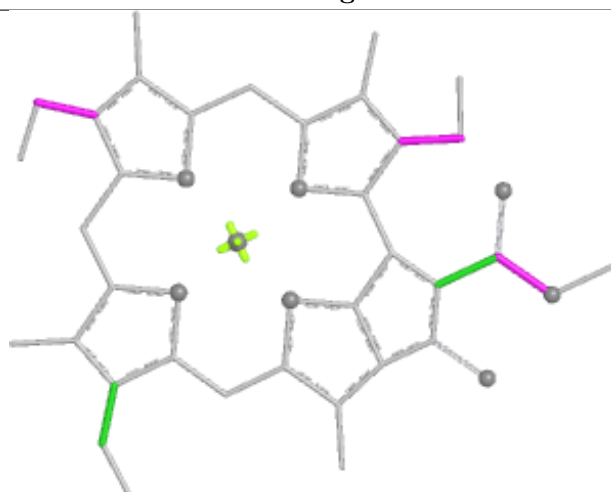
Ligand CLA h 615



Bond lengths



Bond angles

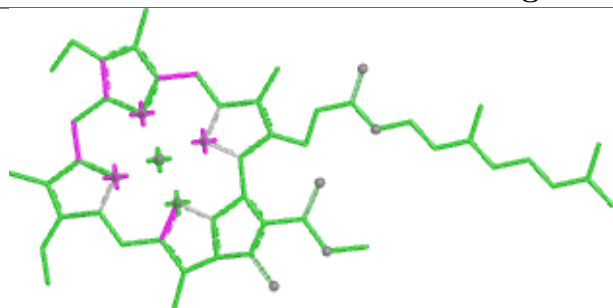


Torsions

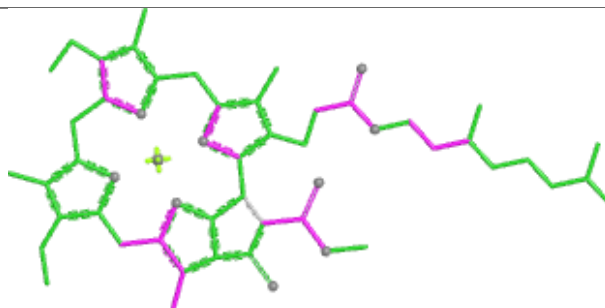


Rings

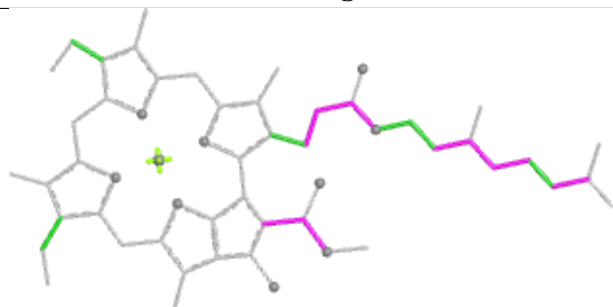
Ligand CLA f 610



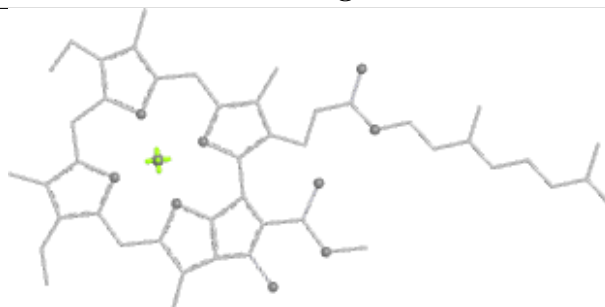
Bond lengths



Bond angles

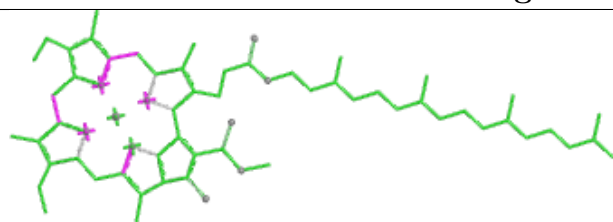


Torsions

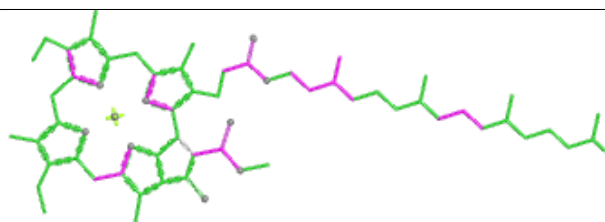


Rings

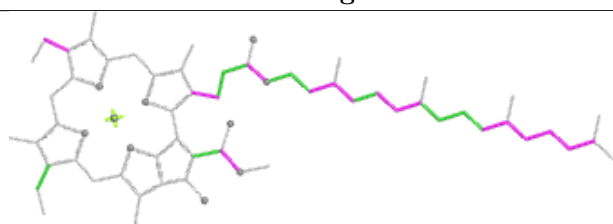
Ligand CLA B 758



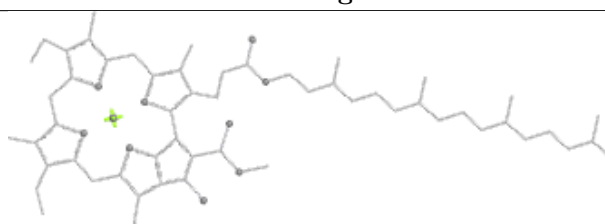
Bond lengths



Bond angles

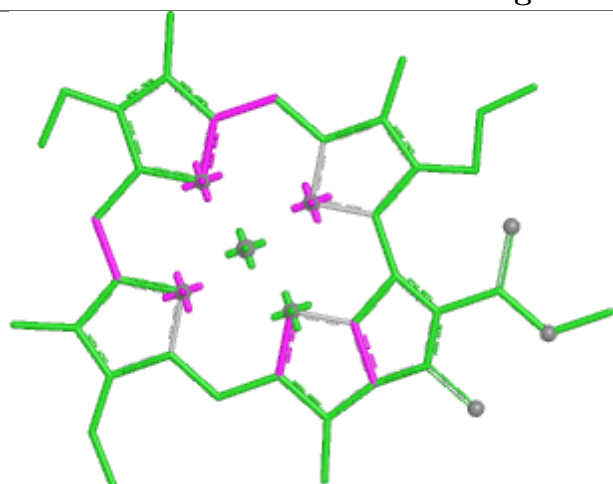


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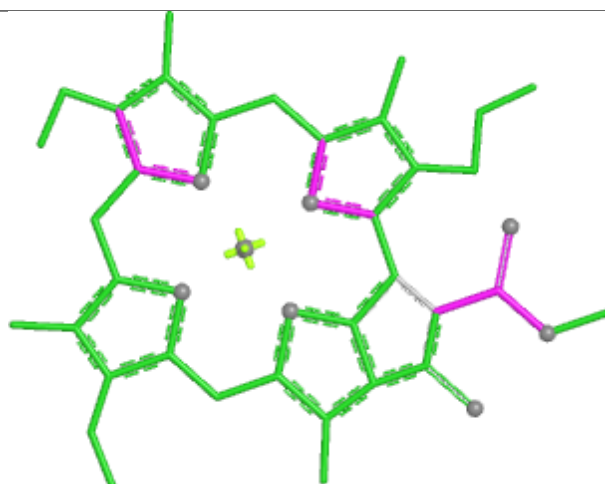


Rings

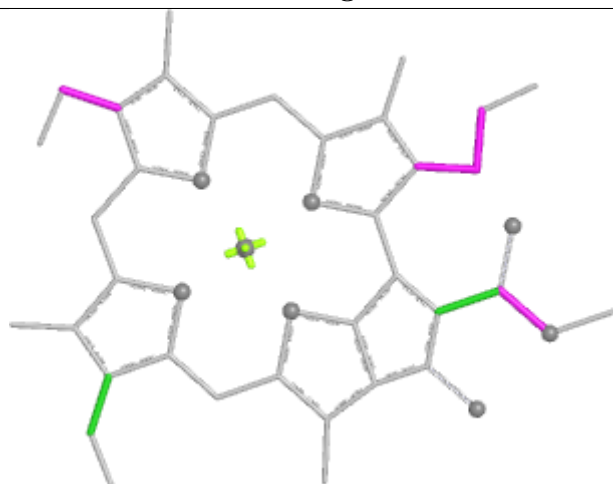
Ligand CLA B 754



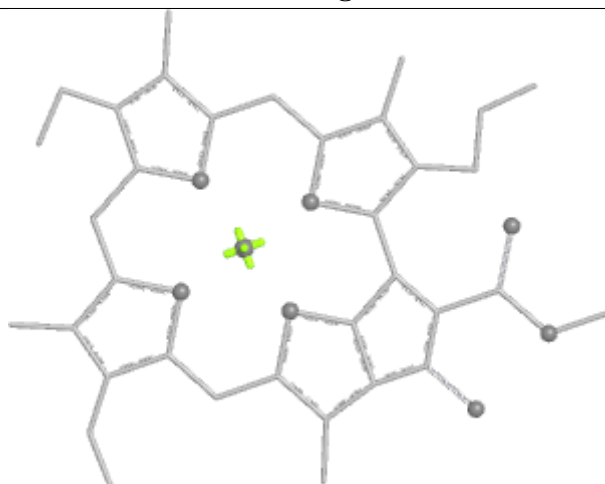
Bond lengths



Bond angles

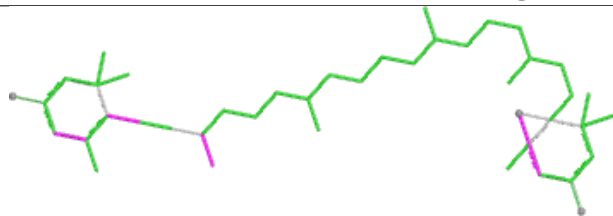


Torsions

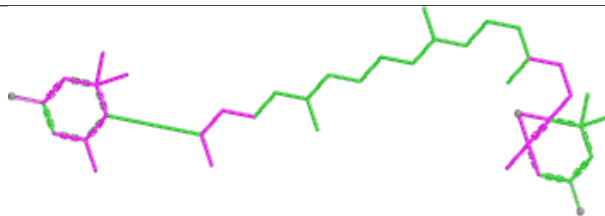


Rings

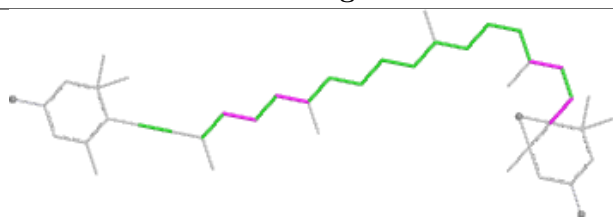
Ligand DD6 m 621



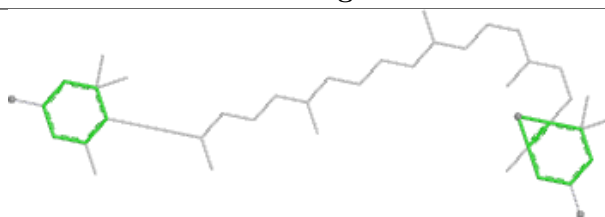
Bond lengths



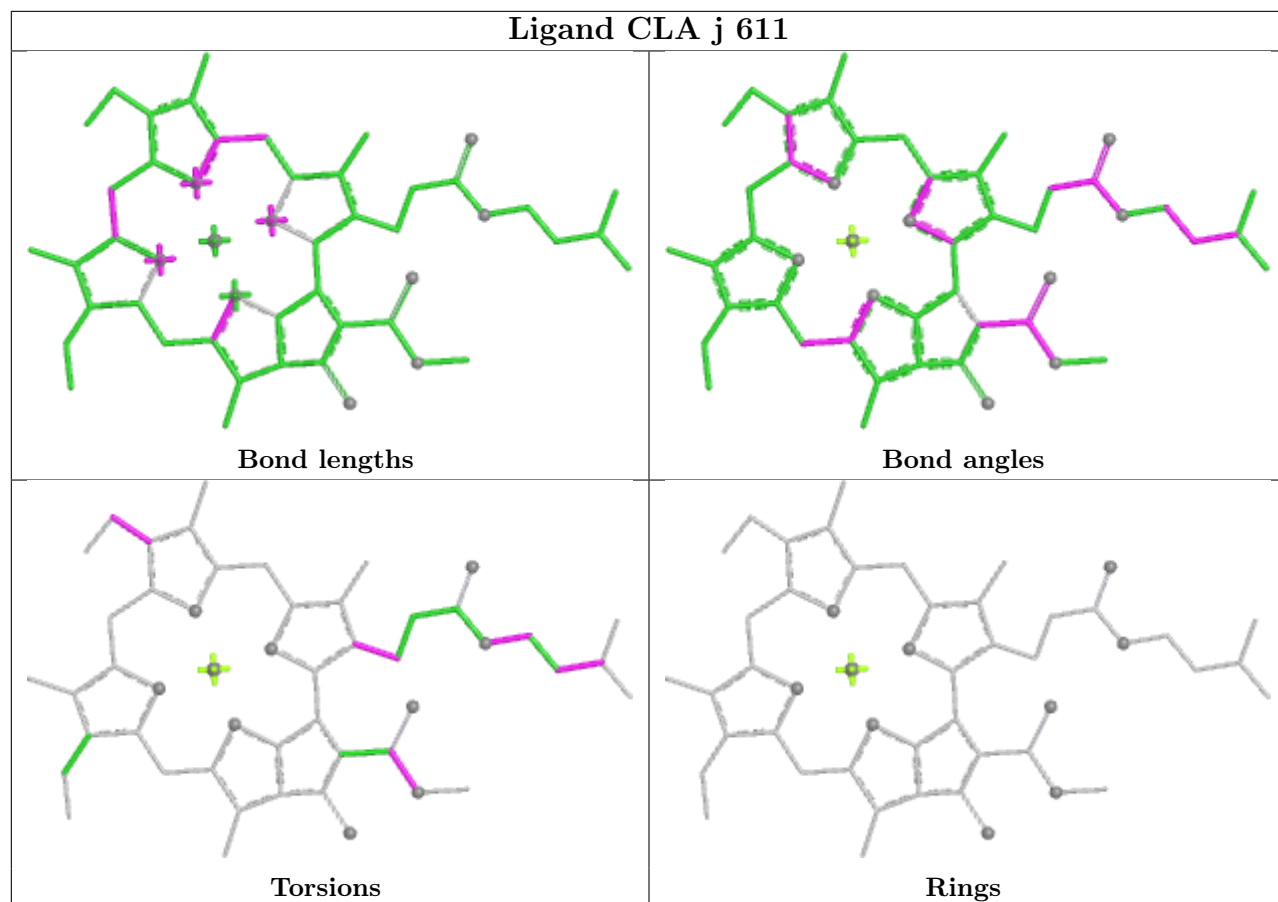
Bond angles



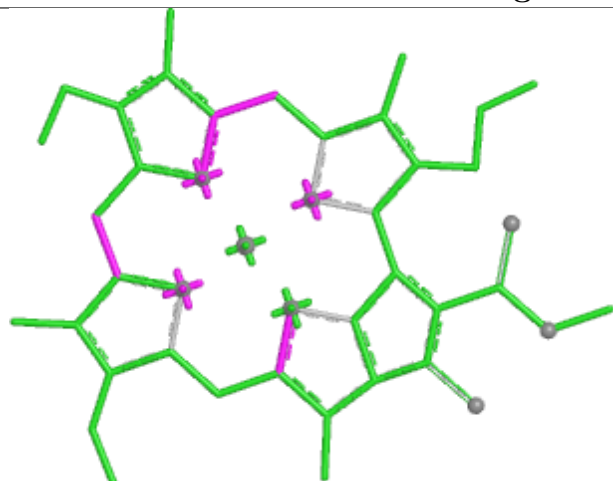
Torsions



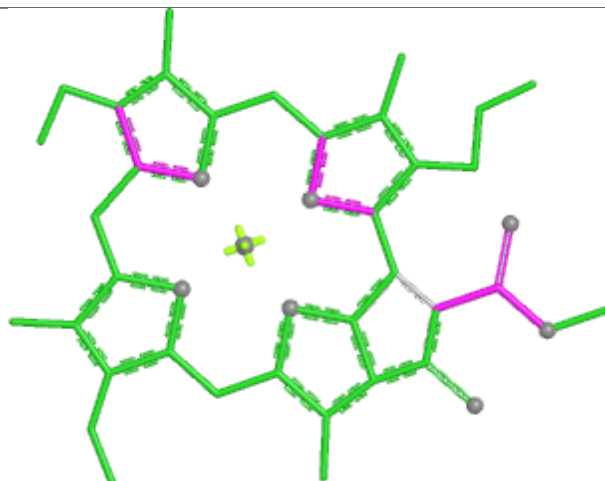
Rings



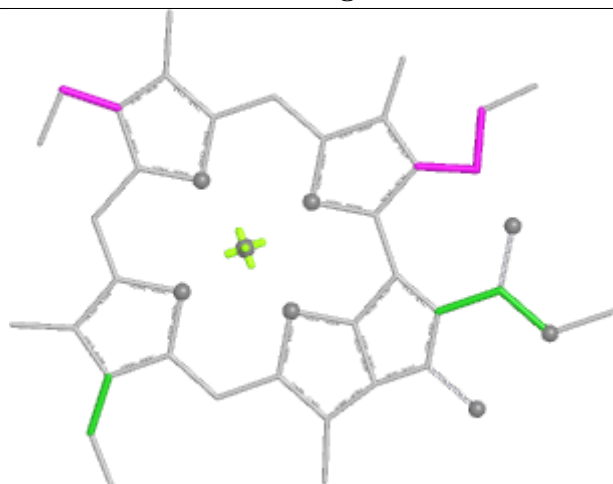
Ligand CLA A 767



Bond lengths



Bond angles

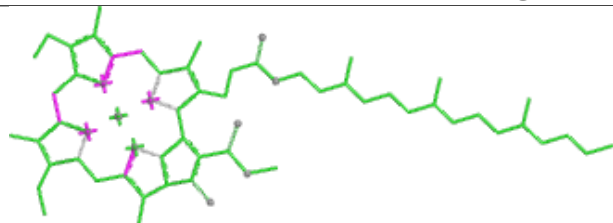


Torsions

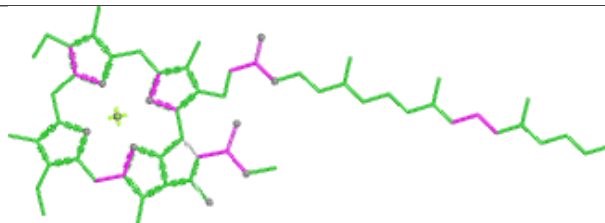


Rings

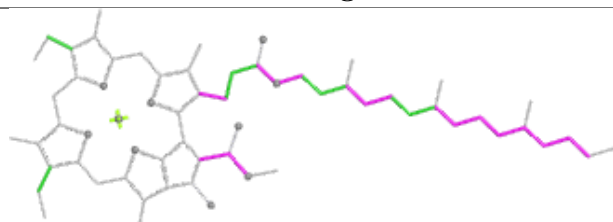
Ligand CLA B 745



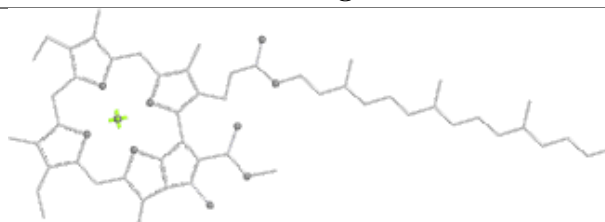
Bond lengths



Bond angles

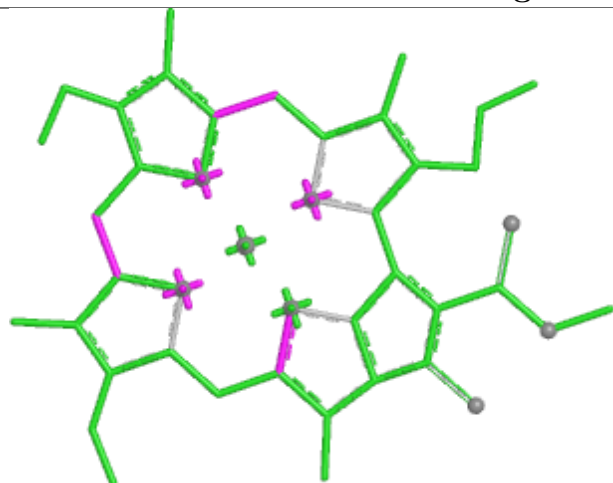


Torsions

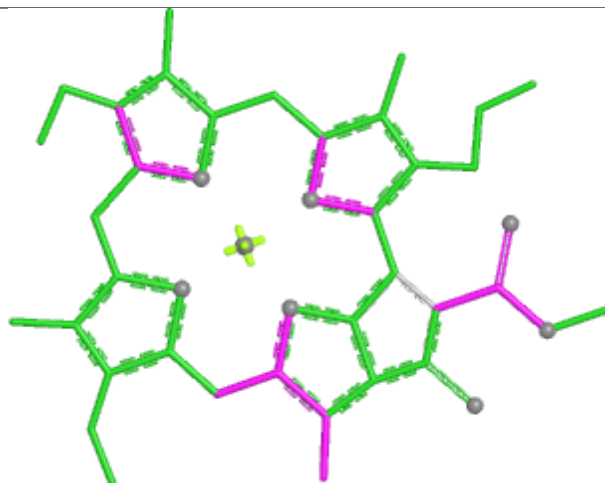


Rings

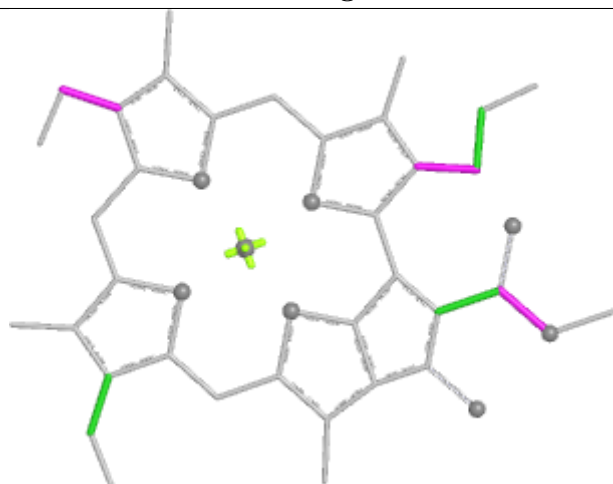
Ligand CLA A 779



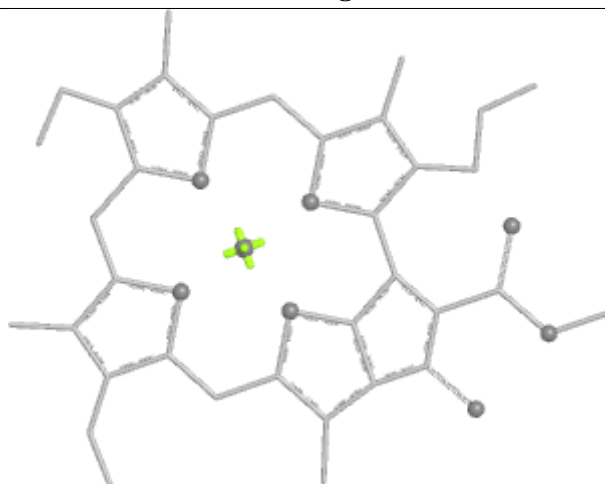
Bond lengths



Bond angles

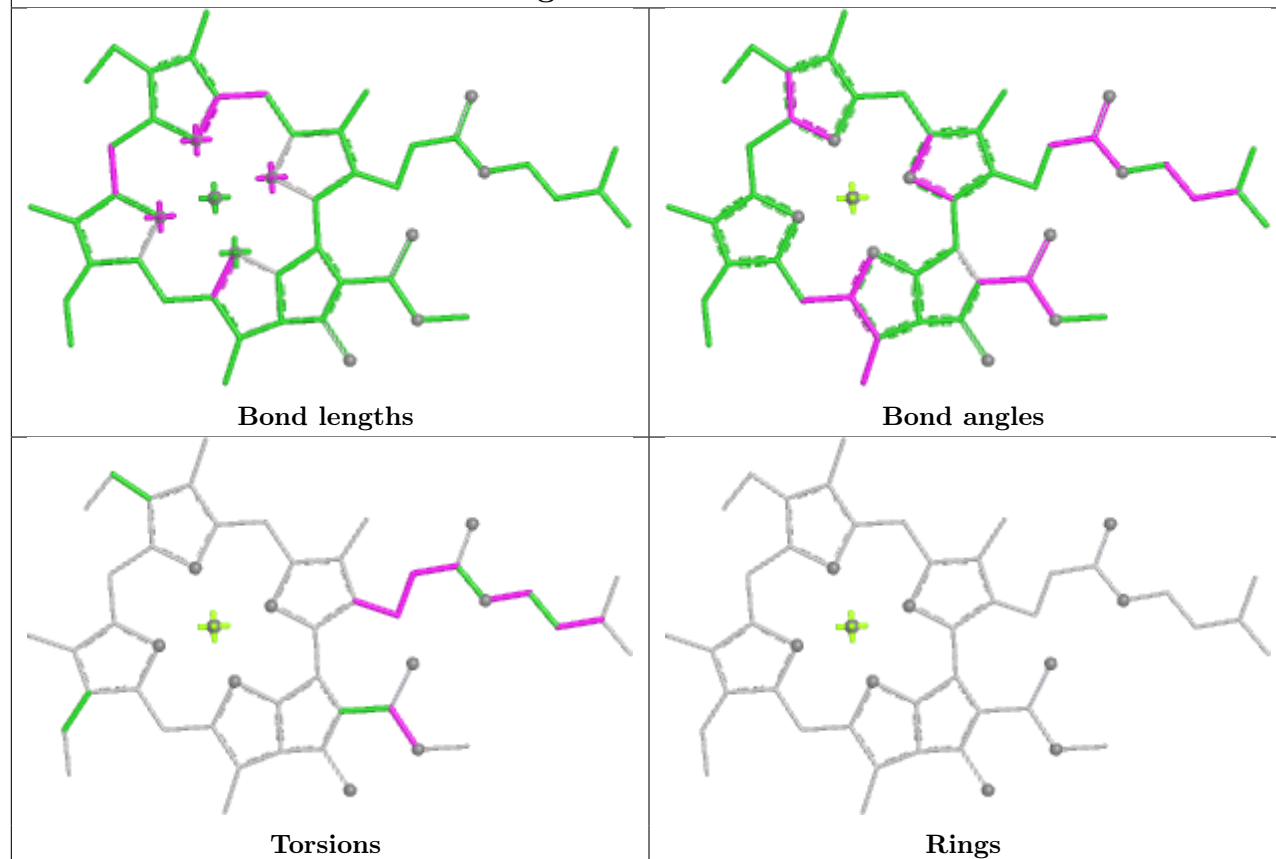


Torsions

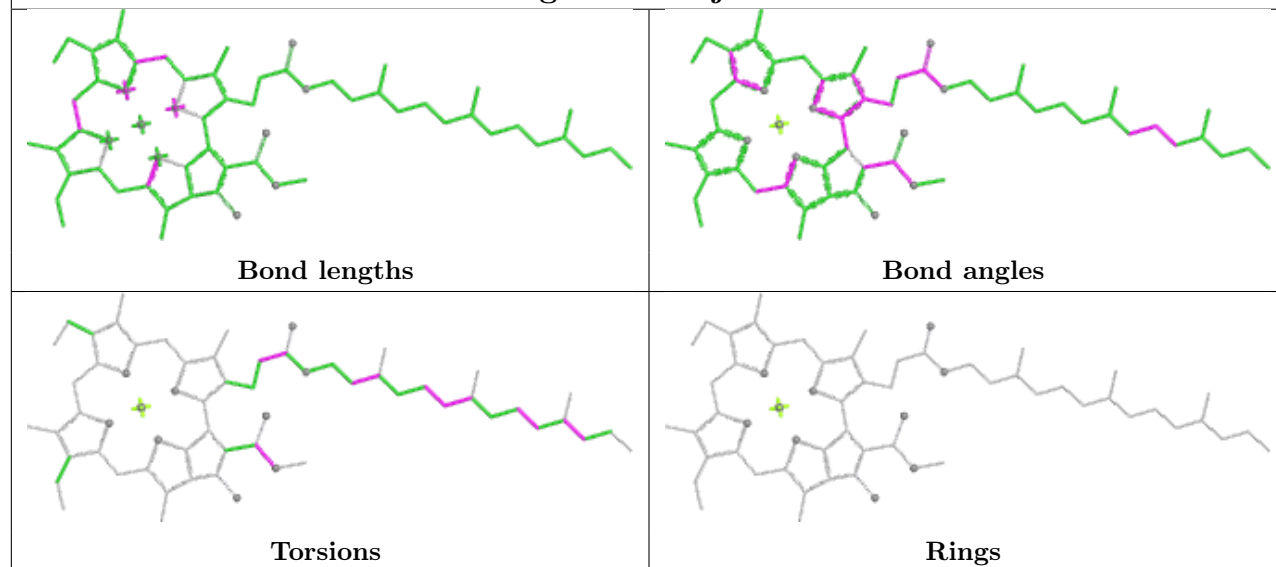


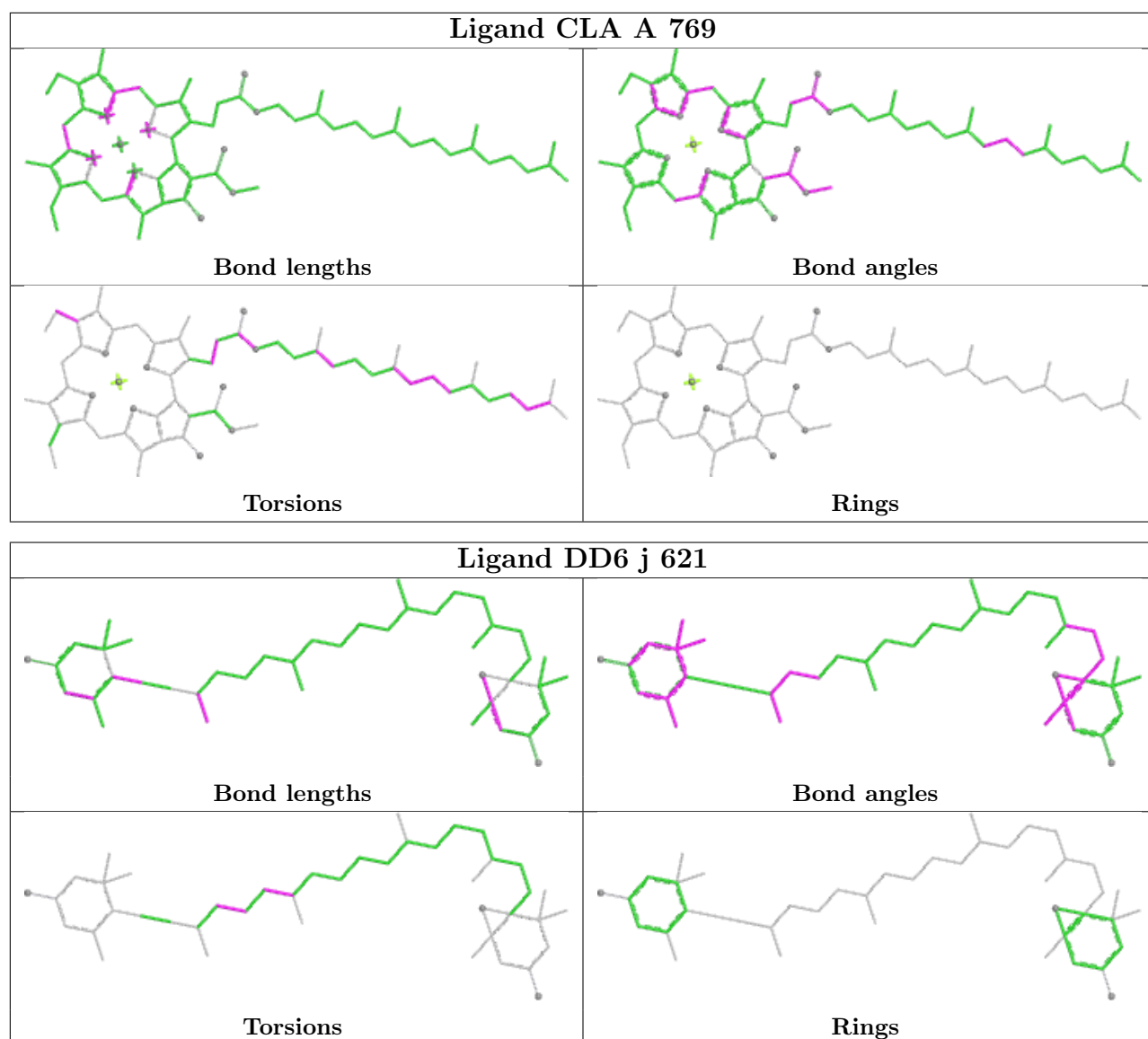
Rings

Ligand CLA c 608

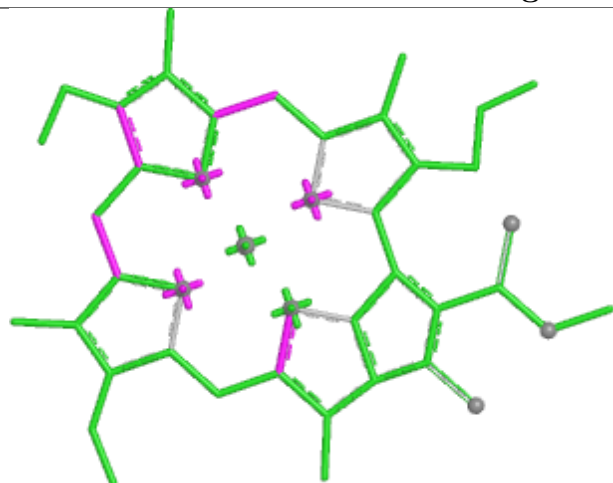


Ligand CLA j 613

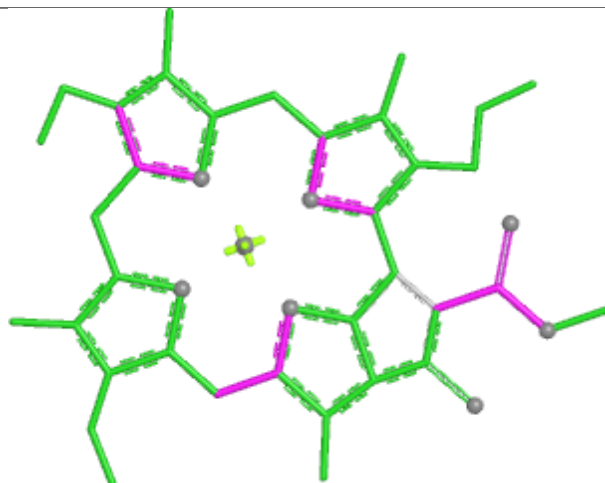




Ligand CLA f 615



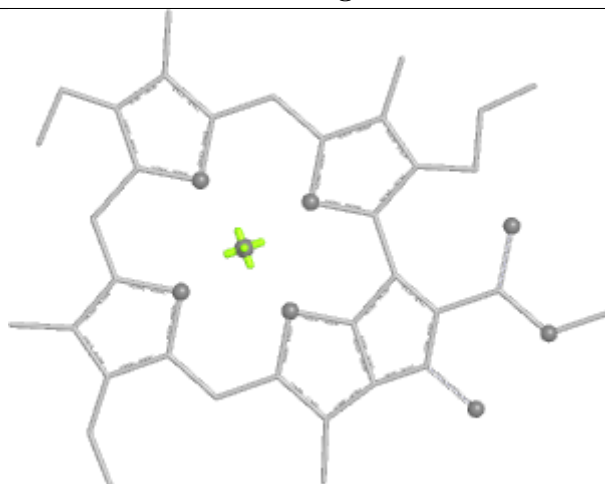
Bond lengths



Bond angles

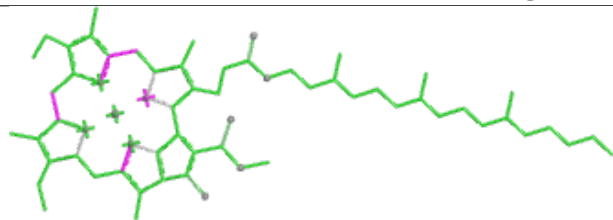


Torsions

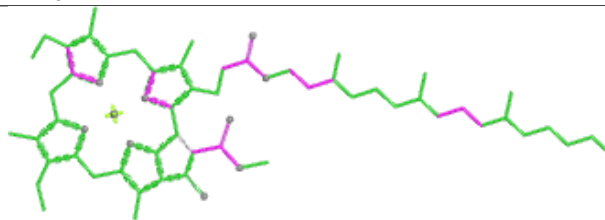


Rings

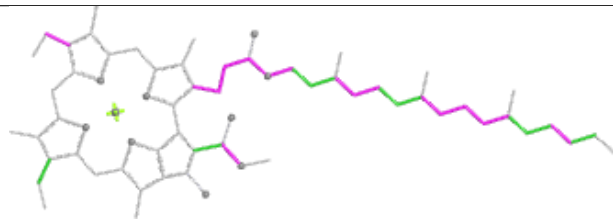
Ligand CLA j 610



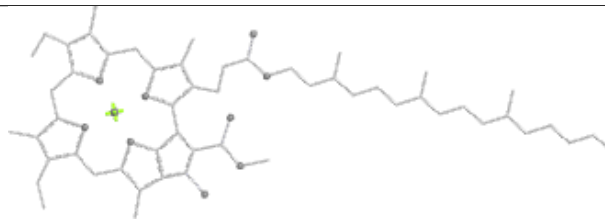
Bond lengths



Bond angles

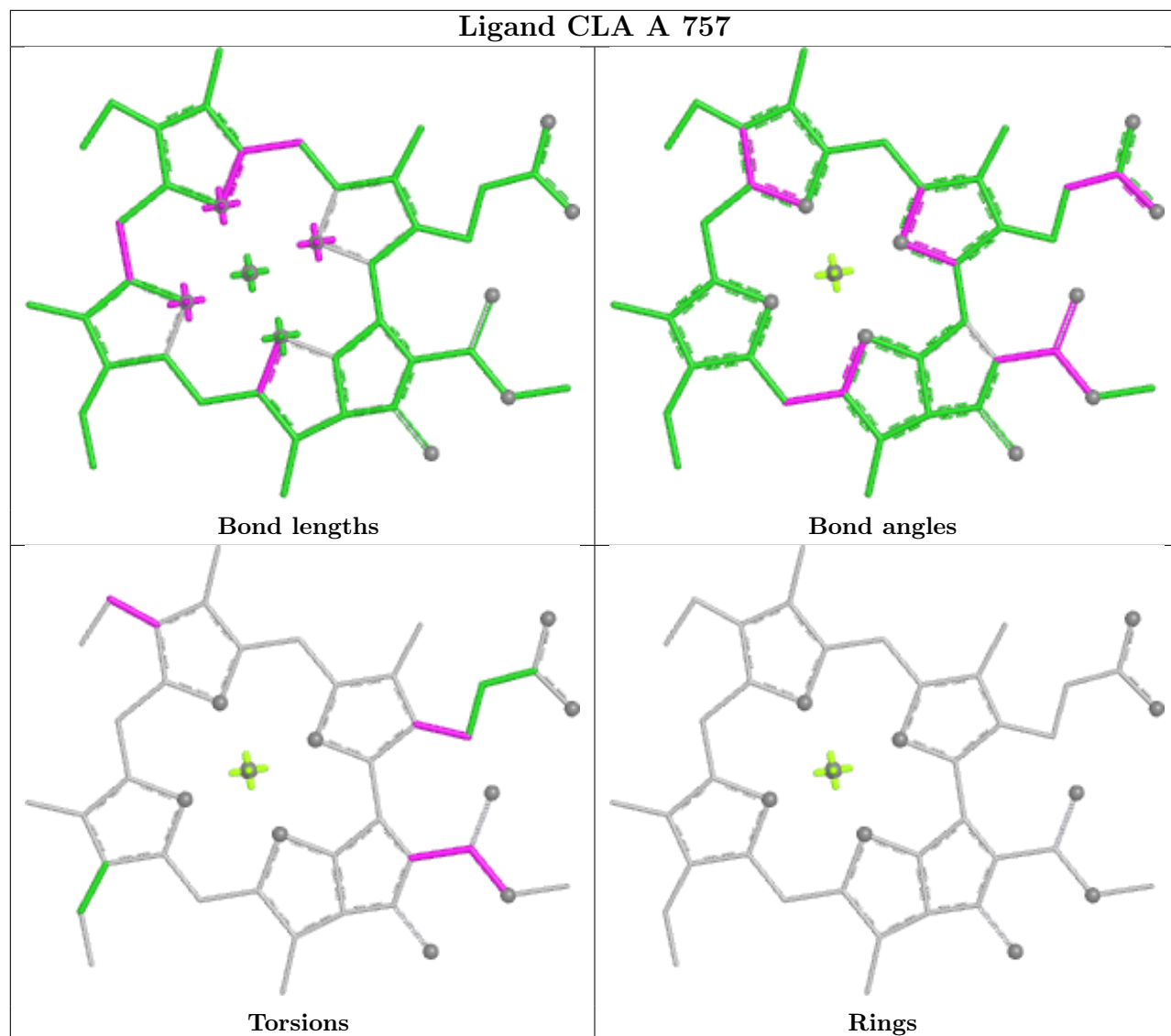


Torsions

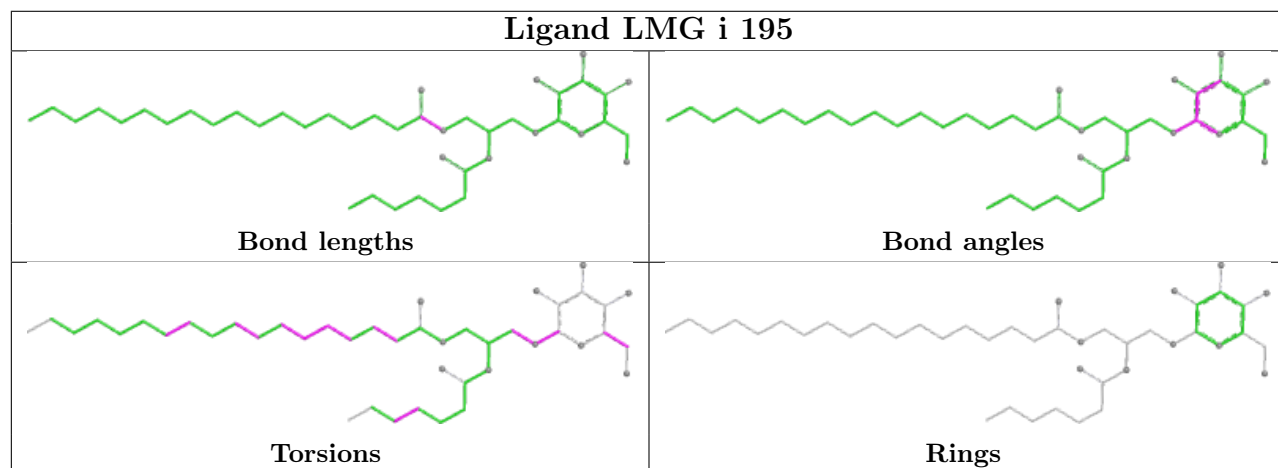


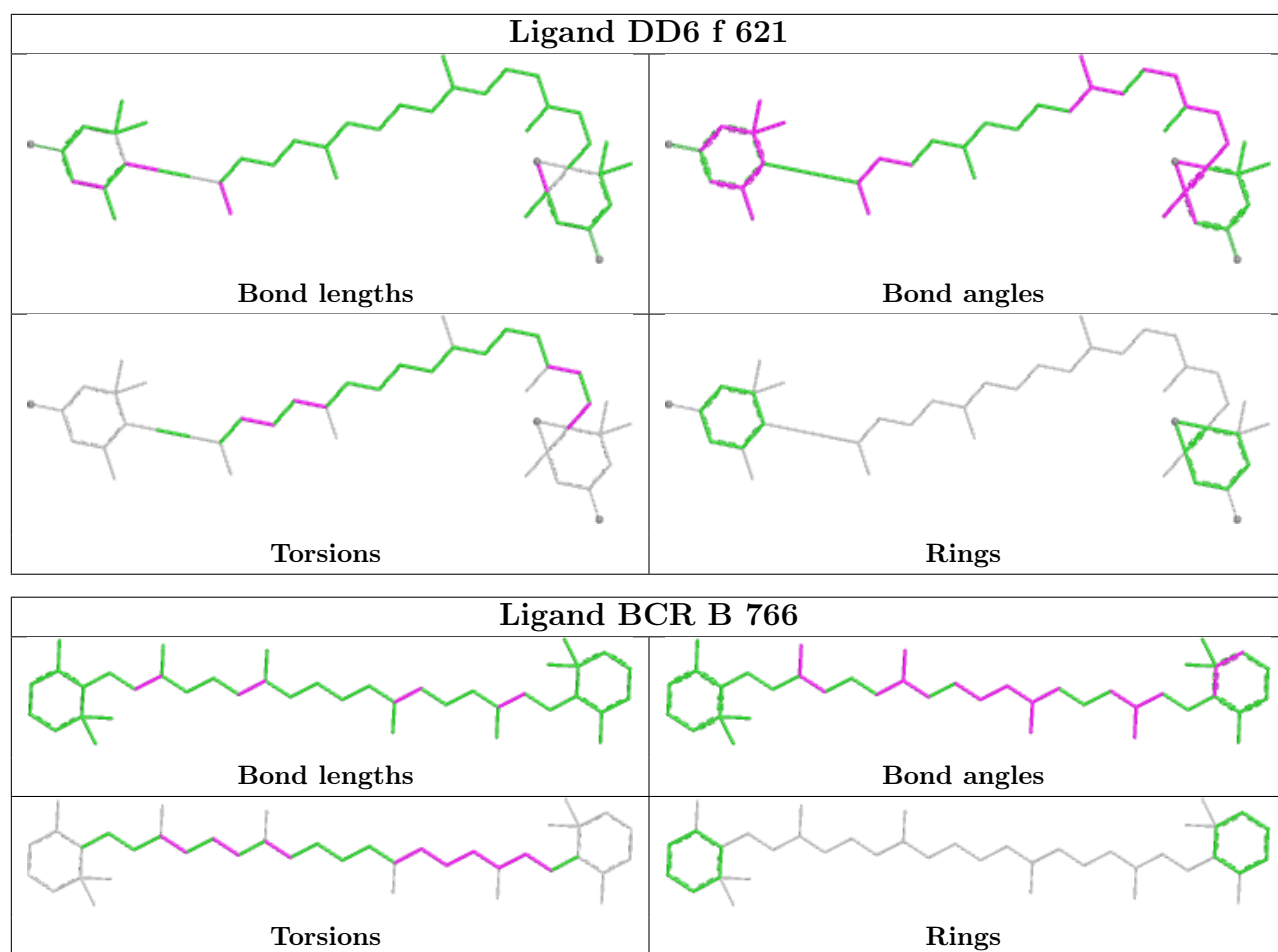
Rings

Ligand CLA A 757

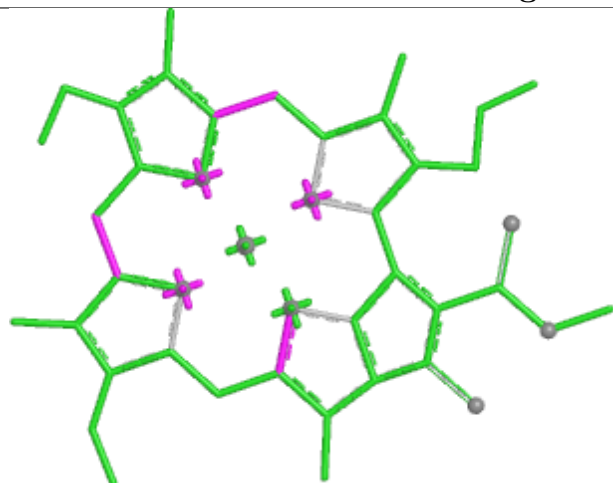


Ligand LMG i 195

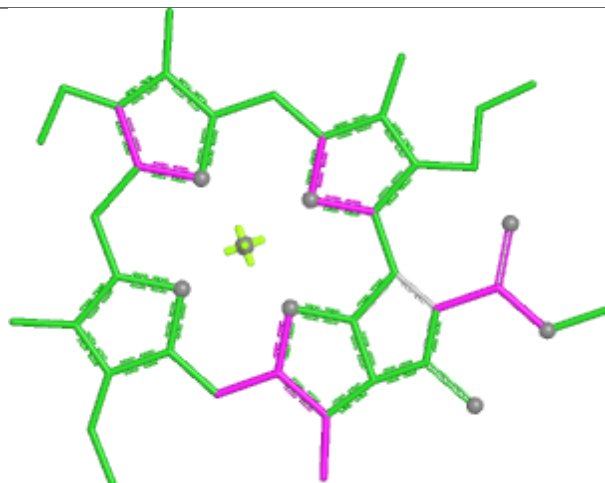




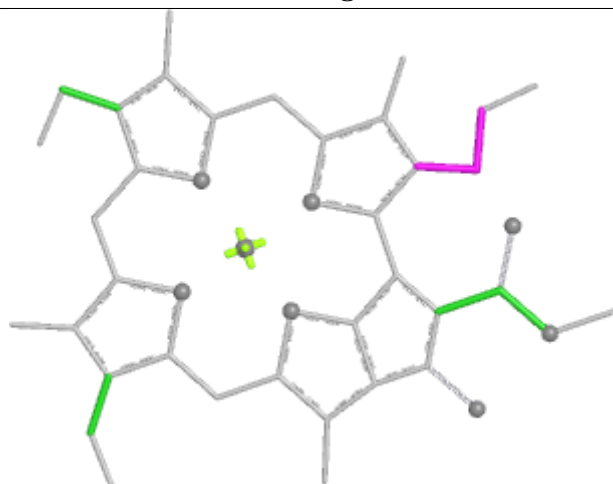
Ligand CLA c 606



Bond lengths



Bond angles

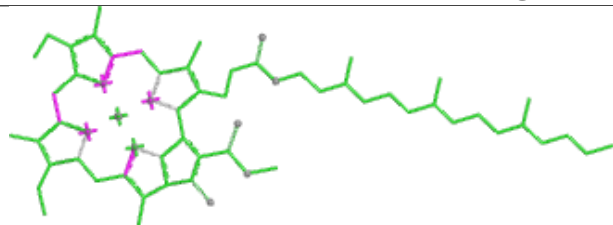


Torsions

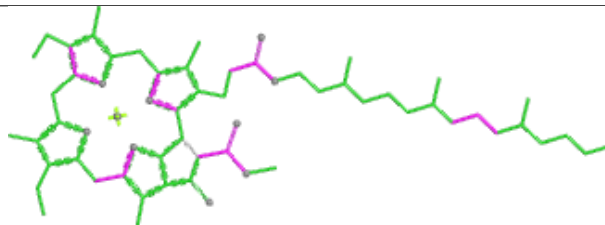


Rings

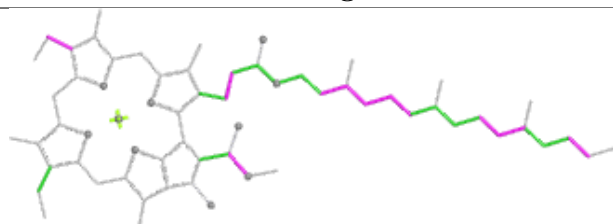
Ligand CLA A 791



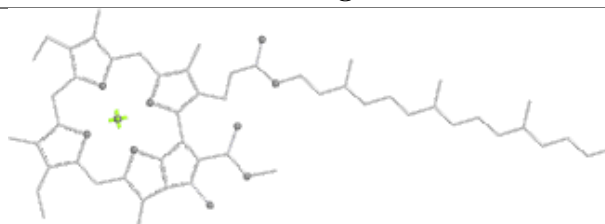
Bond lengths



Bond angles

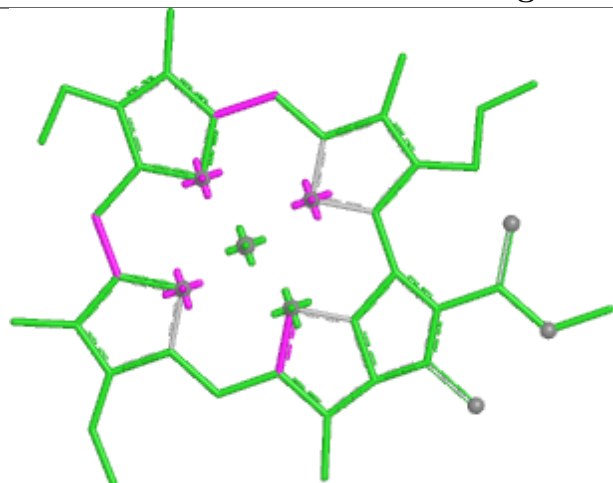


Torsions

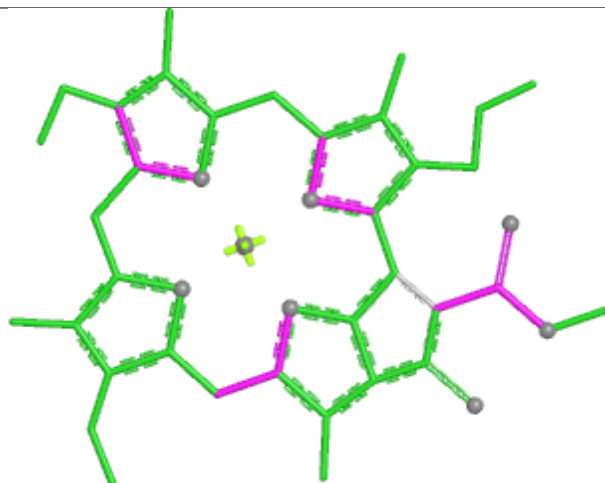


Rings

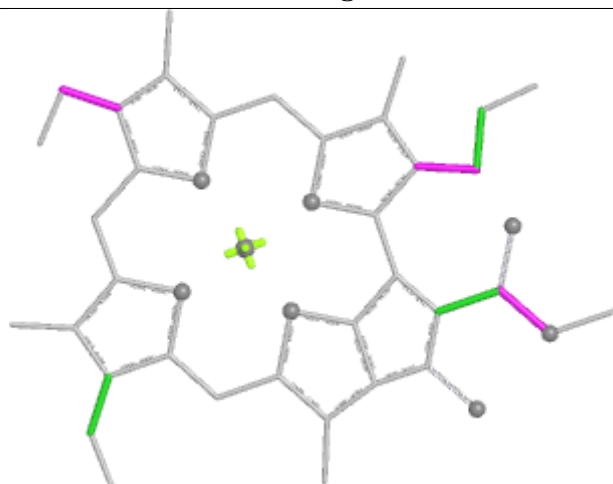
Ligand CLA h 611



Bond lengths



Bond angles

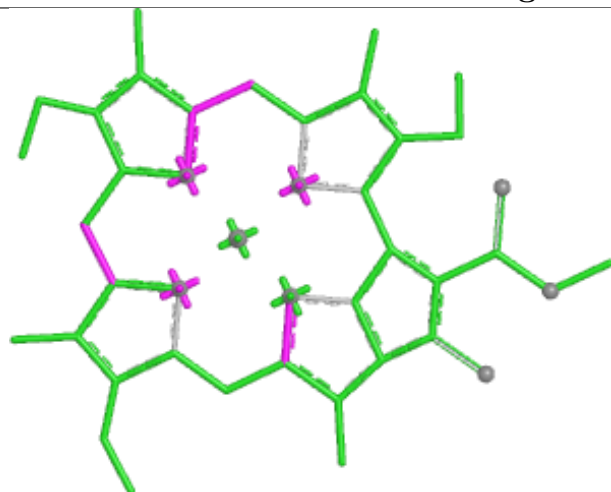


Torsions

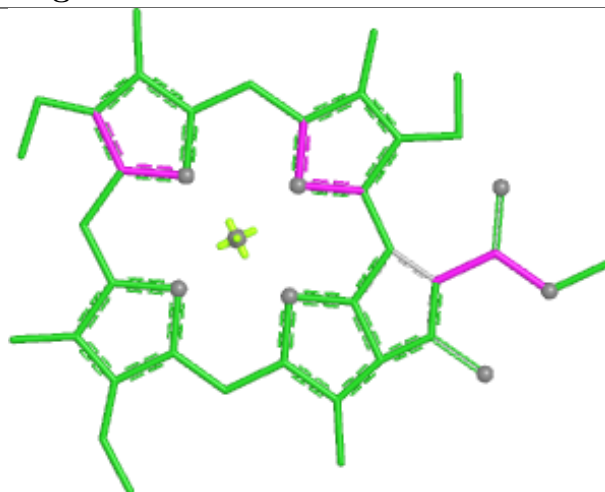


Rings

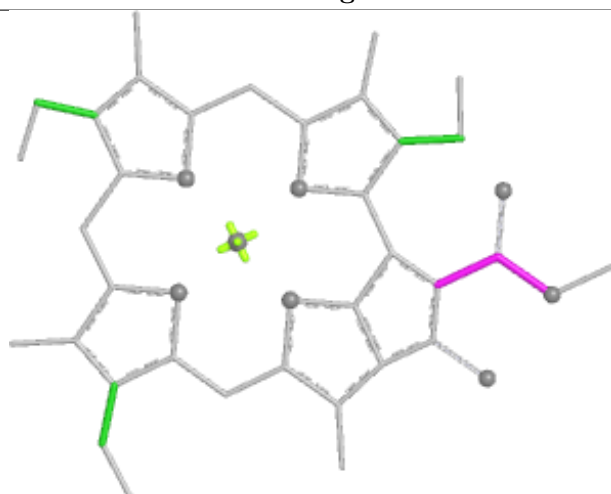
Ligand CLA g 612



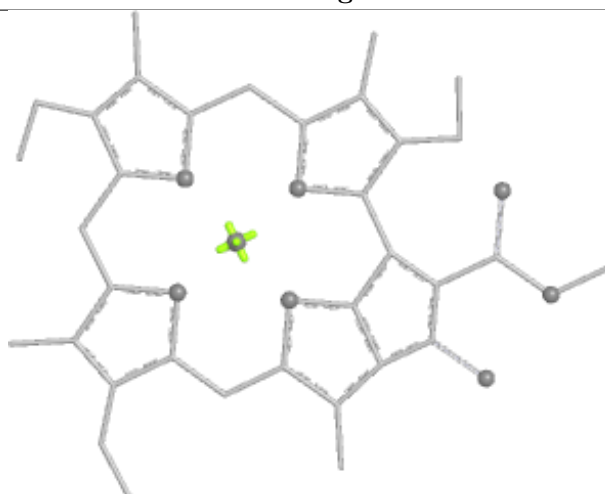
Bond lengths



Bond angles

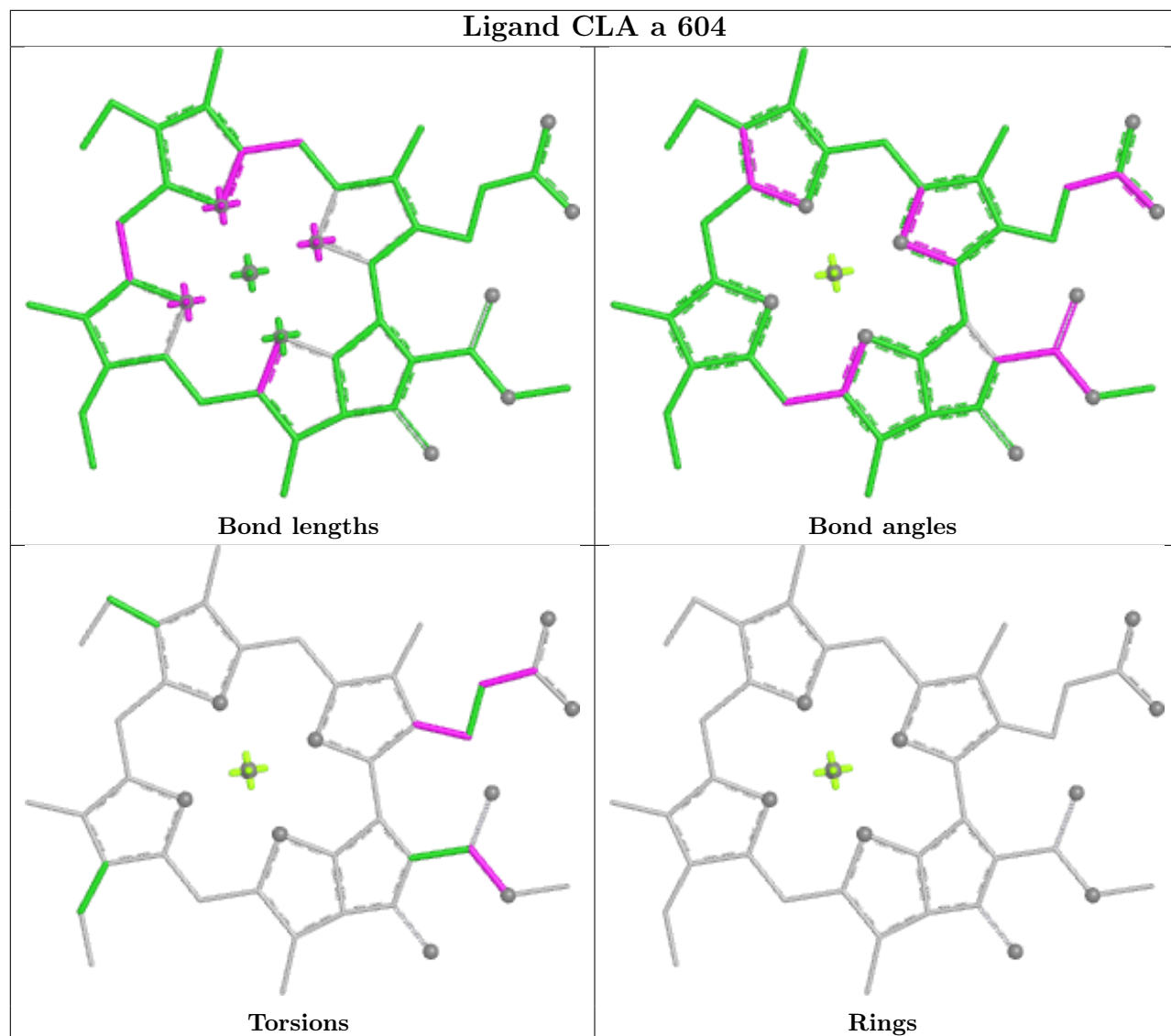


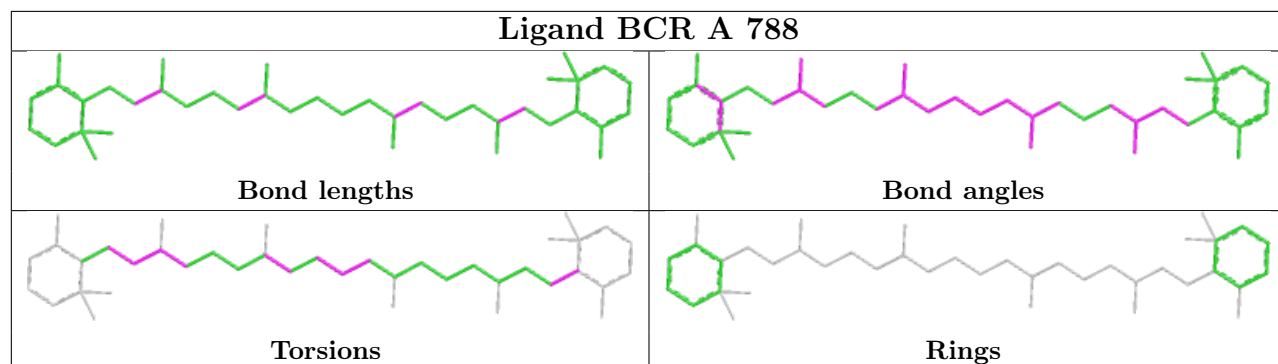
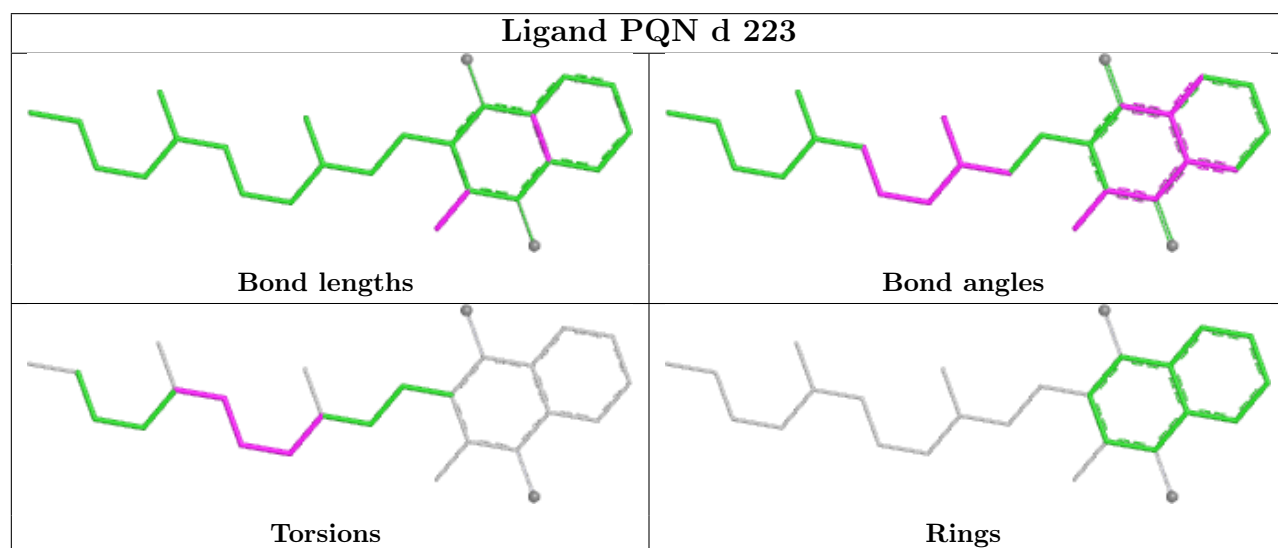
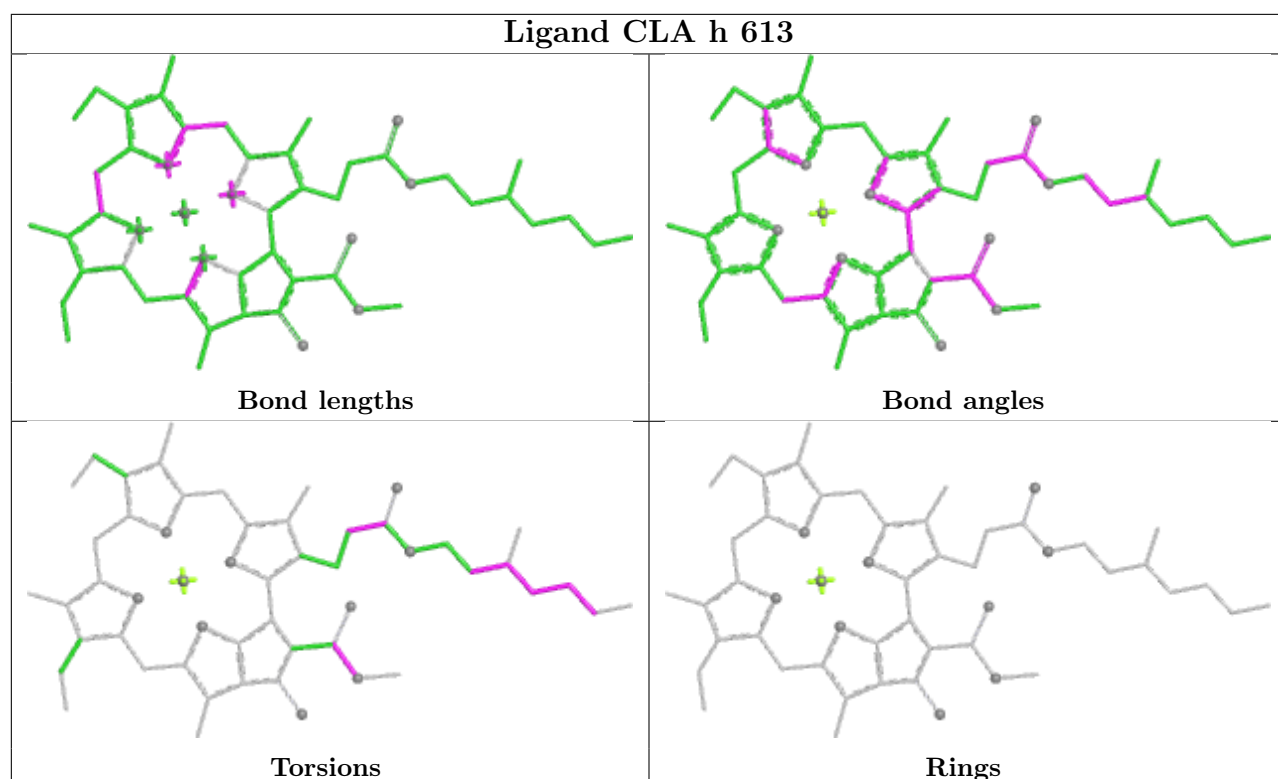
Torsions

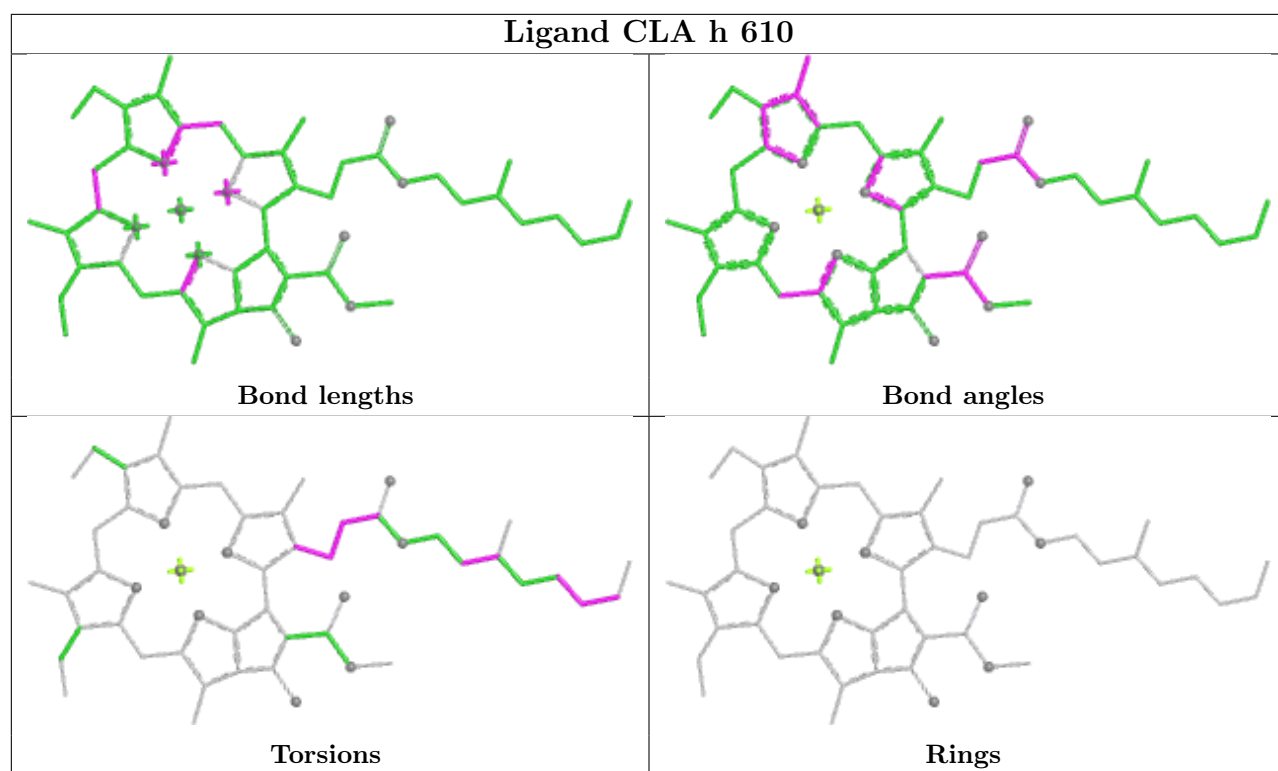


Rings

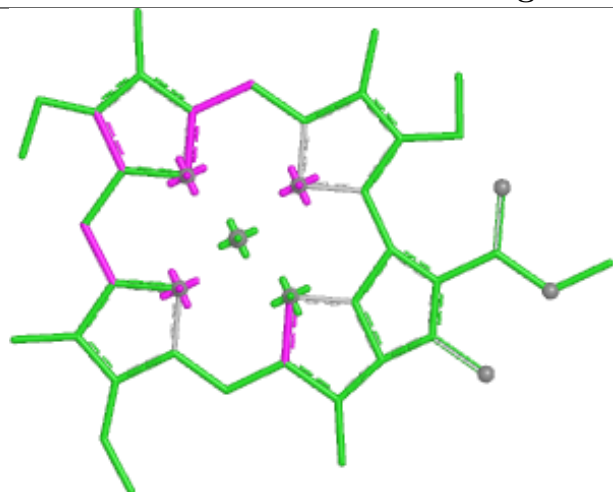
Ligand CLA a 604



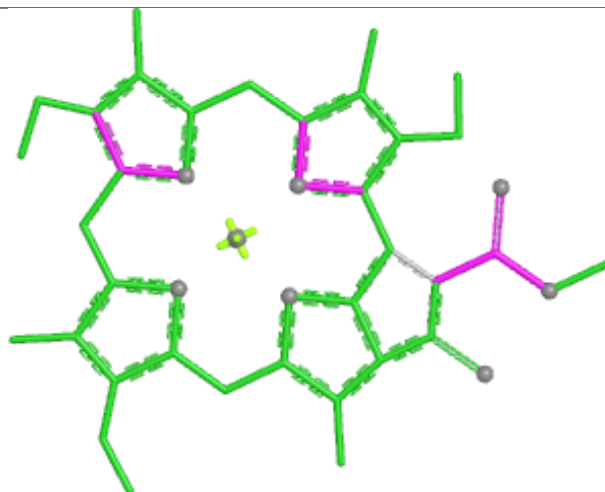




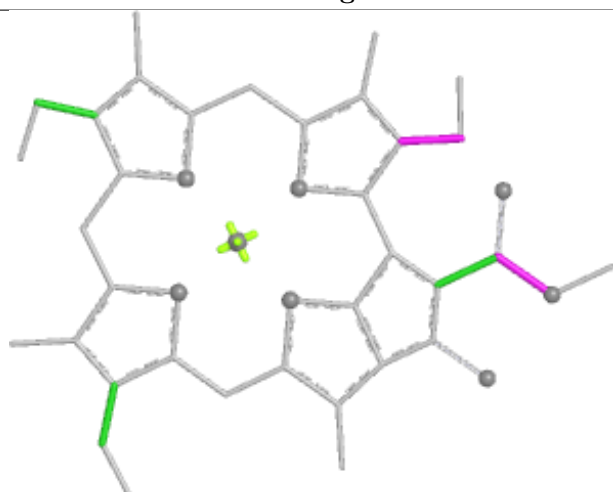
Ligand CLA n 613



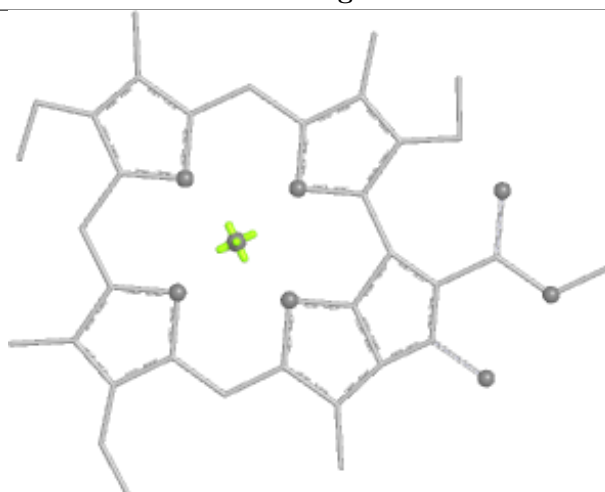
Bond lengths



Bond angles

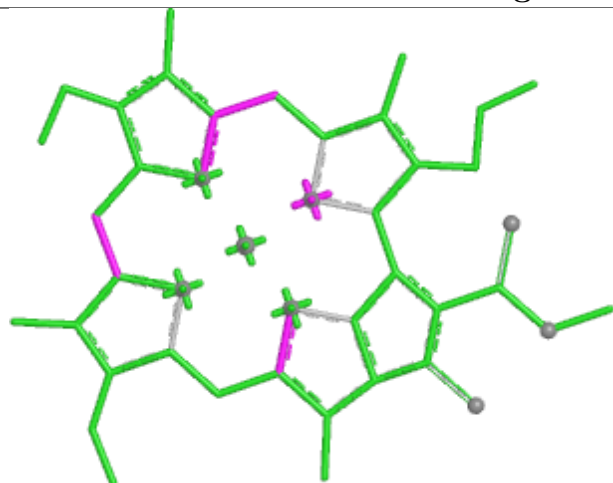


Torsions

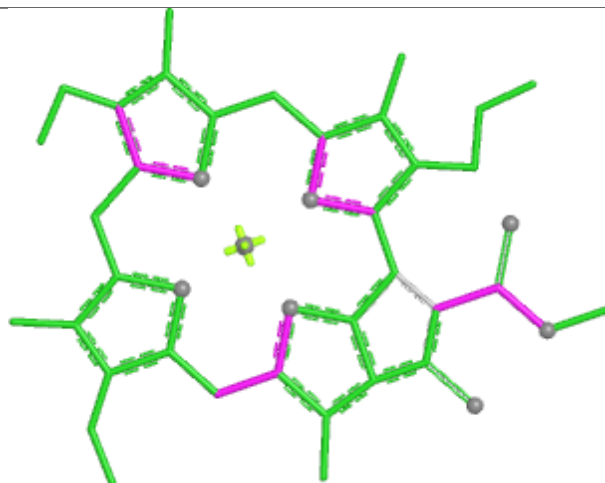


Rings

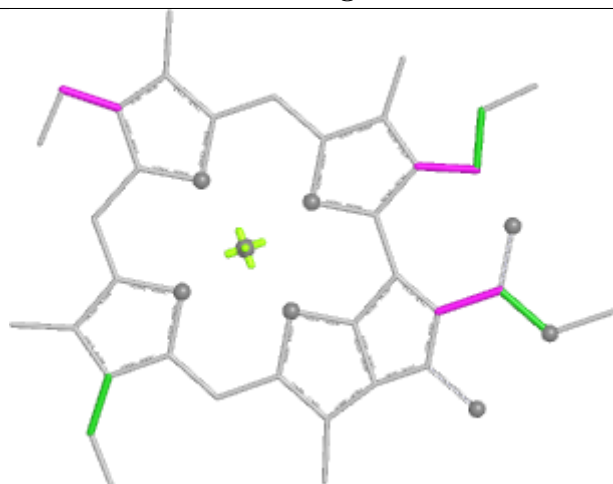
Ligand CLA A 802



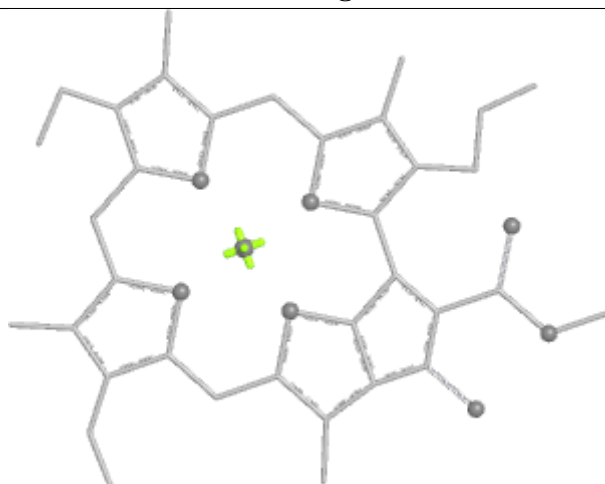
Bond lengths



Bond angles

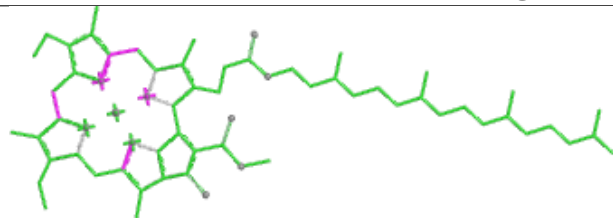


Torsions

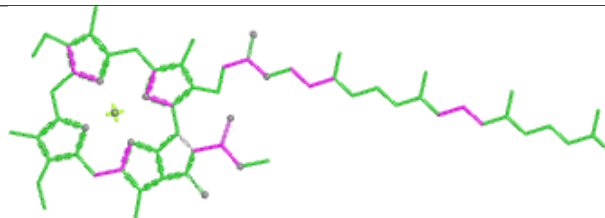


Rings

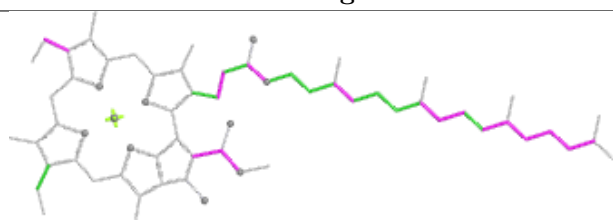
Ligand CLA A 763



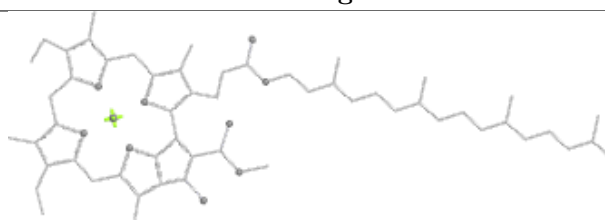
Bond lengths



Bond angles

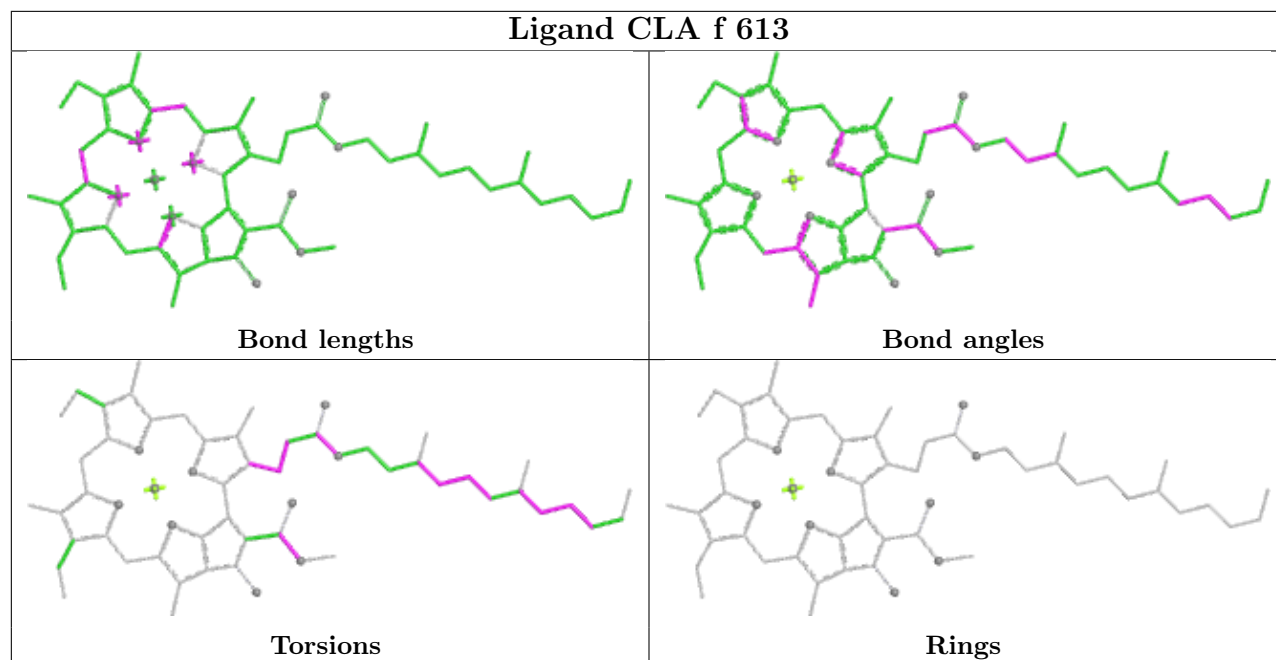


Torsions

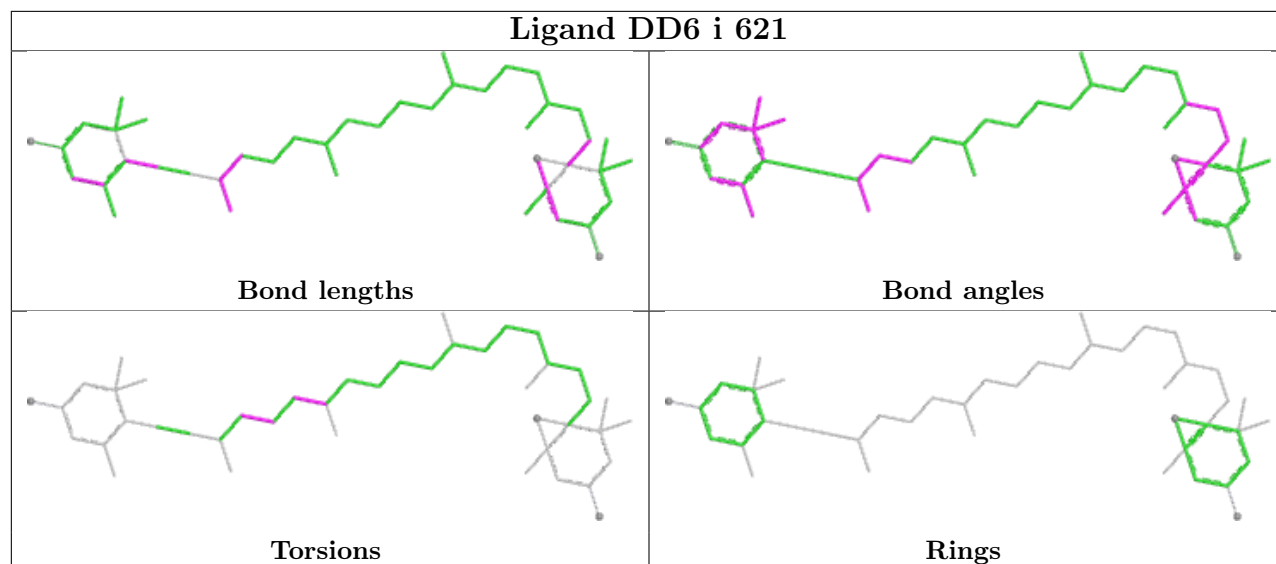


Rings

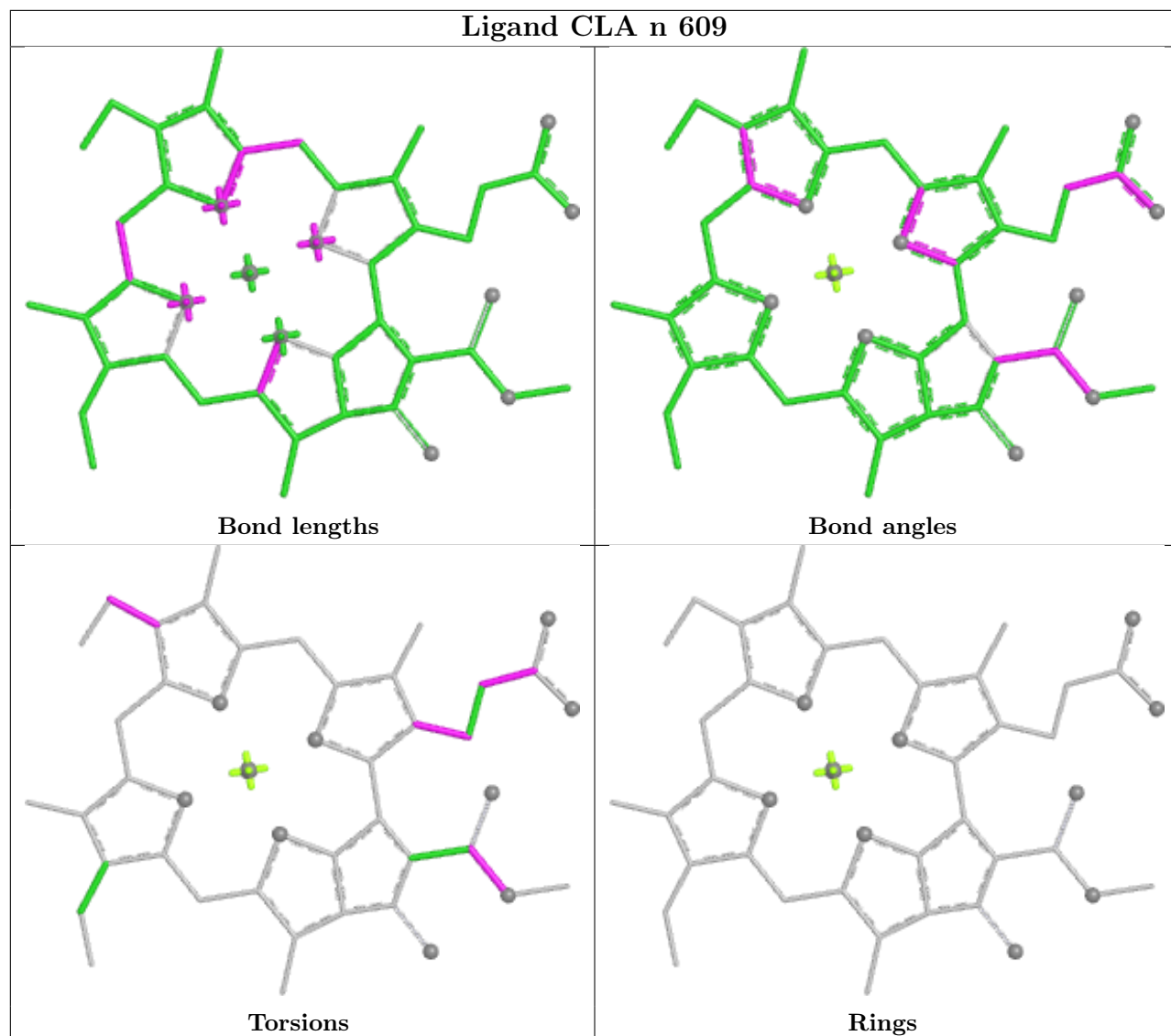
Ligand CLA f 613



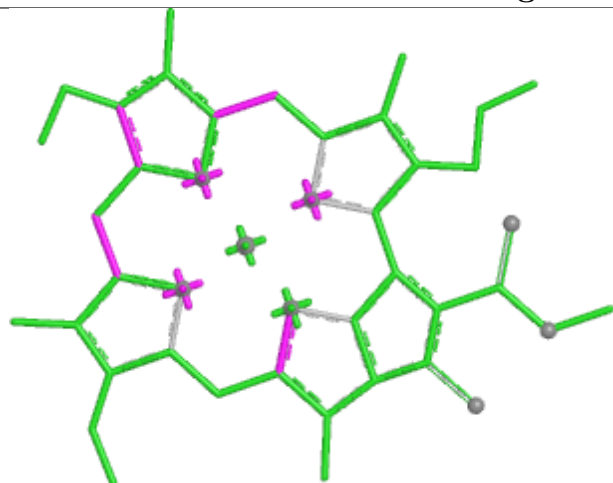
Ligand DD6 i 621



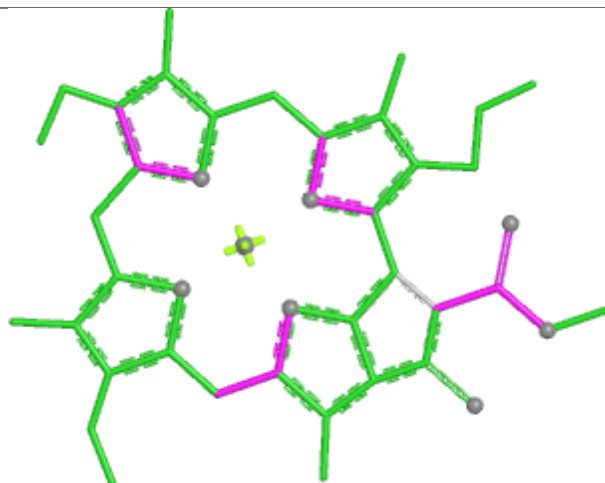
Ligand CLA n 609



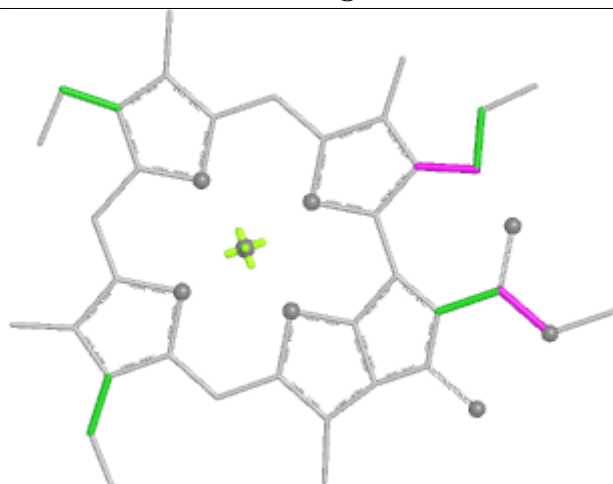
Ligand CLA k 601



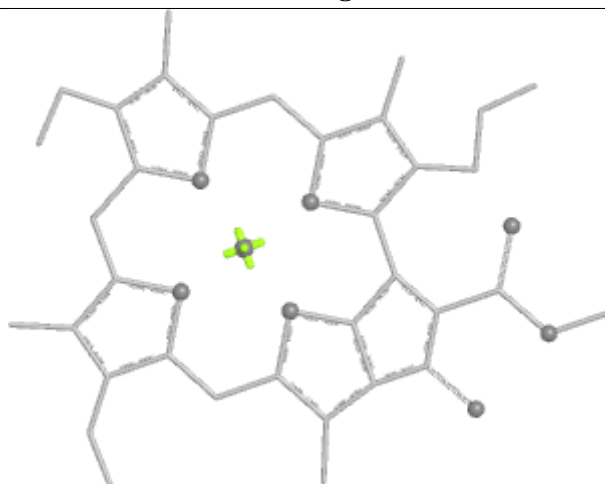
Bond lengths



Bond angles

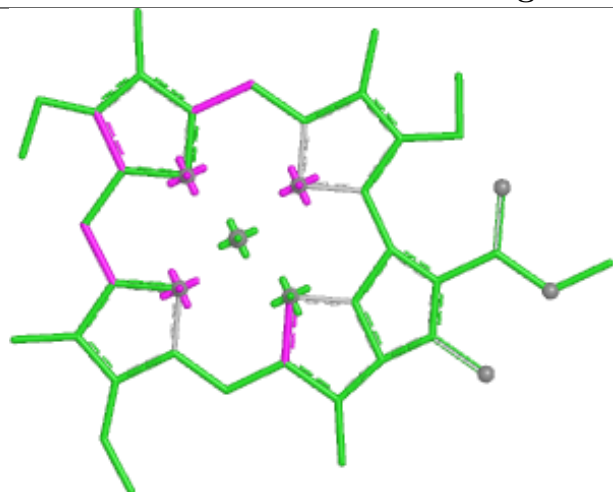


Torsions

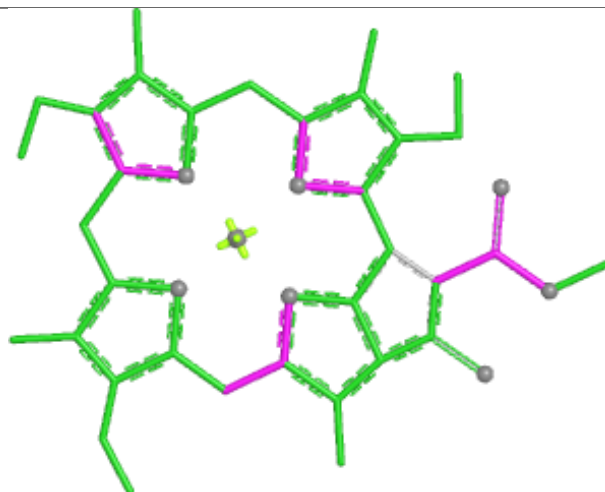


Rings

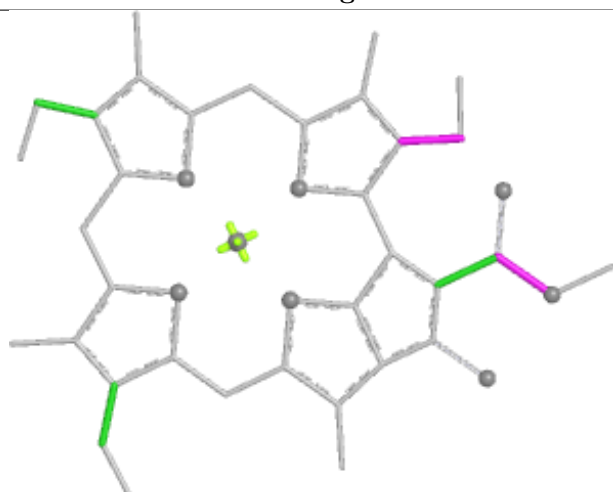
Ligand CLA n 607



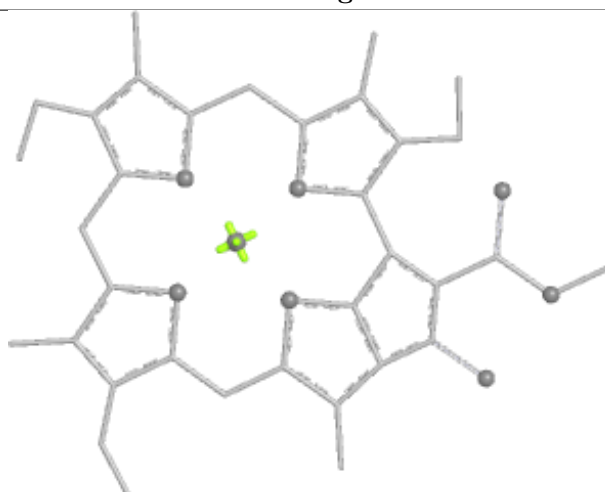
Bond lengths



Bond angles

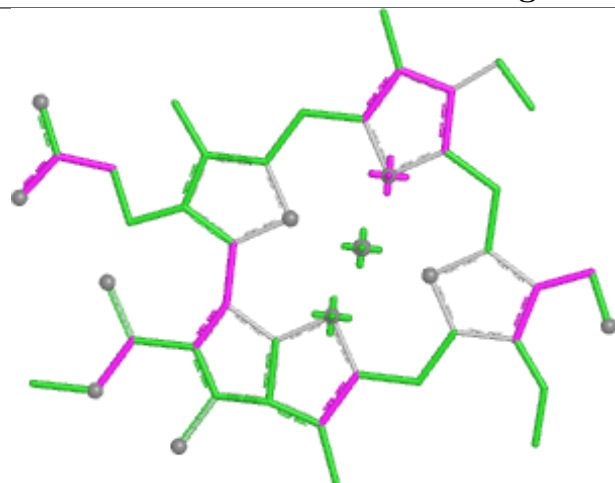


Torsions

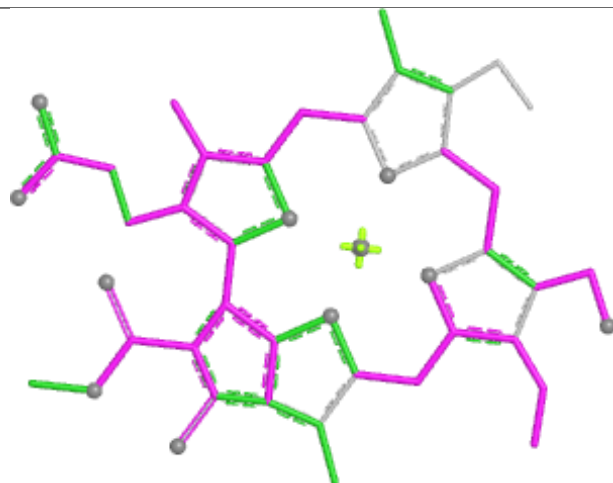


Rings

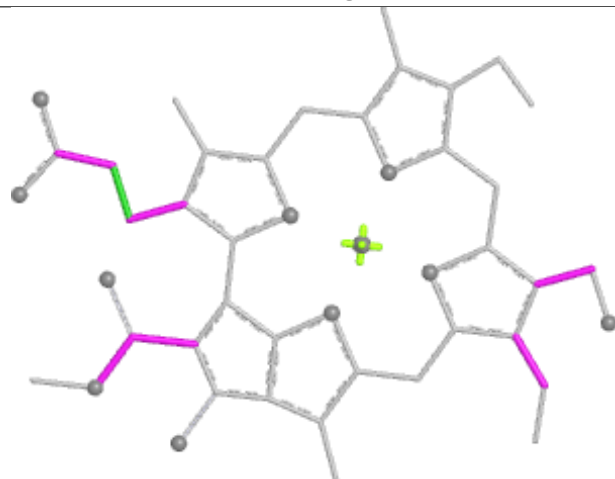
Ligand CHL d 606



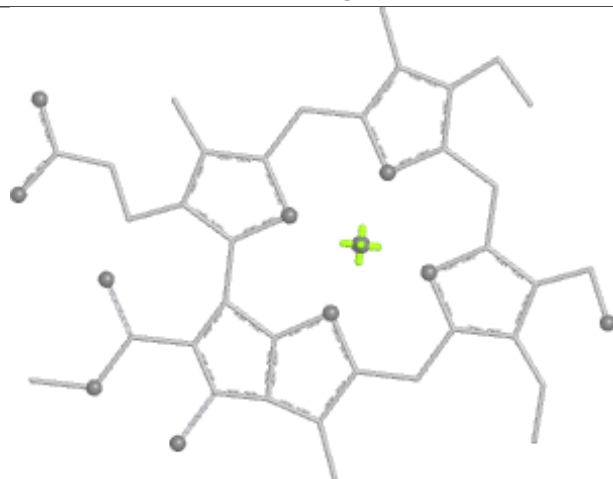
Bond lengths



Bond angles

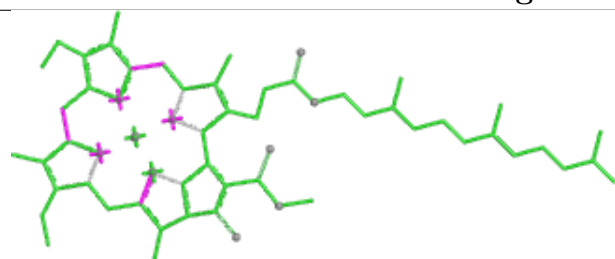


Torsions

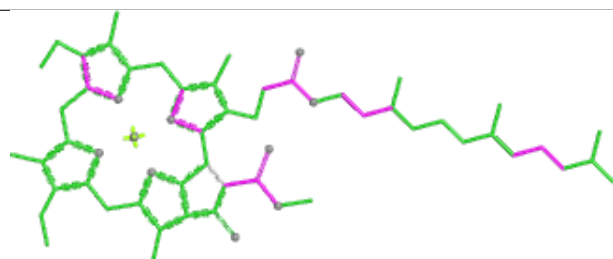


Rings

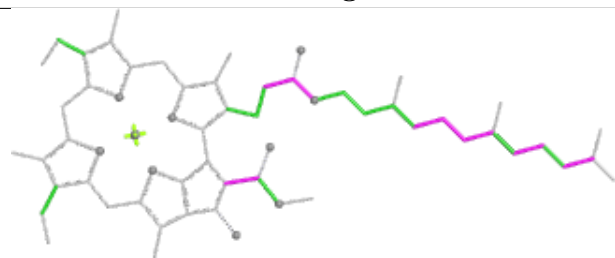
Ligand CLA A 759



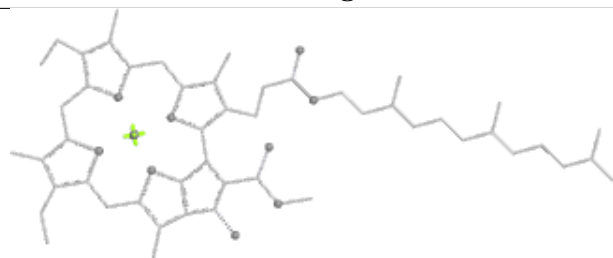
Bond lengths



Bond angles

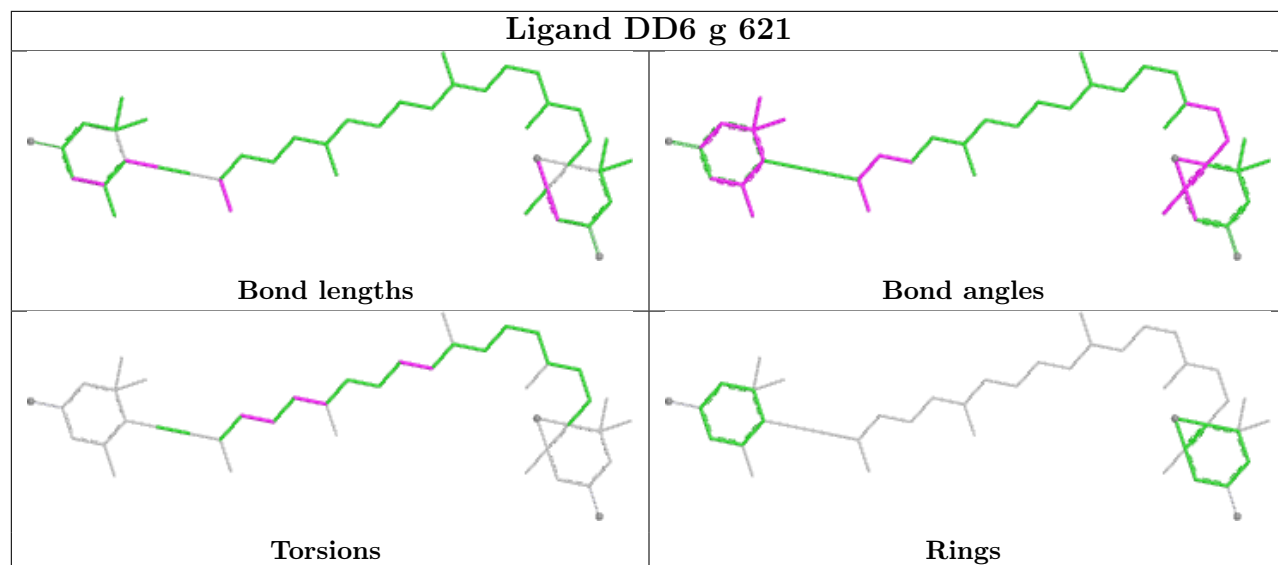


Torsions

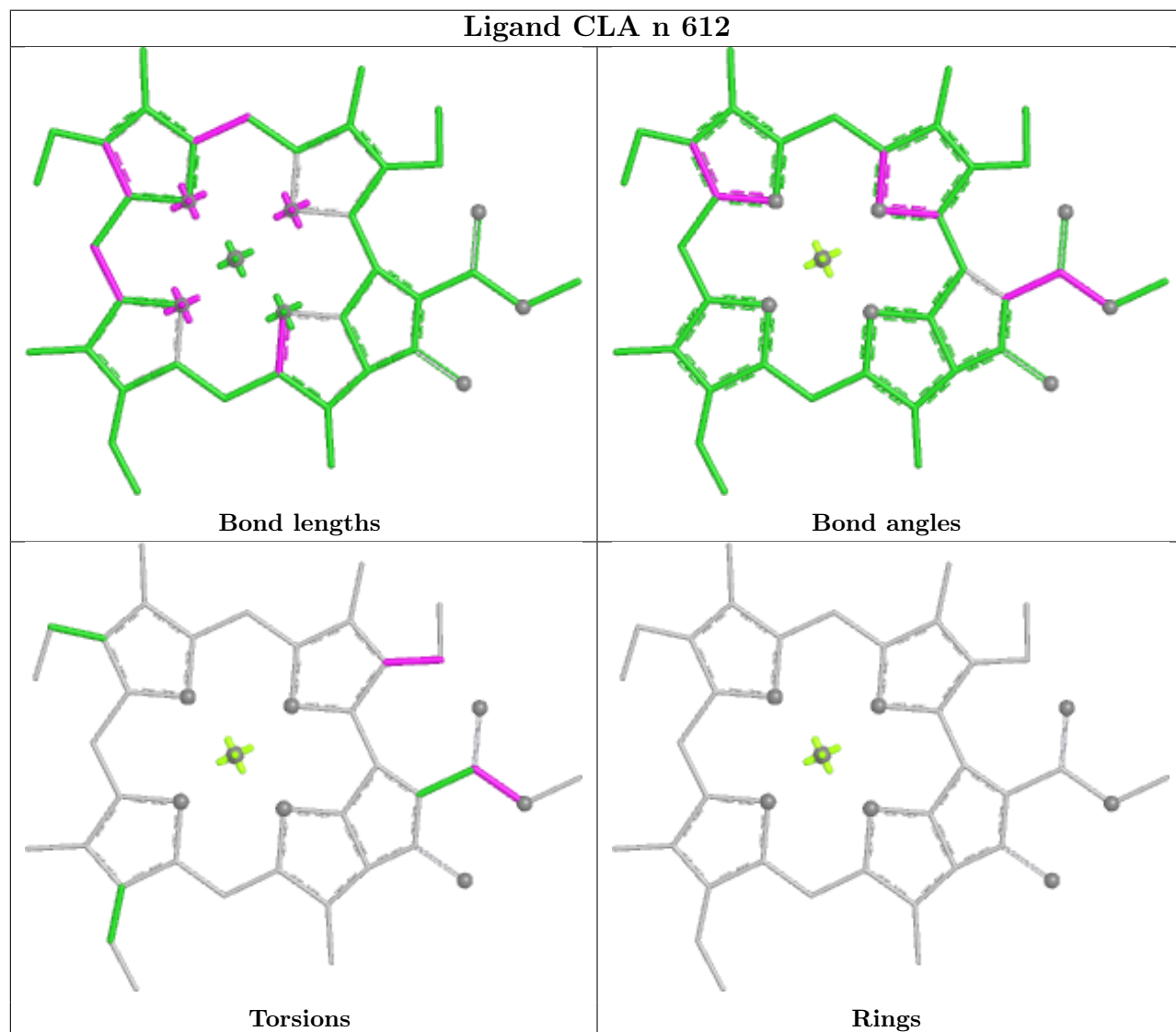


Rings

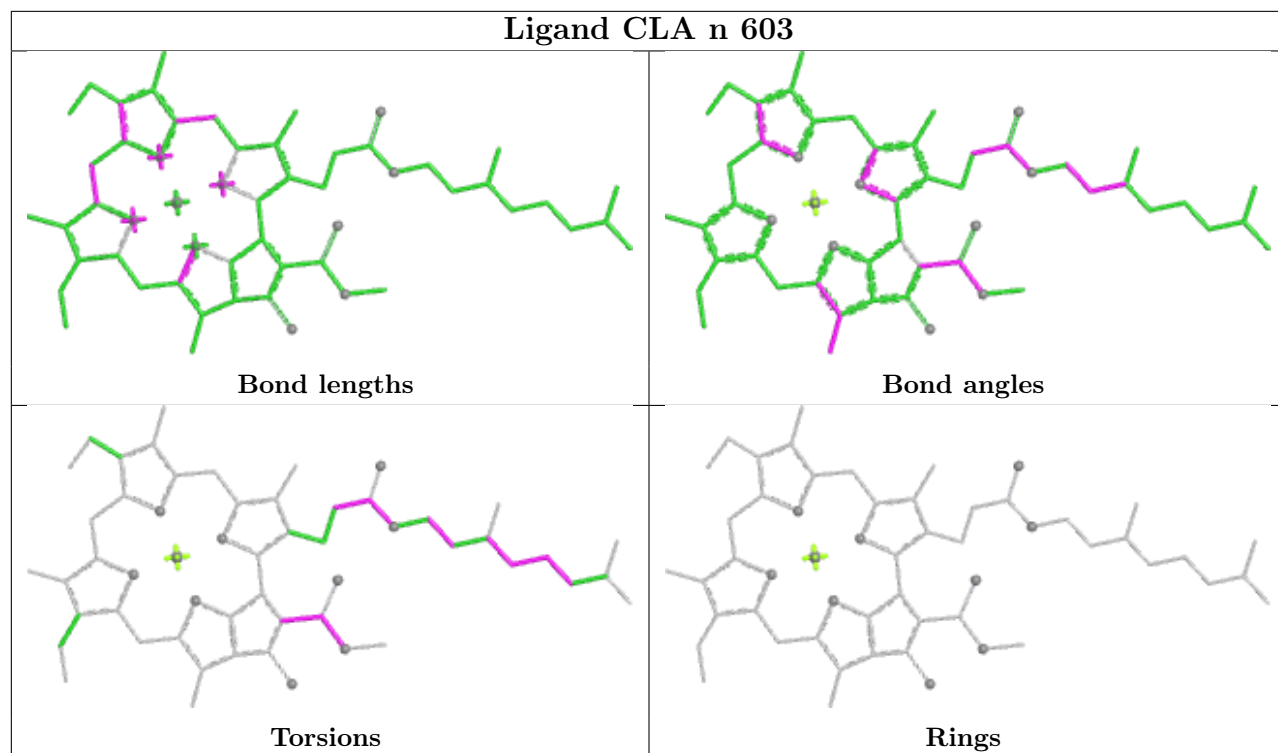
Ligand DD6 g 621



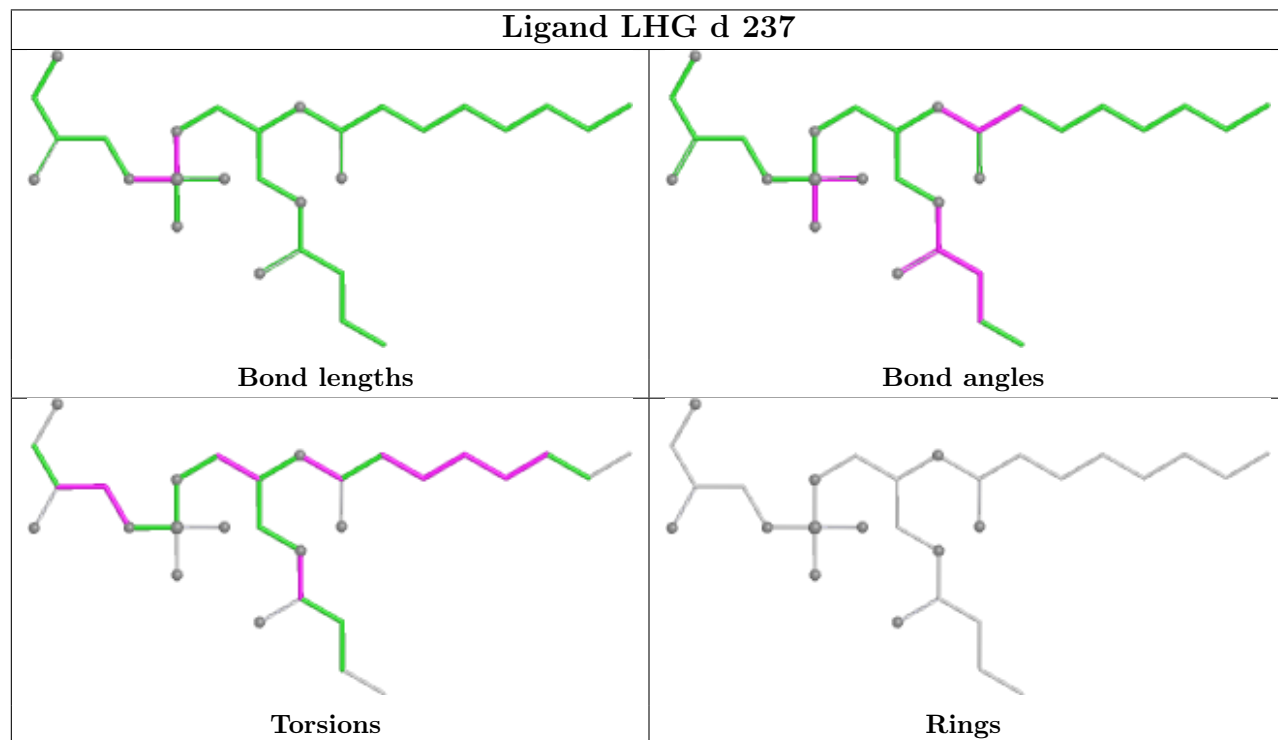
Ligand CLA n 612

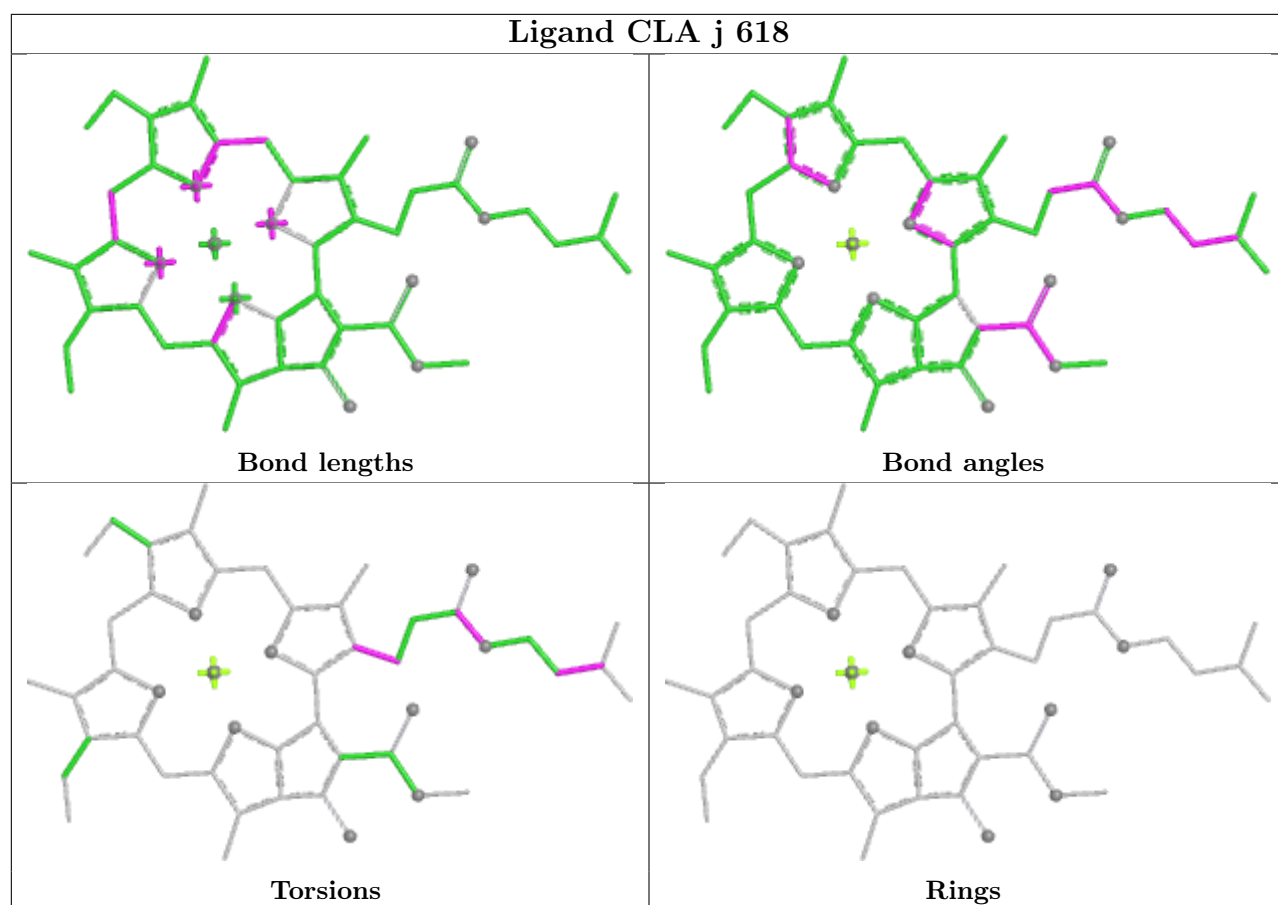


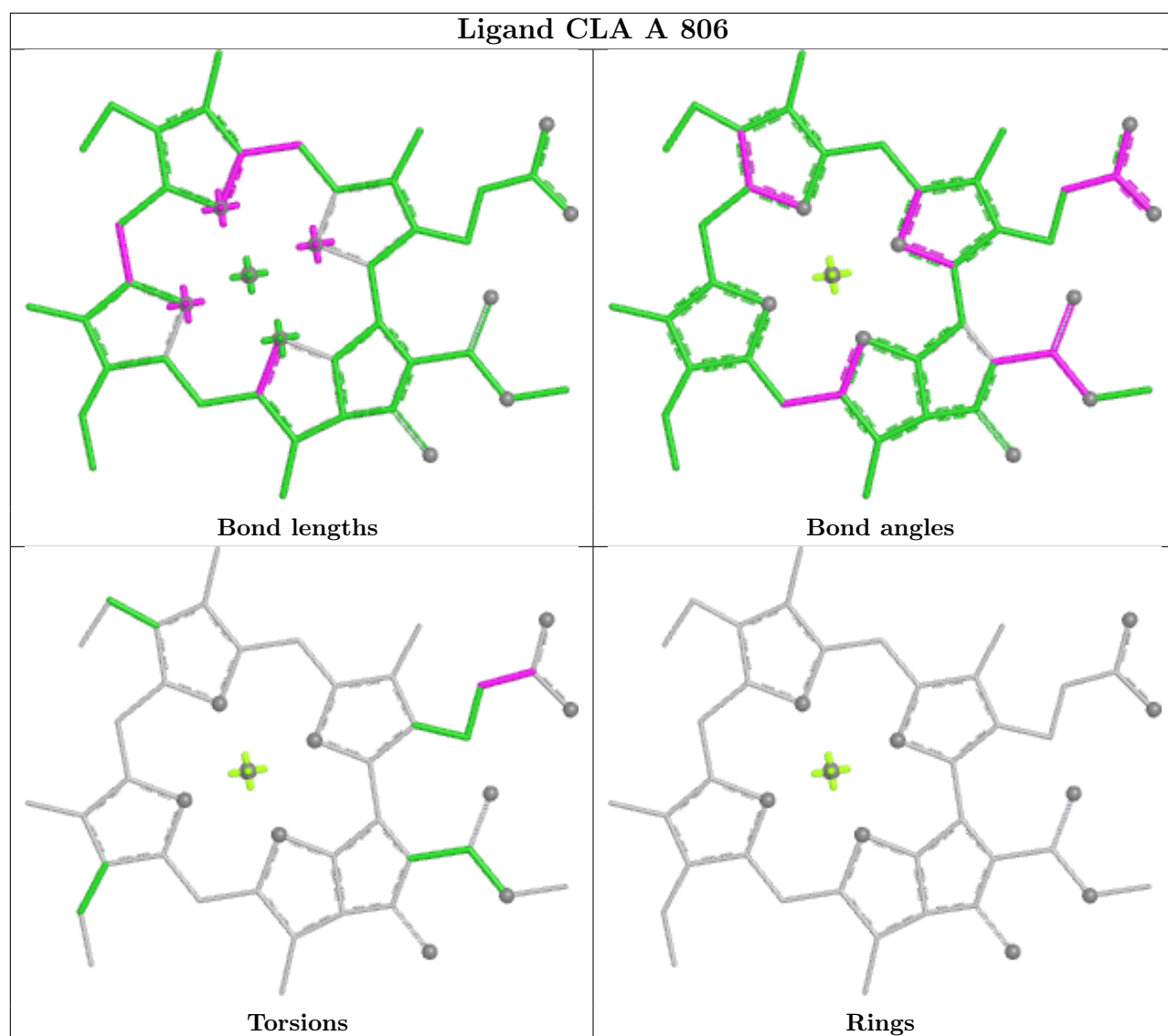
Ligand CLA n 603



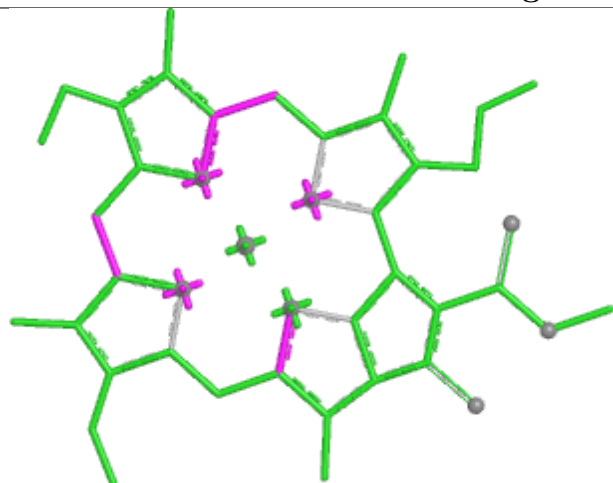
Ligand LHG d 237



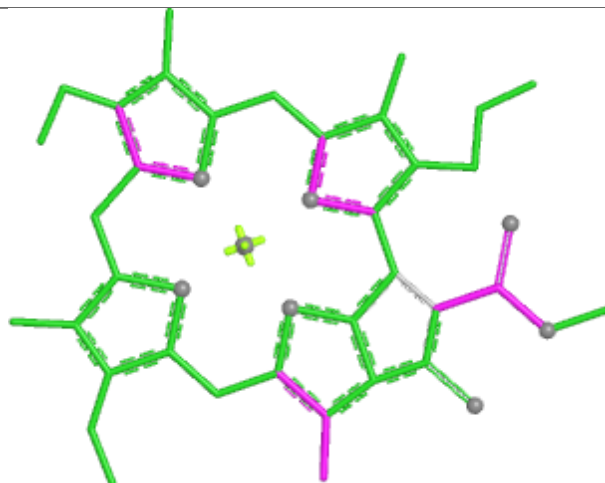




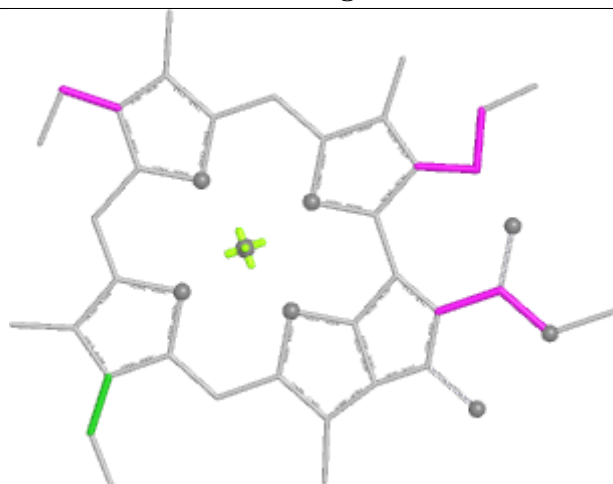
Ligand CLA i 603



Bond lengths



Bond angles

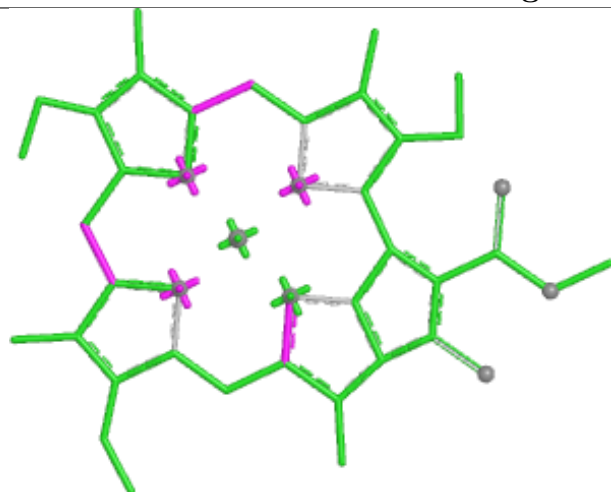


Torsions

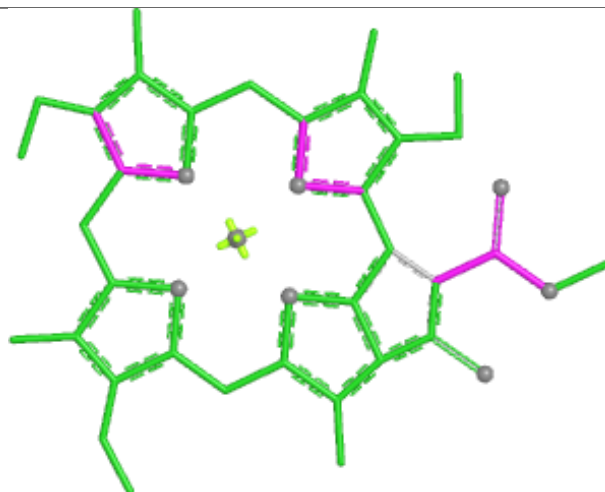


Rings

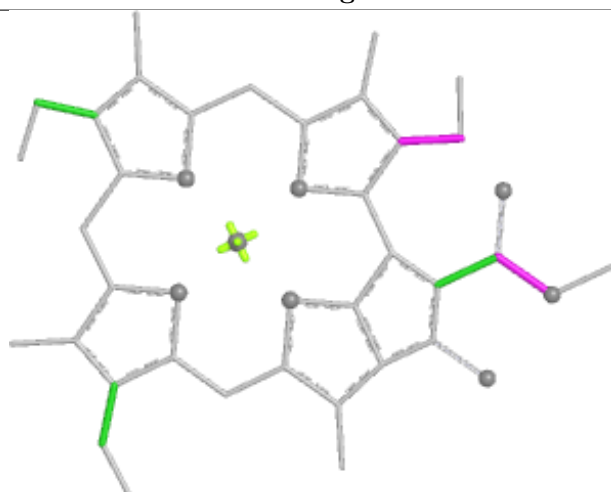
Ligand CLA f 612



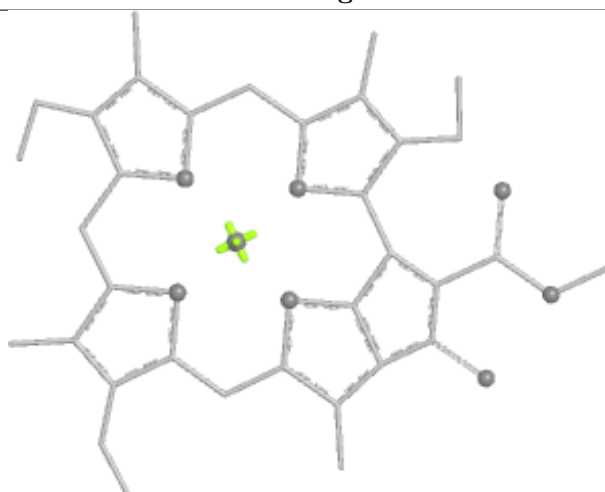
Bond lengths



Bond angles

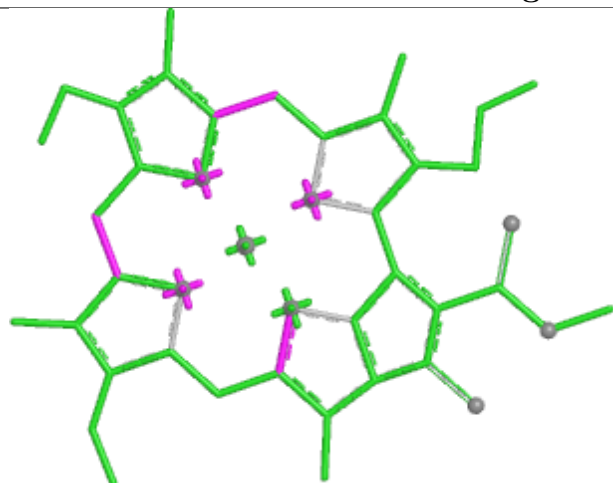


Torsions

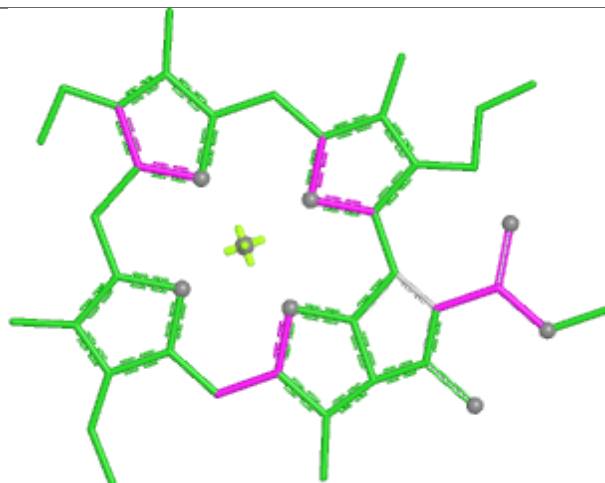


Rings

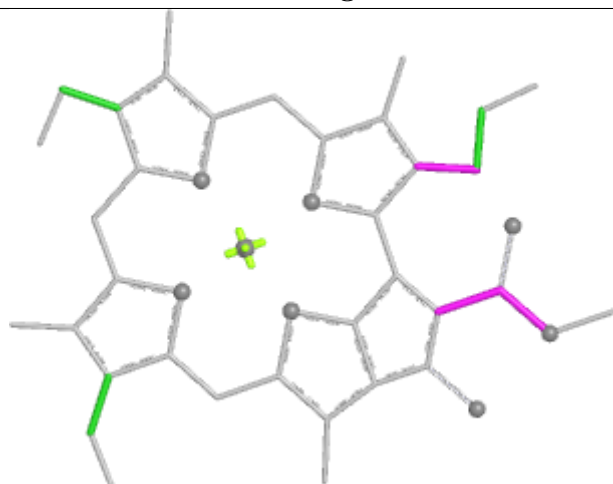
Ligand CLA i 611



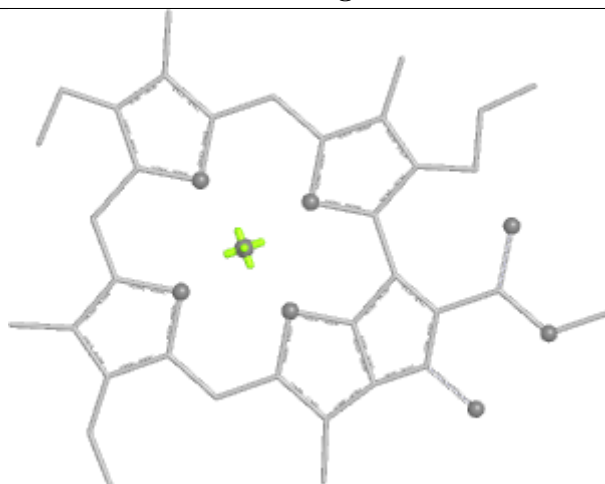
Bond lengths



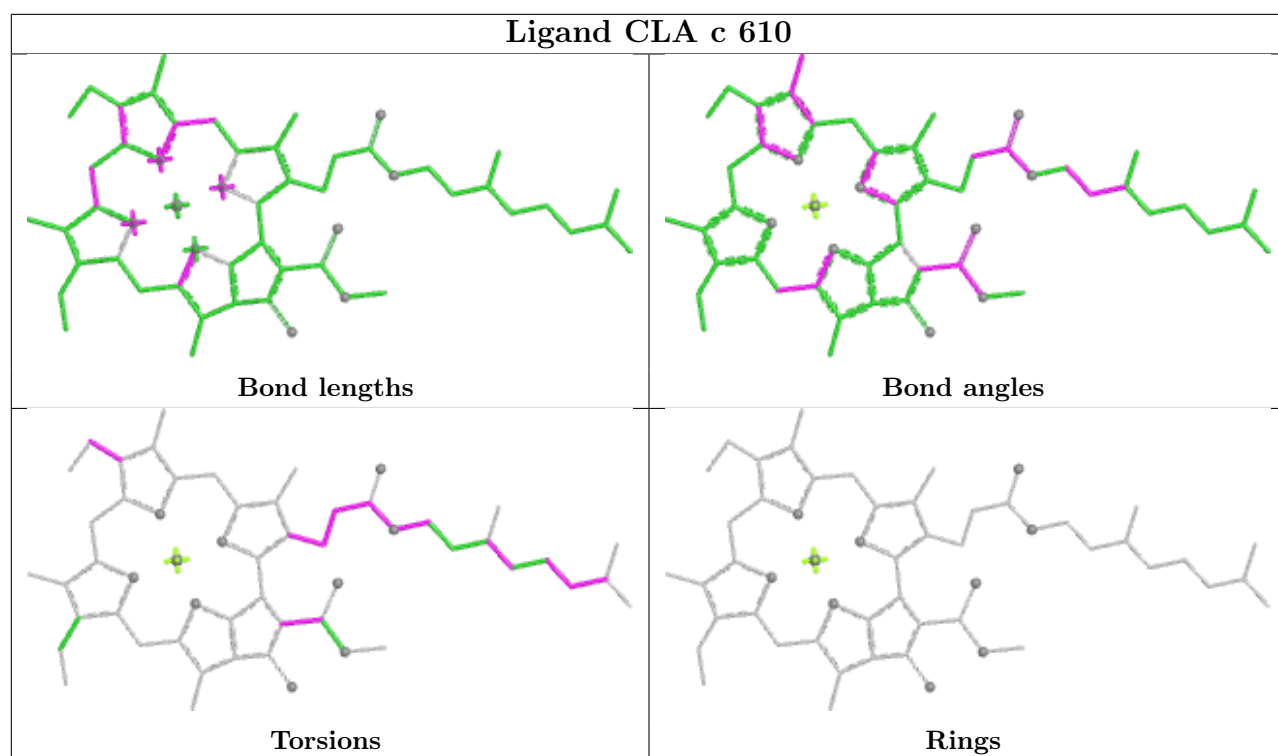
Bond angles



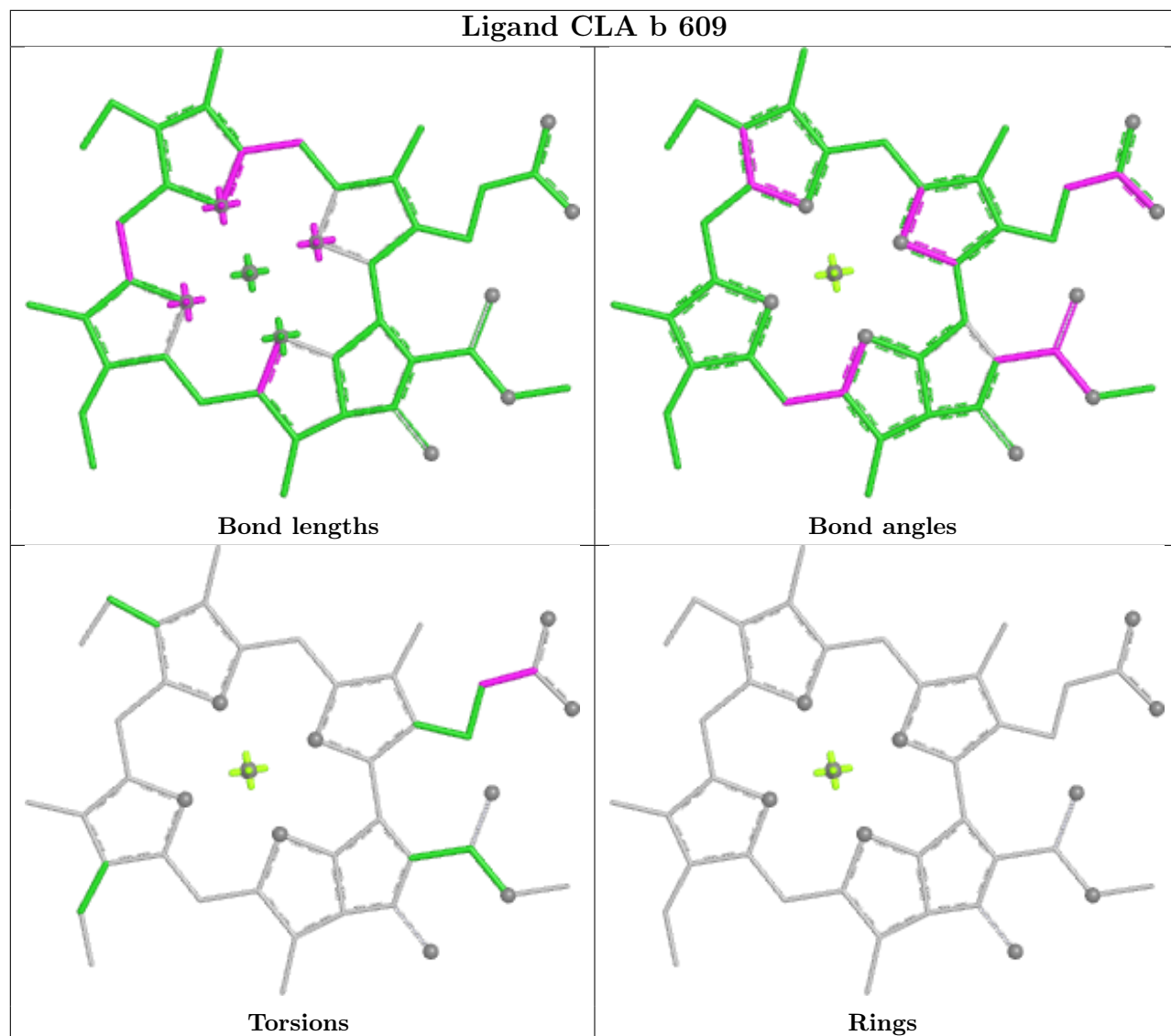
Torsions

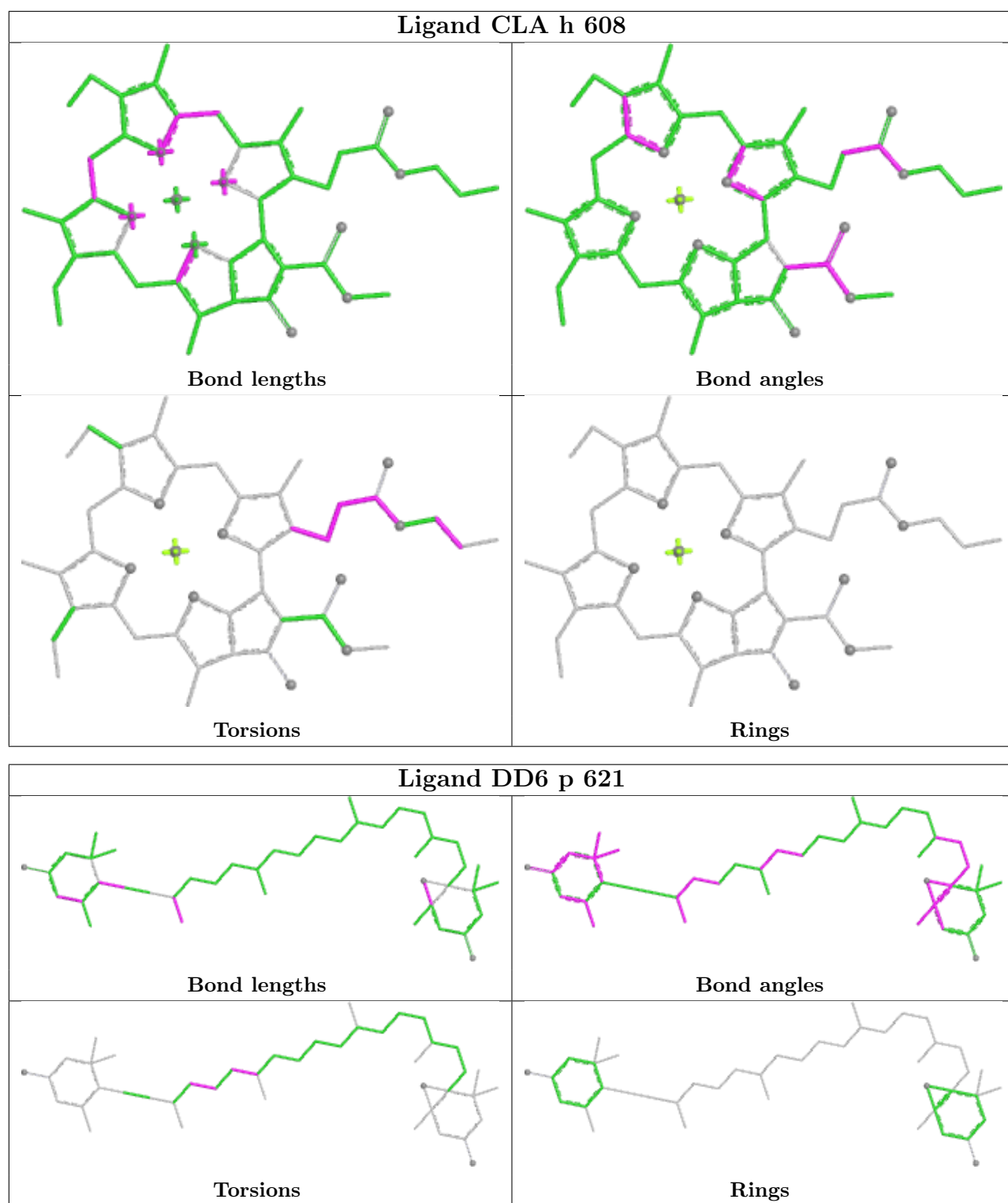


Rings

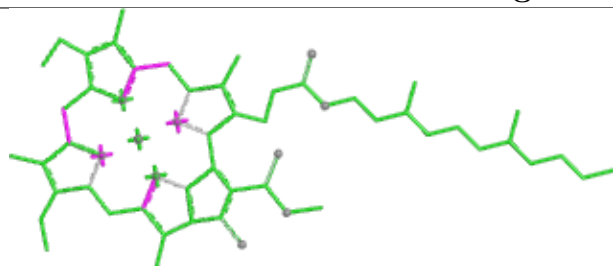


Ligand CLA b 609

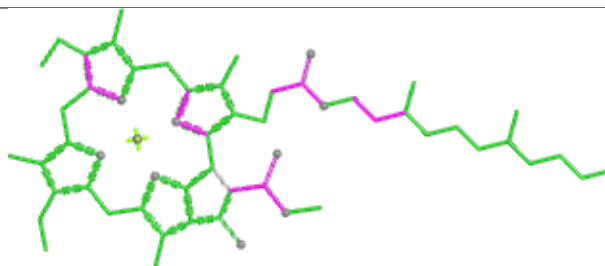




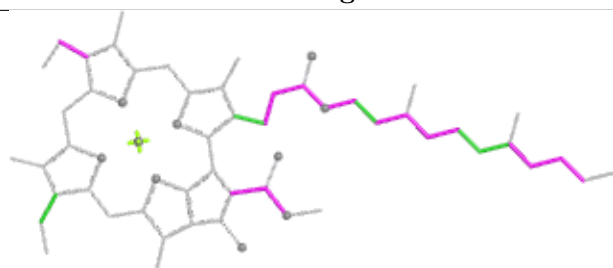
Ligand CLA A 766



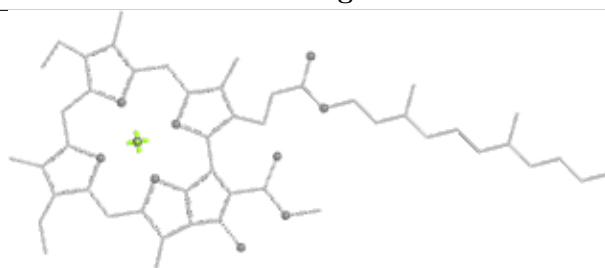
Bond lengths



Bond angles

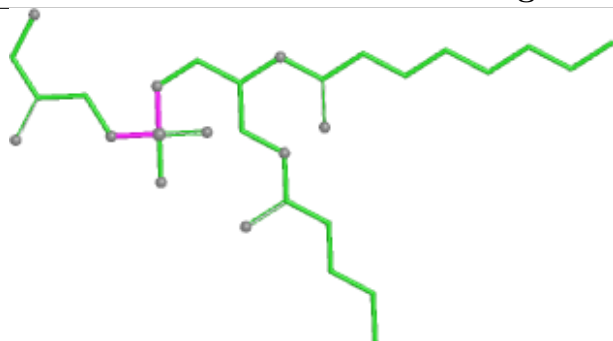


Torsions

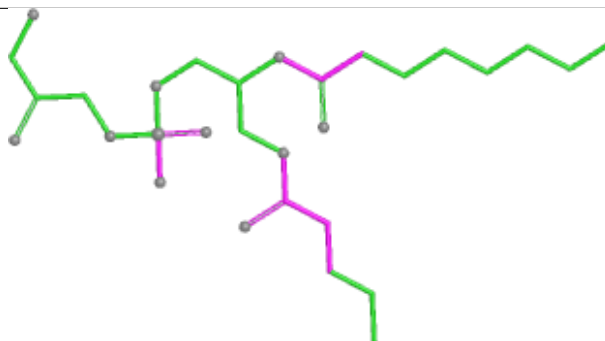


Rings

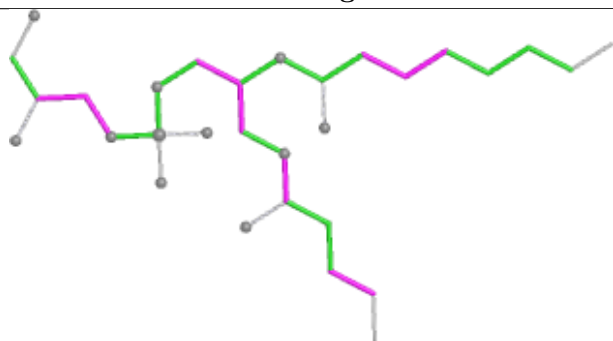
Ligand LHG c 243



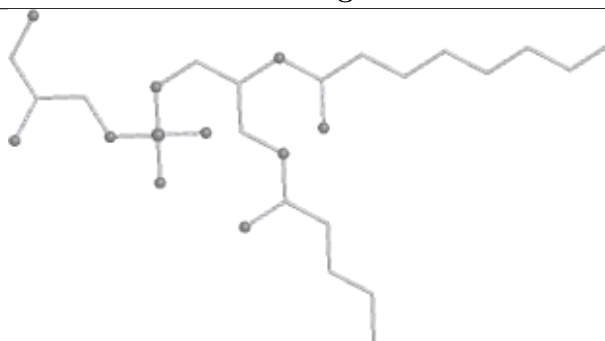
Bond lengths



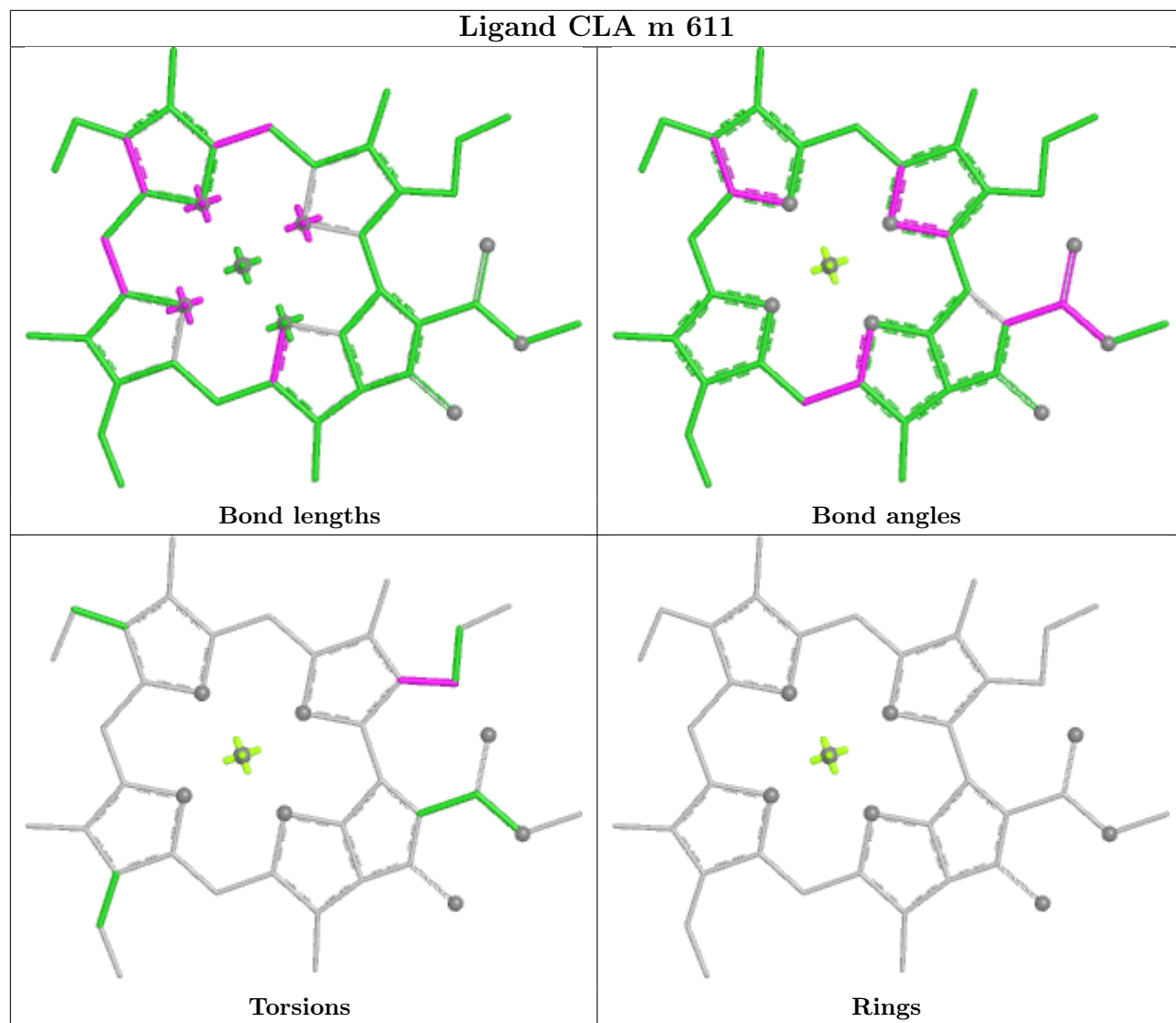
Bond angles



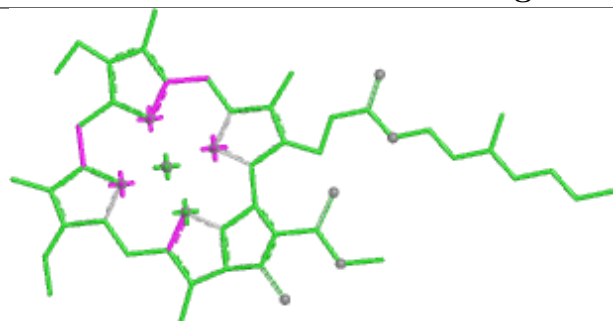
Torsions



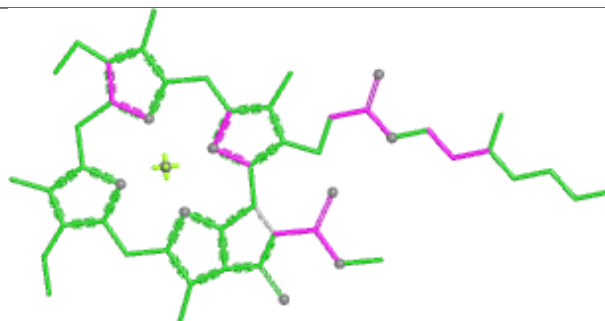
Rings



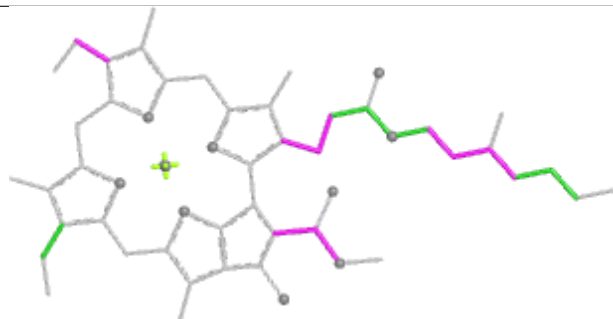
Ligand CLA B 771



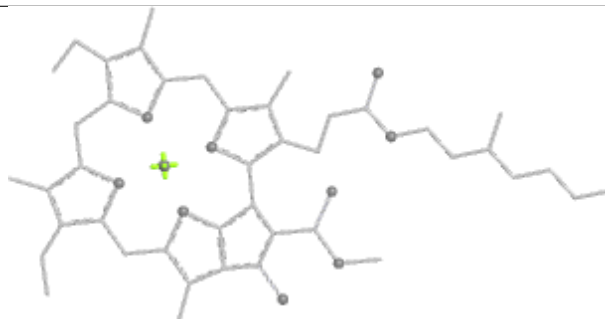
Bond lengths



Bond angles

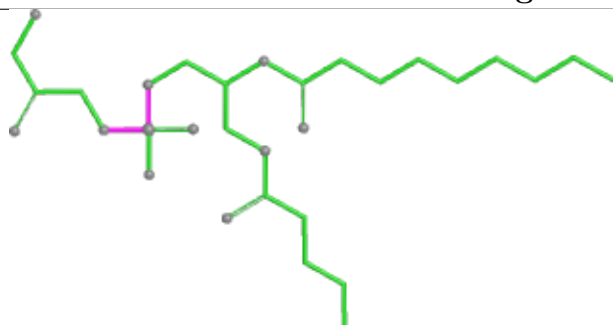


Torsions

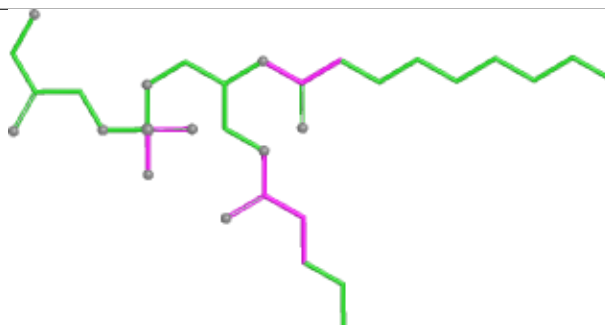


Rings

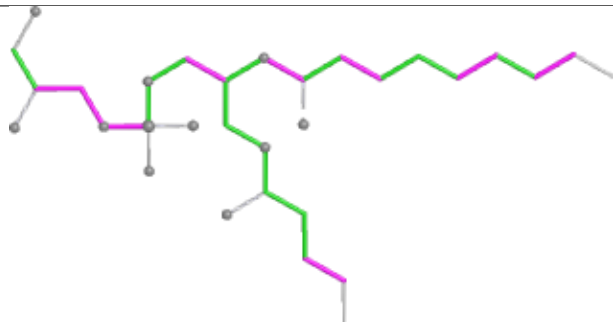
Ligand LHG h 190



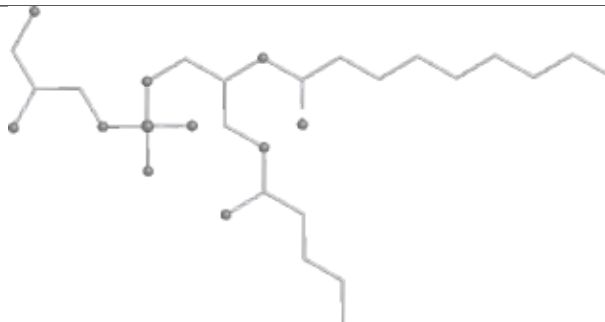
Bond lengths



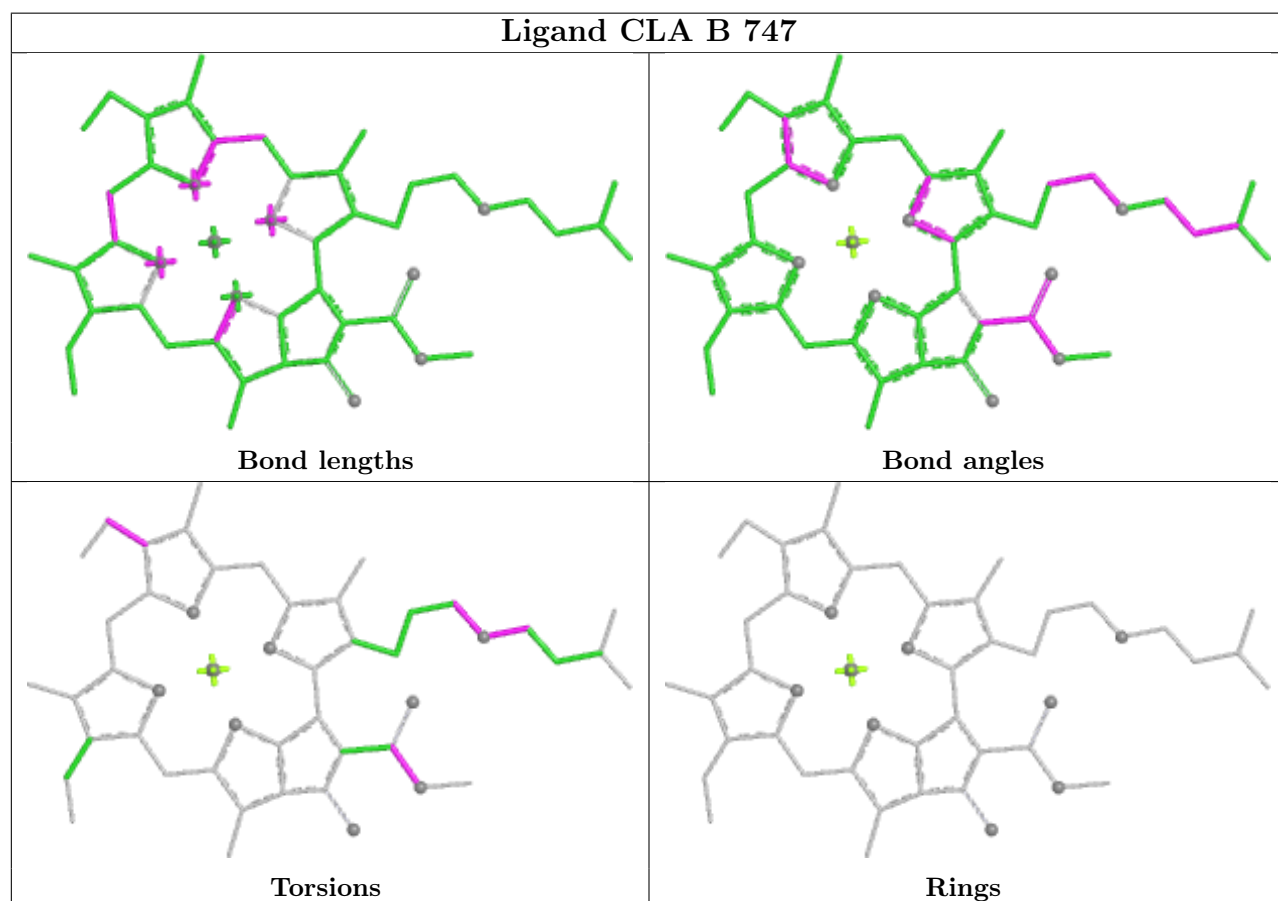
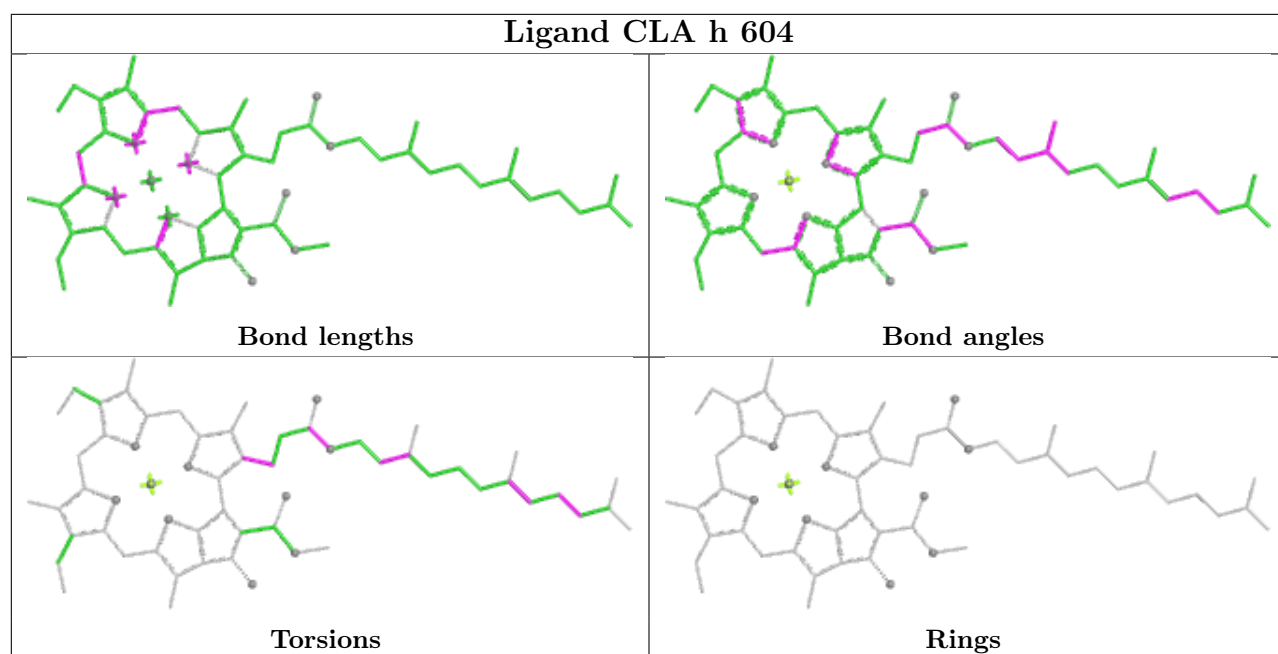
Bond angles

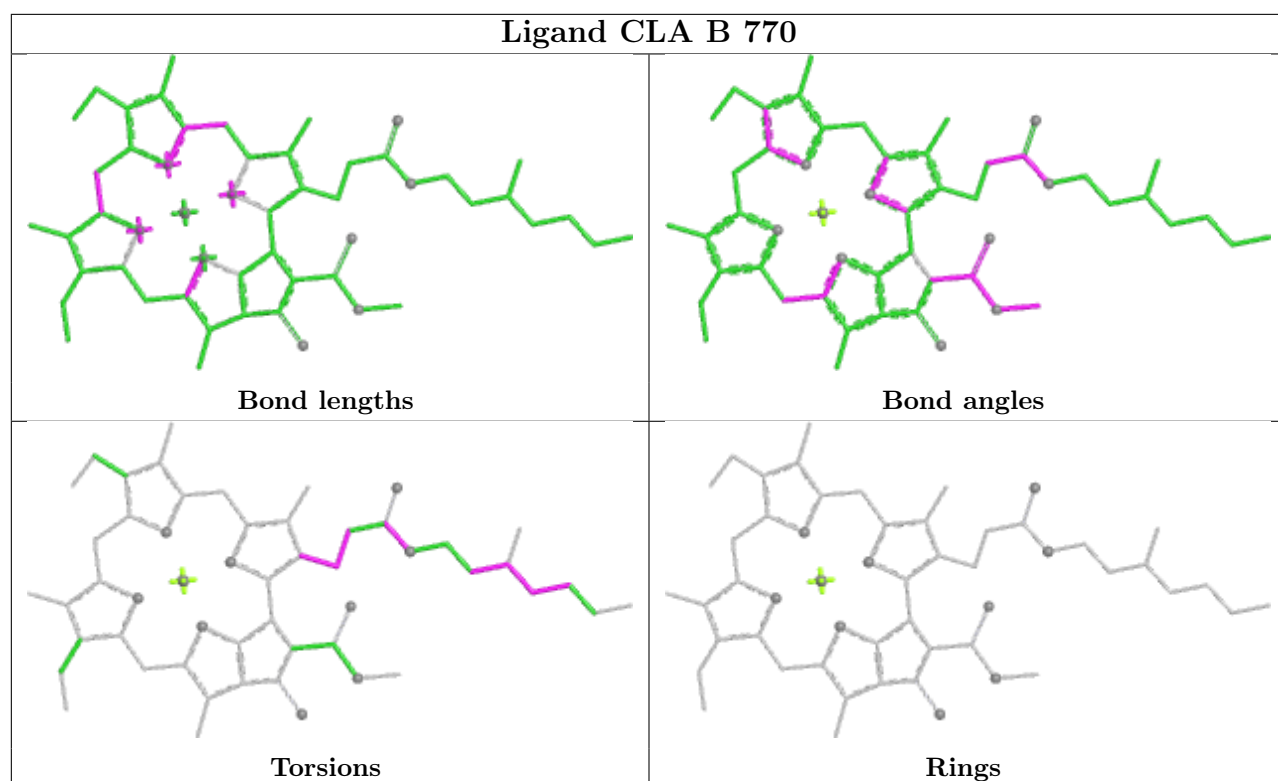


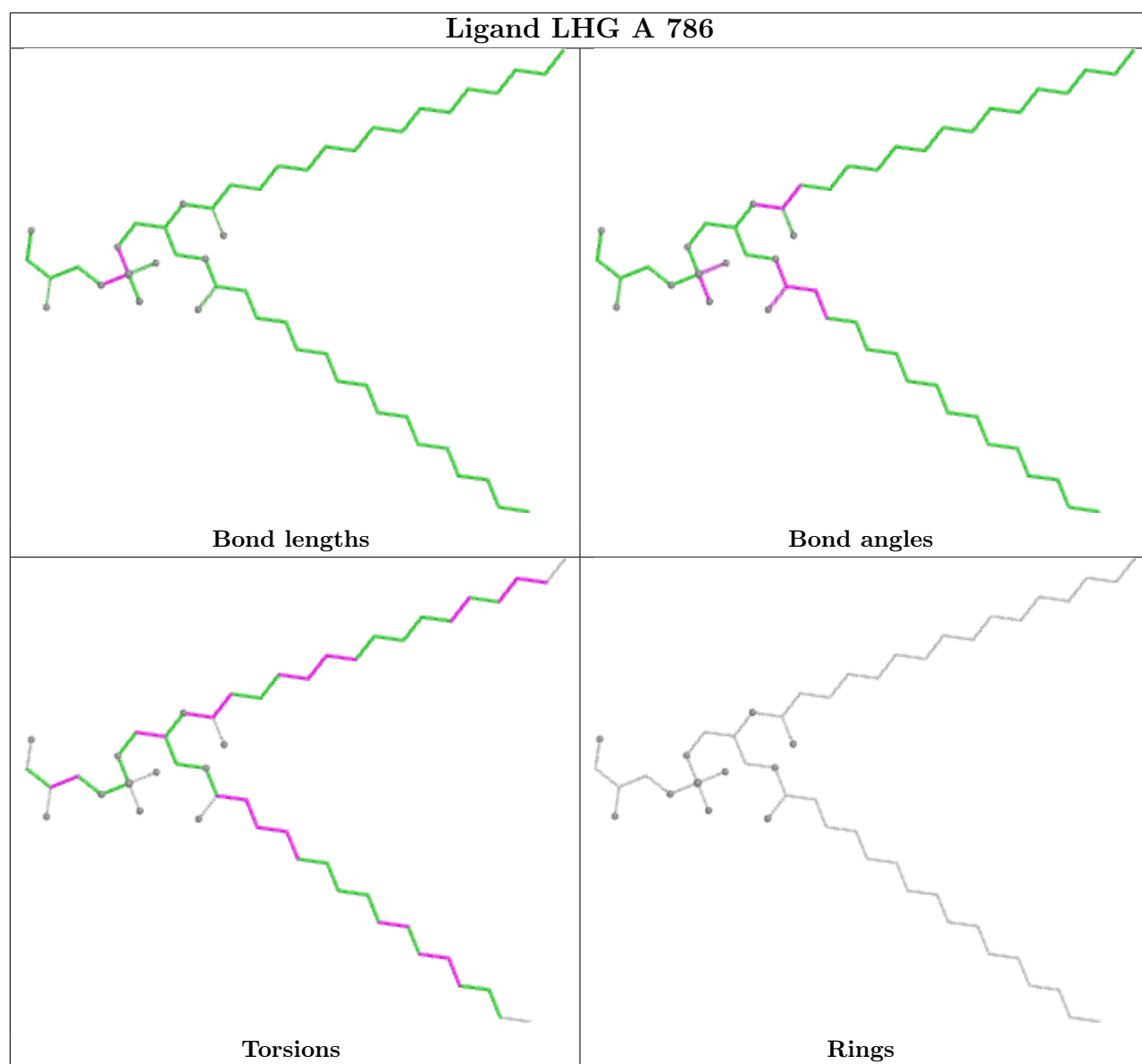
Torsions



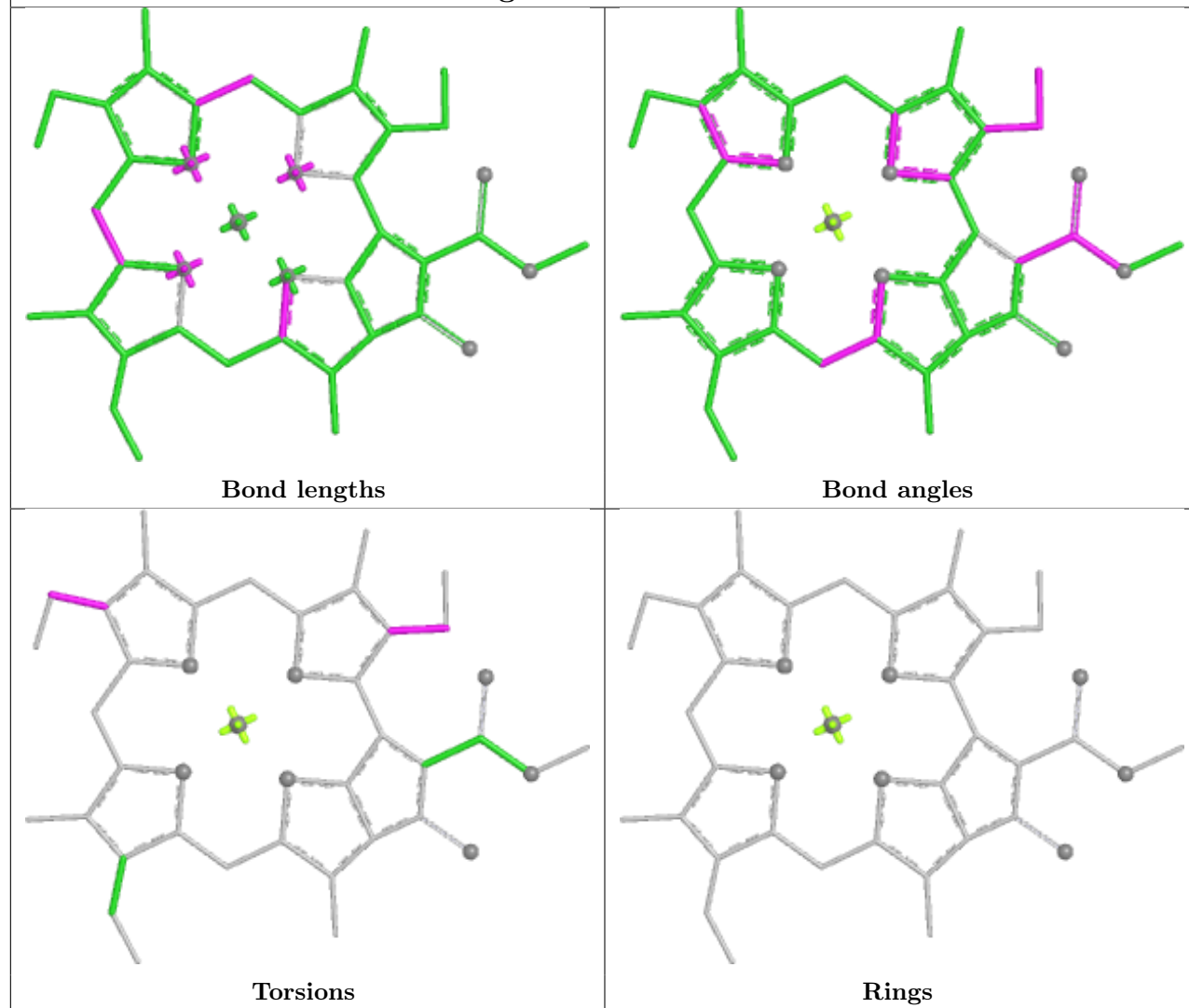
Rings



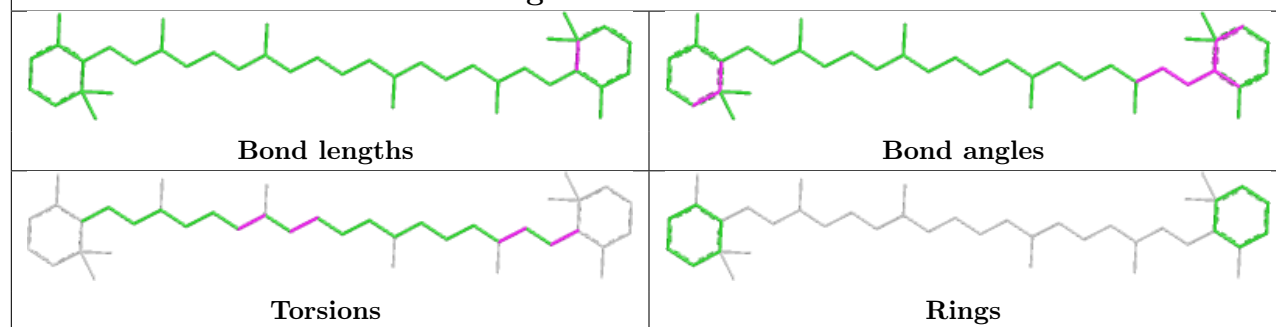


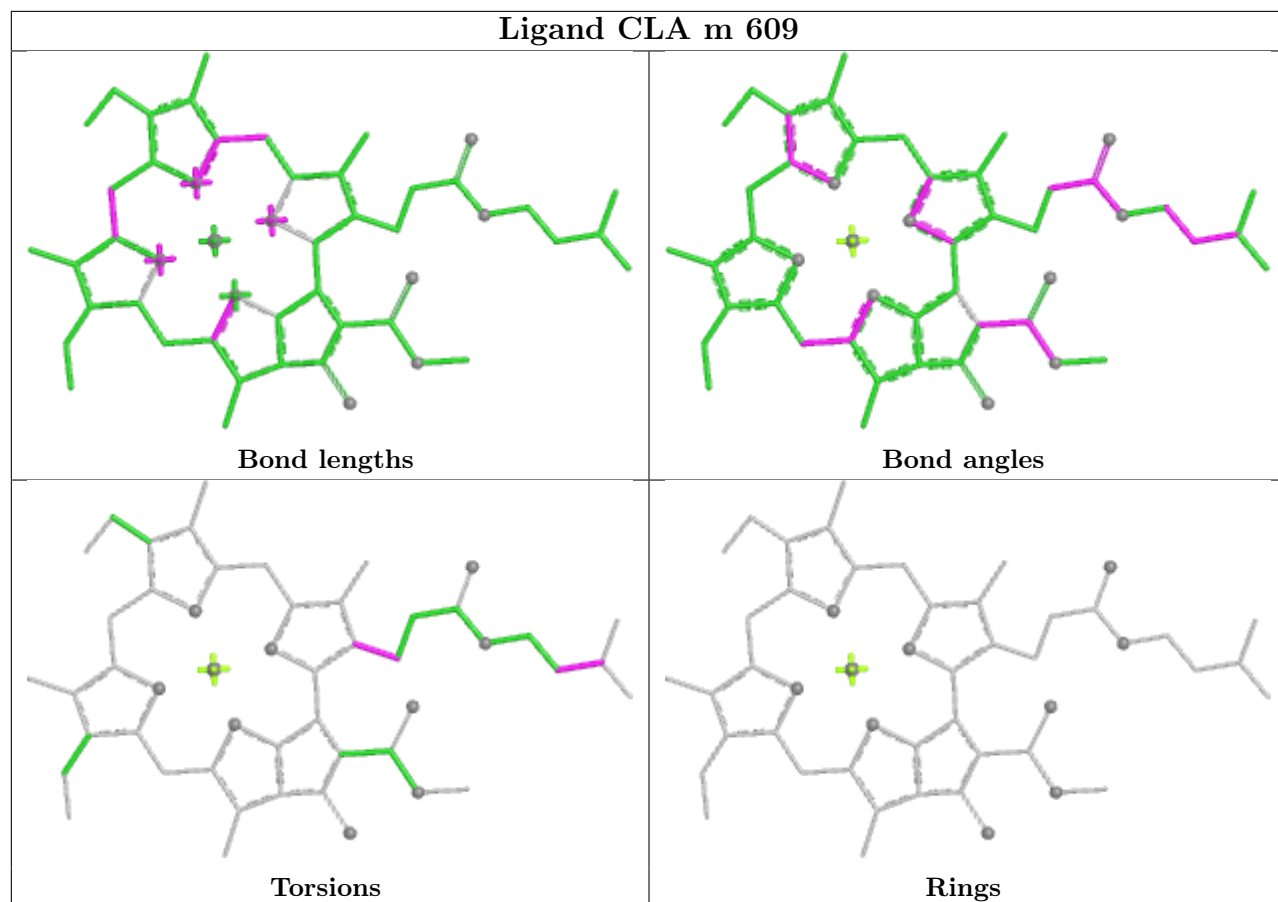


Ligand CLA b 610

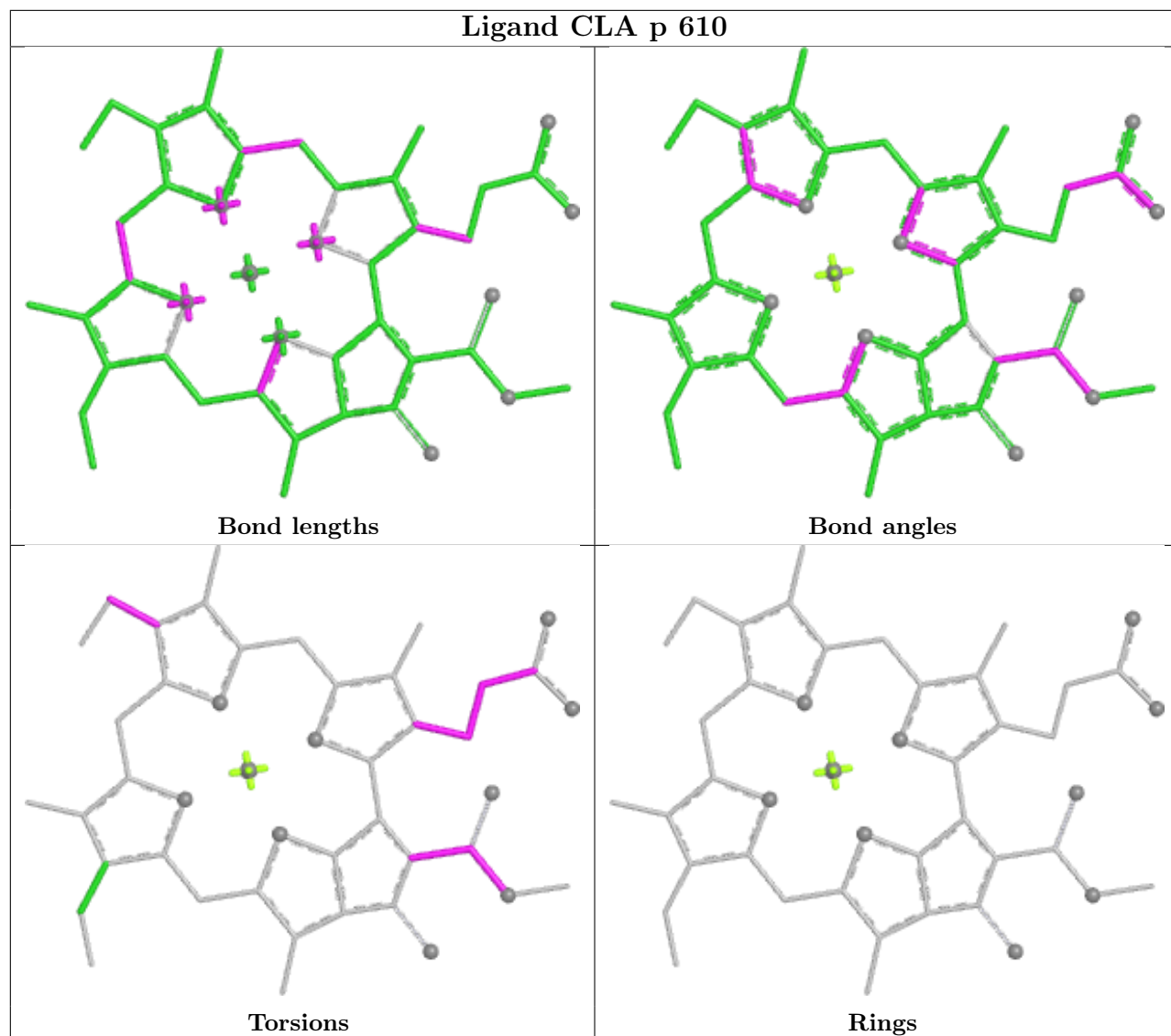


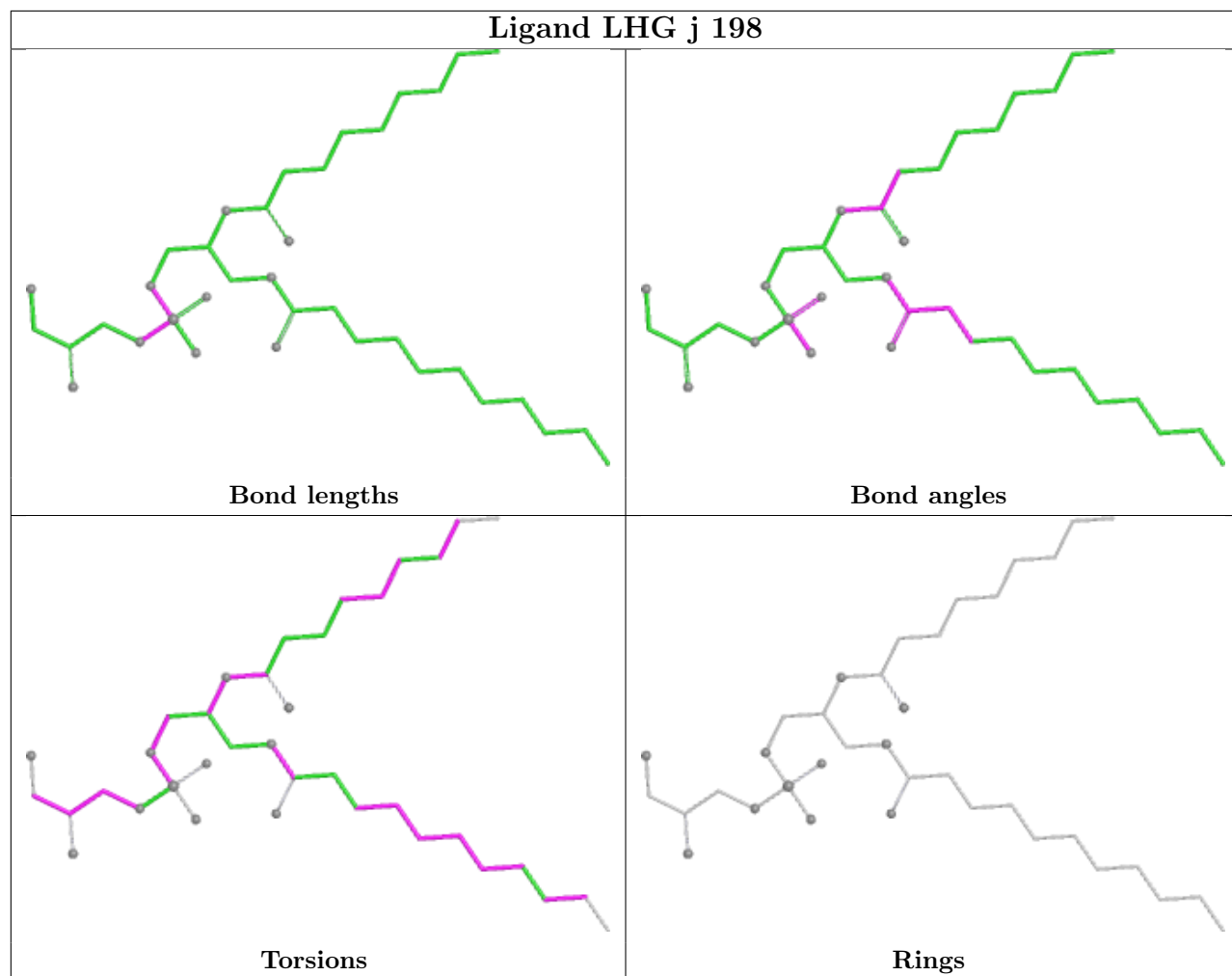
Ligand BCR M 201



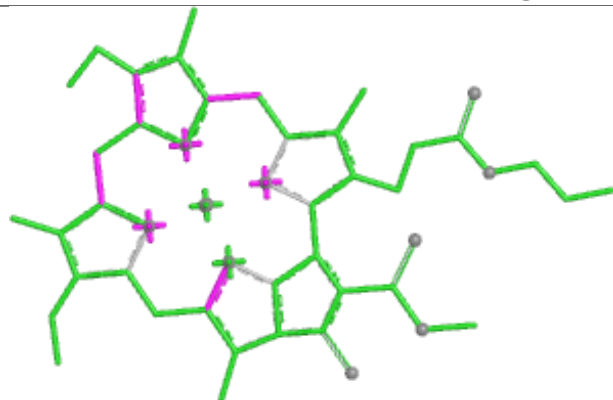


Ligand CLA p 610

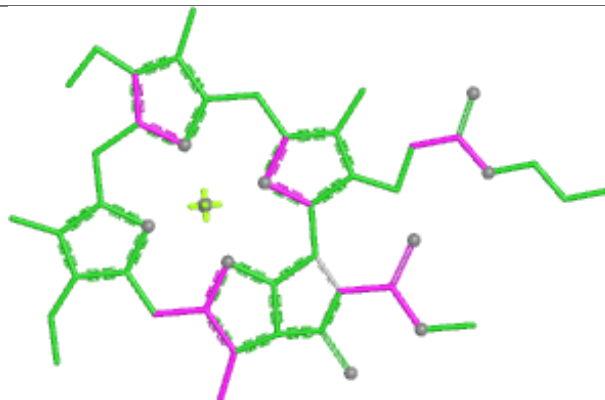




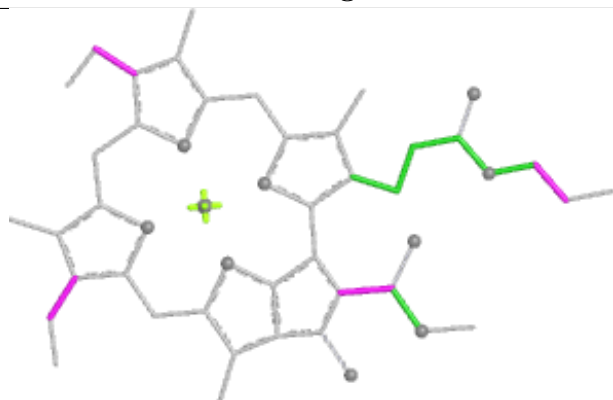
Ligand CLA n 604



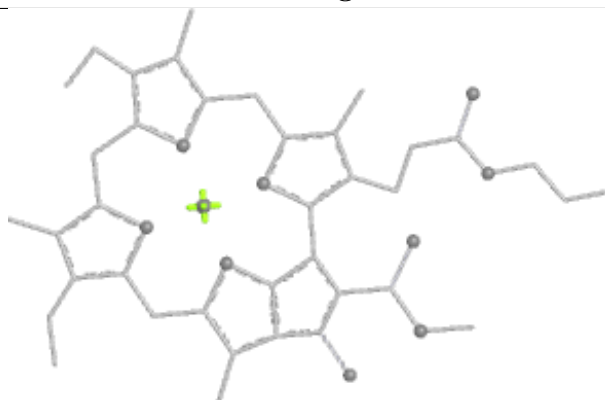
Bond lengths



Bond angles

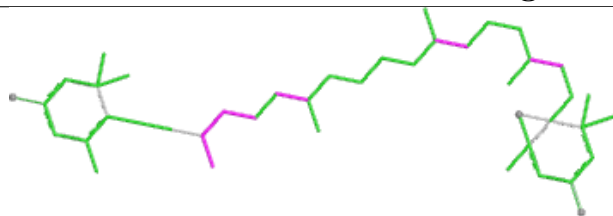


Torsions

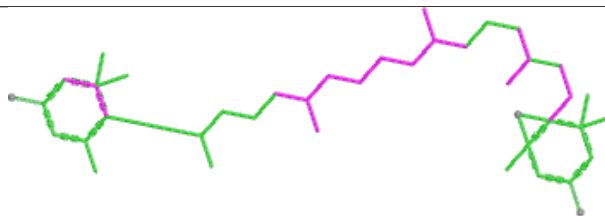


Rings

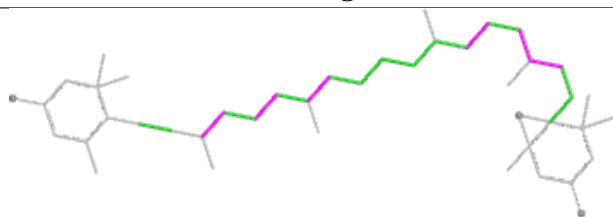
Ligand DD6 e 620



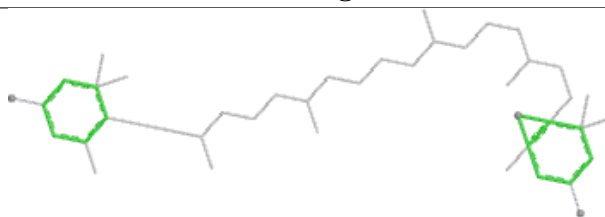
Bond lengths



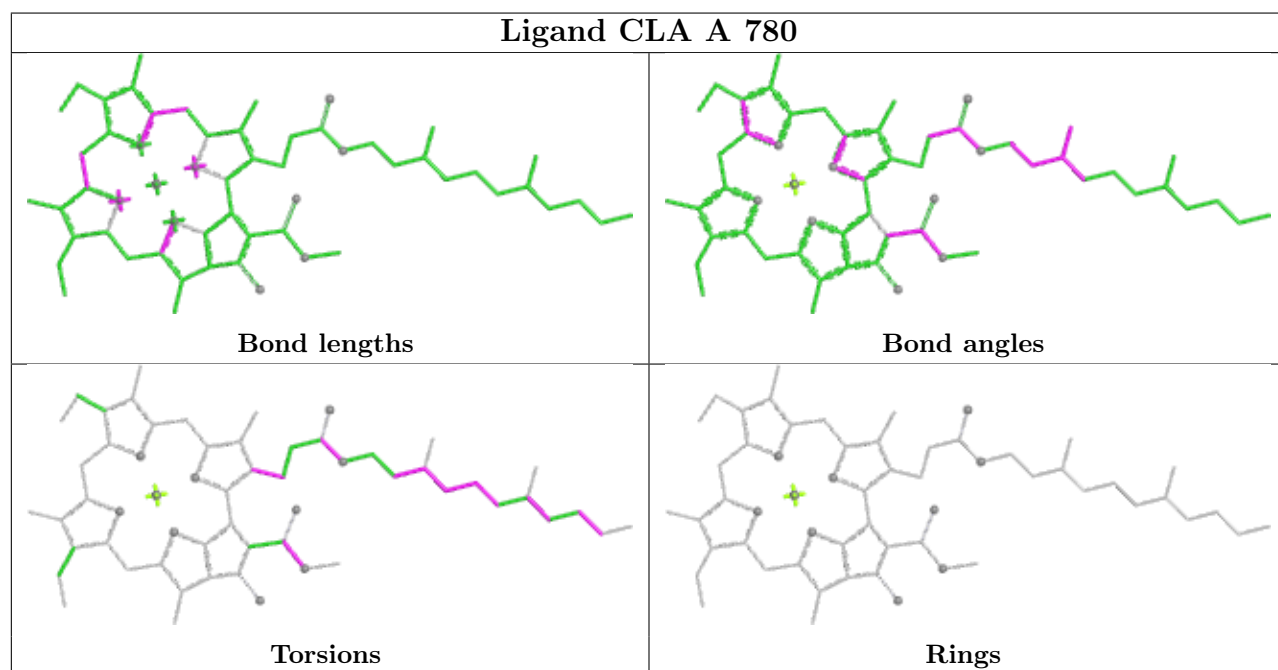
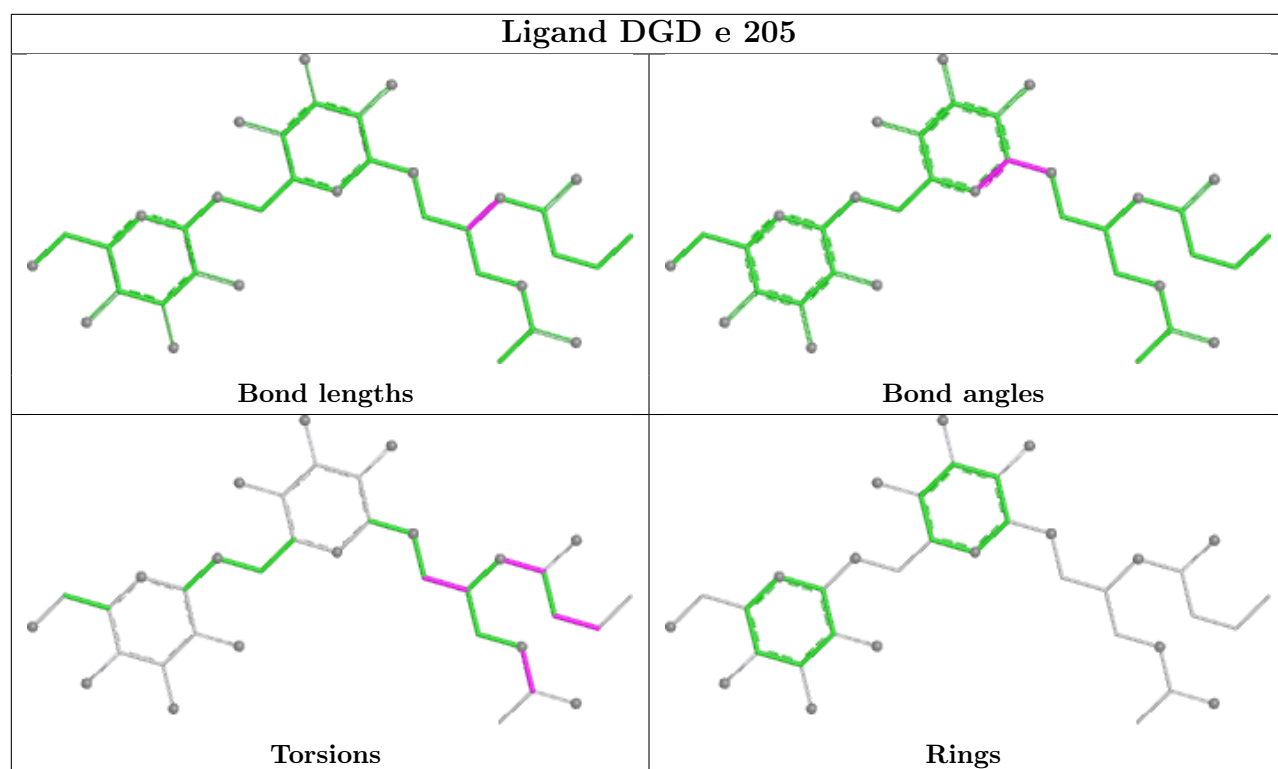
Bond angles



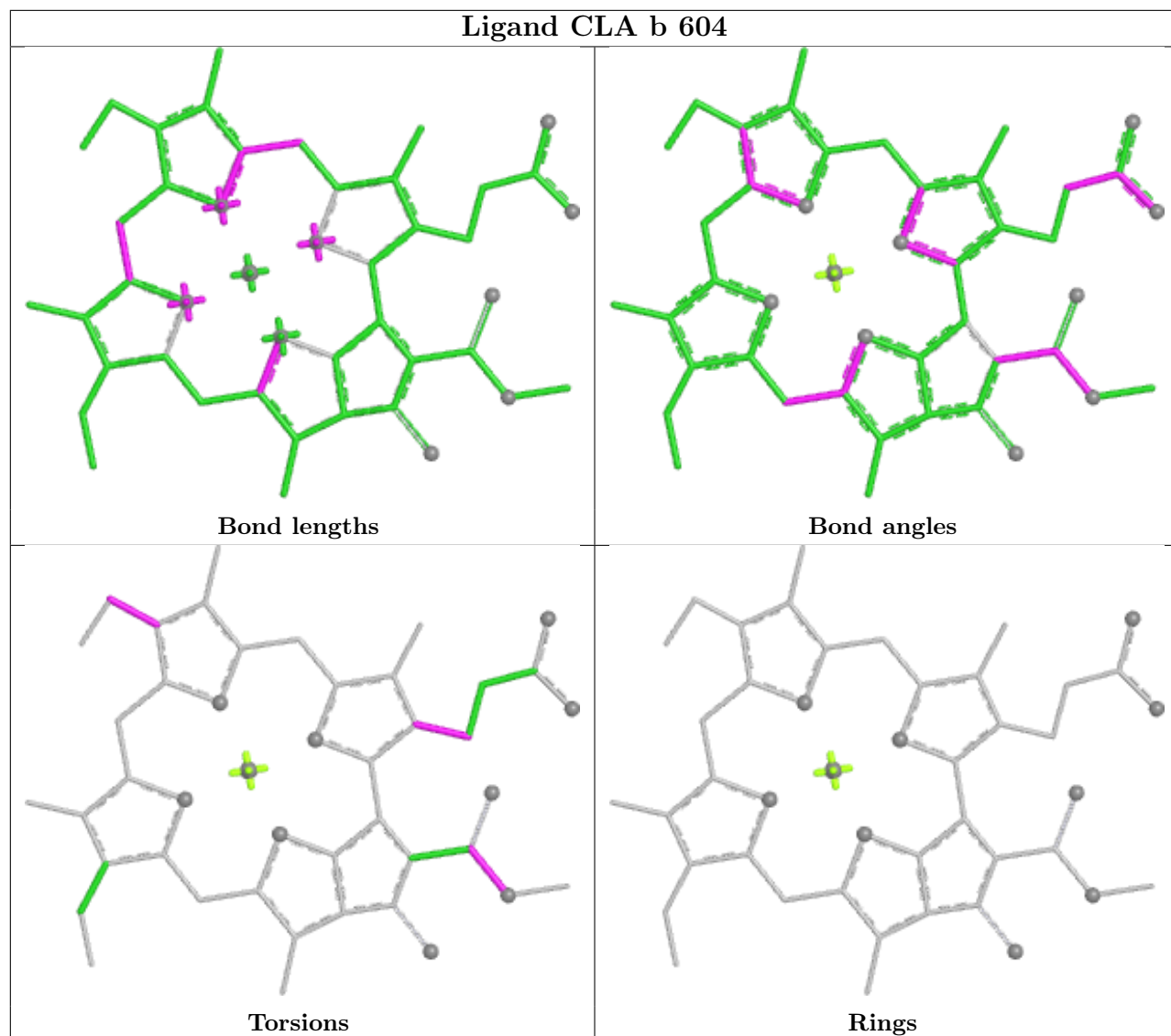
Torsions



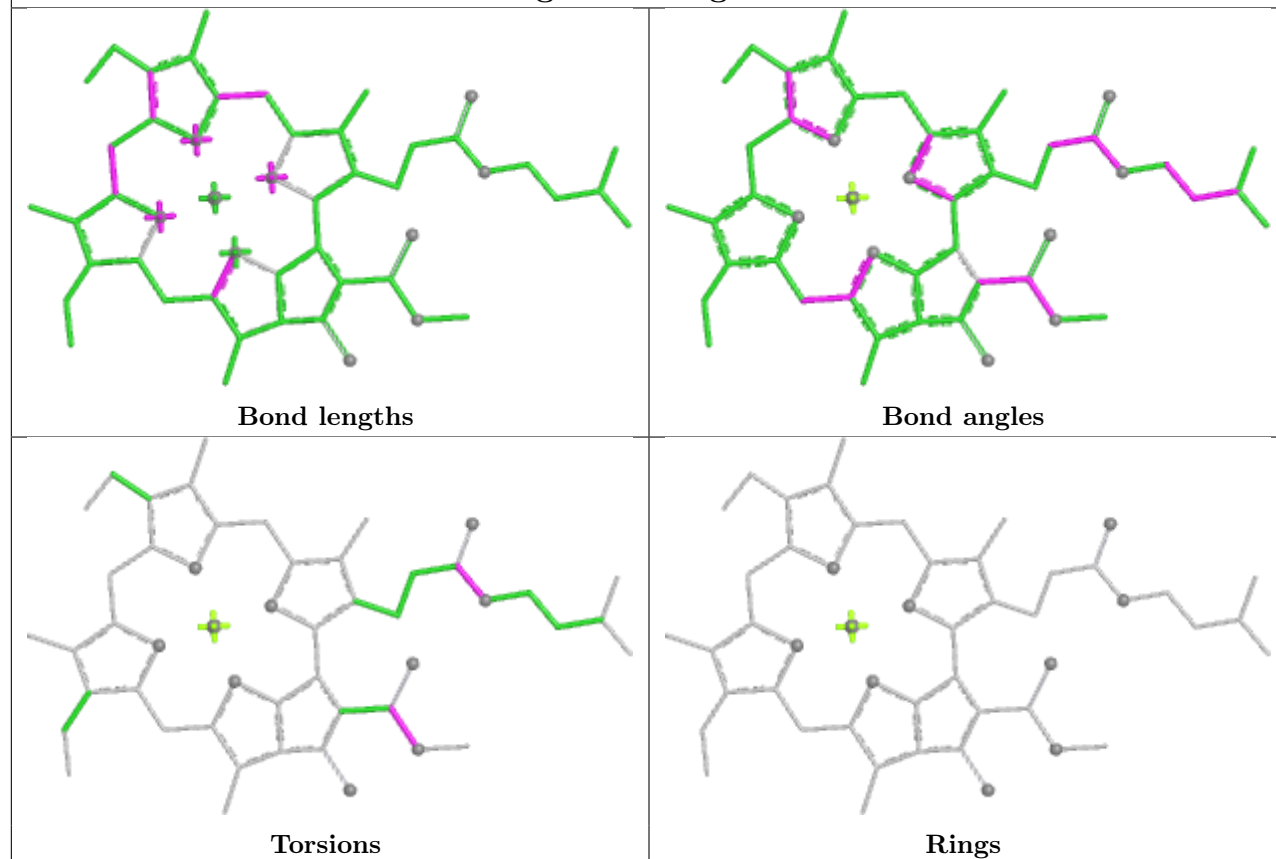
Rings



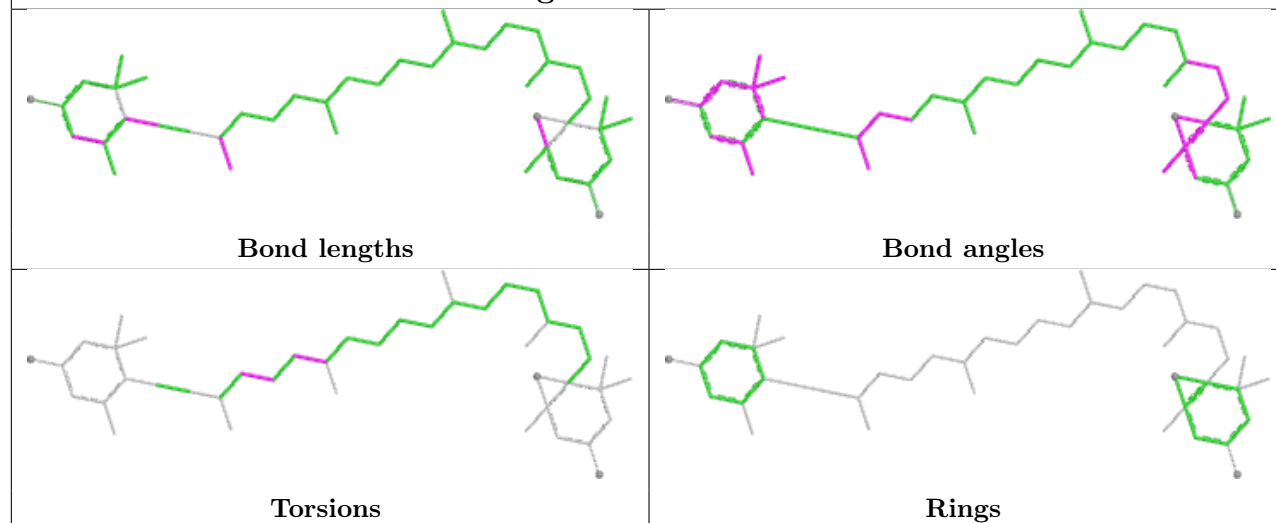
Ligand CLA b 604

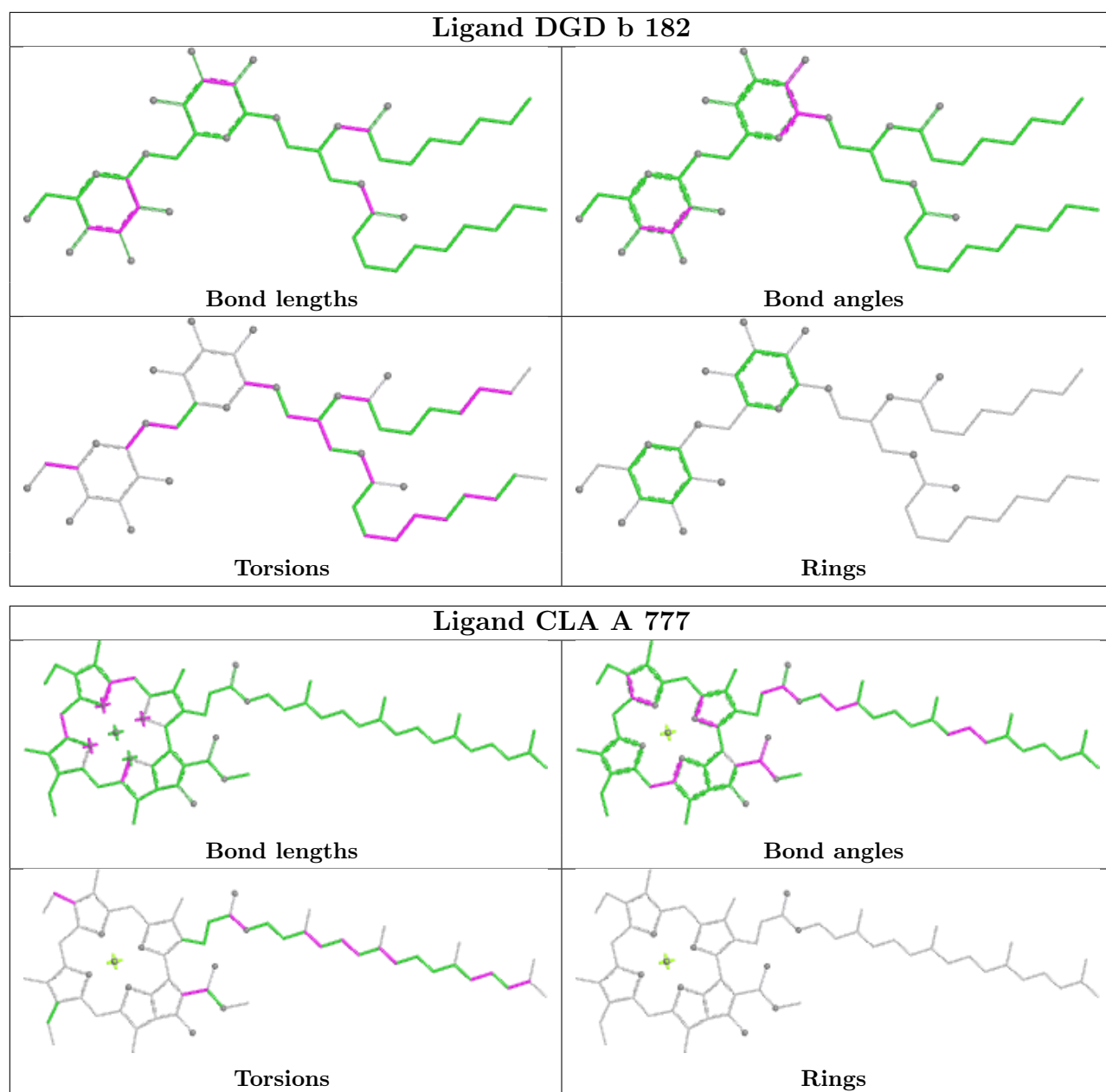


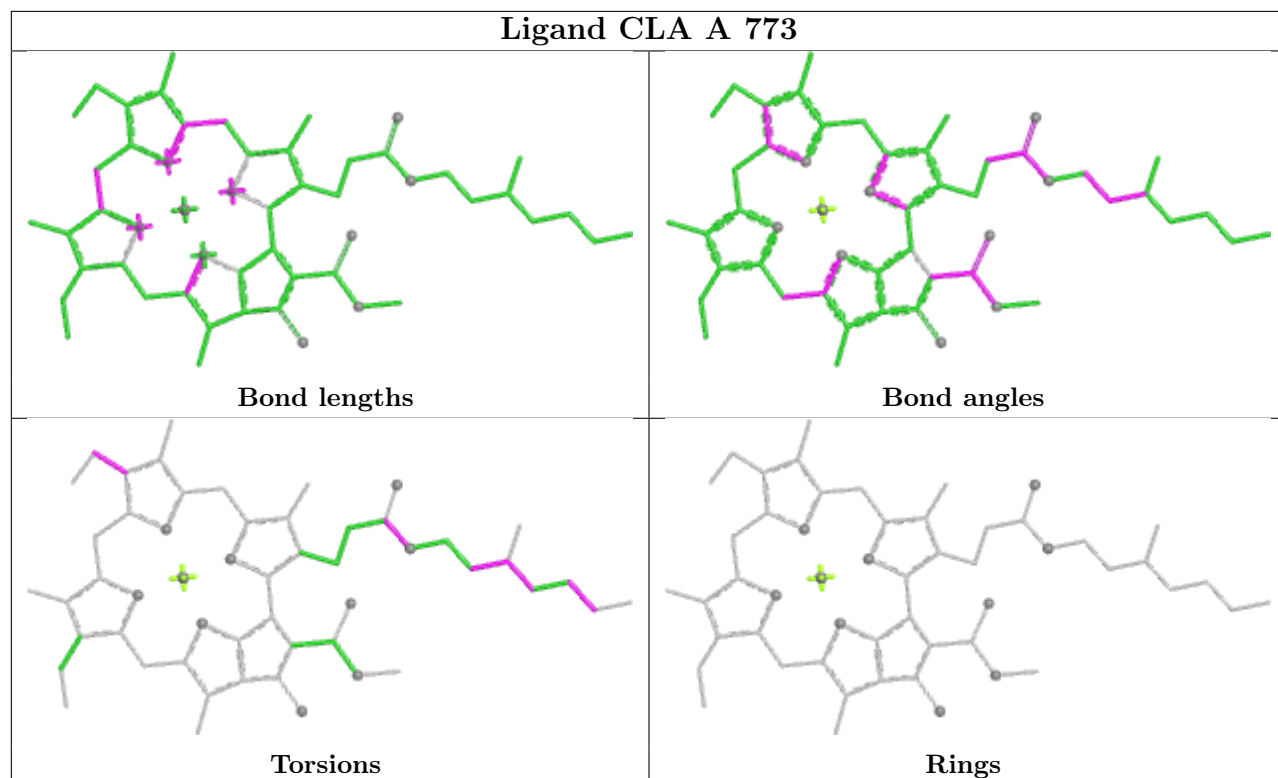
Ligand CLA g 609



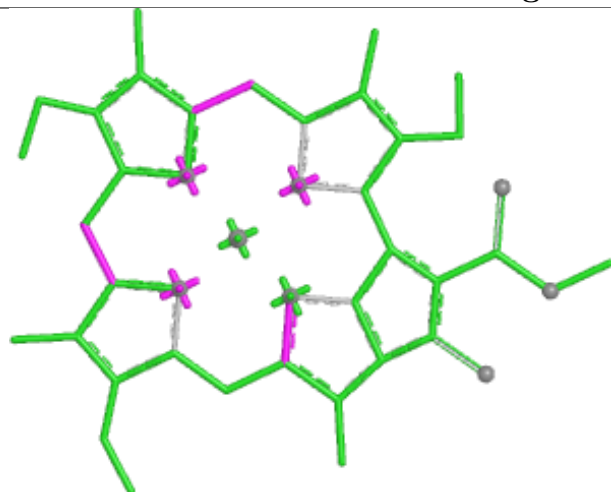
Ligand DD6 o 621



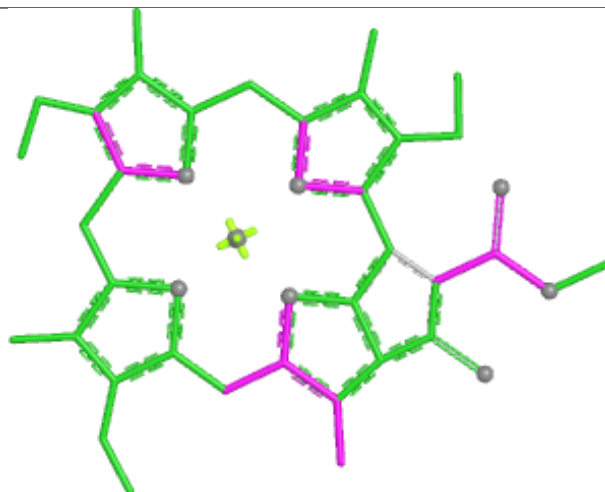




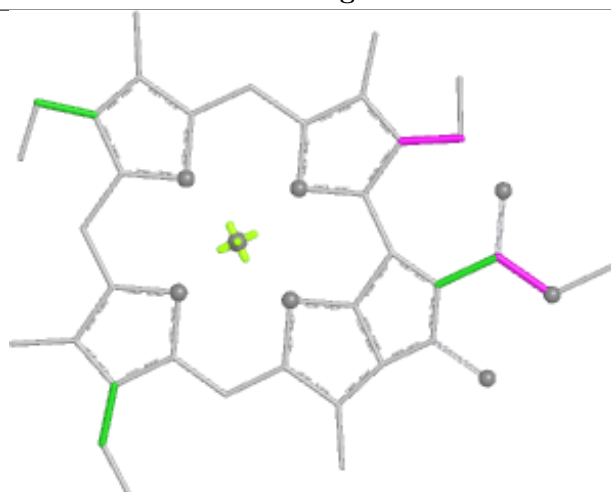
Ligand CLA 1 614



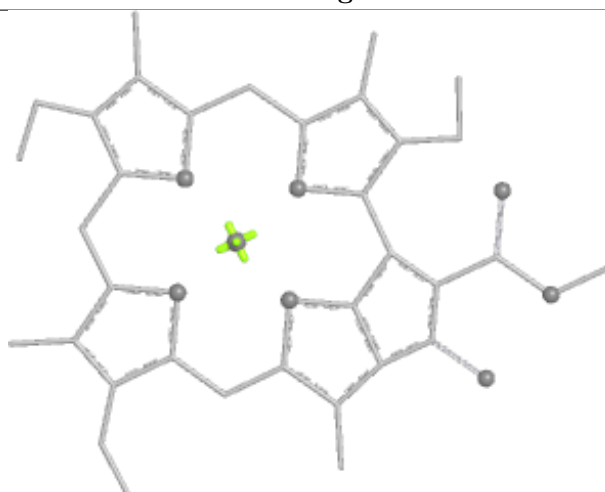
Bond lengths



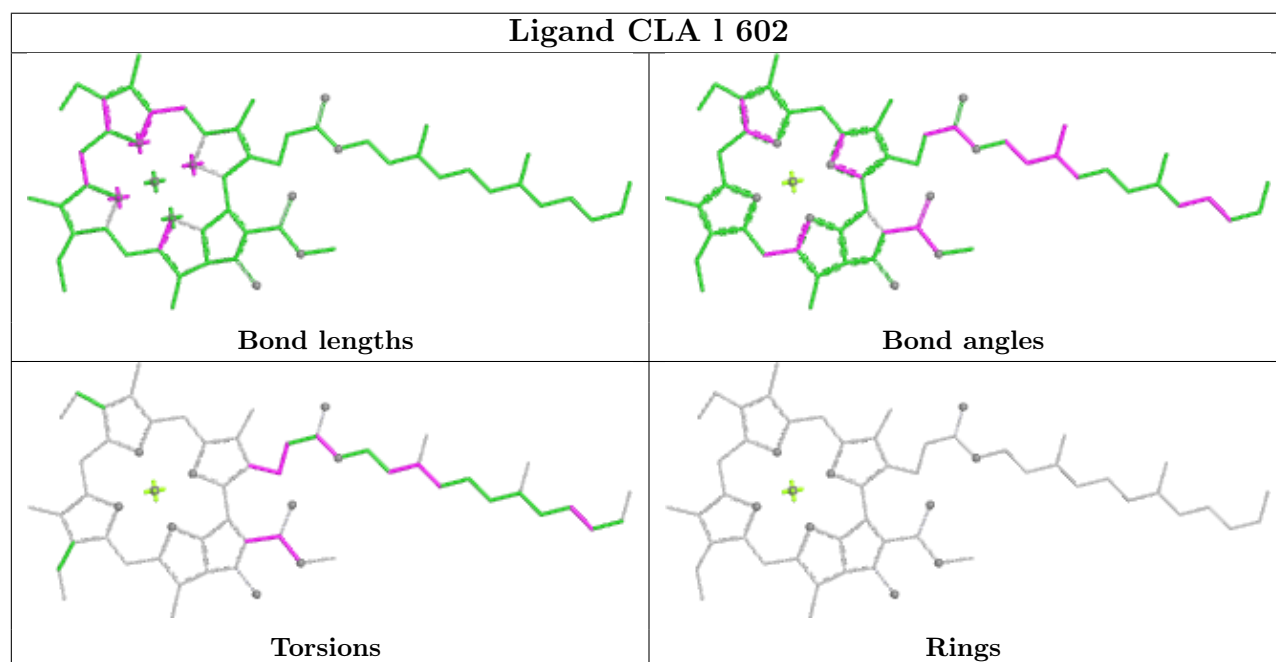
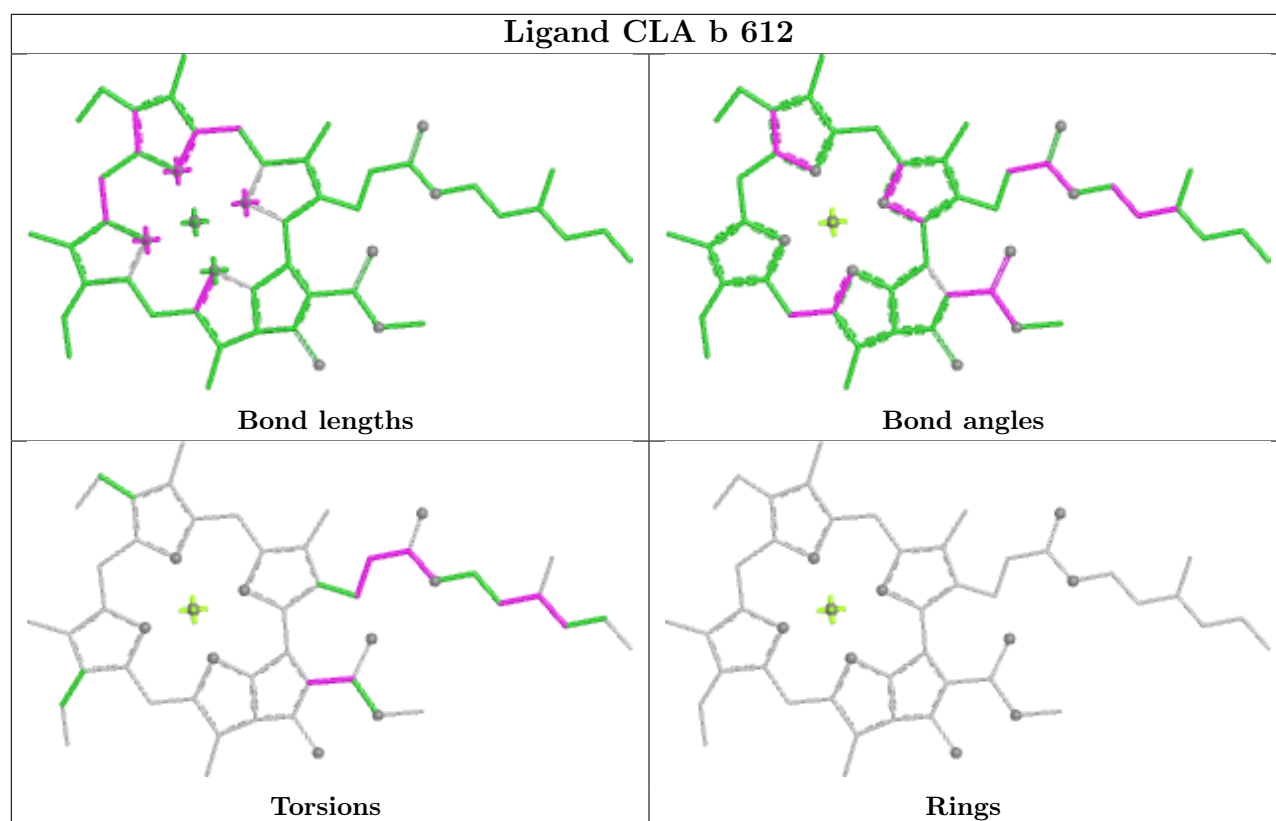
Bond angles

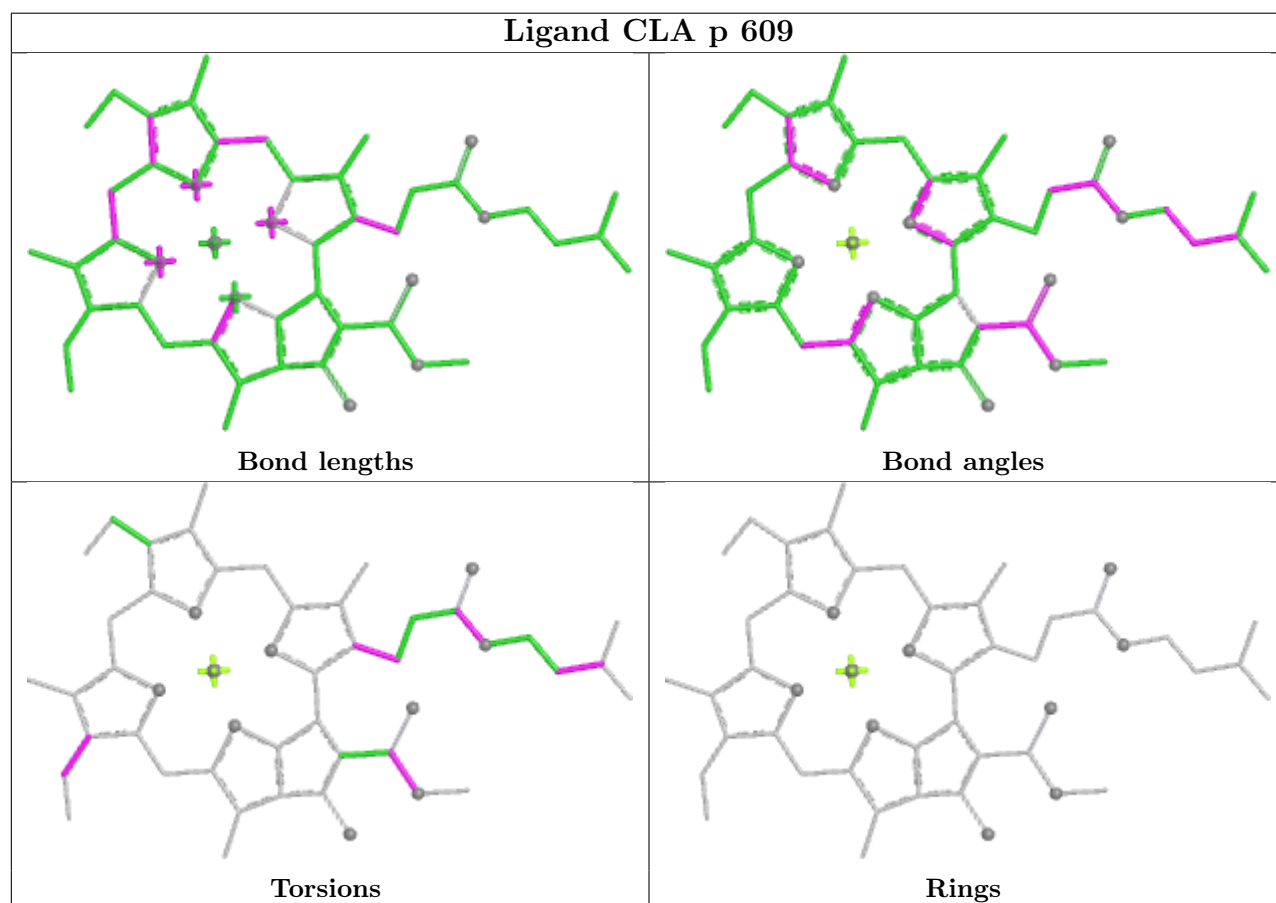
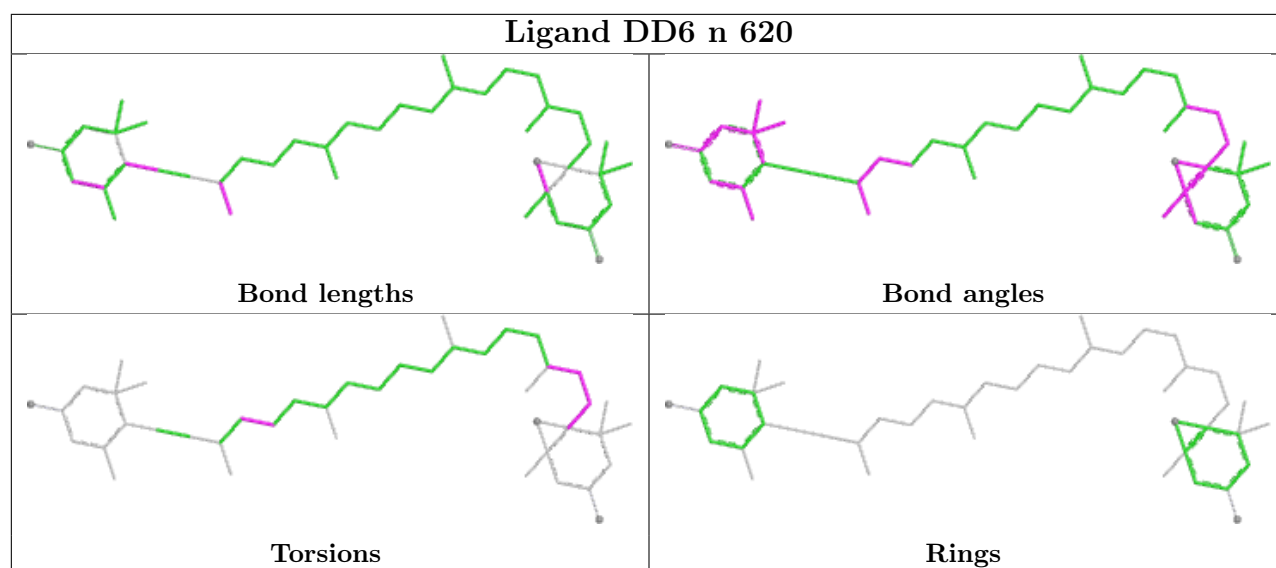


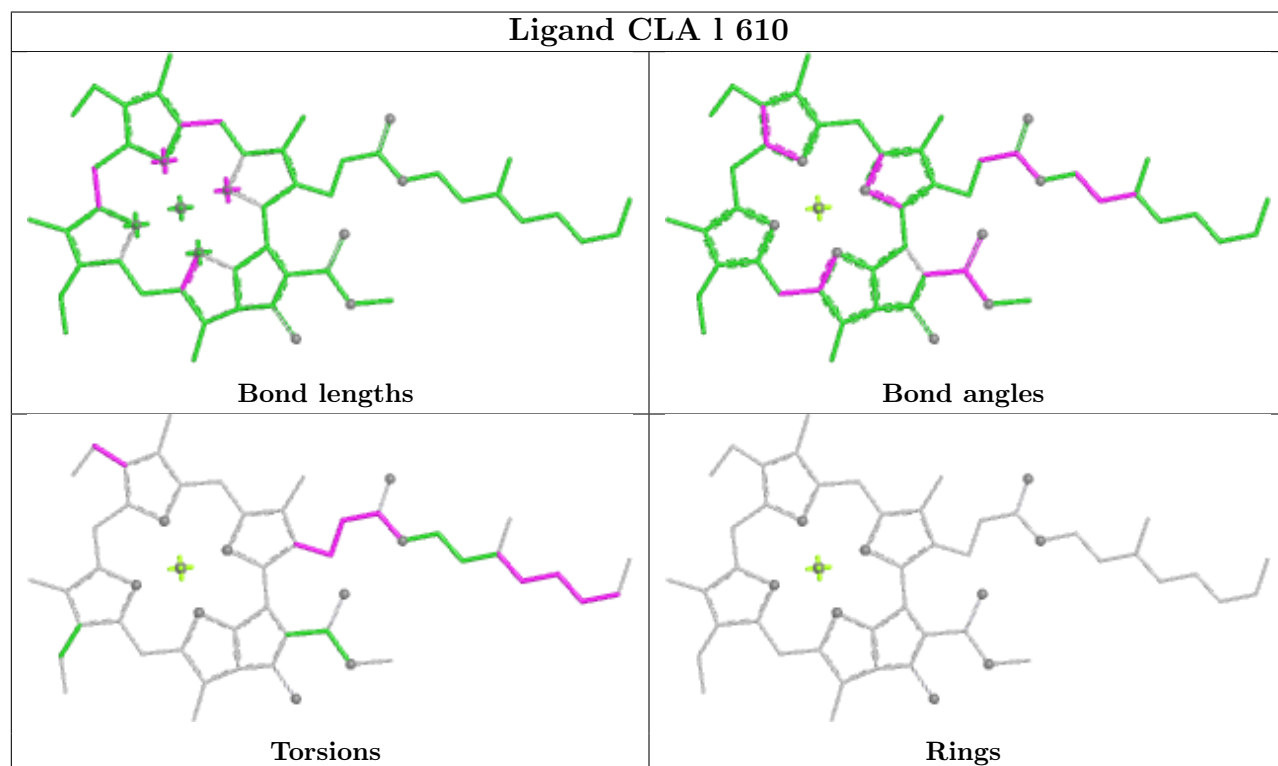
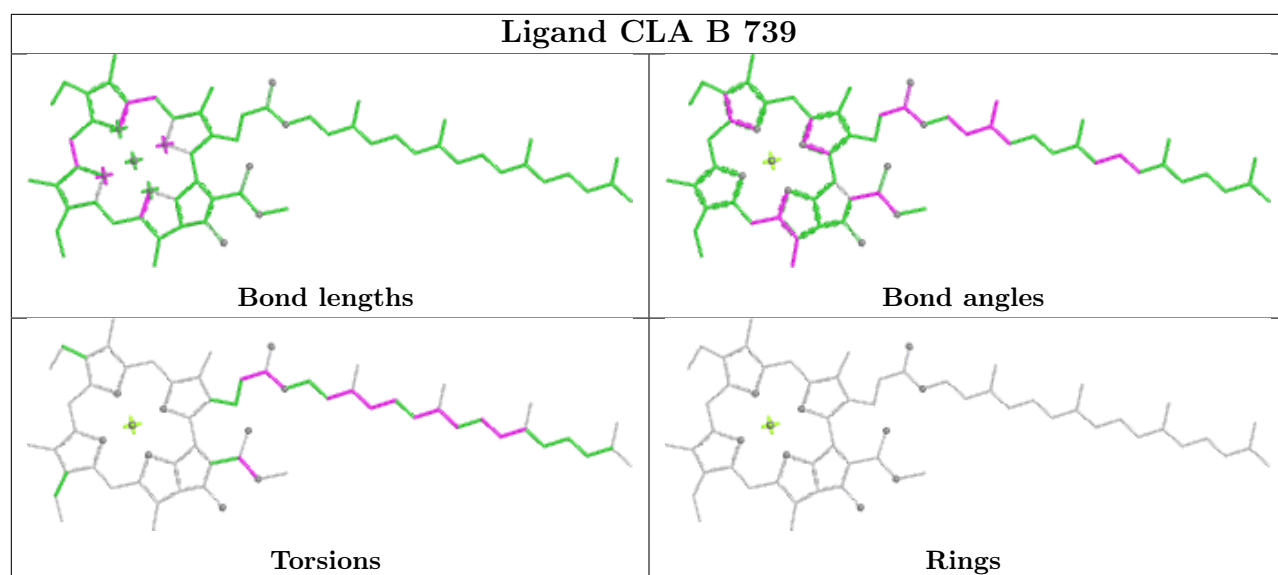
Torsions

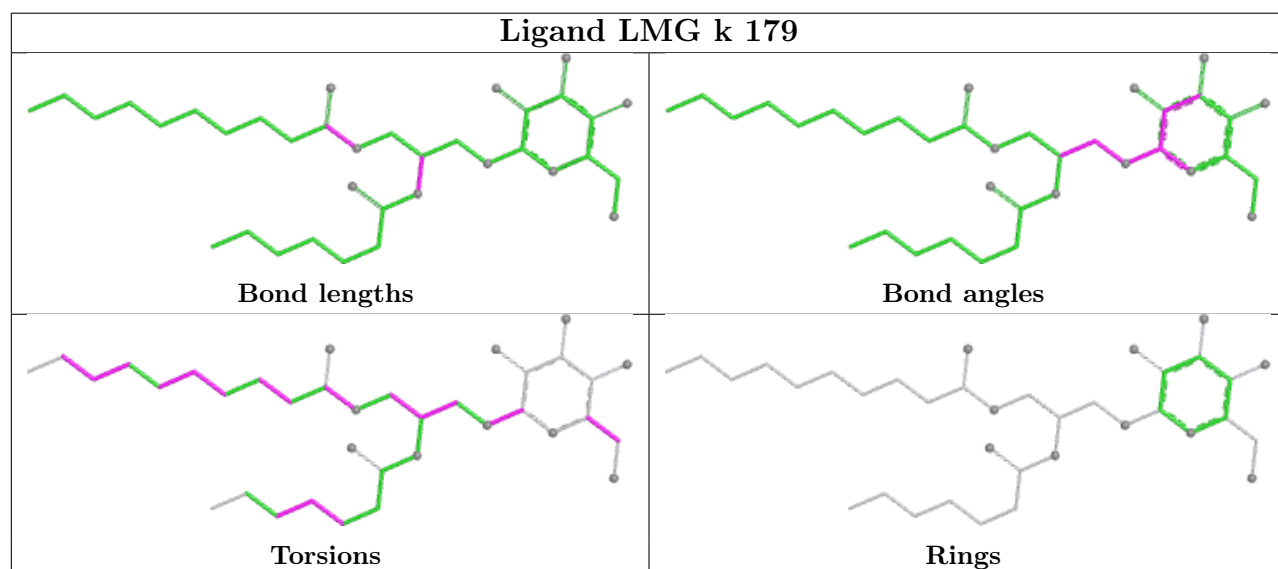
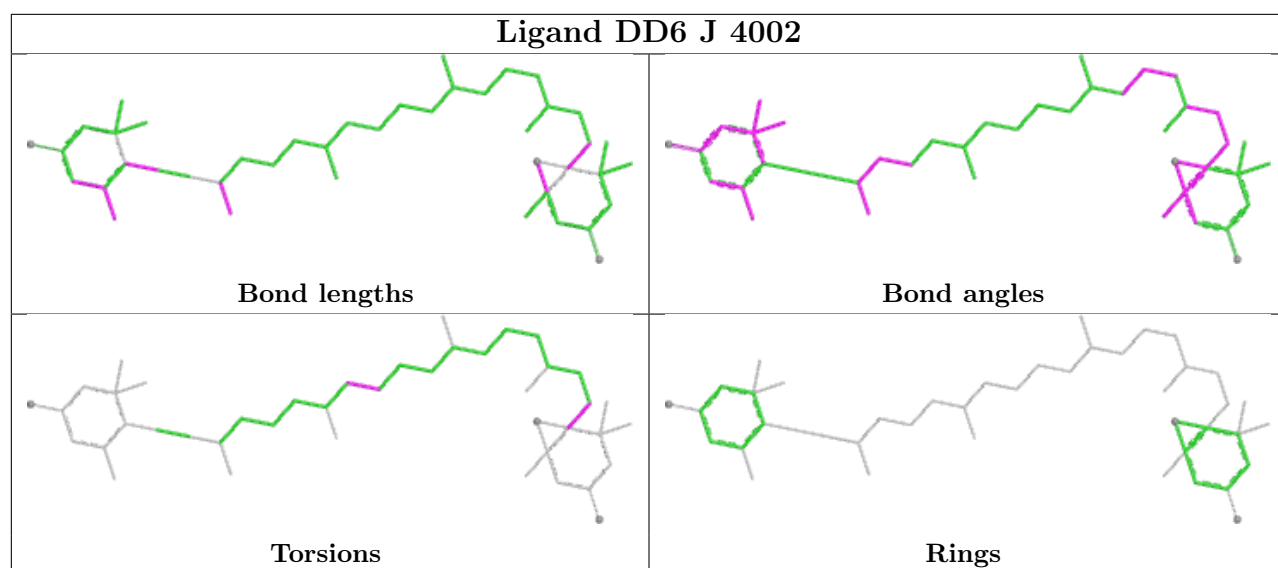


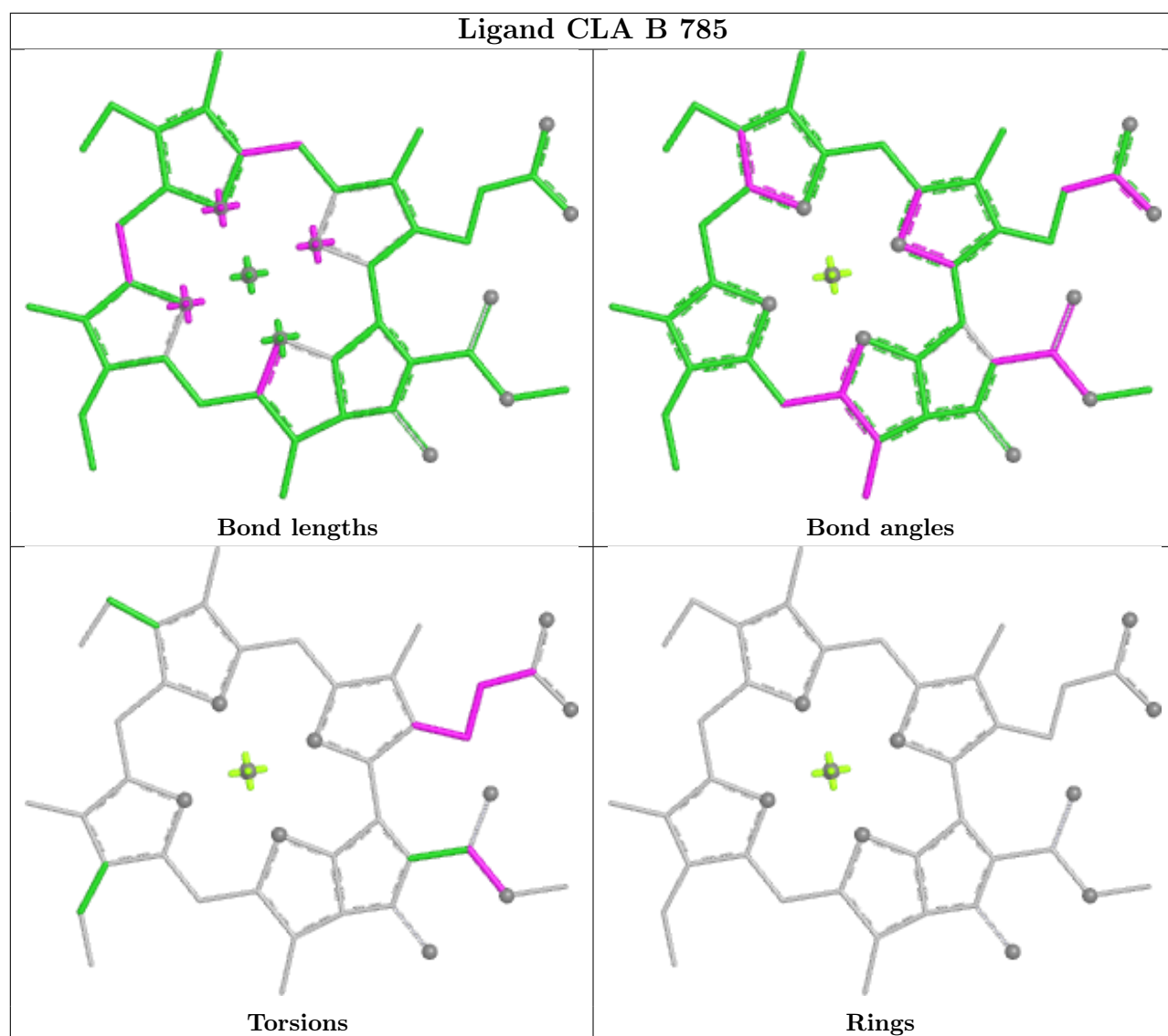
Rings

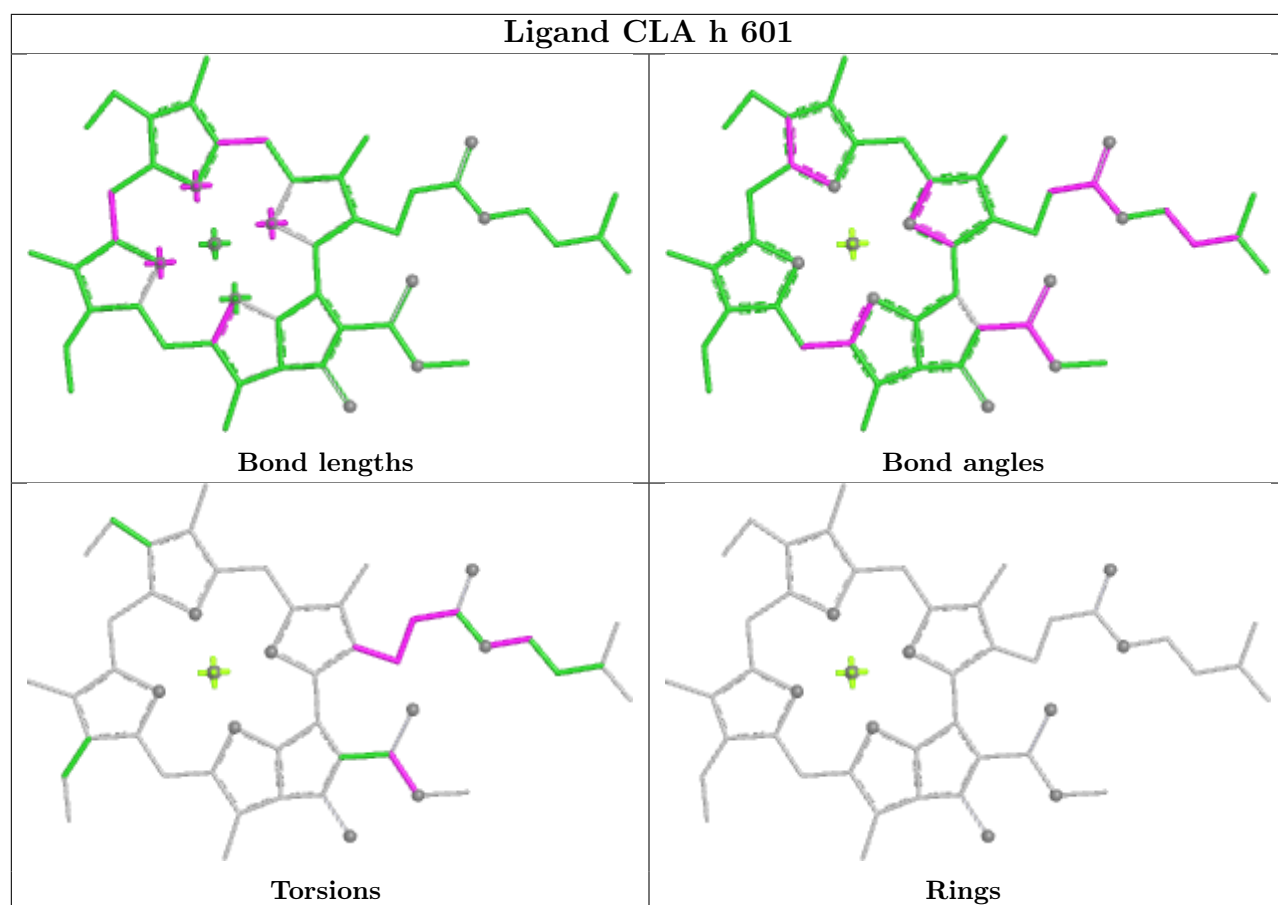




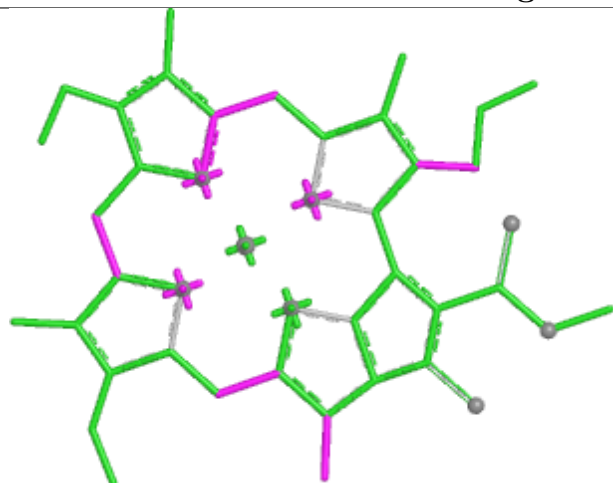




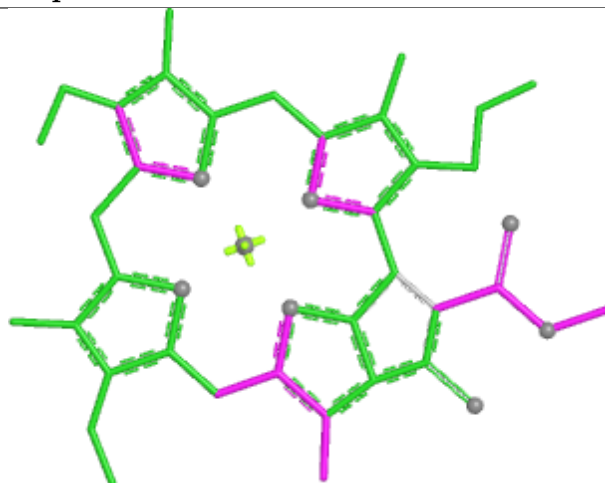




Ligand CLA p 602



Bond lengths



Bond angles

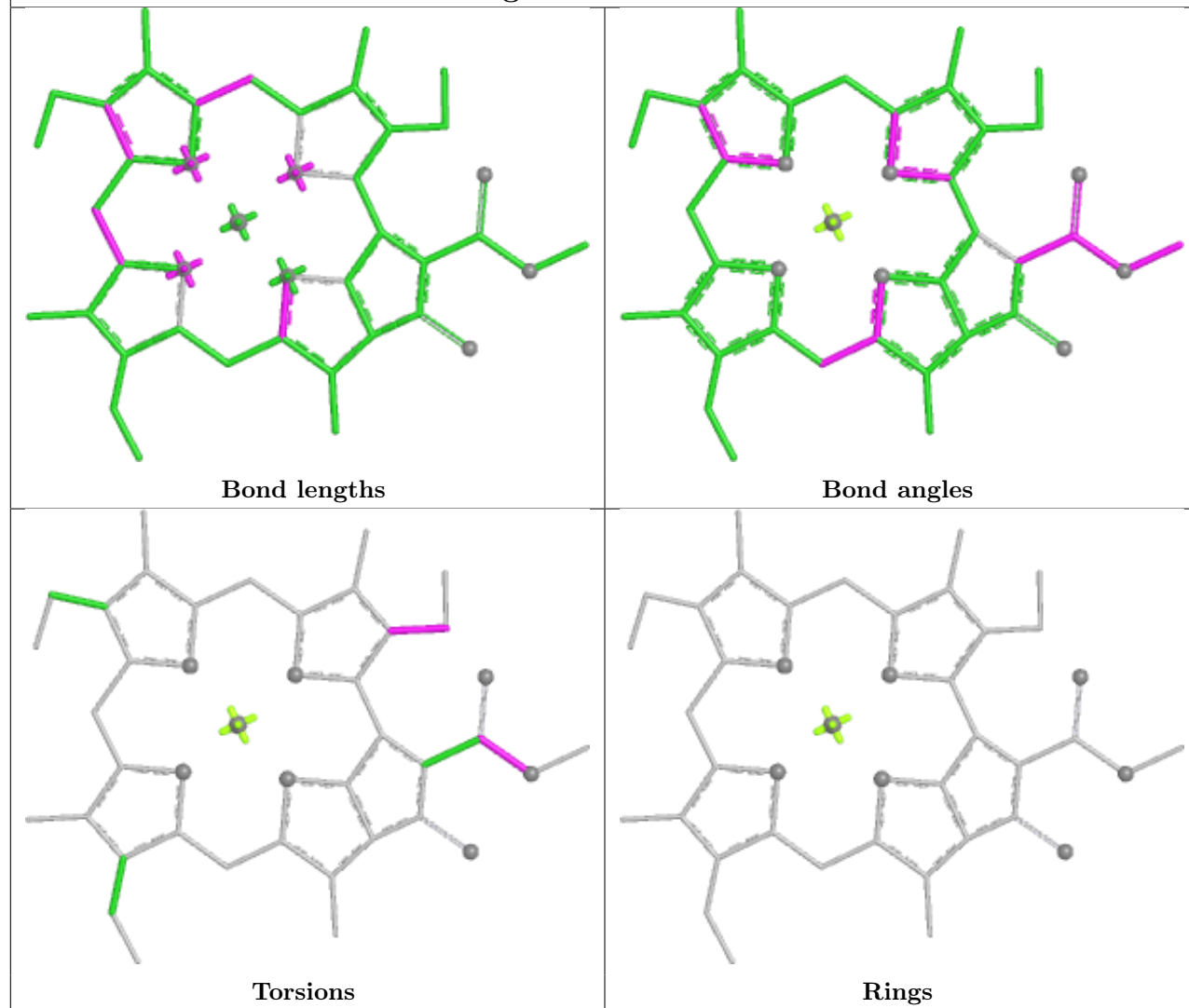


Torsions

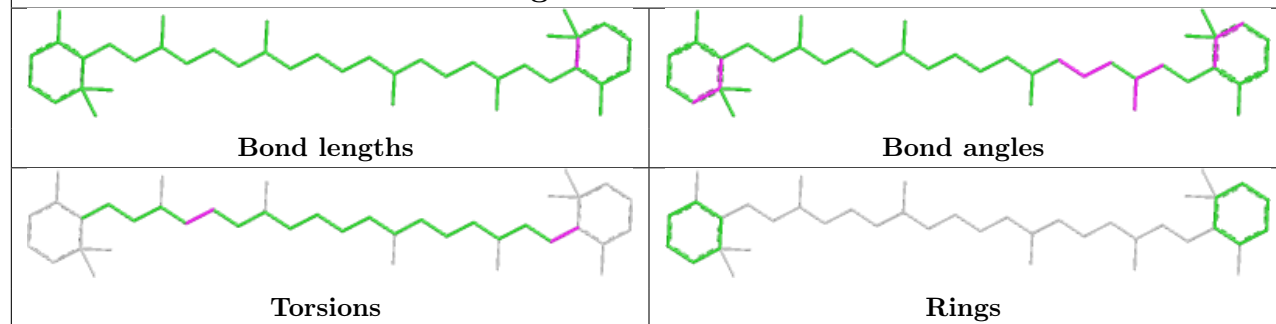


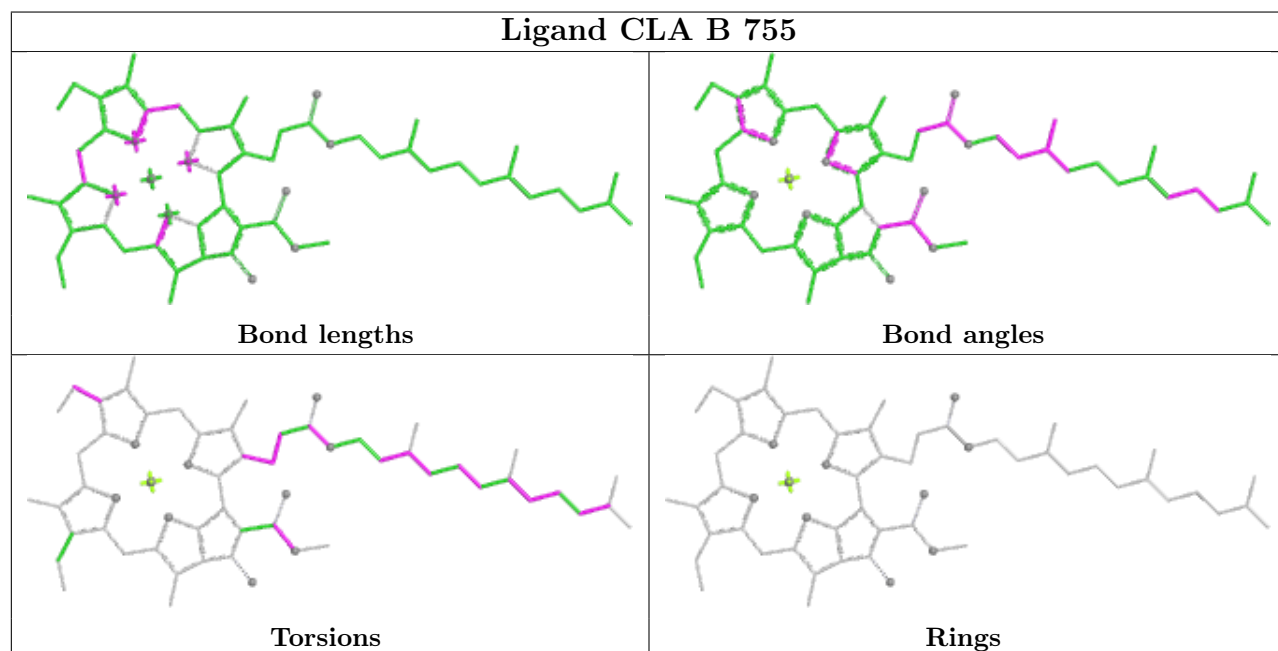
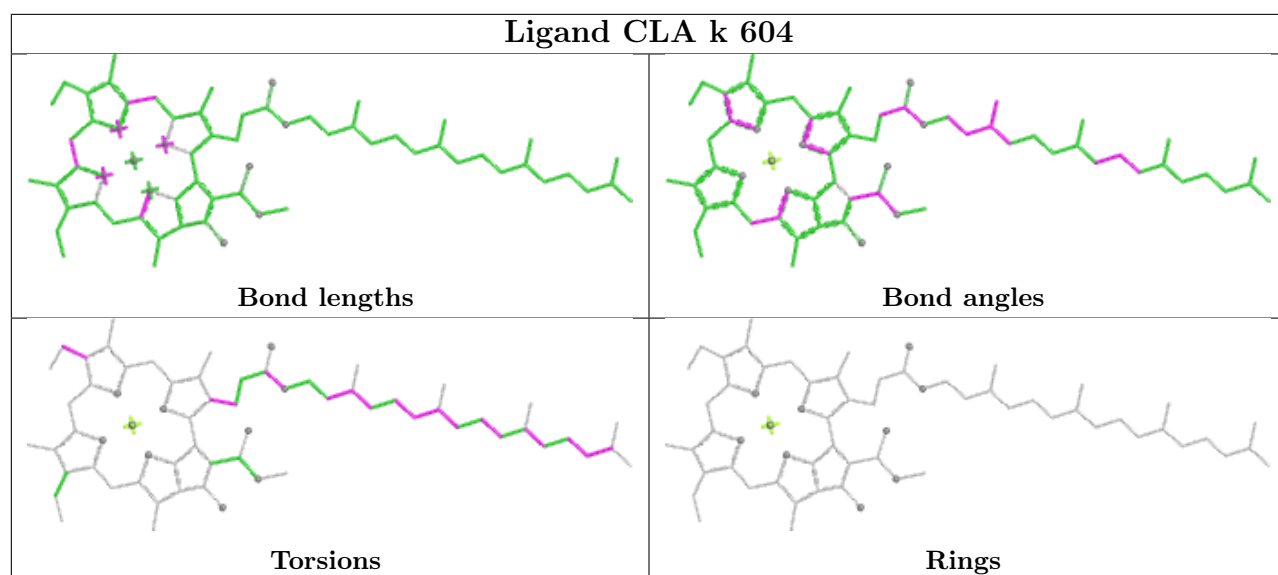
Rings

Ligand CLA f 604

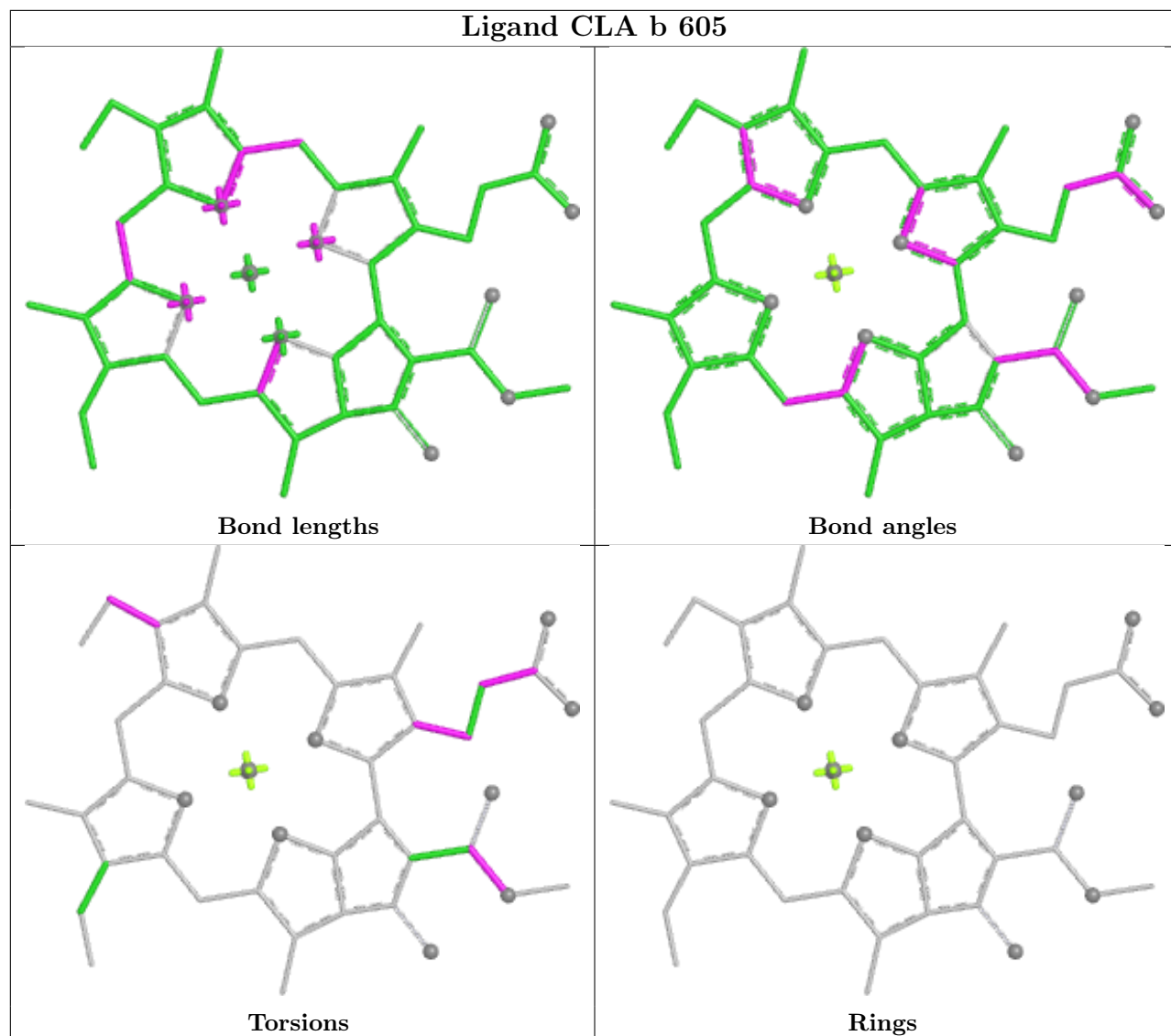


Ligand BCR B 763

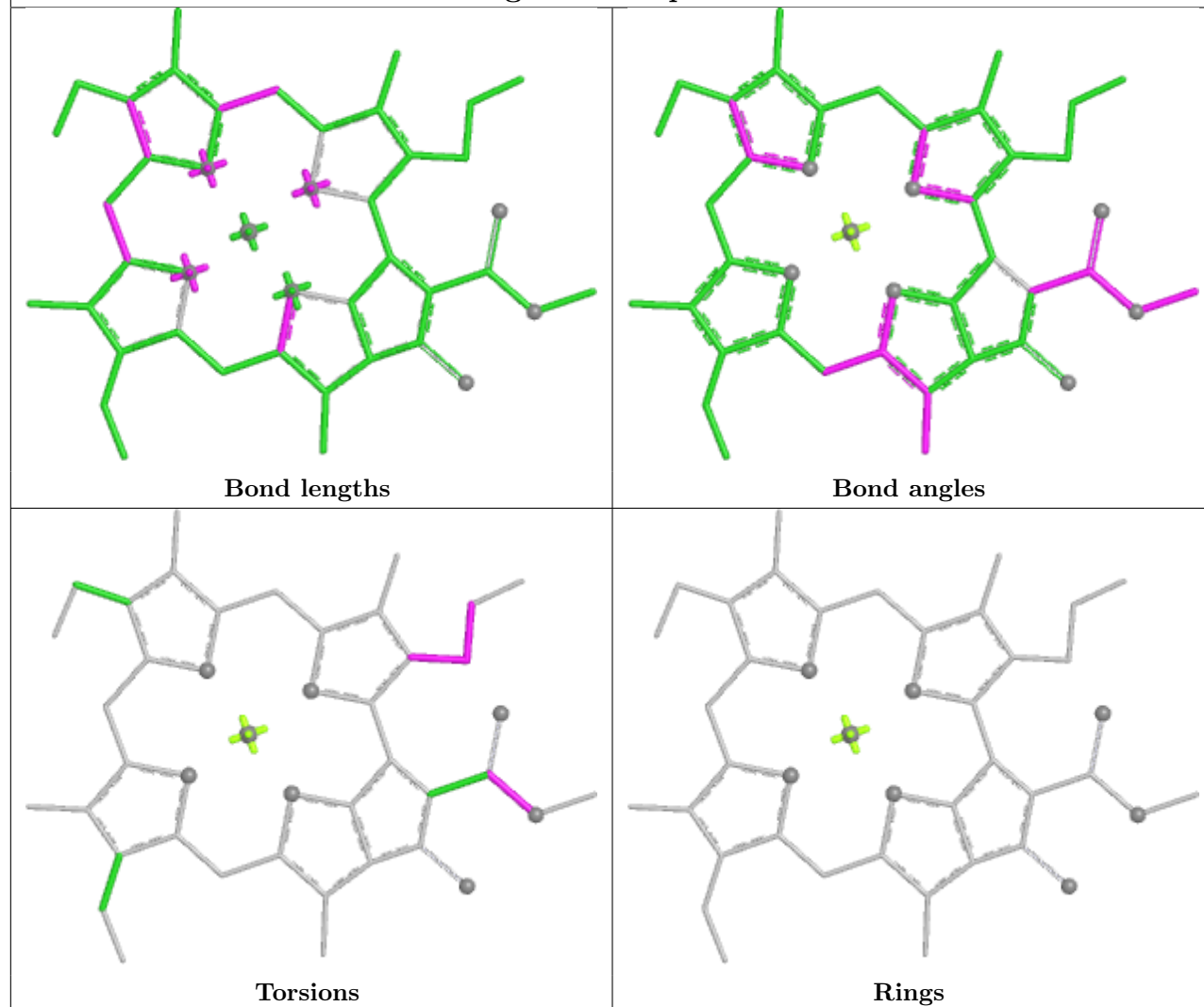




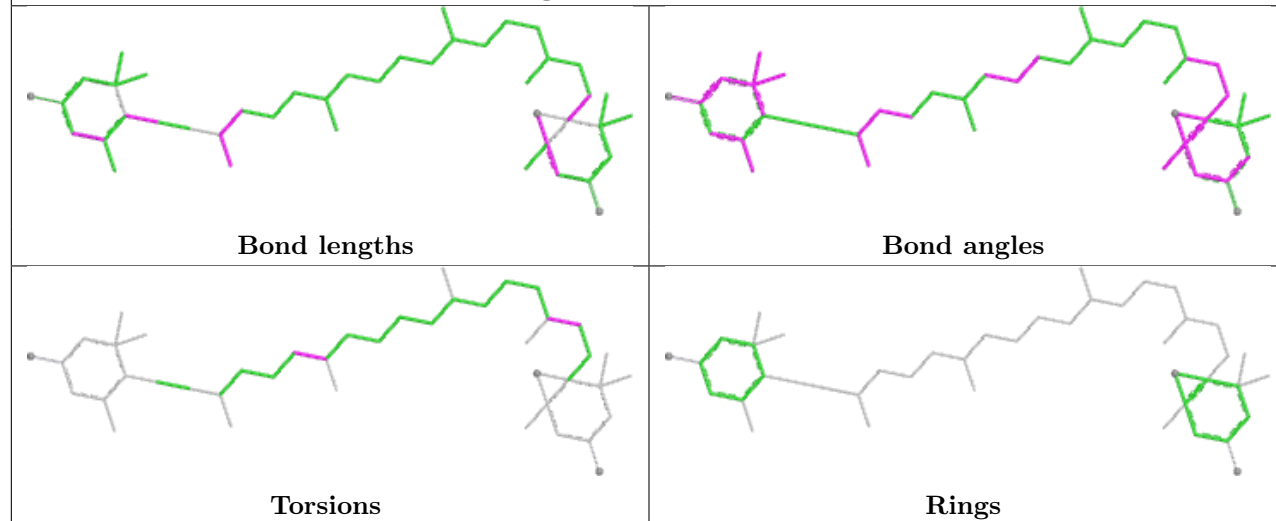
Ligand CLA b 605



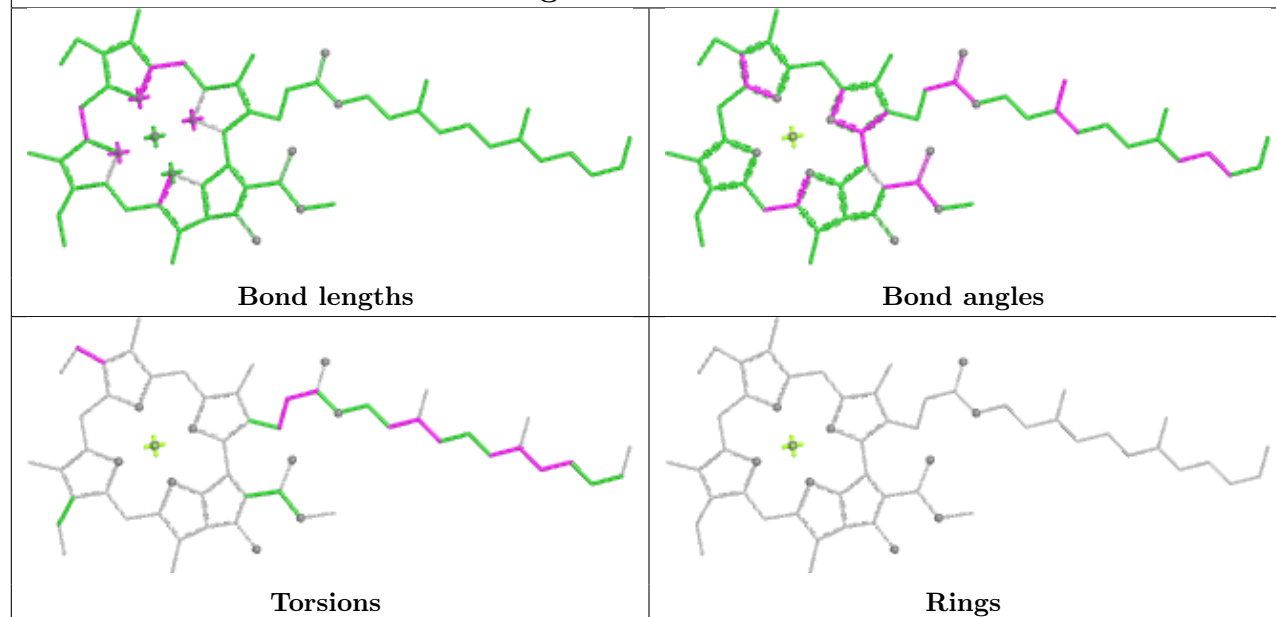
Ligand CLA p 613



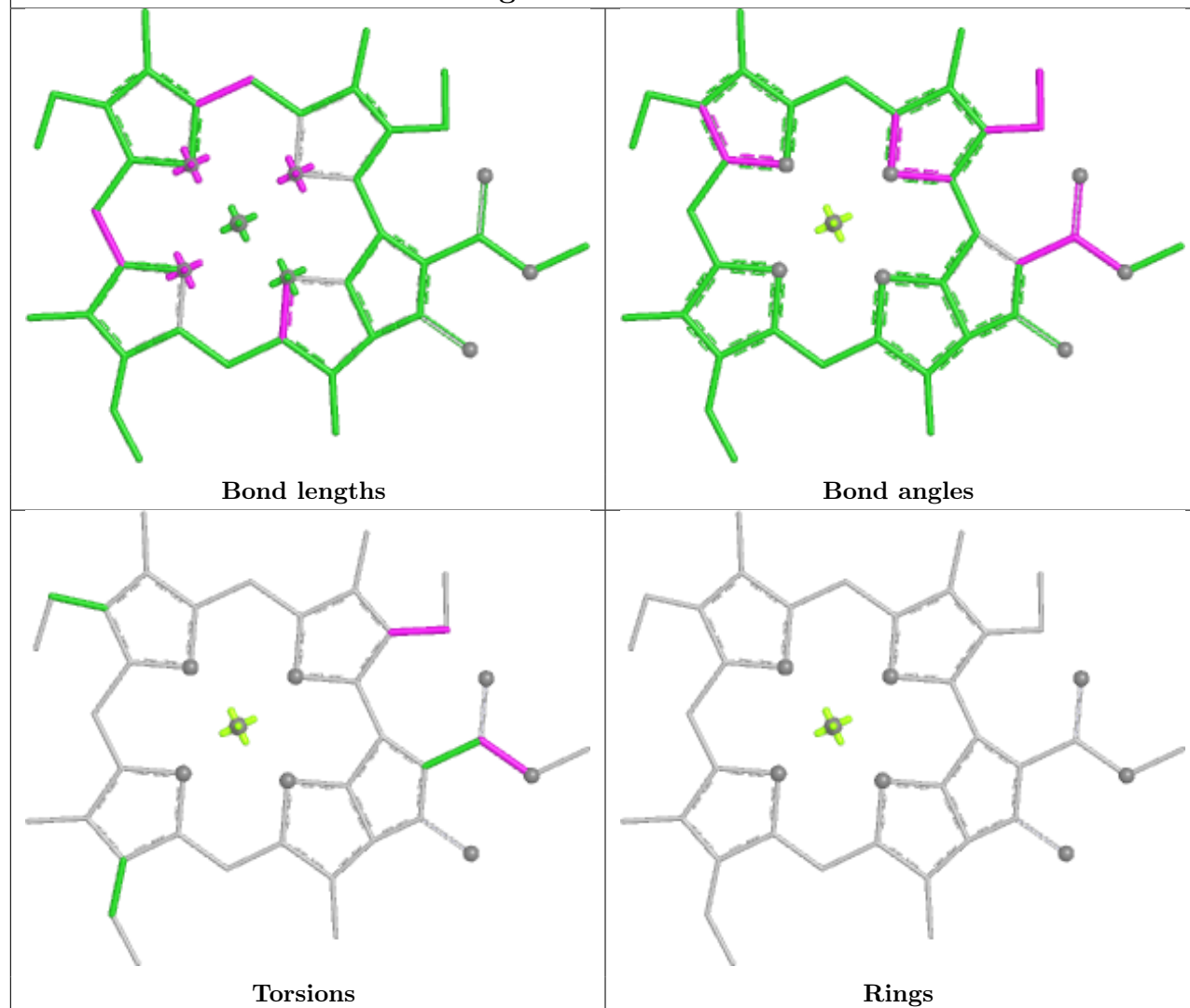
Ligand DD6 c 620



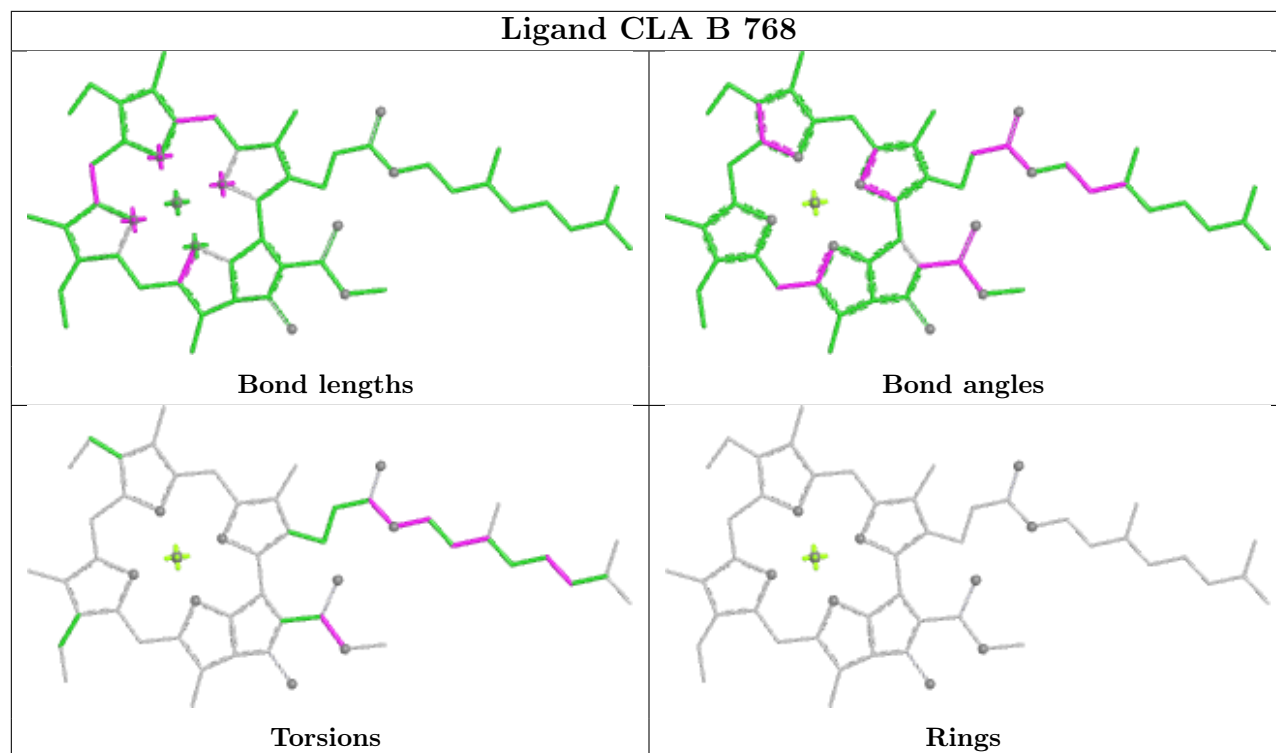
Ligand CLA i 613



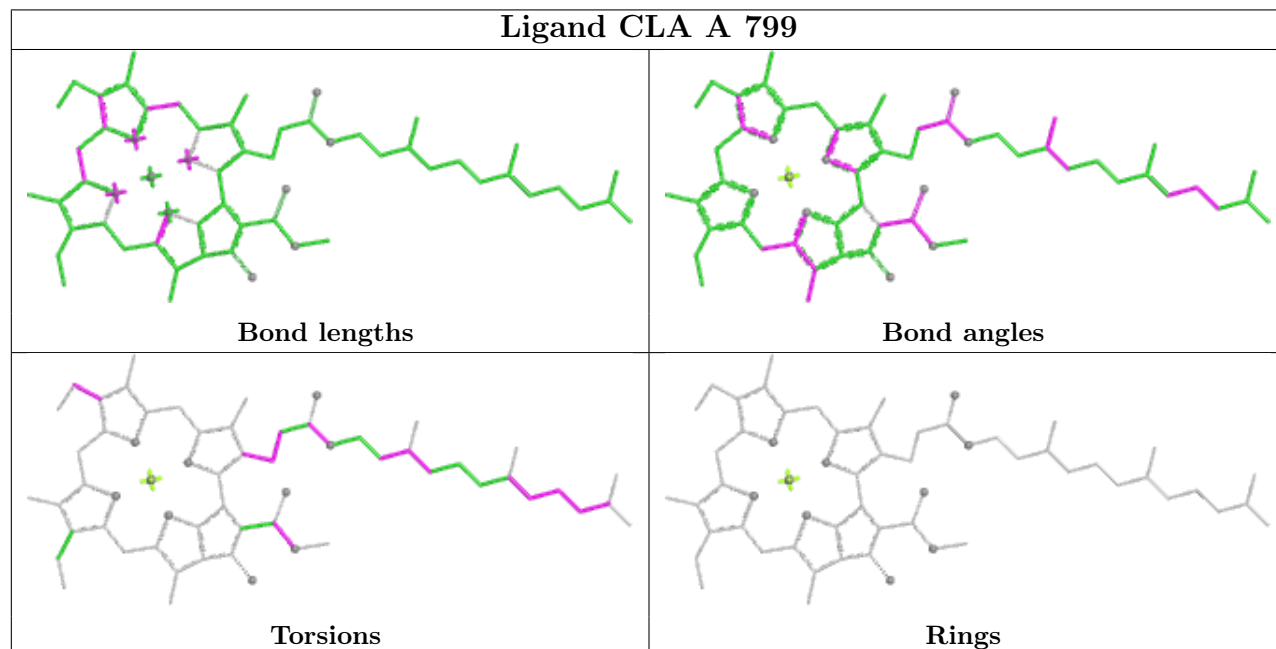
Ligand CLA n 605

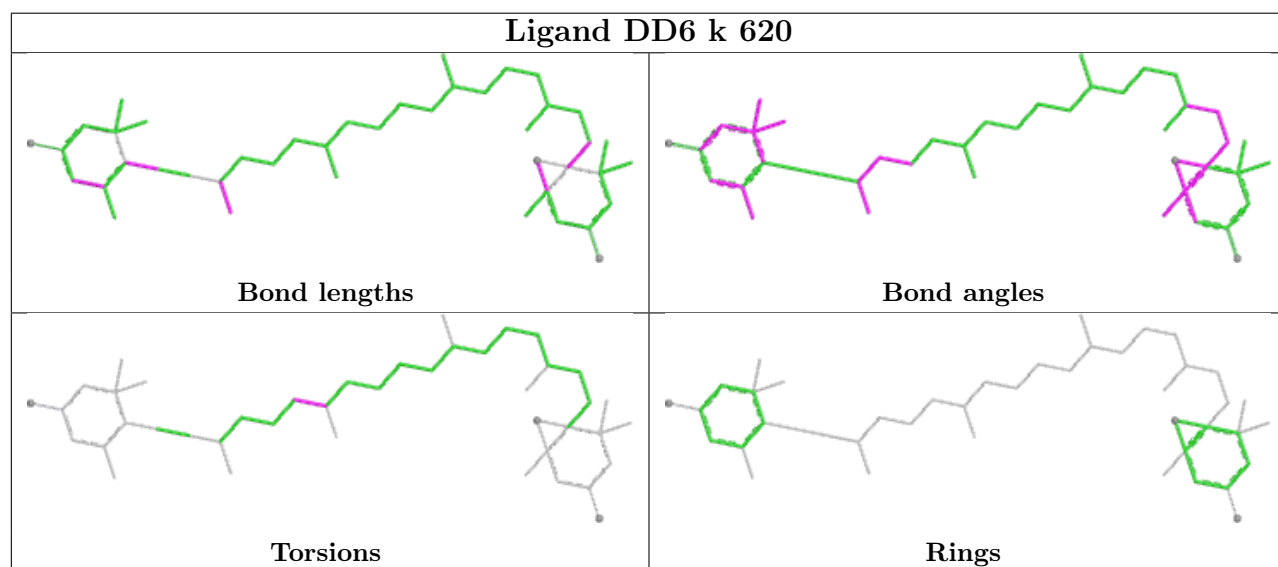
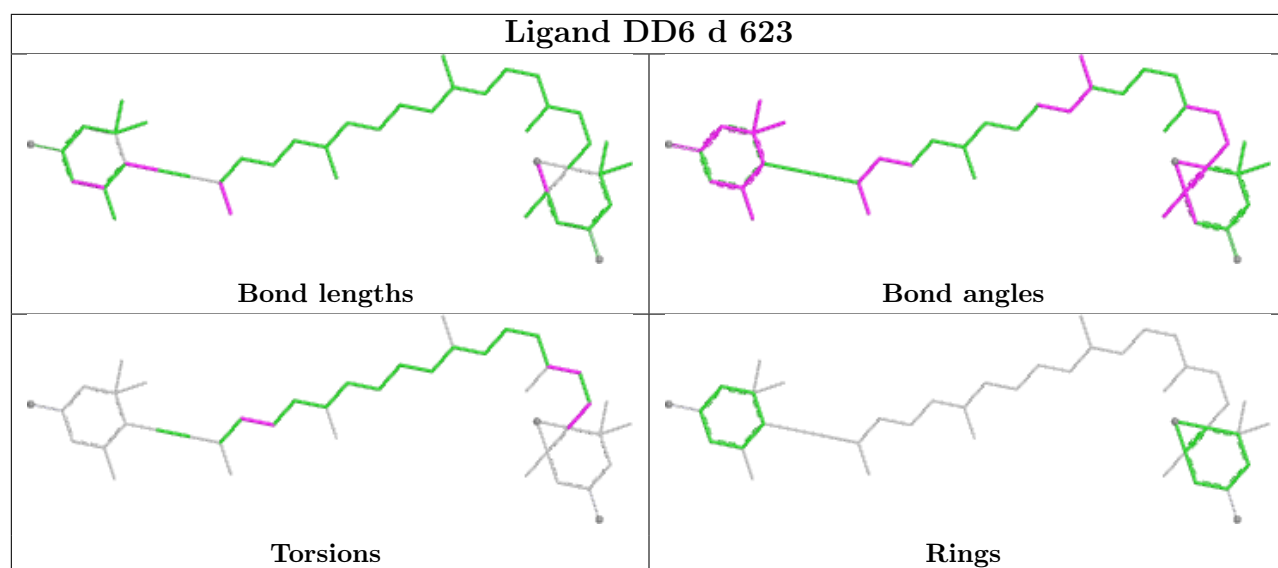


Ligand CLA B 768

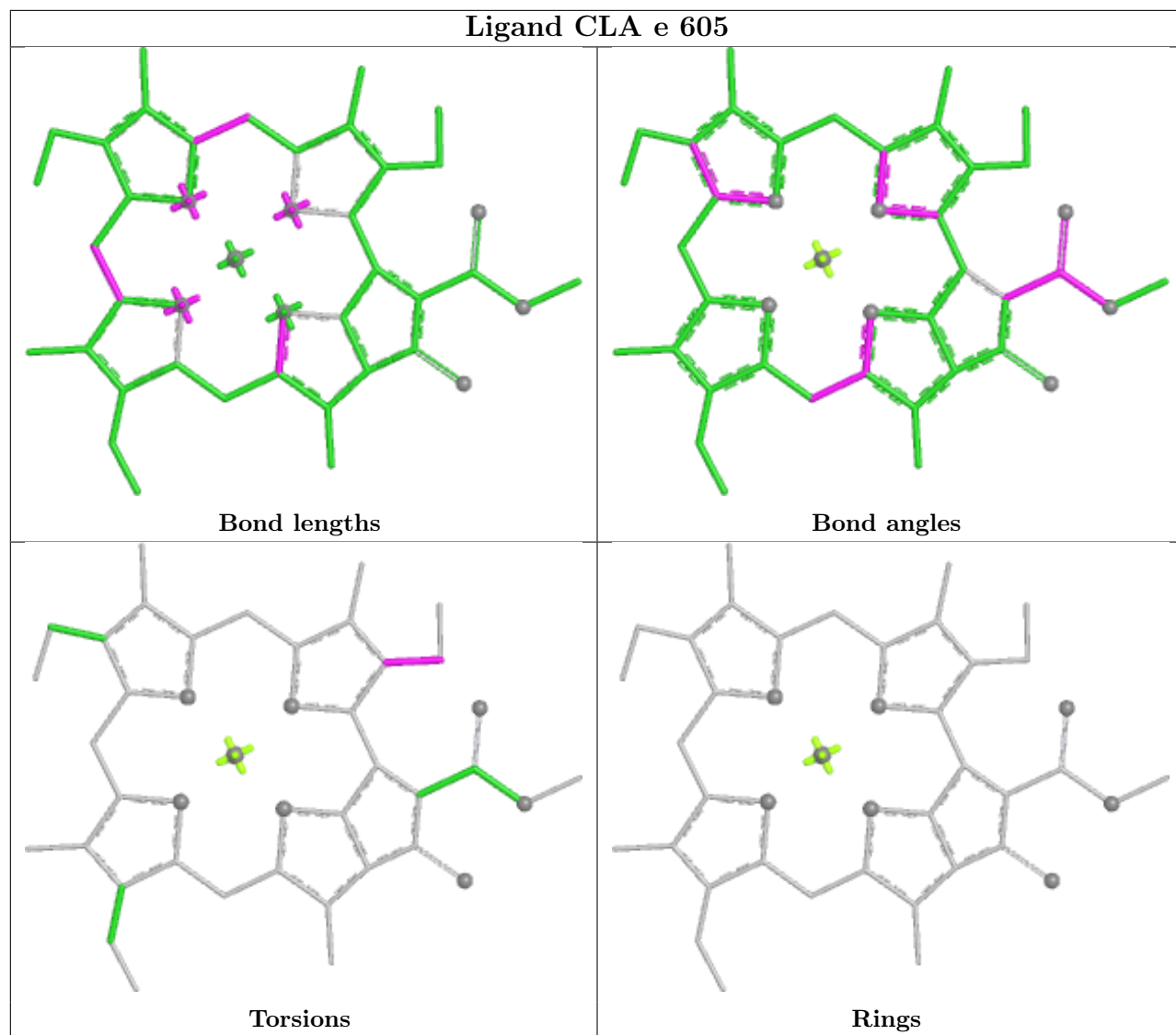


Ligand CLA A 799

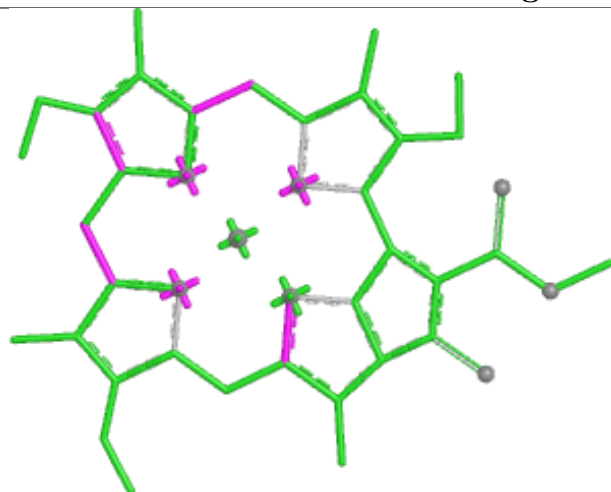




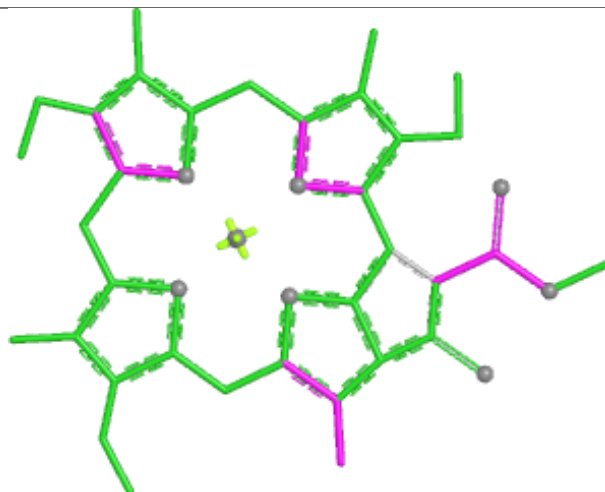
Ligand CLA e 605



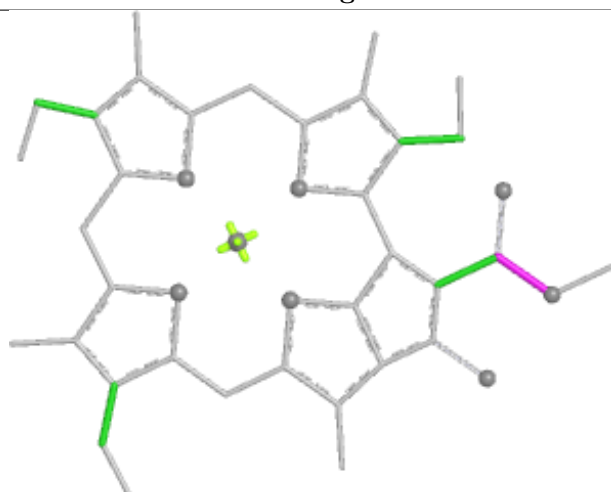
Ligand CLA f 608



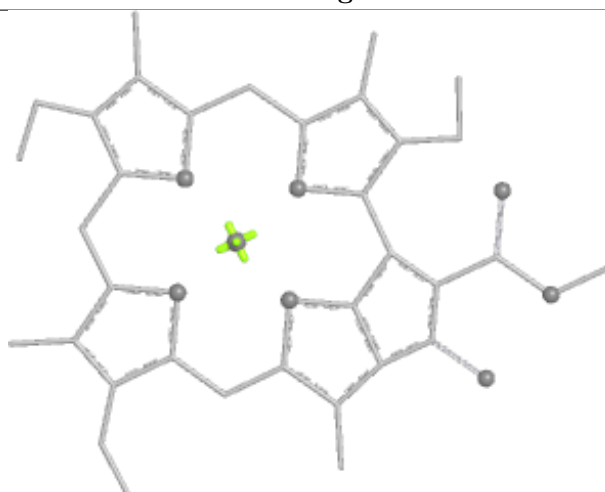
Bond lengths



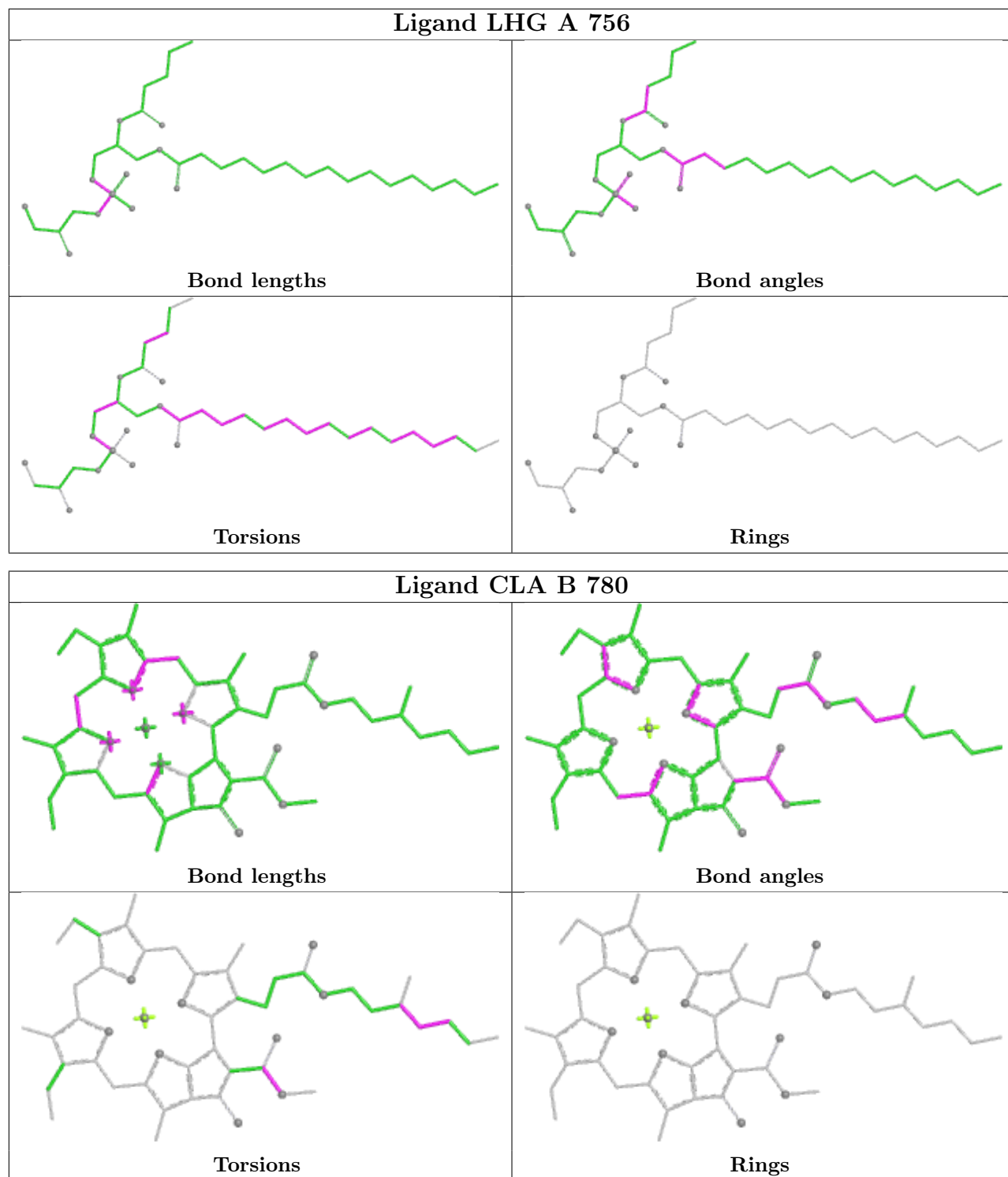
Bond angles



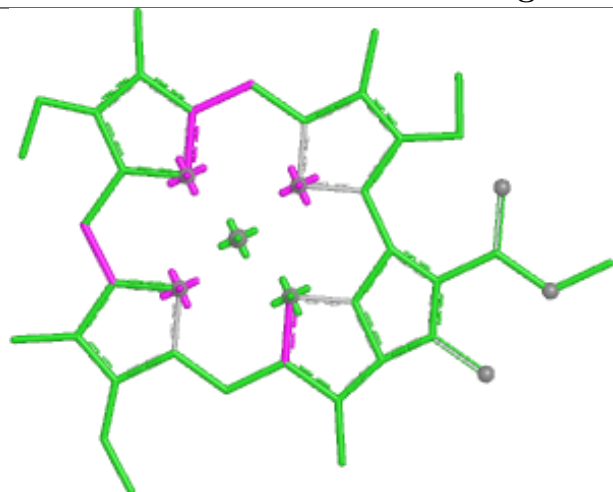
Torsions



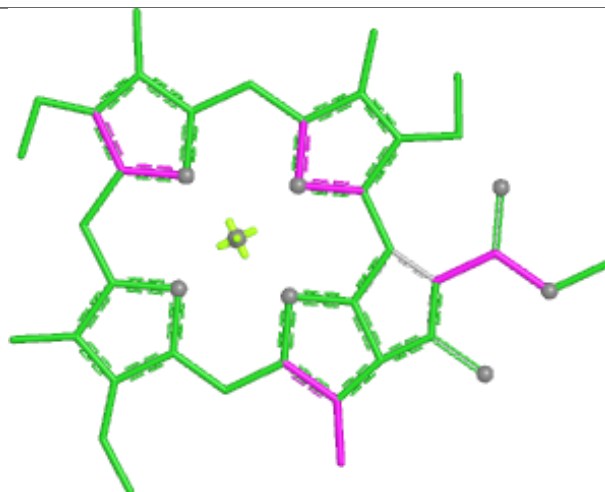
Rings



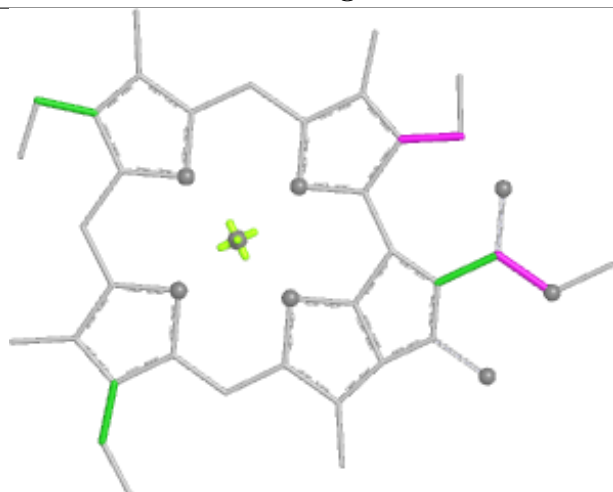
Ligand CLA k 603



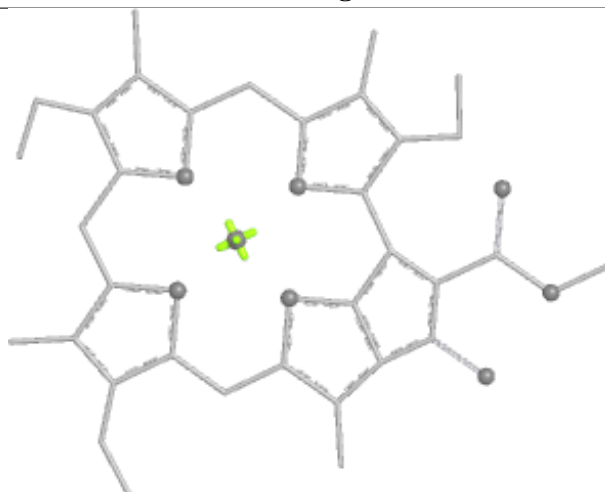
Bond lengths



Bond angles

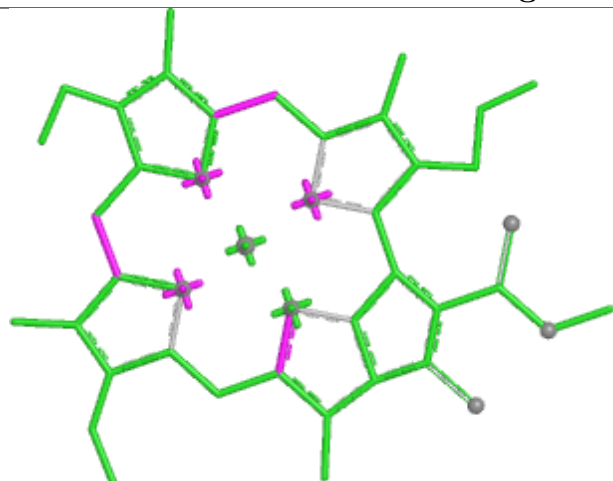


Torsions

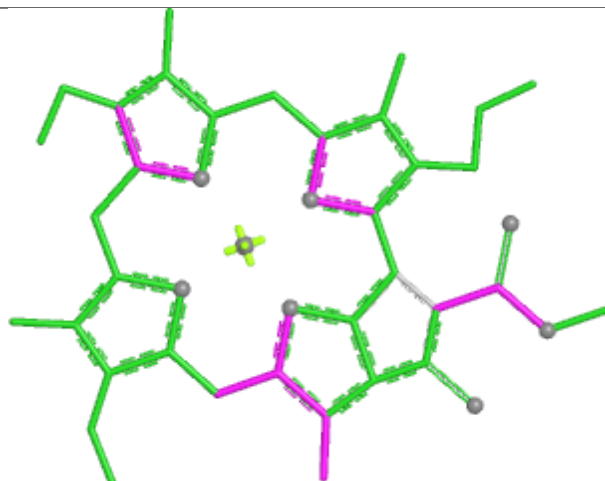


Rings

Ligand CLA e 607



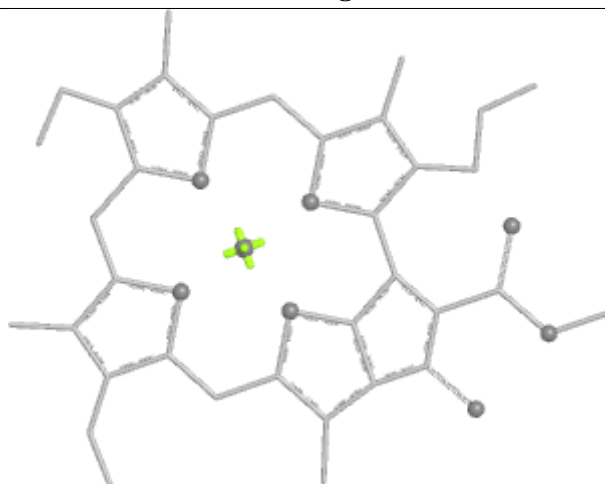
Bond lengths



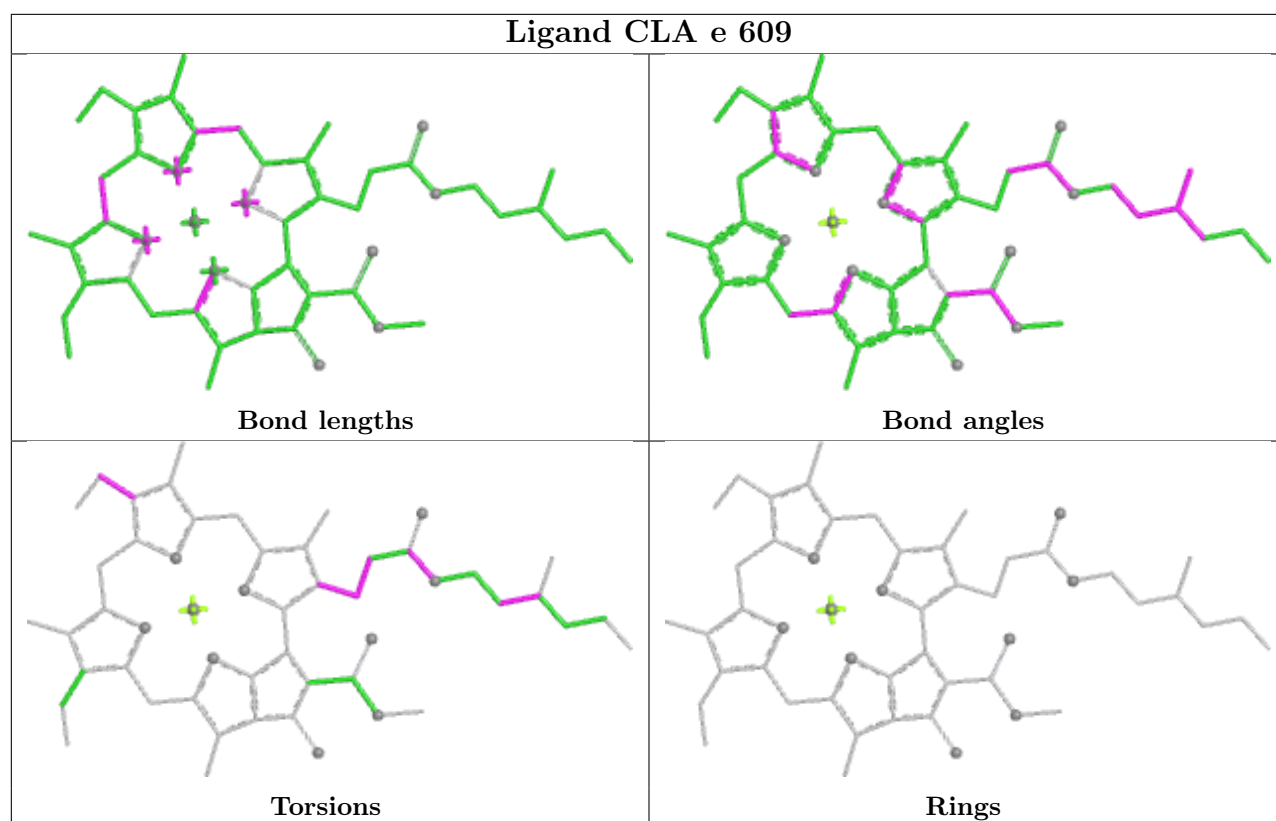
Bond angles



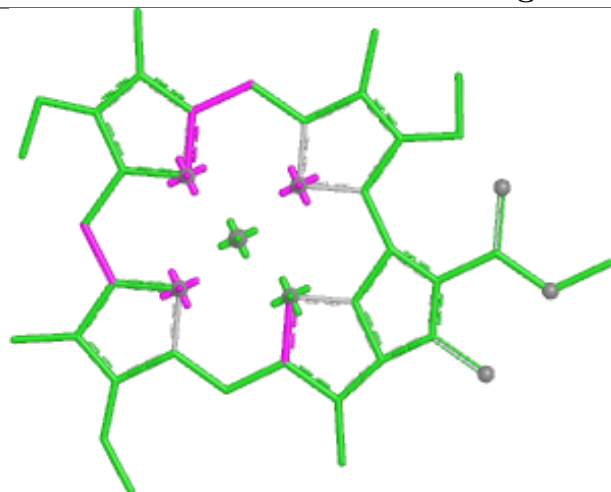
Torsions



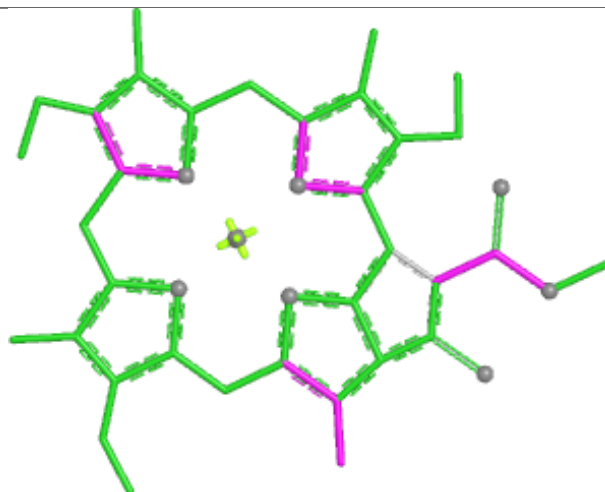
Rings



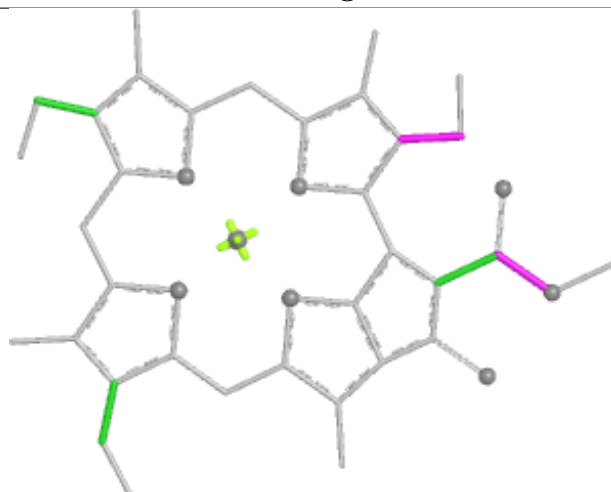
Ligand CLA d 603



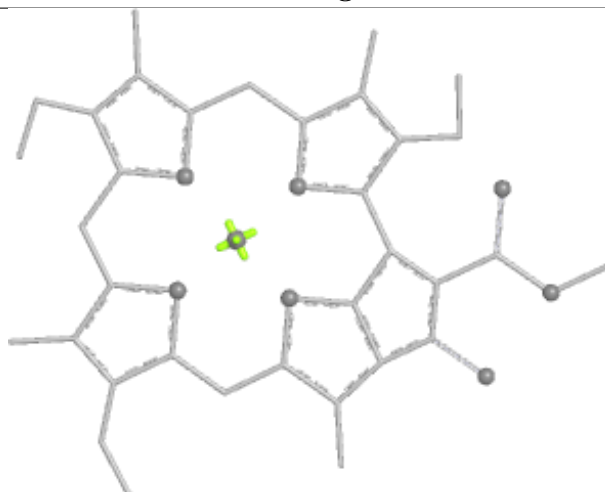
Bond lengths



Bond angles

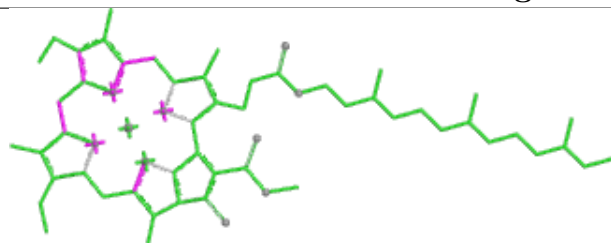


Torsions

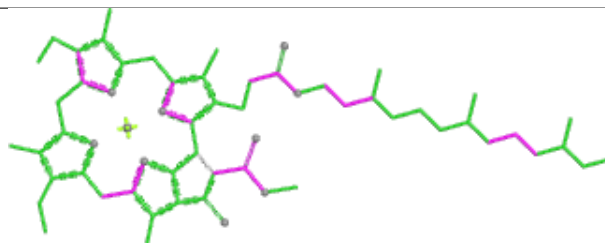


Rings

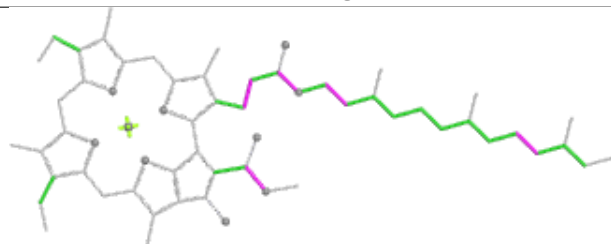
Ligand CLA B 773



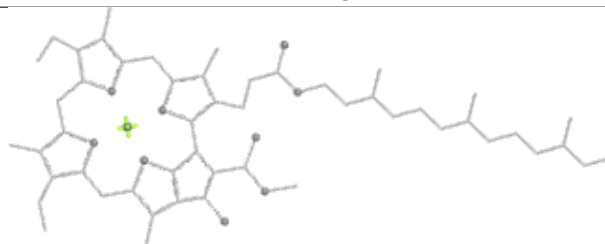
Bond lengths



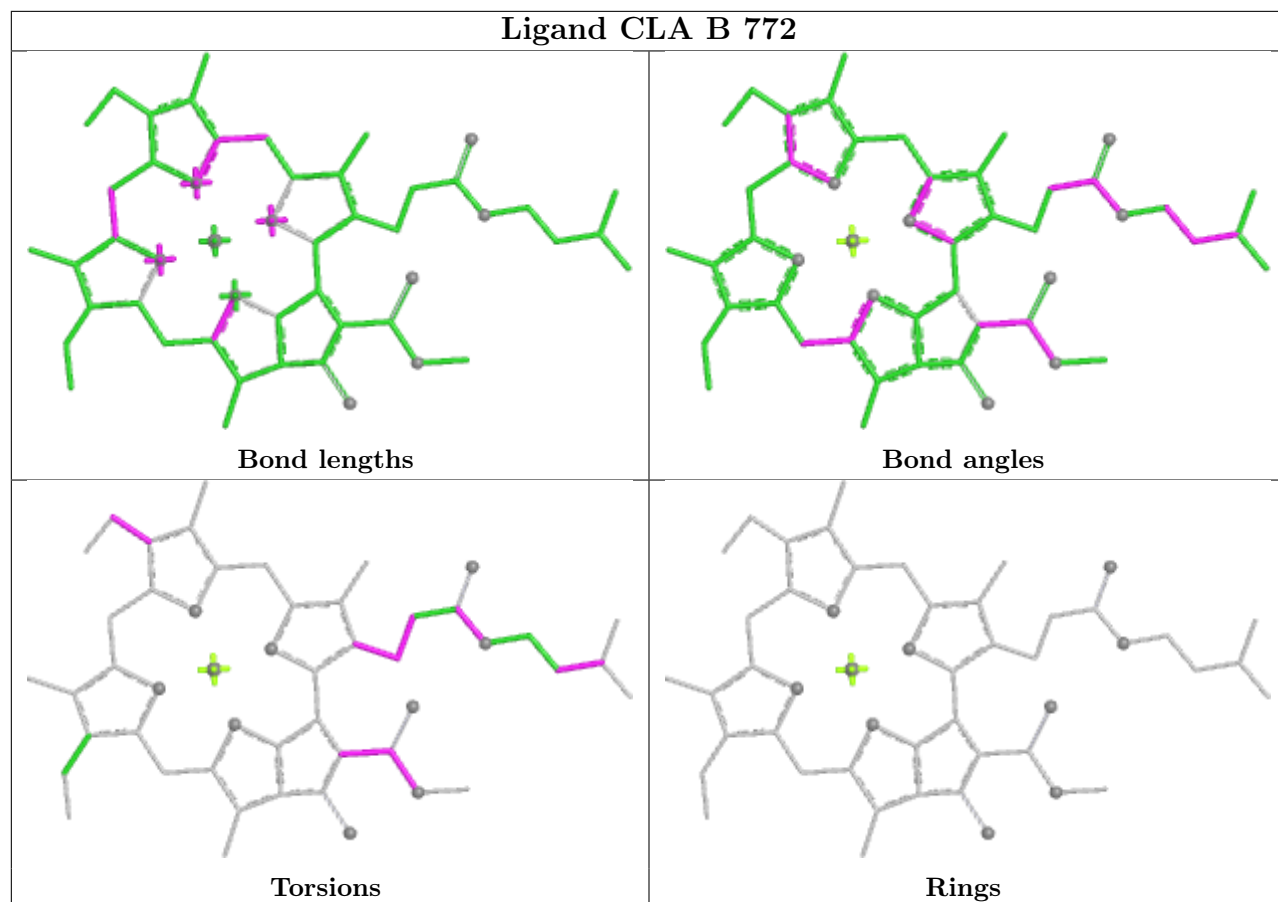
Bond angles

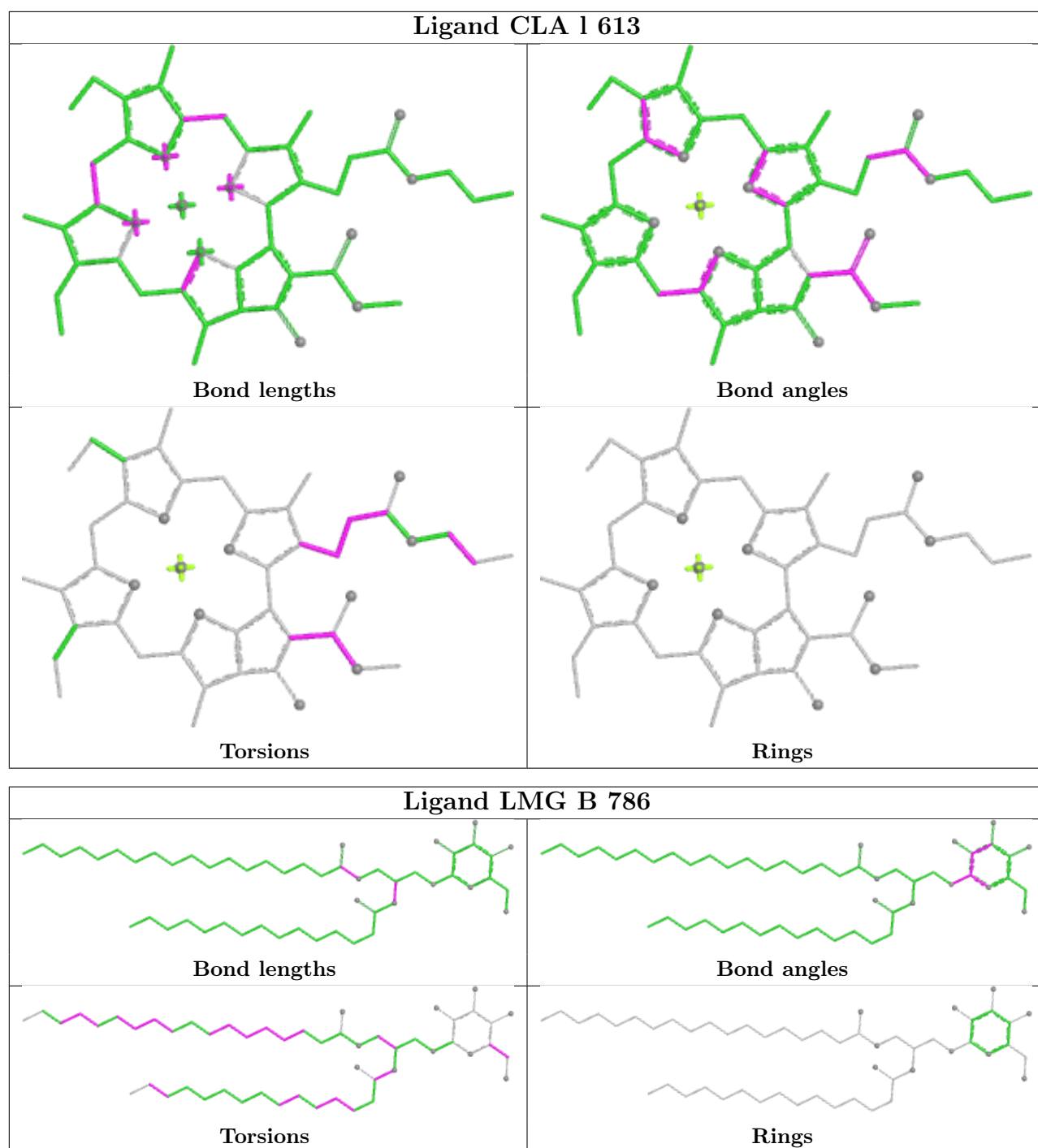


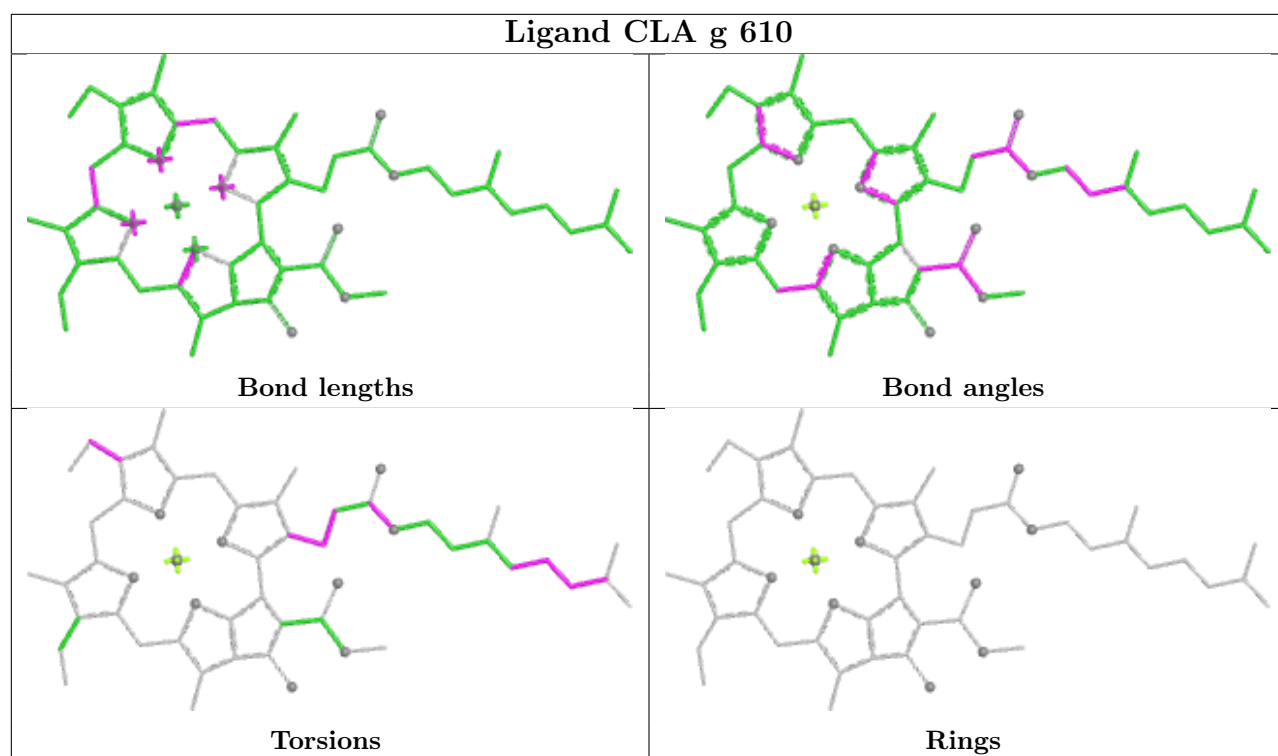
Torsions



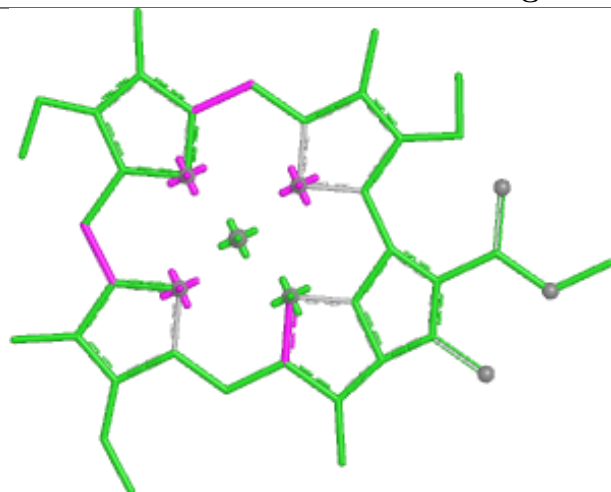
Rings



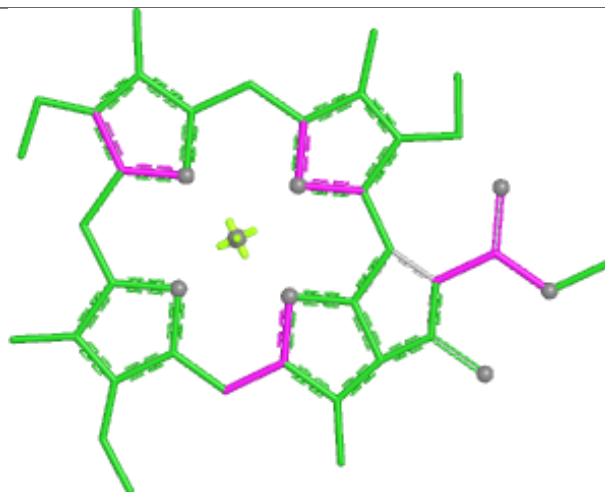




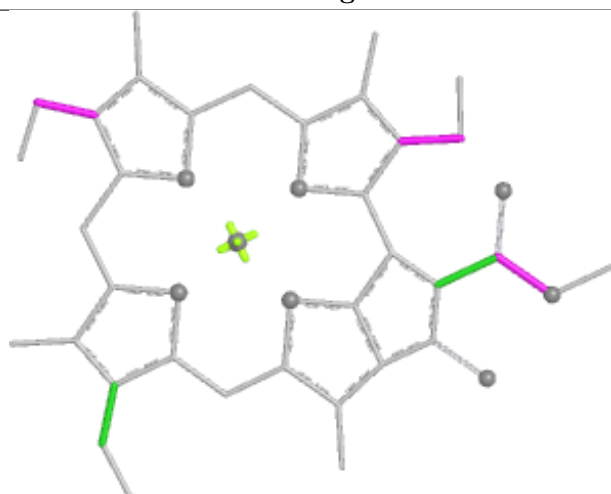
Ligand CLA f 601



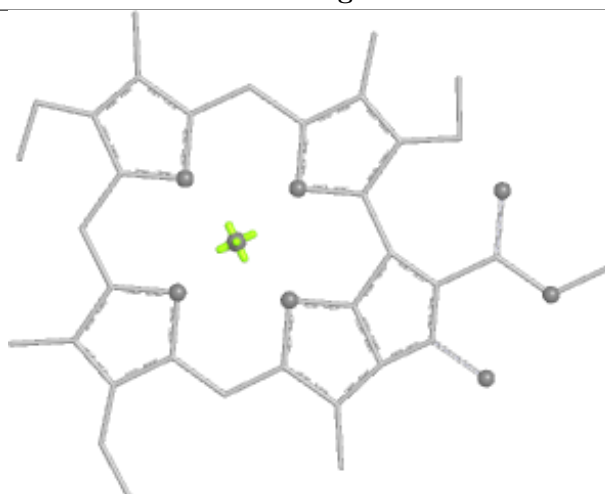
Bond lengths



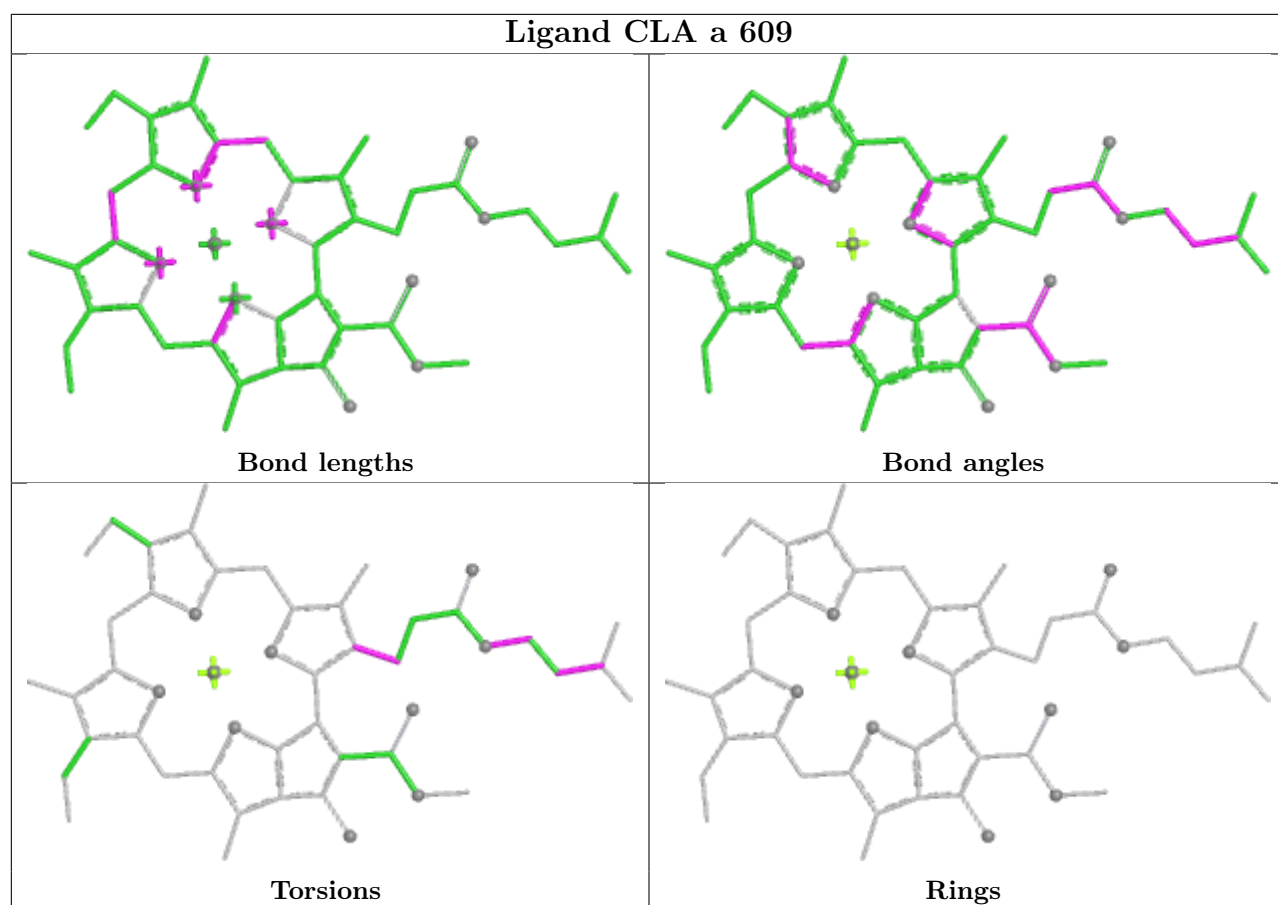
Bond angles



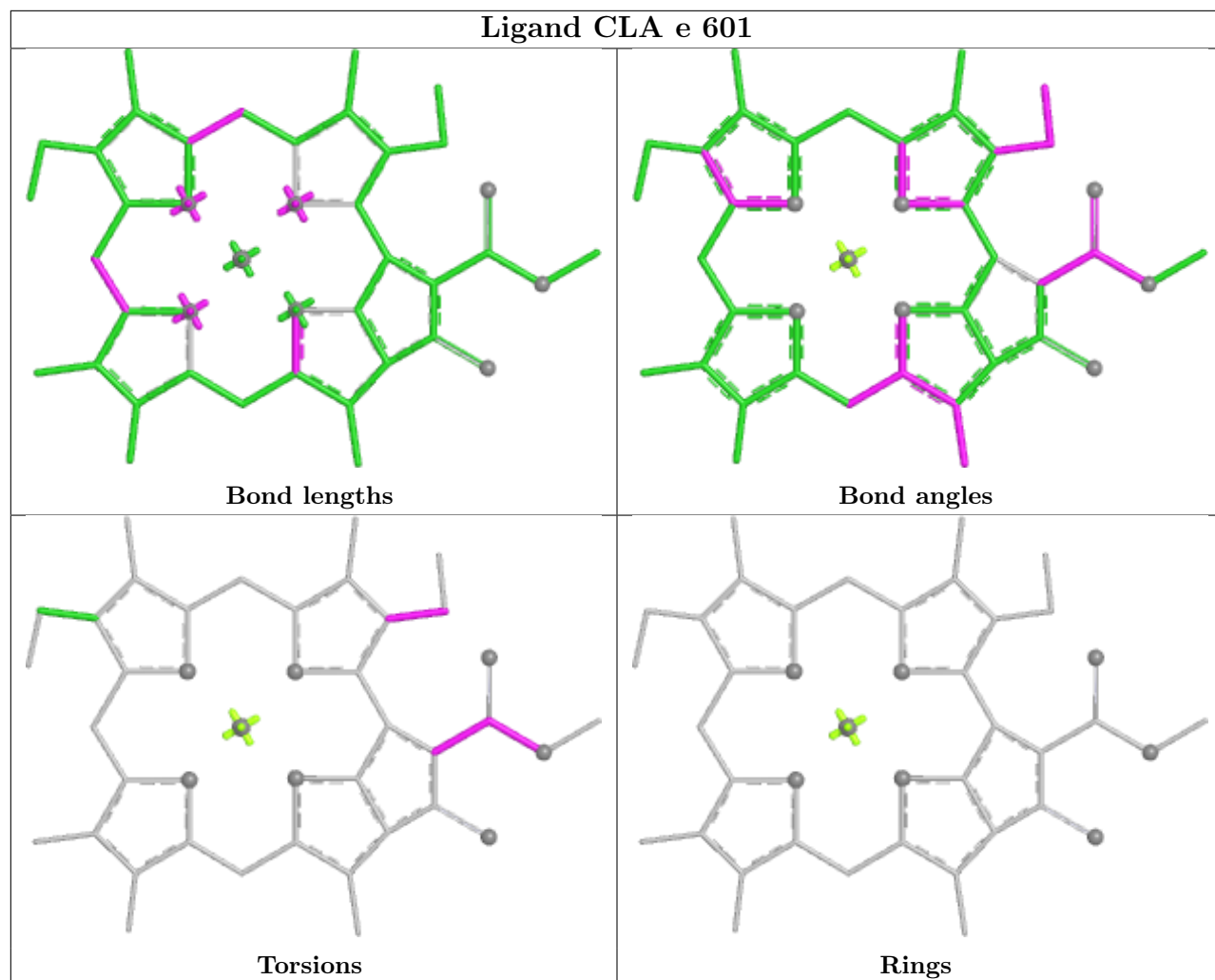
Torsions



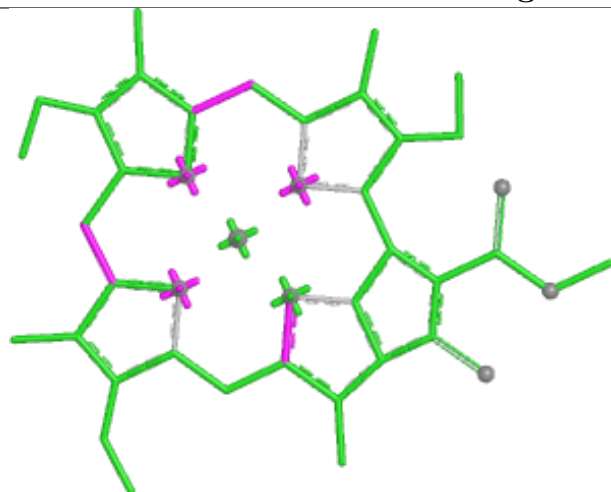
Rings



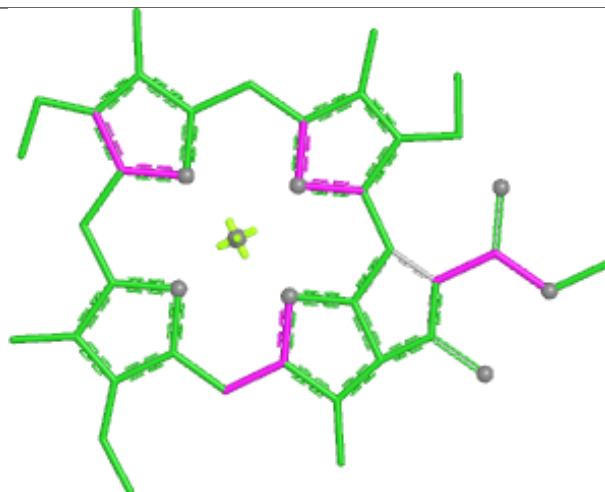
Ligand CLA e 601



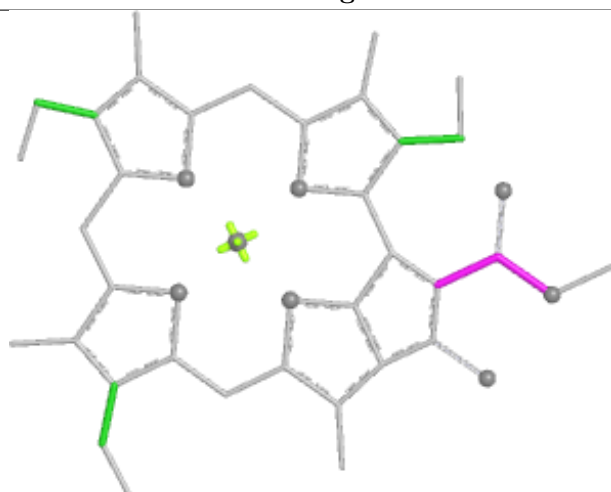
Ligand CLA b 611



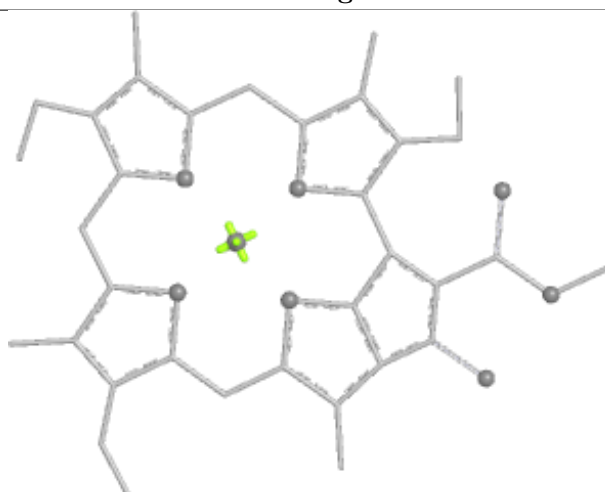
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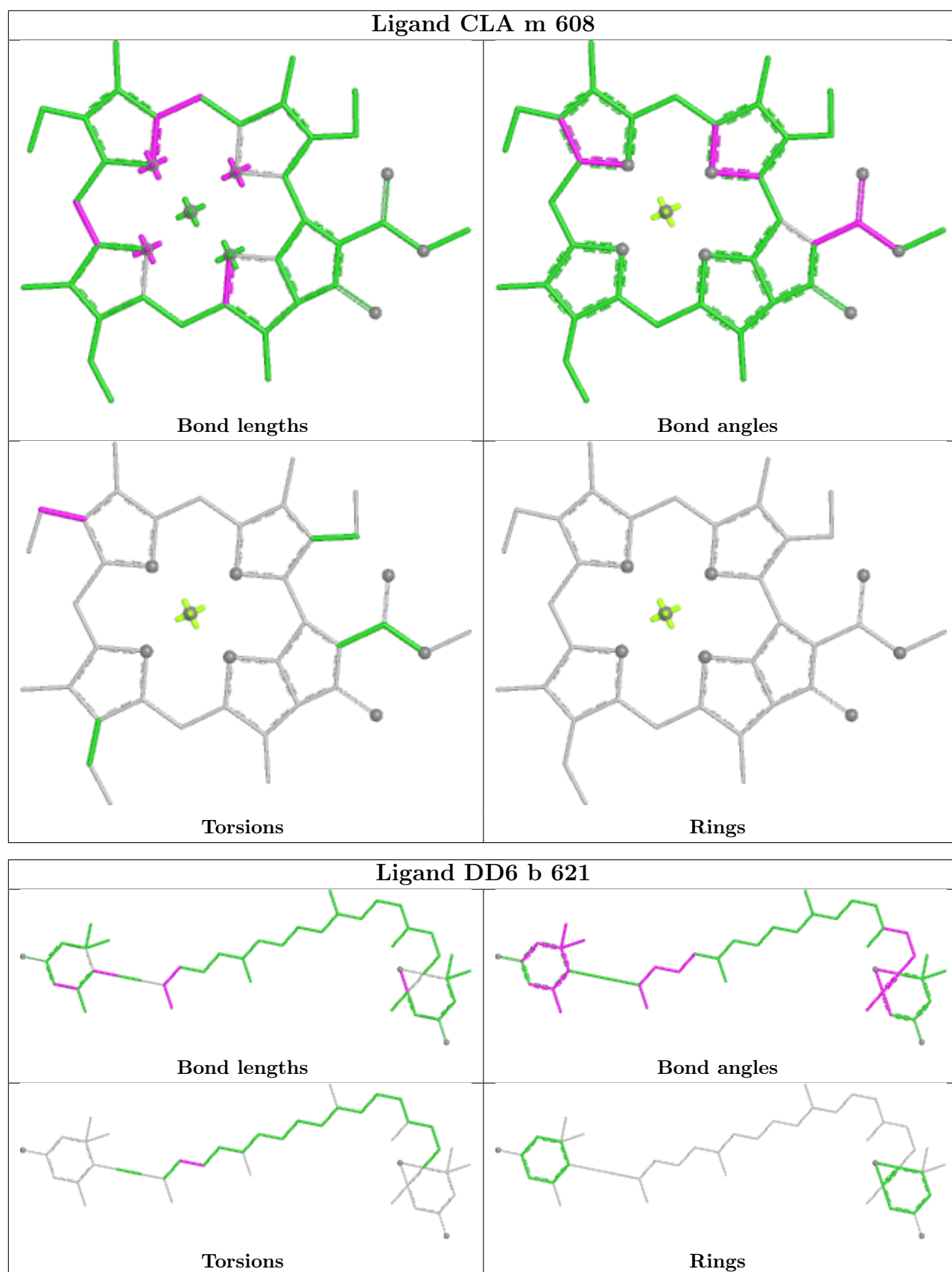
Bond angles



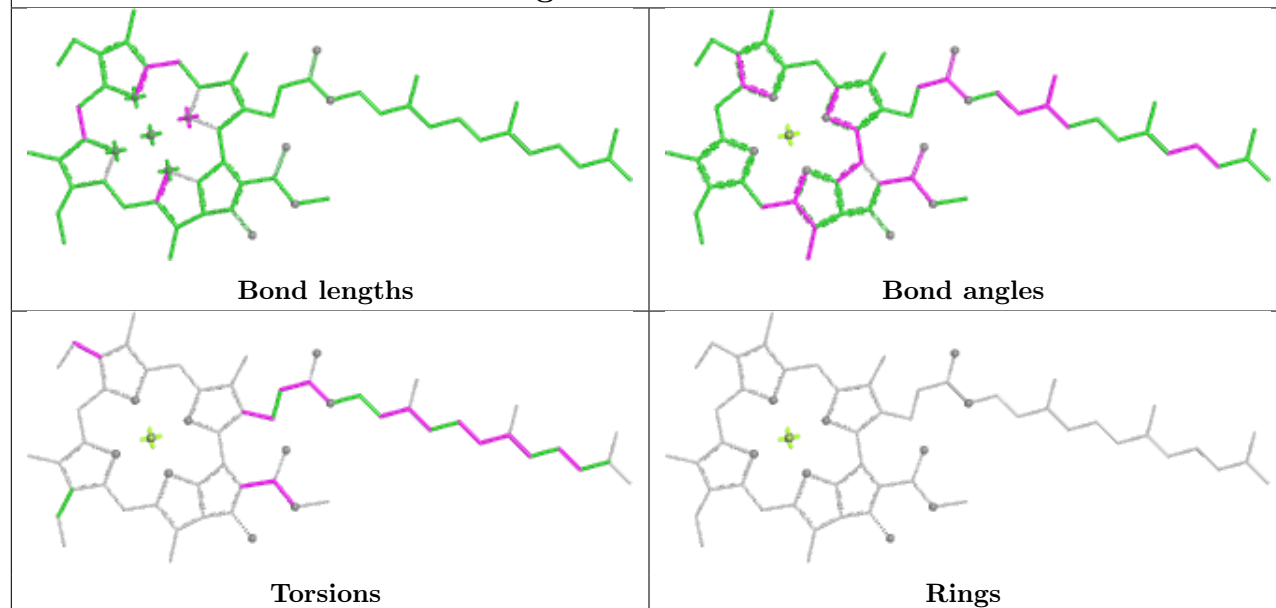
Torsions



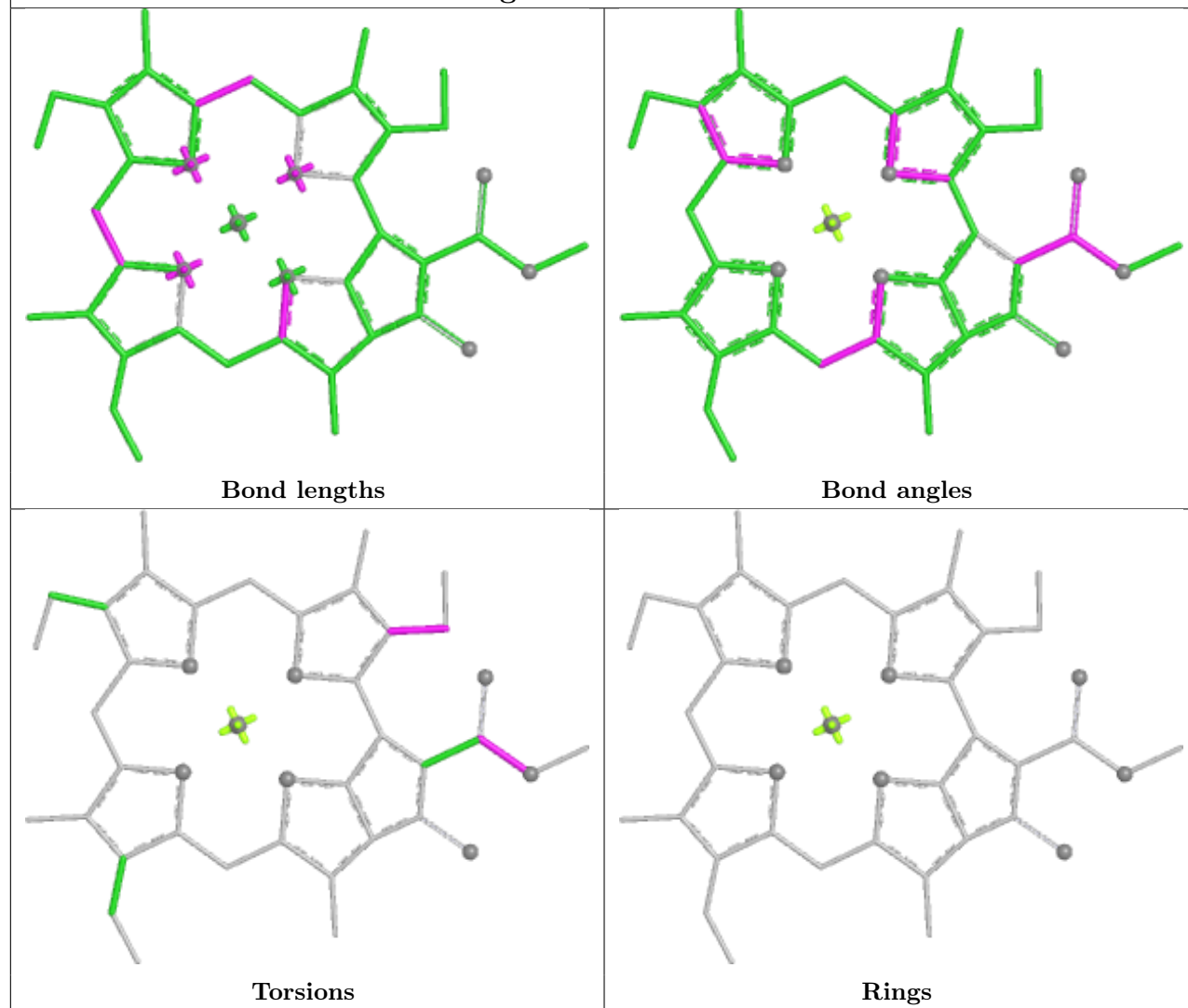
Rings

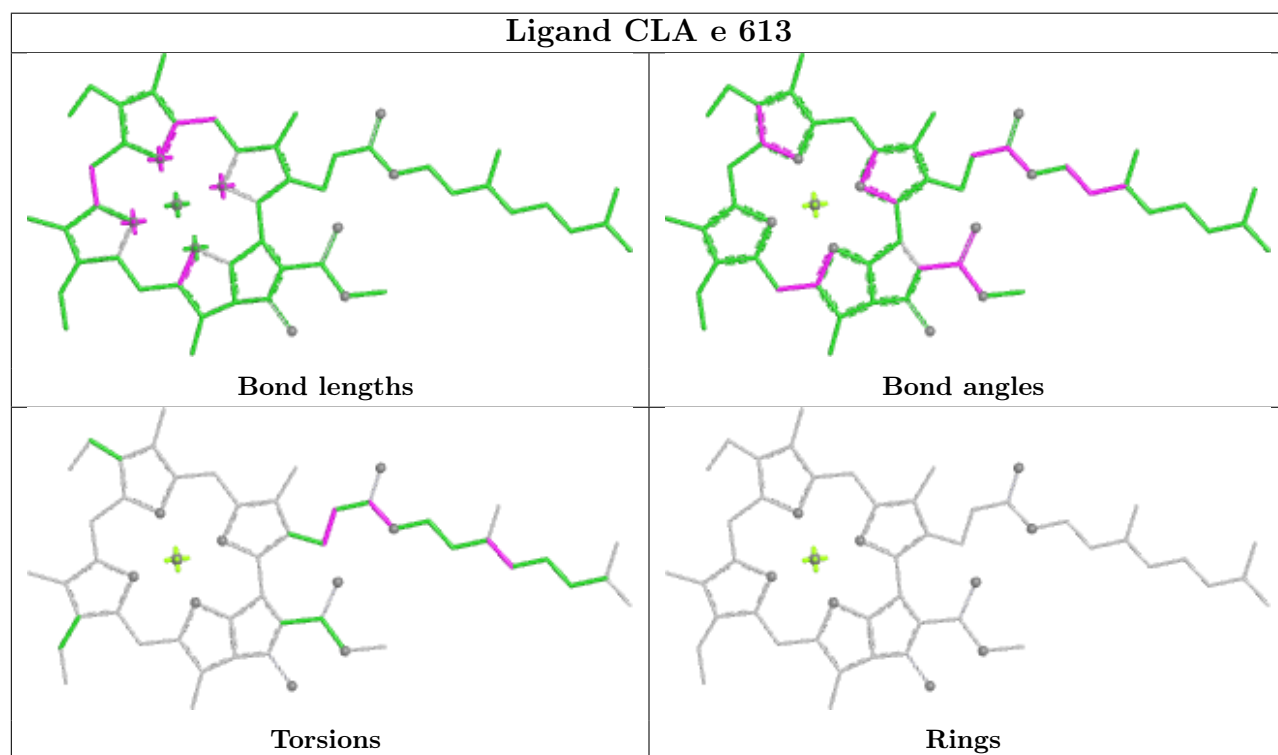
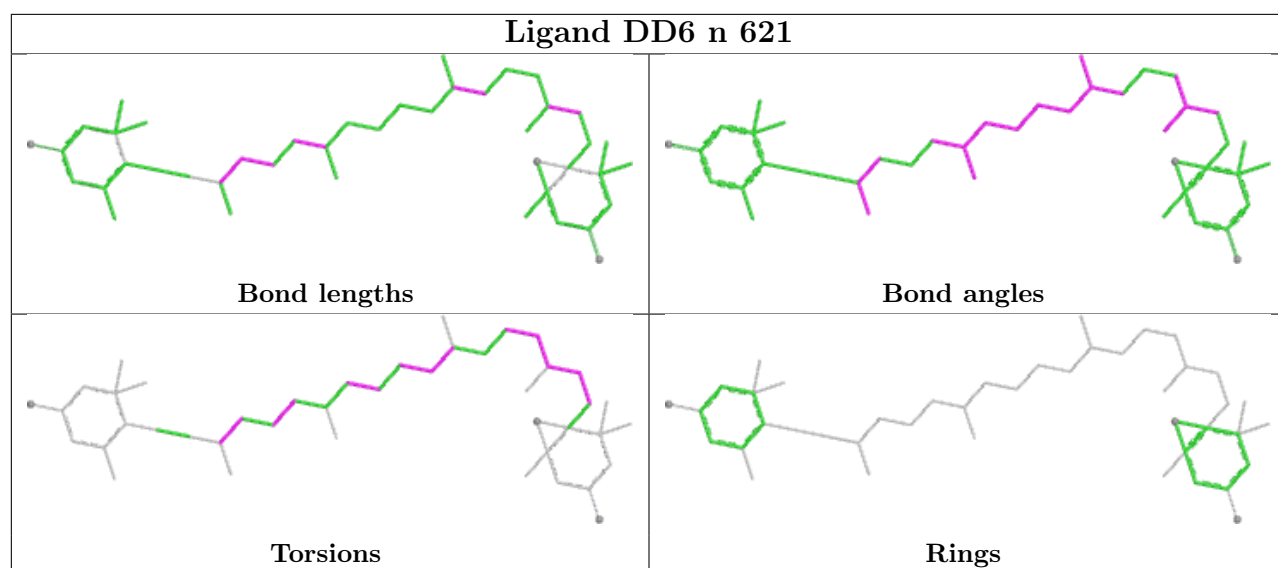


Ligand CLA a 602

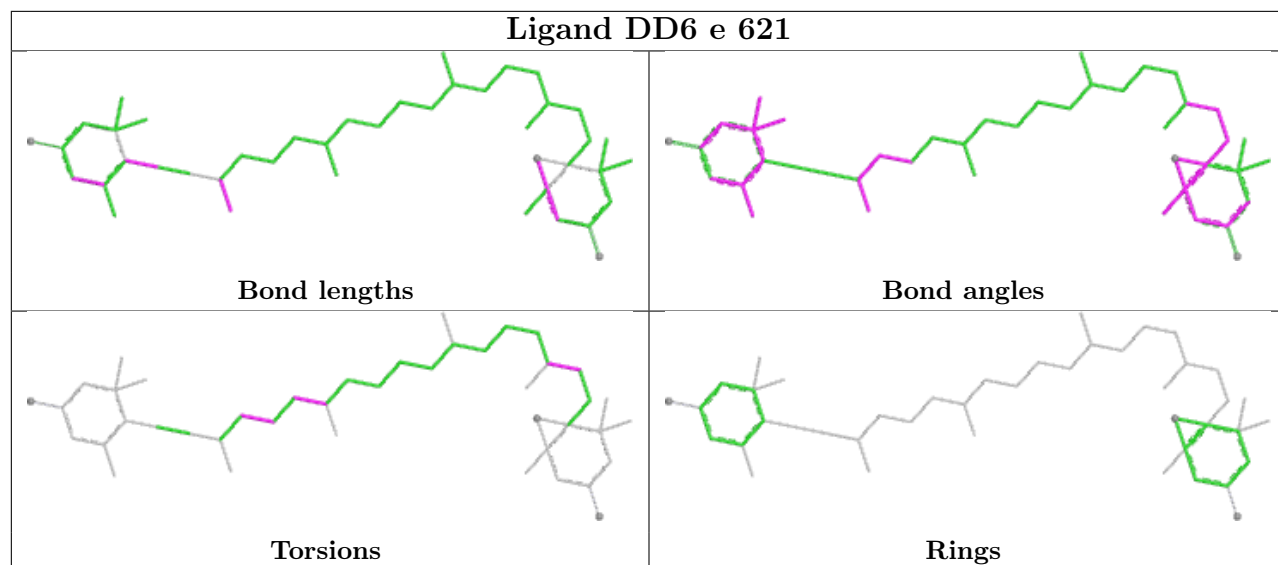


Ligand CLA e 611

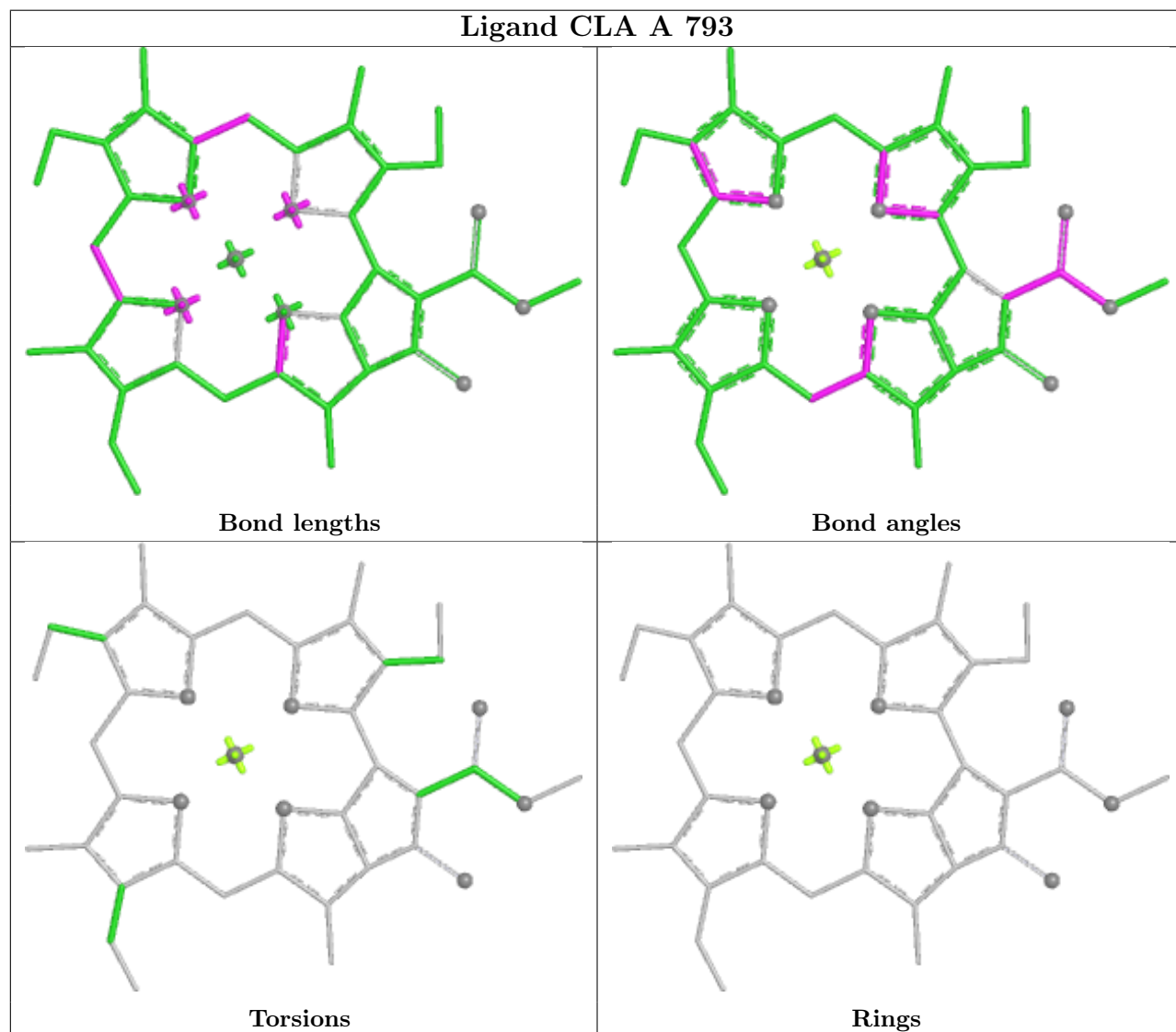




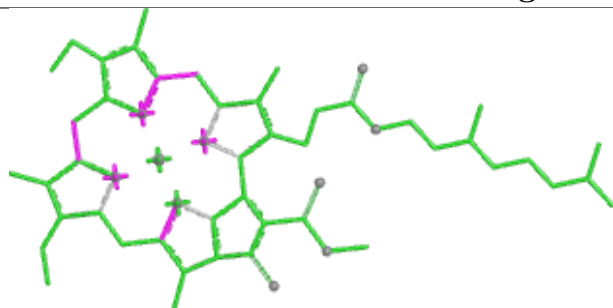
Ligand DD6 e 621



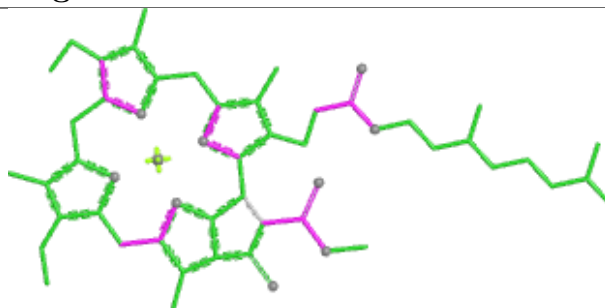
Ligand CLA A 793



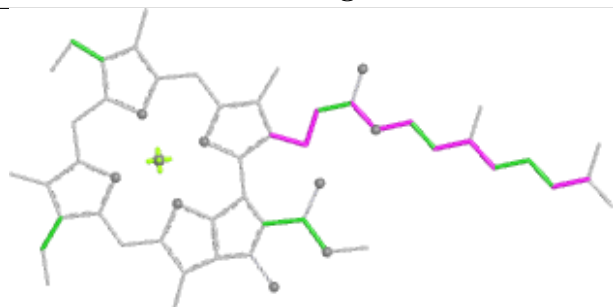
Ligand CLA g 613



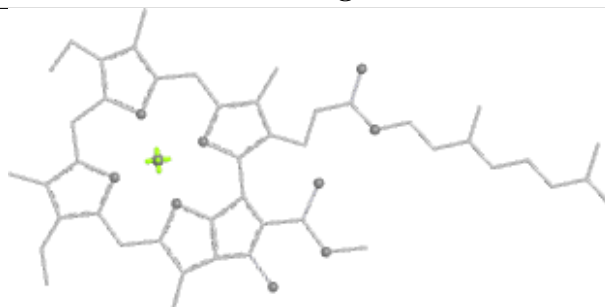
Bond lengths



Bond angles

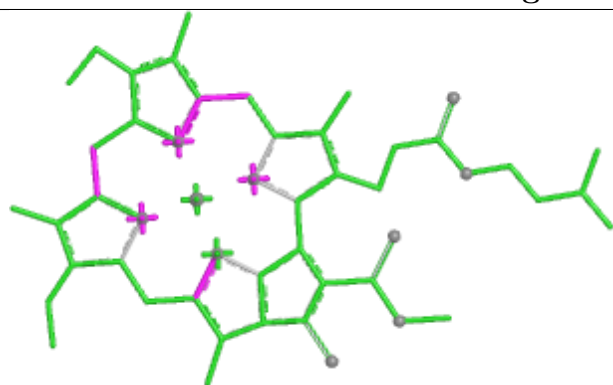


Torsions

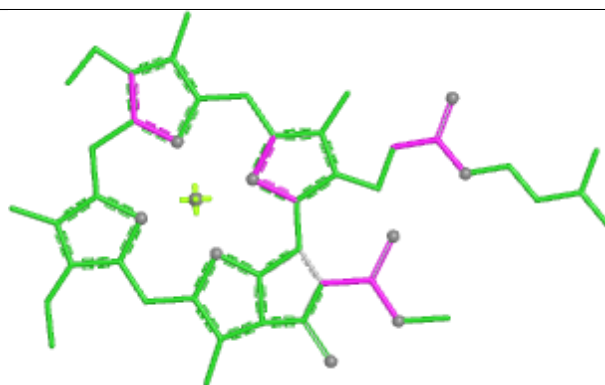


Rings

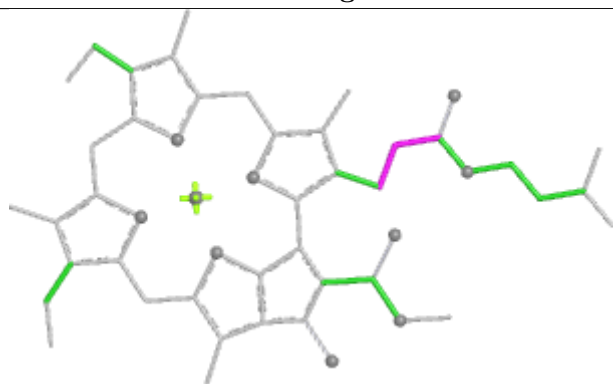
Ligand CLA i 615



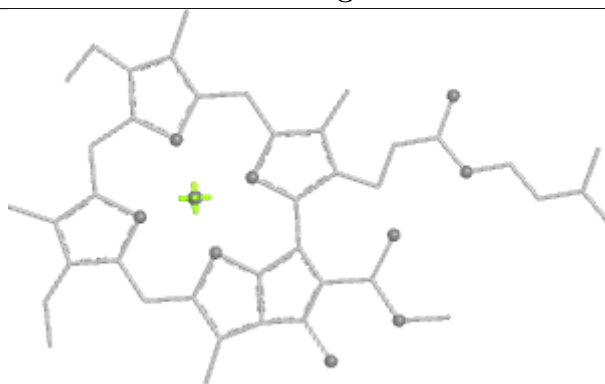
Bond lengths



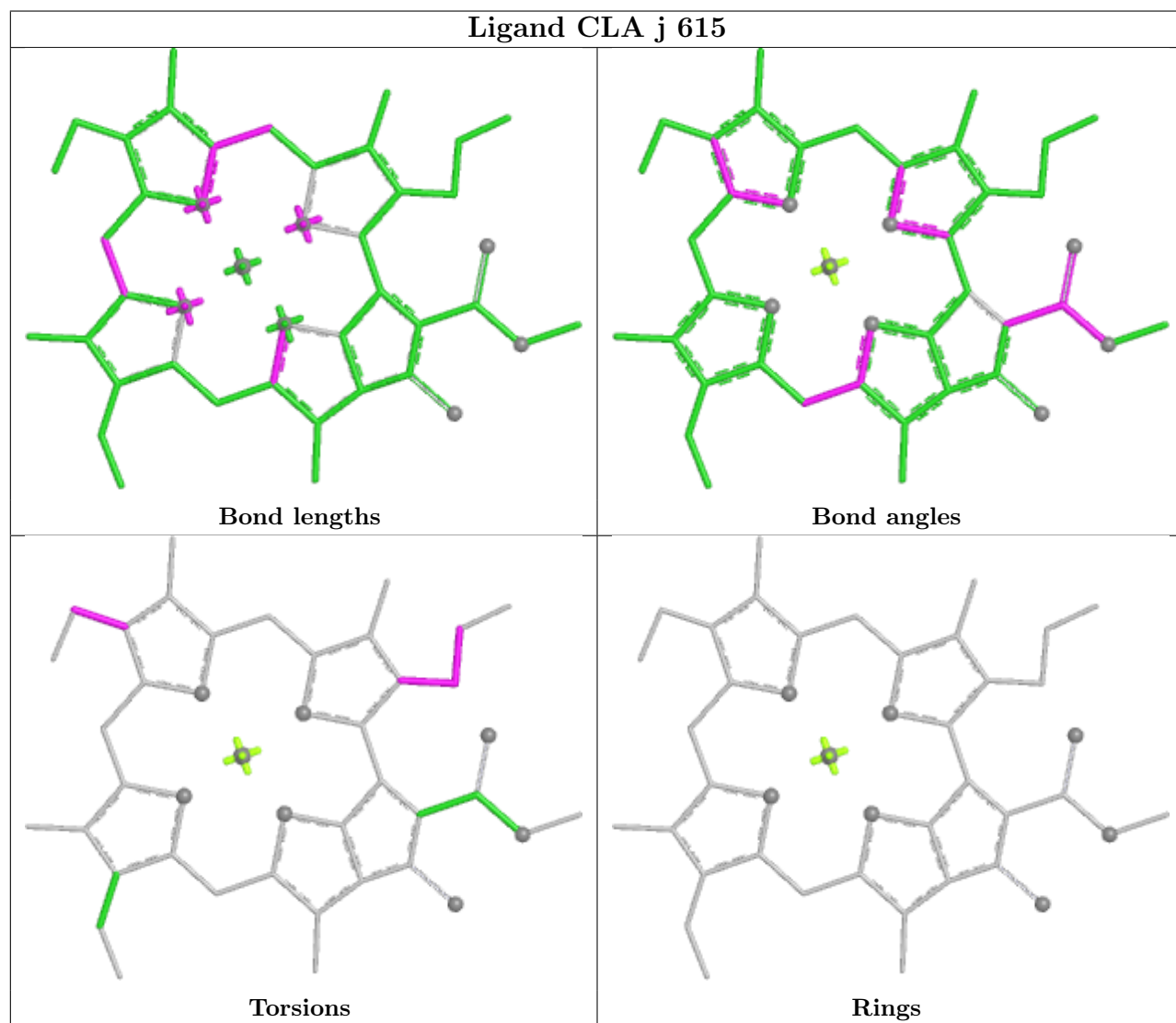
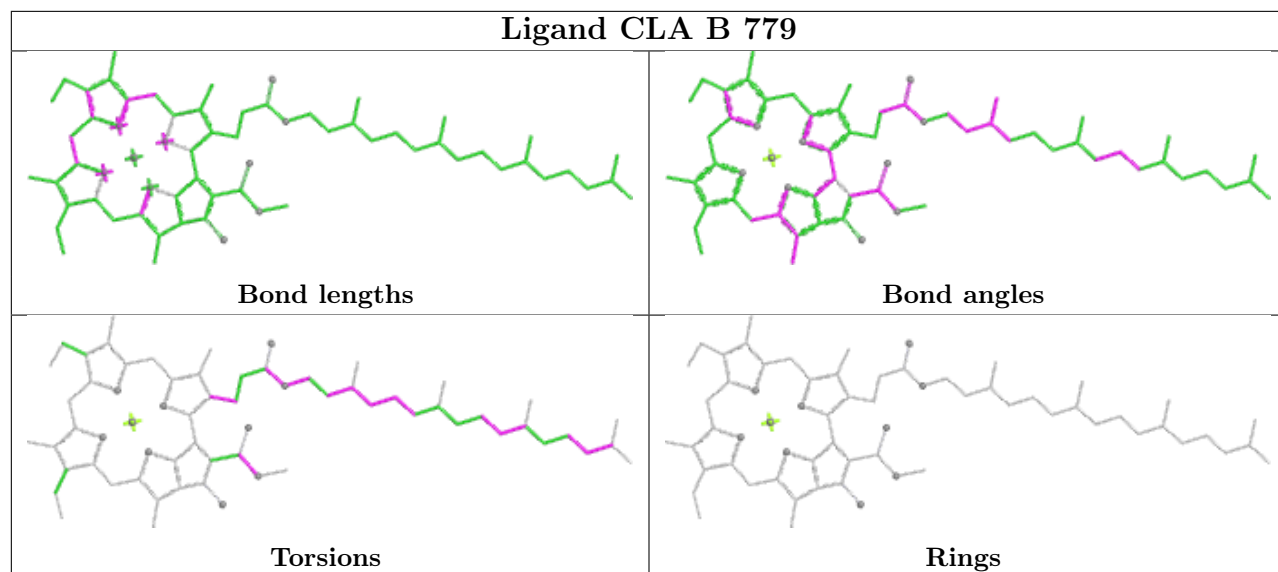
Bond angles



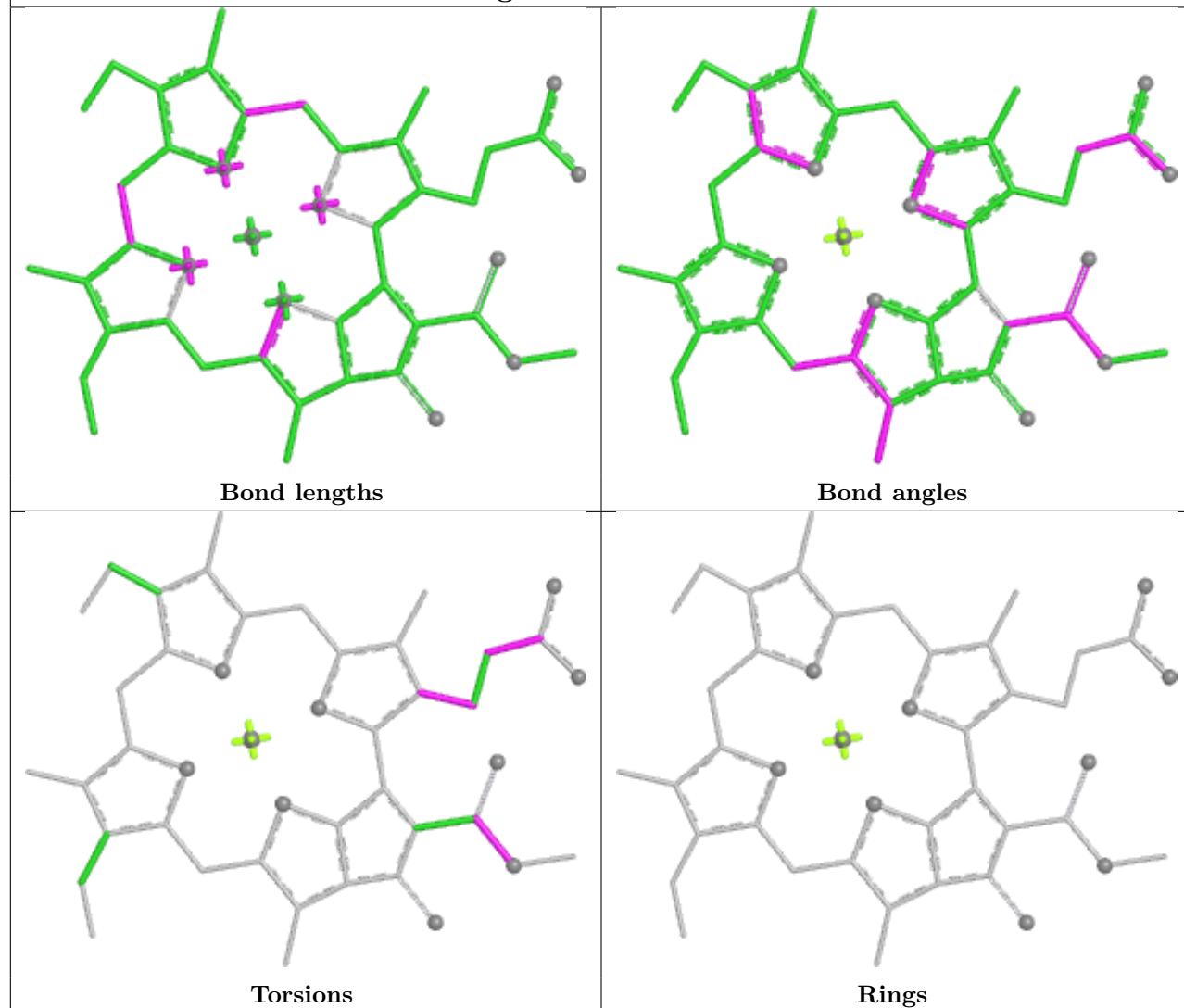
Torsions



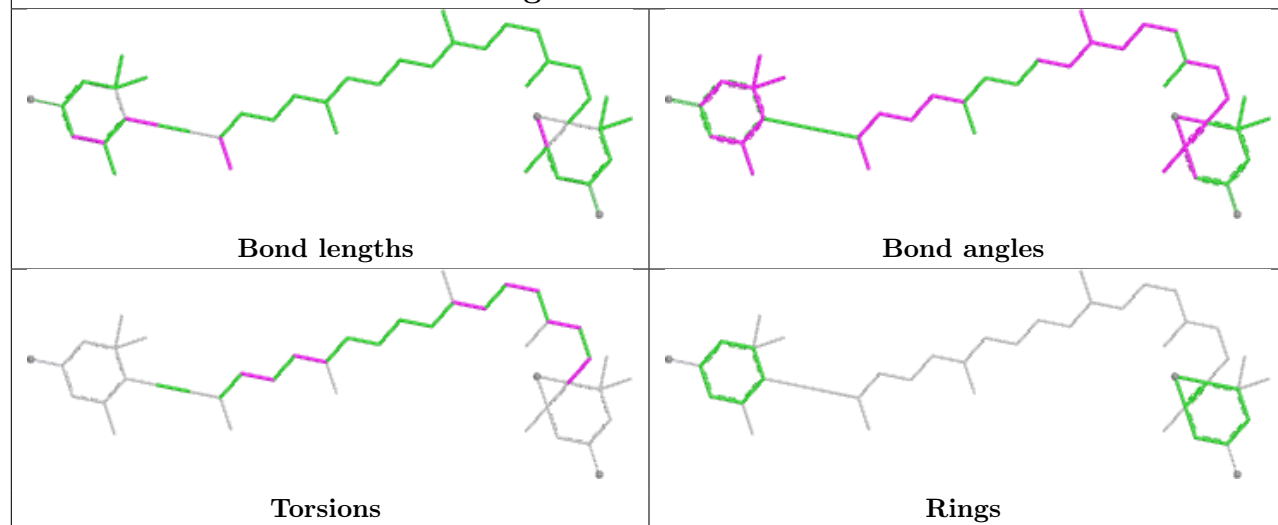
Rings



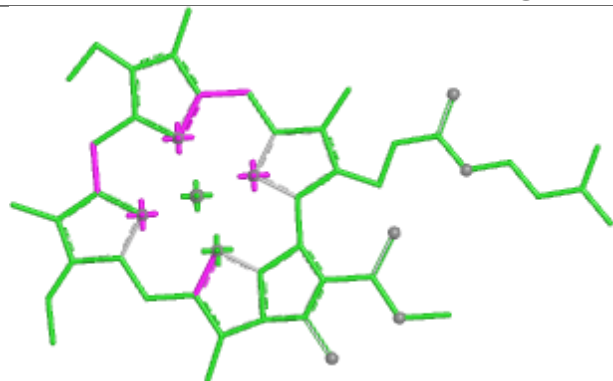
Ligand CLA o 609



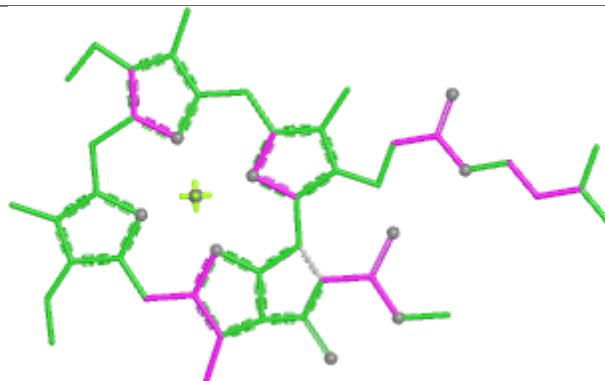
Ligand DD6 A 4008



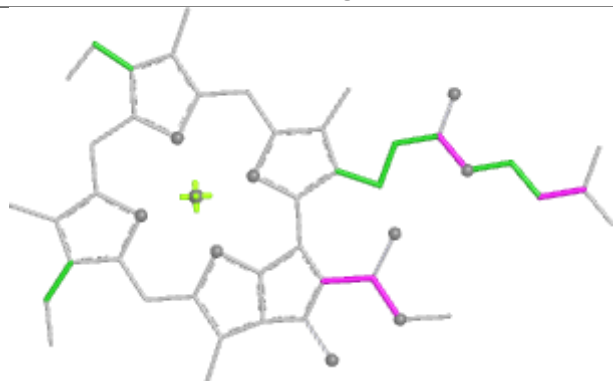
Ligand CLA d 601



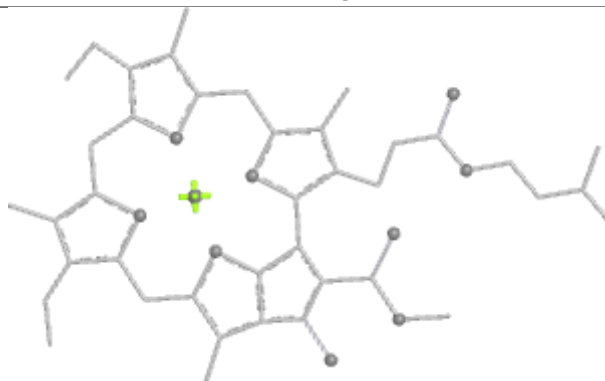
Bond lengths



Bond angles

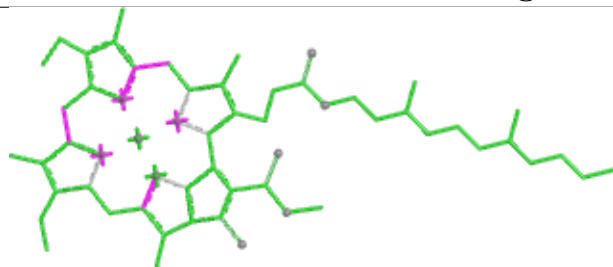


Torsions

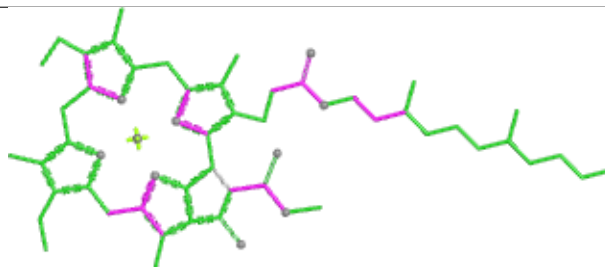


Rings

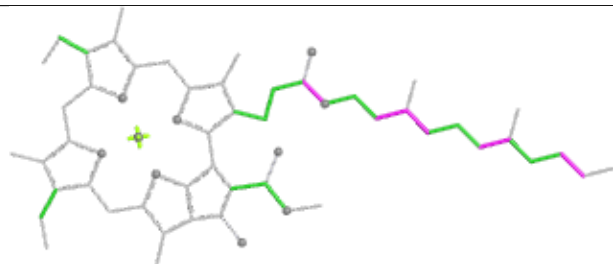
Ligand CLA h 612



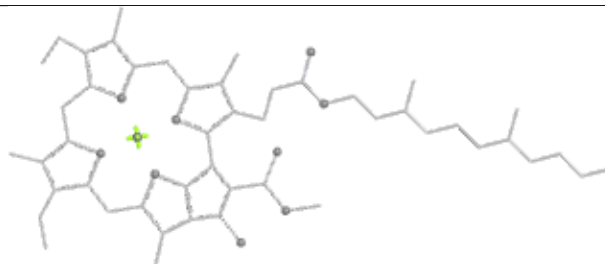
Bond lengths



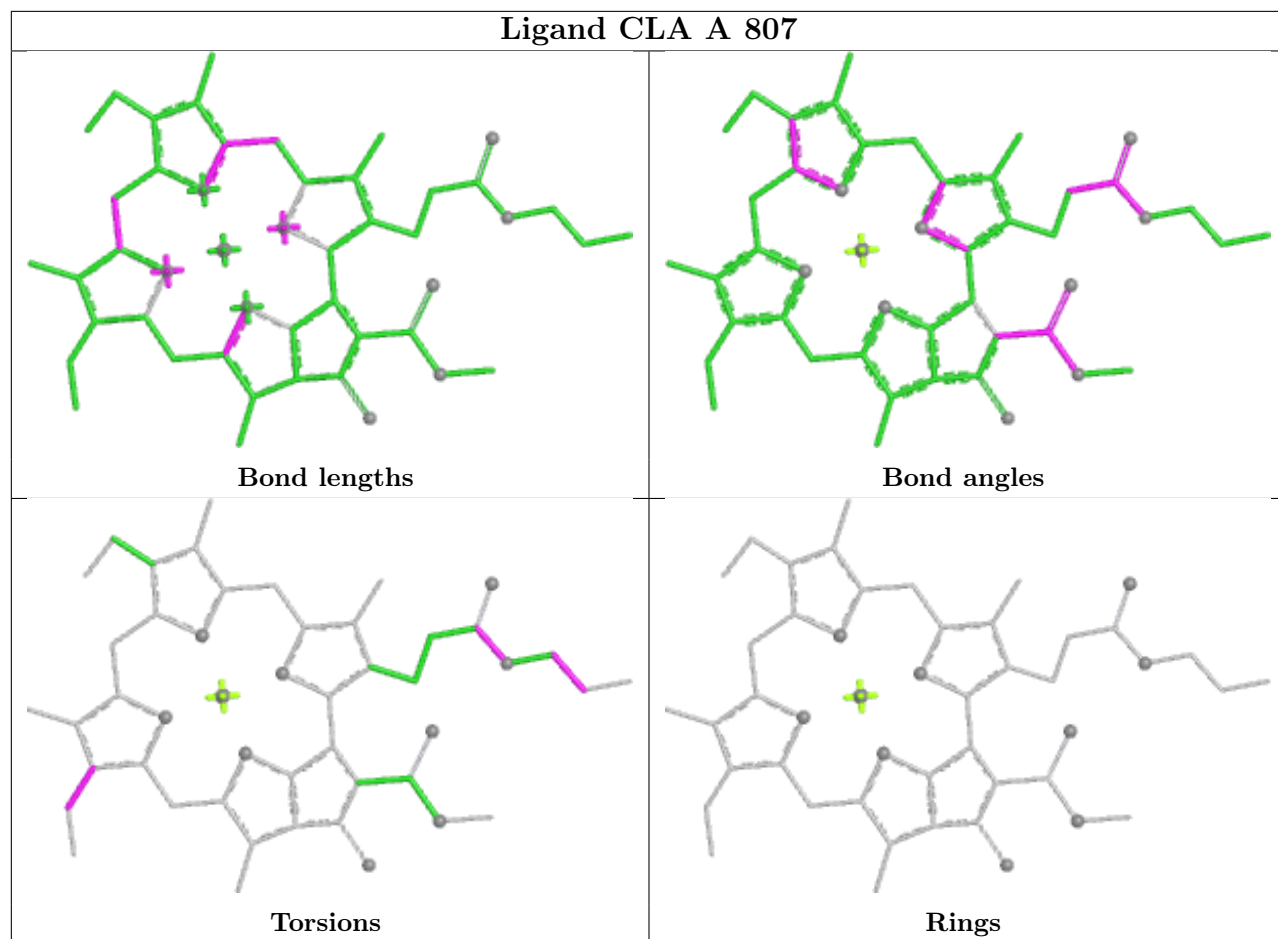
Bond angles



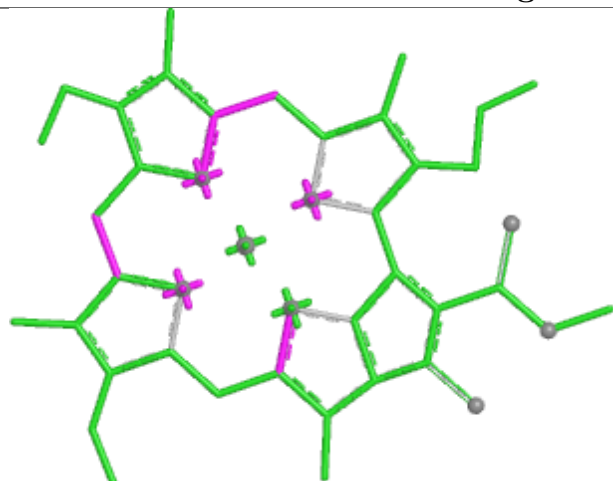
Torsions



Rings



Ligand CLA h 603



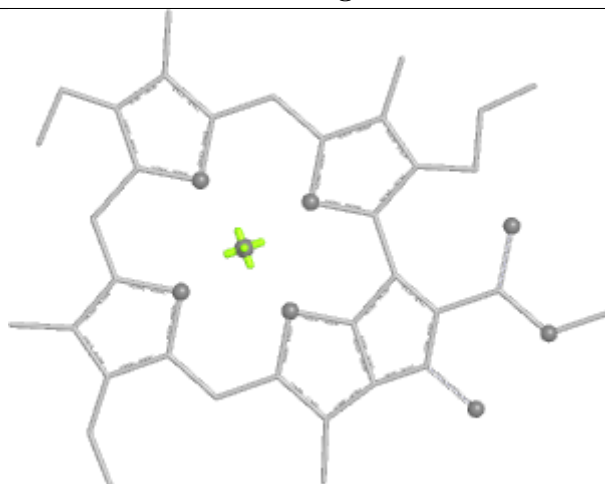
Bond lengths



Bond angles

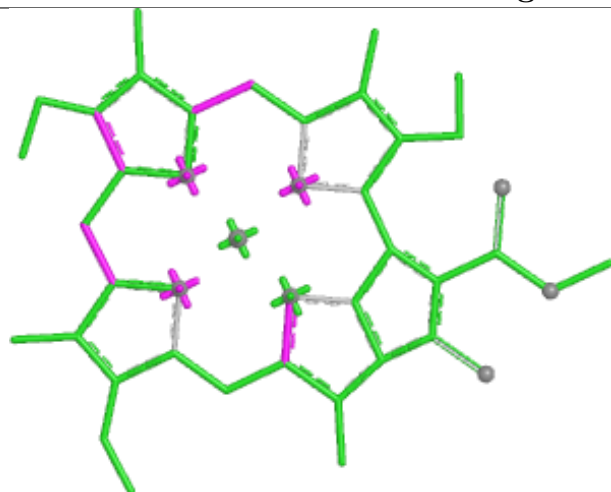


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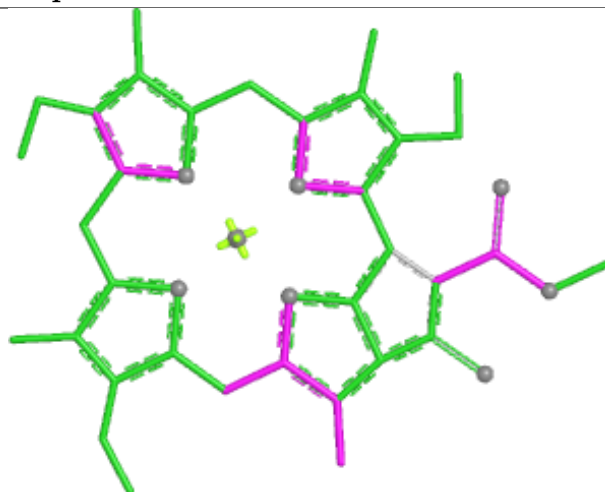


Rings

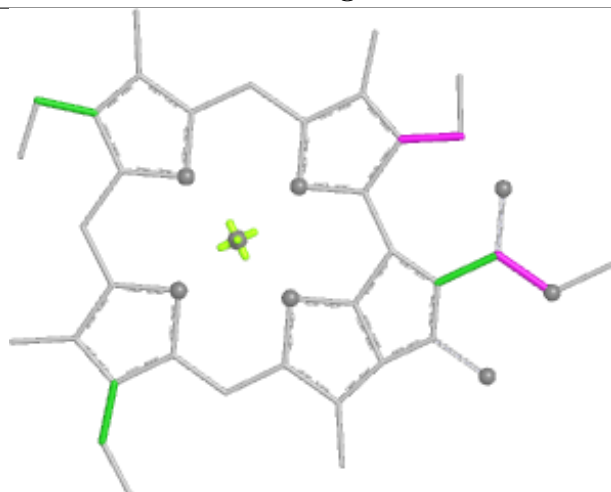
Ligand CLA p 601



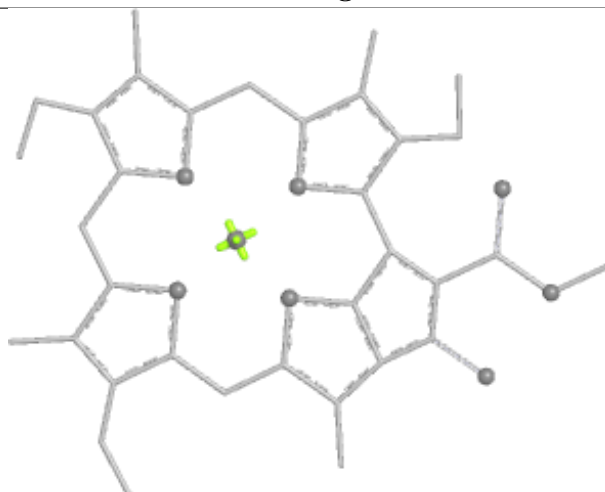
Bond lengths



Bond angles

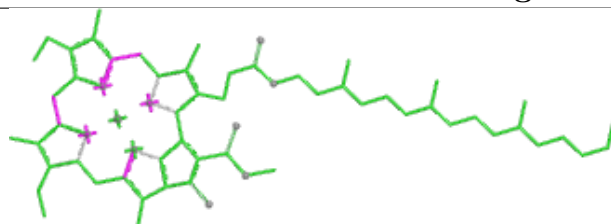


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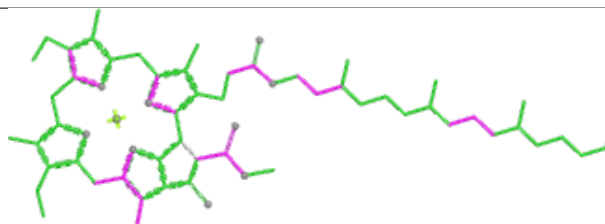


Rings

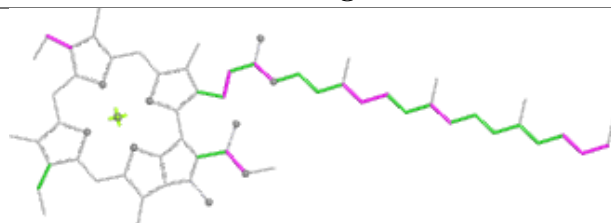
Ligand CLA B 746



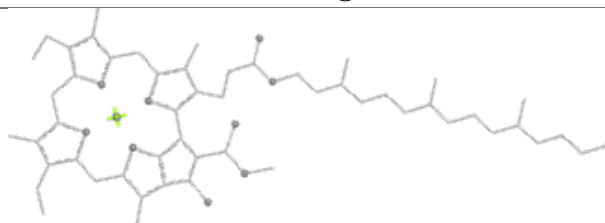
Bond lengths



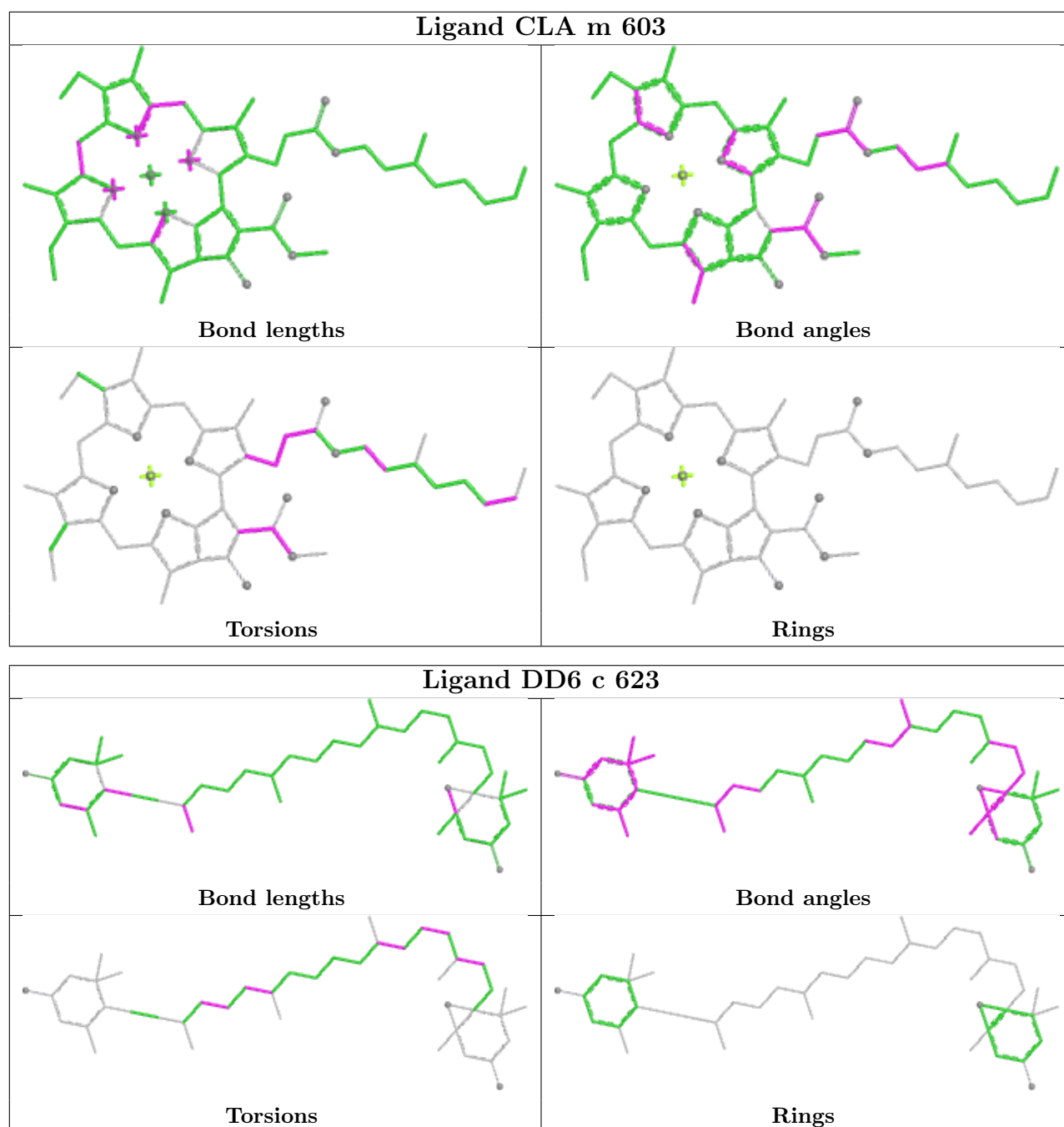
Bond angles



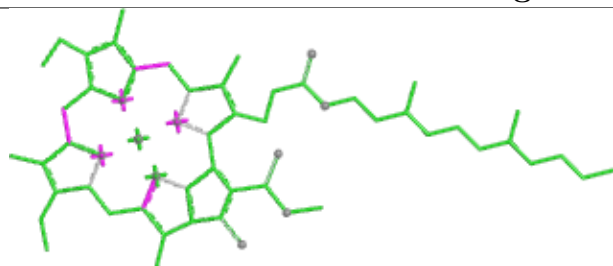
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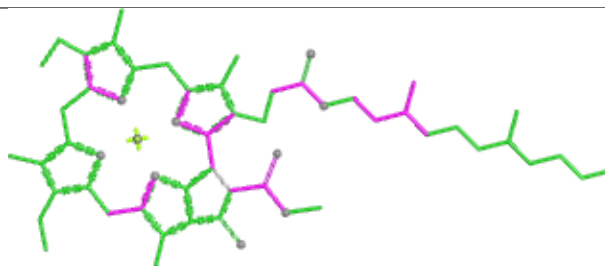
Rings



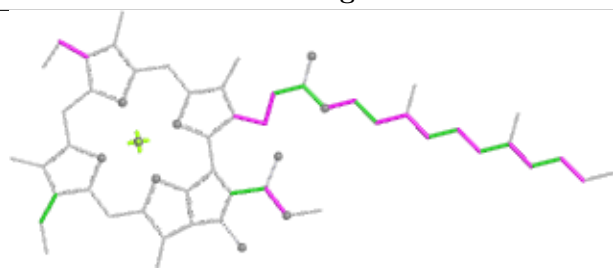
Ligand CLA A 775



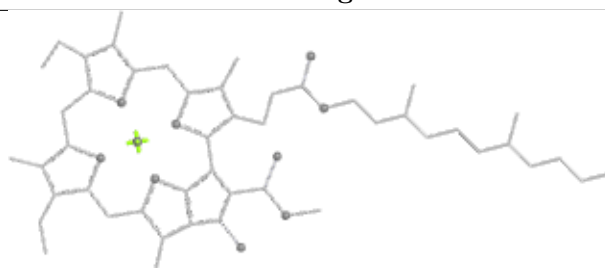
Bond lengths



Bond angles

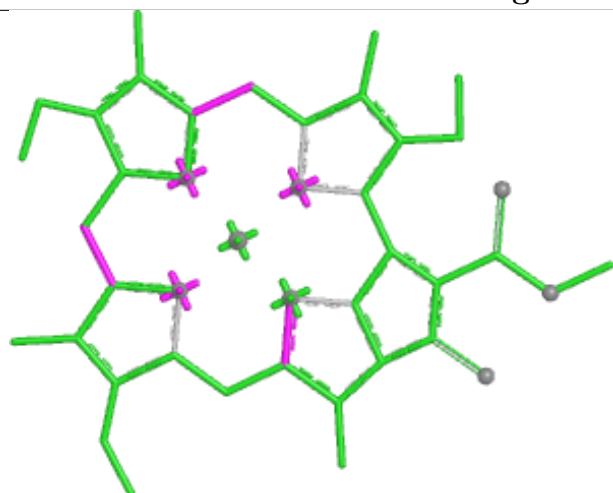


Torsions



Rings

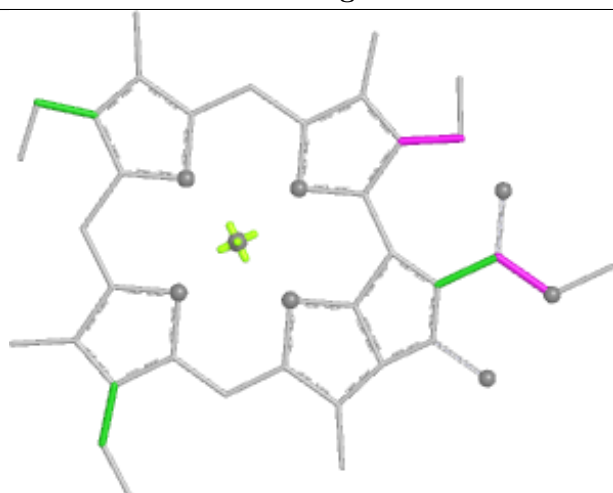
Ligand CLA m 601



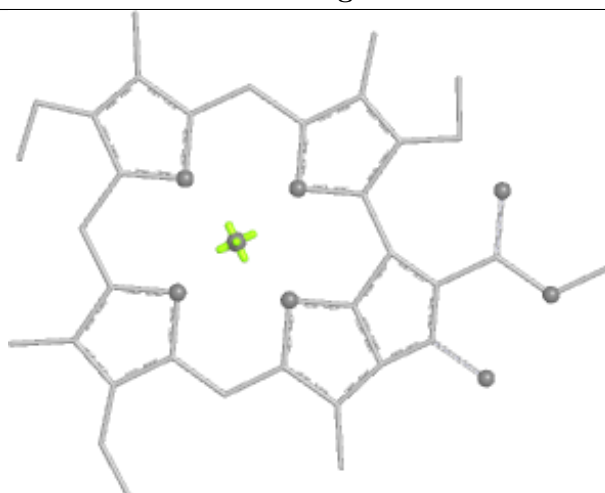
Bond lengths



Bond angles

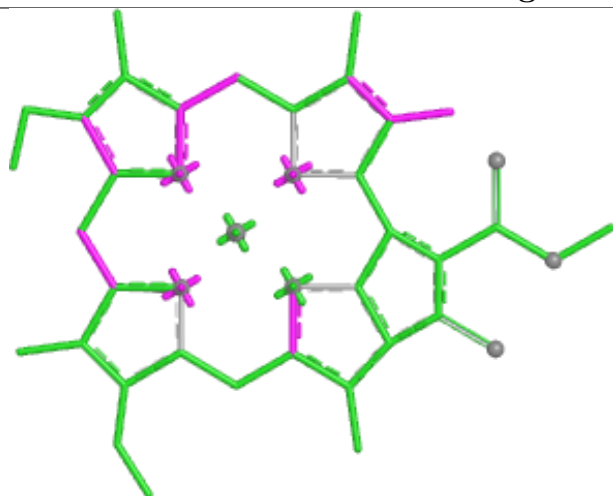


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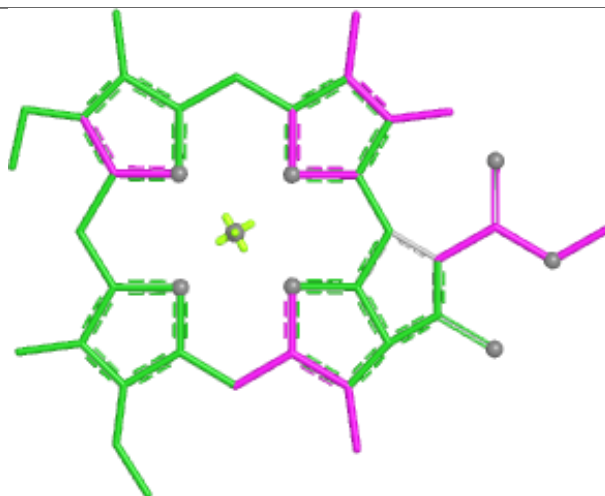


Rings

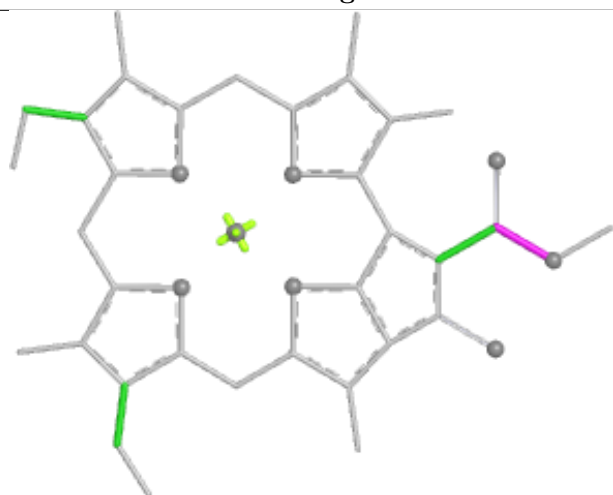
Ligand CLA o 601



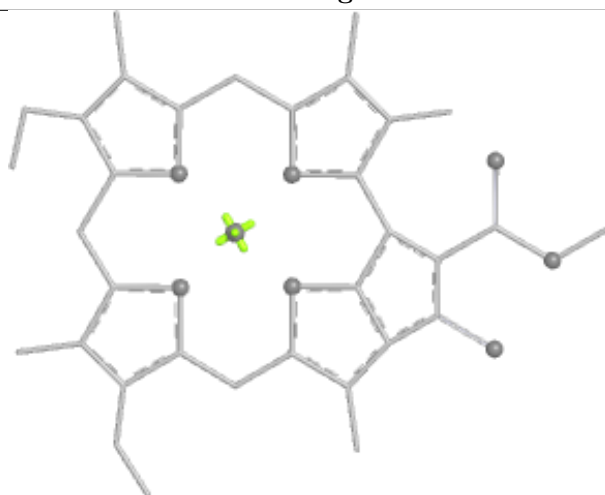
Bond lengths



Bond angles

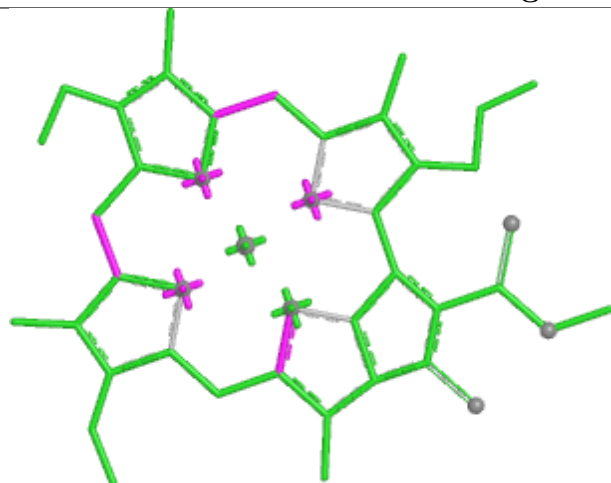


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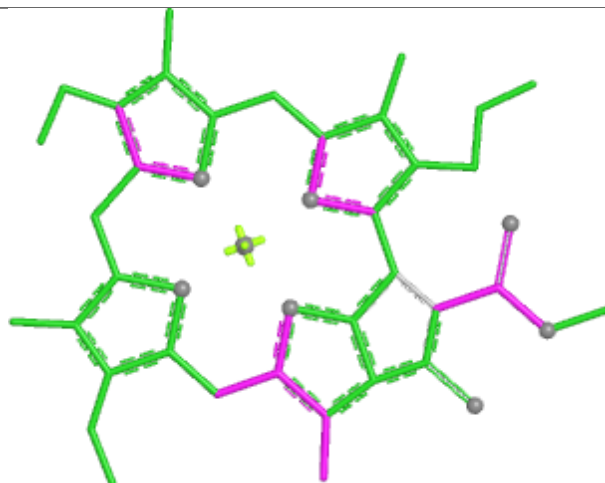


Rings

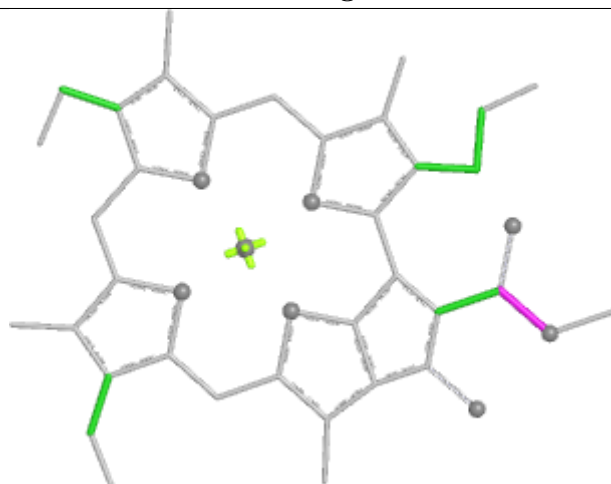
Ligand CLA f 603



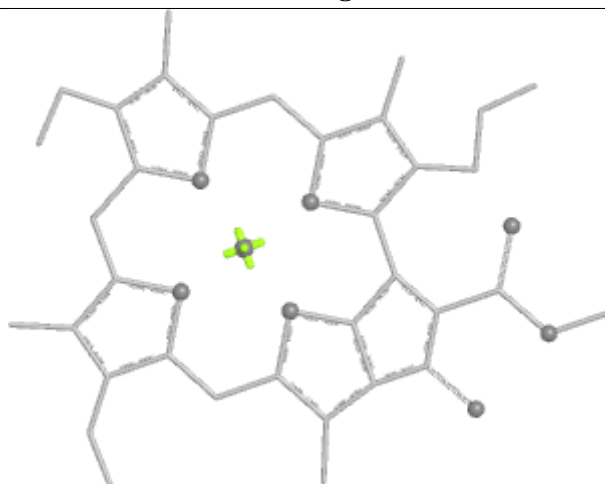
Bond lengths



Bond angles

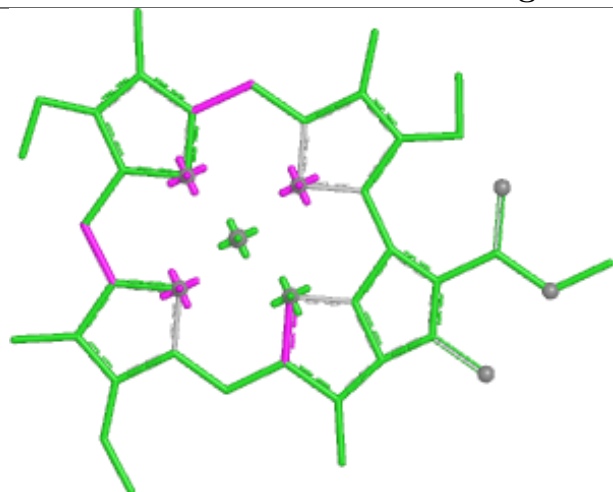


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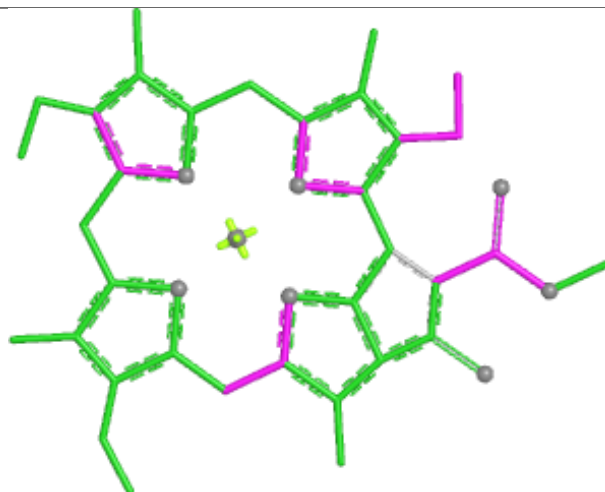


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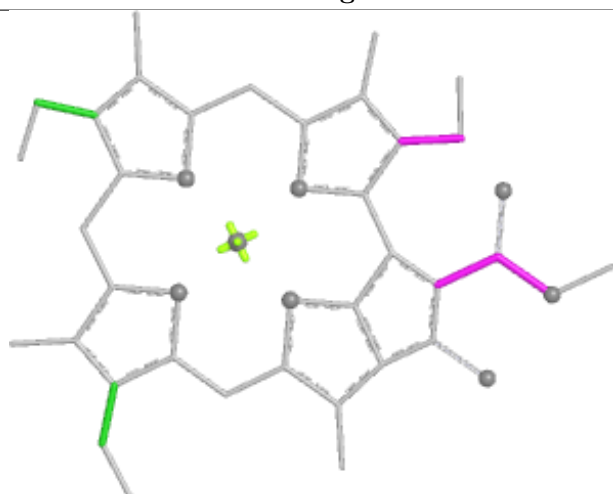
Ligand CLA o 613



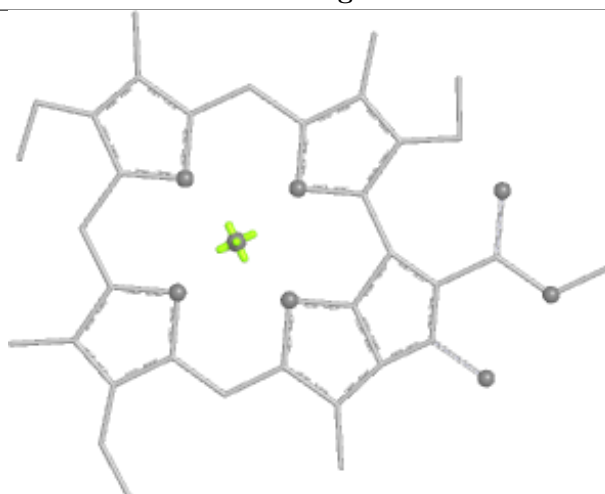
Bond lengths



Bond angles

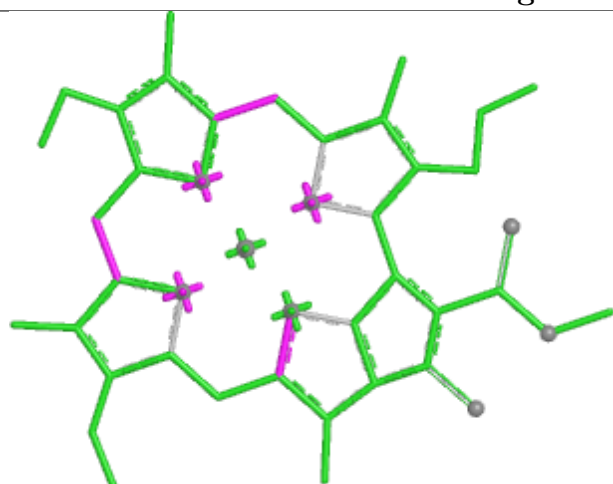


Torsions



Rings

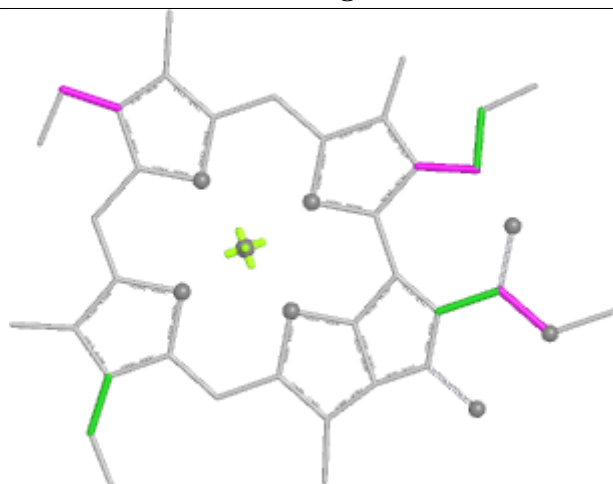
Ligand CLA h 614



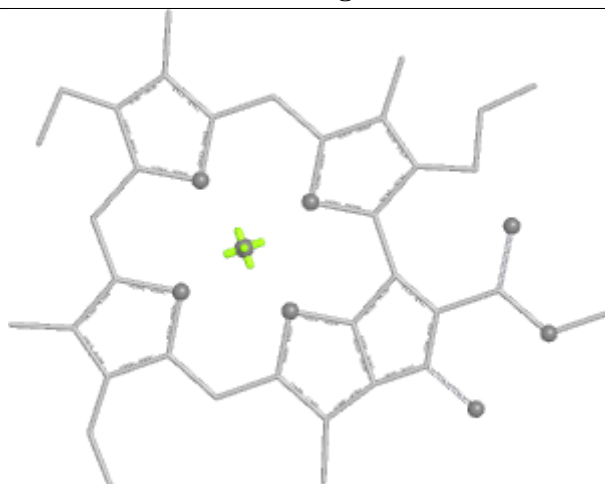
Bond lengths



Bond angles

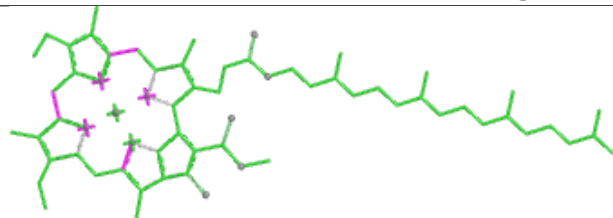


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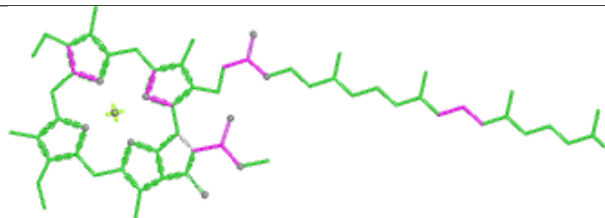


Rings

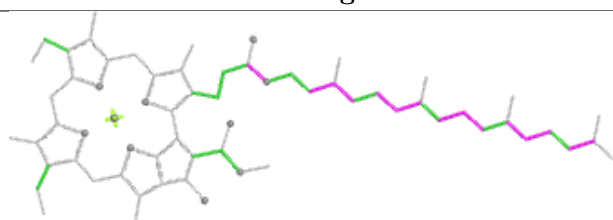
Ligand CLA B 752



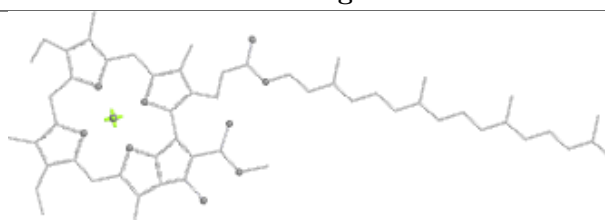
Bond lengths



Bond angles

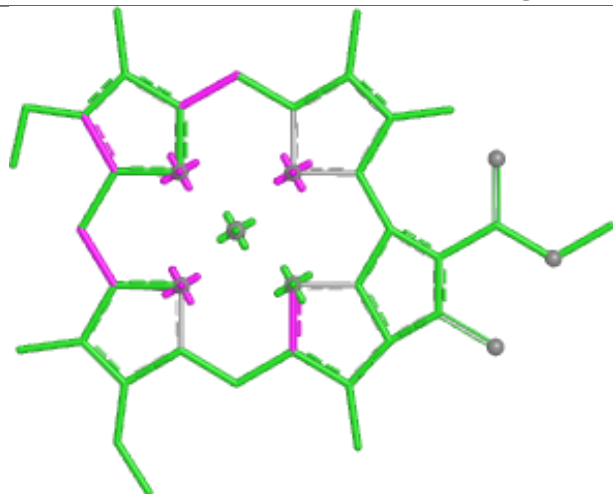


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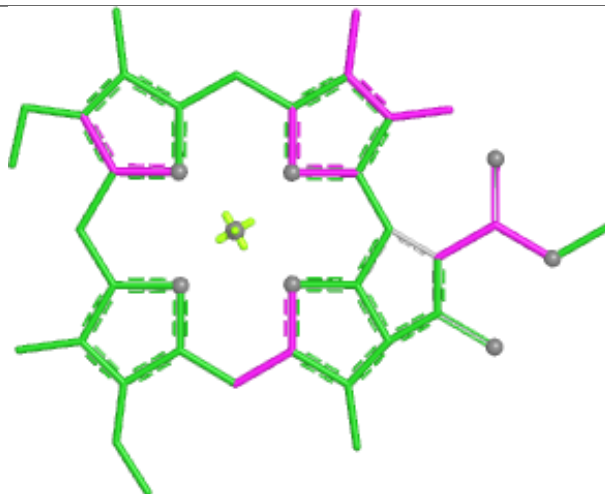


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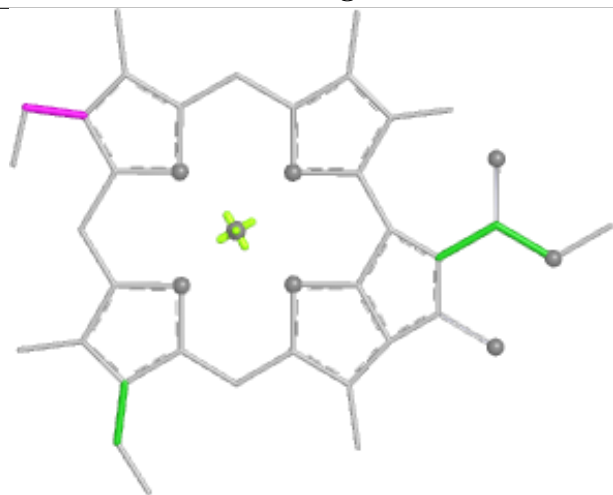
Ligand CLA n 610



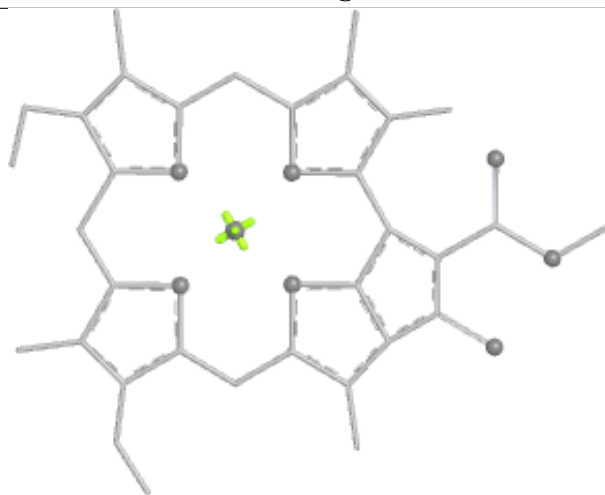
Bond lengths



Bond angles

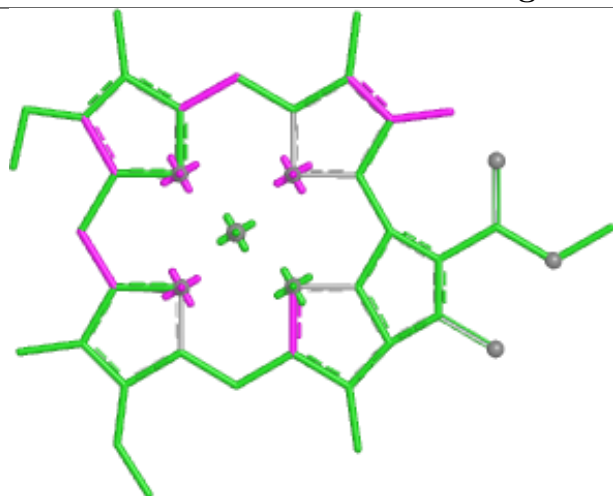


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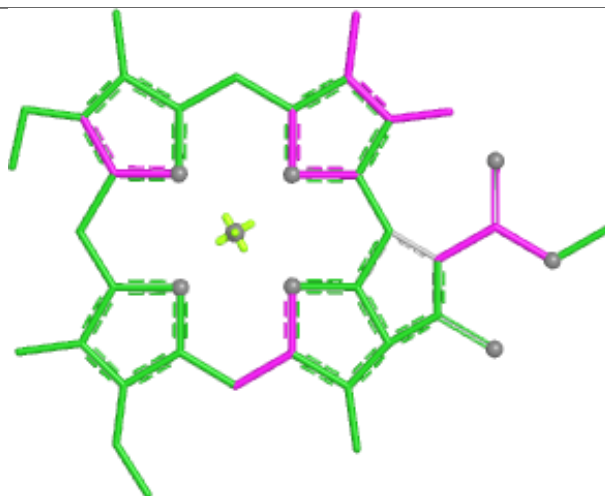


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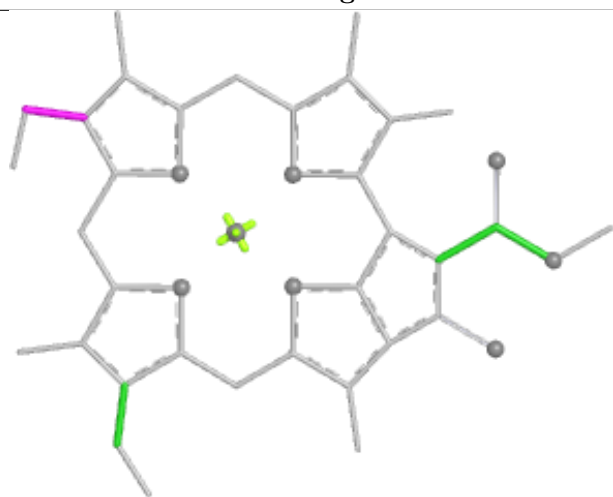
Ligand CLA o 610



Bond lengths



Bond angles

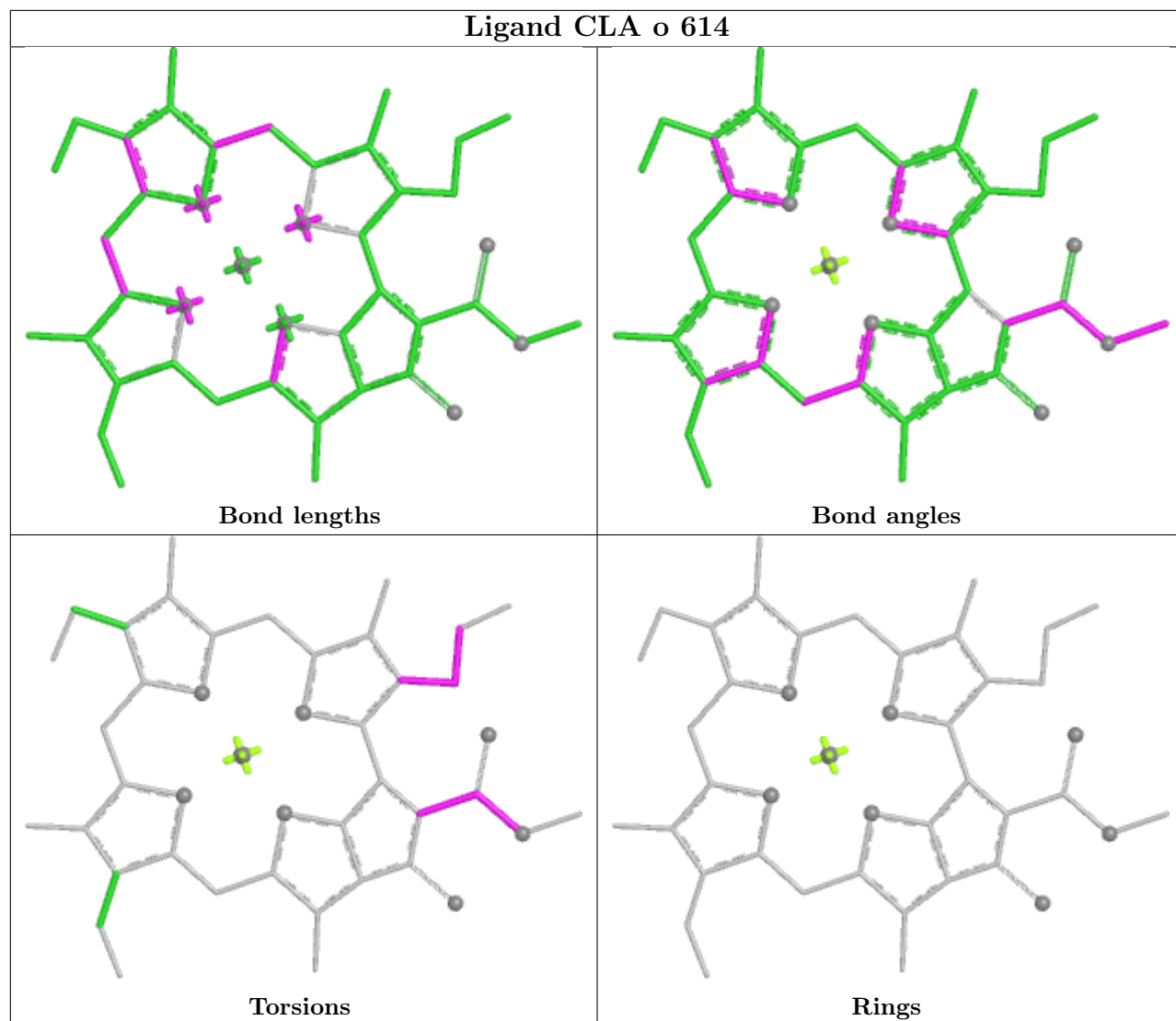


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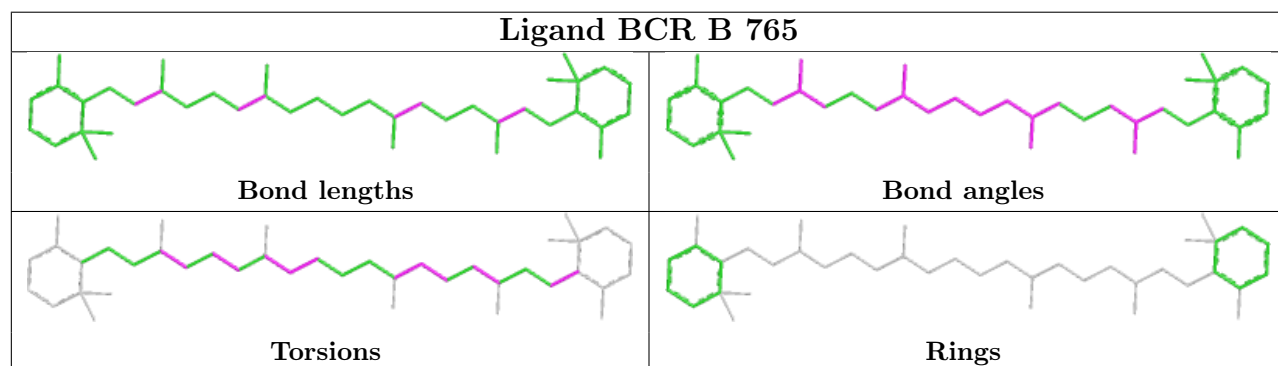


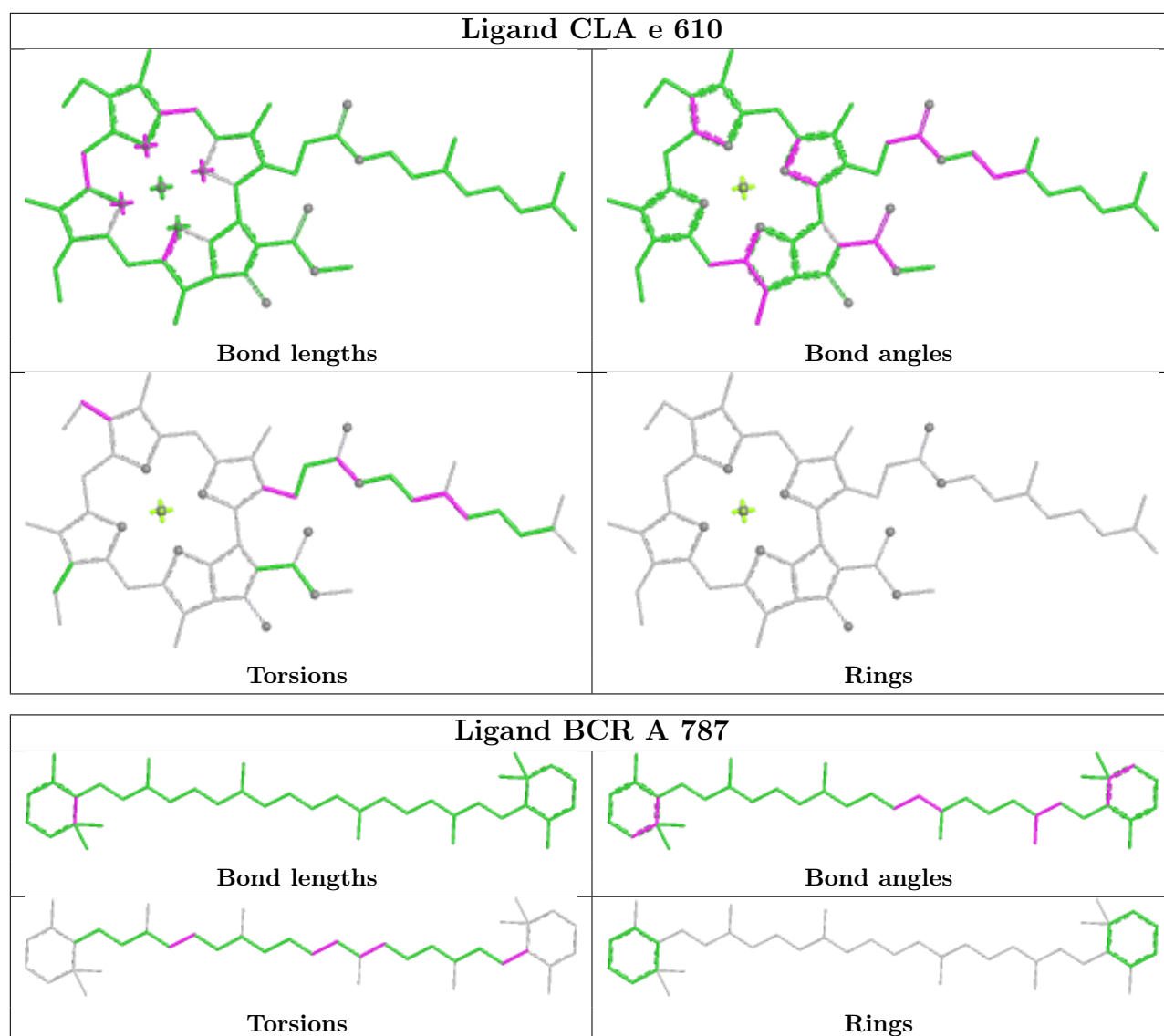
Rings

Ligand CLA o 614

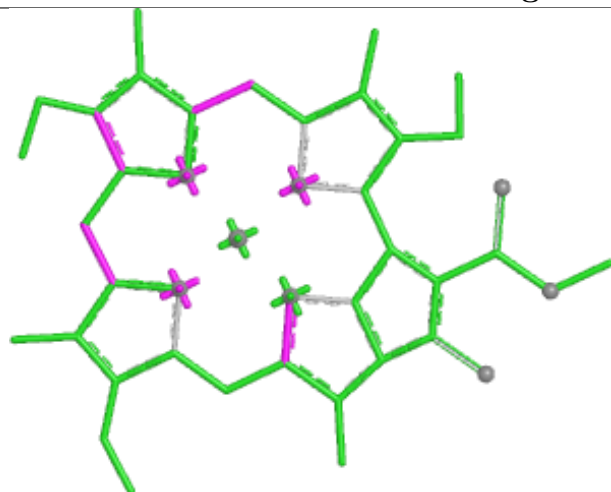


Ligand BCR B 765

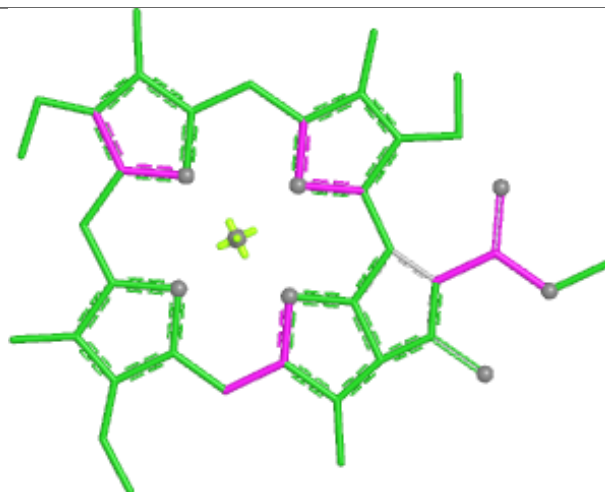




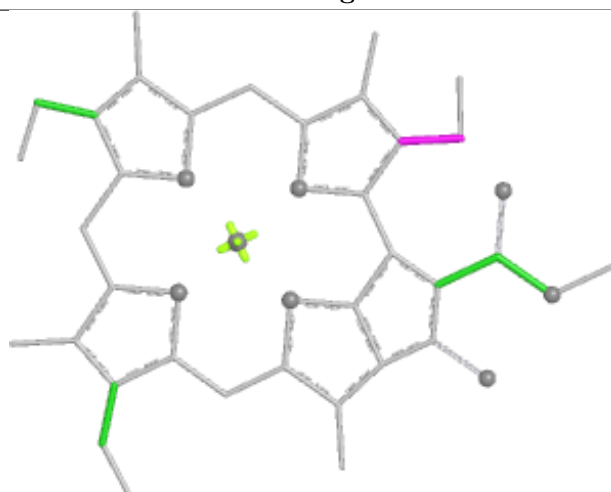
Ligand CLA f 611



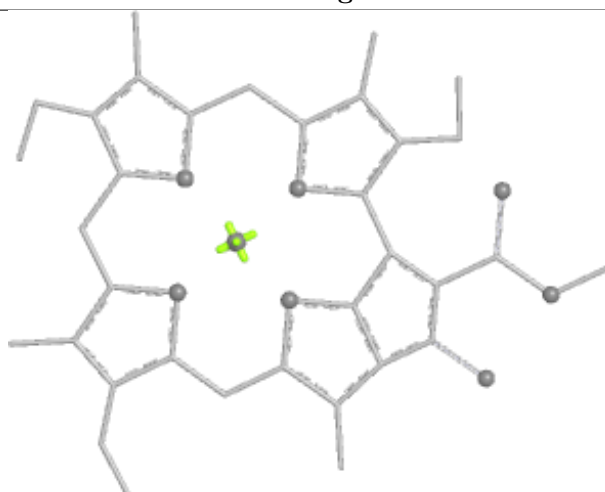
Bond lengths



Bond angles

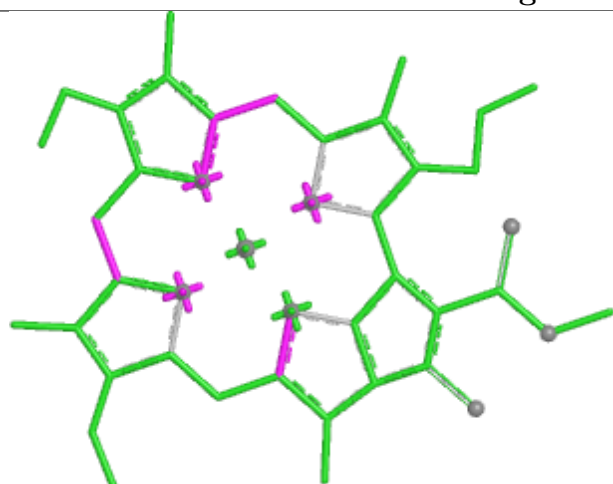


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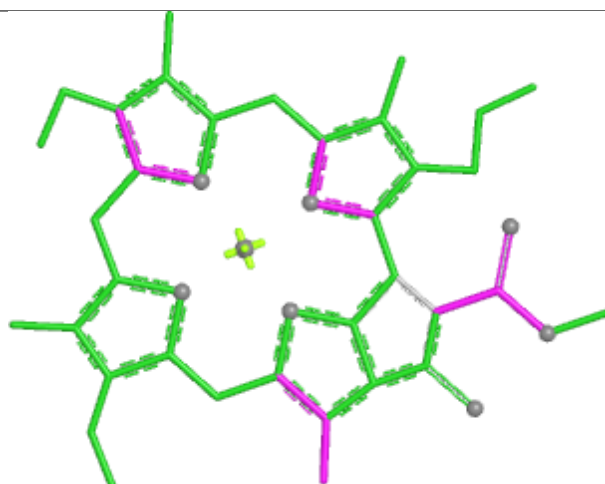


Rings

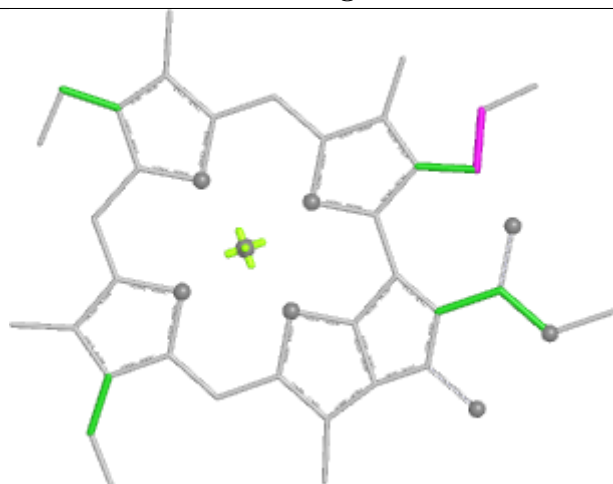
Ligand CLA e 612



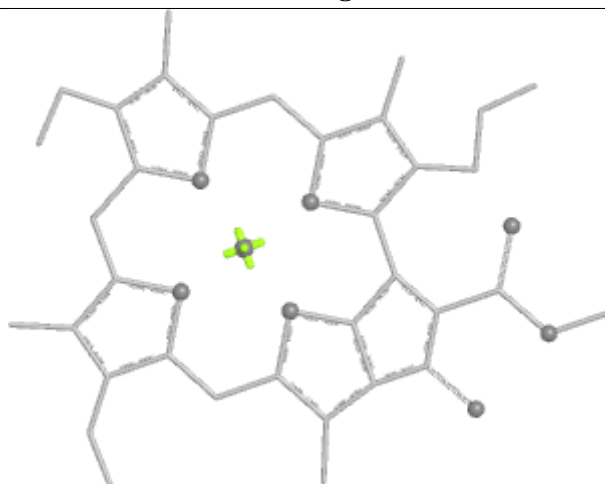
Bond lengths



Bond angles

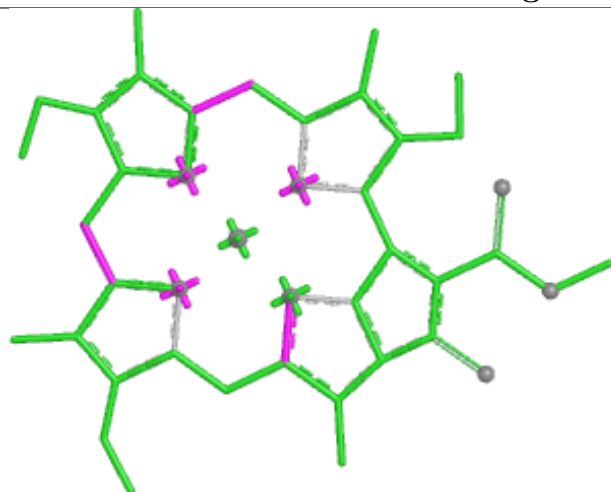


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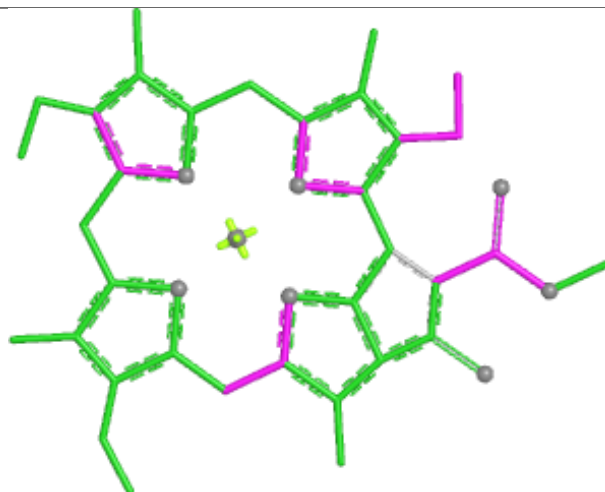


Rings

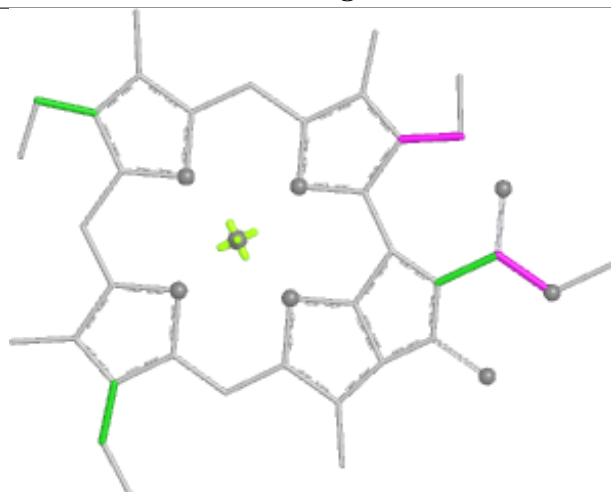
Ligand CLA 1 601



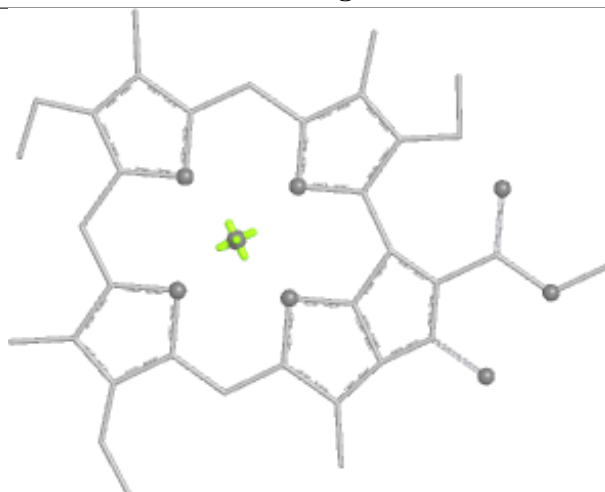
Bond lengths



Bond angles

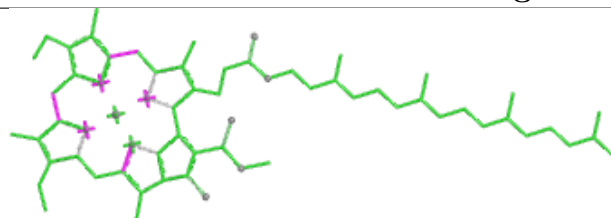


Torsions

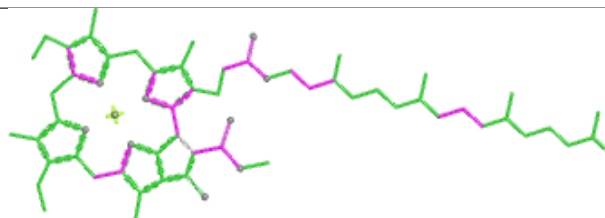


Rings

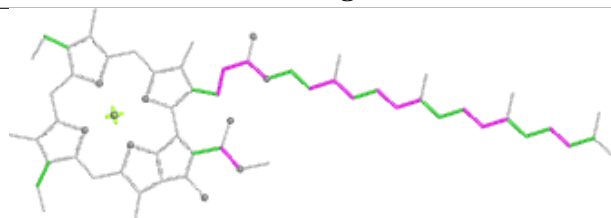
Ligand CLA A 784



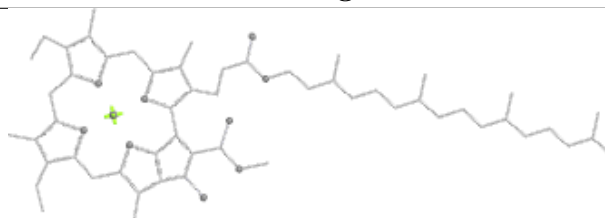
Bond lengths



Bond angles

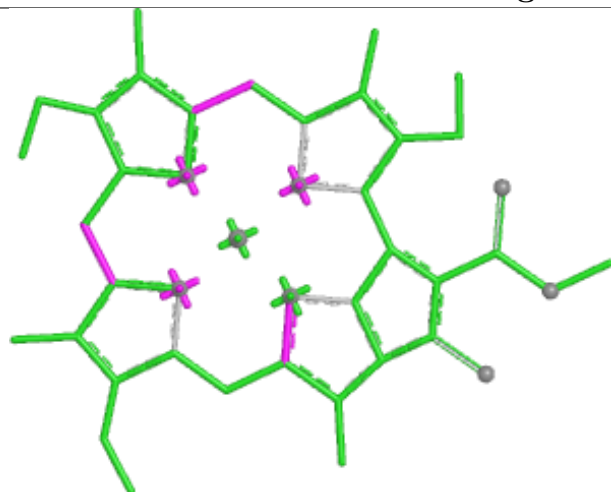


Torsions

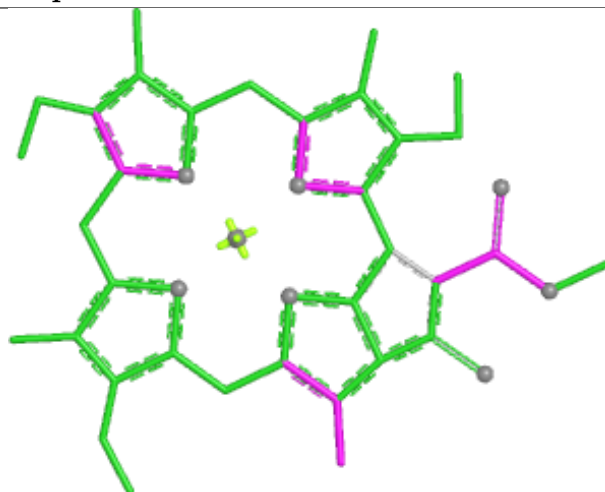


Rings

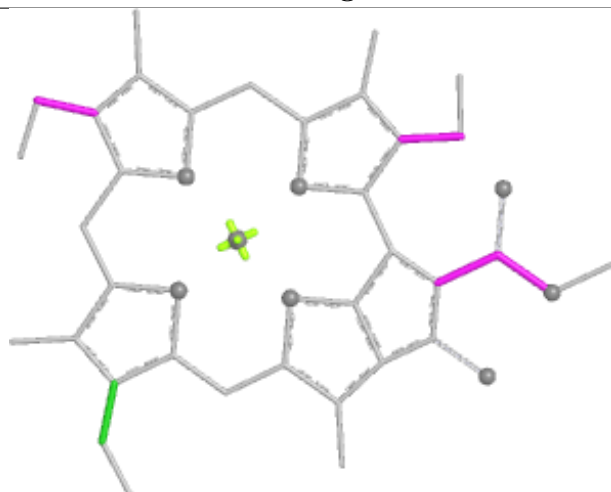
Ligand CLA p 608



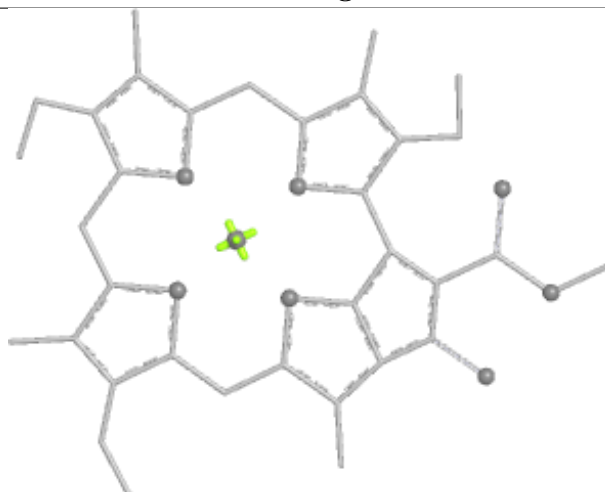
Bond lengths



Bond angles

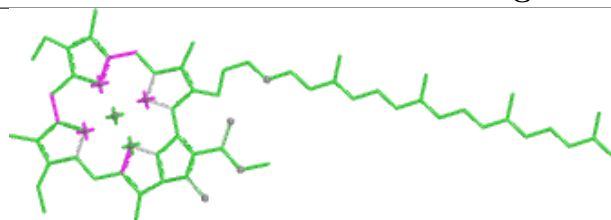


Torsions

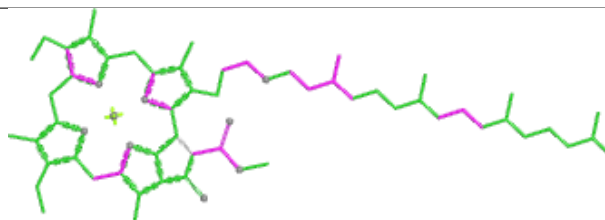


Rings

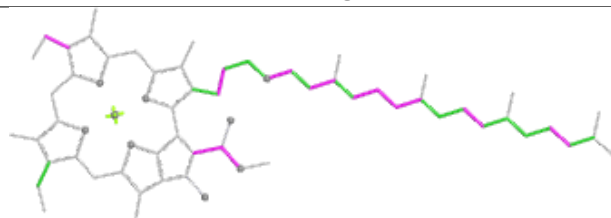
Ligand CLA A 772



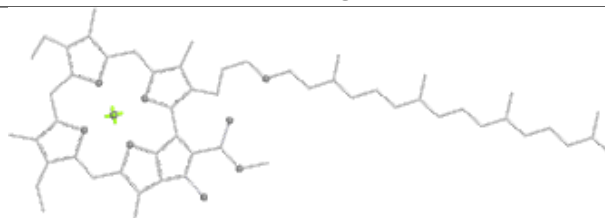
Bond lengths



Bond angles

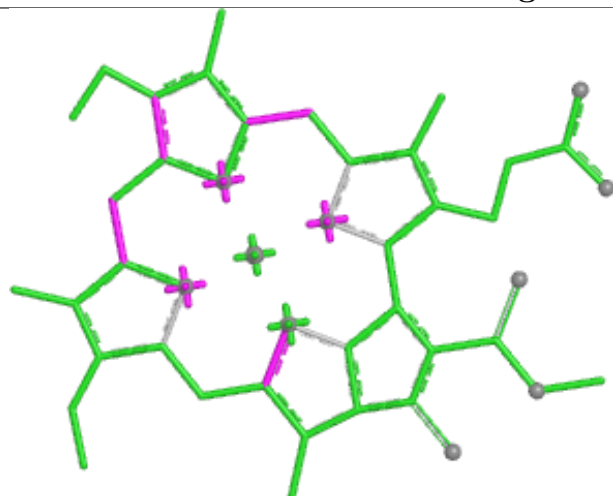


Torsions

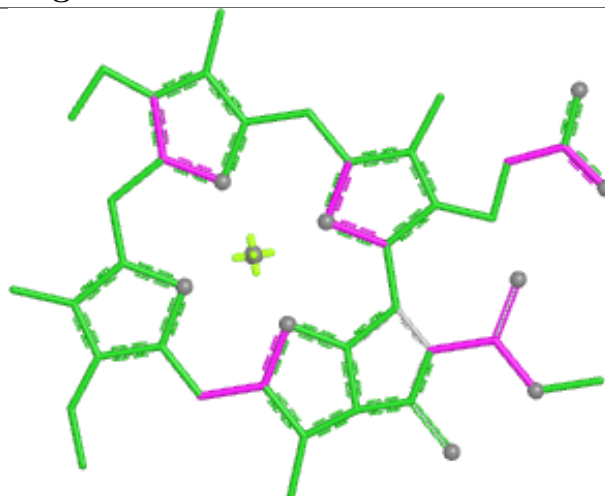


Rings

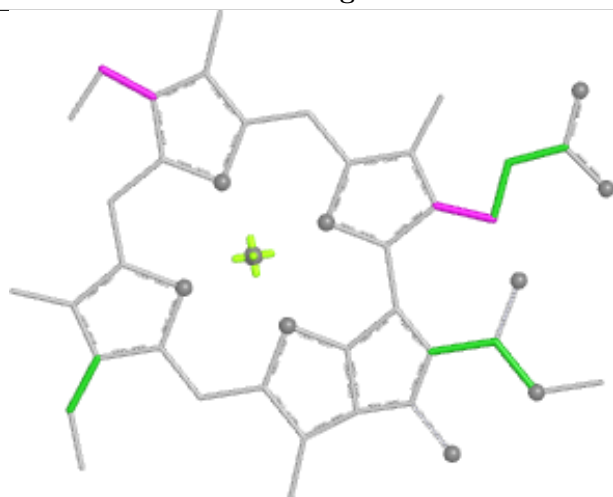
Ligand CLA g 618



Bond lengths



Bond angles

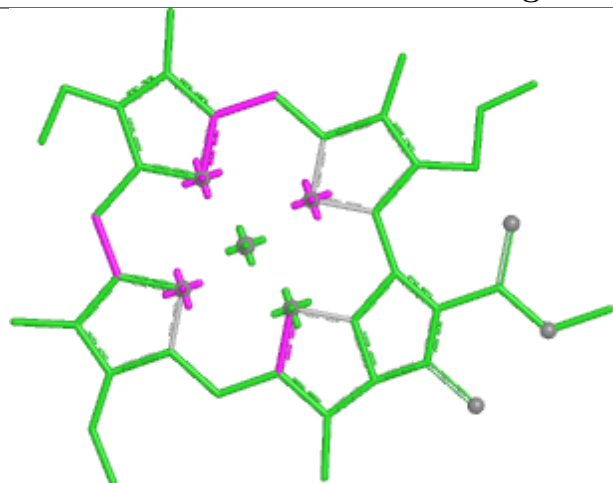


Torsions

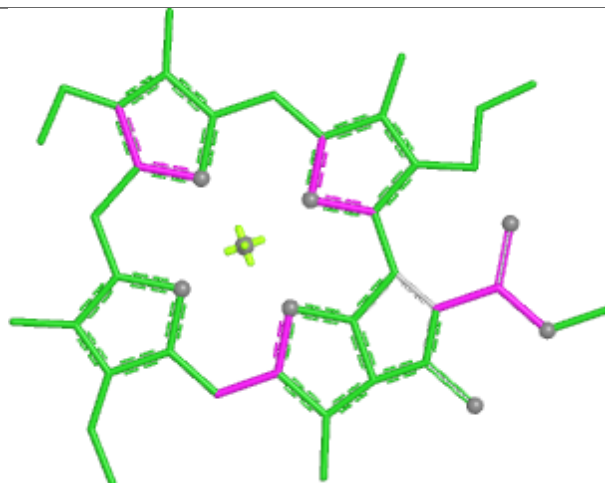


Rings

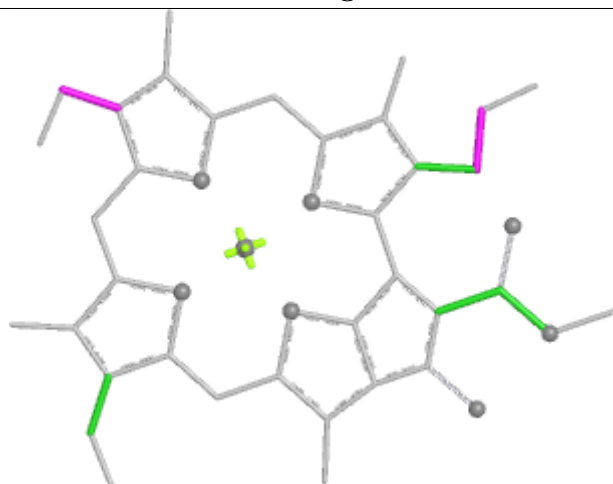
Ligand CLA i 604



Bond lengths



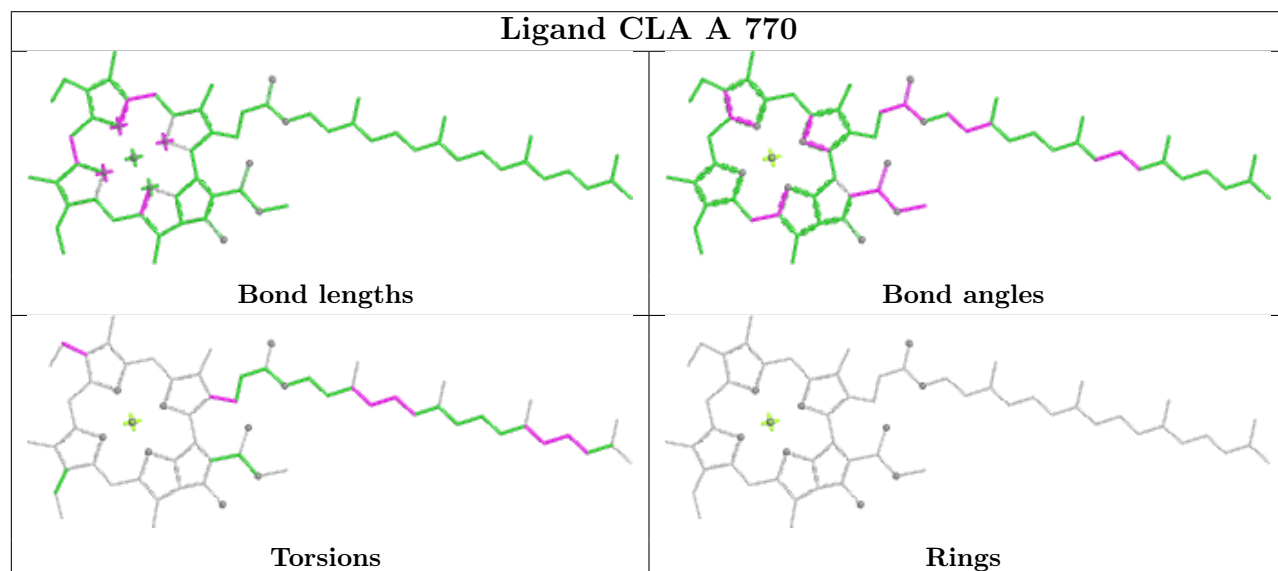
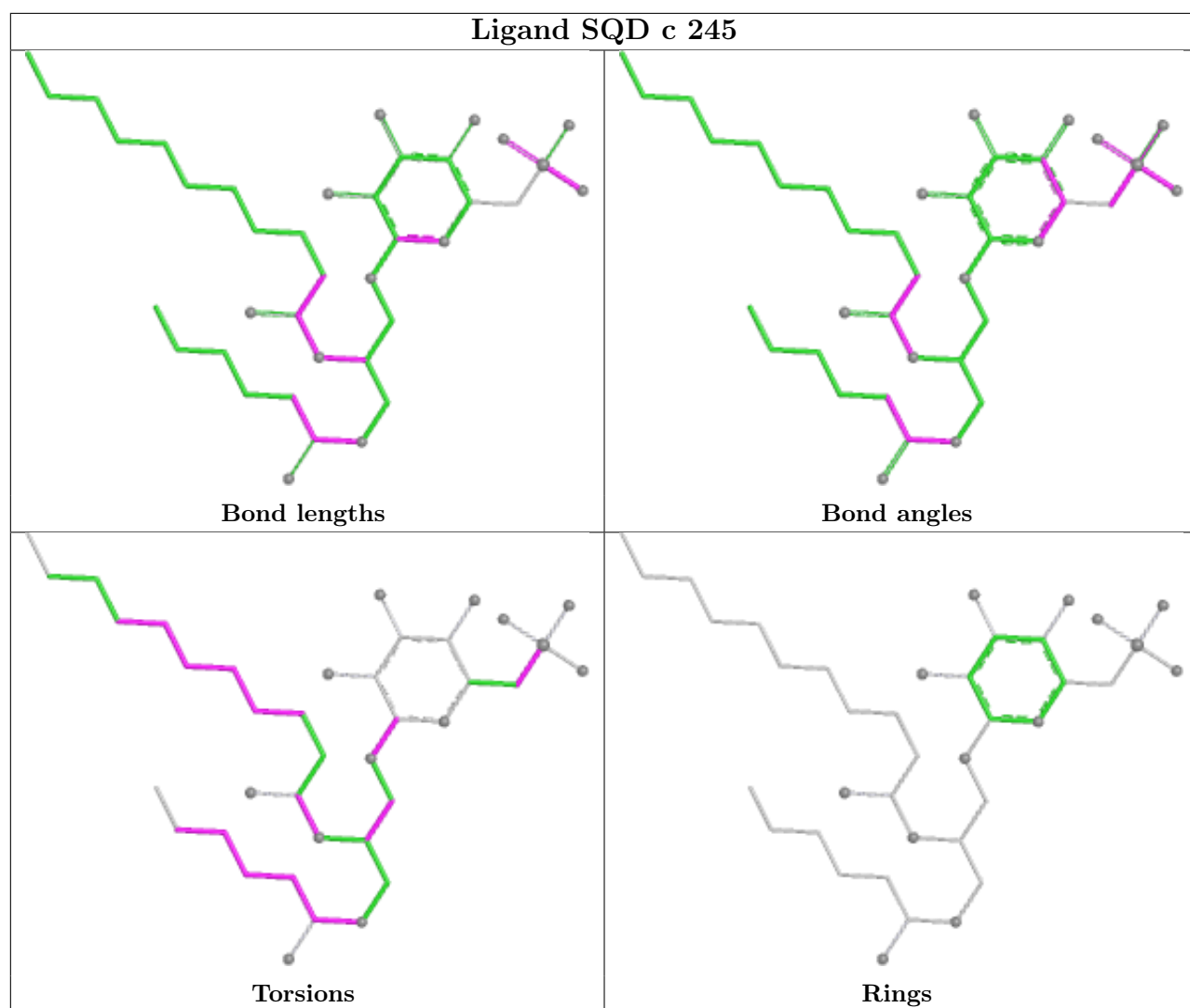
Bond angles



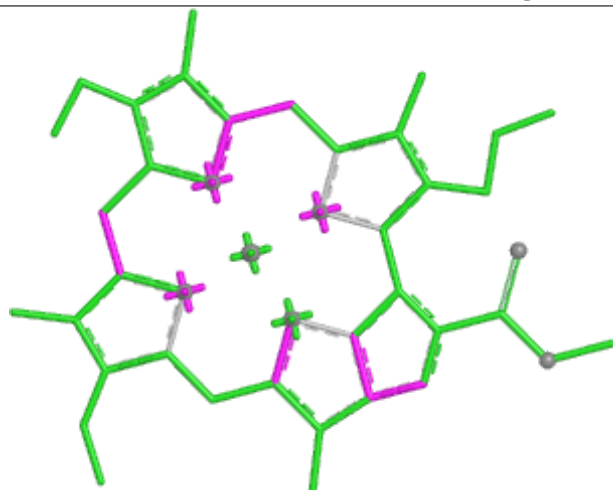
Torsions



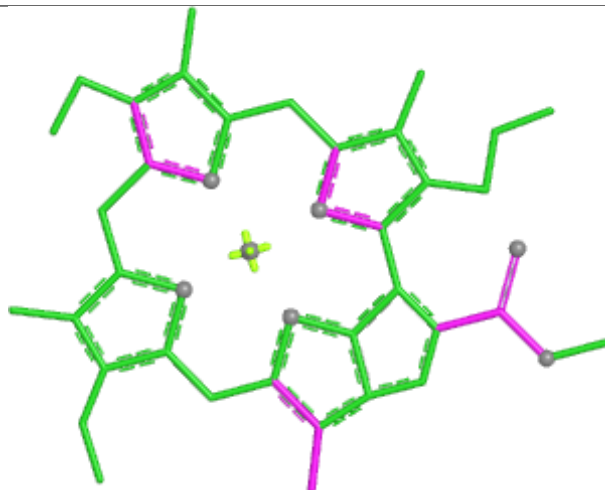
Rings



Ligand CLA o 612



Bond lengths



Bond angles

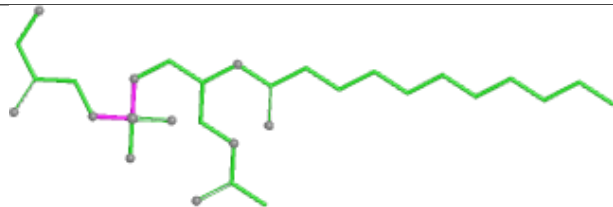


Torsions

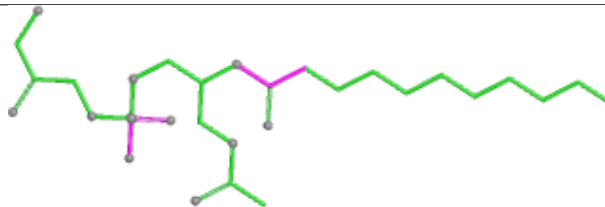


Rings

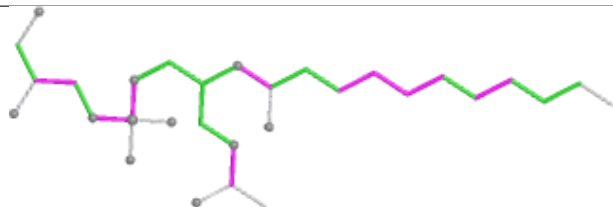
Ligand LHG h 189



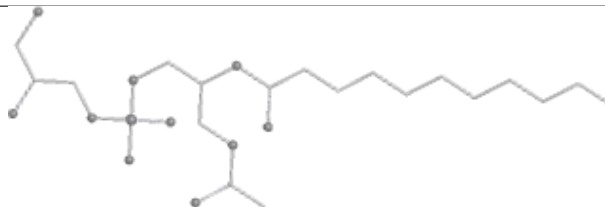
Bond lengths



Bond angles

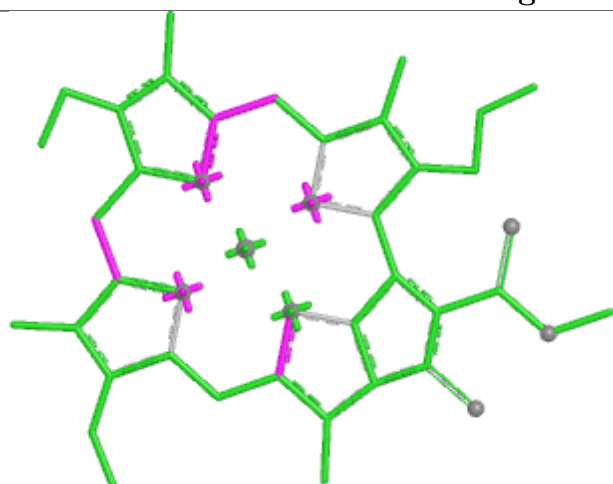


Torsions

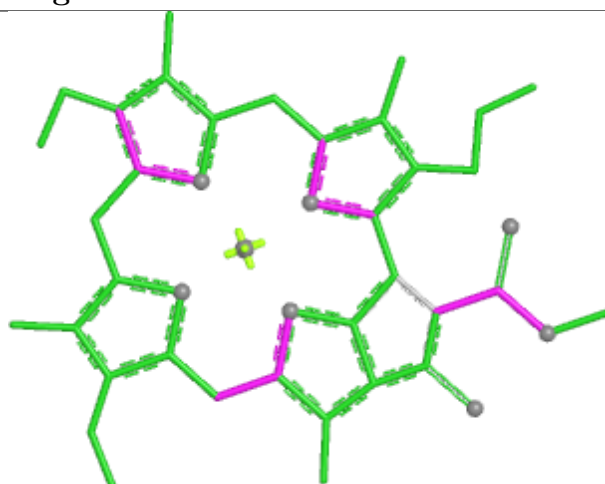


Rings

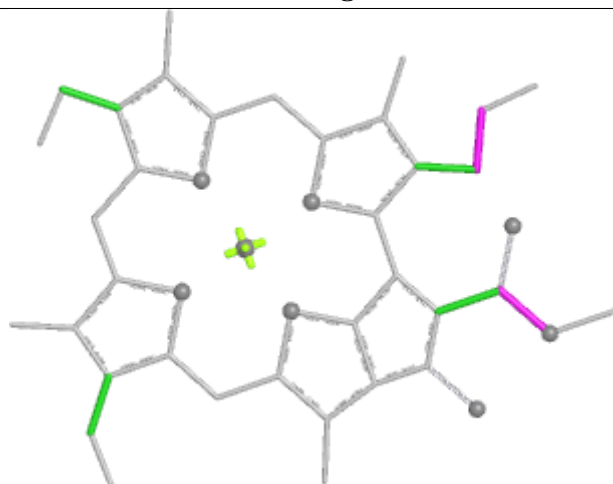
Ligand CLA g 604



Bond lengths



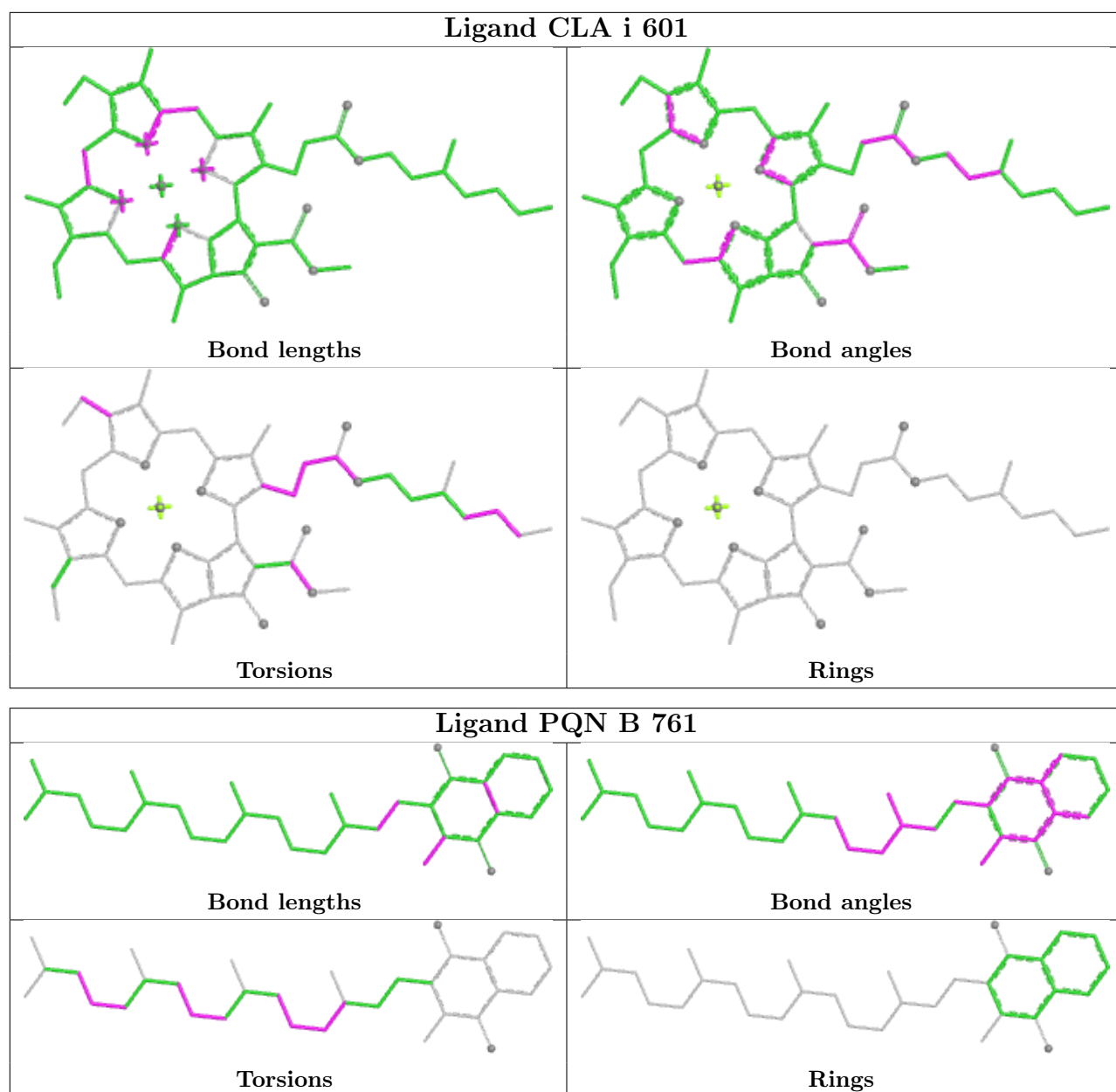
Bond angles



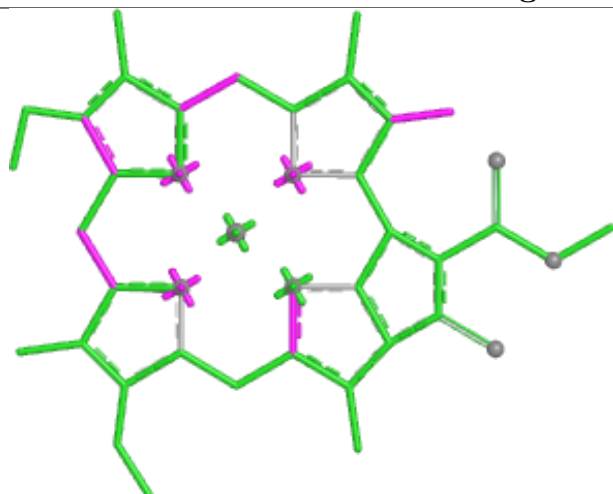
Torsions



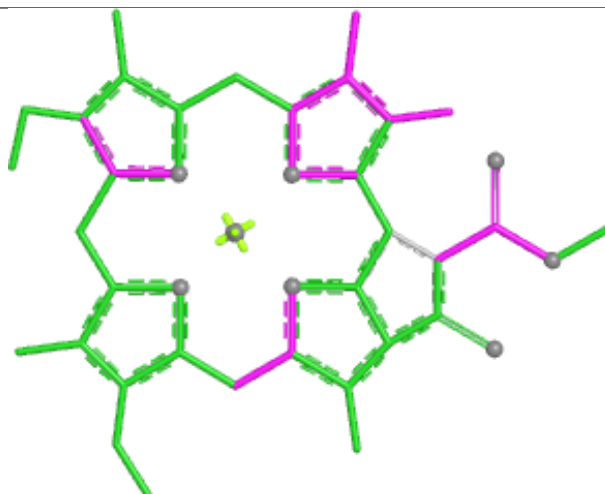
Rings



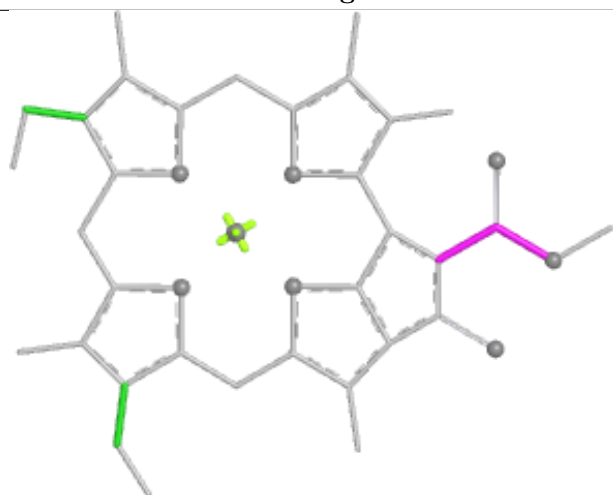
Ligand CLA c 619



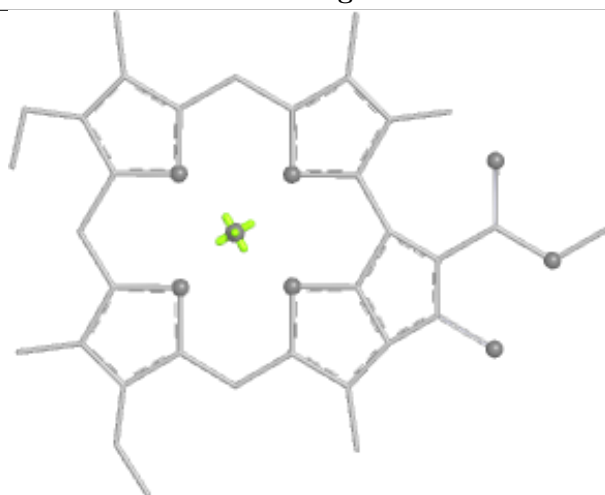
Bond lengths



Bond angles

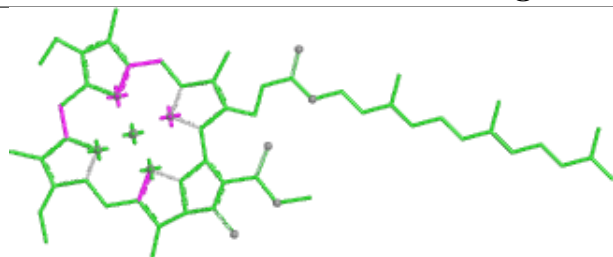


Torsions

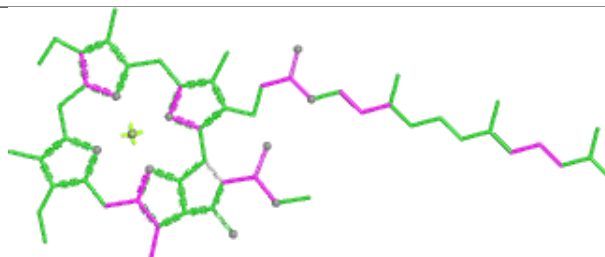


Rings

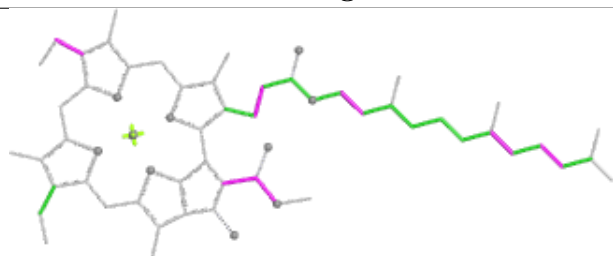
Ligand CLA B 750



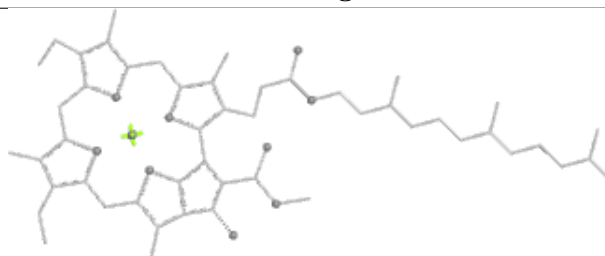
Bond lengths



Bond angles

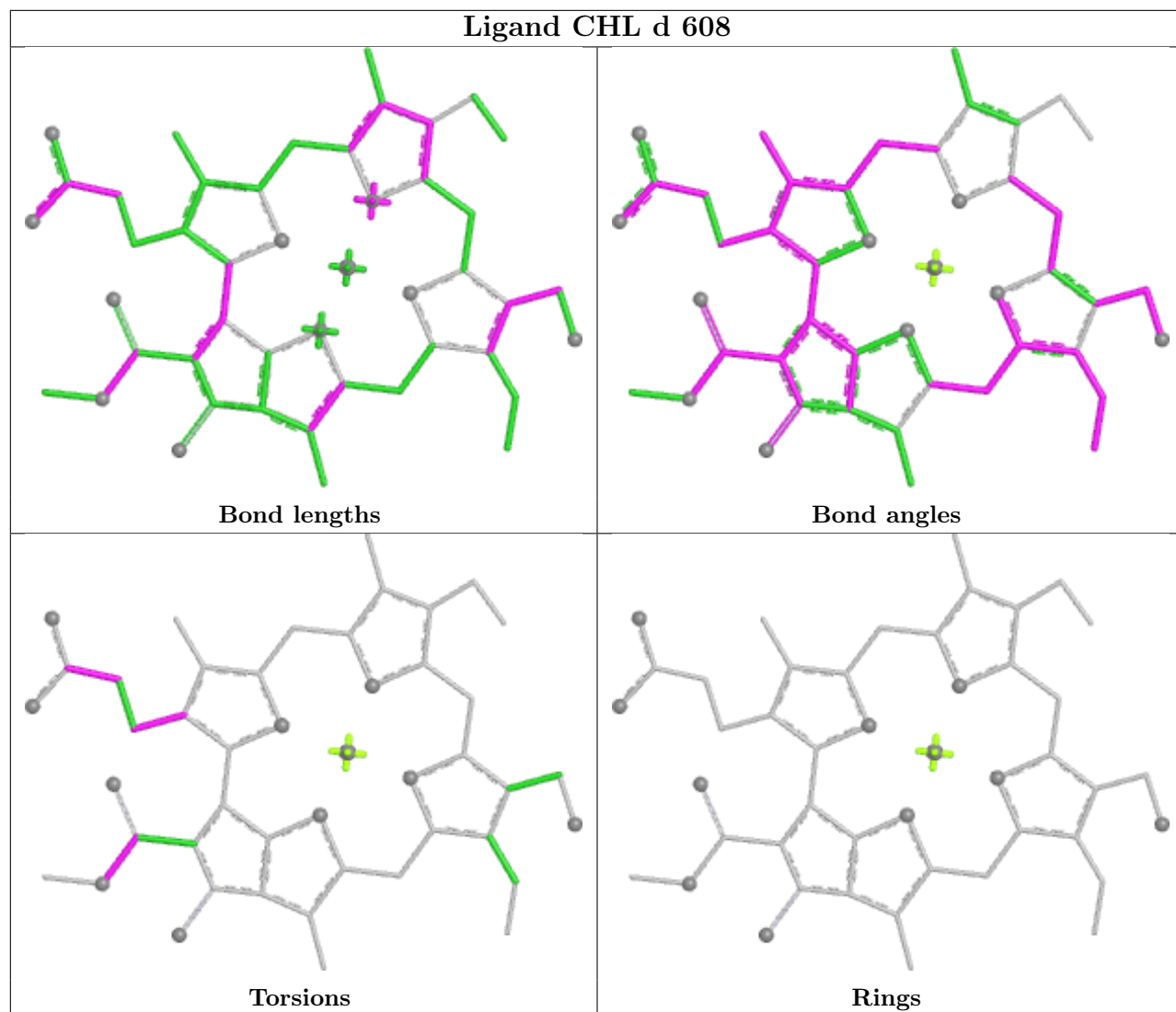


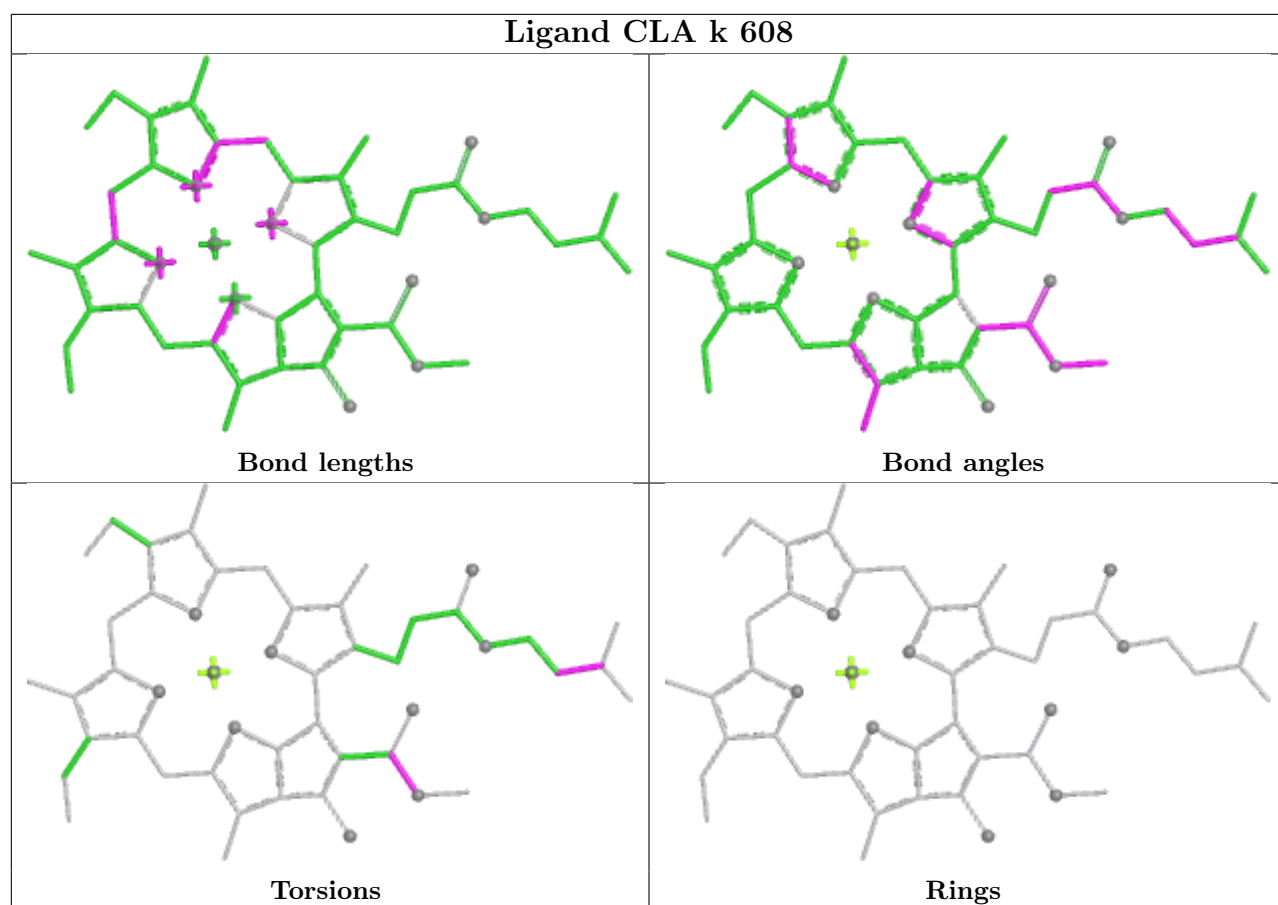
Torsions



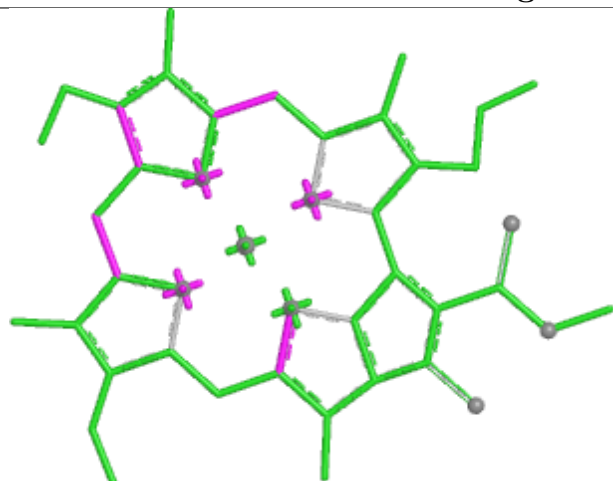
Rings

Ligand CHL d 608

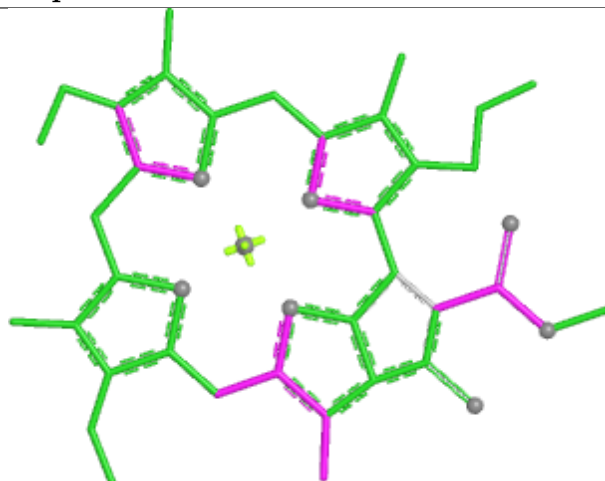




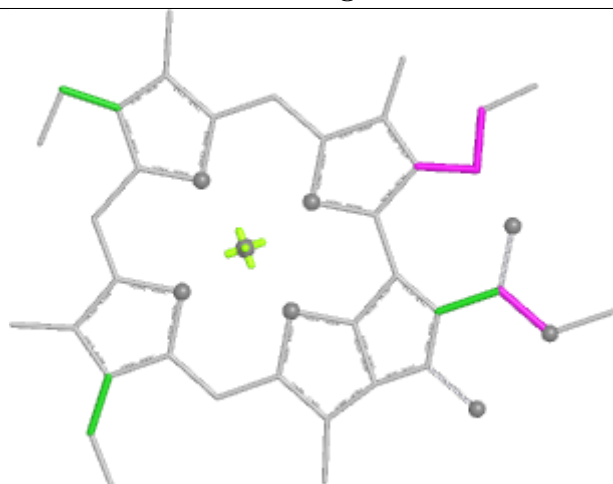
Ligand CLA p 604



Bond lengths



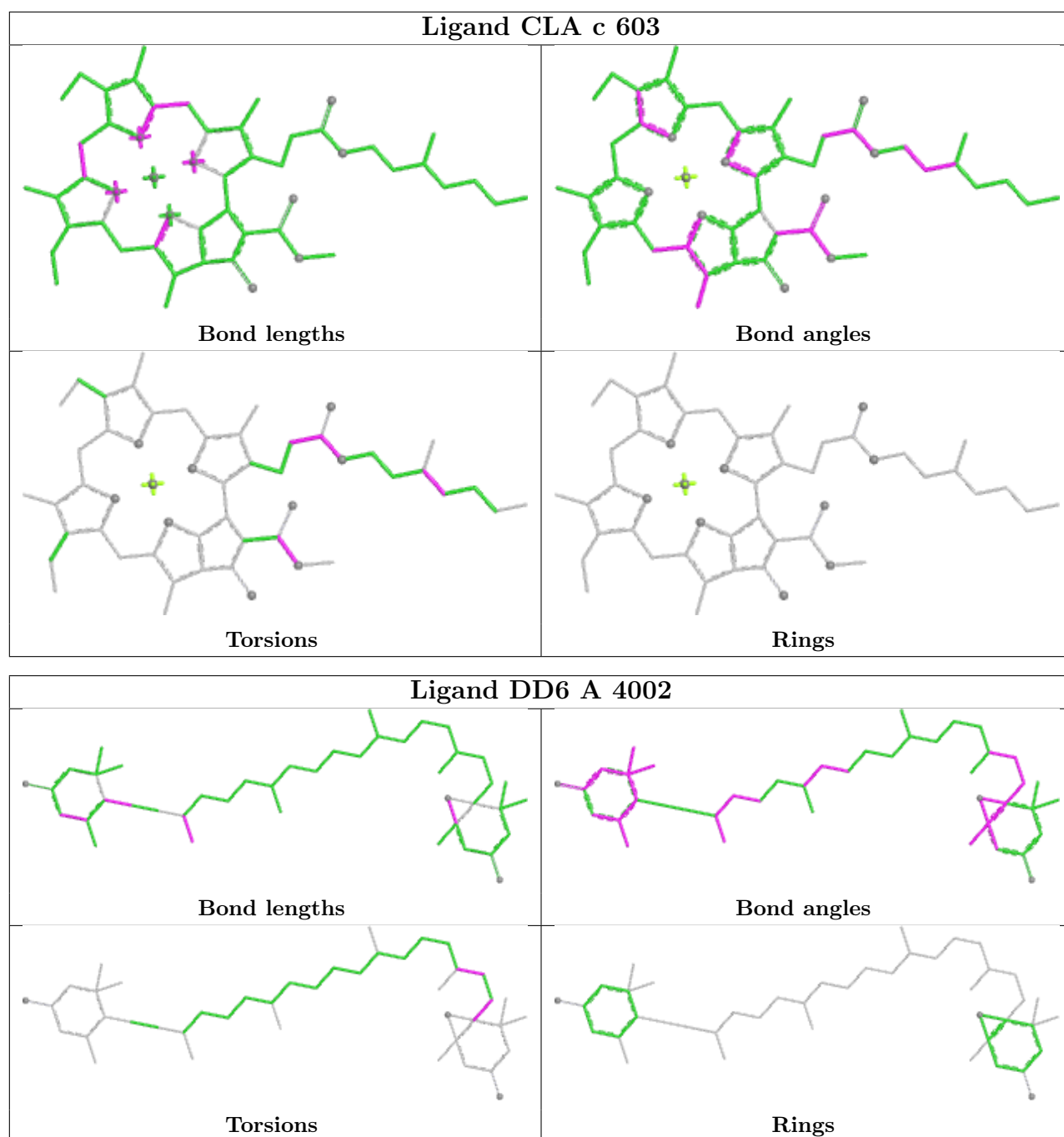
Bond angles

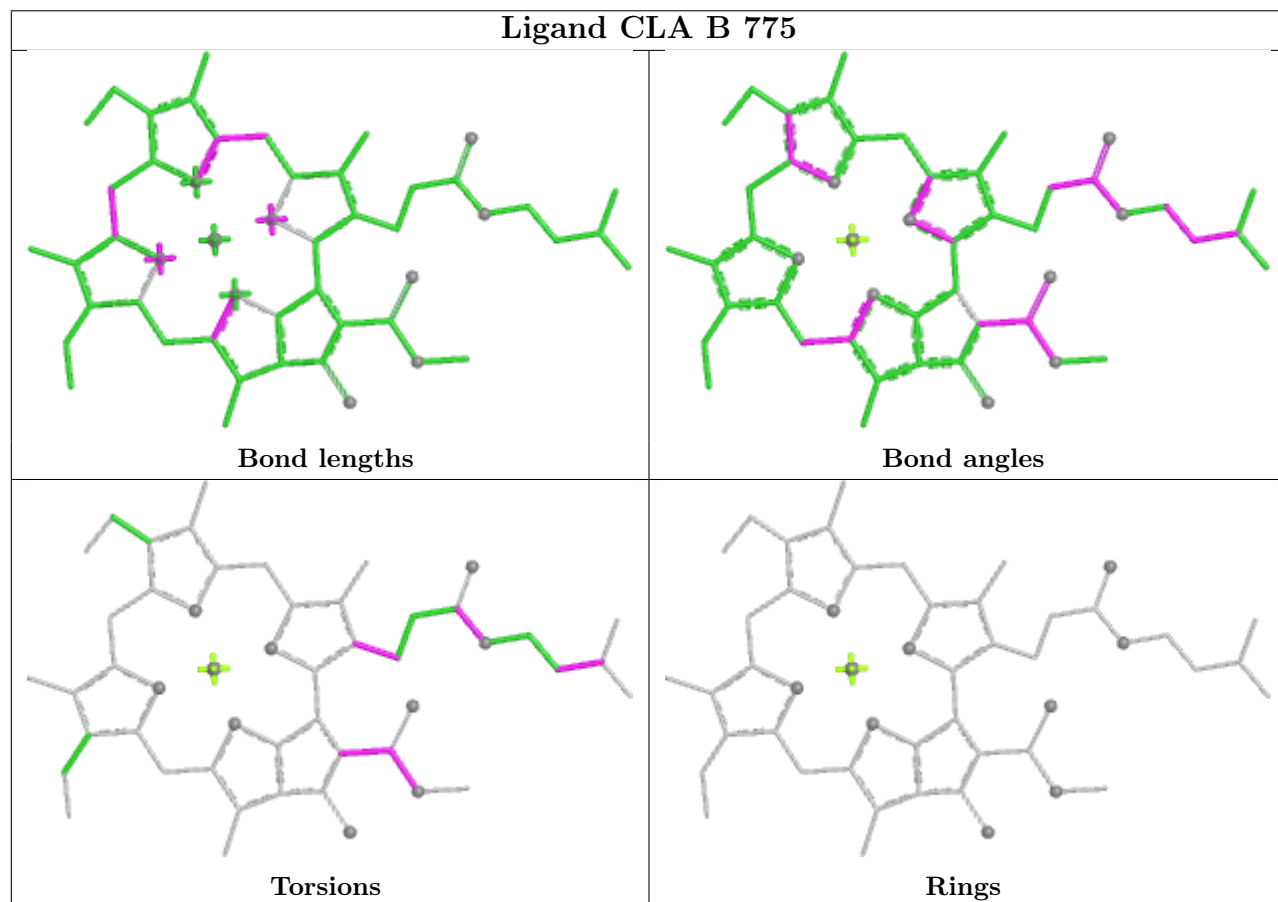
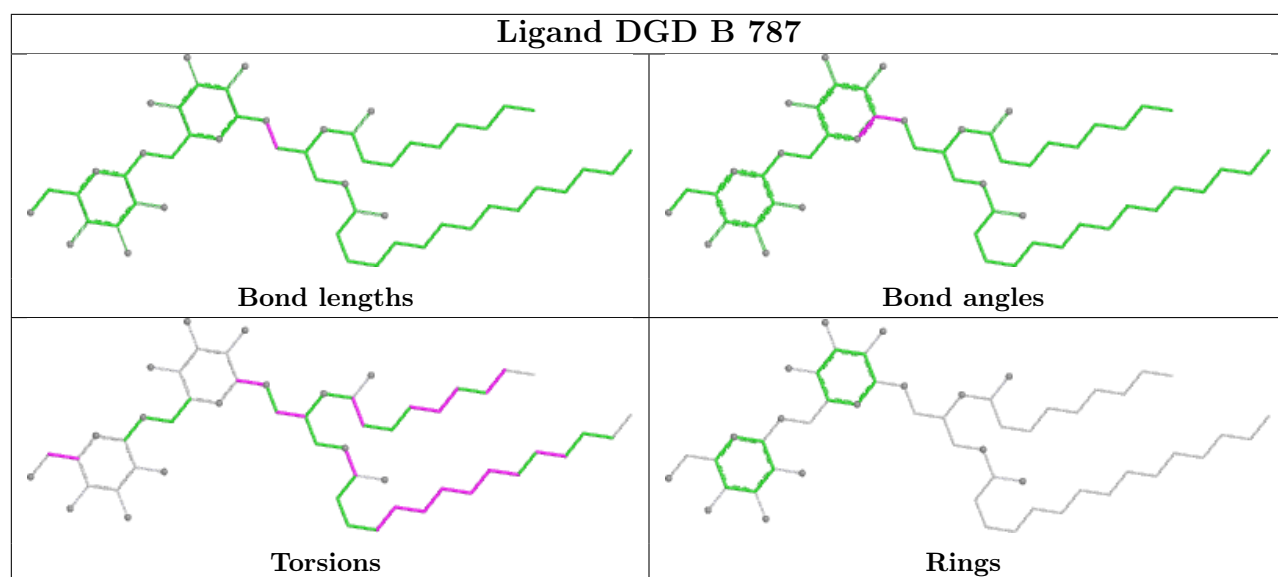


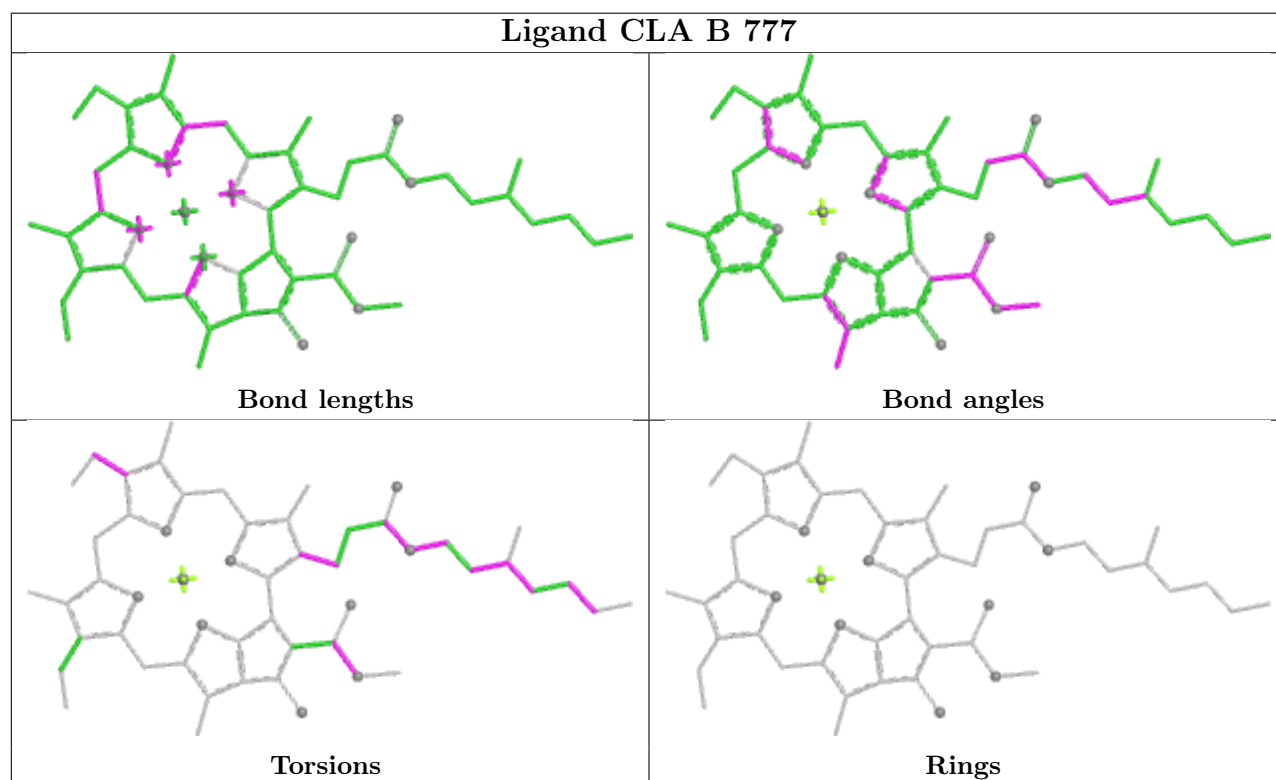
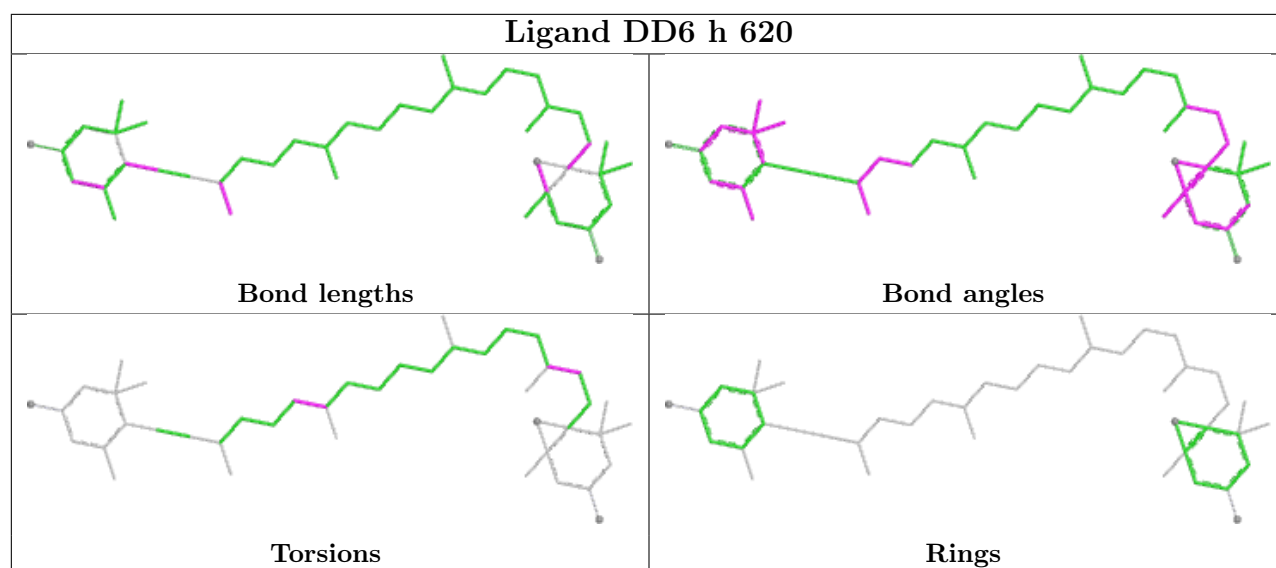
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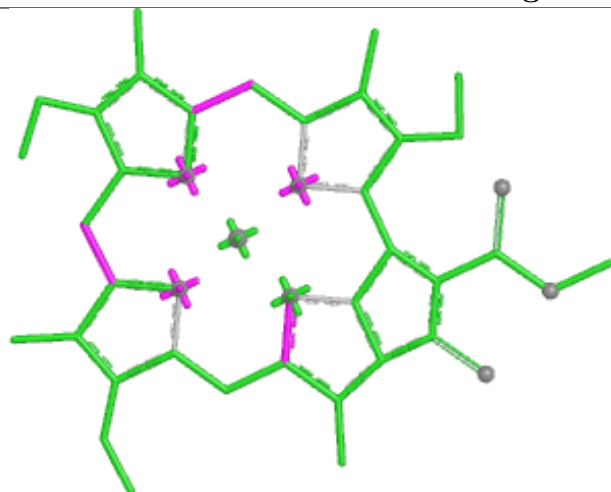
Rings



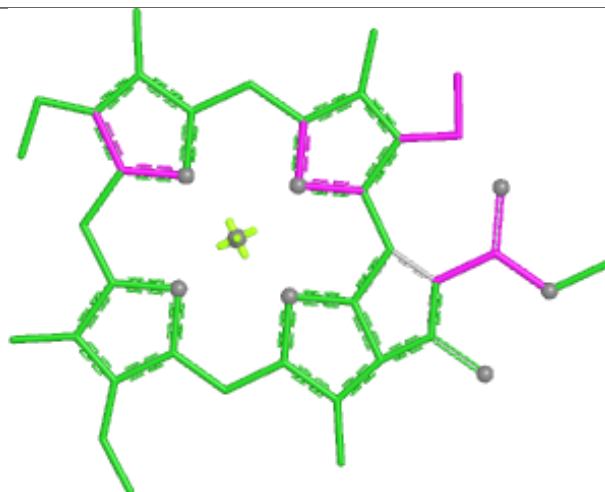




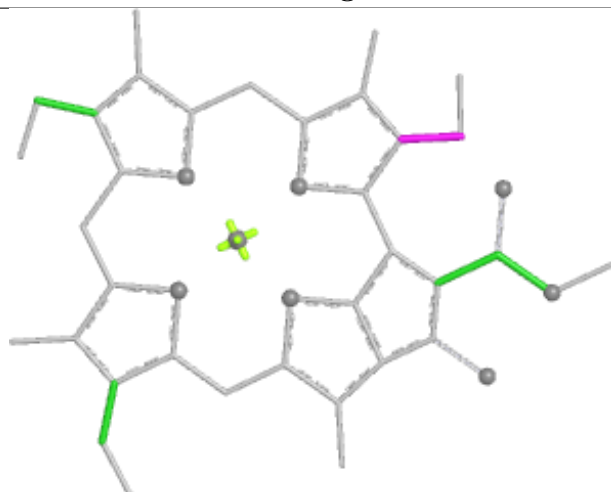
Ligand CLA i 614



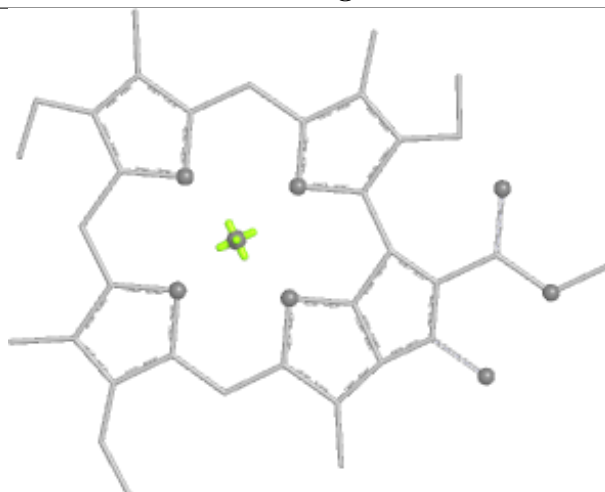
Bond lengths



Bond angles

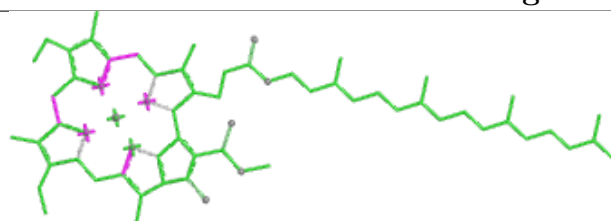


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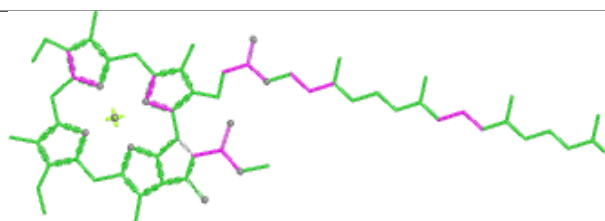


Rings

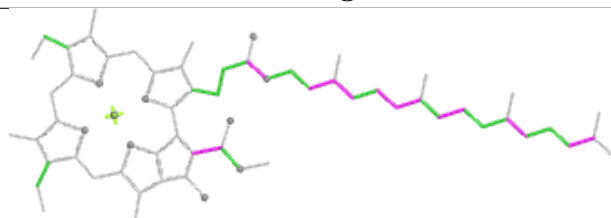
Ligand CLA i 608



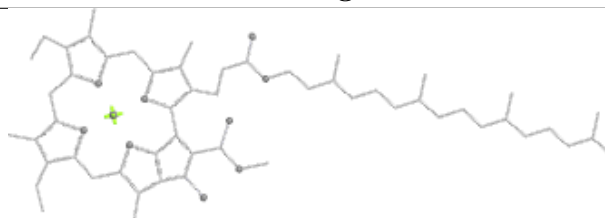
Bond lengths



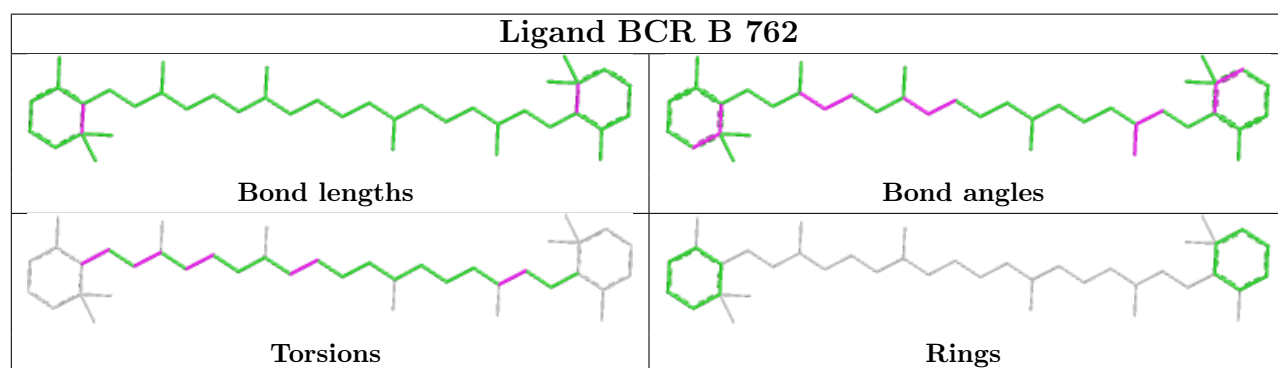
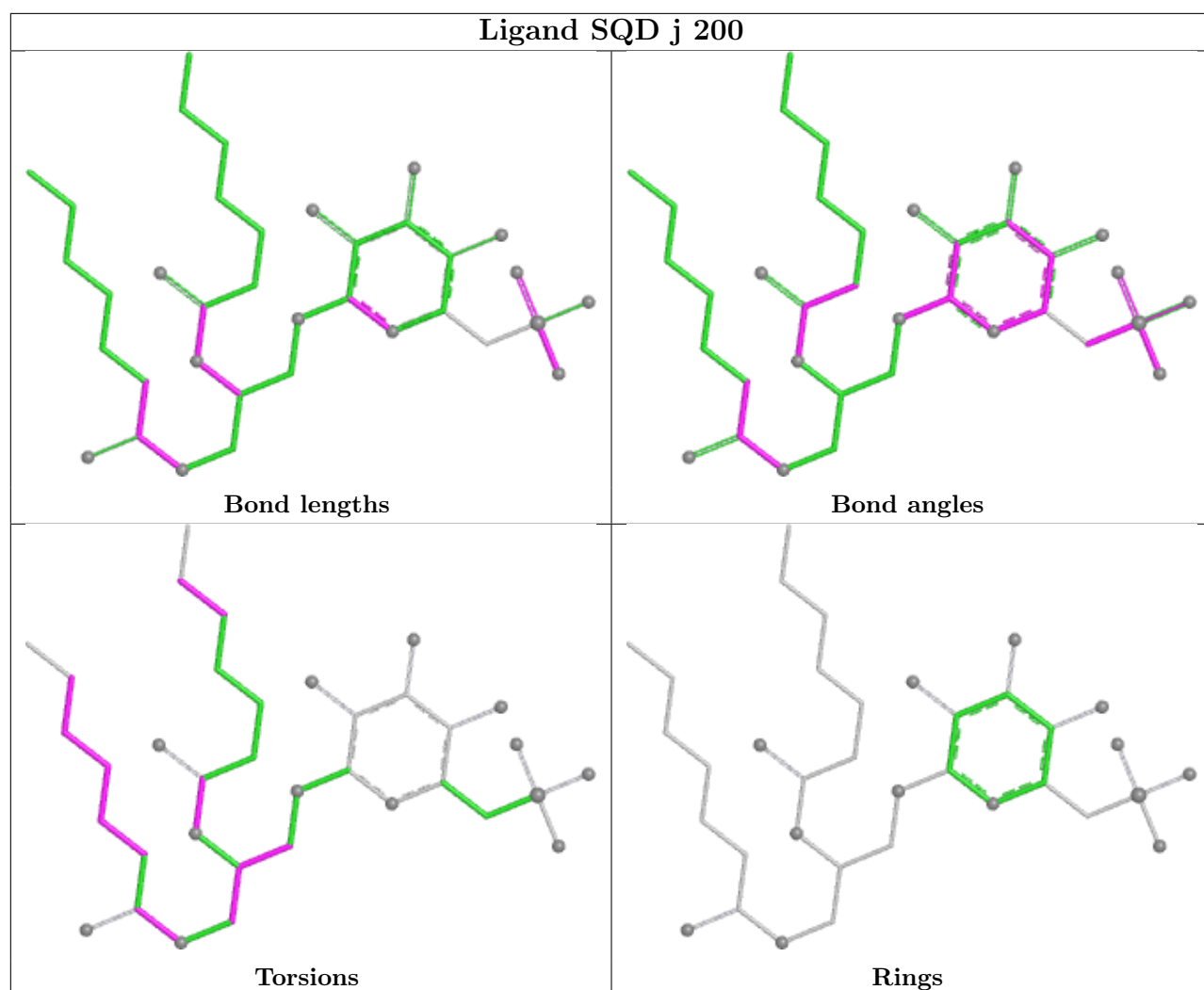
Bond angles



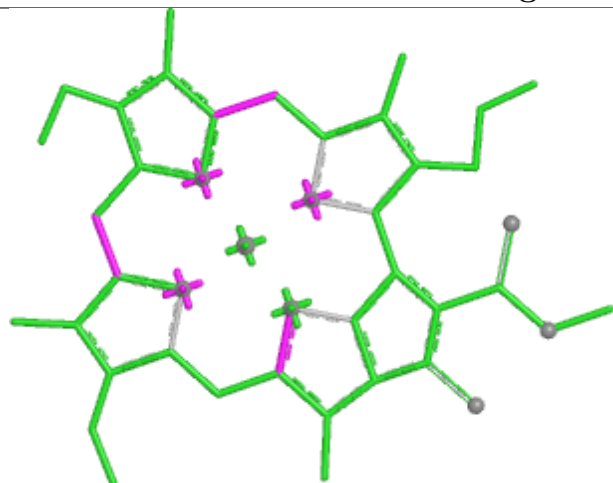
Torsions



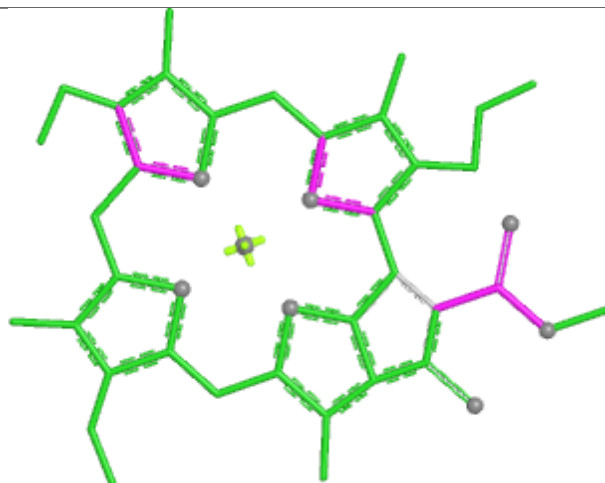
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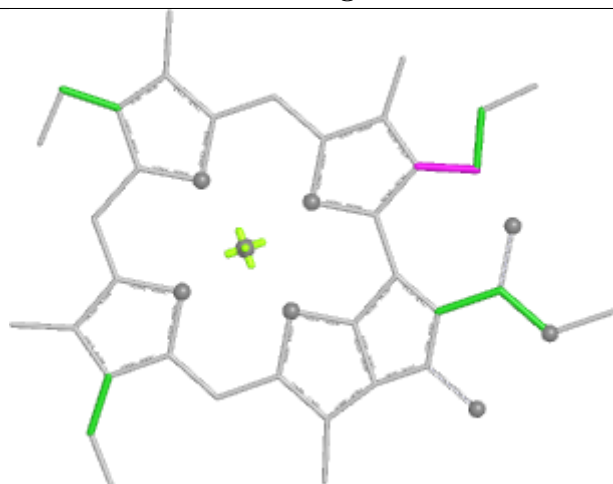
Ligand CLA c 611



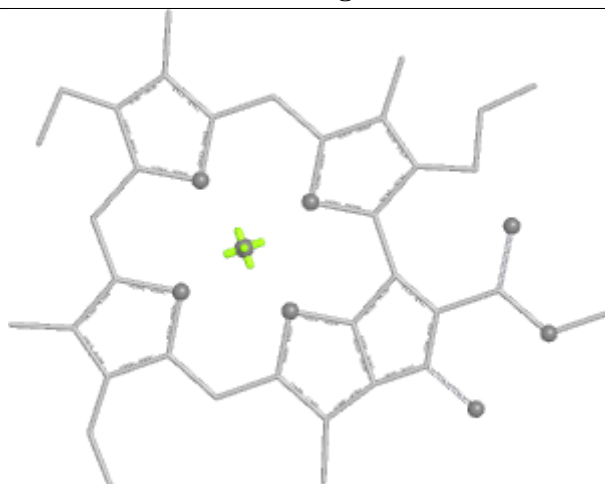
Bond lengths



Bond angles

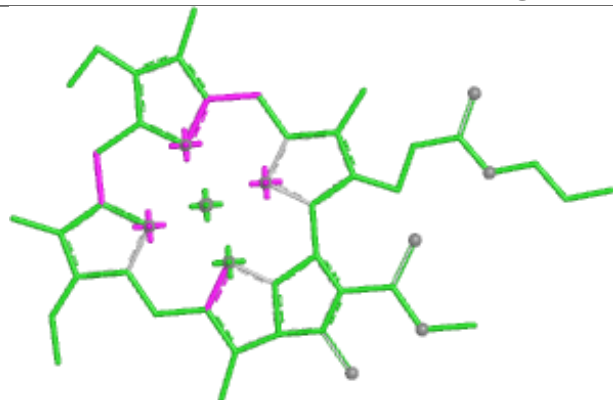


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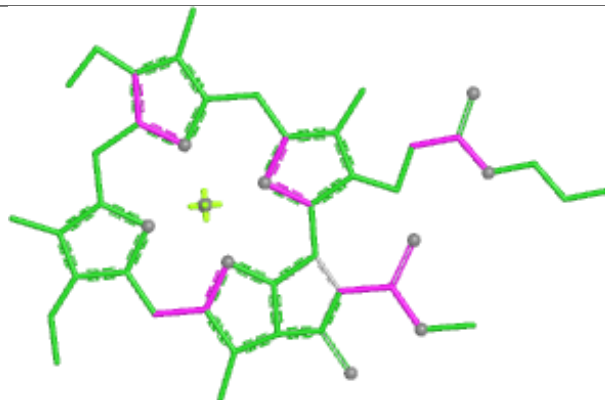


Rings

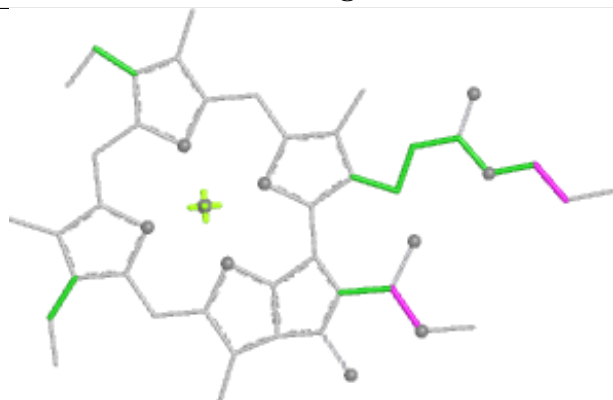
Ligand CLA A 782



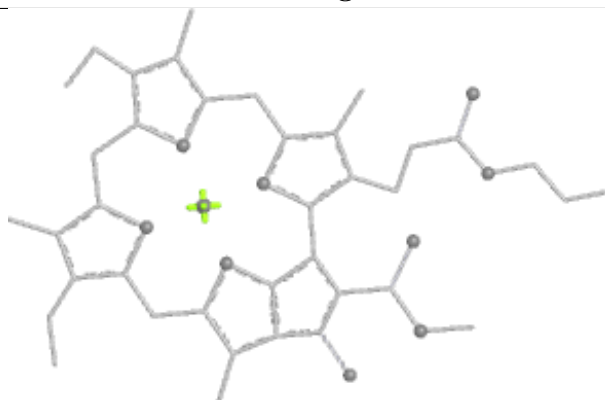
Bond lengths



Bond angles

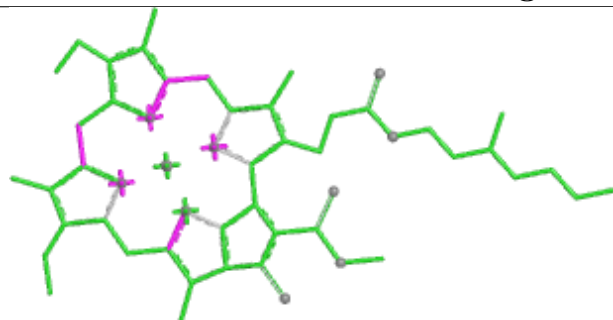


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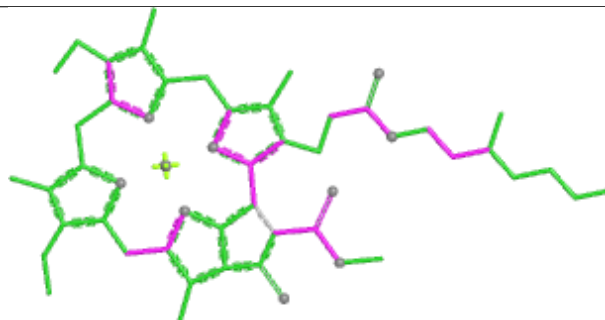


Rings

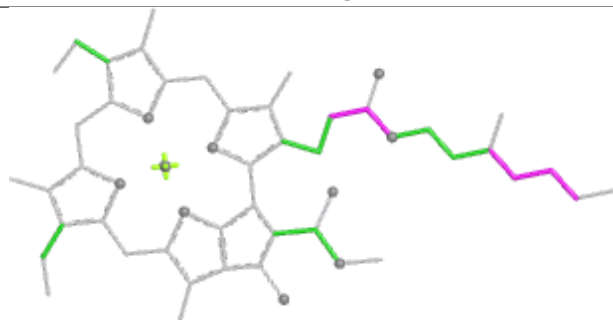
Ligand CLA a 603



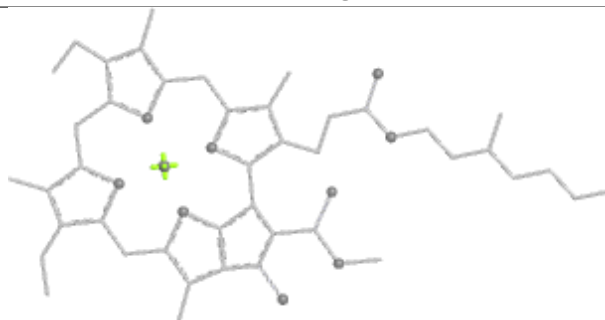
Bond lengths



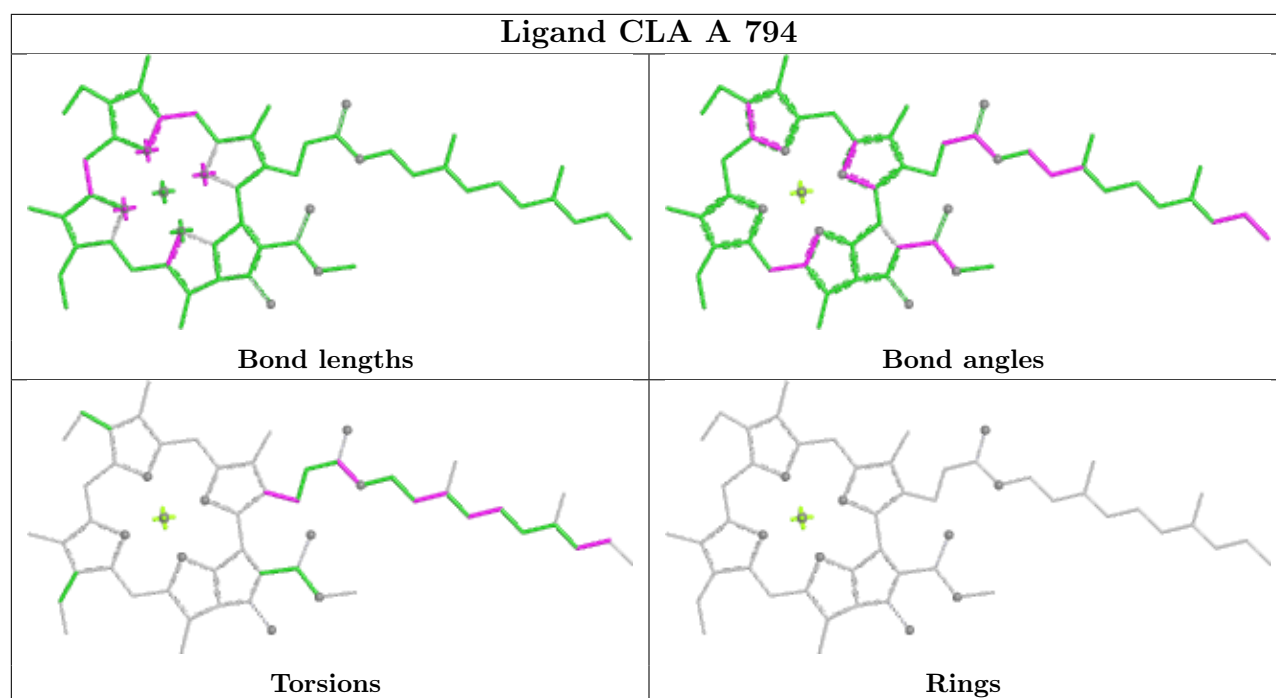
Bond angles

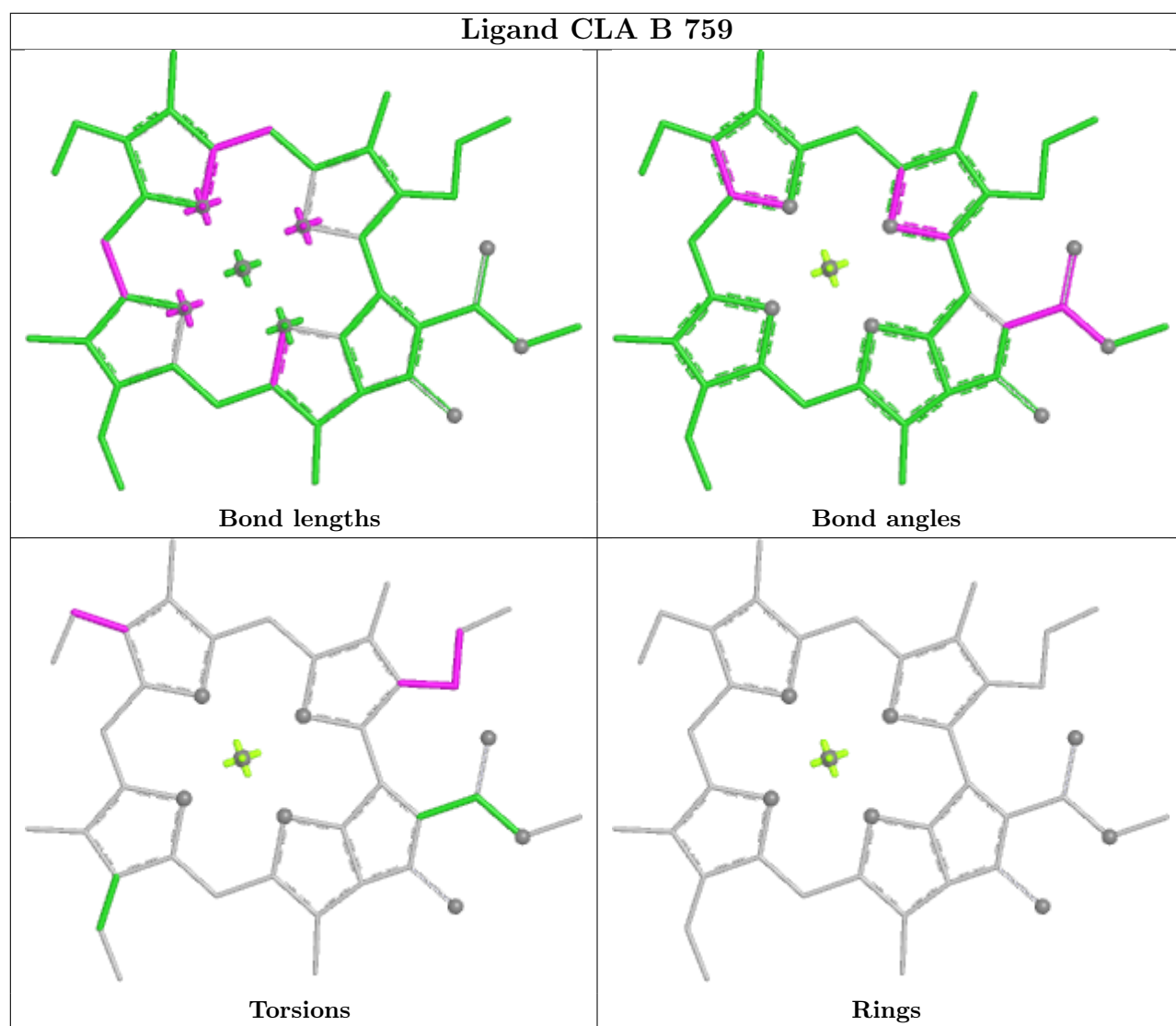


Torsions

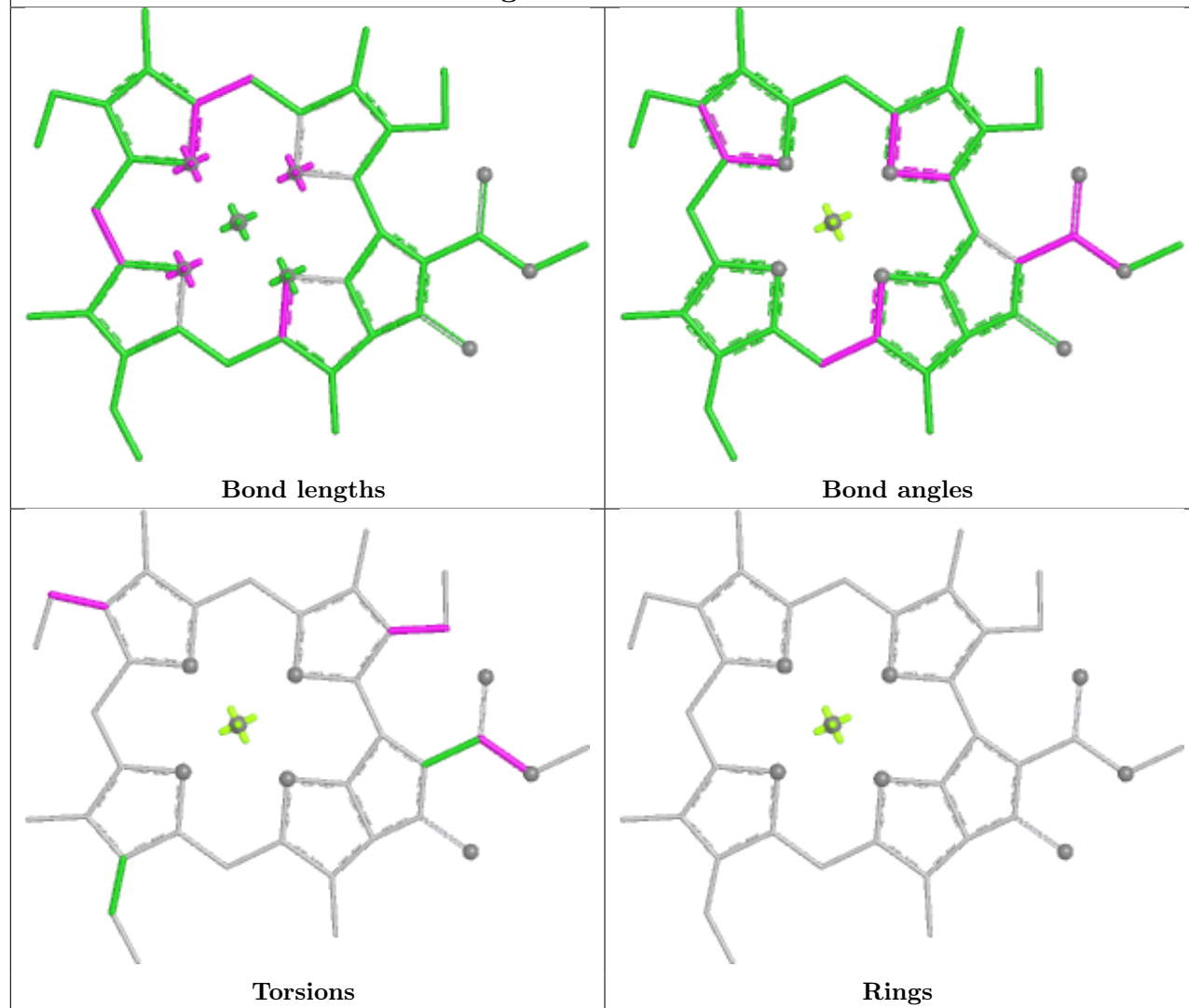


Rings

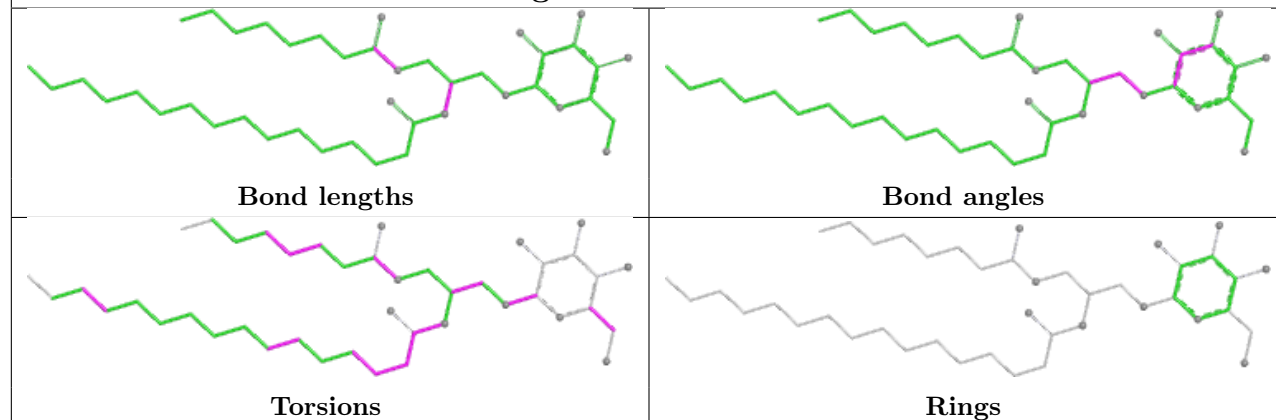


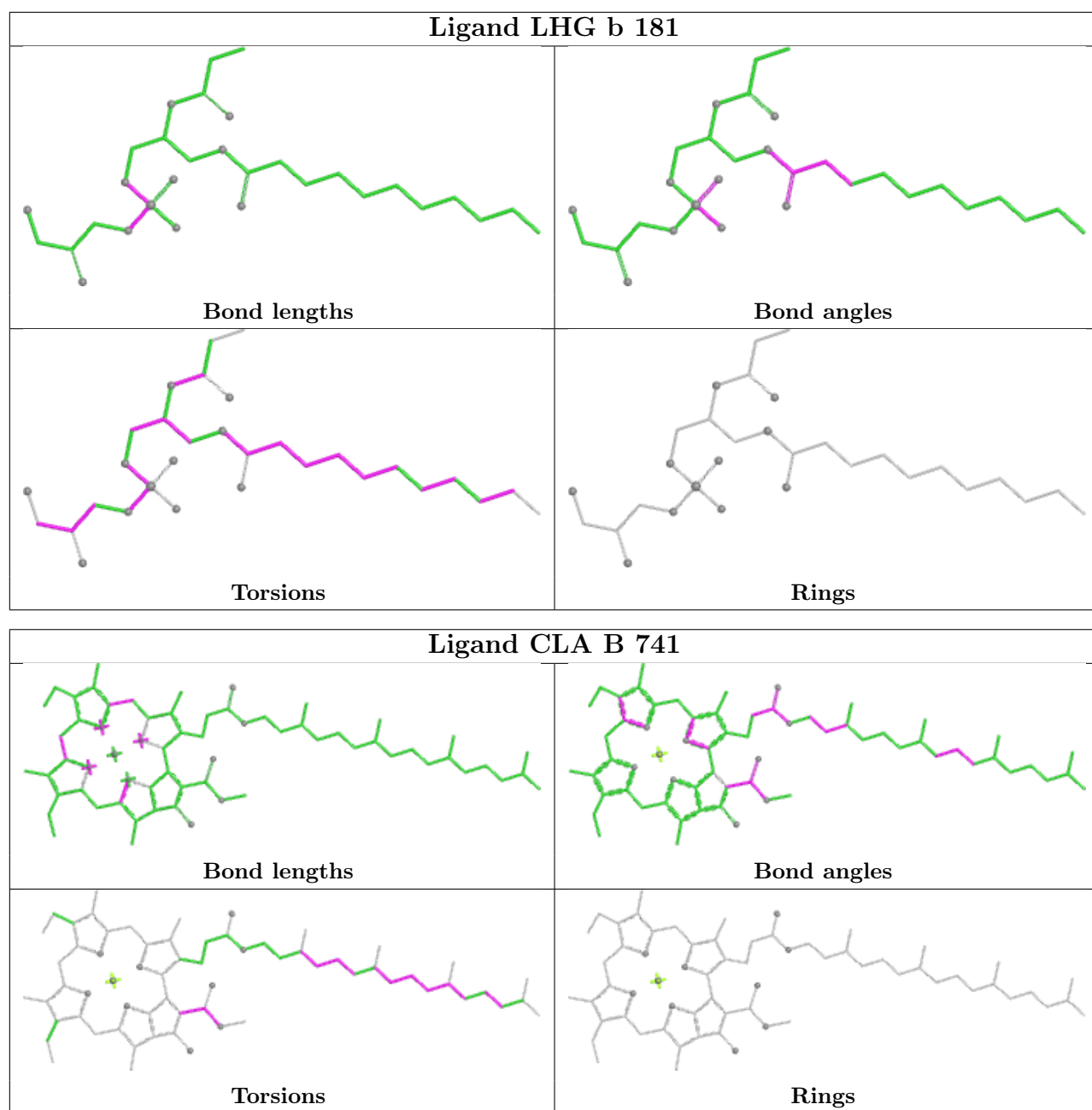


Ligand CLA c 614

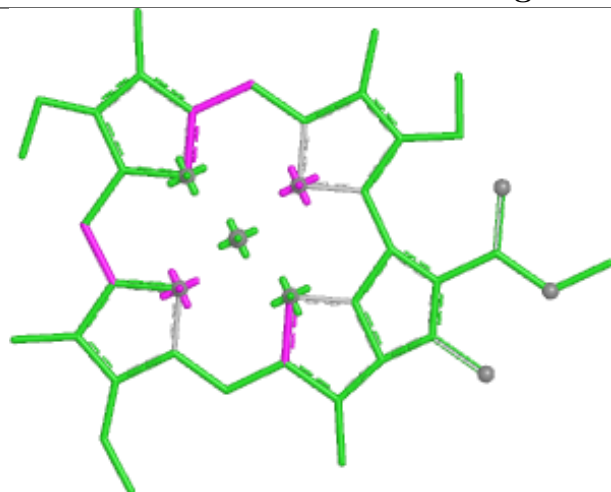


Ligand LMG a 182

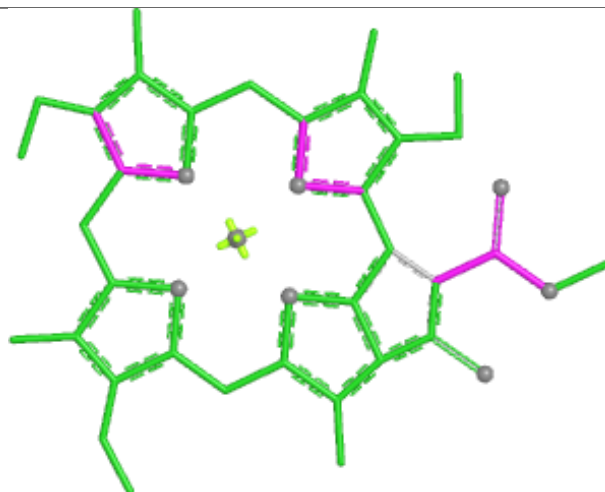




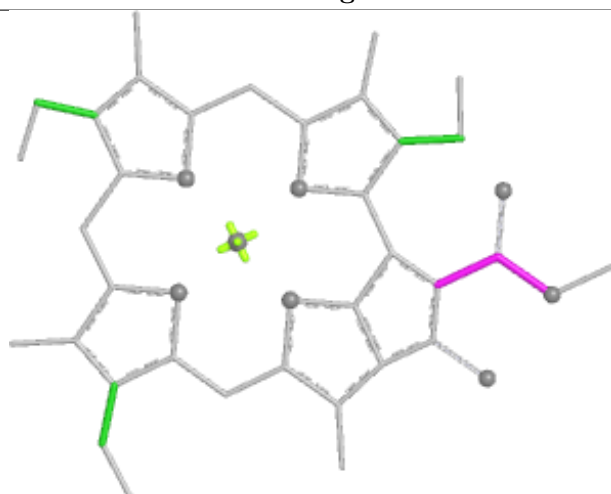
Ligand CLA B 743



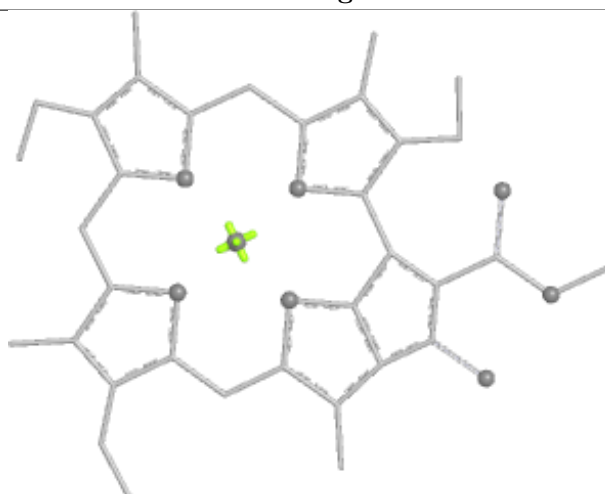
Bond lengths



Bond angles

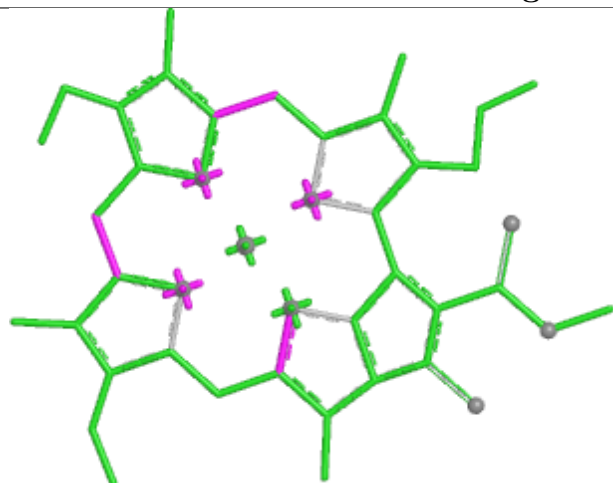


Torsions

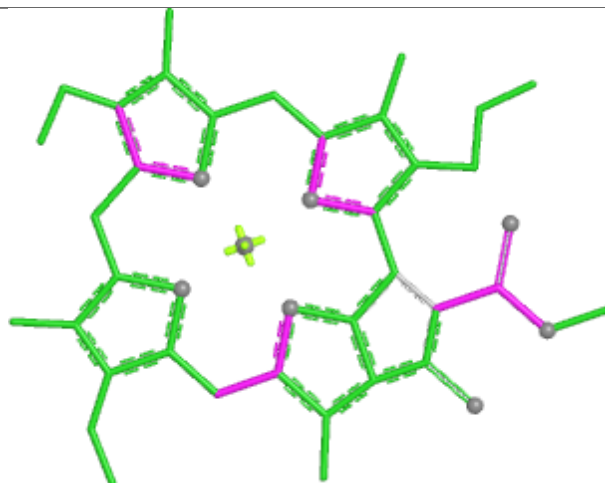


Rings

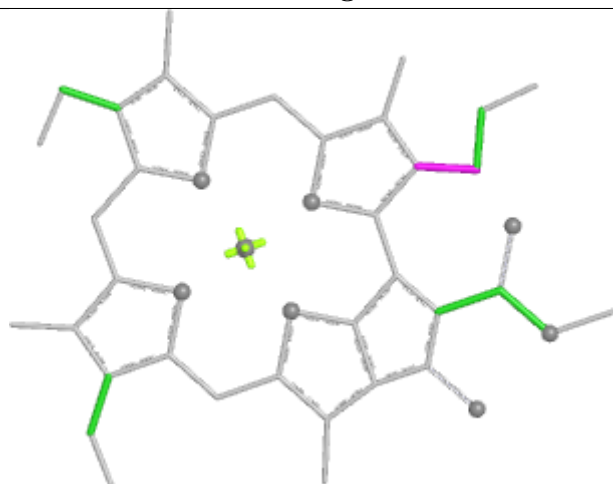
Ligand CLA 1 604



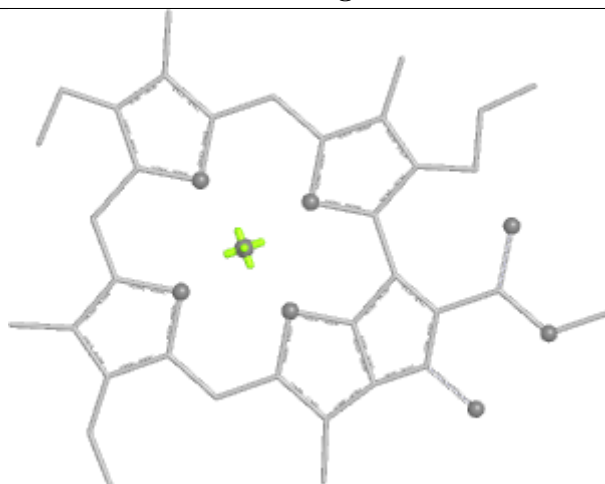
Bond lengths



Bond angles

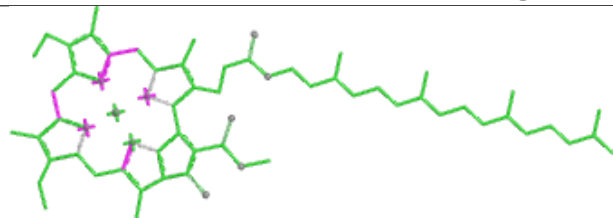


Torsions

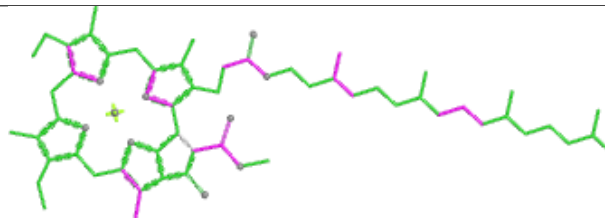


Rings

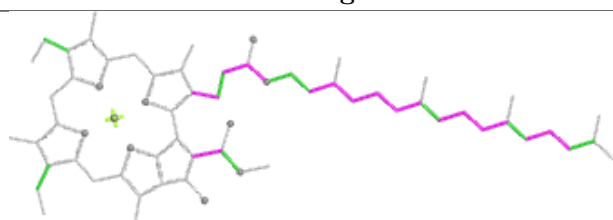
Ligand CLA B 784



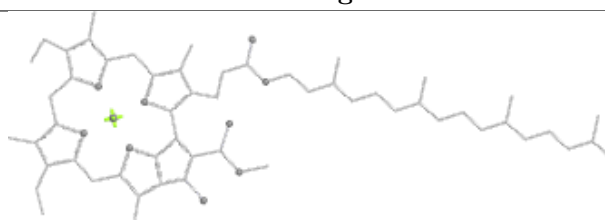
Bond lengths



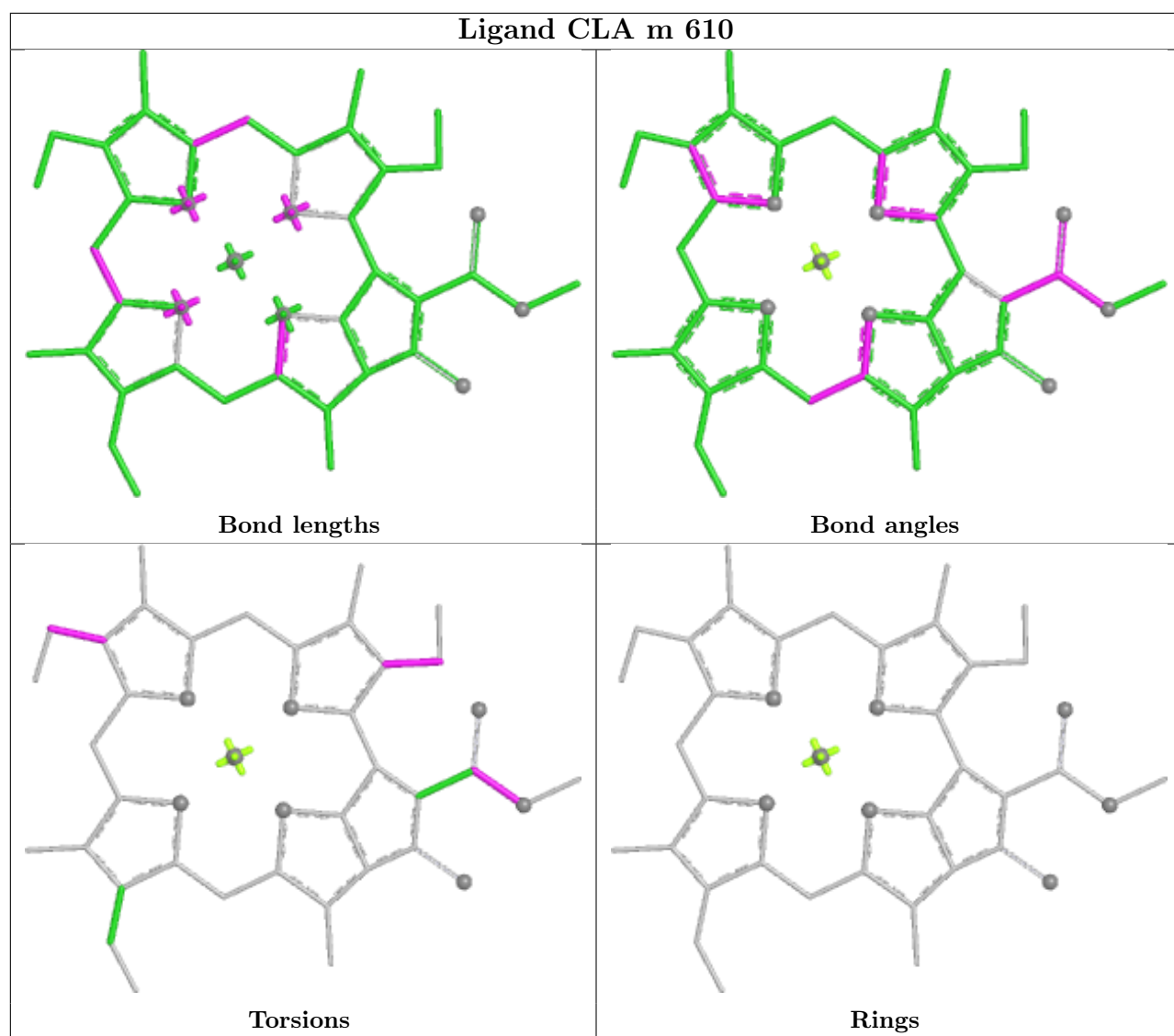
Bond angles

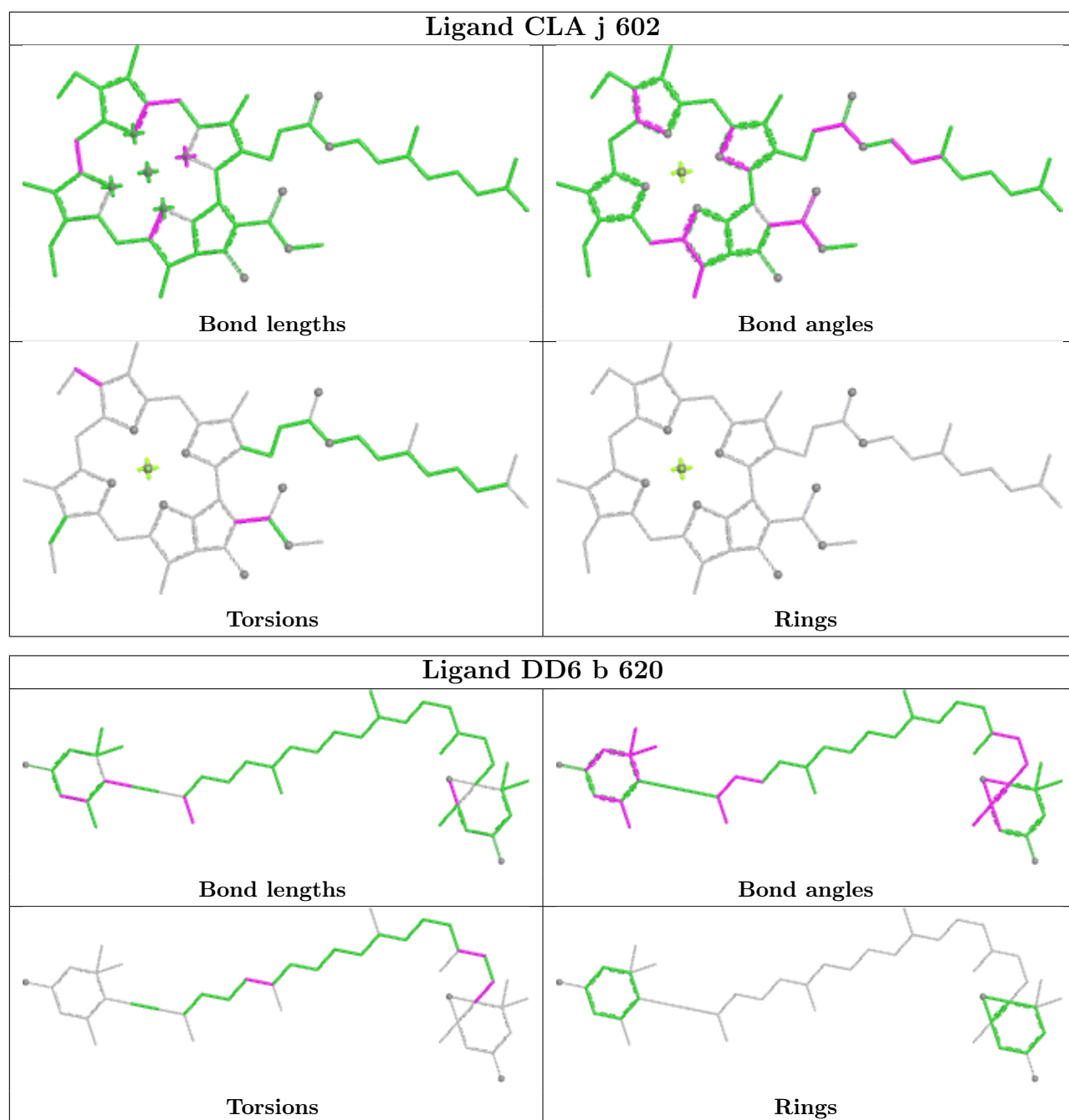


Torsions

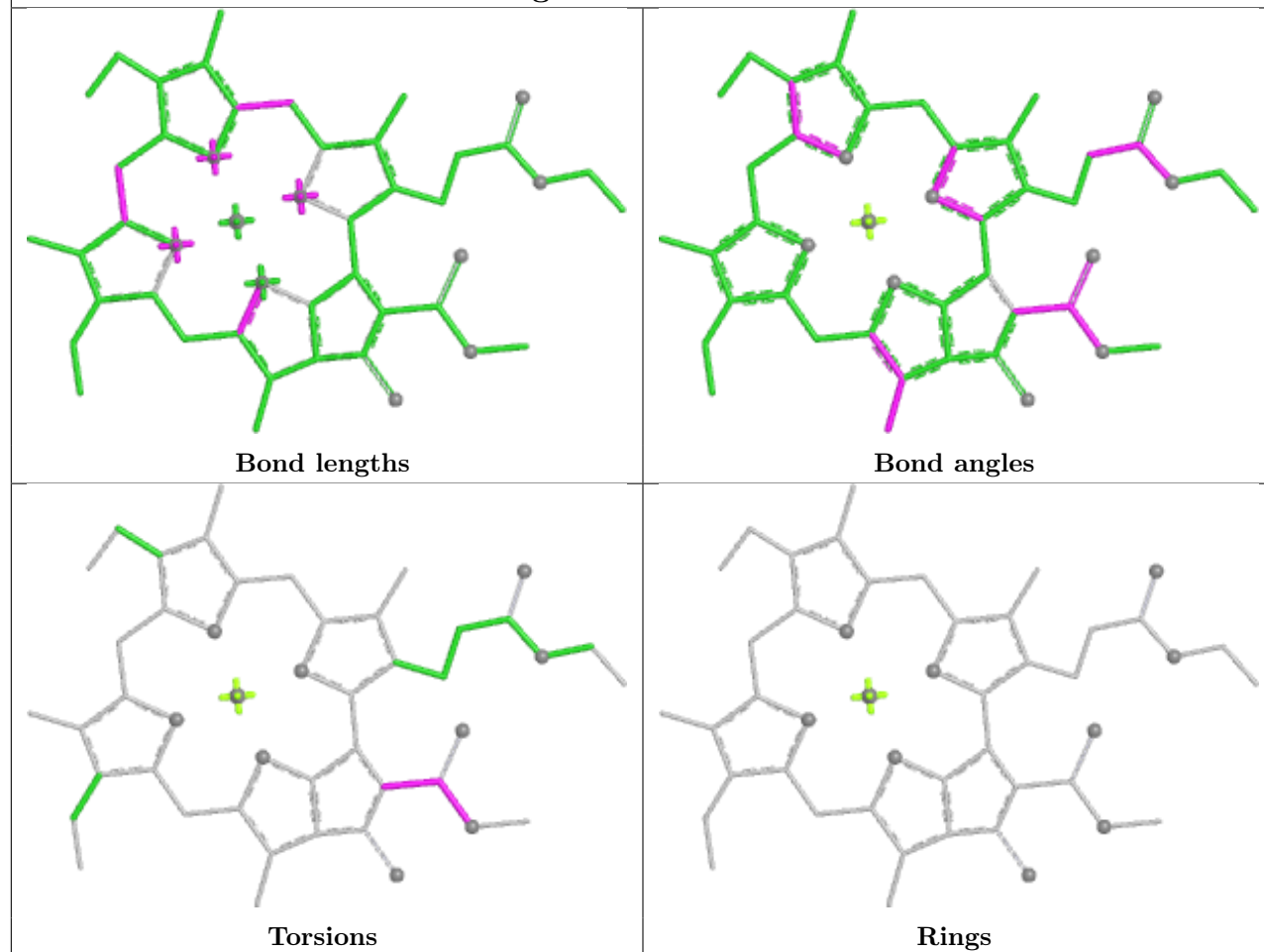


Rings

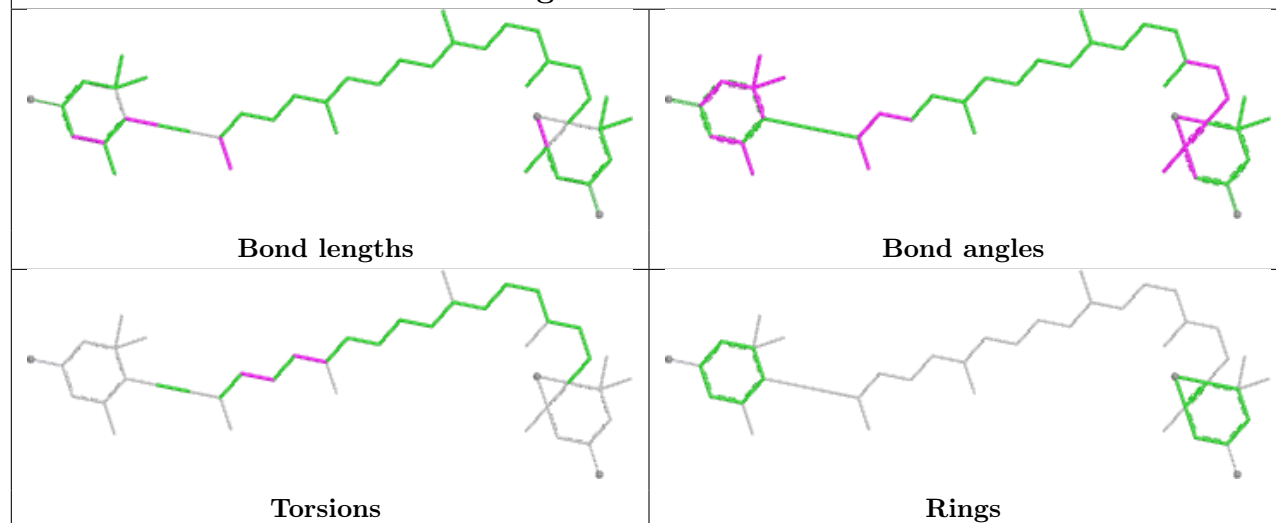


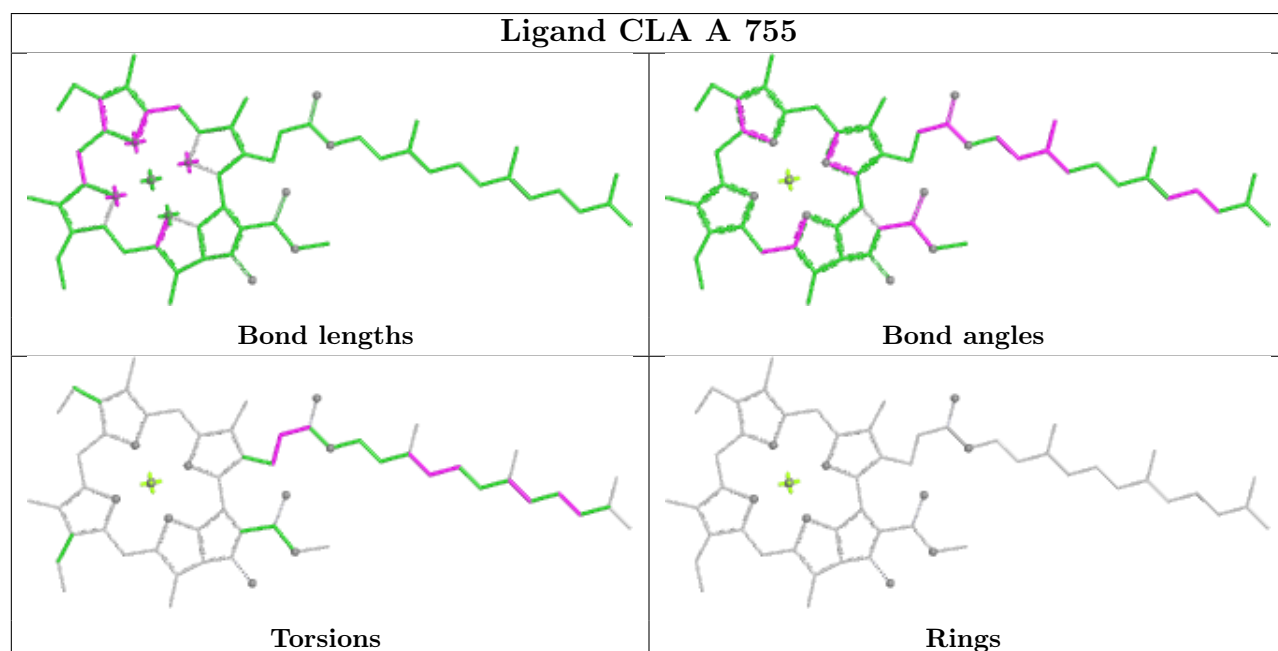
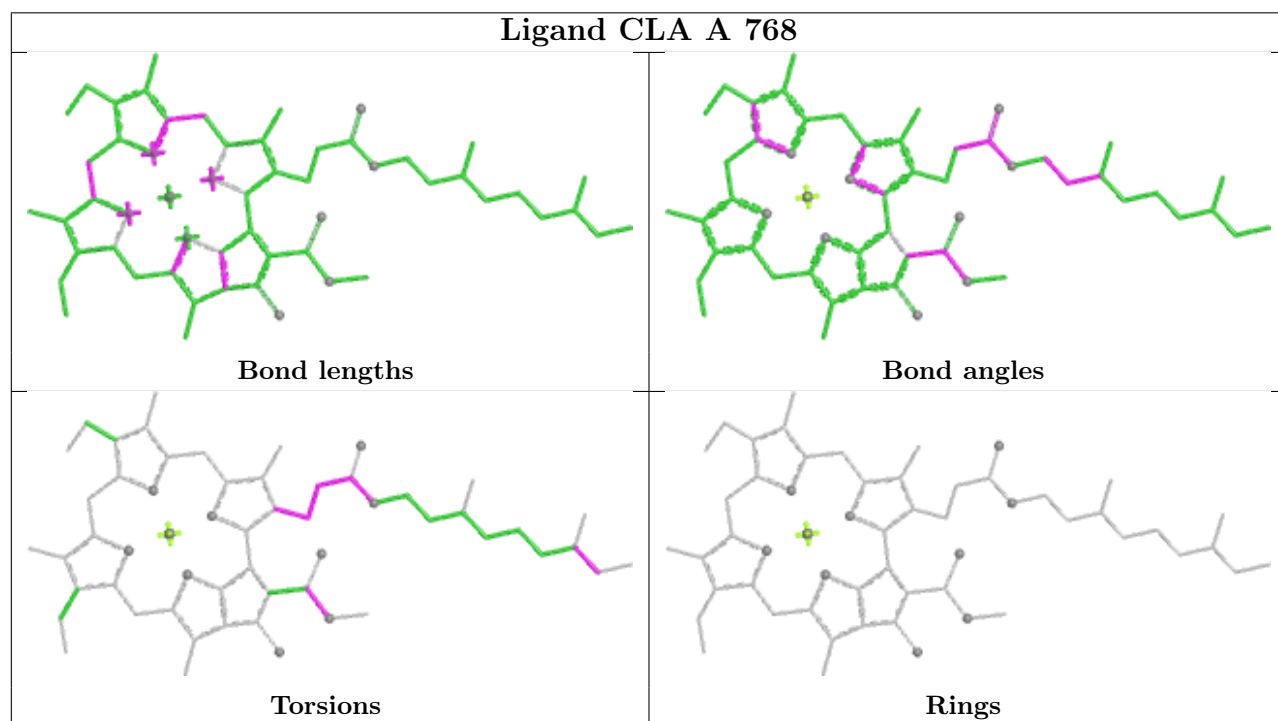
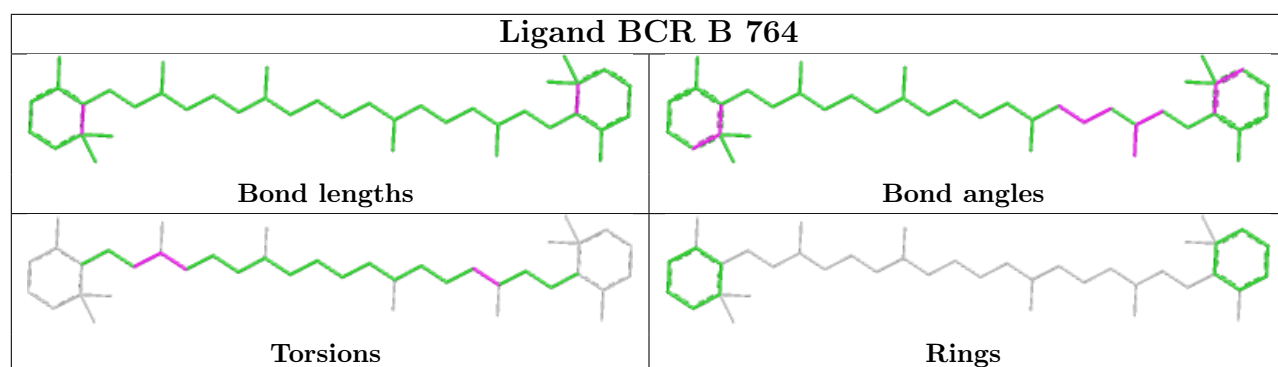


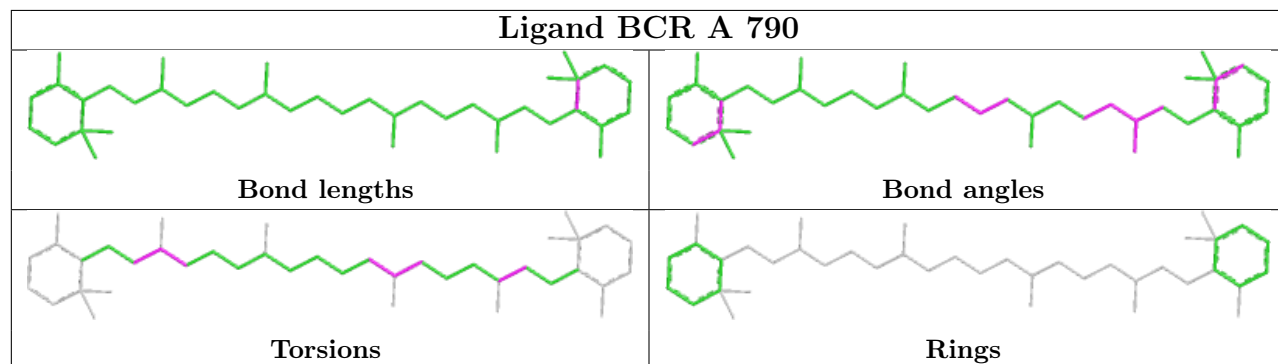
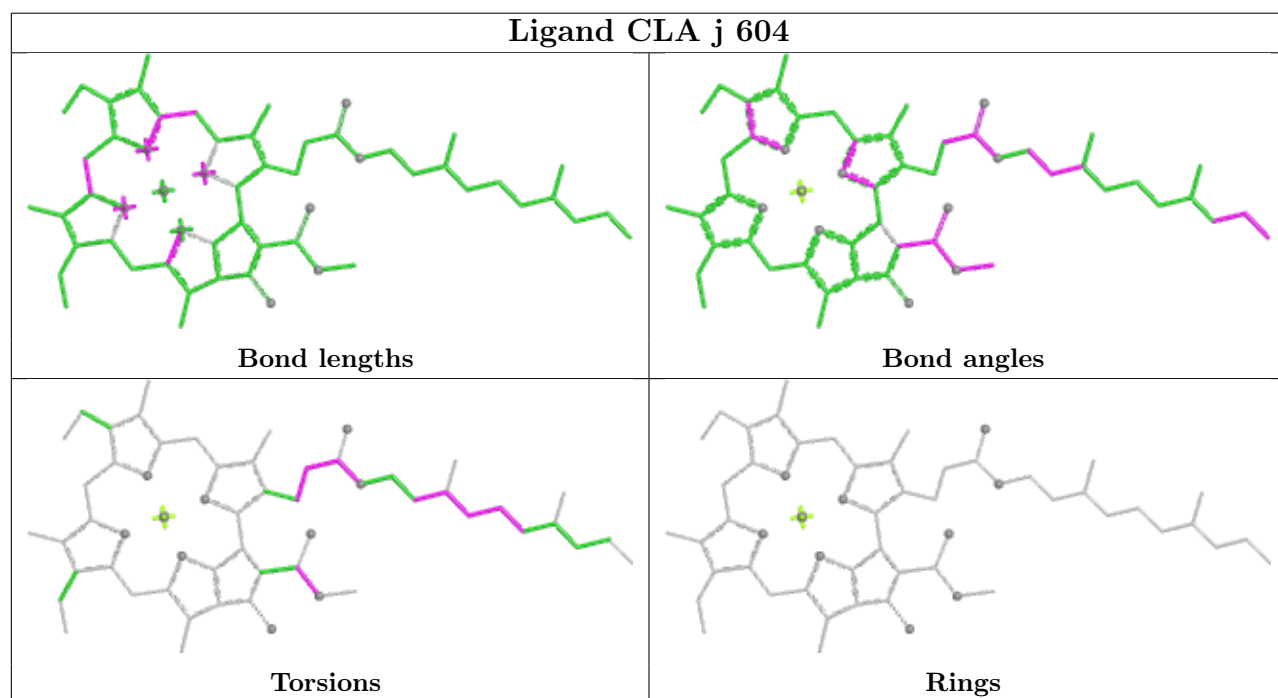
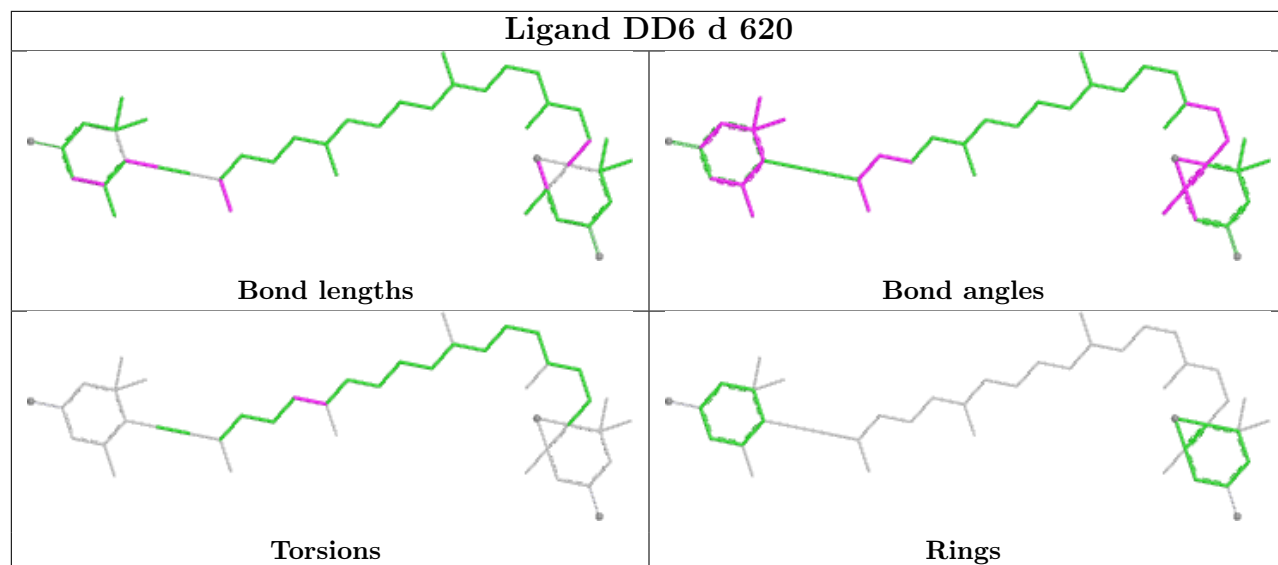
Ligand CLA c 616



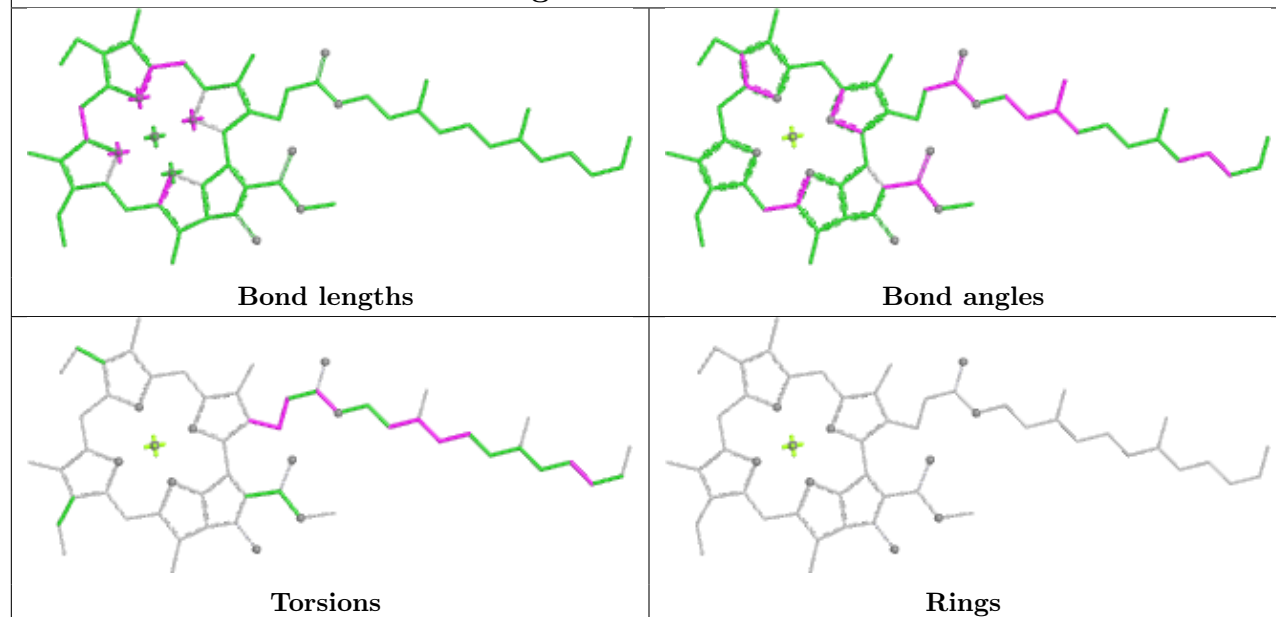
Ligand DD6 k 621



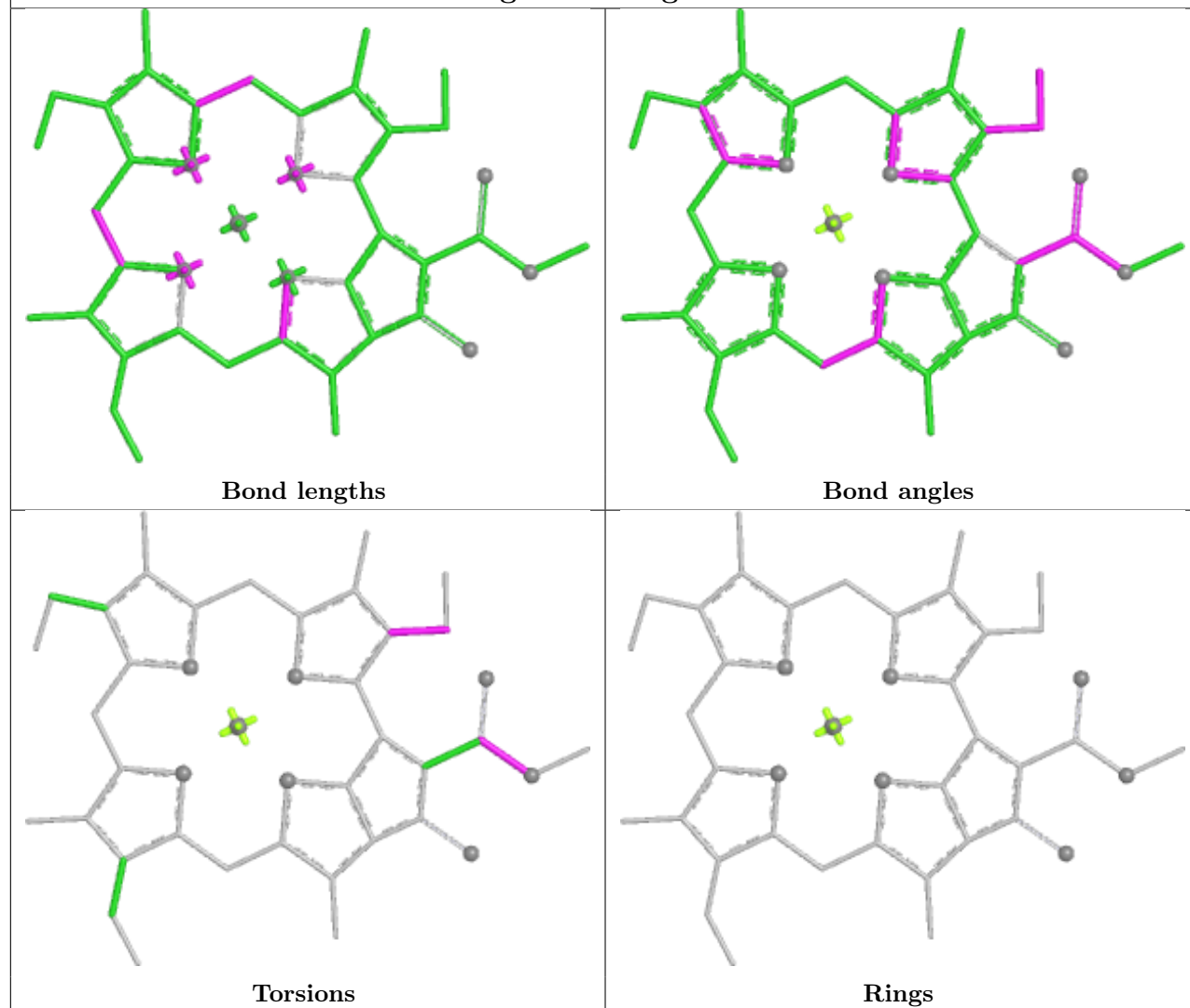


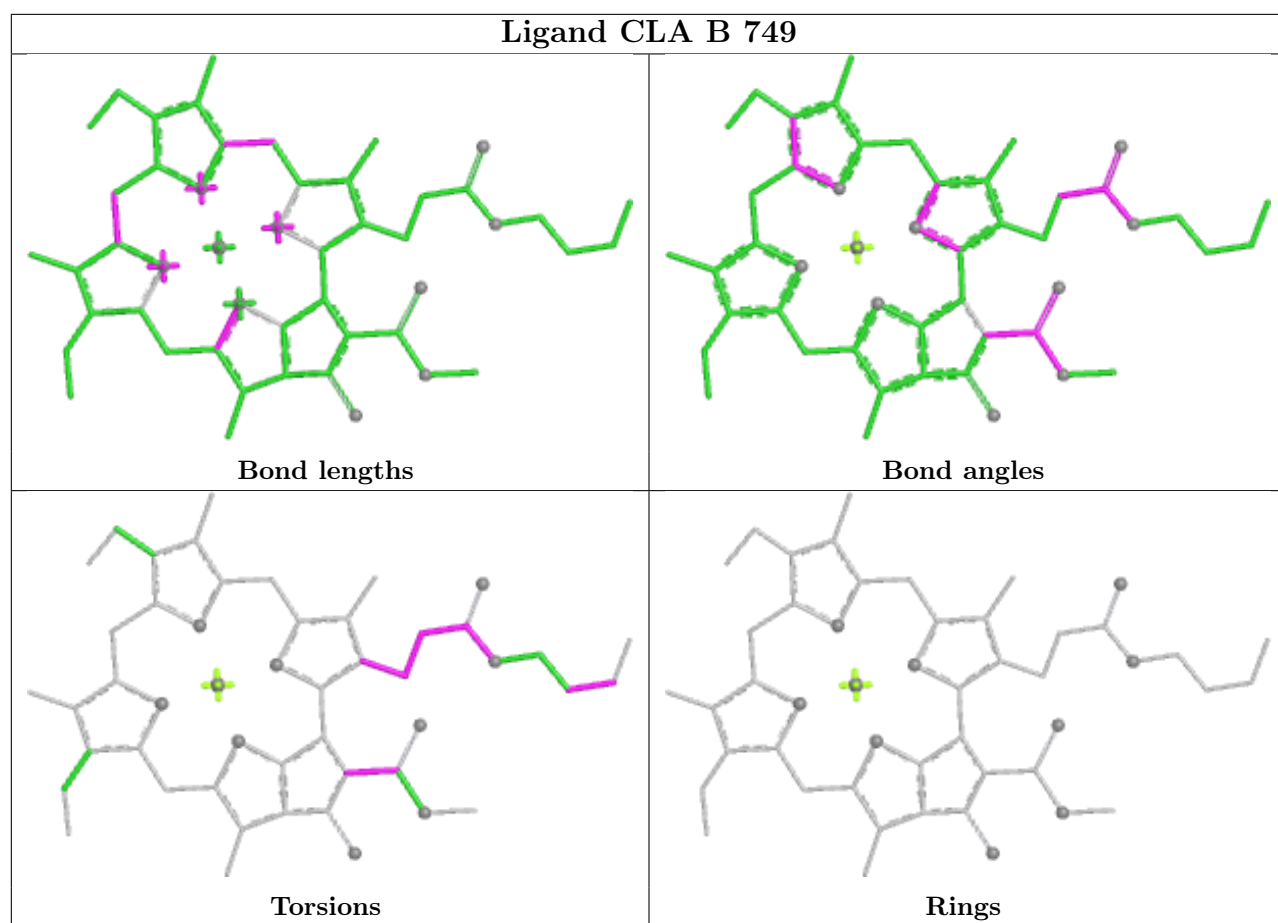


Ligand CLA A 765

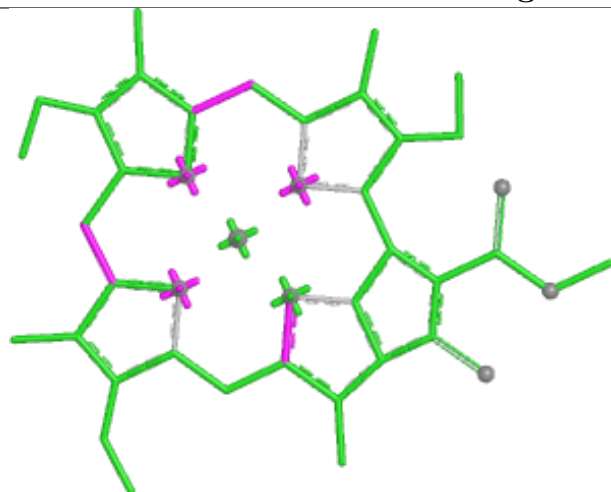


Ligand CLA g 614

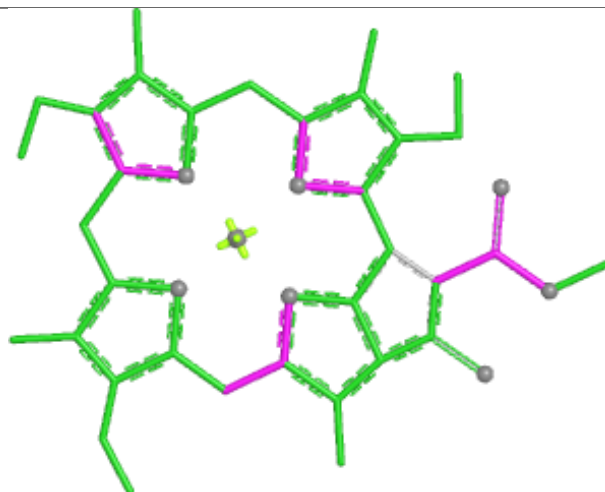




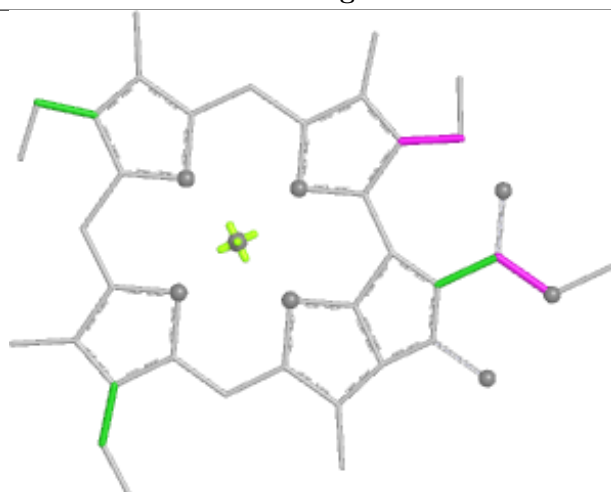
Ligand CLA d 614



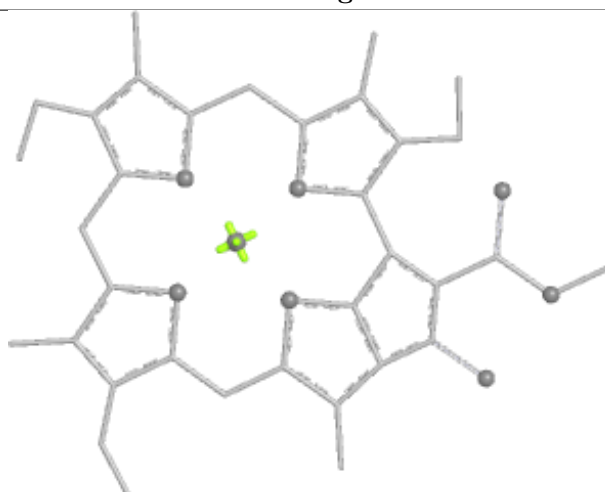
Bond lengths



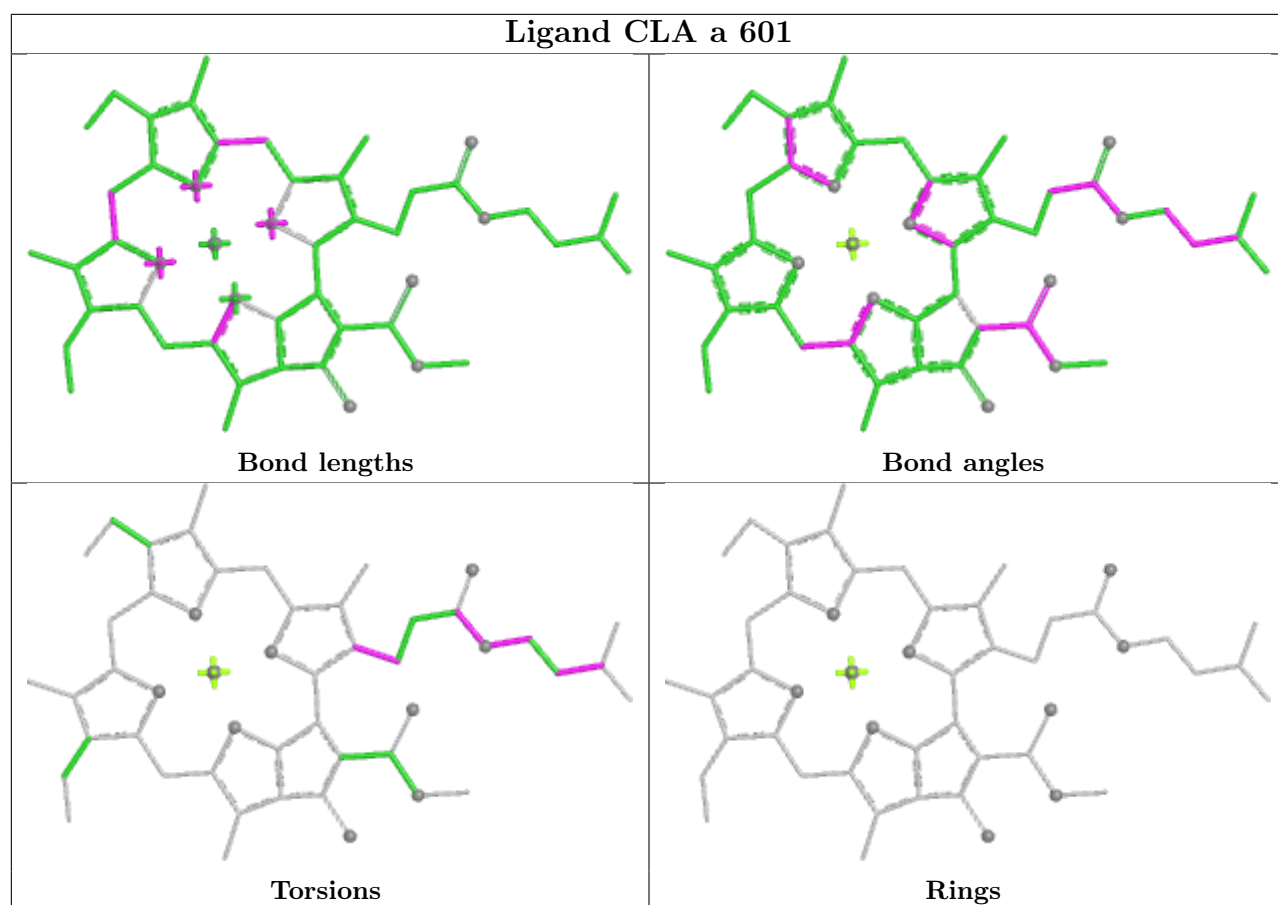
Bond angles



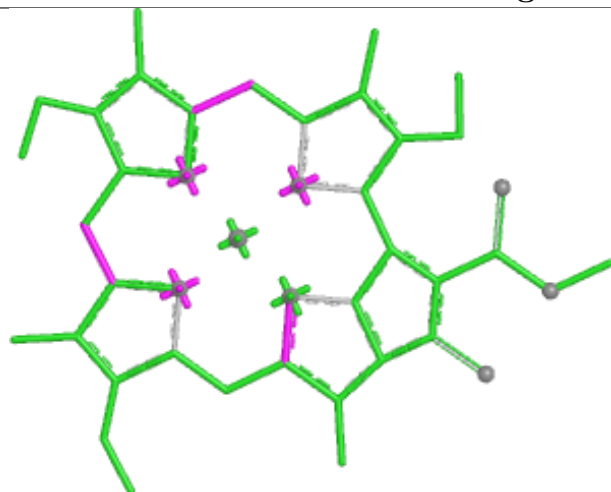
Torsions



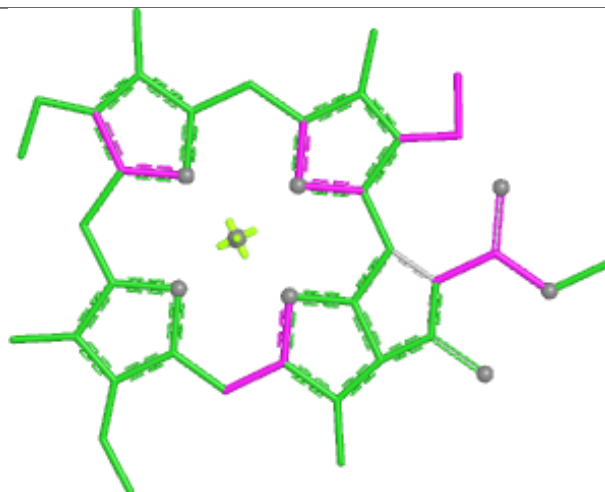
Rings



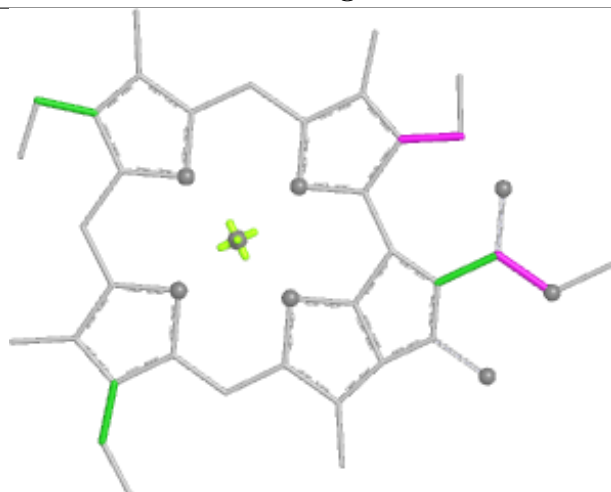
Ligand CLA b 613



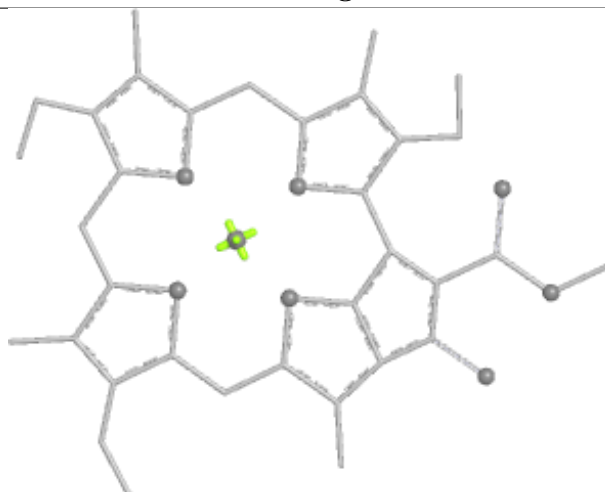
Bond lengths



Bond angles

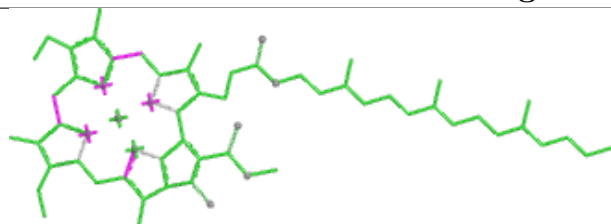


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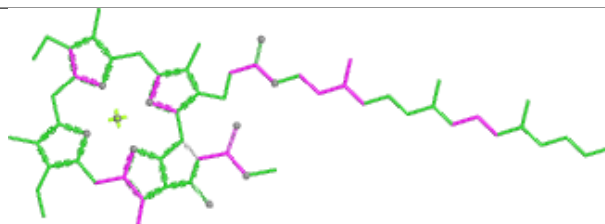


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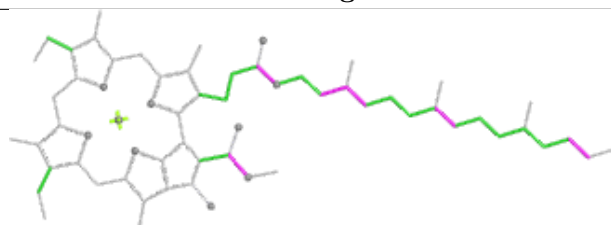
Ligand CLA a 619



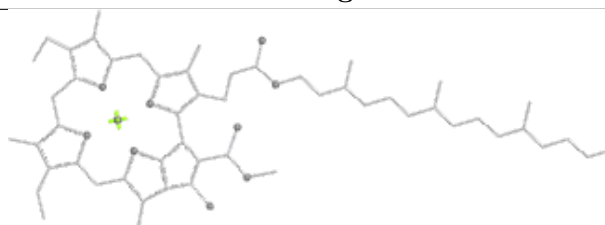
Bond lengths



Bond angles

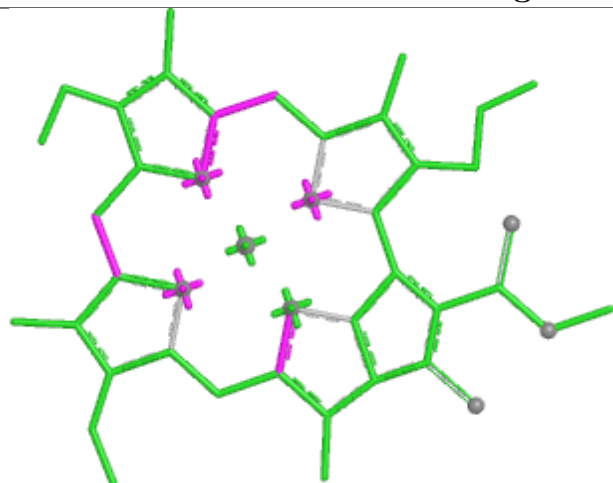


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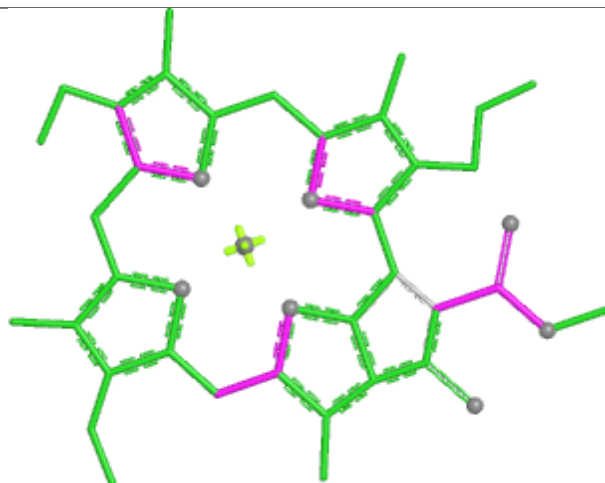


Rings

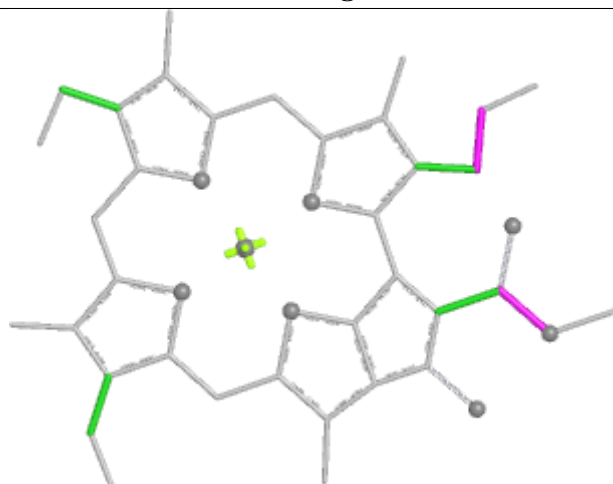
Ligand CLA A 778



Bond lengths



Bond angles

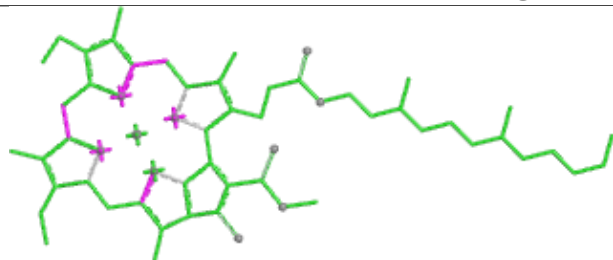


Torsions

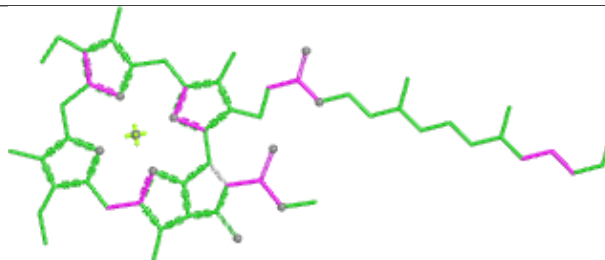


Rings

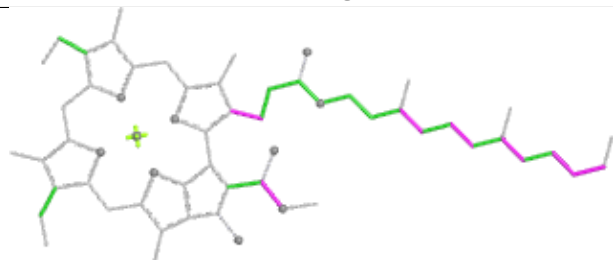
Ligand CLA B 748



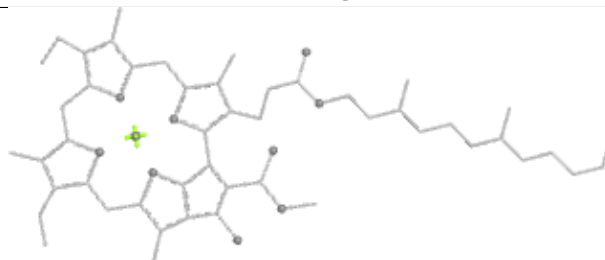
Bond lengths



Bond angles

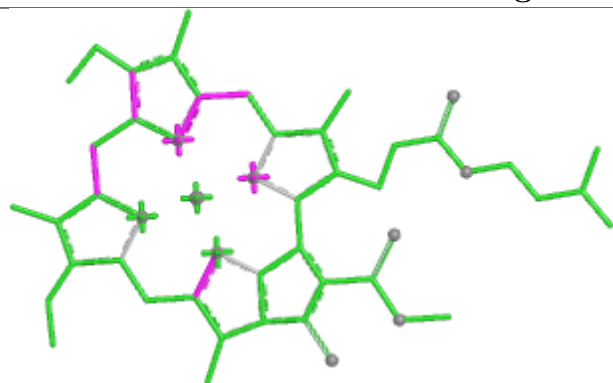


Torsions

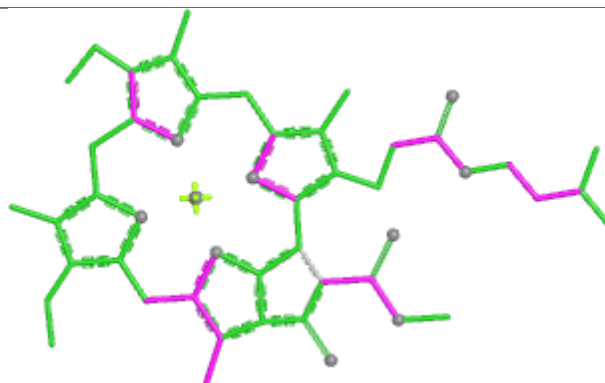


Rings

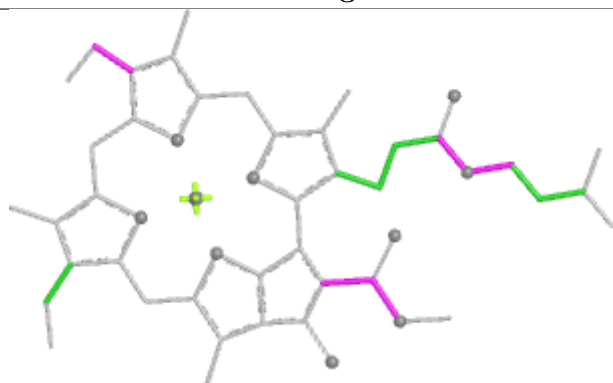
Ligand CLA B 751



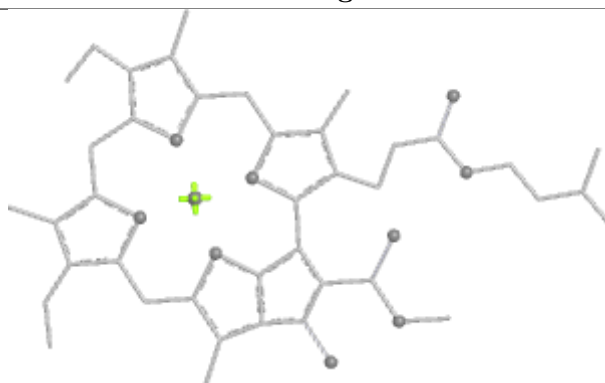
Bond lengths



Bond angles

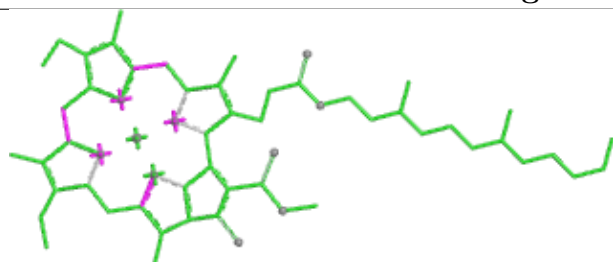


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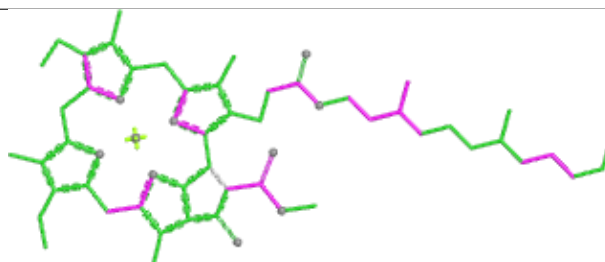


Rings

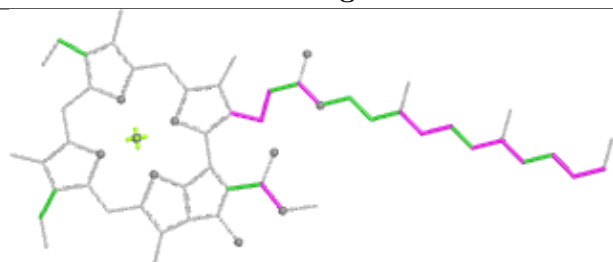
Ligand CLA f 602



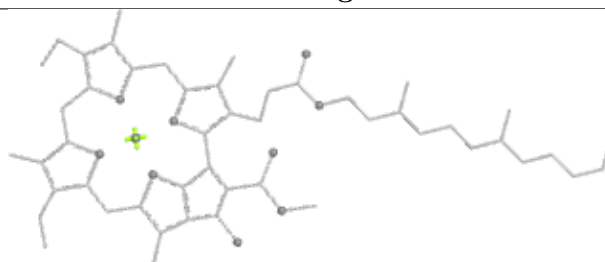
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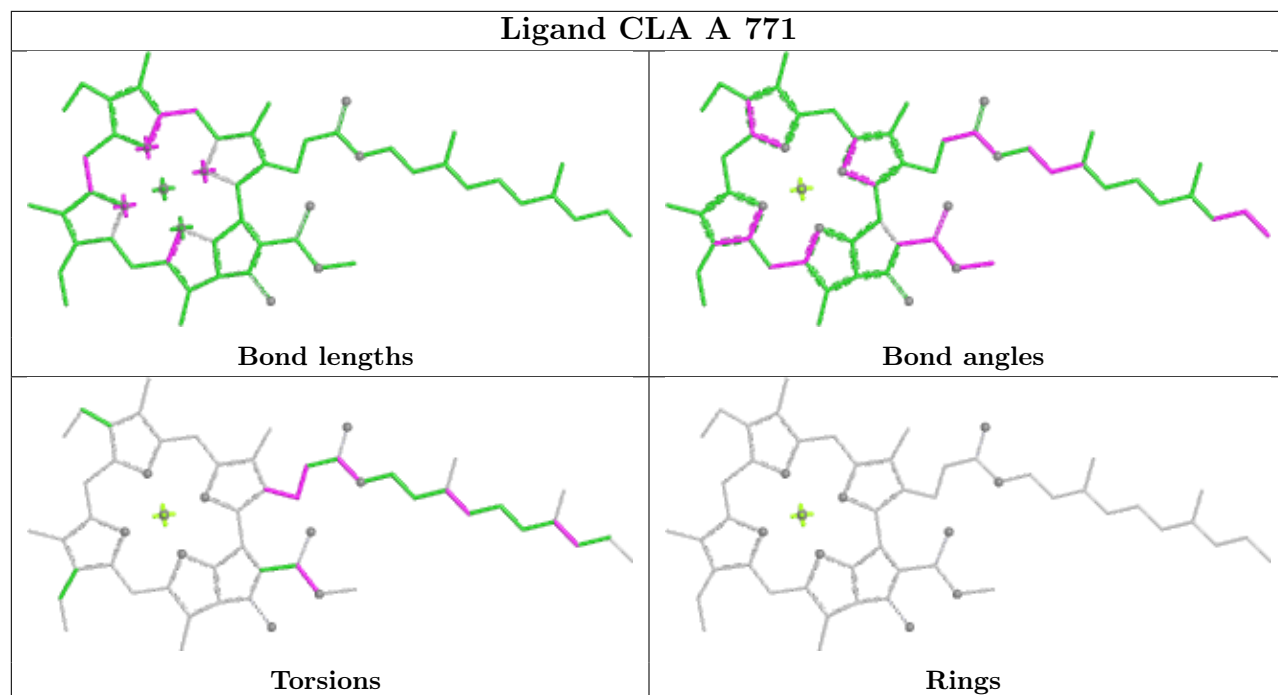
Bond angles



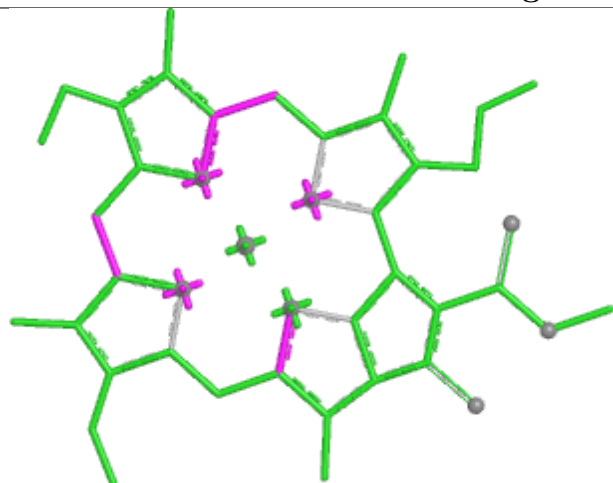
Torsions



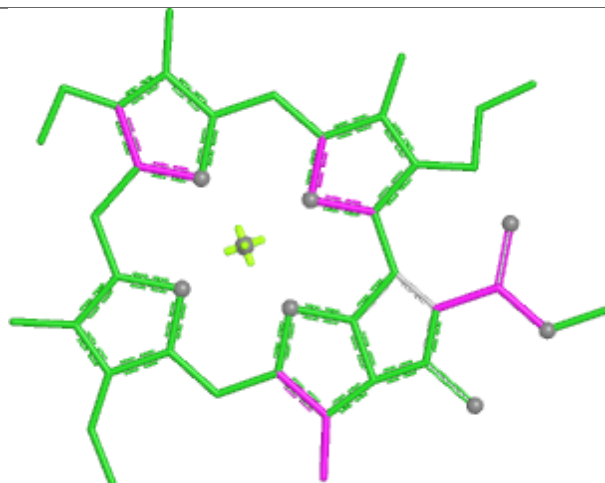
Rings



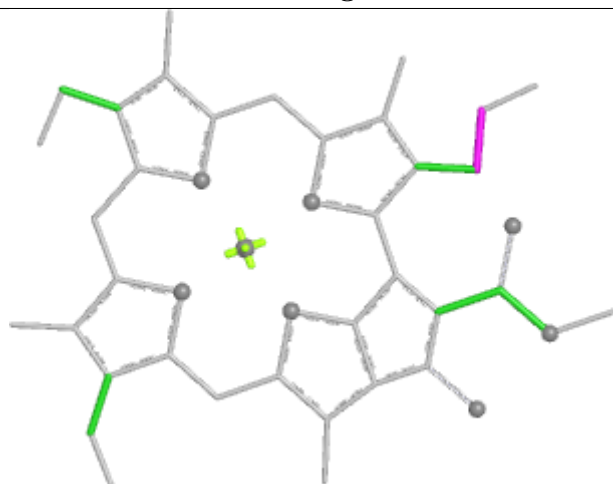
Ligand CLA 1 603



Bond lengths



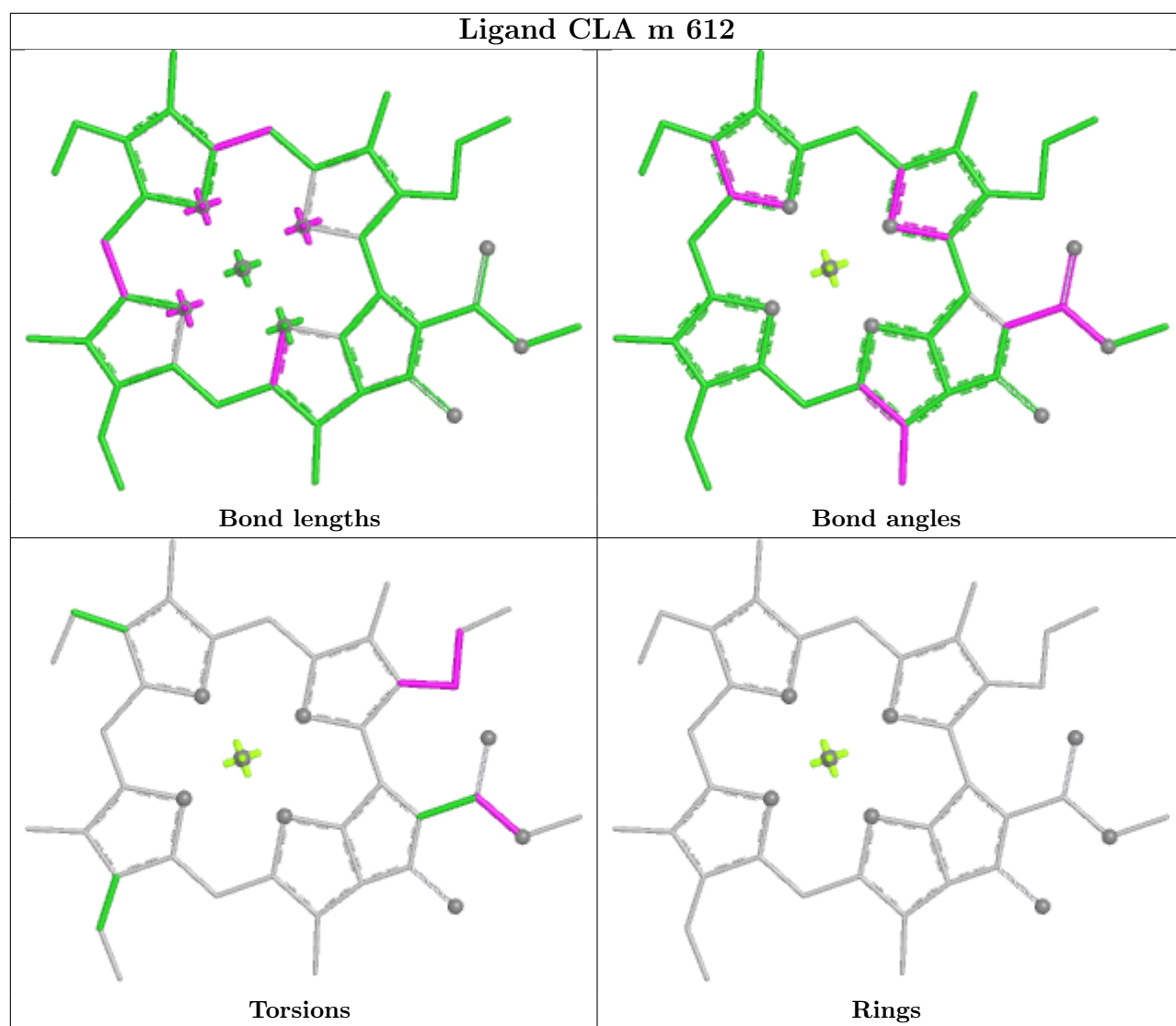
Bond angles

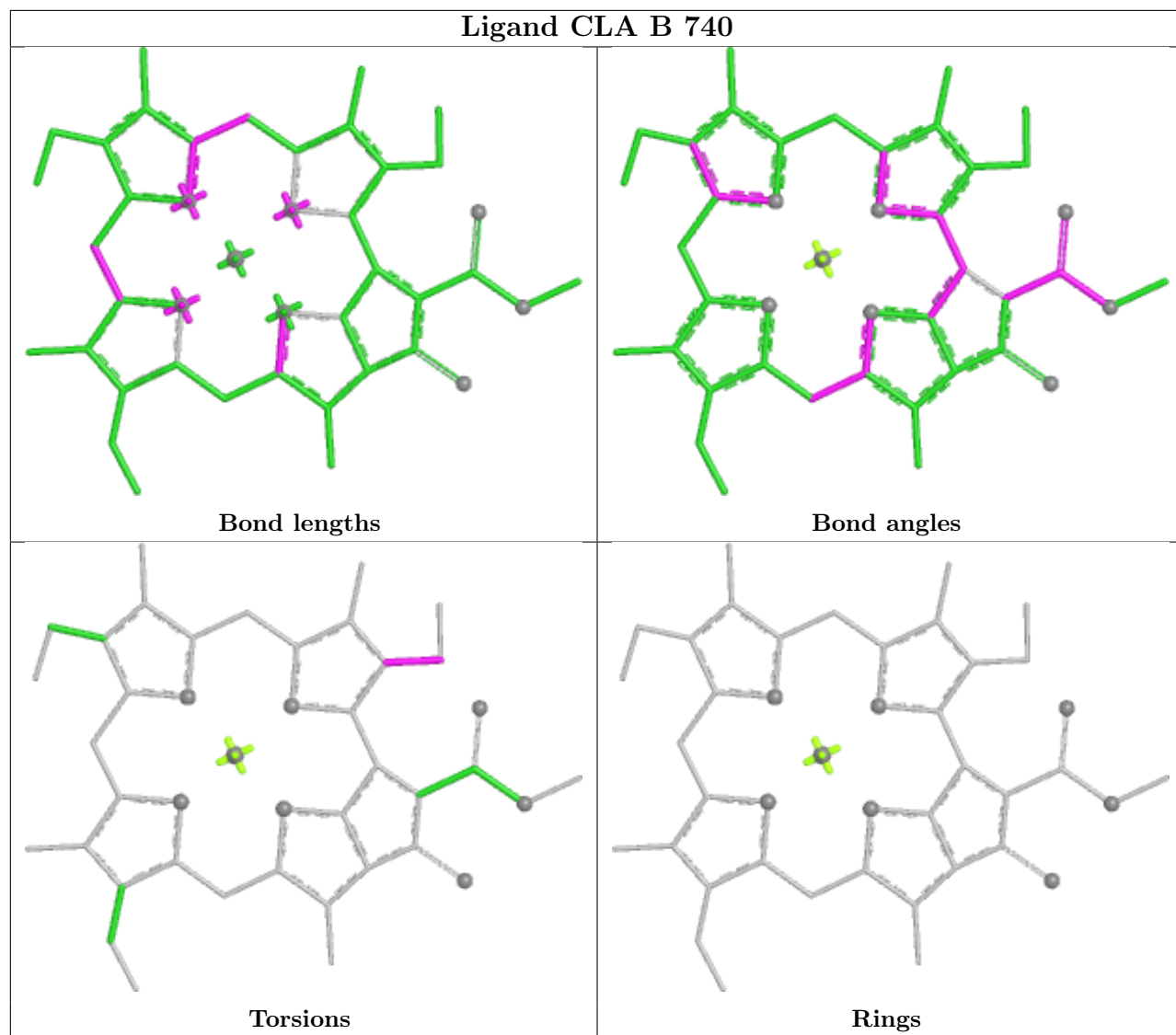


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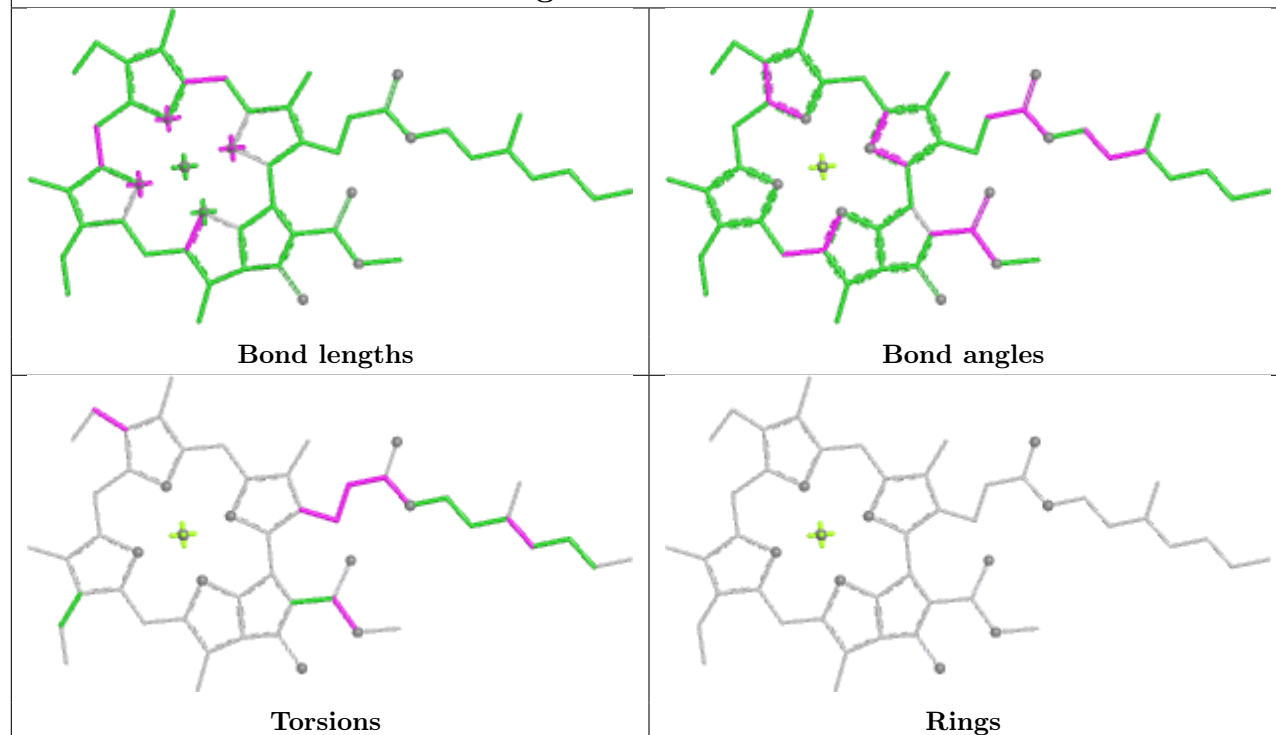


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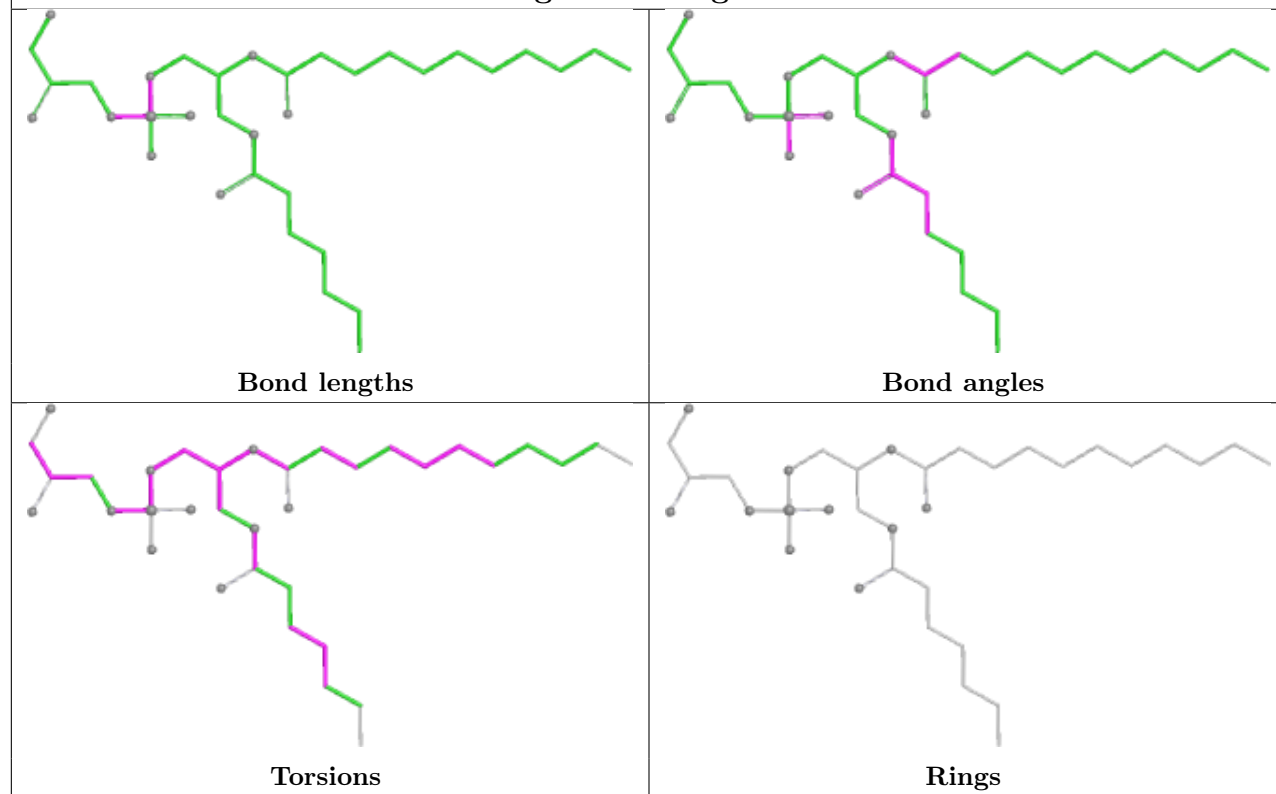




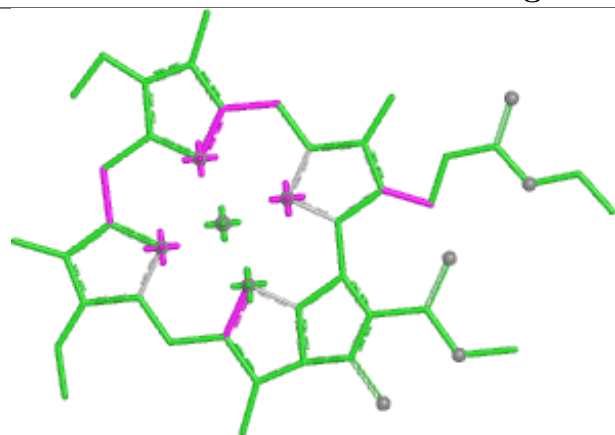
Ligand CLA a 608



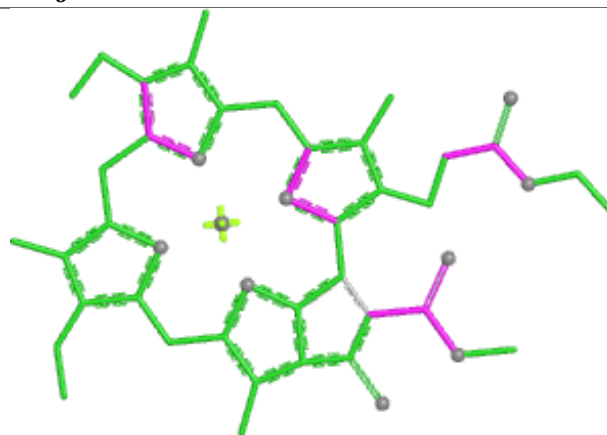
Ligand LHG g 189



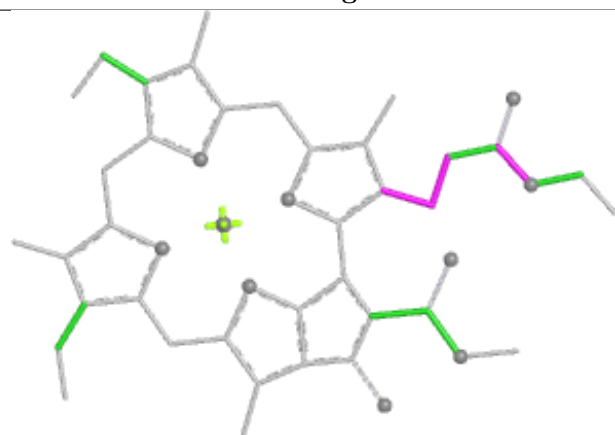
Ligand CLA j 608



Bond lengths



Bond angles

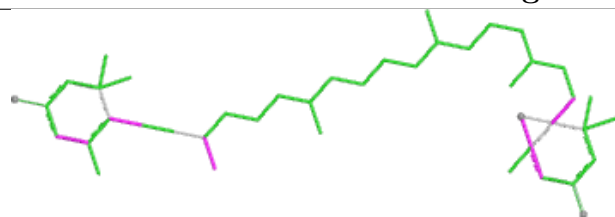


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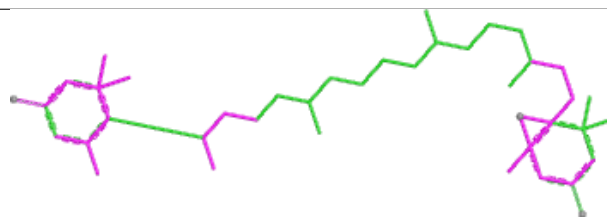


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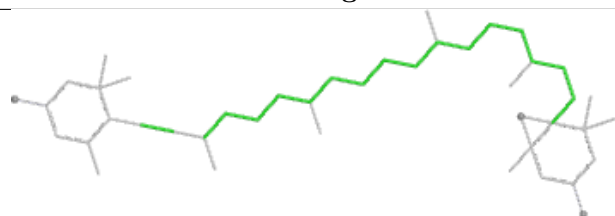
Ligand DD6 c 621



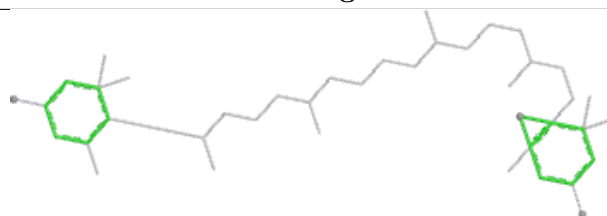
Bond lengths



Bond angles

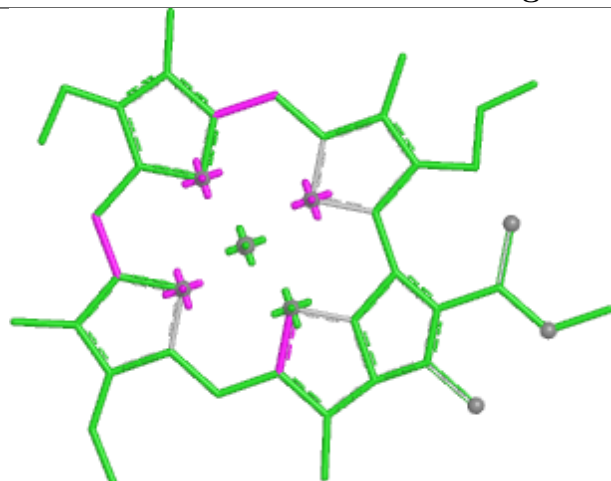


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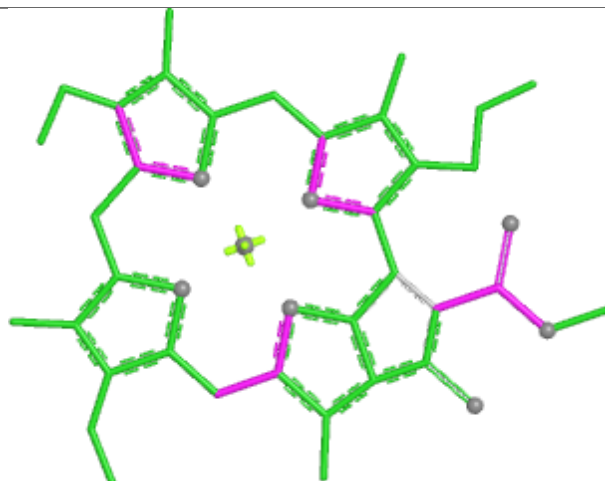


Rings

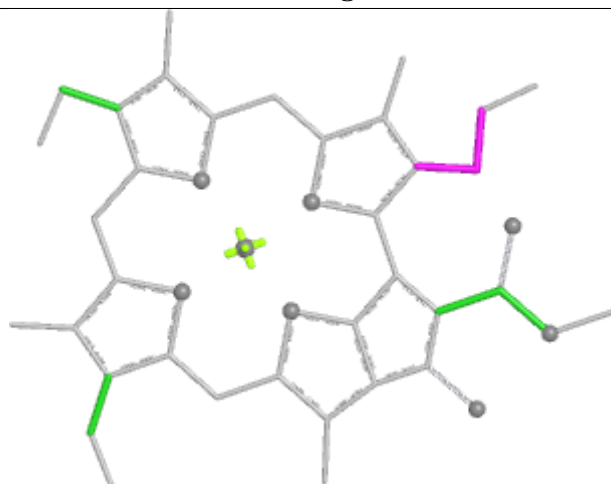
Ligand CLA 1 611



Bond lengths



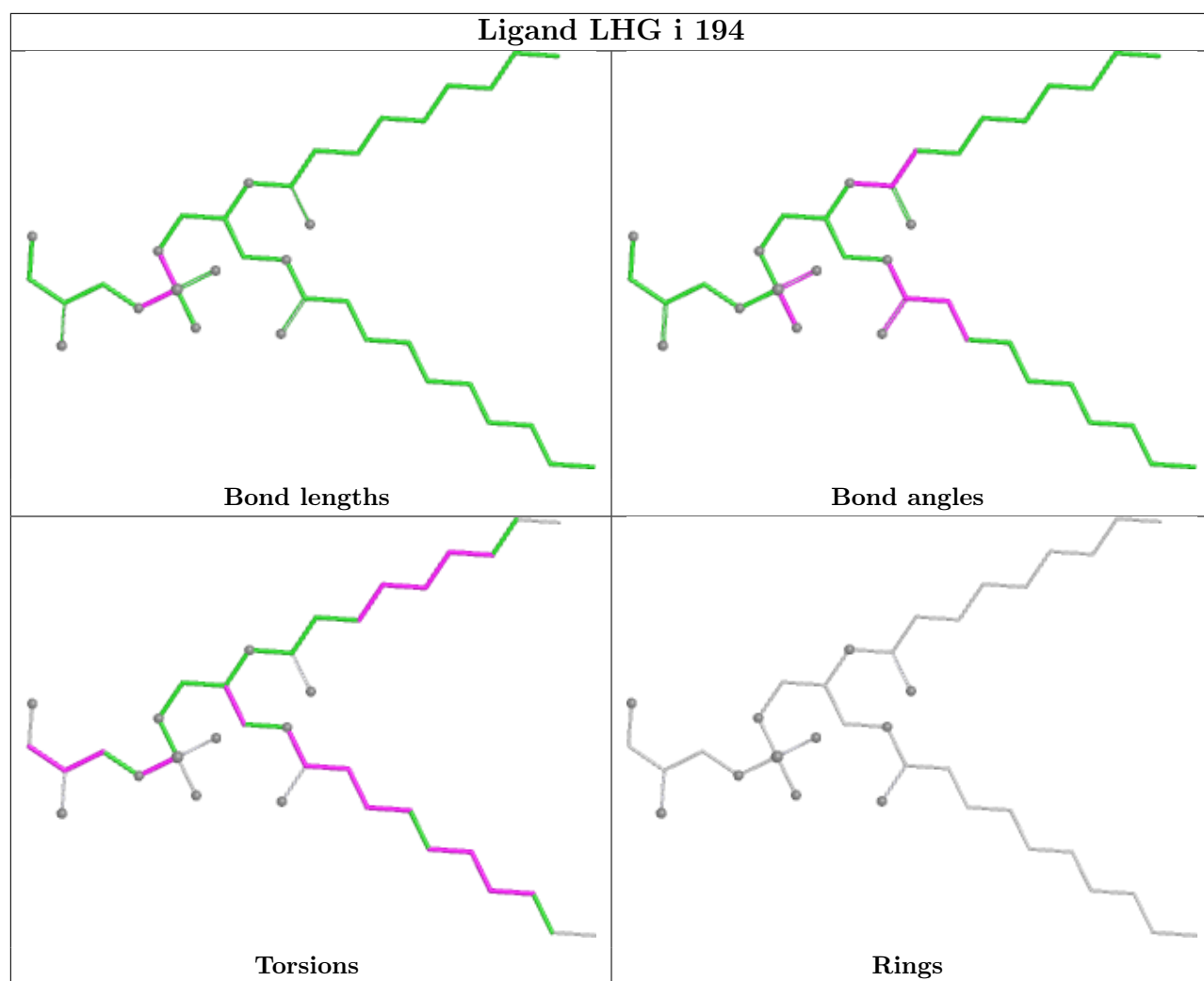
Bond angles



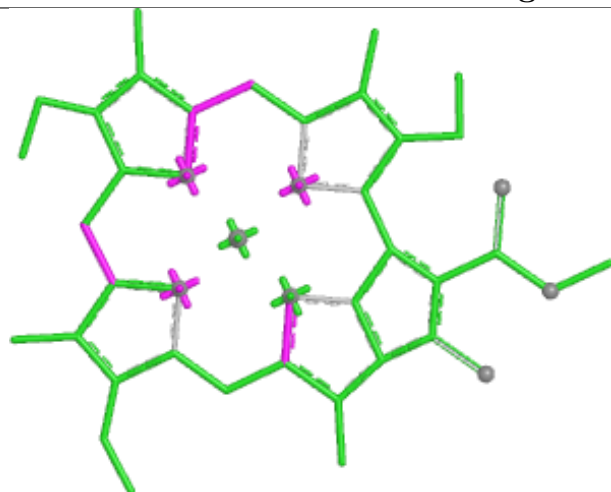
Torsions



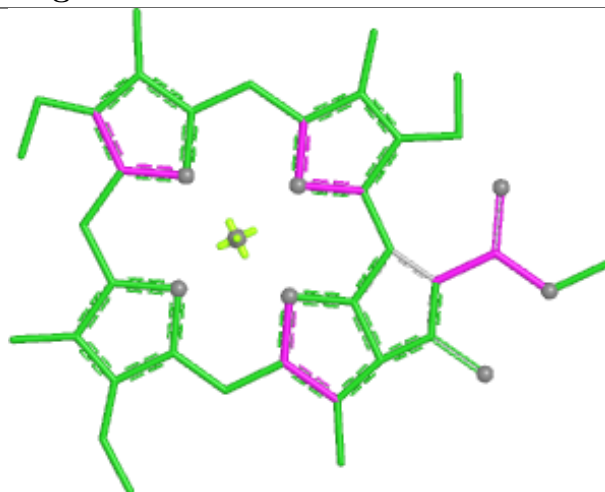
Rings



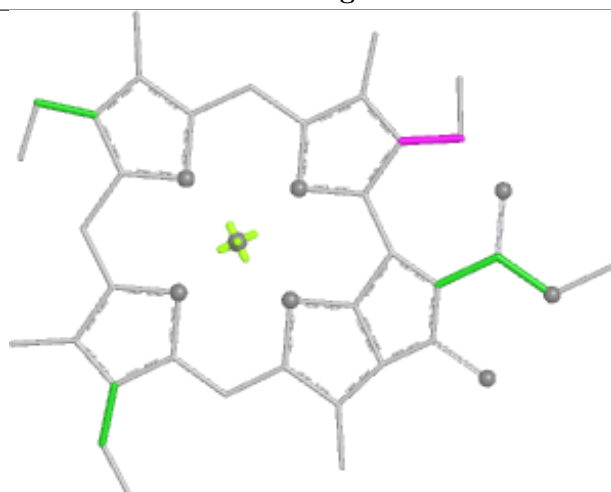
Ligand CLA g 603



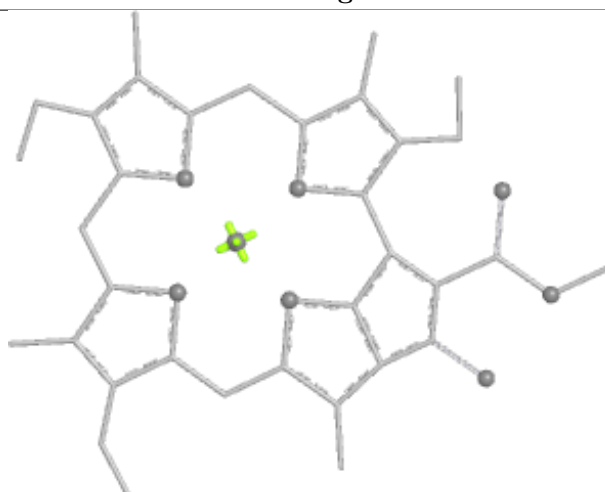
Bond lengths



Bond angles

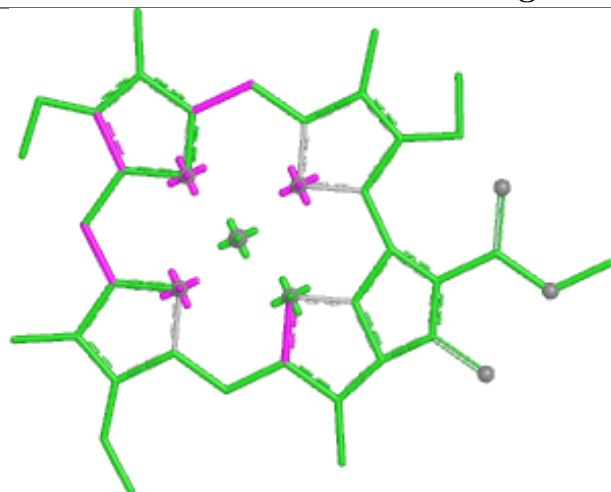


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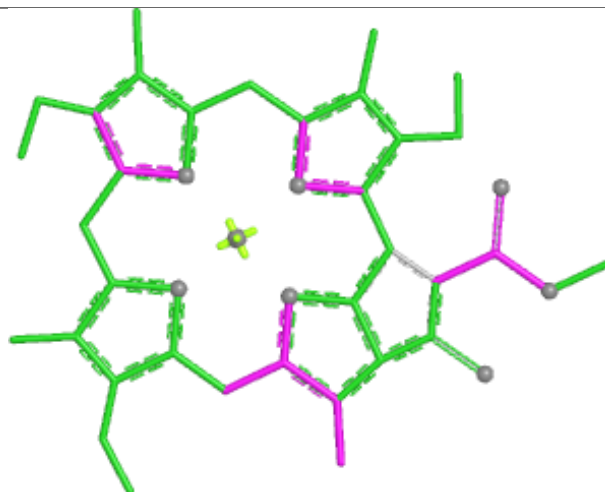


Rings

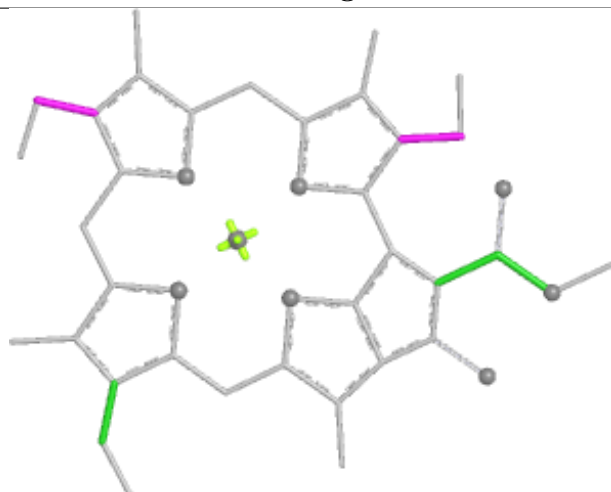
Ligand CLA o 604



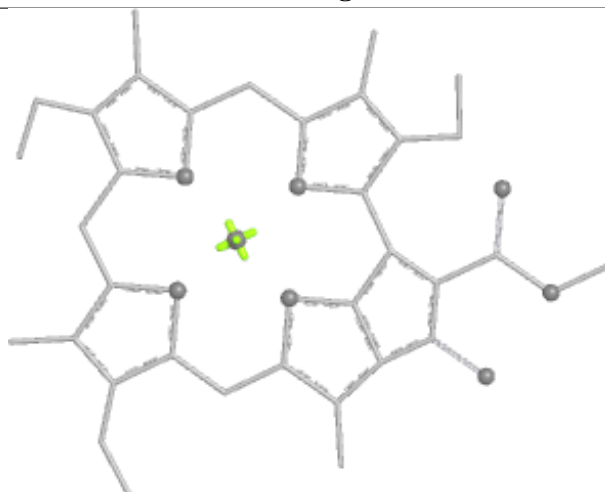
Bond lengths



Bond angles

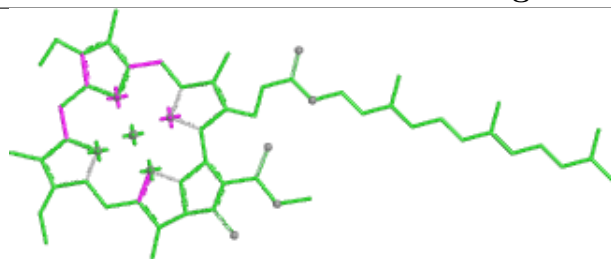


Torsions

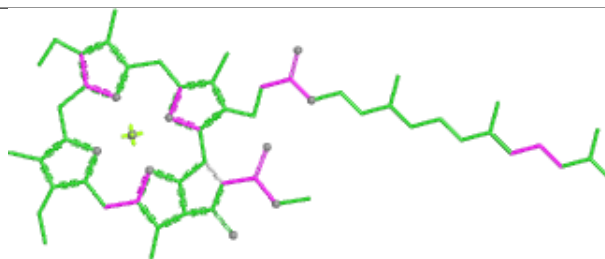


Rings

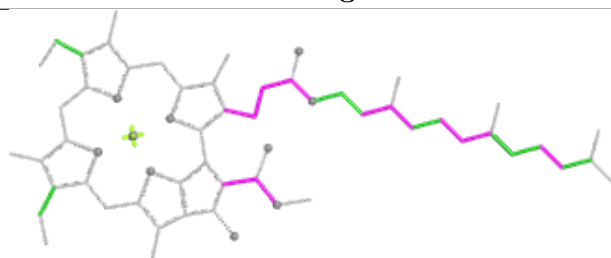
Ligand CLA m 602



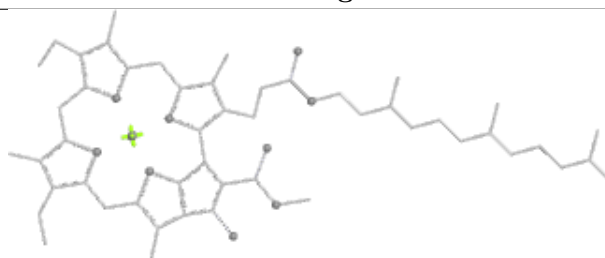
Bond lengths



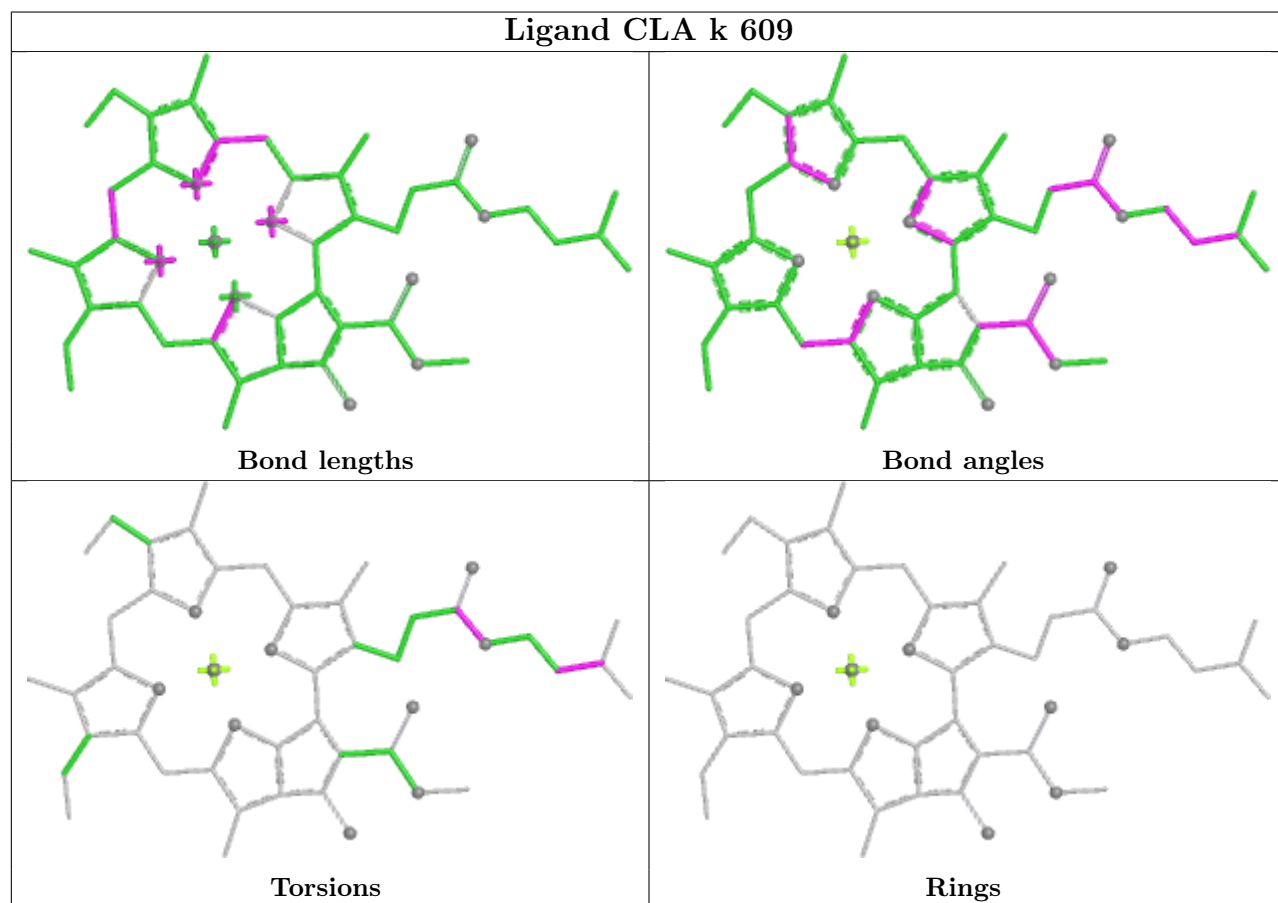
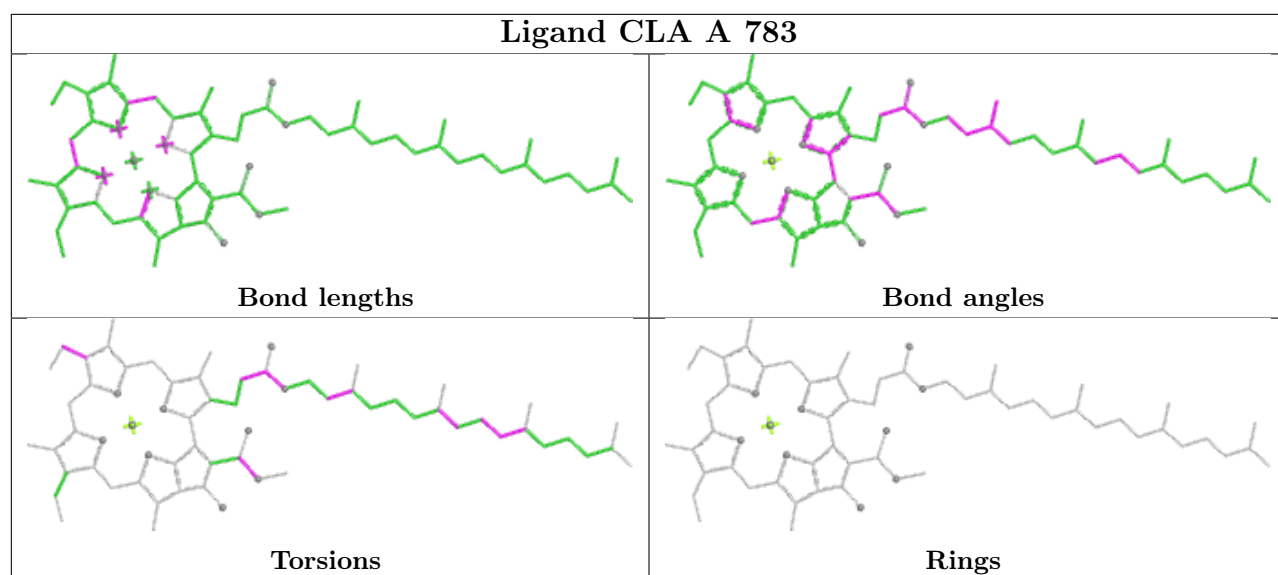
Bond angles

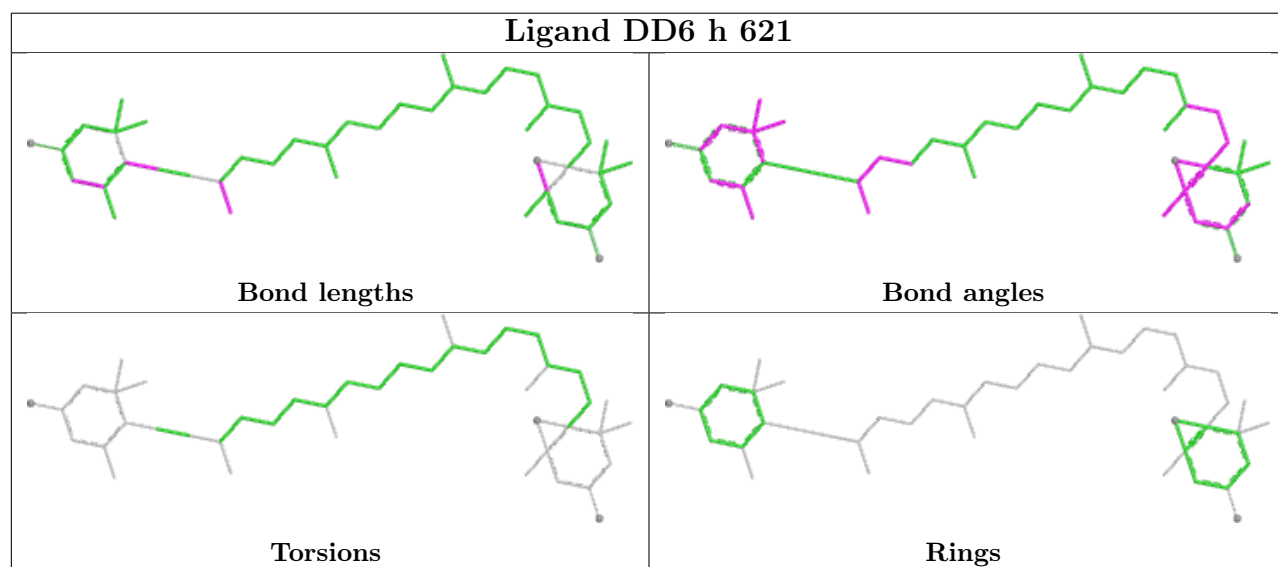
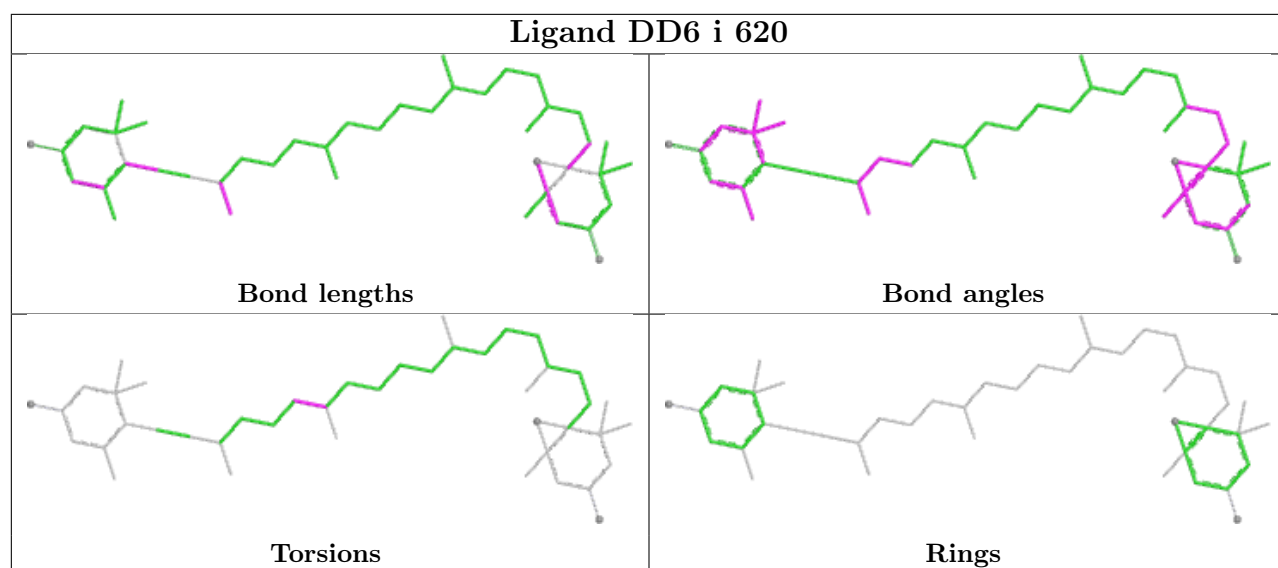


Torsions

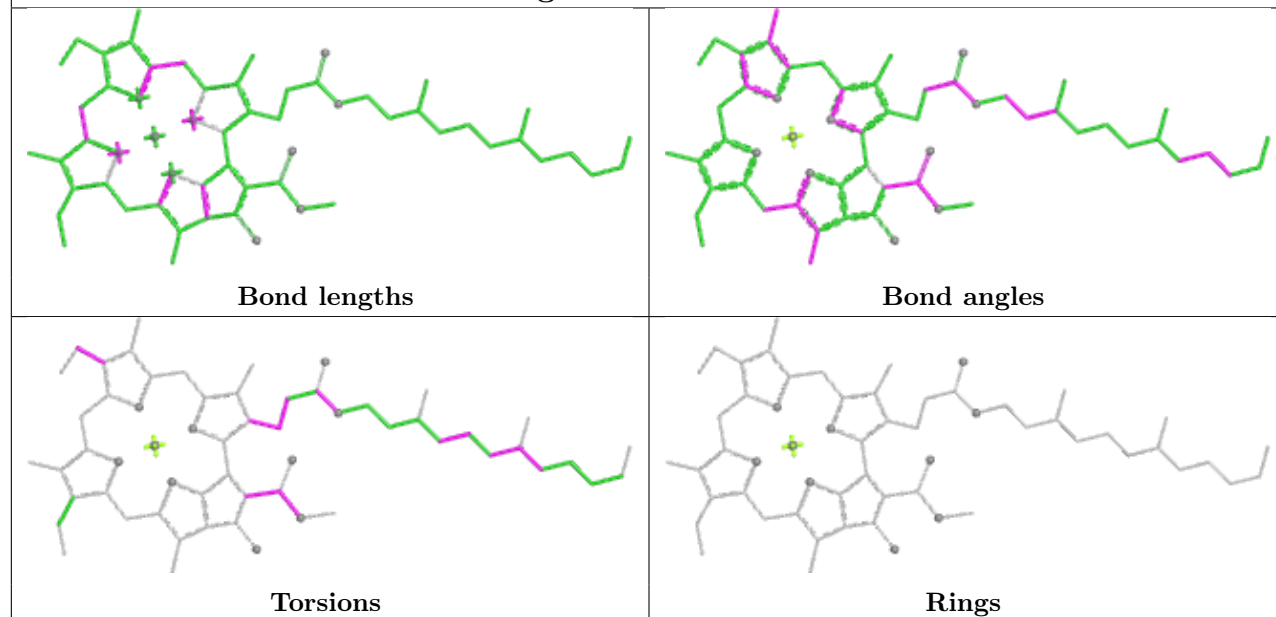


Rings

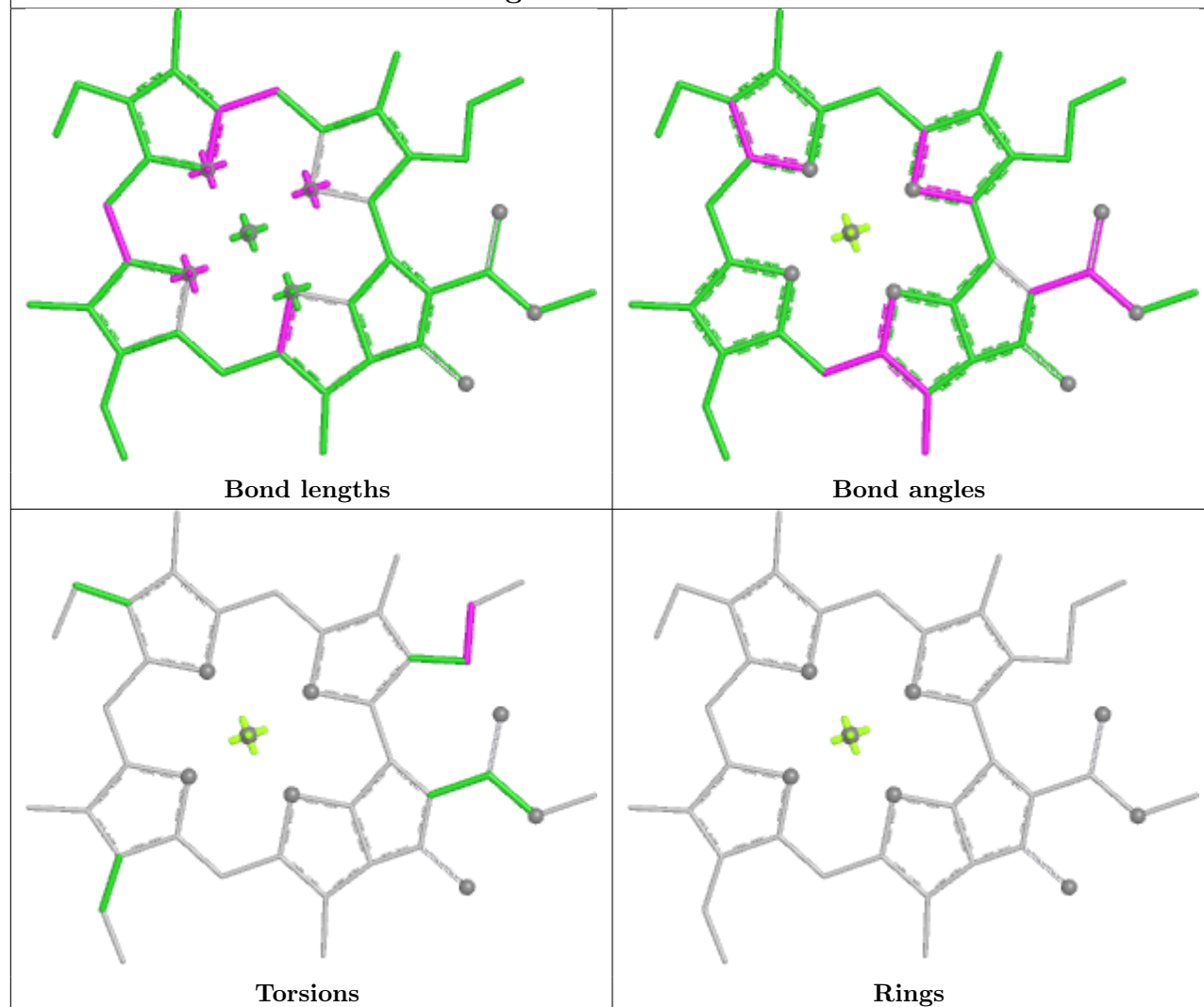




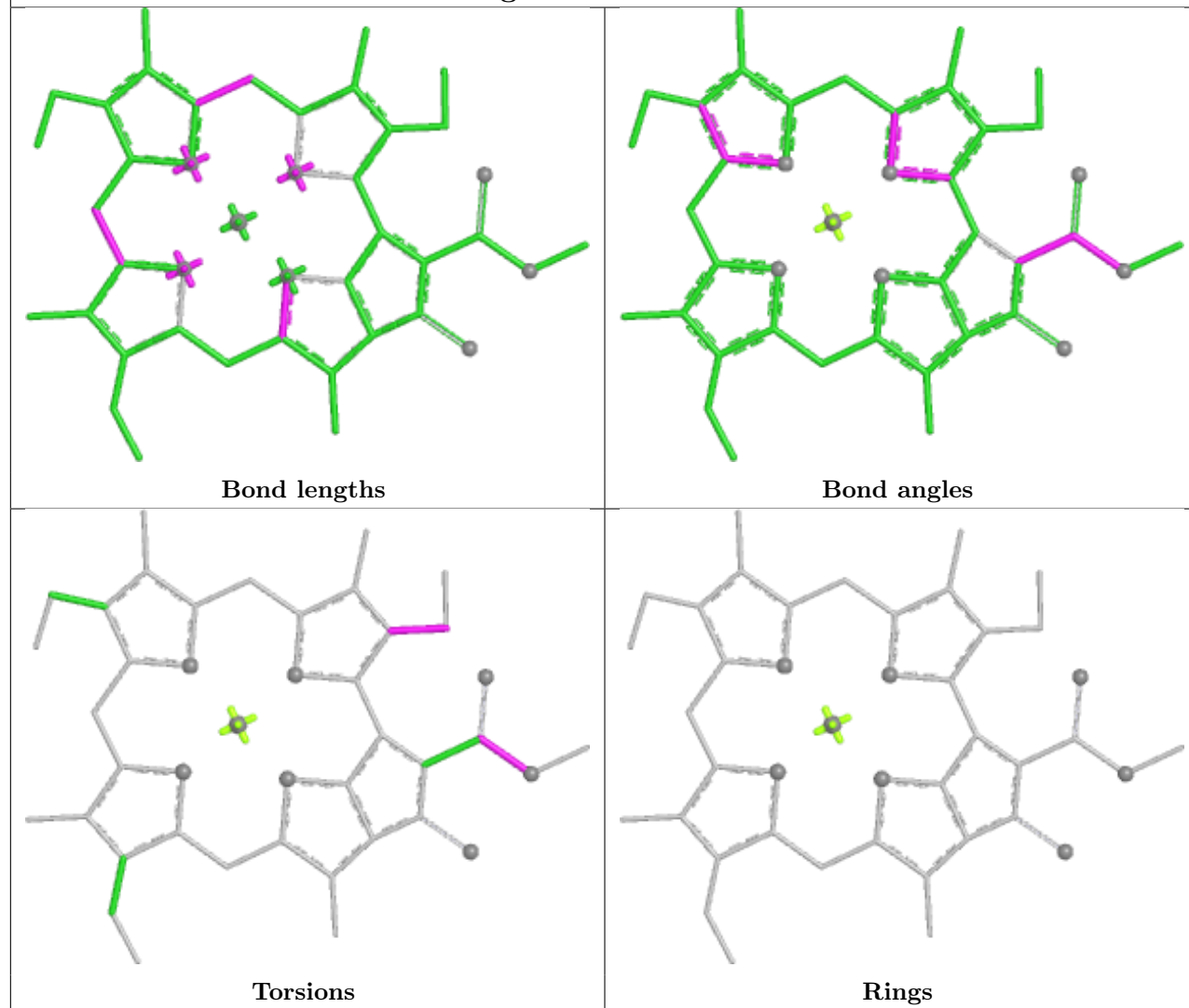
Ligand CLA c 602



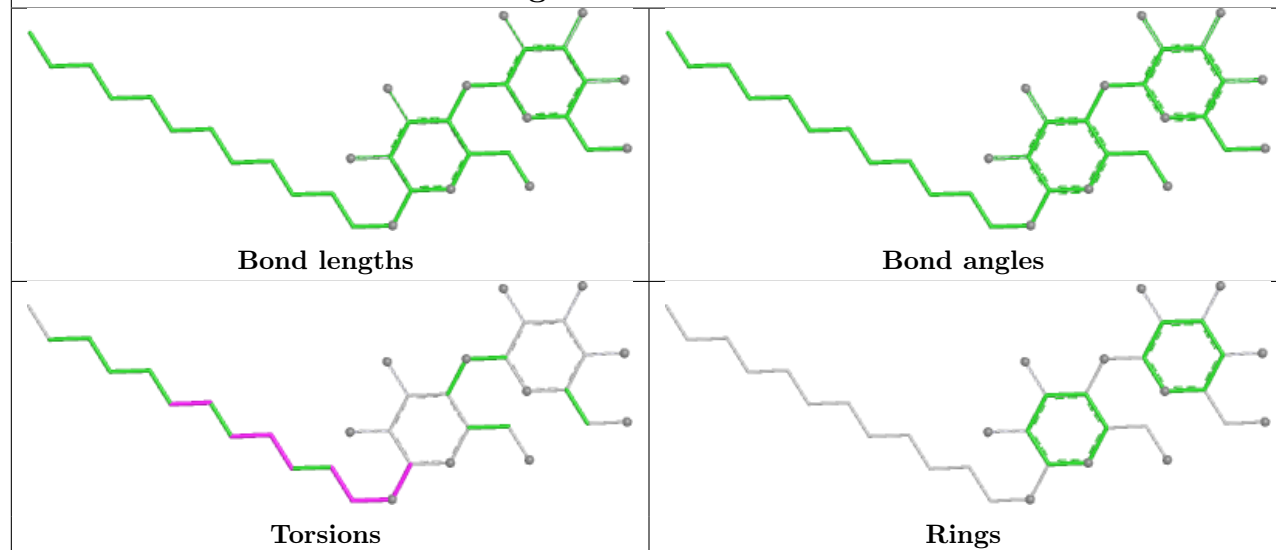
Ligand CLA k 612



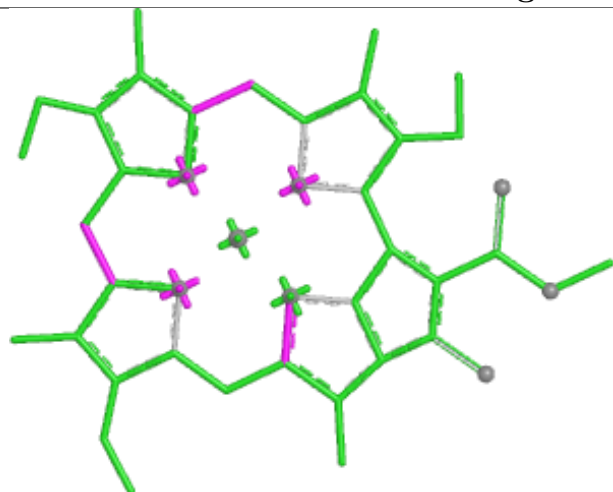
Ligand CLA e 614



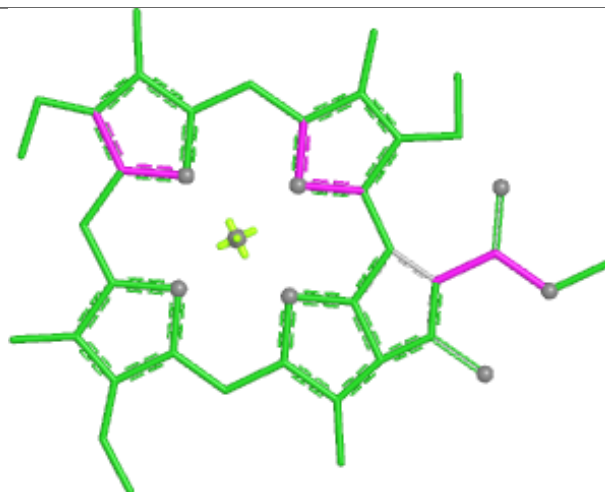
Ligand LMT A 754



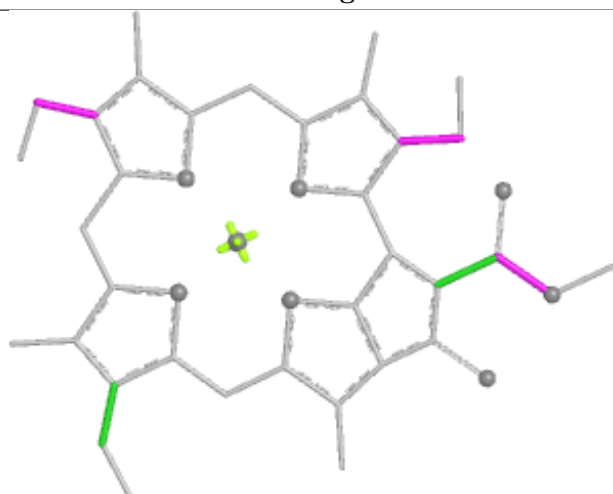
Ligand CLA n 606



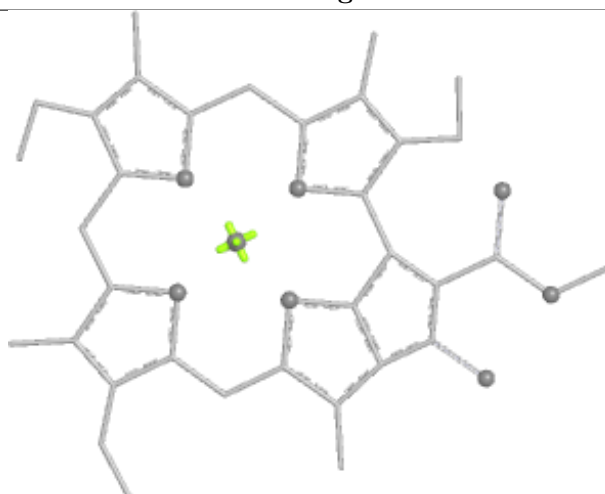
Bond lengths



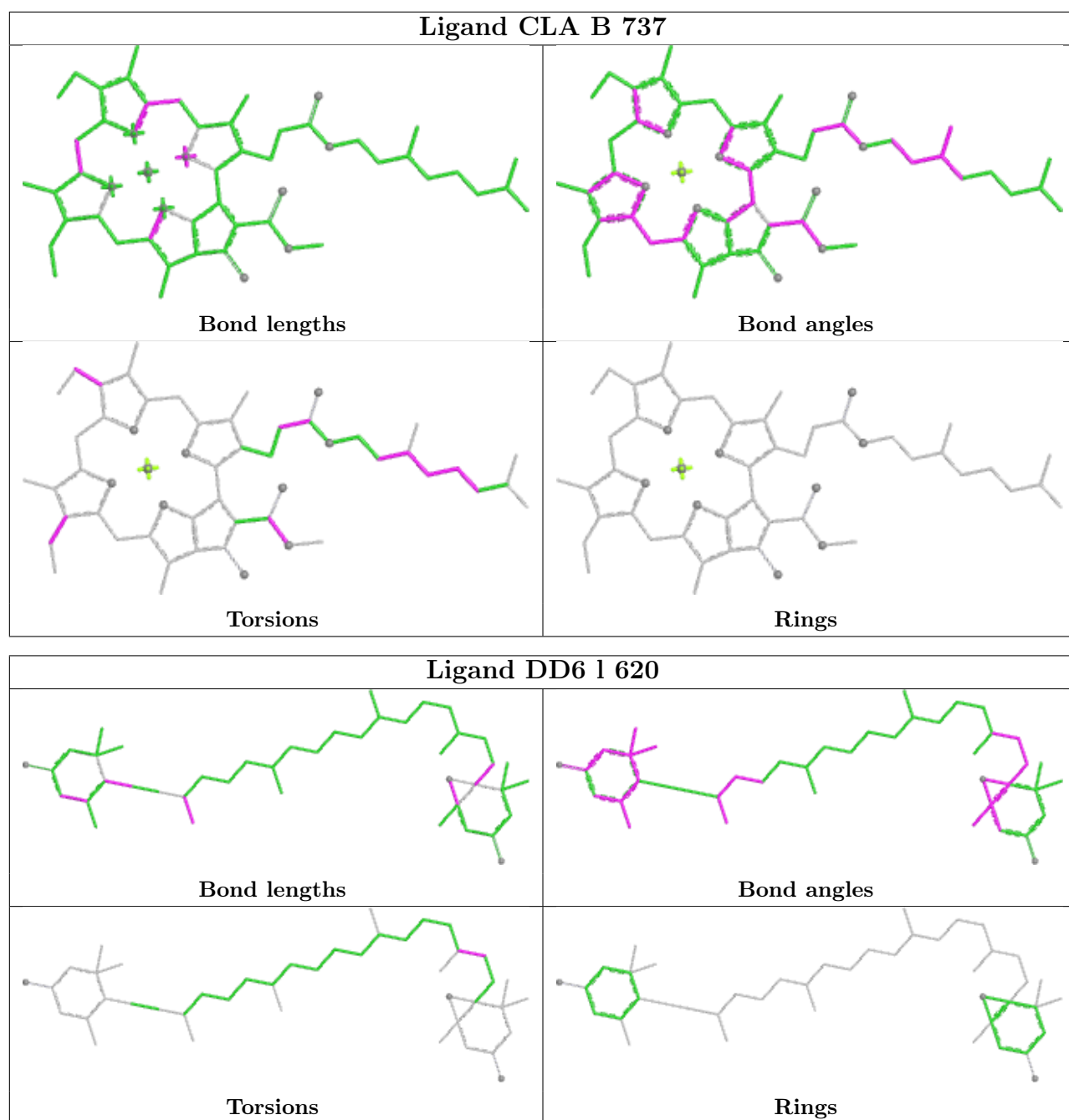
Bond angles



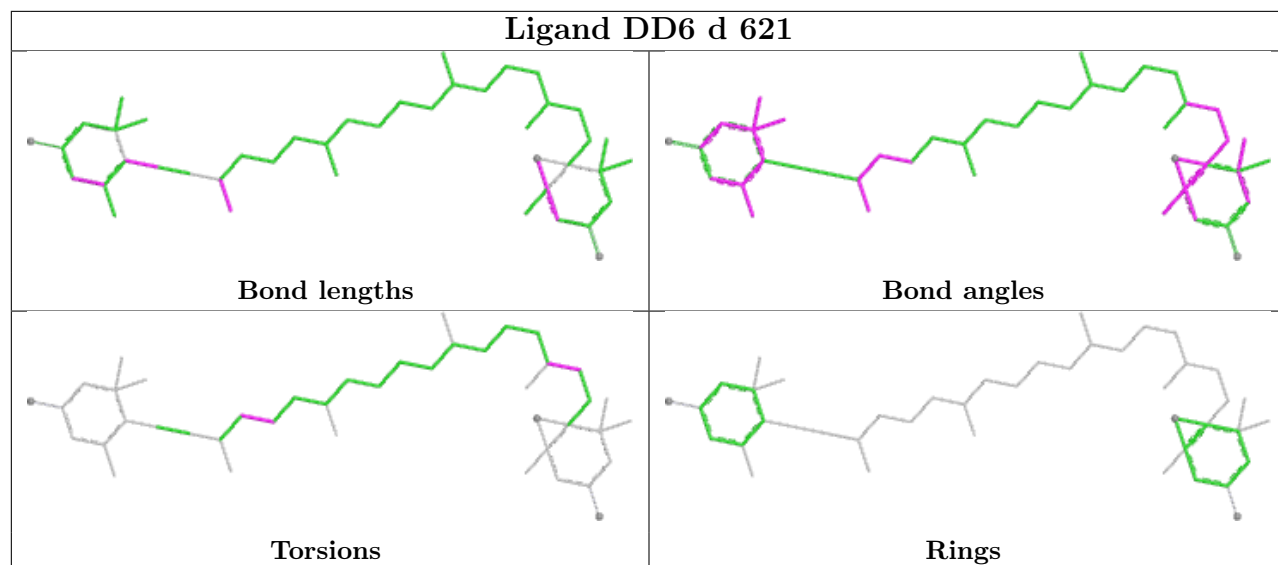
Torsions



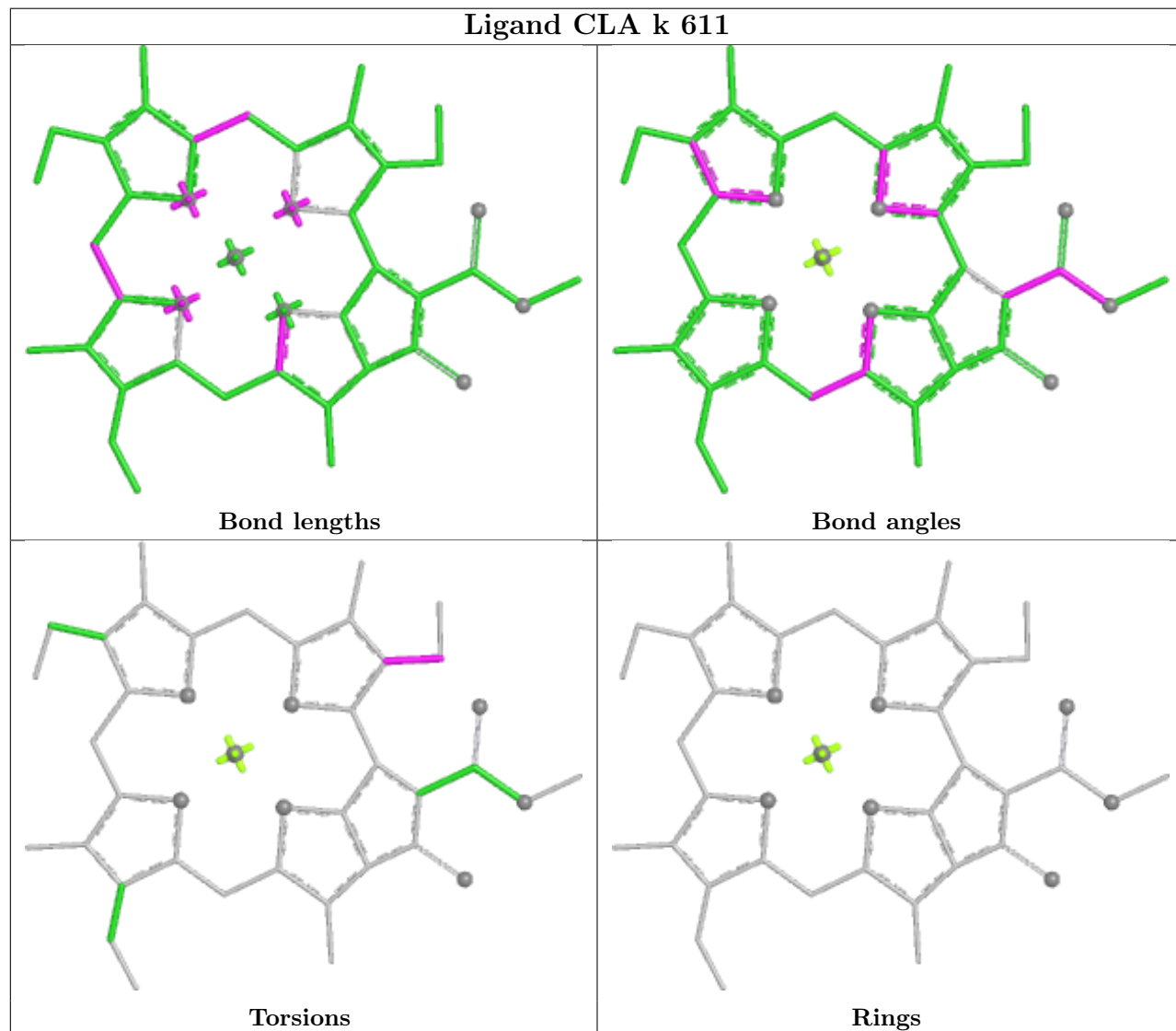
Rings



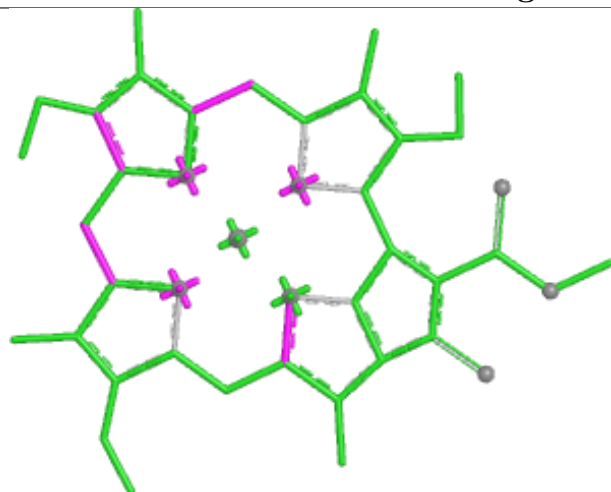
Ligand DD6 d 621



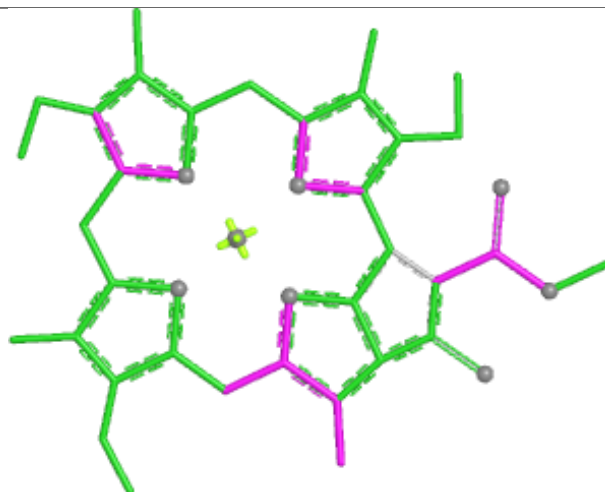
Ligand CLA k 611



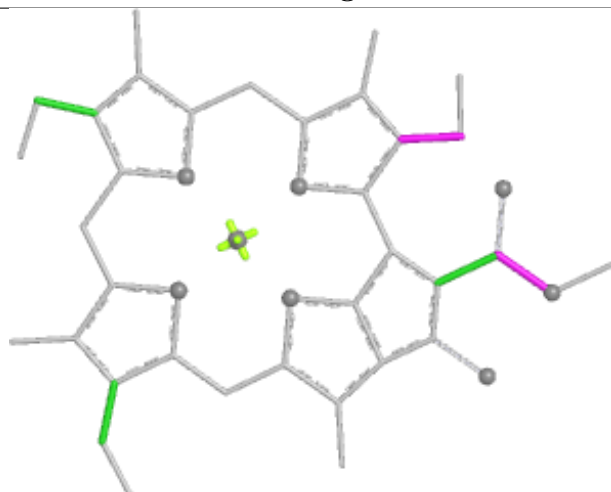
Ligand CLA b 601



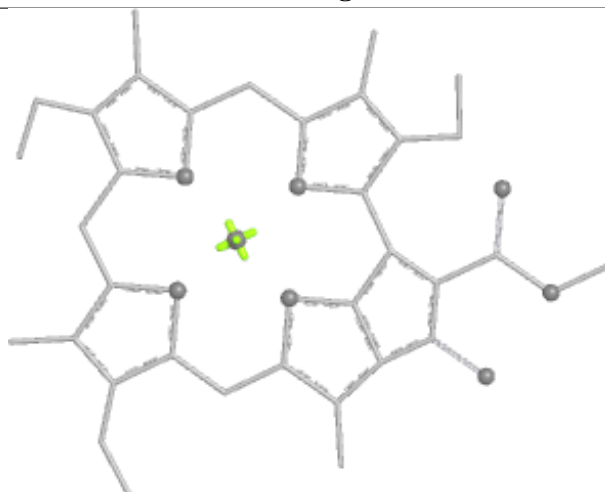
Bond lengths



Bond angles

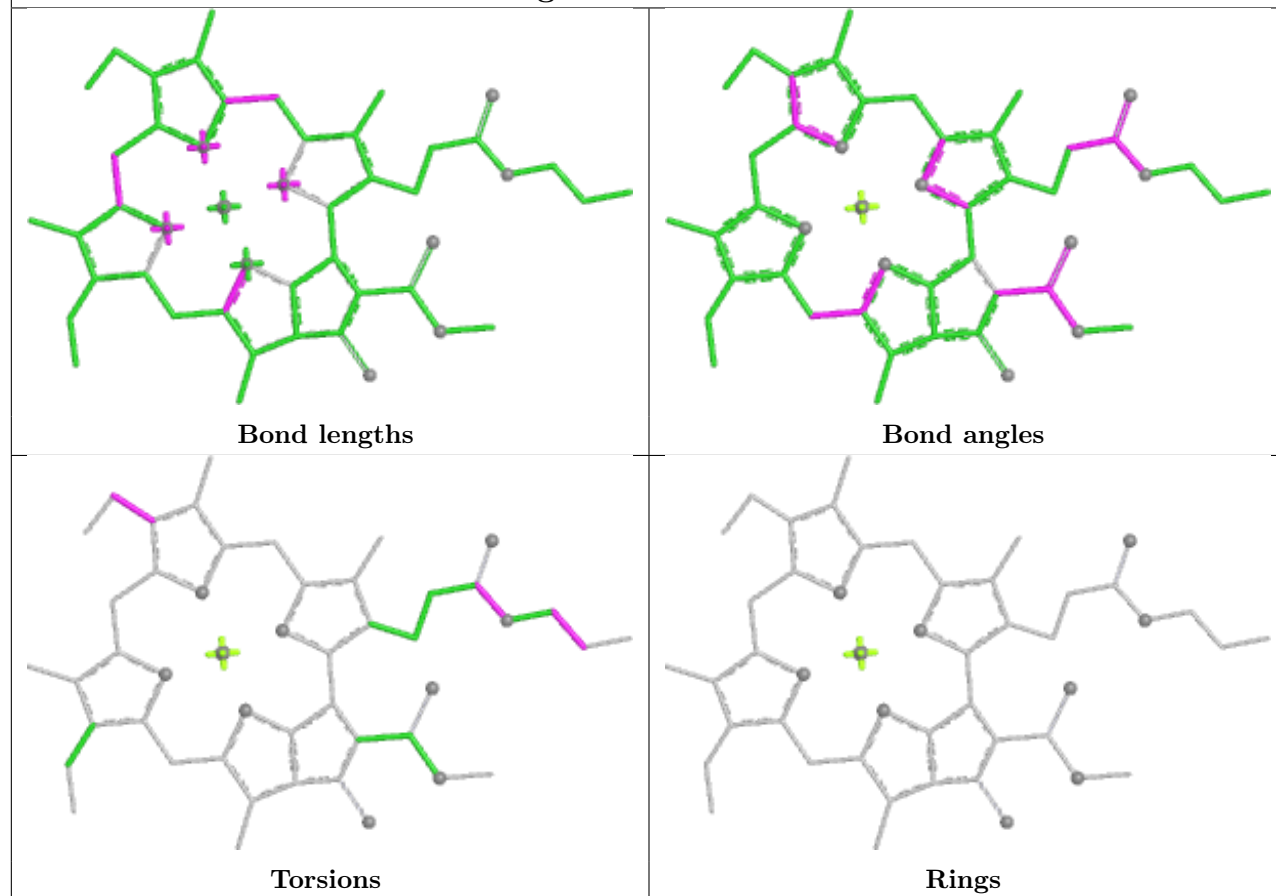


Torsions

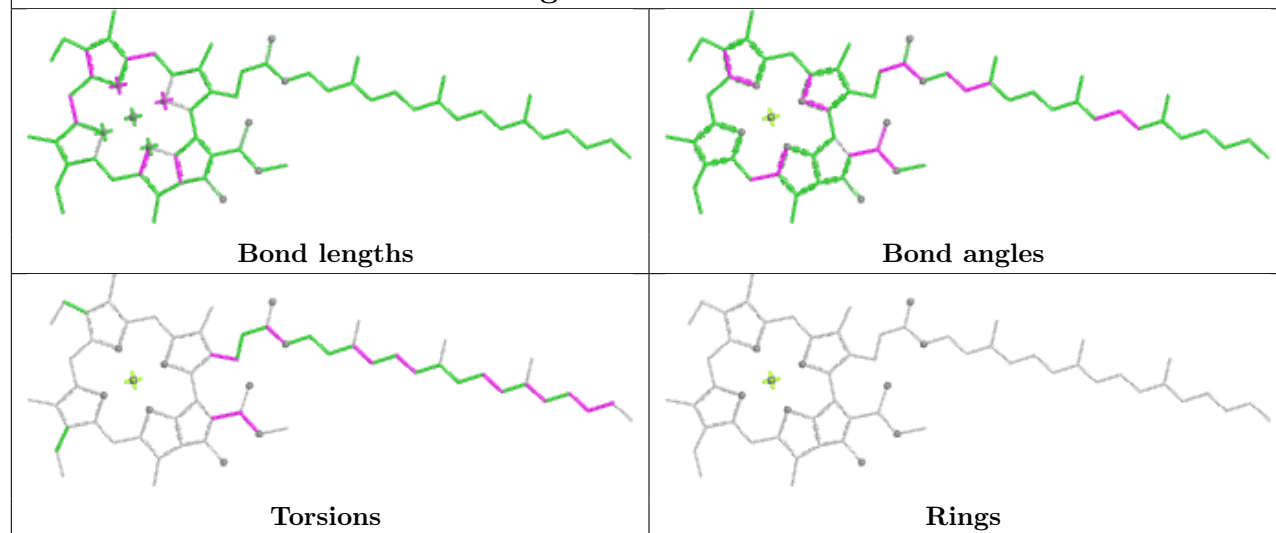


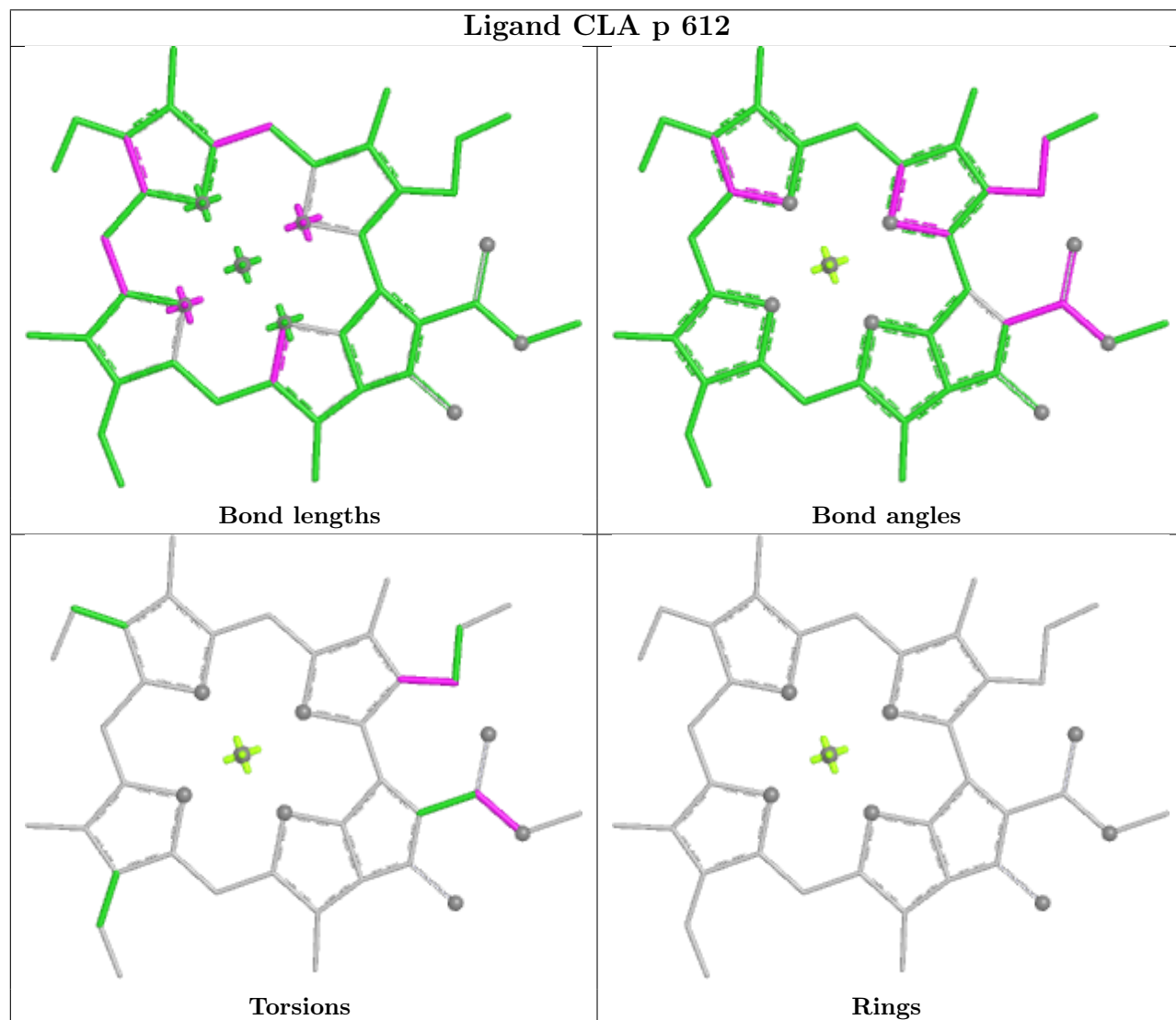
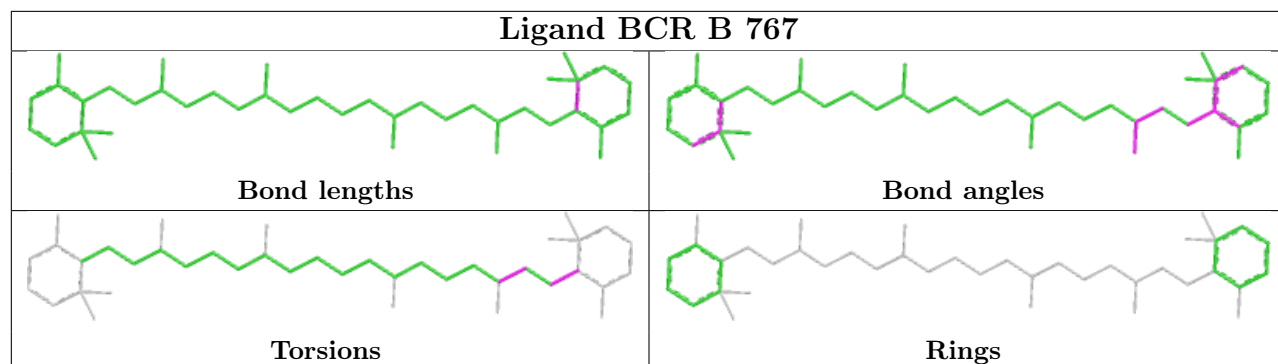
Rings

Ligand CLA c 604

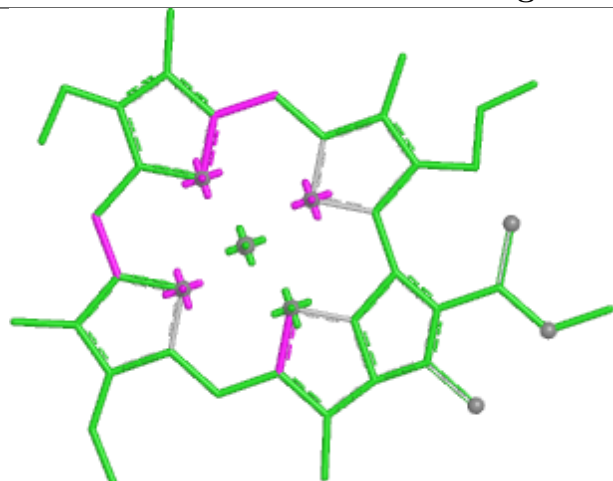


Ligand CLA i 602

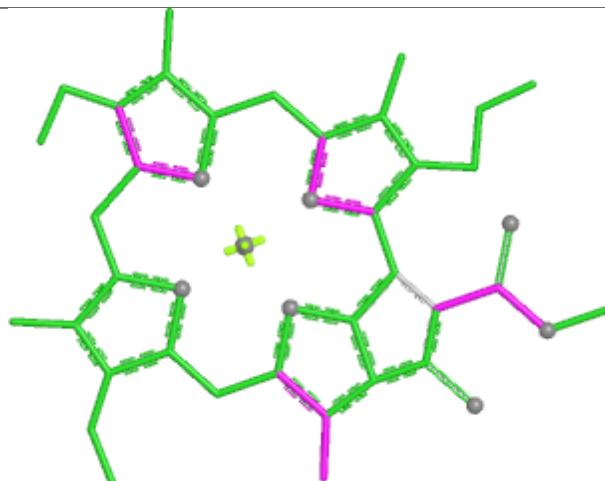




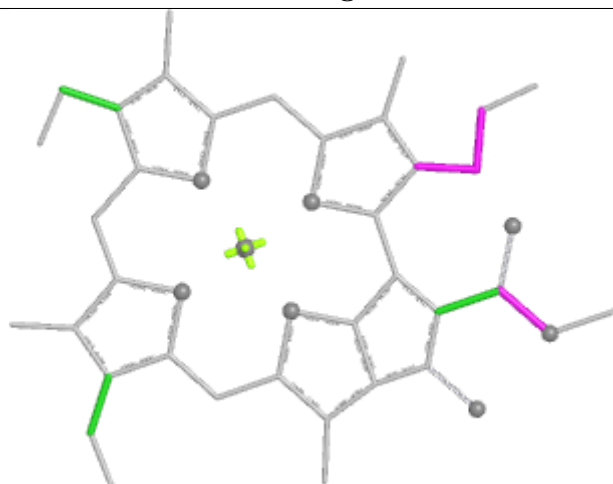
Ligand CLA b 603



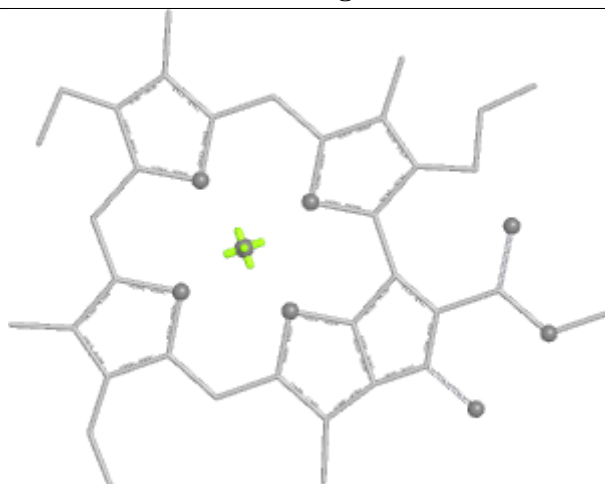
Bond lengths



Bond angles

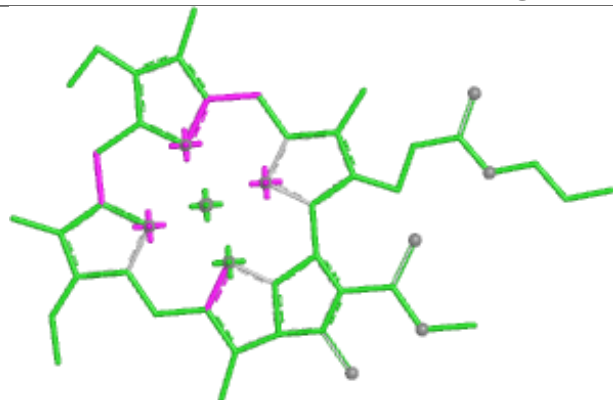


Torsions

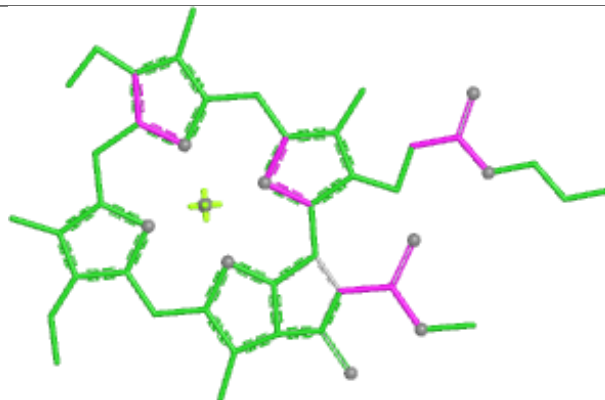


Rings

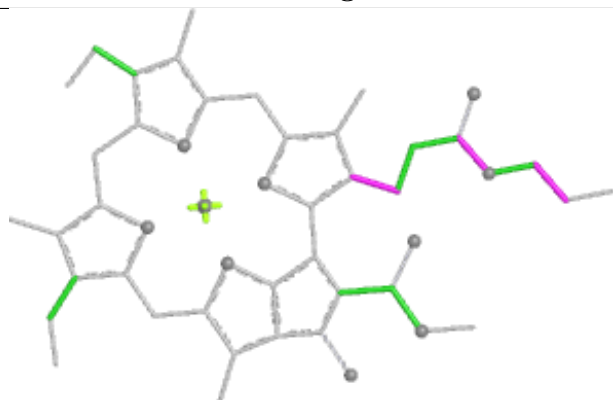
Ligand CLA A 800



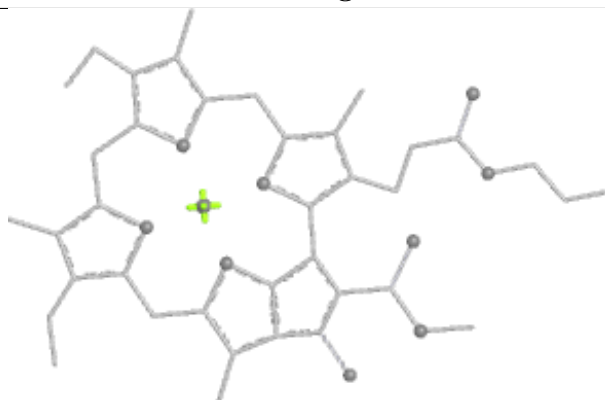
Bond lengths



Bond angles

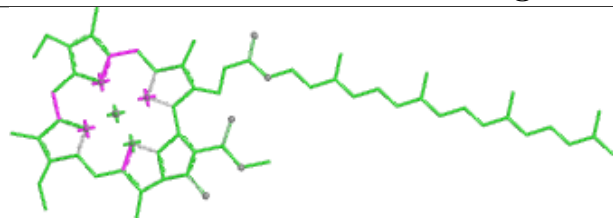


Torsions

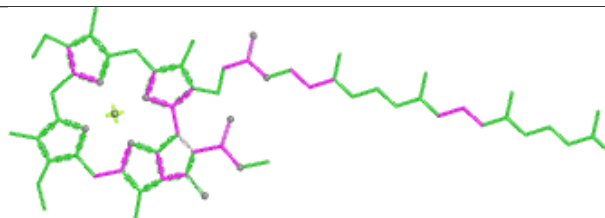


Rings

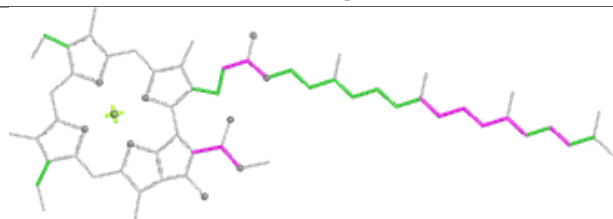
Ligand CLA A 752



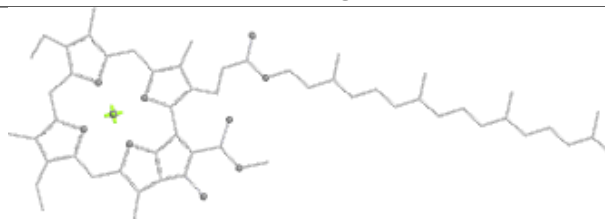
Bond lengths



Bond angles

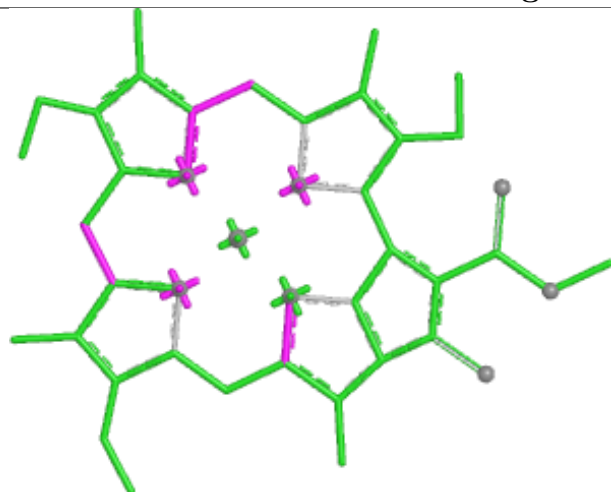


Torsions

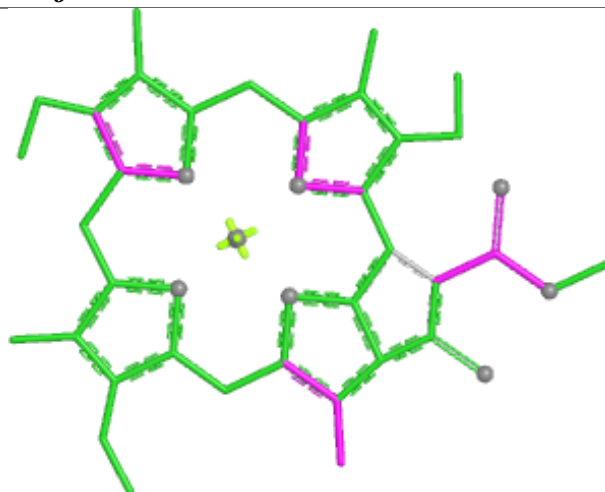


Rings

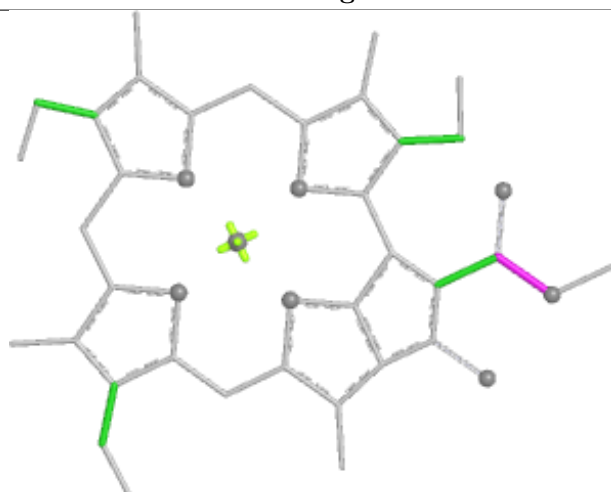
Ligand CLA j 603



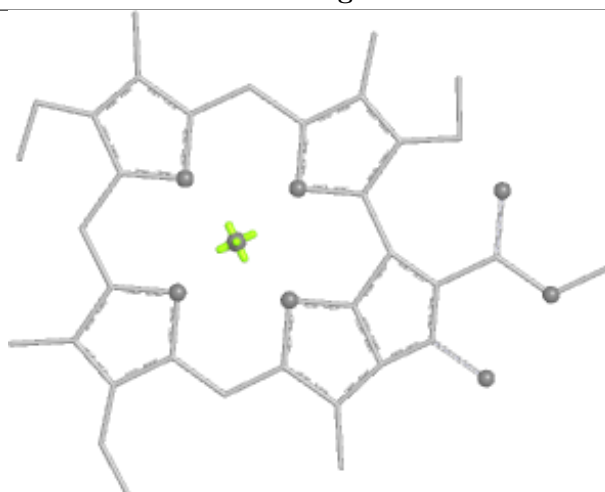
Bond lengths



Bond angles

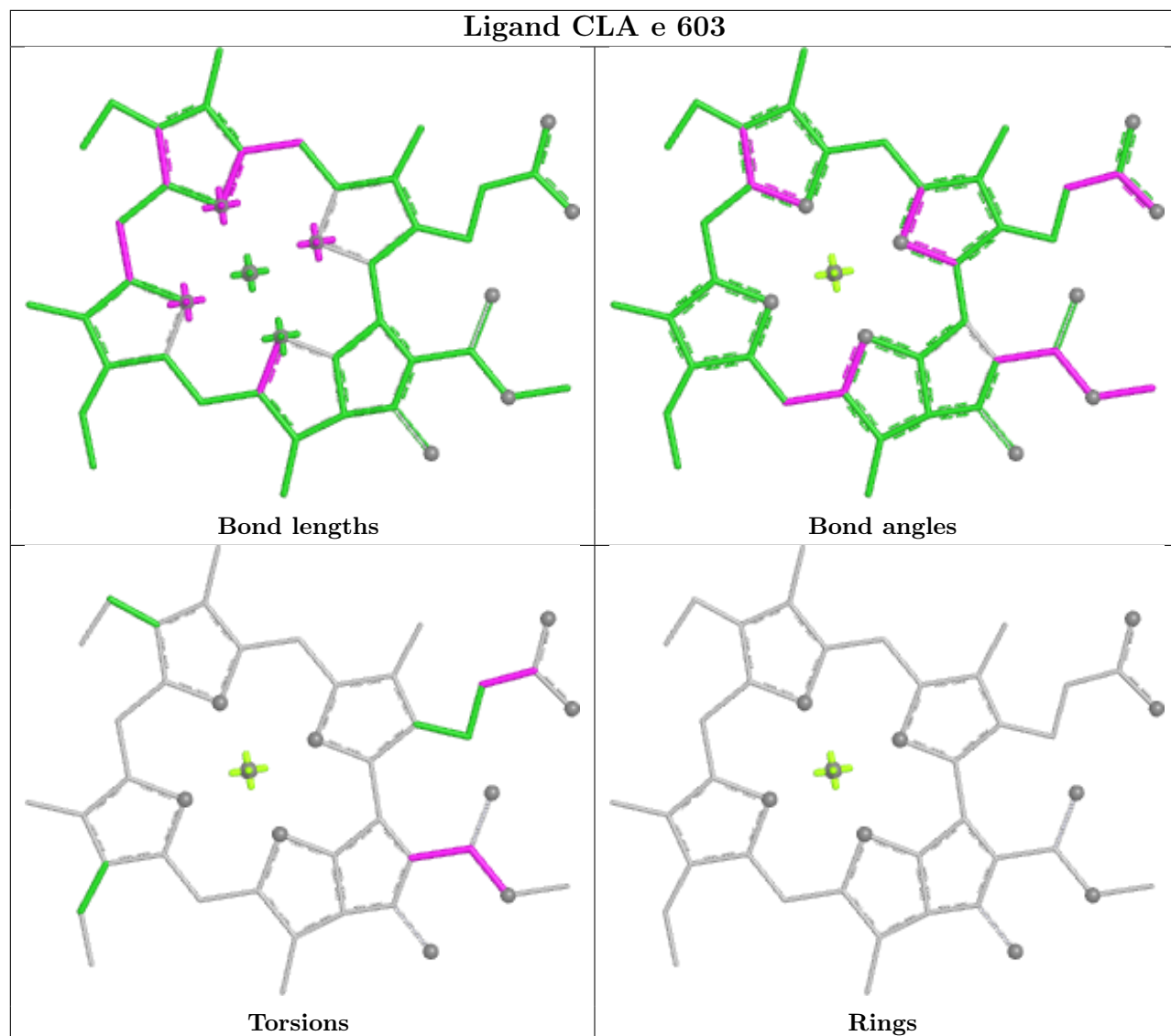


Torsions

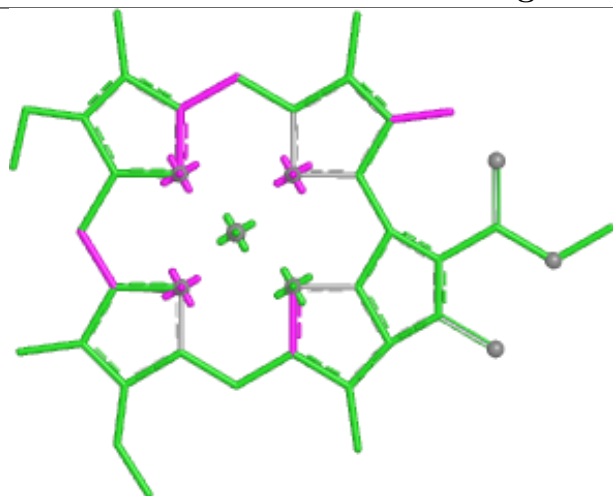


Rings

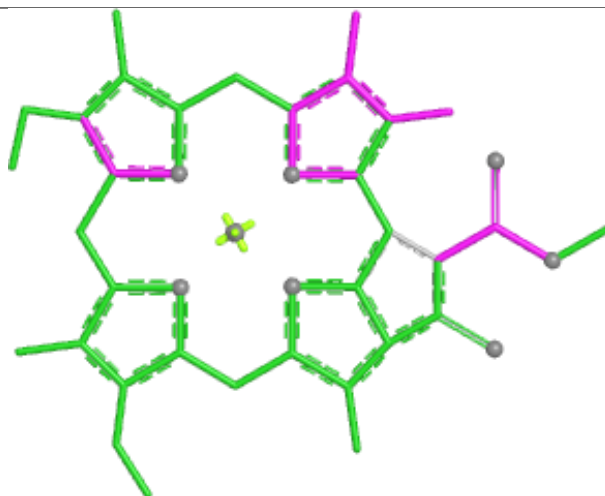
Ligand CLA e 603



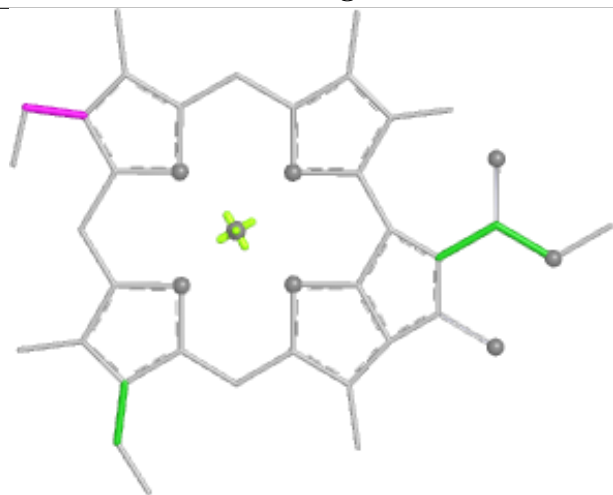
Ligand CLA b 608



Bond lengths



Bond angles

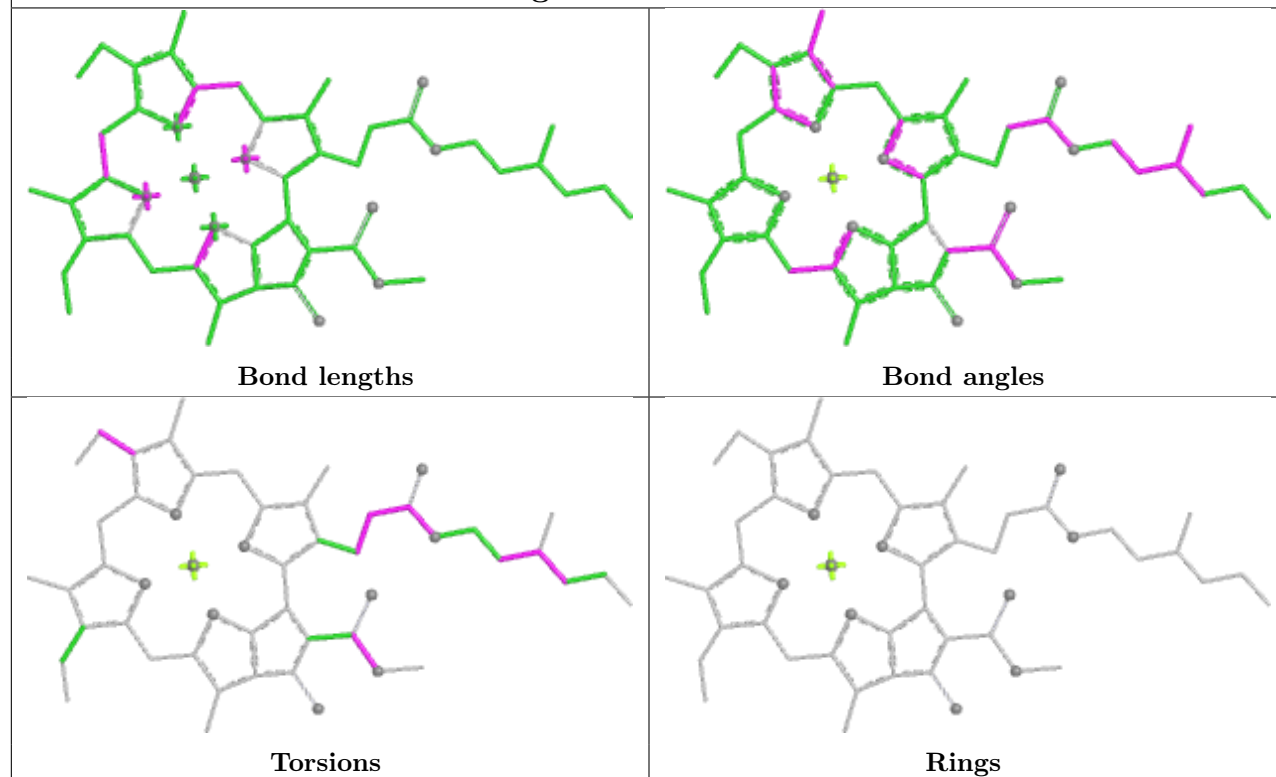


Torsions

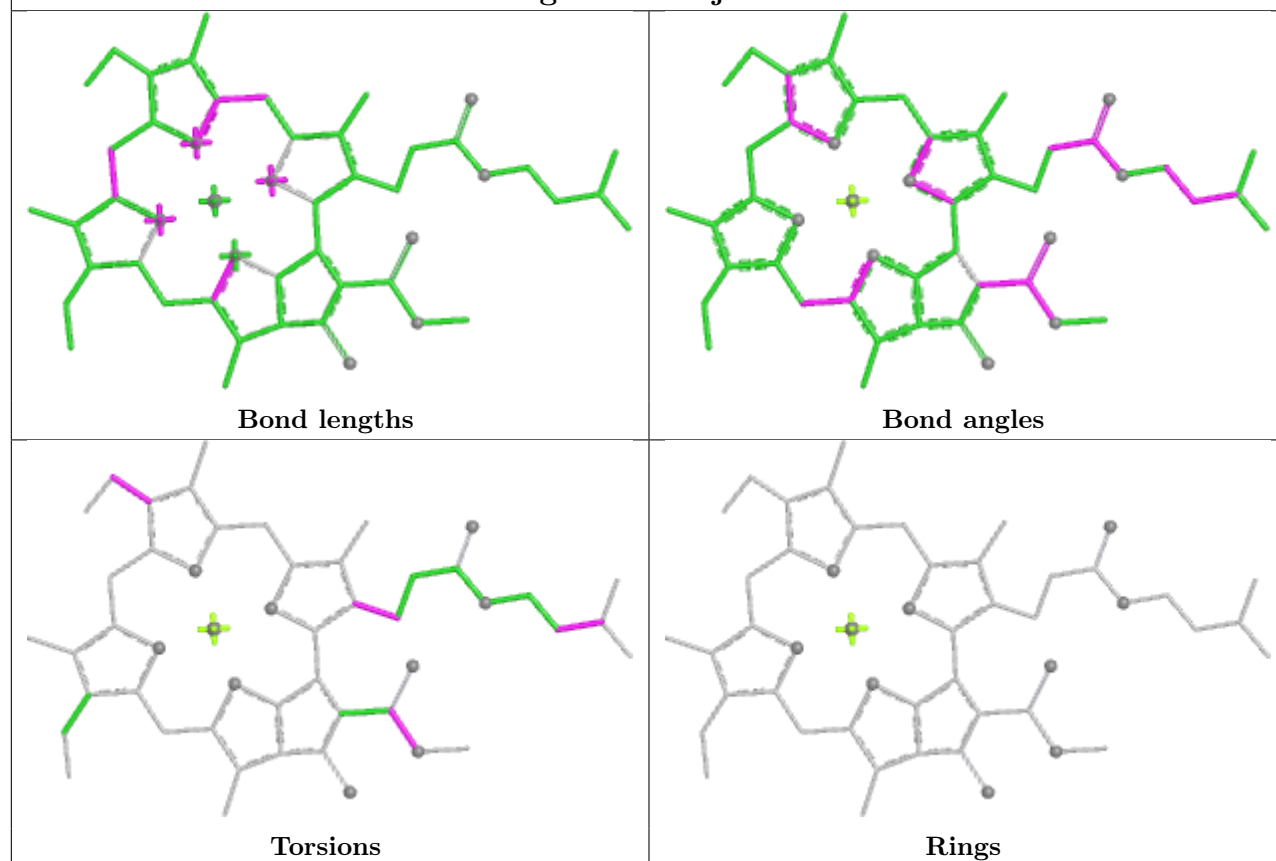


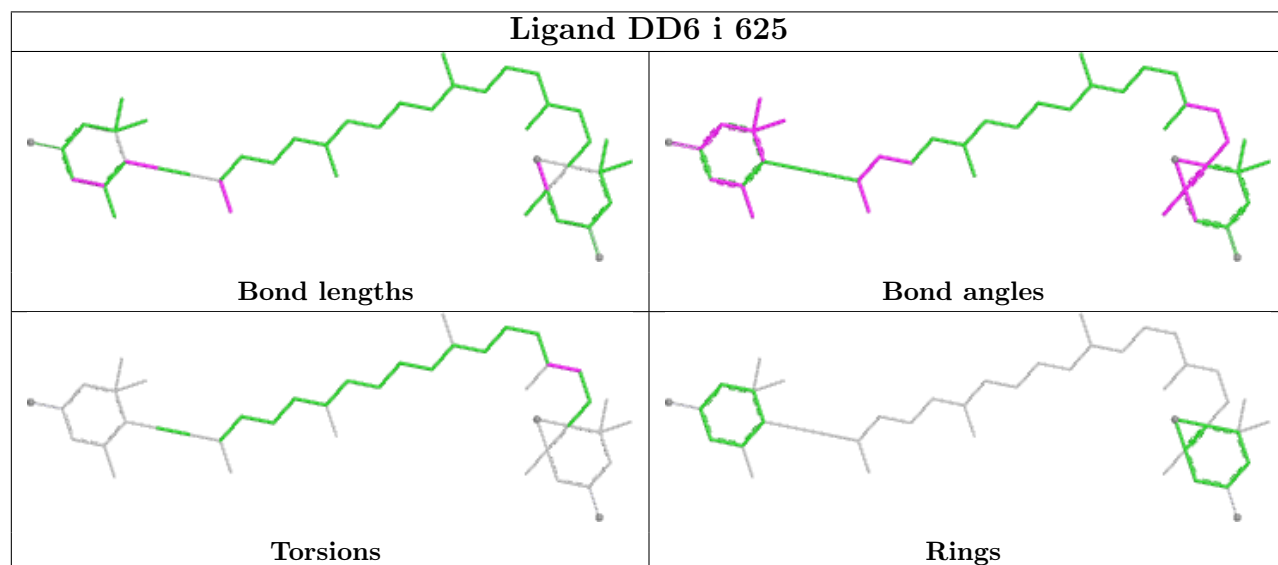
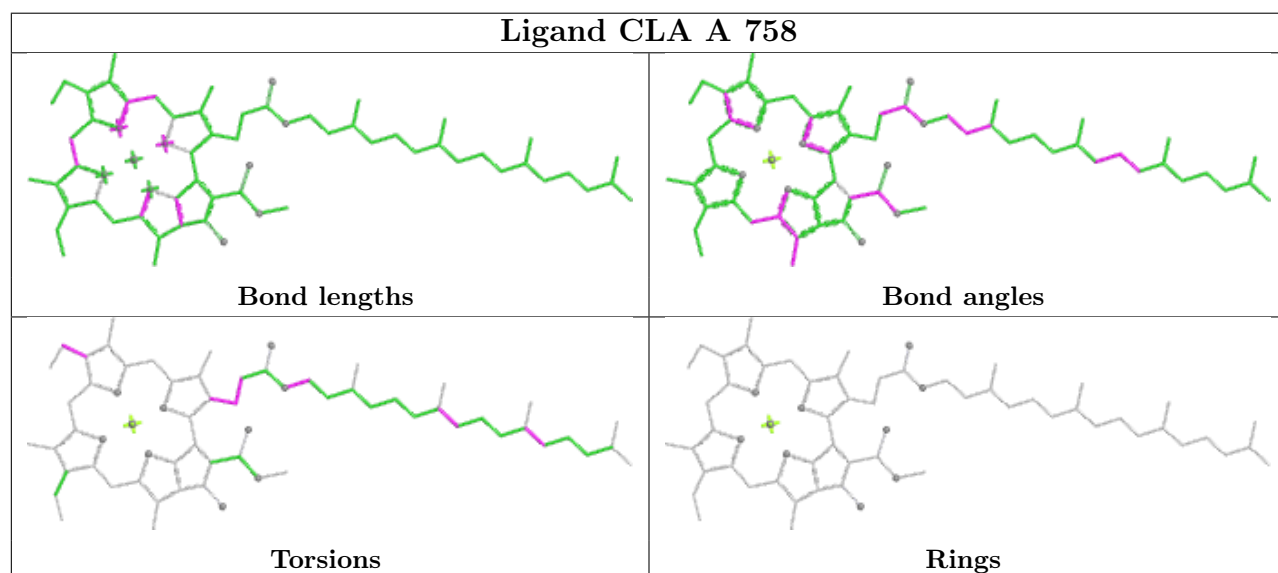
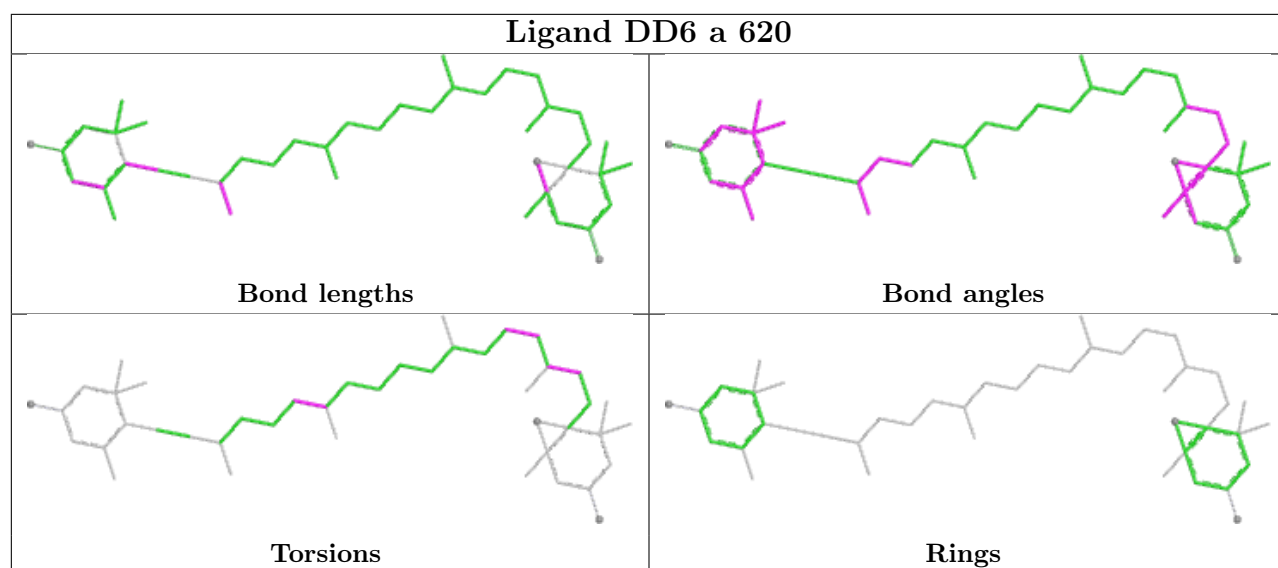
Rings

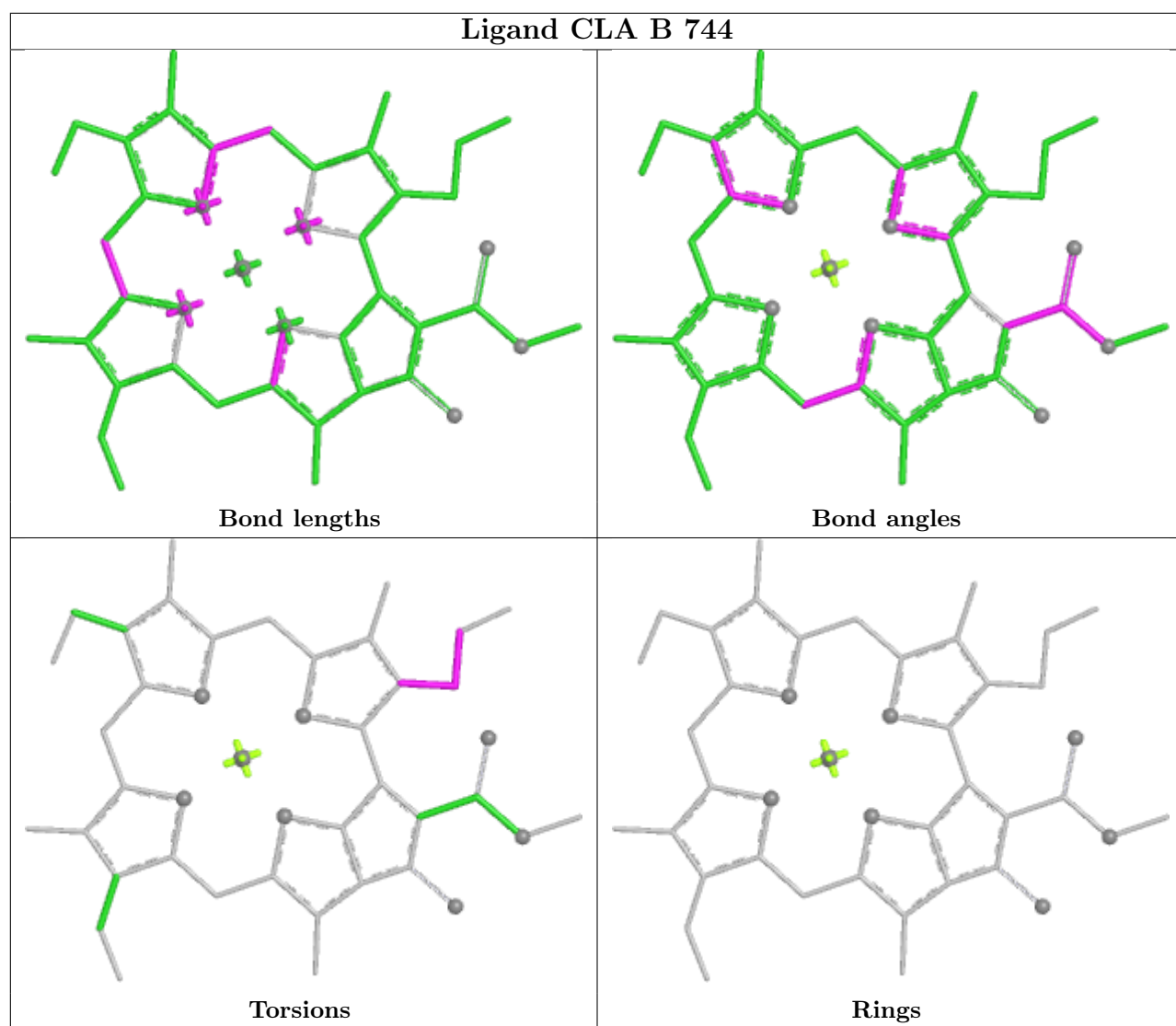
Ligand CLA A 798



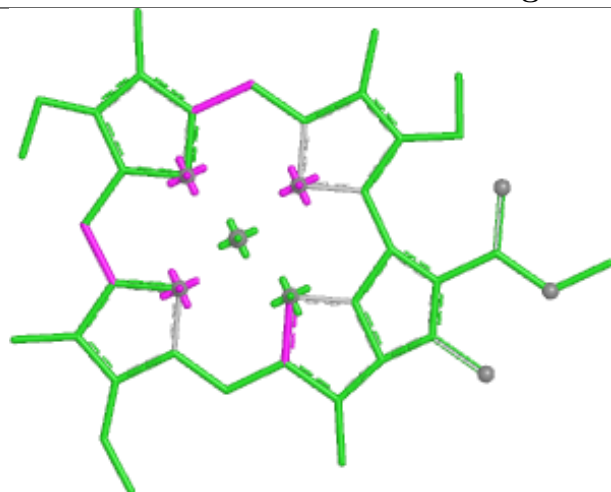
Ligand CLA j 601



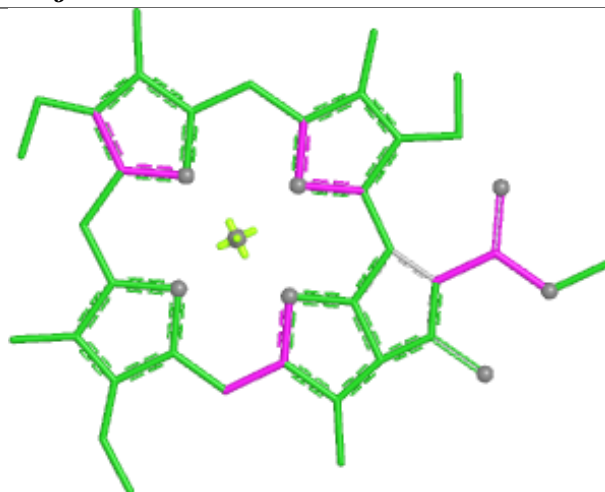




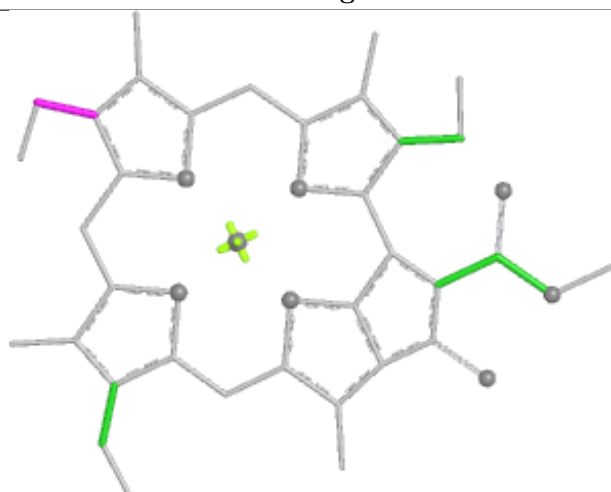
Ligand CLA j 614



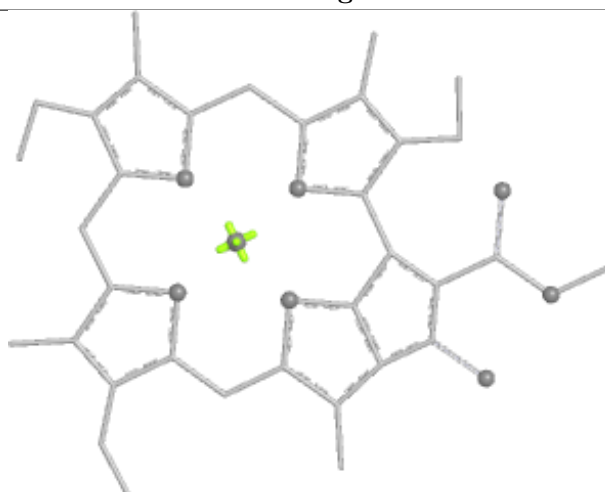
Bond lengths



Bond angles

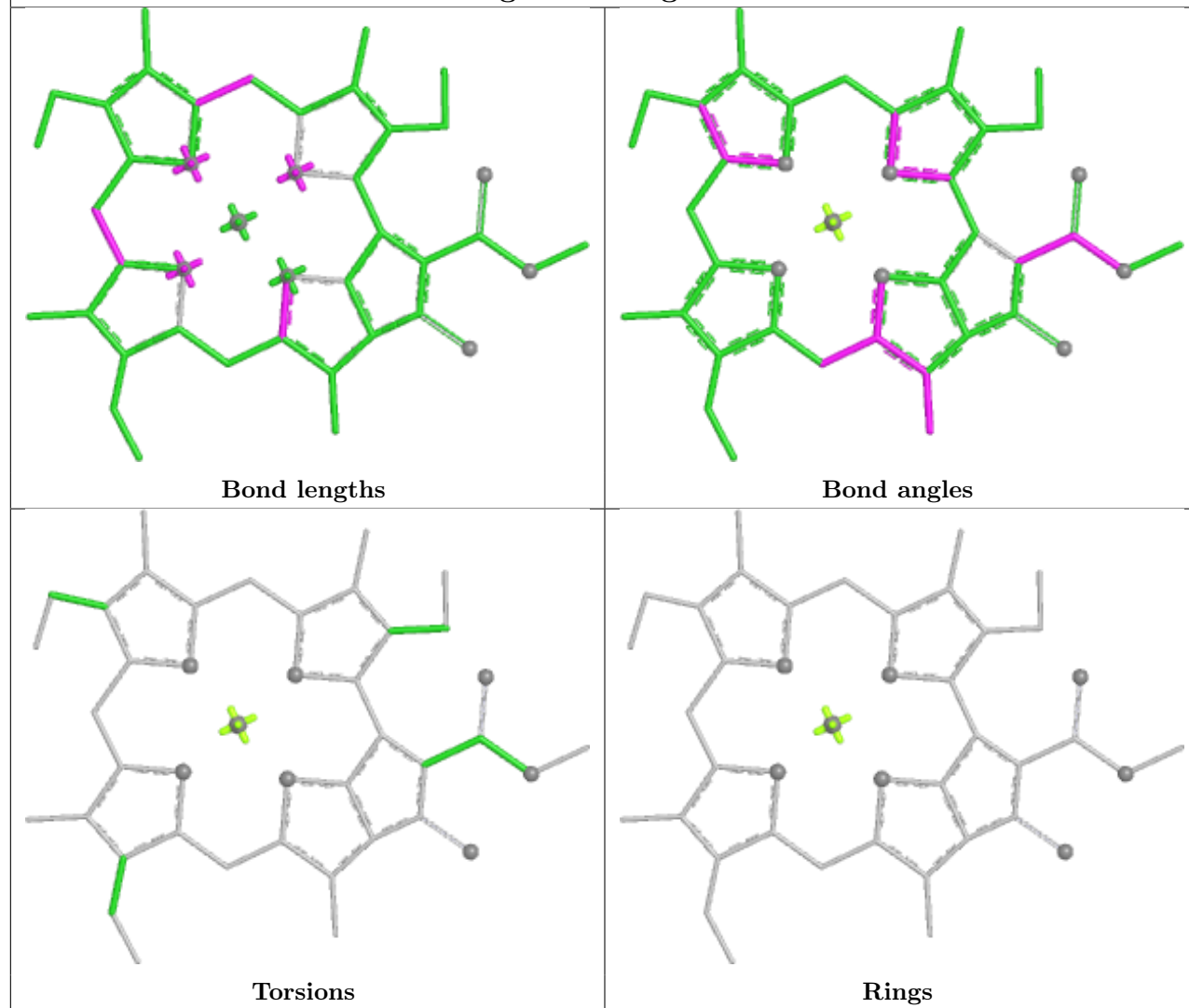


Torsions

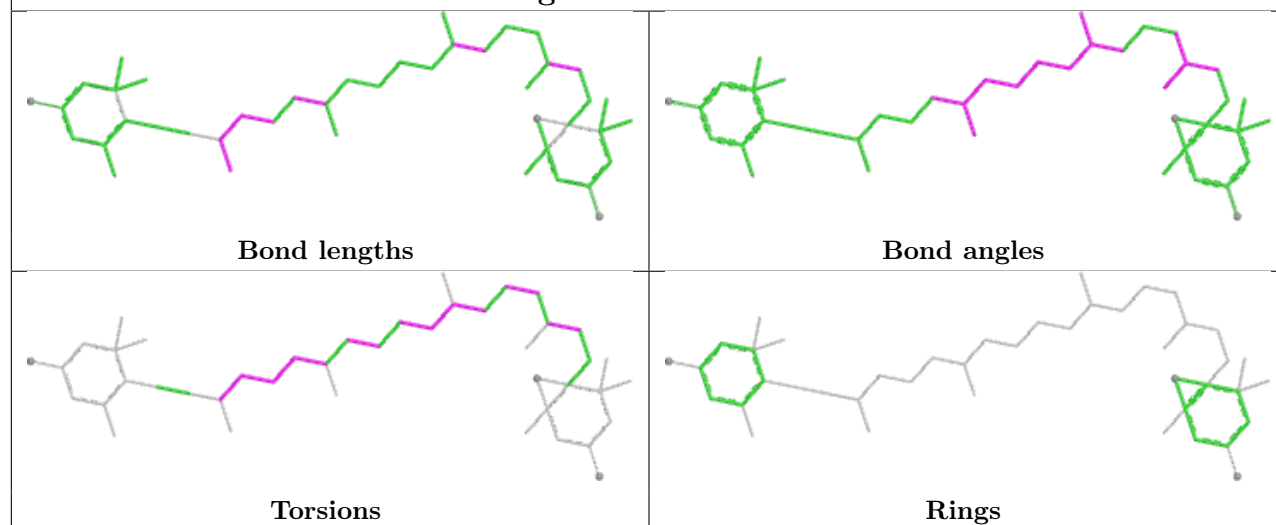


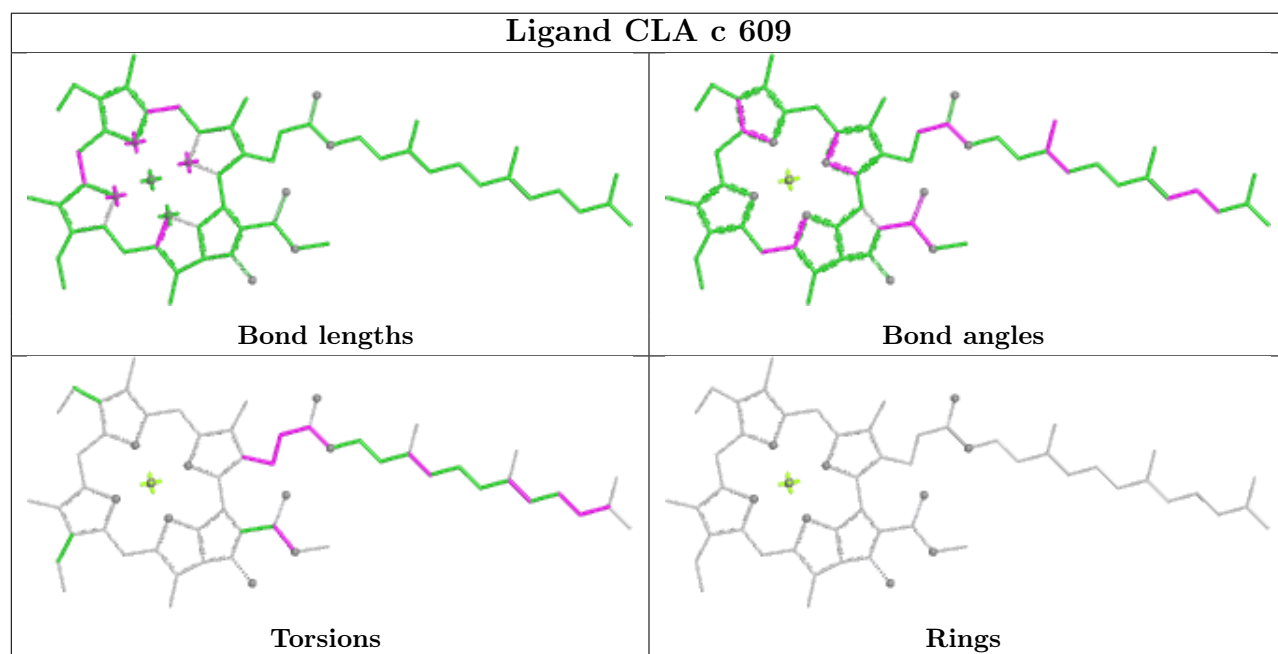
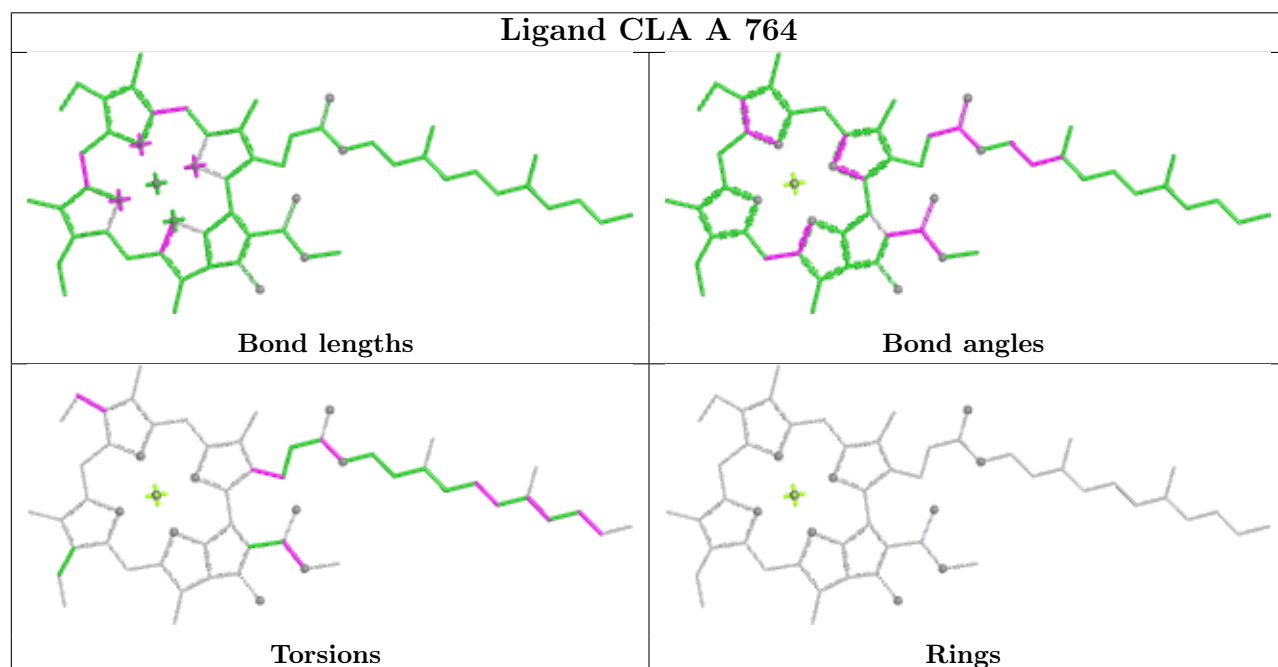
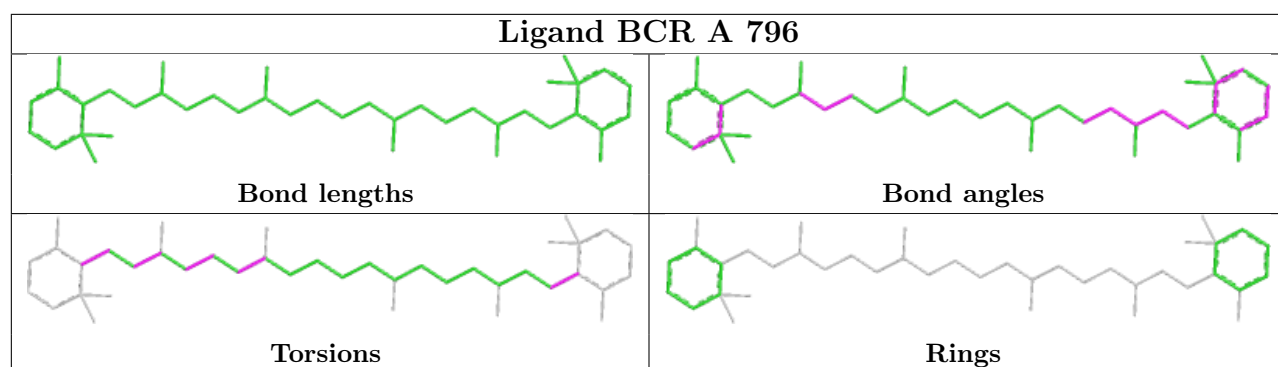
Rings

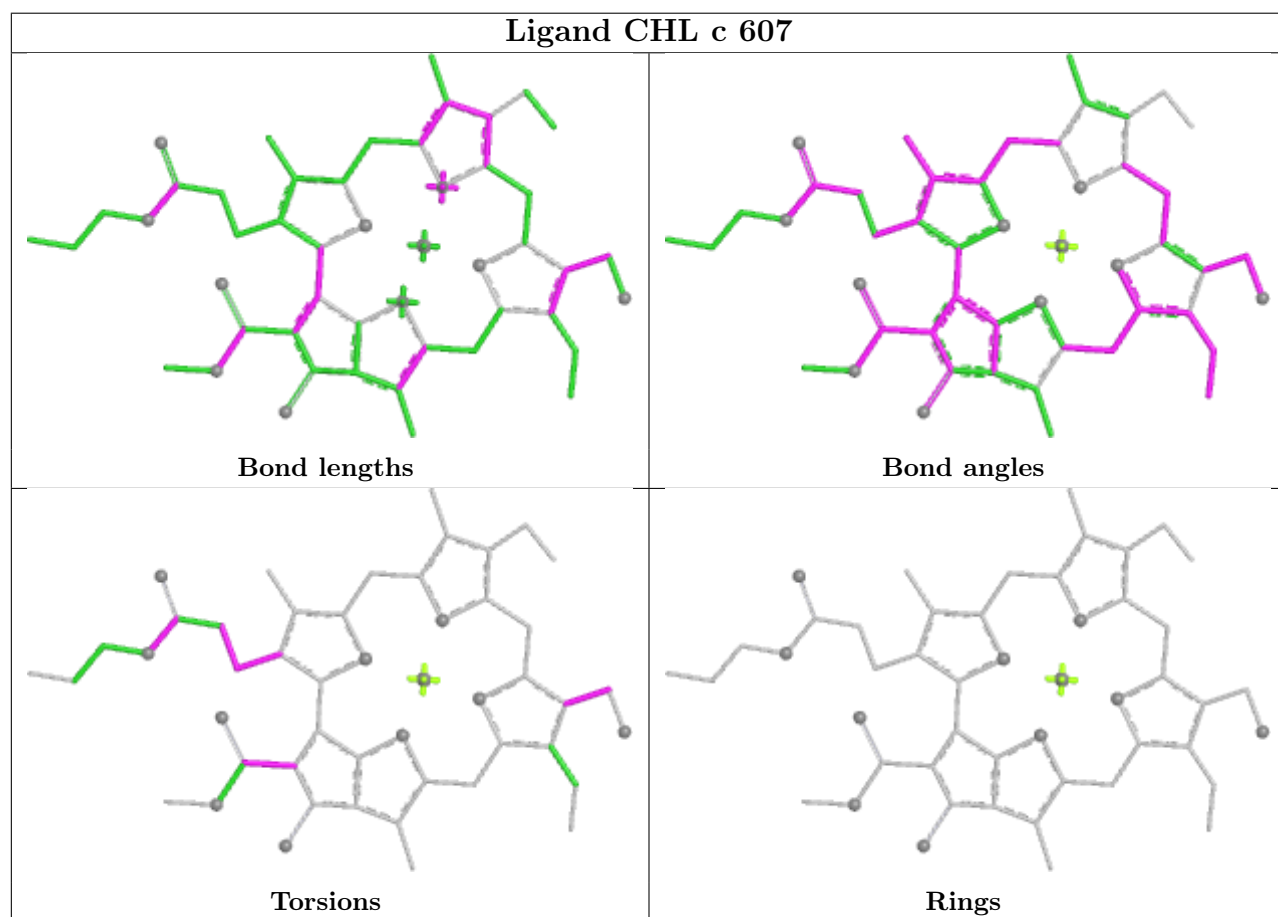
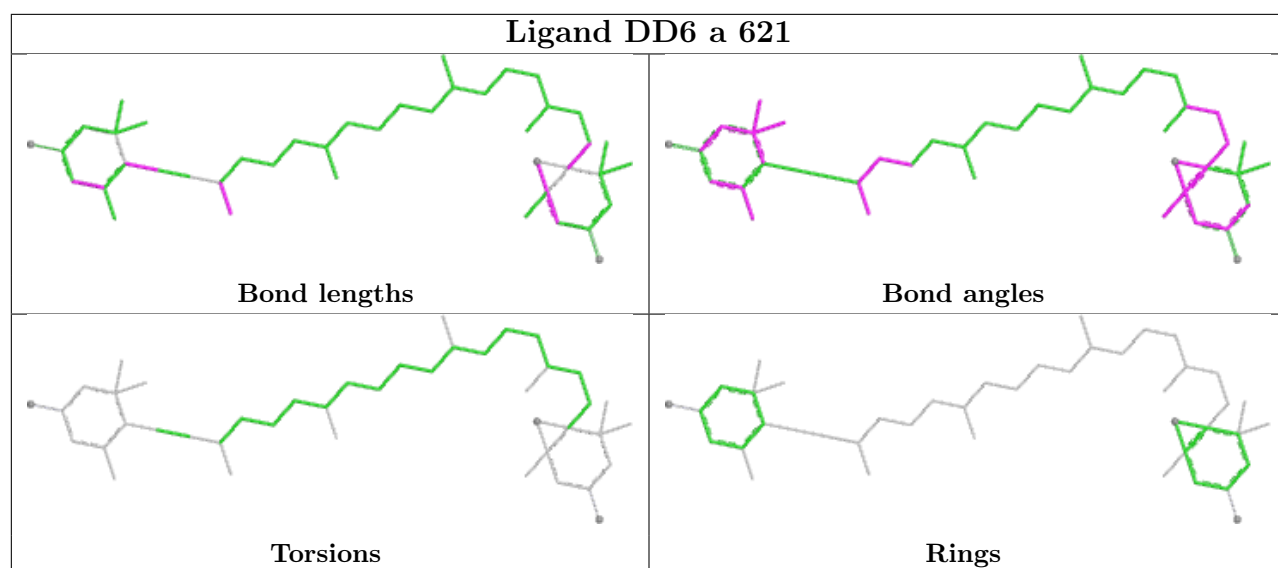
Ligand CLA g 615

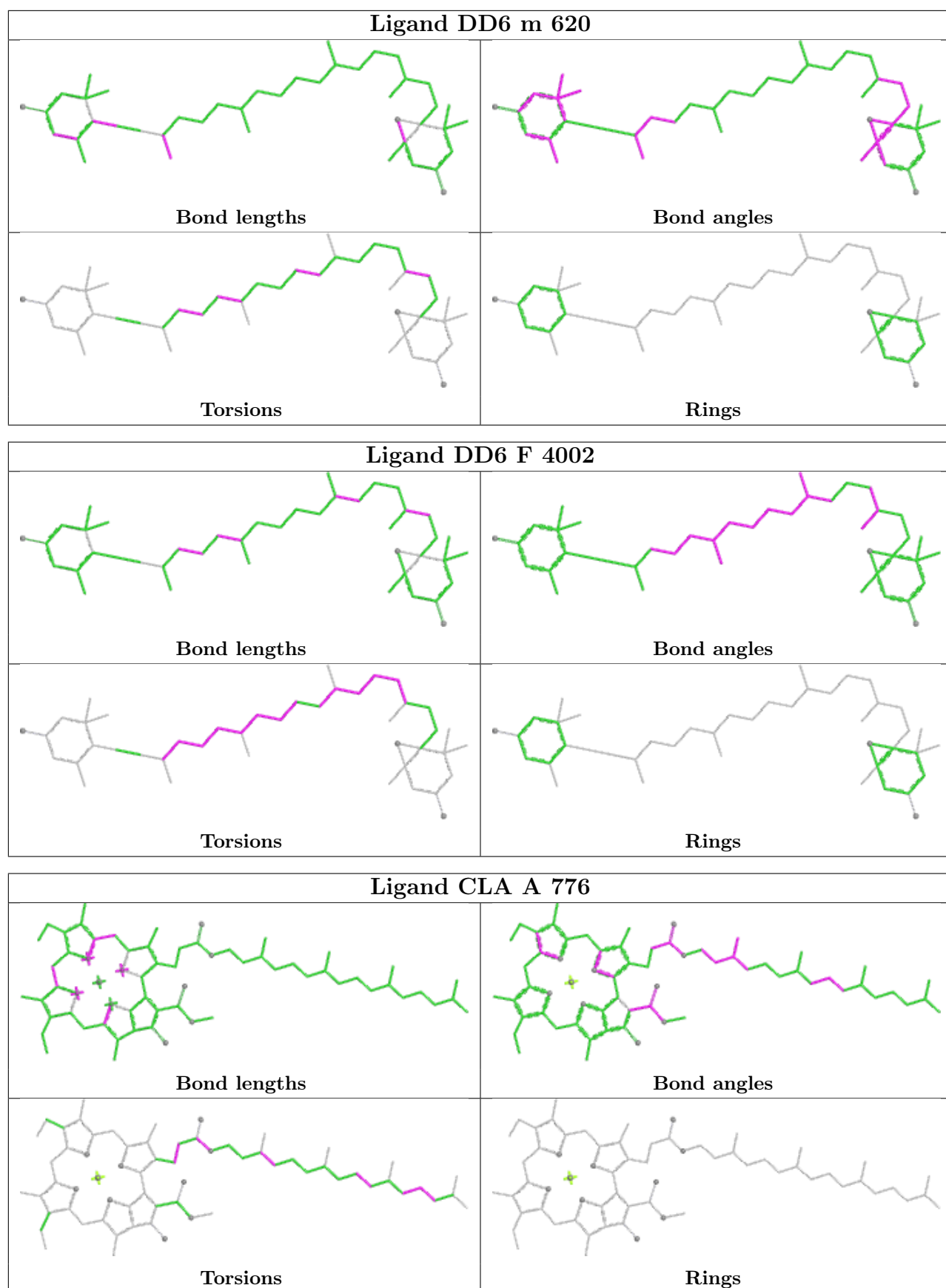


Ligand DD6 c 624

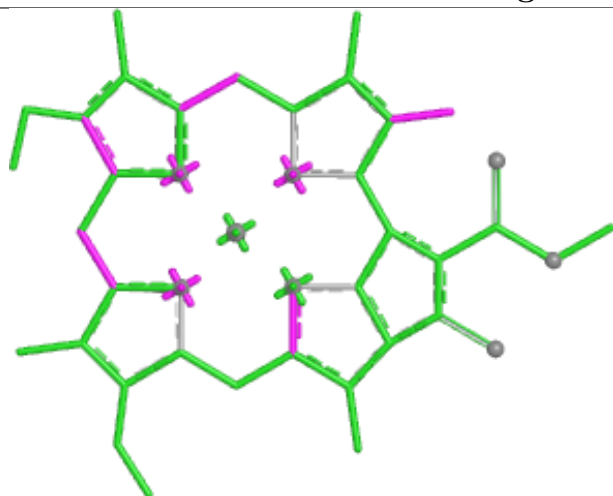




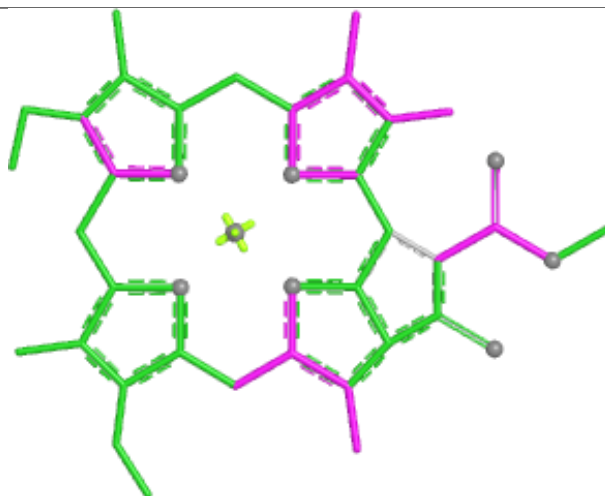




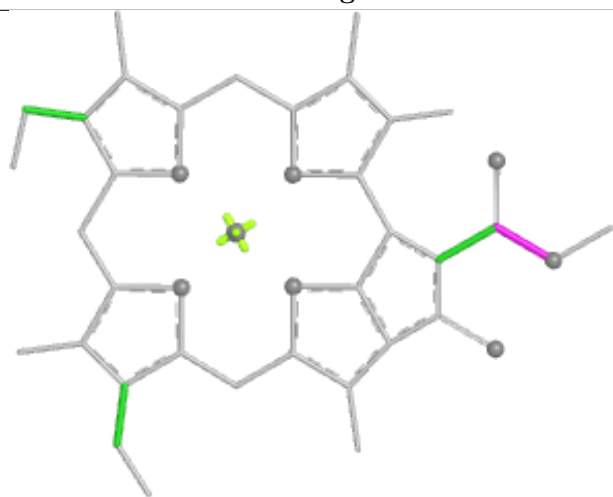
Ligand CLA n 608



Bond lengths



Bond angles

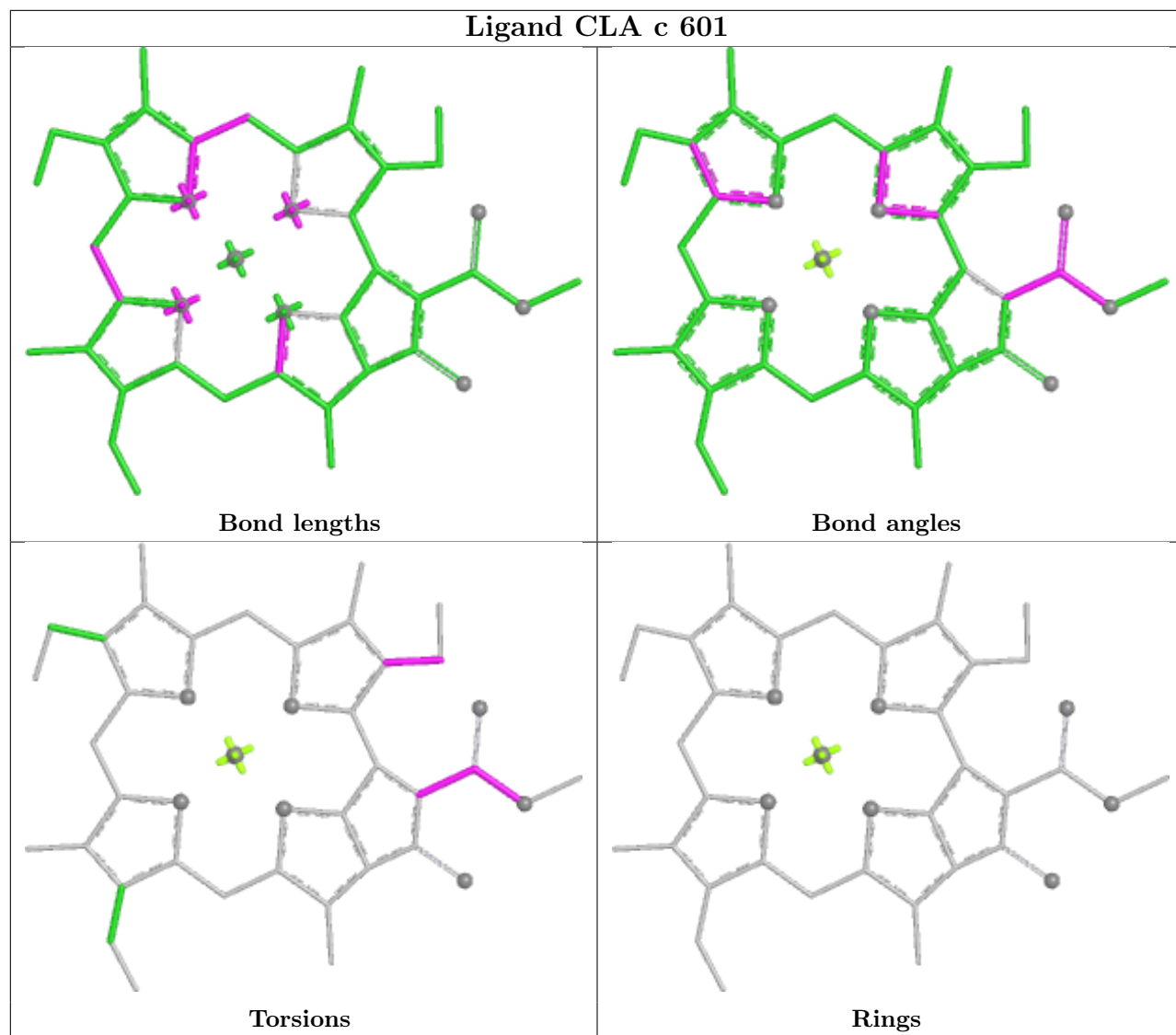


Torsions

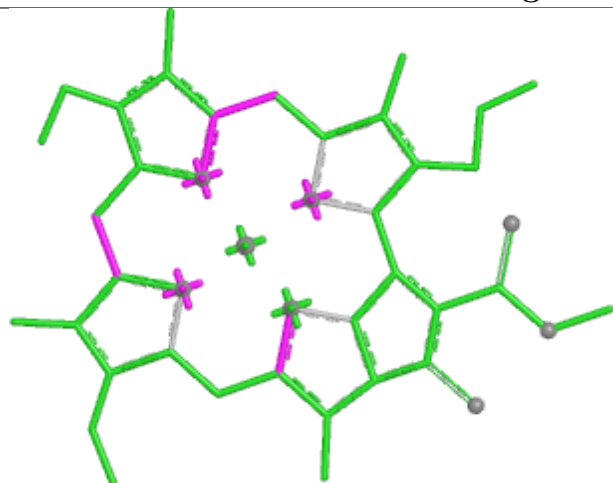


Rings

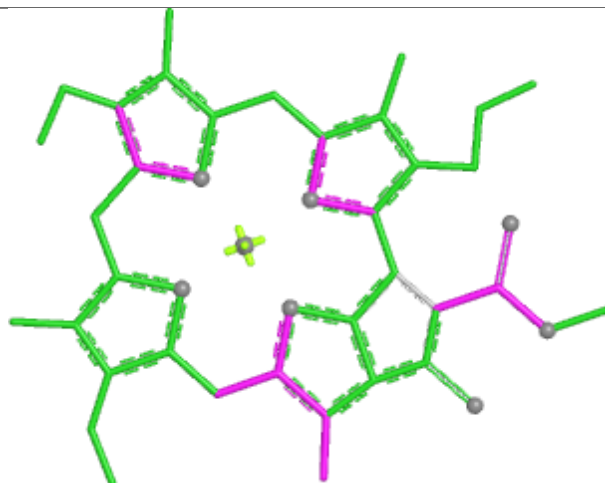
Ligand CLA c 601



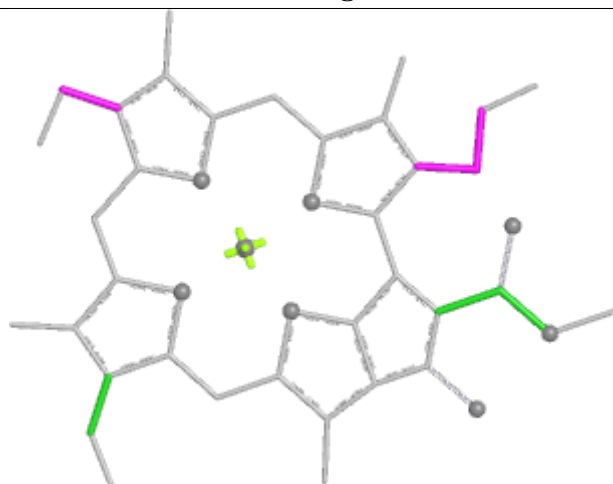
Ligand CLA 1 608



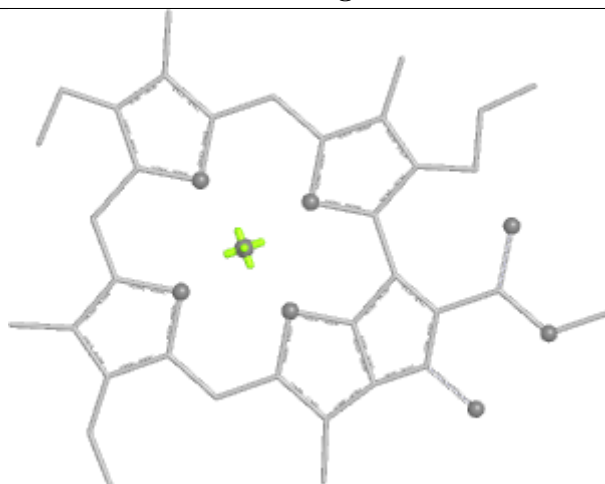
Bond lengths



Bond angles

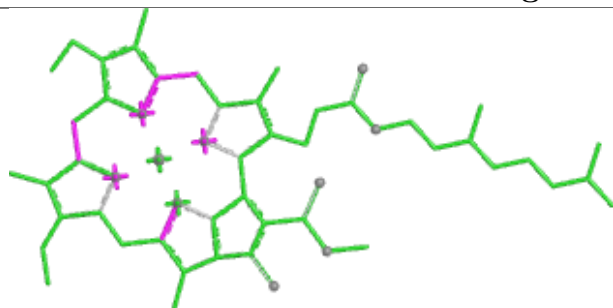


Torsions

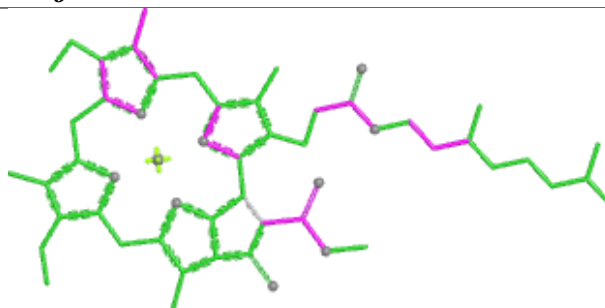


Rings

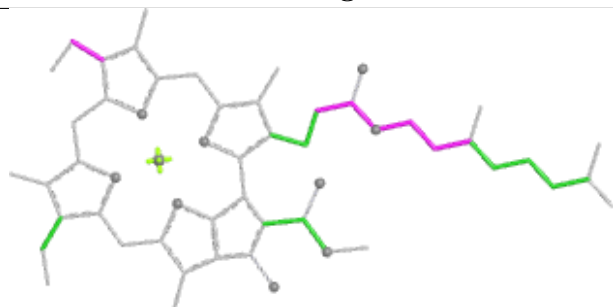
Ligand CLA j 612



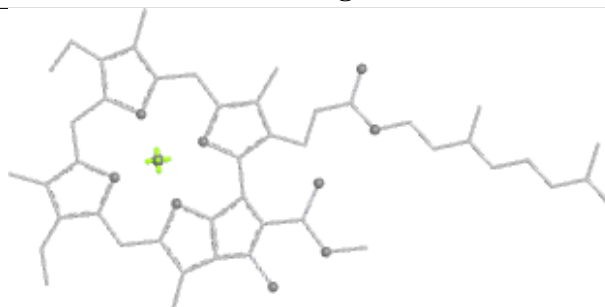
Bond lengths



Bond angles

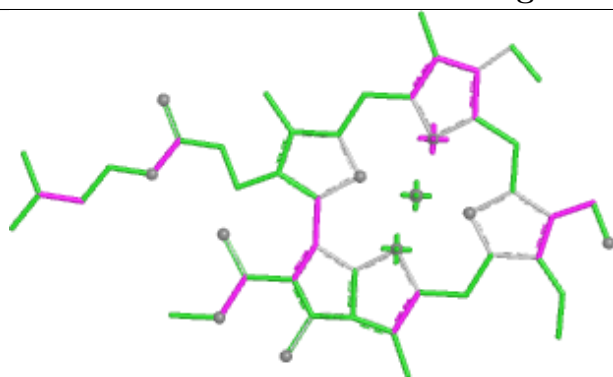


Torsions

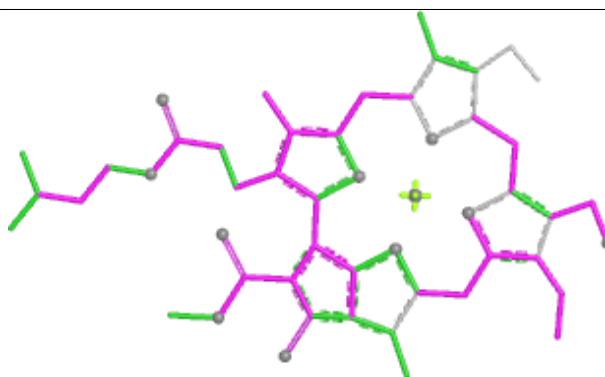


Rings

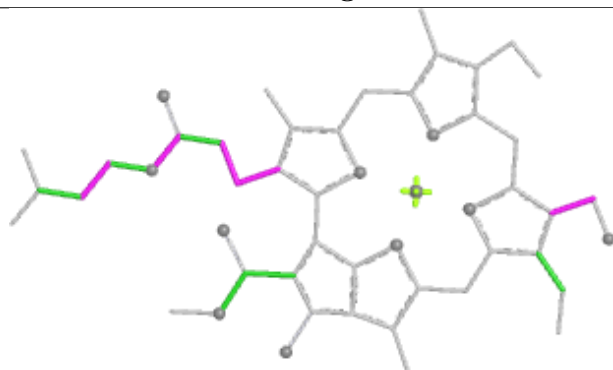
Ligand CHL d 605



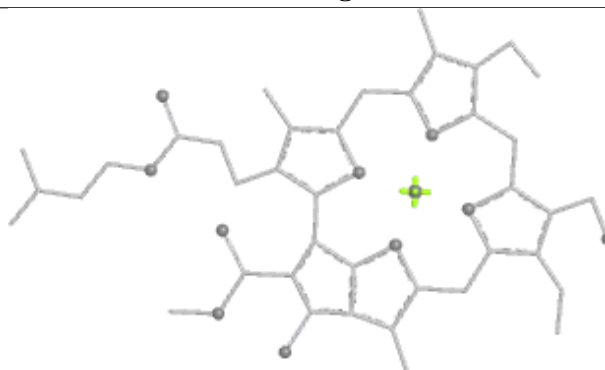
Bond lengths



Bond angles

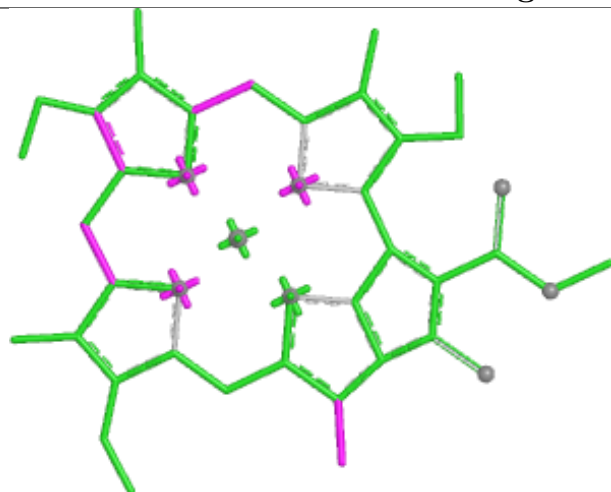


Torsions

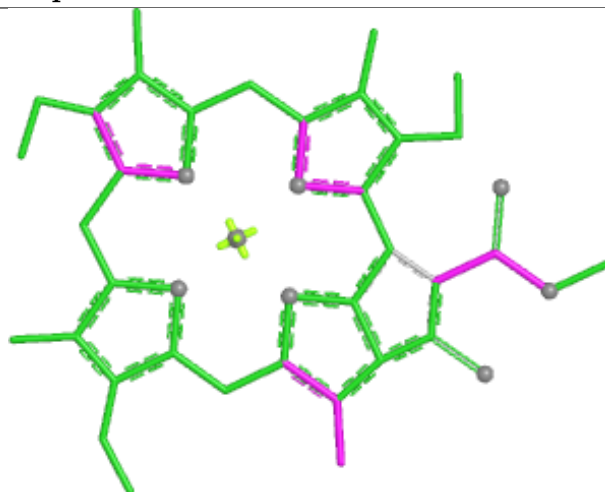


Rings

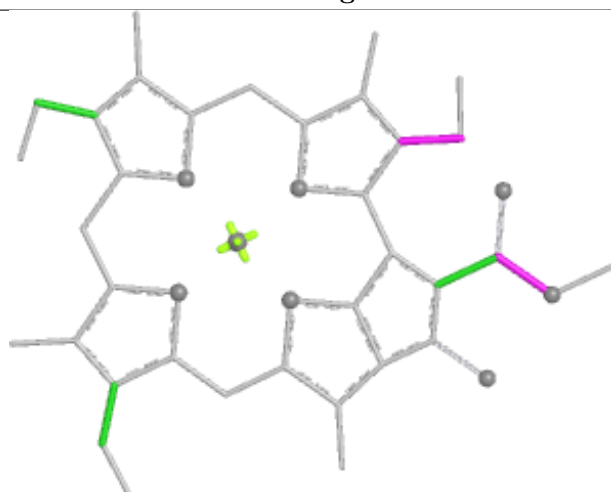
Ligand CLA p 603



Bond lengths



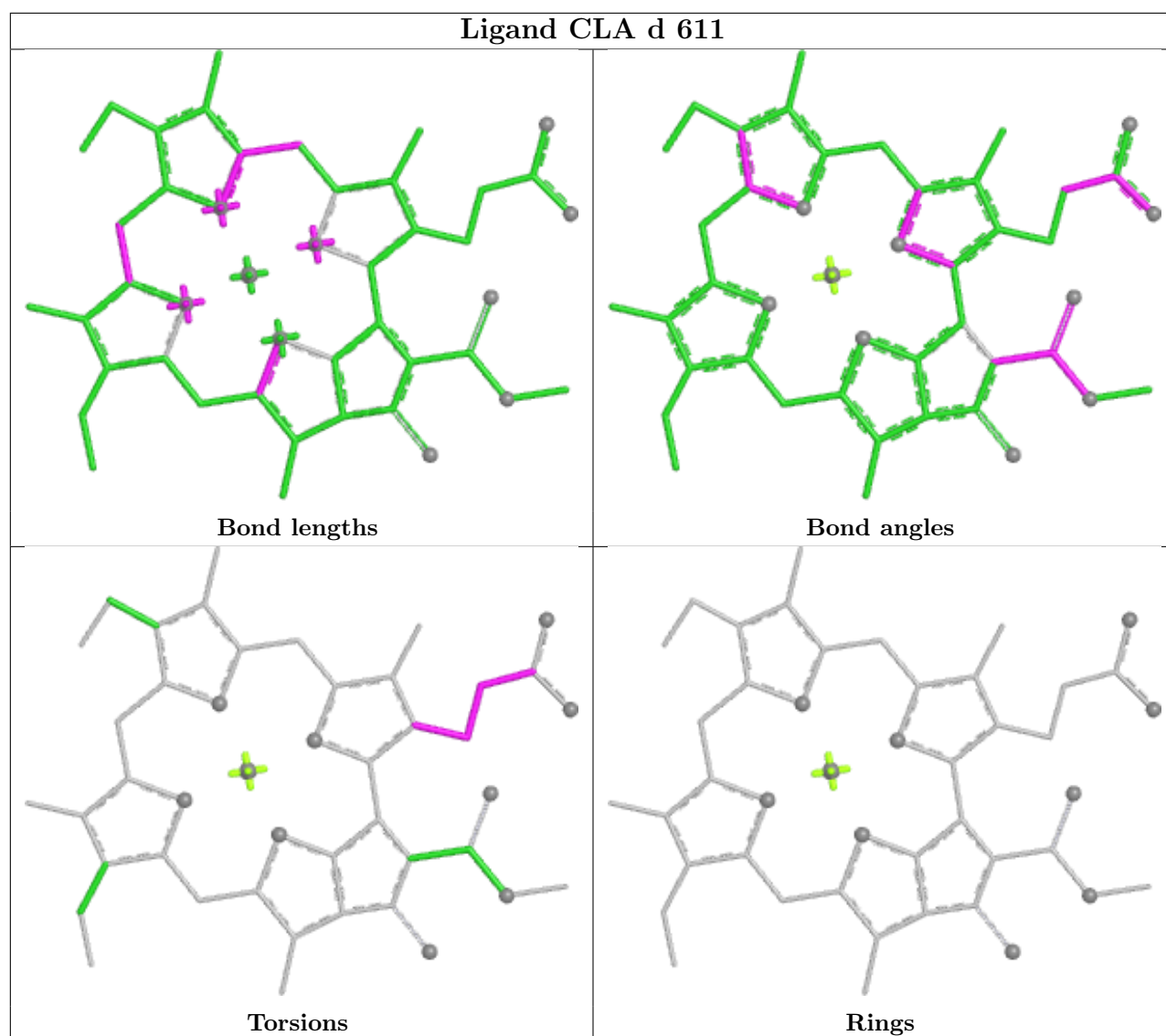
Bond angles



Torsions



Rings



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.

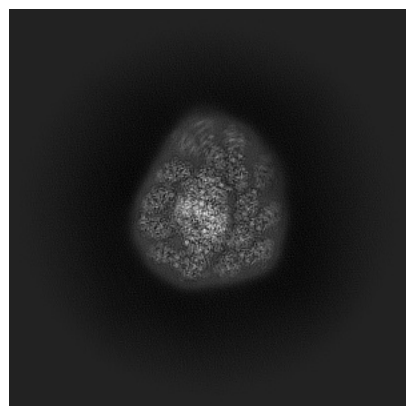
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64823. These allow visual inspection of the internal detail of the map and identification of artifacts.

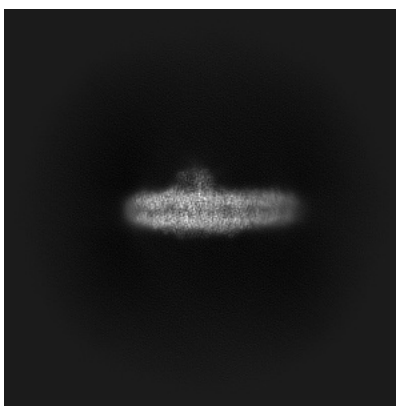
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X

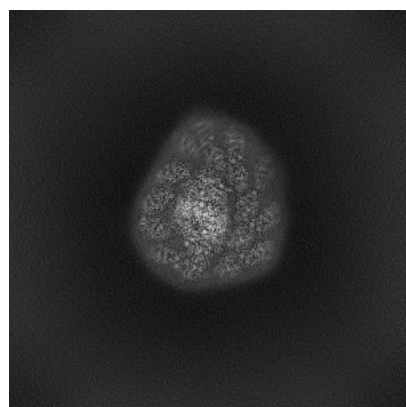


Y

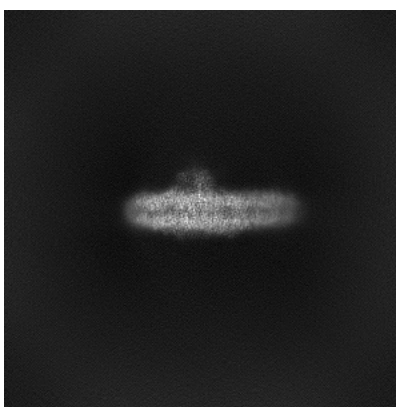


Z

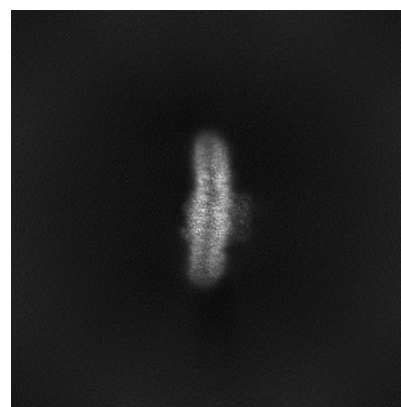
6.1.2 Raw map



X



Y

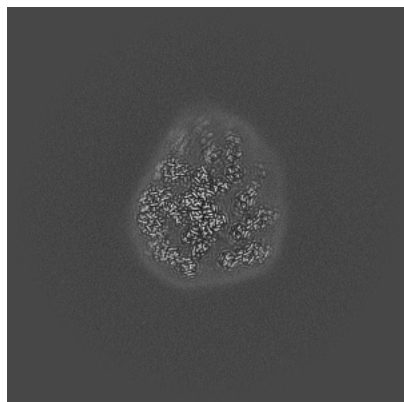


Z

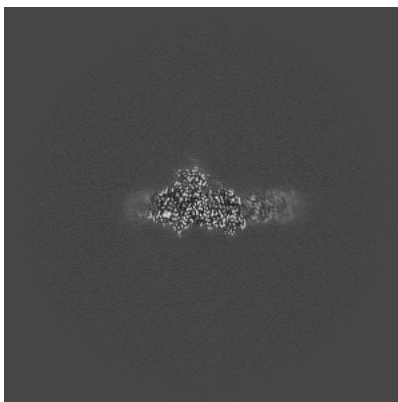
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

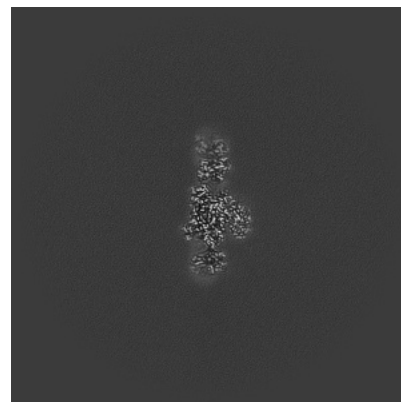
6.2.1 Primary map



X Index: 256

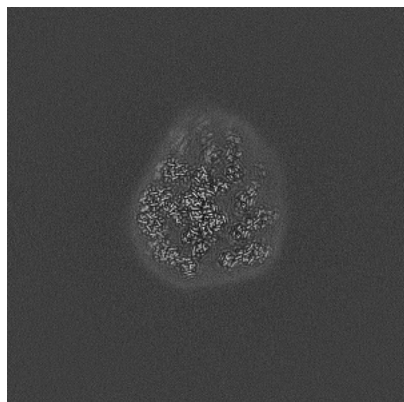


Y Index: 256

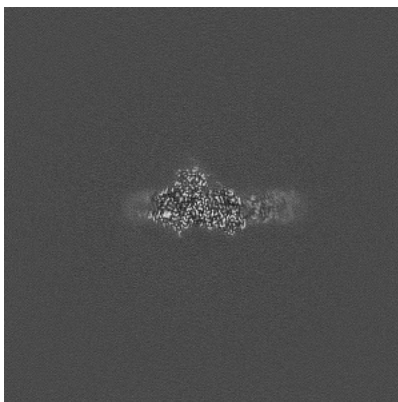


Z Index: 256

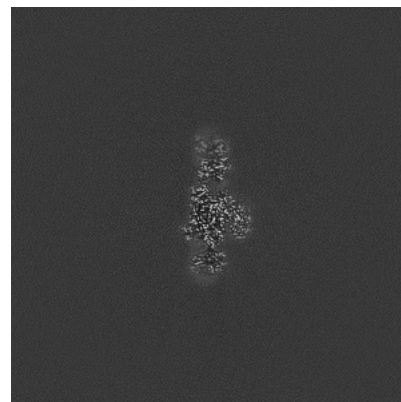
6.2.2 Raw map



X Index: 256



Y Index: 256

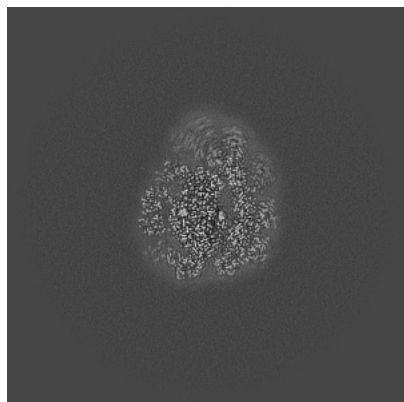


Z Index: 256

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

6.3 Largest variance slices [i](#)

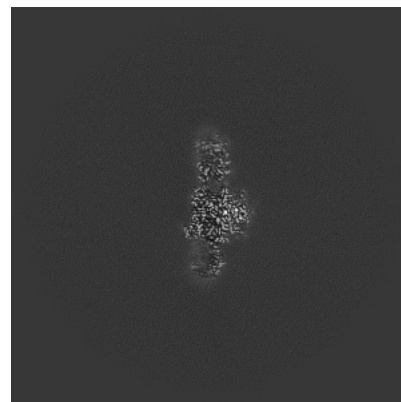
6.3.1 Primary map



X Index: 267

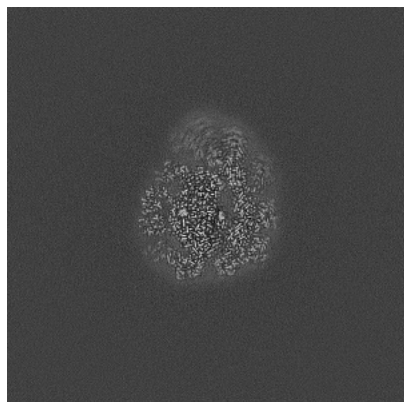


Y Index: 249



Z Index: 250

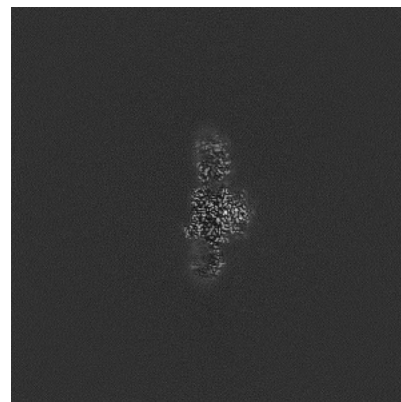
6.3.2 Raw map



X Index: 267



Y Index: 249

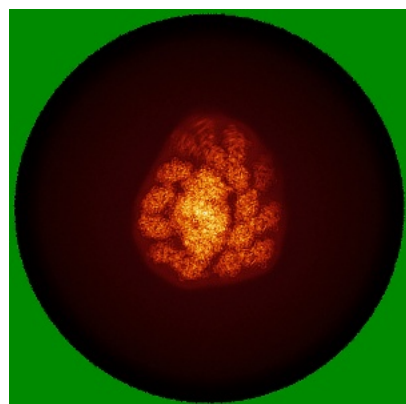


Z Index: 250

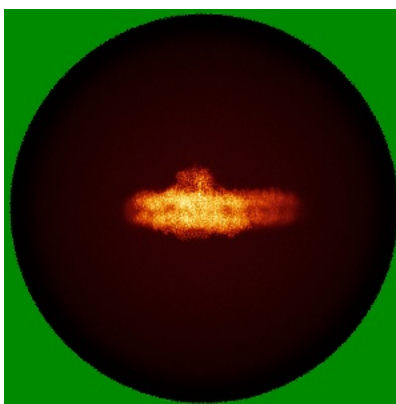
The images above show the largest variance slices of the map in three orthogonal directions.

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

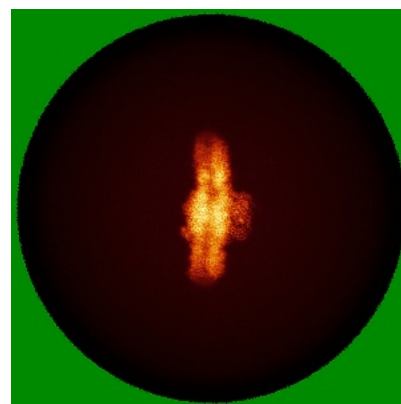
6.4.1 Primary map



X

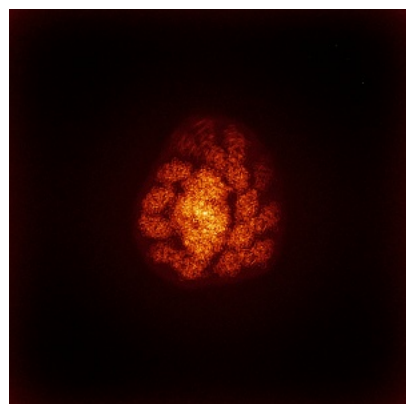


Y

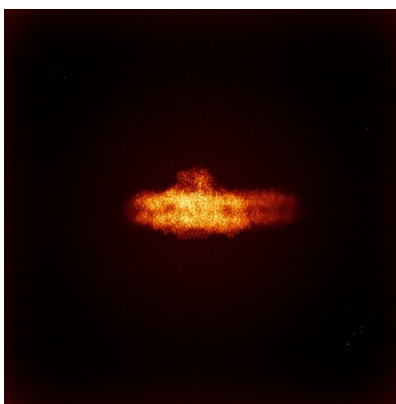


Z

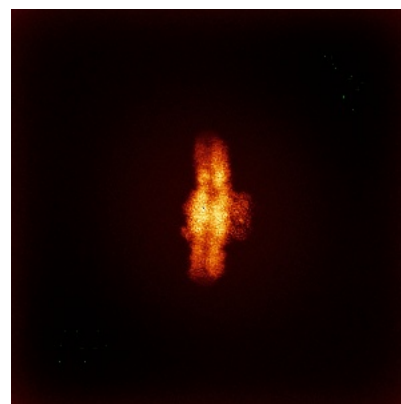
6.4.2 Raw map



X



Y

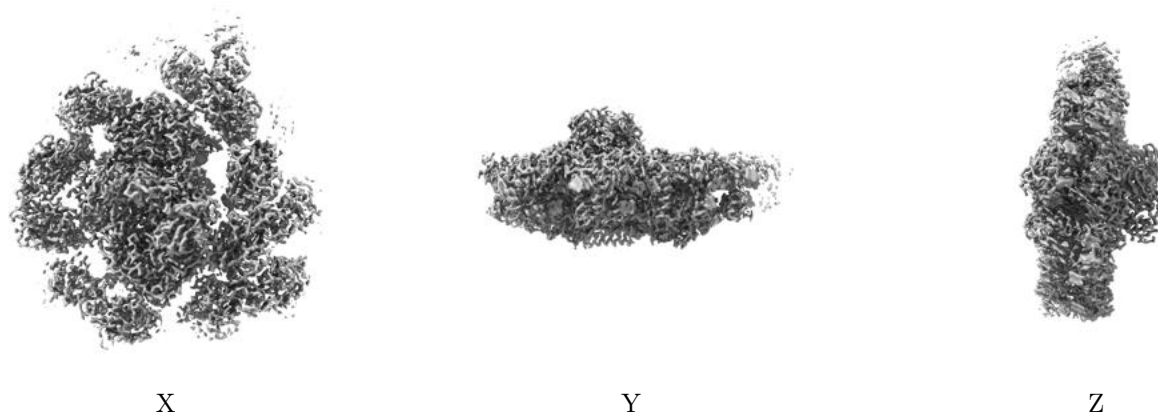


Z

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.

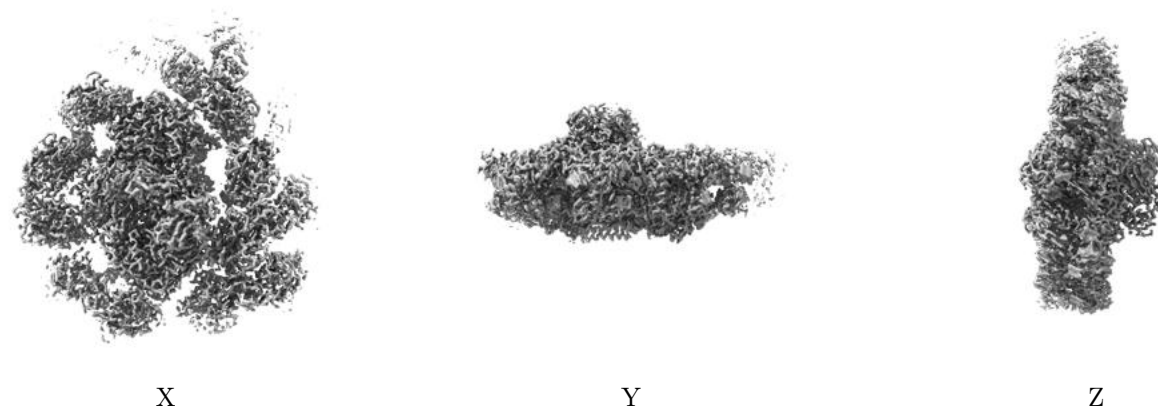
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. 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.

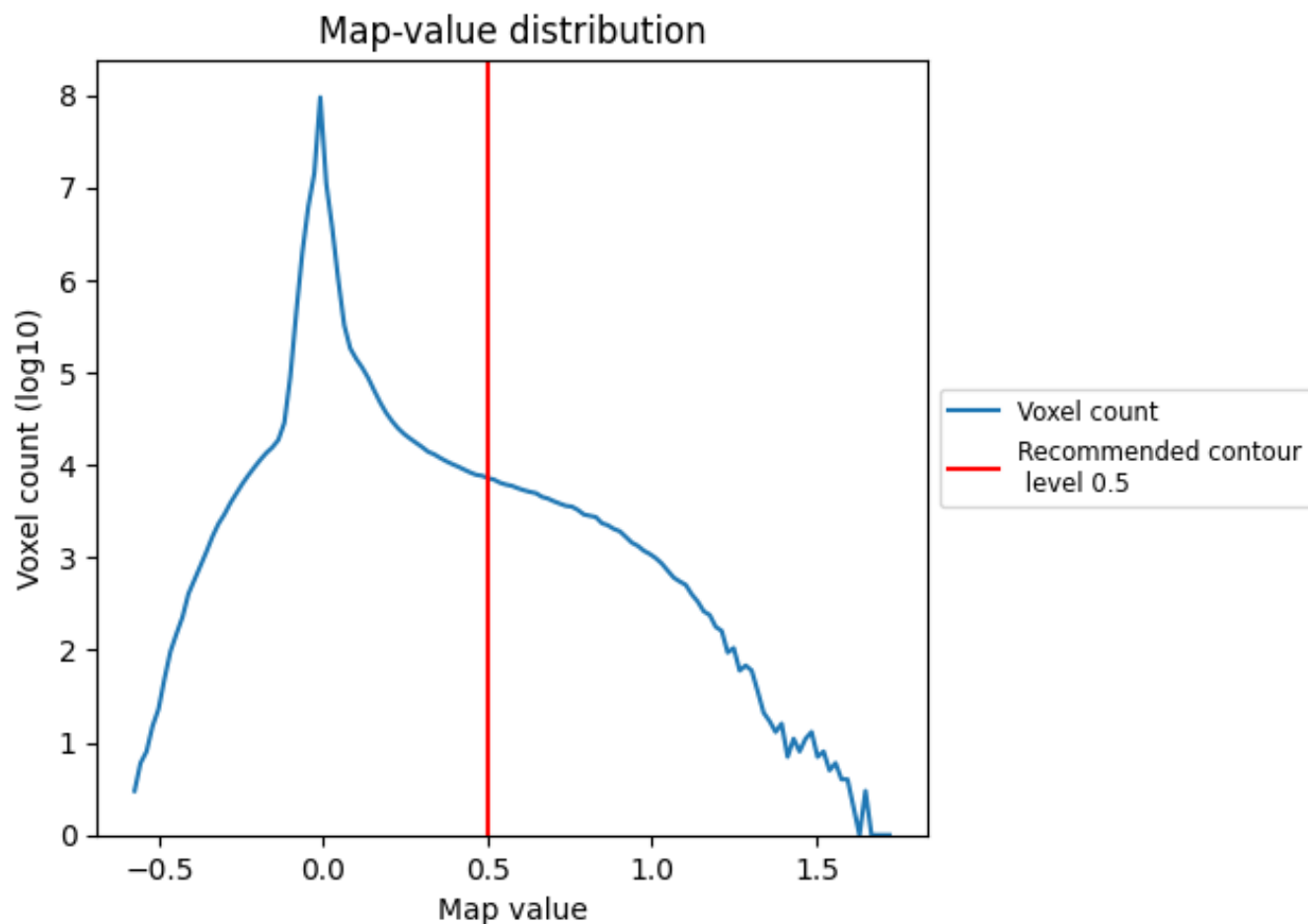
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

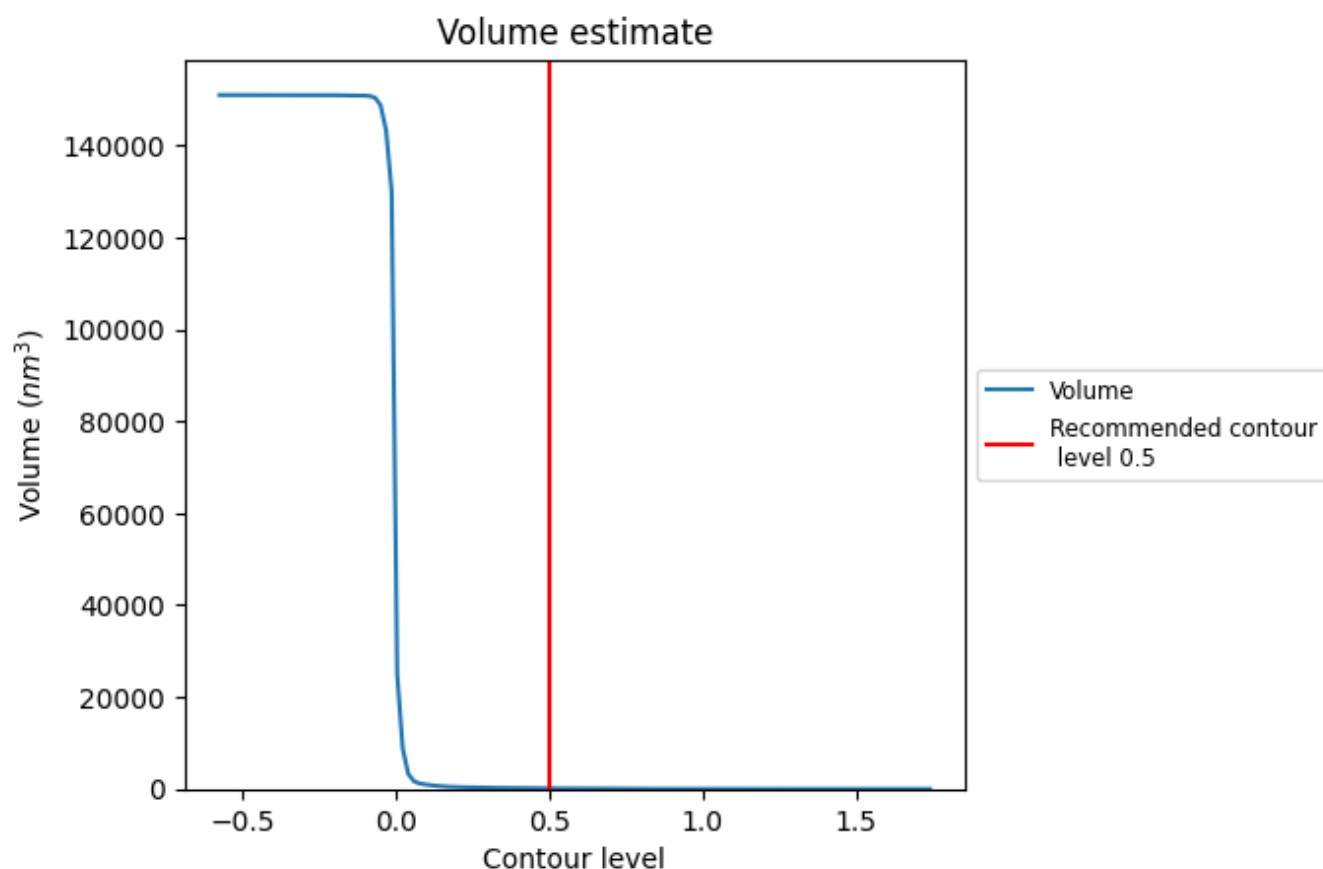
This section contains the results of statistical analysis of the map.

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.

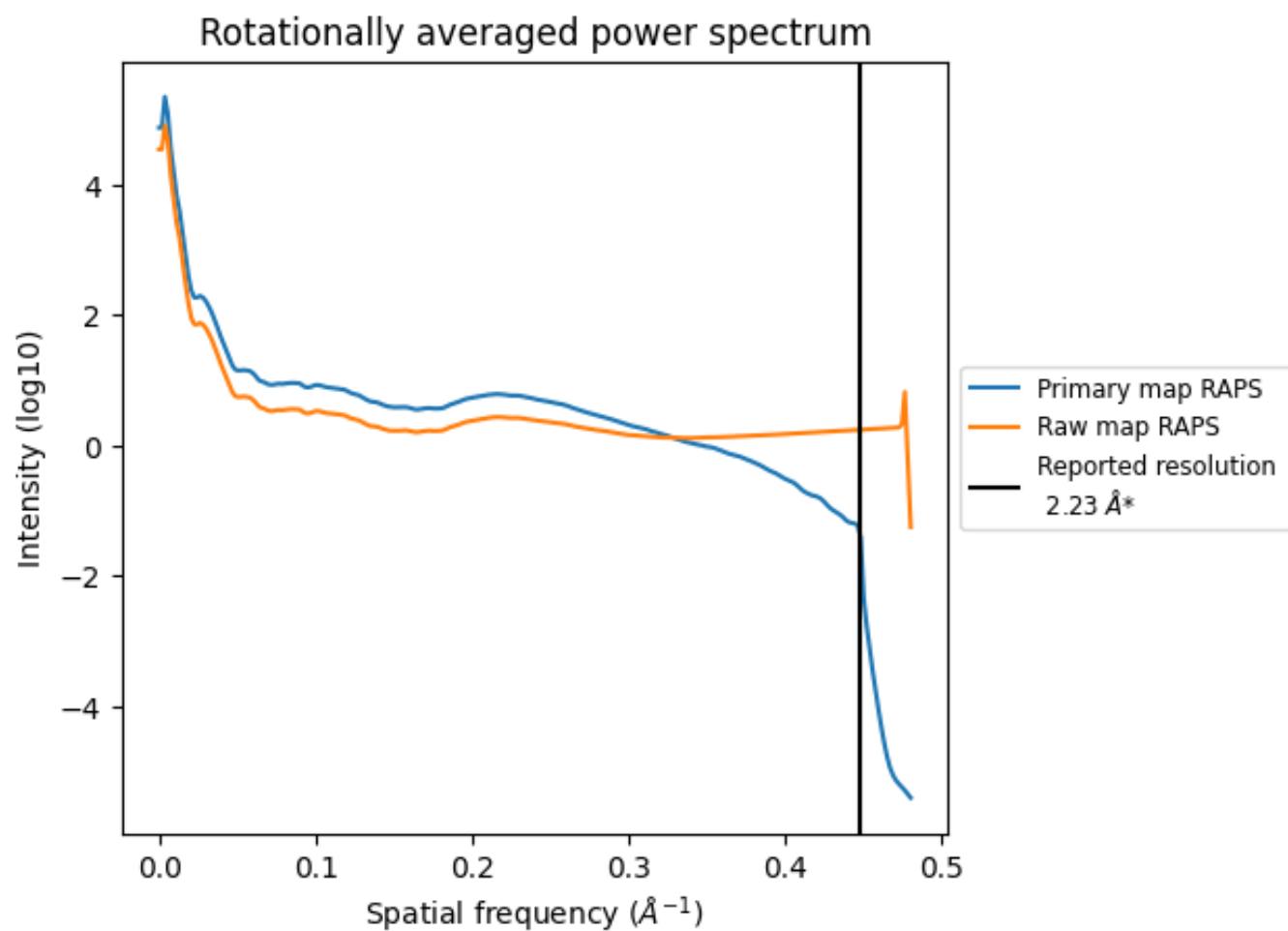
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 125 nm³; this corresponds to an approximate mass of 113 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 ⓘ

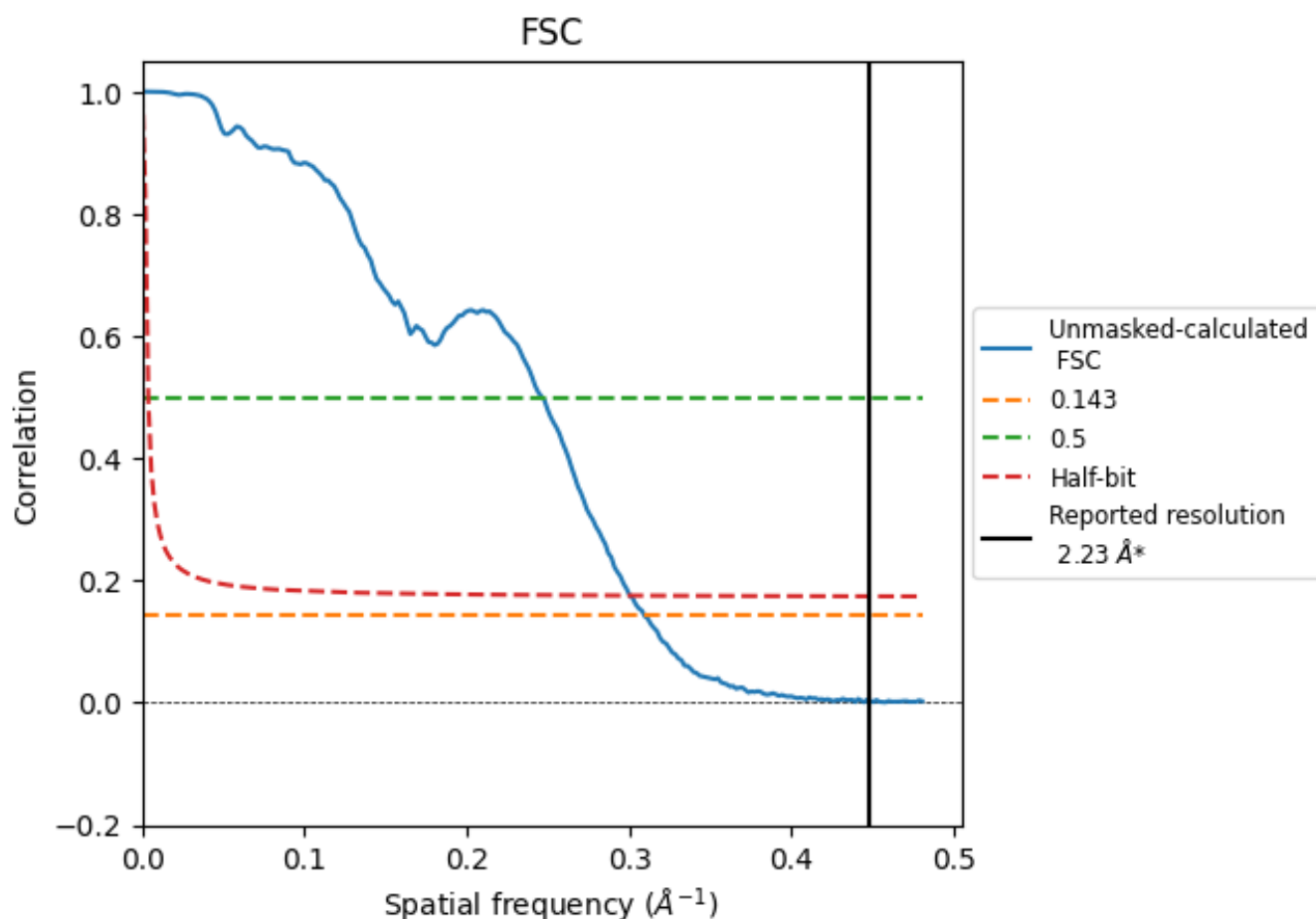


*Reported resolution corresponds to spatial frequency of 0.448 Å⁻¹

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 0.448 \AA^{-1}

8.2 Resolution estimates [i](#)

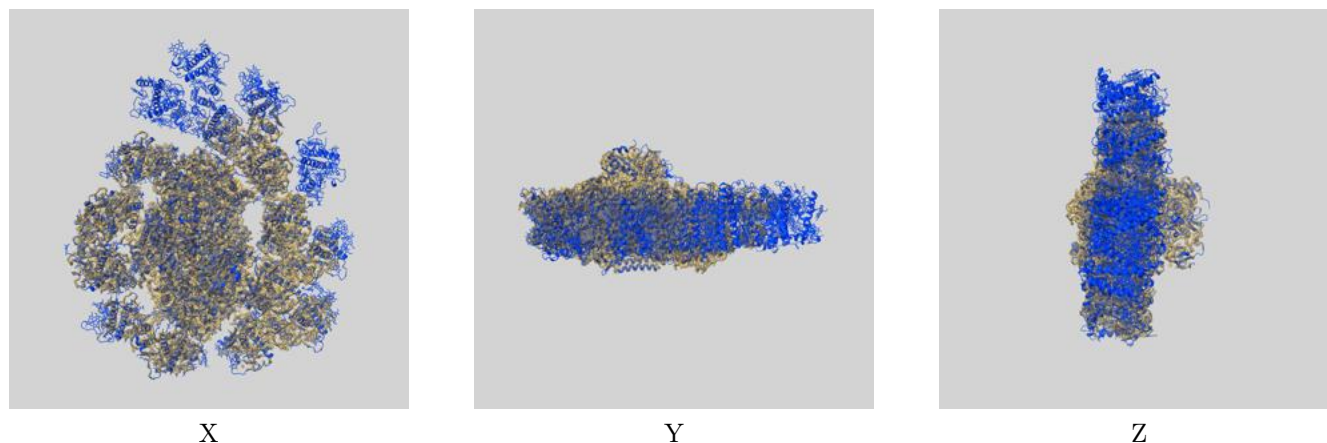
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.23	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.23	4.06	3.33

*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 3.23 differs from the reported value 2.23 by more than 10 %

9 Map-model fit [i](#)

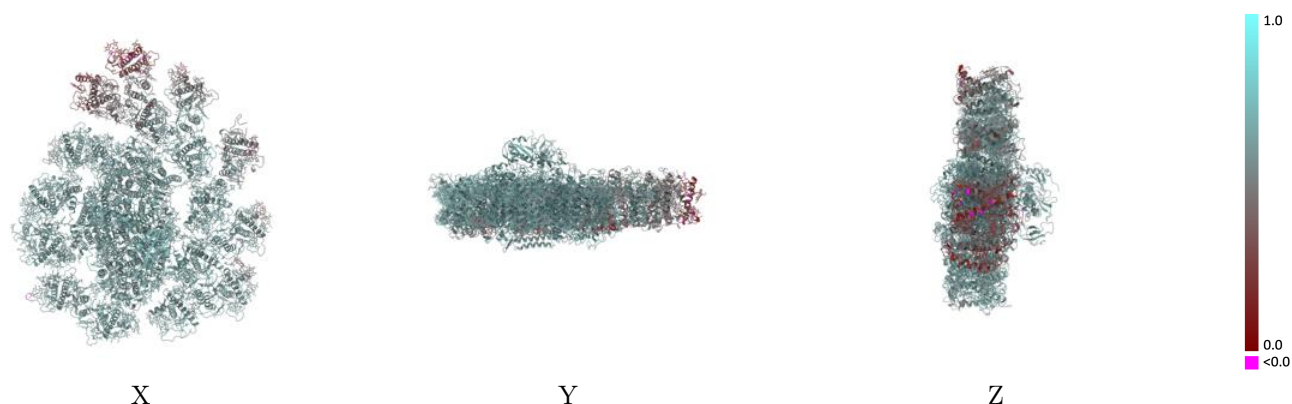
This section contains information regarding the fit between EMDB map EMD-64823 and PDB model 9V7T. Per-residue inclusion information can be found in section [3](#) on page [38](#).

9.1 Map-model overlay [i](#)



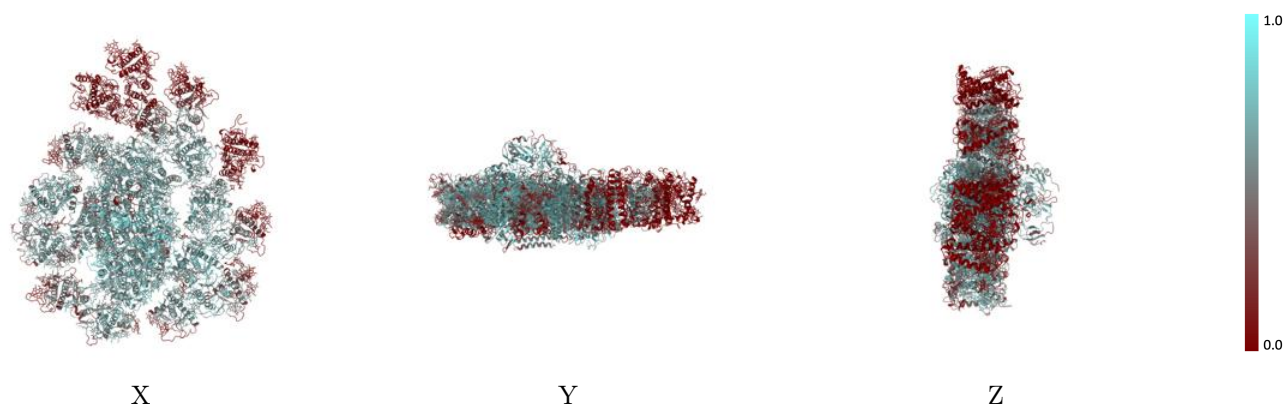
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



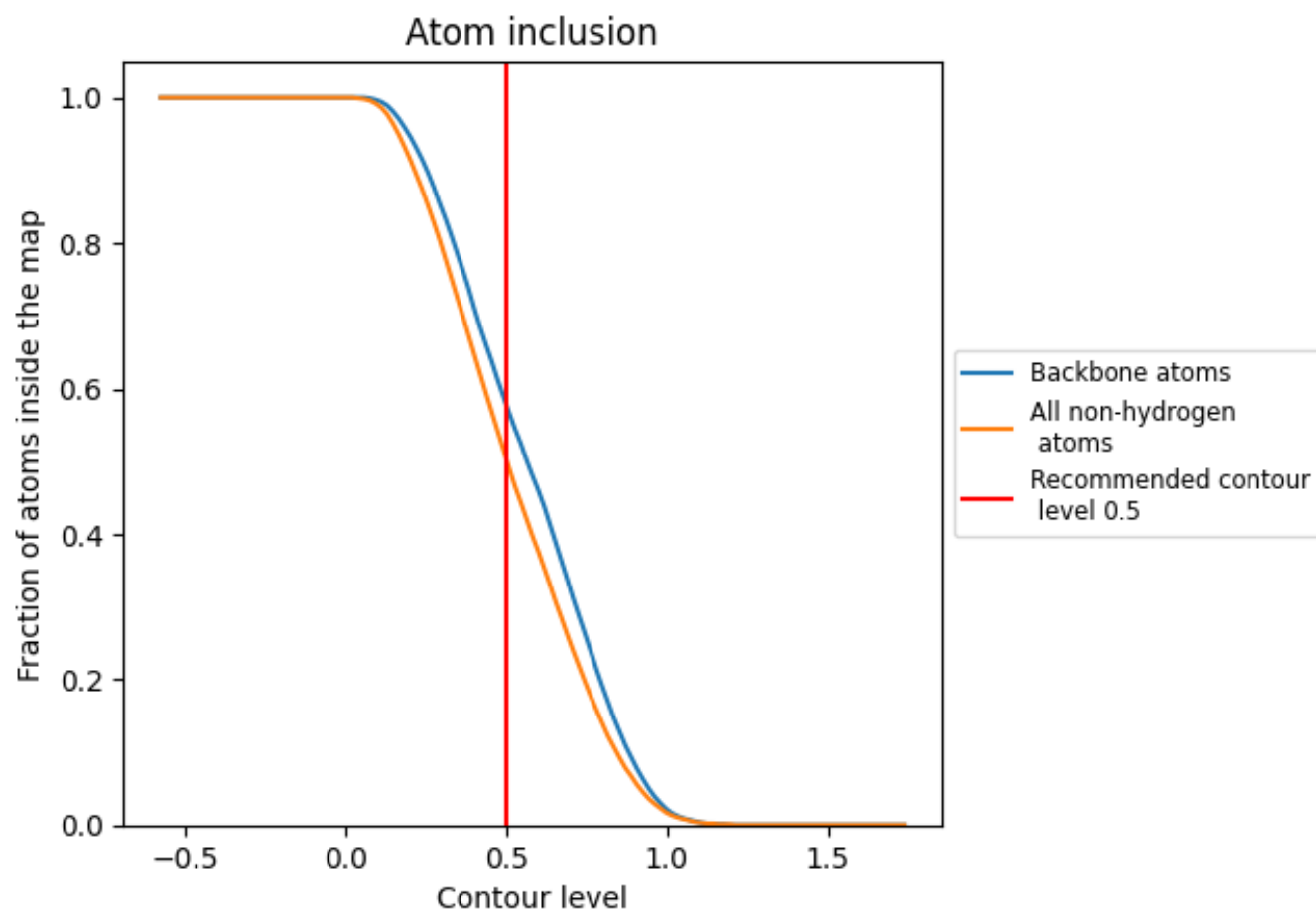
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).



















































9.4 Atom inclusion [i](#)



At the recommended contour level, 58% of all backbone atoms, 50% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5050	 0.6030
A	 0.7370	 0.6620
B	 0.7200	 0.6600
C	 0.7380	 0.6460
D	 0.4870	 0.6250
E	 0.5280	 0.6170
F	 0.5750	 0.6420
J	 0.6550	 0.6550
M	 0.5350	 0.6370
a	 0.5050	 0.6250
b	 0.3480	 0.5970
c	 0.4990	 0.6240
d	 0.5540	 0.6300
e	 0.4480	 0.6170
f	 0.0030	 0.3560
g	 0.2530	 0.5450
h	 0.5780	 0.6320
i	 0.5940	 0.6340
j	 0.6730	 0.6500
k	 0.4950	 0.6240
l	 0.3890	 0.5840
m	 0.2650	 0.5670
n	 0.0050	 0.4830
o	 0.1340	 0.5040
p	 0.0000	 0.2870

