



Full wwPDB EM Validation Report ⓘ

Oct 27, 2024 – 07:44 PM JST

PDB ID : 7XQP
EMDB ID : EMD-33401
Title : PSI-LHCI-LHCII-Lhcb9 supercomplex of *Physcomitrella patens*
Authors : Zhang, S.; Tang, K.L.; Li, X.Y.; Wang, W.D.; Yan, Q.J.; Shen, L.L.; Kuang, T.Y.; Han, G.Y.; Shen, J.R.; Zhang, X.
Deposited on : 2022-05-08
Resolution : 2.68 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.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

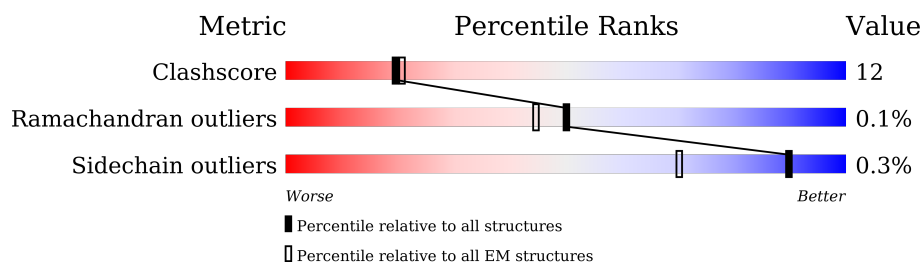
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.68 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	742	87% 13%
2	B	733	85% 15%
3	C	80	81% 19%
4	D	141	87% 13%
5	E	62	85% 15%
6	F	159	90% 10%
7	G	98	5% 84% 16%
8	H	95	93% 7%

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Mol	Chain	Length	Quality of chain
9	I	34	
10	J	41	
11	K	81	
12	L	163	
13	M	32	
14	O	89	
15	1	192	
15	5	192	
16	2	211	
16	6	211	
17	3	216	
17	7	216	
18	4	205	
18	8	205	
19	9	225	
20	a	227	
20	b	227	
20	c	227	

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
21	CLA	1	303	X	-	-	-
21	CLA	1	304	X	-	-	-
21	CLA	1	305	X	-	-	-
21	CLA	1	306	X	-	-	-
21	CLA	1	308	X	-	-	-
21	CLA	1	309	X	-	-	-
21	CLA	1	310	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	1	311	X	-	-	-
21	CLA	1	312	X	-	-	-
21	CLA	1	313	X	-	-	-
21	CLA	1	314	X	-	-	-
21	CLA	1	315	X	-	-	-
21	CLA	1	316	X	-	-	-
21	CLA	2	603	X	-	-	-
21	CLA	2	604	X	-	-	-
21	CLA	2	608	X	-	-	-
21	CLA	2	609	X	-	X	-
21	CLA	2	610	X	-	-	-
21	CLA	2	611	X	-	-	-
21	CLA	2	612	X	-	-	-
21	CLA	2	613	X	-	-	-
21	CLA	3	401	X	-	-	-
21	CLA	3	402	X	-	-	-
21	CLA	3	403	X	-	-	-
21	CLA	3	404	X	-	-	-
21	CLA	3	405	X	-	-	-
21	CLA	3	406	X	-	-	-
21	CLA	3	408	X	-	-	-
21	CLA	3	409	X	-	X	-
21	CLA	3	410	X	-	-	-
21	CLA	3	411	X	-	-	-
21	CLA	3	412	X	-	-	-
21	CLA	3	413	X	-	-	-
21	CLA	3	414	X	-	-	-
21	CLA	3	415	X	-	-	-
21	CLA	4	601	X	-	-	-
21	CLA	4	602	X	-	-	-
21	CLA	4	603	X	-	-	-
21	CLA	4	604	X	-	-	-
21	CLA	4	608	X	-	-	-
21	CLA	4	610	X	-	-	-
21	CLA	4	611	X	-	-	-
21	CLA	4	612	X	-	-	-
21	CLA	4	613	X	-	-	-
21	CLA	5	602	X	-	-	-
21	CLA	5	603	X	-	-	-
21	CLA	5	604	X	-	-	-
21	CLA	5	605	X	-	-	-
21	CLA	5	607	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	5	608	X	-	-	-
21	CLA	5	609	X	-	-	-
21	CLA	5	610	X	-	-	-
21	CLA	5	611	X	-	-	-
21	CLA	5	612	X	-	-	-
21	CLA	5	613	X	-	-	-
21	CLA	5	614	X	-	-	-
21	CLA	6	603	X	-	-	-
21	CLA	6	604	X	-	-	-
21	CLA	6	608	X	-	-	-
21	CLA	6	609	X	-	-	-
21	CLA	6	610	X	-	-	-
21	CLA	6	611	X	-	-	-
21	CLA	6	612	X	-	-	-
21	CLA	6	613	X	-	-	-
21	CLA	7	401	X	-	-	-
21	CLA	7	402	X	-	-	-
21	CLA	7	403	X	-	-	-
21	CLA	7	404	X	-	-	-
21	CLA	7	405	X	-	-	-
21	CLA	7	408	X	-	-	-
21	CLA	7	409	X	-	-	-
21	CLA	7	410	X	-	-	-
21	CLA	7	411	X	-	-	-
21	CLA	7	412	X	-	-	-
21	CLA	7	413	X	-	-	-
21	CLA	7	414	X	-	-	-
21	CLA	8	601	X	-	-	-
21	CLA	8	602	X	-	-	-
21	CLA	8	603	X	-	-	-
21	CLA	8	604	X	-	-	-
21	CLA	8	608	X	-	-	-
21	CLA	8	609	X	-	X	-
21	CLA	8	610	X	-	-	-
21	CLA	8	611	X	-	-	-
21	CLA	8	612	X	-	-	-
21	CLA	8	618	X	-	-	-
21	CLA	9	602	X	-	-	-
21	CLA	9	603	X	-	-	-
21	CLA	9	604	X	-	-	-
21	CLA	9	610	X	-	-	-
21	CLA	9	611	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	9	612	X	-	-	-
21	CLA	9	613	X	-	-	-
21	CLA	A	802	X	-	-	-
21	CLA	A	803	X	-	-	-
21	CLA	A	804	X	-	-	-
21	CLA	A	805	X	-	-	-
21	CLA	A	806	X	-	-	-
21	CLA	A	807	X	-	-	-
21	CLA	A	808	X	-	-	-
21	CLA	A	809	X	-	-	-
21	CLA	A	810	X	-	-	-
21	CLA	A	811	X	-	-	-
21	CLA	A	812	X	-	-	-
21	CLA	A	813	X	-	-	-
21	CLA	A	814	X	-	-	-
21	CLA	A	815	X	-	-	-
21	CLA	A	816	X	-	-	-
21	CLA	A	817	X	-	-	-
21	CLA	A	818	X	-	-	-
21	CLA	A	819	X	-	-	-
21	CLA	A	820	X	-	-	-
21	CLA	A	821	X	-	-	-
21	CLA	A	822	X	-	-	-
21	CLA	A	823	X	-	-	-
21	CLA	A	824	X	-	-	-
21	CLA	A	825	X	-	-	-
21	CLA	A	826	X	-	-	-
21	CLA	A	827	X	-	-	-
21	CLA	A	828	X	-	-	-
21	CLA	A	829	X	-	-	-
21	CLA	A	830	X	-	-	-
21	CLA	A	831	X	-	-	-
21	CLA	A	832	X	-	-	-
21	CLA	A	833	X	-	-	-
21	CLA	A	834	X	-	-	-
21	CLA	A	835	X	-	-	-
21	CLA	A	836	X	-	-	-
21	CLA	A	837	X	-	-	-
21	CLA	A	838	X	-	-	-
21	CLA	A	839	X	-	-	-
21	CLA	A	840	X	-	-	-
21	CLA	A	841	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	A	842	X	-	-	-
21	CLA	A	852	X	-	-	-
21	CLA	B	801	X	-	-	-
21	CLA	B	802	X	-	-	-
21	CLA	B	803	X	-	-	-
21	CLA	B	804	X	-	-	-
21	CLA	B	805	X	-	-	-
21	CLA	B	806	X	-	-	-
21	CLA	B	807	X	-	-	-
21	CLA	B	808	X	-	-	-
21	CLA	B	809	X	-	-	-
21	CLA	B	810	X	-	-	-
21	CLA	B	811	X	-	-	-
21	CLA	B	812	X	-	-	-
21	CLA	B	813	X	-	-	-
21	CLA	B	814	X	-	-	-
21	CLA	B	815	X	-	-	-
21	CLA	B	816	X	-	-	-
21	CLA	B	817	X	-	-	-
21	CLA	B	818	X	-	-	-
21	CLA	B	819	X	-	-	-
21	CLA	B	820	X	-	-	-
21	CLA	B	821	X	-	-	-
21	CLA	B	822	X	-	-	-
21	CLA	B	823	X	-	-	-
21	CLA	B	824	X	-	-	-
21	CLA	B	825	X	-	-	-
21	CLA	B	826	X	-	-	-
21	CLA	B	827	X	-	-	-
21	CLA	B	828	X	-	-	-
21	CLA	B	829	X	-	-	-
21	CLA	B	830	X	-	-	-
21	CLA	B	831	X	-	-	-
21	CLA	B	832	X	-	-	-
21	CLA	B	833	X	-	-	-
21	CLA	B	834	X	-	-	-
21	CLA	B	835	X	-	-	-
21	CLA	B	836	X	-	-	-
21	CLA	B	837	X	-	-	-
21	CLA	B	838	X	-	-	-
21	CLA	B	839	X	-	-	-
21	CLA	B	840	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	F	302	X	-	-	-
21	CLA	F	304	X	-	-	-
21	CLA	F	305	X	-	-	-
21	CLA	G	202	X	-	-	-
21	CLA	G	203	X	-	-	-
21	CLA	G	204	X	-	-	-
21	CLA	H	201	X	-	-	-
21	CLA	J	102	X	-	-	-
21	CLA	K	201	X	-	-	-
21	CLA	K	202	X	-	-	-
21	CLA	K	203	X	-	-	-
21	CLA	K	204	X	-	-	-
21	CLA	L	302	X	-	-	-
21	CLA	L	303	X	-	-	-
21	CLA	L	304	X	-	-	-
21	CLA	O	201	X	-	-	-
21	CLA	O	202	X	-	-	-
21	CLA	O	203	X	-	-	-
21	CLA	O	204	X	-	-	-
21	CLA	a	602	X	-	-	-
21	CLA	a	603	X	-	-	-
21	CLA	a	604	X	-	-	-
21	CLA	a	610	X	-	-	-
21	CLA	a	611	X	-	-	-
21	CLA	a	612	X	-	-	-
21	CLA	a	613	X	-	-	-
21	CLA	a	614	X	-	-	-
21	CLA	b	303	X	-	-	-
21	CLA	b	304	X	-	-	-
21	CLA	b	305	X	-	-	-
21	CLA	b	311	X	-	-	-
21	CLA	b	312	X	-	-	-
21	CLA	b	313	X	-	-	-
21	CLA	b	314	X	-	-	-
21	CLA	b	315	X	-	-	-
21	CLA	c	602	X	-	-	-
21	CLA	c	603	X	-	-	-
21	CLA	c	604	X	-	-	-
21	CLA	c	610	X	-	-	-
21	CLA	c	611	X	-	-	-
21	CLA	c	612	X	-	-	-
21	CLA	c	613	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	c	614	X	-	-	-
24	BCR	K	205	-	-	X	-
29	CHL	1	302	X	-	-	-
29	CHL	1	307	X	-	-	-
29	CHL	2	601	X	-	-	-
29	CHL	2	602	X	-	-	-
29	CHL	2	605	X	-	-	-
29	CHL	2	606	X	-	-	-
29	CHL	2	607	X	-	-	-
29	CHL	2	614	X	-	-	-
29	CHL	3	407	X	-	-	-
29	CHL	4	605	X	-	-	-
29	CHL	4	606	X	-	-	-
29	CHL	4	607	X	-	-	-
29	CHL	4	614	X	-	-	-
29	CHL	5	601	X	-	-	-
29	CHL	5	606	X	-	-	-
29	CHL	6	601	X	-	-	-
29	CHL	6	602	X	-	-	-
29	CHL	6	605	X	-	-	-
29	CHL	6	606	X	-	-	-
29	CHL	6	607	X	-	-	-
29	CHL	6	614	X	-	-	-
29	CHL	7	406	X	-	-	-
29	CHL	8	605	X	-	-	-
29	CHL	8	606	X	-	-	-
29	CHL	8	607	X	-	-	-
29	CHL	8	613	X	-	-	-
29	CHL	9	601	X	-	-	-
29	CHL	9	605	X	-	-	-
29	CHL	9	606	X	-	-	-
29	CHL	9	607	X	-	-	-
29	CHL	9	608	X	-	-	-
29	CHL	9	609	X	-	-	-
29	CHL	a	601	X	-	-	-
29	CHL	a	605	X	-	-	-
29	CHL	a	606	X	-	-	-
29	CHL	a	607	X	-	-	-
29	CHL	a	608	X	-	-	-
29	CHL	a	609	X	-	-	-
29	CHL	b	302	X	-	-	-
29	CHL	b	306	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CHL	b	307	X	-	-	-
29	CHL	b	308	X	-	-	-
29	CHL	b	309	X	-	-	-
29	CHL	b	310	X	-	-	-
29	CHL	c	601	X	-	-	-
29	CHL	c	605	X	-	-	-
29	CHL	c	606	X	-	-	-
29	CHL	c	607	X	-	-	-
29	CHL	c	608	X	-	-	-
29	CHL	c	609	X	-	-	-

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 56417 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	742	Total	C	N	O	S	0	0
			5836	3827	993	997	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	733	Total	C	N	O	S	0	0
			5849	3839	996	998	16		

- 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
			595	365	103	116	11		

- Molecule 4 is a protein called Predicted protein PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	141	Total	C	N	O	S	0	0
			1104	707	196	198	3		

- Molecule 5 is a protein called PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	62	Total	C	N	O	0	0
			487	309	87	91		

- Molecule 6 is a protein called PSI-F.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	159	Total	C	N	O	S	0	0
			1230	796	210	221	3		

- Molecule 7 is a protein called PSI-G.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	98	Total	C	N	O	0	0
			749	483	128	138		

- Molecule 8 is a protein called PsaH photosystem I reaction center subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	95	Total	C	N	O	S	0	0
			740	476	125	138	1		

- Molecule 9 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	34	Total	C	N	O	S	0	0
			266	181	35	48	2		

- Molecule 10 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	41	Total	C	N	O	S	0	0
			325	222	48	54	1		

- Molecule 11 is a protein called PsaK.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	81	Total	C	N	O	S	0	0
			566	356	98	109	3		

- Molecule 12 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	163	Total	C	N	O	S	0	0
			1229	808	197	222	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	32	Total	C	N	O	S	0	0
			238	155	38	44	1		

- Molecule 14 is a protein called PsaO.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	89	Total	C	N	O	S	0	0
			702	472	115	114	1		

- Molecule 15 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	1	192	Total	C	N	O	S	0	0
			1478	965	247	265	1		
15	5	192	Total	C	N	O	S	0	0
			1475	962	247	265	1		

- Molecule 16 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	2	211	Total	C	N	O	S	0	0
			1632	1062	274	292	4		
16	6	205	Total	C	N	O	S	0	0
			1587	1035	265	283	4		

- Molecule 17 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	3	216	Total	C	N	O	S	0	0
			1670	1094	269	300	7		
17	7	213	Total	C	N	O	S	0	0
			1644	1076	265	296	7		

- Molecule 18 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	4	205	Total	C	N	O	S	0	0
			1592	1033	266	288	5		
18	8	204	Total	C	N	O	S	0	0
			1585	1029	265	286	5		

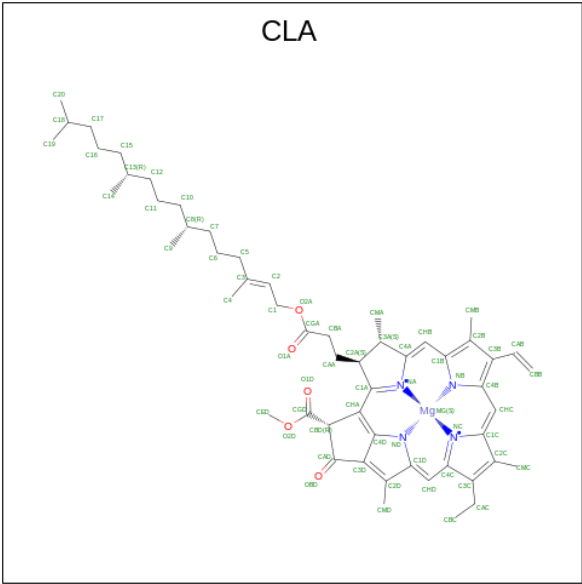
- Molecule 19 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	9	225	Total	C	N	O	S	0	0
			1747	1139	287	312	9		

- Molecule 20 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace	
20	a	218	Total	C	N	O	S	0	0	
			1651	1069	268	309	5			
20	b	218	Total	C	N	O	S	0	0	
			1651	1069	268	309	5			
20	c	227	Total	C	N	O	P	S	0	0
			1727	1110	284	327	1	5		

- Molecule 21 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
21	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
21	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
21	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 53	C 43	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 63	C 53	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
21	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
21	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
21	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	F	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
21	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	F	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
21	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	G	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
21	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
21	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	K	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
21	K	1	Total 44	C 34	Mg 1	N 4	O 5	0
21	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	L	1	Total 42	C 34	Mg 1	N 4	O 3	0
21	O	1	Total 42	C 34	Mg 1	N 4	O 3	0
21	O	1	Total 38	C 30	Mg 1	N 4	O 3	0
21	O	1	Total 50	C 42	Mg 1	N 4	O 3	0
21	O	1	Total 40	C 32	Mg 1	N 4	O 3	0
21	1	1	Total 61	C 51	Mg 1	N 4	O 5	0
21	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	1	1	Total 49	C 39	Mg 1	N 4	O 5	0
21	1	1	Total 40	C 32	Mg 1	N 4	O 3	0
21	1	1	Total 44	C 34	Mg 1	N 4	O 5	0
21	1	1	Total 41	C 33	Mg 1	N 4	O 3	0
21	1	1	Total 43	C 33	Mg 1	N 4	O 5	0
21	1	1	Total 38	C 30	Mg 1	N 4	O 3	0
21	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	1	1	Total 38	C 30	Mg 1	N 4	O 3	0
21	1	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
21	1	1	Total 43	C 33	Mg 1	N 4	O 5	0
21	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	2	1	Total 51	C 42	Mg 1	N 4	O 4	0
21	2	1	Total 42	C 34	Mg 1	N 4	O 3	0
21	2	1	Total 41	C 33	Mg 1	N 4	O 3	0
21	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	2	1	Total 42	C 34	Mg 1	N 4	O 3	0
21	3	1	Total 40	C 32	Mg 1	N 4	O 3	0
21	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	3	1	Total 42	C 32	Mg 1	N 4	O 5	0
21	3	1	Total 41	C 33	Mg 1	N 4	O 3	0
21	3	1	Total 40	C 32	Mg 1	N 4	O 3	0
21	3	1	Total 59	C 49	Mg 1	N 4	O 5	0
21	3	1	Total 52	C 42	Mg 1	N 4	O 5	0
21	3	1	Total 40	C 32	Mg 1	N 4	O 3	0
21	3	1	Total 43	C 35	Mg 1	N 4	O 3	0
21	3	1	Total 54	C 44	Mg 1	N 4	O 5	0
21	3	1	Total 40	C 32	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
21	3	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
21	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
21	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
21	4	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
21	4	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
21	5	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
21	5	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
21	5	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
21	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
21	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	5	1	Total 38	C 30	Mg 1	N 4	O 3	0
21	5	1	Total 43	C 33	Mg 1	N 4	O 5	0
21	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	6	1	Total 42	C 34	Mg 1	N 4	O 3	0
21	6	1	Total 42	C 34	Mg 1	N 4	O 3	0
21	6	1	Total 41	C 33	Mg 1	N 4	O 3	0
21	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	6	1	Total 42	C 34	Mg 1	N 4	O 3	0
21	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	7	1	Total 42	C 32	Mg 1	N 4	O 5	0
21	7	1	Total 41	C 33	Mg 1	N 4	O 3	0
21	7	1	Total 40	C 32	Mg 1	N 4	O 3	0
21	7	1	Total 44	C 34	Mg 1	N 4	O 5	0
21	7	1	Total 41	C 33	Mg 1	N 4	O 3	0
21	7	1	Total 40	C 32	Mg 1	N 4	O 3	0
21	7	1	Total 43	C 35	Mg 1	N 4	O 3	0
21	7	1	Total 54	C 44	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
21	7	1	Total 40	C 32	Mg 1	N 4	O 3	0
21	7	1	Total 36	C 30	Mg 1	N 4	O 1	0
21	7	1	Total 40	C 32	Mg 1	N 4	O 3	0
21	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	8	1	Total 58	C 48	Mg 1	N 4	O 5	0
21	8	1	Total 44	C 34	Mg 1	N 4	O 5	0
21	8	1	Total 43	C 34	Mg 1	N 4	O 4	0
21	8	1	Total 43	C 34	Mg 1	N 4	O 4	0
21	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	8	1	Total 44	C 34	Mg 1	N 4	O 5	0
21	8	1	Total 54	C 45	Mg 1	N 4	O 4	0
21	8	1	Total 43	C 35	Mg 1	N 4	O 3	0
21	8	1	Total 41	C 33	Mg 1	N 4	O 3	0
21	9	1	Total 53	C 43	Mg 1	N 4	O 5	0
21	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	9	1	Total 54	C 44	Mg 1	N 4	O 5	0
21	9	1	Total 57	C 47	Mg 1	N 4	O 5	0
21	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	9	1	Total 53	C 43	Mg 1	N 4	O 5	0
21	a	1	Total 60	C 50	Mg 1	N 4	O 5	0

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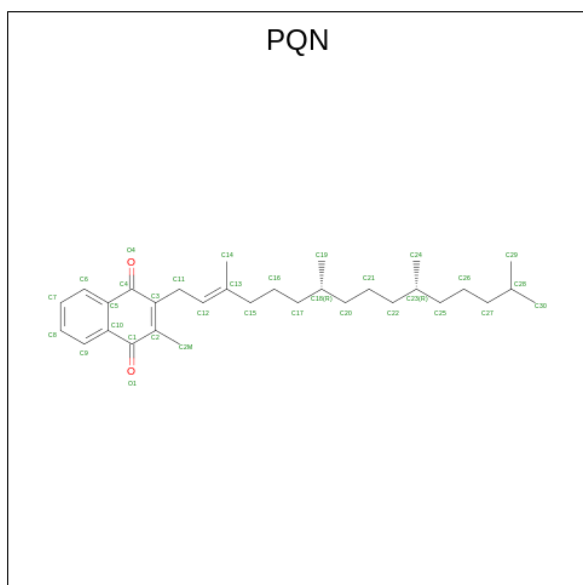
Mol	Chain	Residues	Atoms					AltConf
21	a	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
21	a	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
21	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	a	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
21	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	a	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
21	a	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
21	b	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
21	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	b	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
21	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	b	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
21	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	c	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	c	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	c	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
21	c	1	Total	C	Mg	N	O	0
			44	35	1	4	4	

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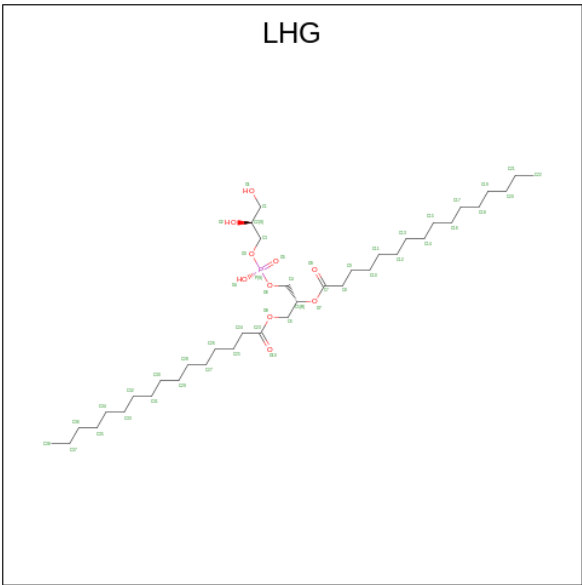
Mol	Chain	Residues	Atoms					AltConf
21	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 22 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



Mol	Chain	Residues	Atoms			AltConf
22	A	1	Total	C	O	0
			33	31	2	
22	B	1	Total	C	O	0
			33	31	2	

- Molecule 23 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



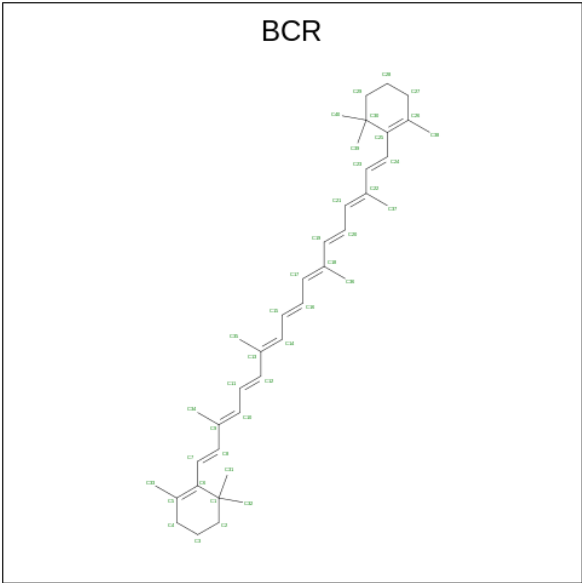
Mol	Chain	Residues	Atoms				AltConf
23	A	1	Total	C	O	P	0
			49	38	10	1	
23	A	1	Total	C	O	P	0
			27	16	10	1	
23	A	1	Total	C	O	P	0
			49	38	10	1	
23	1	1	Total	C	O	P	0
			23	12	10	1	
23	1	1	Total	C	O	P	0
			28	17	10	1	
23	2	1	Total	C	O	P	0
			35	24	10	1	
23	4	1	Total	C	O	P	0
			37	26	10	1	
23	4	1	Total	C	O	P	0
			49	38	10	1	
23	5	1	Total	C	O	P	0
			28	17	10	1	
23	6	1	Total	C	O	P	0
			35	24	10	1	
23	8	1	Total	C	O	P	0
			37	26	10	1	
23	9	1	Total	C	O	P	0
			49	38	10	1	
23	a	1	Total	C	O	P	0
			49	38	10	1	
23	b	1	Total	C	O	P	0
			49	38	10	1	

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Mol	Chain	Residues	Atoms				AltConf
23	c	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 24 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



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

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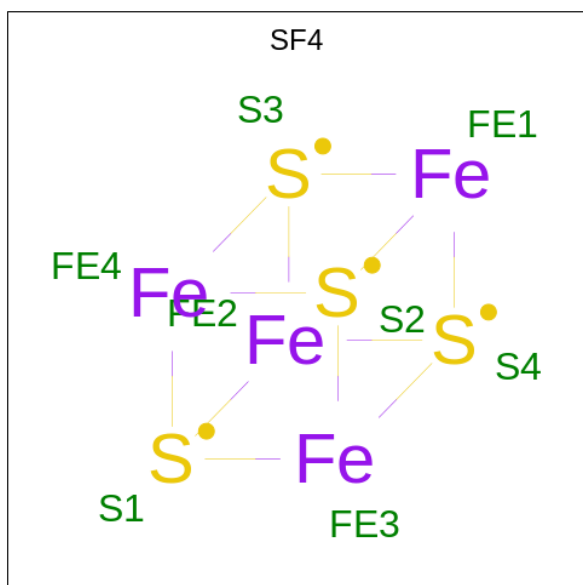
Mol	Chain	Residues	Atoms	AltConf
24	B	1	Total C 40 40	0
24	F	1	Total C 40 40	0
24	F	1	Total C 40 40	0
24	G	1	Total C 40 40	0
24	G	1	Total C 40 40	0
24	I	1	Total C 40 40	0
24	J	1	Total C 40 40	0
24	J	1	Total C 40 40	0
24	J	1	Total C 40 40	0
24	K	1	Total C 40 40	0
24	L	1	Total C 40 40	0
24	L	1	Total C 40 40	0
24	L	1	Total C 40 40	0
24	M	1	Total C 40 40	0
24	O	1	Total C 40 40	0
24	2	1	Total C 40 40	0
24	3	1	Total C 40 40	0
24	3	1	Total C 40 40	0
24	4	1	Total C 40 40	0
24	6	1	Total C 40 40	0
24	7	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
24	7	1	Total C 40 40	0
24	8	1	Total C 40 40	0

- Molecule 25 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



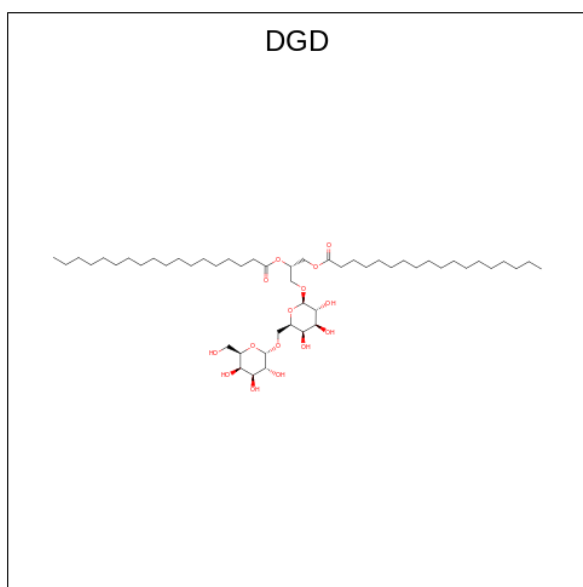
Mol	Chain	Residues	Atoms	AltConf
25	A	1	Total Fe S 8 4 4	0
25	C	1	Total Fe S 8 4 4	0
25	C	1	Total Fe S 8 4 4	0

- Molecule 26 is DODECYL-ALPHA-D-MALTOSIDE (three-letter code: LMU) (formula: $\text{C}_{24}\text{H}_{46}\text{O}_{11}$) (labeled as "Ligand of Interest" by depositor).



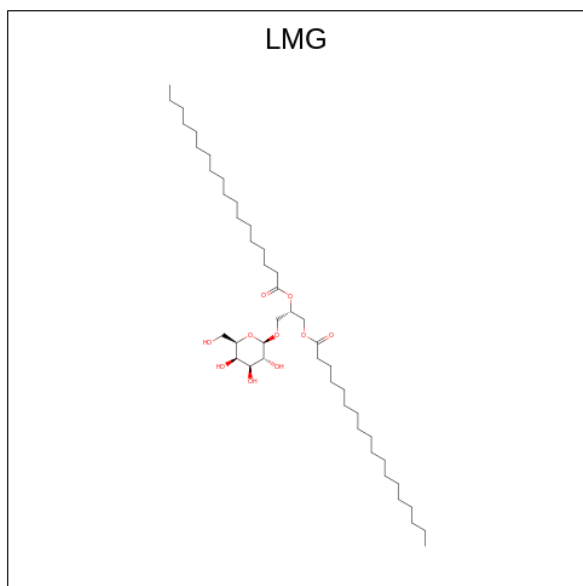
Mol	Chain	Residues	Atoms			AltConf
26	A	1	Total 35	C 24	O 11	0
26	A	1	Total 35	C 24	O 11	0
26	O	1	Total 35	C 24	O 11	0
26	3	1	Total 35	C 24	O 11	0
26	b	1	Total 35	C 24	O 11	0

- Molecule 27 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C₅₁H₉₆O₁₅).



Mol	Chain	Residues	Atoms			AltConf
27	B	1	Total	C	O	0
			66	51	15	

- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



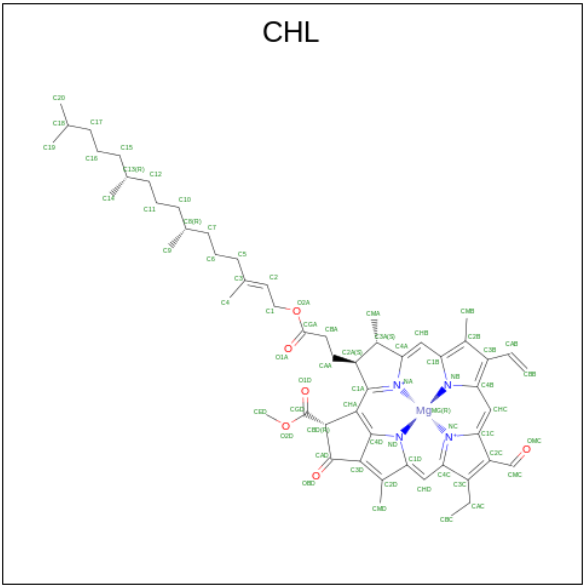
Mol	Chain	Residues	Atoms			AltConf
28	G	1	Total	C	O	0
			55	45	10	
28	J	1	Total	C	O	0
			30	20	10	

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Mol	Chain	Residues	Atoms			AltConf
28	2	1	Total	C	O	0
			13	7	6	
28	6	1	Total	C	O	0
			13	7	6	

- Molecule 29 is CHLOROPHYLL B (three-letter code: CHL) (formula: C₅₅H₇₀MgN₄O₆).



Mol	Chain	Residues	Atoms					AltConf
29	1	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
29	1	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
29	2	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
29	2	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
29	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	2	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
29	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	

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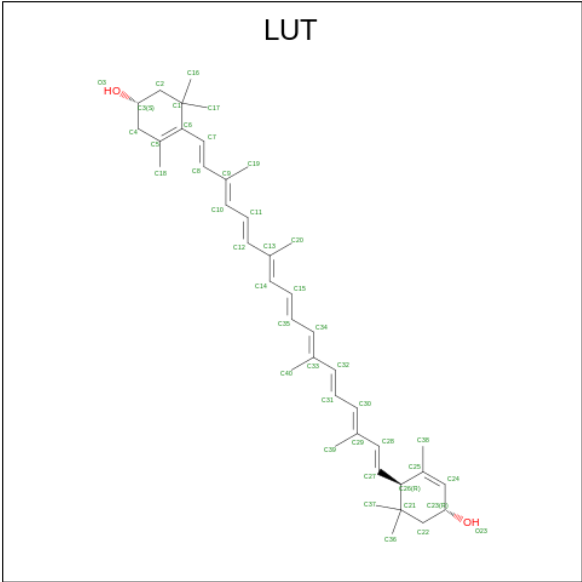
Mol	Chain	Residues	Atoms					AltConf
29	4	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
29	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
29	4	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
29	5	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	5	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	6	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
29	6	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
29	6	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	6	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	6	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
29	6	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	7	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
29	8	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
29	8	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	8	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
29	8	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
29	9	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
29	9	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	9	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	9	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
29	9	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	9	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	a	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	a	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
29	a	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	a	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
29	a	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	a	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	b	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	b	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	b	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	b	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
29	b	1	Total	C	Mg	N	O	0
			49	38	1	4	6	
29	b	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
29	c	1	Total	C	Mg	N	O	0
			49	38	1	4	6	
29	c	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
29	c	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	c	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	c	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	c	1	Total	C	Mg	N	O	0
			44	33	1	4	6	

- Molecule 30 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C₄₀H₅₆O₂).



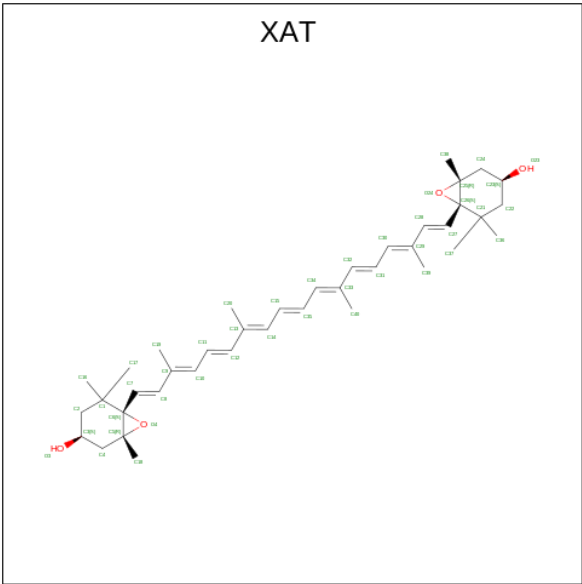
Mol	Chain	Residues	Atoms			AltConf
30	1	1	Total	C	O	0
			42	40	2	
30	2	1	Total	C	O	0
			42	40	2	
30	3	1	Total	C	O	0
			42	40	2	
30	4	1	Total	C	O	0
			42	40	2	
30	5	1	Total	C	O	0
			42	40	2	
30	6	1	Total	C	O	0
			42	40	2	
30	7	1	Total	C	O	0
			42	40	2	
30	8	1	Total	C	O	0
			42	40	2	
30	9	1	Total	C	O	0
			42	40	2	
30	9	1	Total	C	O	0
			42	40	2	
30	a	1	Total	C	O	0
			42	40	2	
30	a	1	Total	C	O	0
			42	40	2	
30	b	1	Total	C	O	0
			42	40	2	
30	b	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms			AltConf
30	c	1	Total	C	O	0
			42	40	2	
30	c	1	Total	C	O	0
			42	40	2	

- Molecule 31 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (three-letter code: XAT) (formula: C₄₀H₅₆O₄).



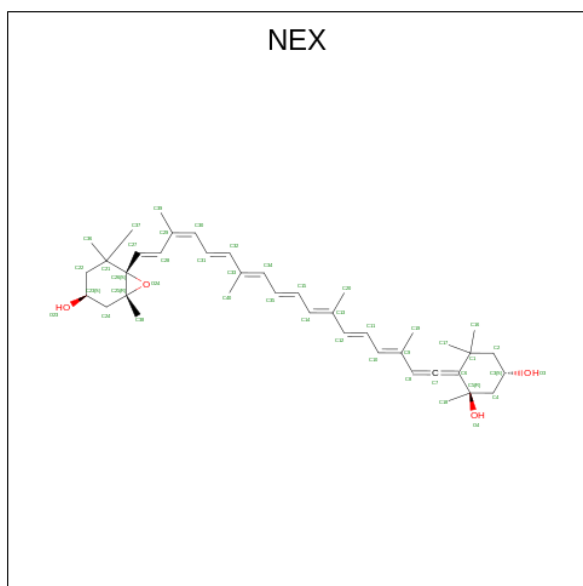
Mol	Chain	Residues	Atoms			AltConf
31	1	1	Total	C	O	0
			44	40	4	
31	2	1	Total	C	O	0
			44	40	4	
31	3	1	Total	C	O	0
			44	40	4	
31	4	1	Total	C	O	0
			44	40	4	
31	5	1	Total	C	O	0
			44	40	4	
31	6	1	Total	C	O	0
			44	40	4	
31	7	1	Total	C	O	0
			44	40	4	
31	8	1	Total	C	O	0
			44	40	4	
31	9	1	Total	C	O	0
			44	40	4	

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Mol	Chain	Residues	Atoms			AltConf
31	a	1	Total	C	O	0
			44	40	4	
31	c	1	Total	C	O	0
			44	40	4	

- Molecule 32 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTA DECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (three-letter code: NEX) (formula: C₄₀H₅₆O₄).

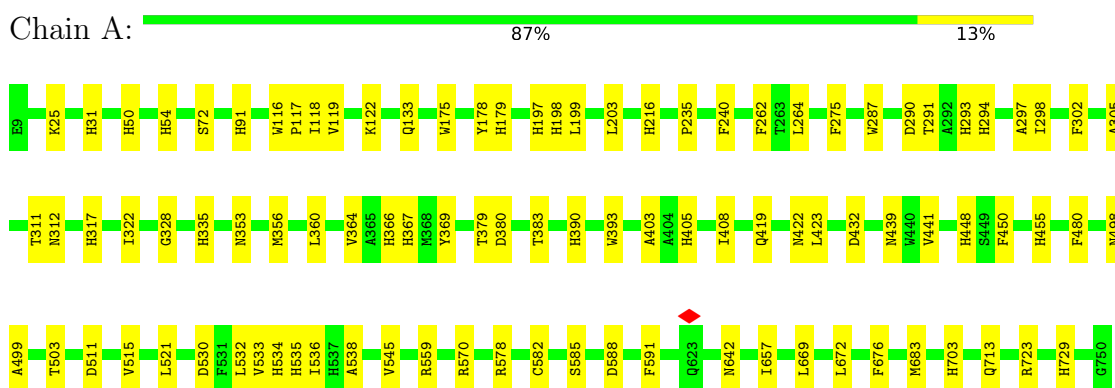


Mol	Chain	Residues	Atoms			AltConf
32	9	1	Total	C	O	0
			44	40	4	
32	b	1	Total	C	O	0
			44	40	4	
32	c	1	Total	C	O	0
			44	40	4	

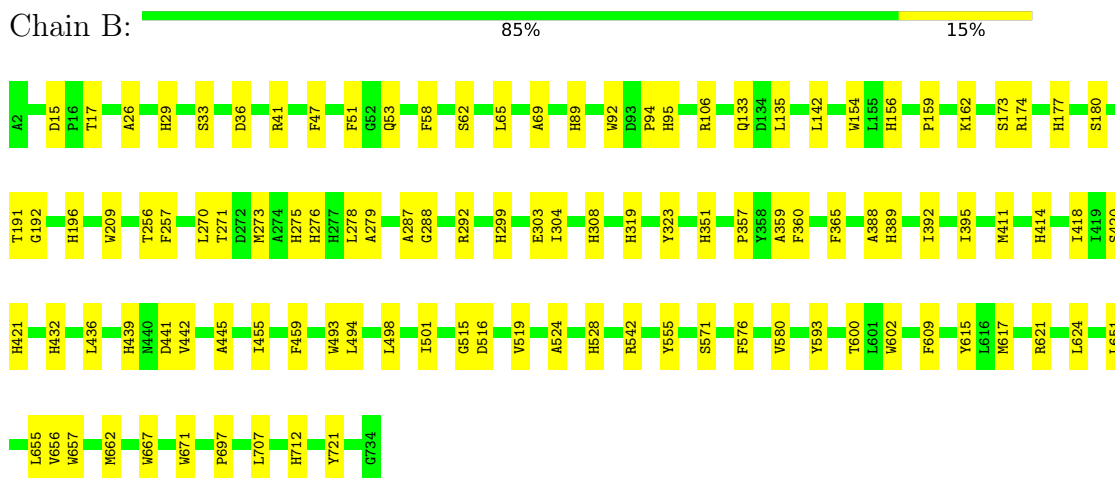
3 Residue-property plots

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.

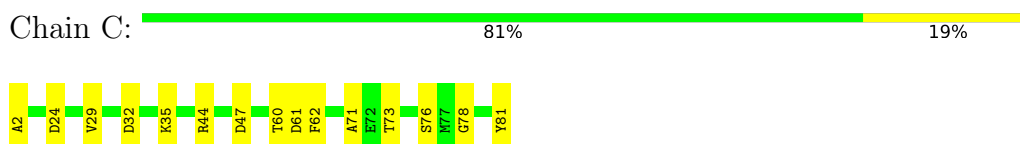
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1




- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



- Molecule 3: Photosystem I iron-sulfur center




- Molecule 4: Predicted protein PsaD

Chain D:  87% 13%




- Molecule 5: PsaE

Chain E:  85% 15%




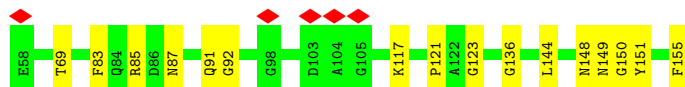
- Molecule 6: PSI-F

Chain F:  90% 10%



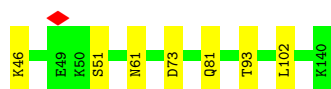
- Molecule 7: PSI-G

Chain G:  5% 84% 16%



- Molecule 8: PsaH photosystem I reaction center subunit

Chain H:  93% 7%




- Molecule 9: Photosystem I reaction center subunit VIII

Chain I:  79% 21%



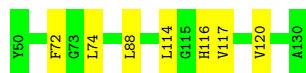
- Molecule 10: Photosystem I reaction center subunit IX

Chain J:  88% 12%




- Molecule 11: PsaK

Chain K:  91% 9%




- Molecule 12: PSI subunit V

Chain L:  89% 11%




- Molecule 13: Photosystem I reaction center subunit XII

Chain M:  81% 19%




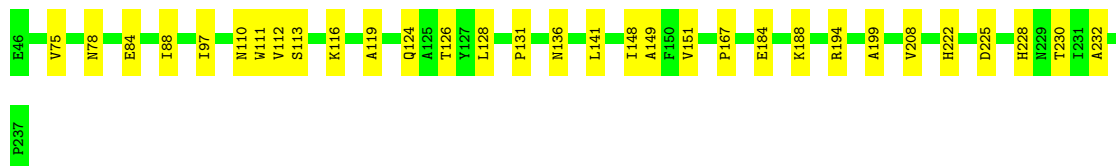
- Molecule 14: PsaO

Chain O:  79% 21%



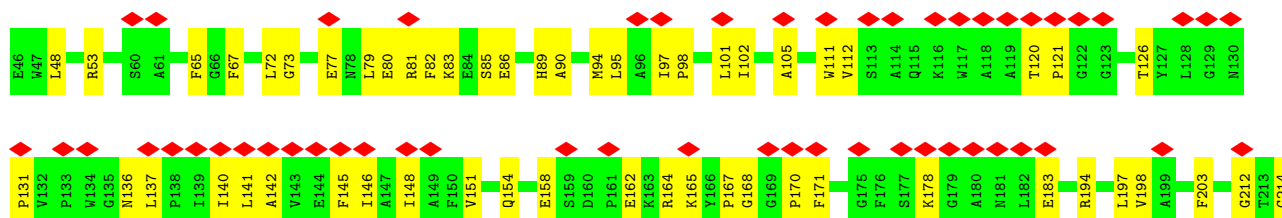
- Molecule 15: Chlorophyll a-b binding protein, chloroplastic

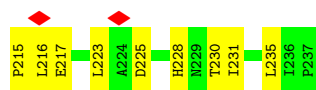
Chain 1:  84% 16%



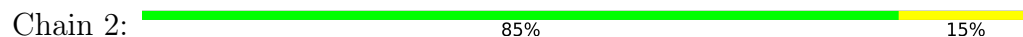
- Molecule 15: Chlorophyll a-b binding protein, chloroplastic

Chain 5:  29% 67% 33%

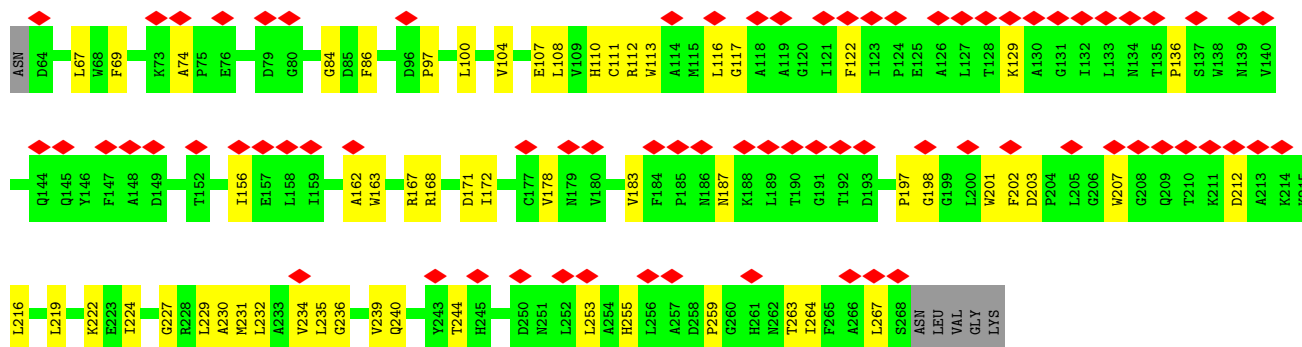




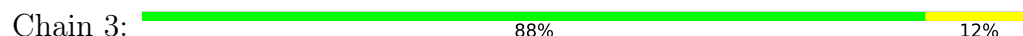
- Molecule 16: Chlorophyll a-b binding protein, chloroplastic



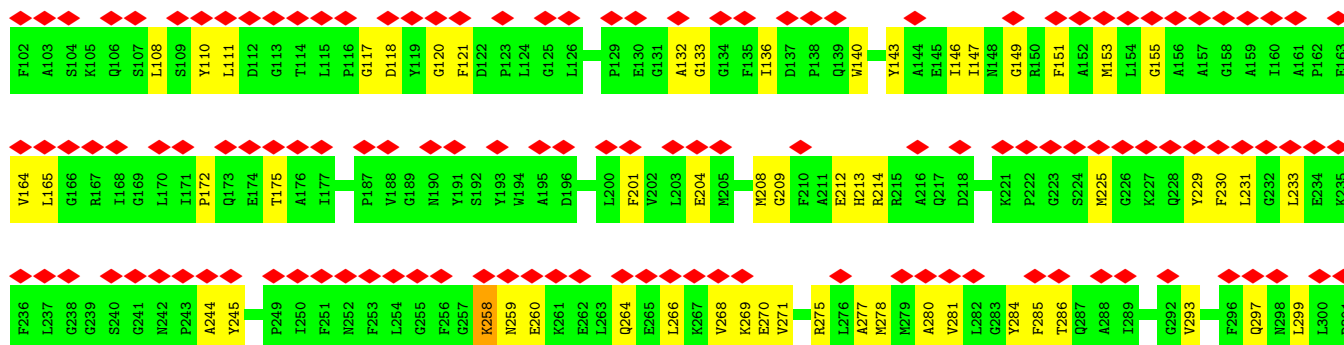
- Molecule 16: Chlorophyll a-b binding protein, chloroplastic

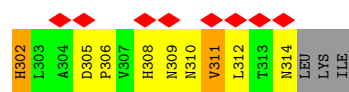


- Molecule 17: Chlorophyll a-b binding protein, chloroplastic

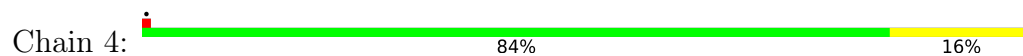


- Molecule 17: Chlorophyll a-b binding protein, chloroplastic

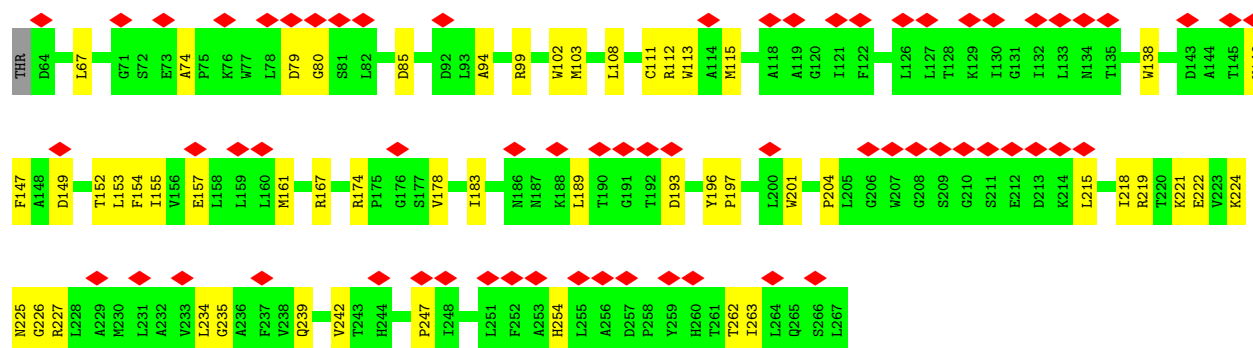
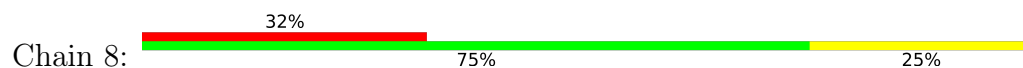




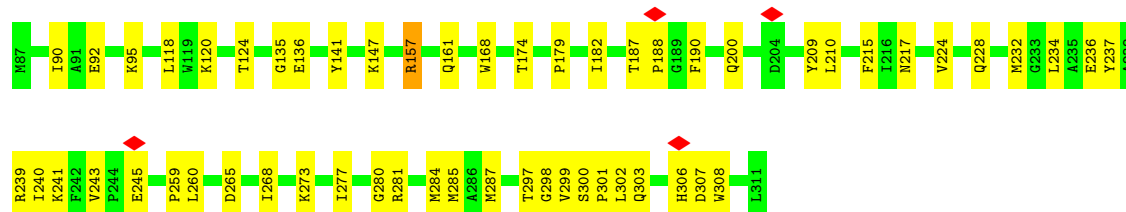
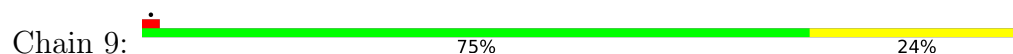
- Molecule 18: Chlorophyll a-b binding protein, chloroplastic



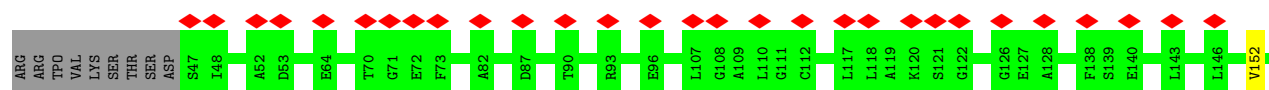
- Molecule 18: Chlorophyll a-b binding protein, chloroplastic

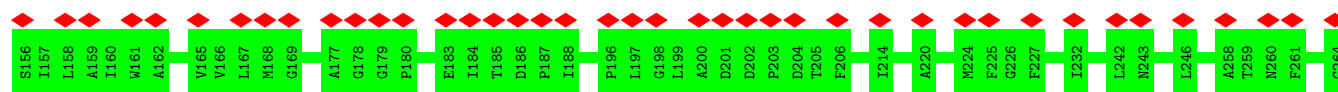


- Molecule 19: Chlorophyll a-b binding protein, chloroplastic



- Molecule 20: Chlorophyll a-b binding protein, chloroplastic





- Molecule 20: Chlorophyll a-b binding protein, chloroplastic



- Molecule 20: Chlorophyll a-b binding protein, chloroplastic



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	83777	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	78	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	4.400	Depositor
Minimum map value	-1.758	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.105	Depositor
Recommended contour level	0.45	Depositor
Map size (Å)	486.72003, 486.72003, 486.72003	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.014, 1.014, 1.014	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, LMU, LMG, TPO, PQN, CHL, XAT, LUT, DGD, SF4, CLA, BCR, NEX

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	0.28	0/6031	0.46	0/8227
2	B	0.30	0/6063	0.48	0/8274
3	C	0.28	0/605	0.55	0/821
4	D	0.28	0/1132	0.54	0/1532
5	E	0.28	0/498	0.51	0/677
6	F	0.27	0/1255	0.48	0/1696
7	G	0.28	0/767	0.50	0/1046
8	H	0.26	0/758	0.48	0/1022
9	I	0.28	0/273	0.41	0/373
10	J	0.26	0/334	0.43	0/457
11	K	0.25	0/572	0.46	0/773
12	L	0.27	0/1264	0.45	0/1727
13	M	0.28	0/239	0.42	0/322
14	O	0.26	0/729	0.47	0/997
15	1	0.28	0/1527	0.47	0/2088
15	5	0.27	0/1524	0.50	0/2084
16	2	0.29	0/1683	0.49	0/2300
16	6	0.25	0/1638	0.45	0/2241
17	3	0.30	0/1721	0.49	0/2335
17	7	0.28	0/1695	0.50	0/2302
18	4	0.26	0/1641	0.45	0/2244
18	8	0.25	0/1634	0.46	0/2234
19	9	0.29	0/1801	0.50	0/2451
20	a	0.27	0/1700	0.47	0/2316
20	b	0.27	0/1700	0.45	0/2316
20	c	0.26	0/1764	0.49	0/2399
All	All	0.28	0/40548	0.48	0/55254

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5836	0	5725	107	0
2	B	5849	0	5623	116	0
3	C	595	0	573	12	0
4	D	1104	0	1112	16	0
5	E	487	0	480	9	0
6	F	1230	0	1282	13	0
7	G	749	0	729	12	0
8	H	740	0	727	7	0
9	I	266	0	274	4	0
10	J	325	0	341	5	0
11	K	566	0	587	7	0
12	L	1229	0	1242	14	0
13	M	238	0	263	4	0
14	O	702	0	697	11	0
15	1	1478	0	1455	26	0
15	5	1475	0	1447	51	0
16	2	1632	0	1603	32	0
16	6	1587	0	1556	57	0
17	3	1670	0	1633	22	0
17	7	1644	0	1599	64	0
18	4	1592	0	1561	32	0
18	8	1585	0	1555	60	0
19	9	1747	0	1721	42	0
20	a	1651	0	1586	0	0
20	b	1651	0	1585	0	0
20	c	1727	0	1661	0	0
21	1	587	0	420	28	0
21	2	366	0	281	37	0
21	3	642	0	487	43	0
21	4	472	0	362	30	0
21	5	531	0	369	29	0
21	6	347	0	253	25	0
21	7	551	0	377	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	8	460	0	348	46	0
21	9	352	0	290	15	0
21	A	2422	0	2311	131	0
21	B	2312	0	2267	120	0
21	F	147	0	123	5	0
21	G	139	0	102	3	0
21	H	45	0	33	2	0
21	J	42	0	31	1	0
21	K	185	0	135	15	0
21	L	132	0	97	5	0
21	O	170	0	116	3	0
21	a	383	0	304	0	0
21	b	391	0	316	0	0
21	c	417	0	367	0	0
22	A	33	0	46	0	0
22	B	33	0	46	3	0
23	1	51	0	42	0	0
23	2	35	0	40	1	0
23	4	86	0	118	6	0
23	5	28	0	26	1	0
23	6	35	0	40	3	0
23	8	37	0	44	3	0
23	9	49	0	74	4	0
23	A	125	0	172	7	0
23	a	49	0	74	0	0
23	b	49	0	74	0	0
23	c	49	0	74	0	0
24	2	40	0	56	6	0
24	3	80	0	112	8	0
24	4	40	0	56	0	0
24	6	40	0	56	14	0
24	7	80	0	112	11	0
24	8	40	0	56	9	0
24	A	240	0	336	21	0
24	B	200	0	280	38	0
24	F	80	0	112	3	0
24	G	80	0	112	6	0
24	I	40	0	56	1	0
24	J	120	0	168	16	0
24	K	40	0	56	23	0
24	L	120	0	168	8	0
24	M	40	0	56	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	O	40	0	56	1	0
25	A	8	0	0	0	0
25	C	16	0	0	0	0
26	3	35	0	46	4	0
26	A	70	0	92	2	0
26	O	35	0	46	0	0
26	b	35	0	46	0	0
27	B	66	0	96	7	0
28	2	13	0	11	0	0
28	6	13	0	11	1	0
28	G	55	0	86	3	0
28	J	30	0	30	0	0
29	1	102	0	74	8	0
29	2	295	0	212	16	0
29	3	40	0	23	2	0
29	4	180	0	116	6	0
29	5	92	0	62	6	0
29	6	286	0	196	17	0
29	7	40	0	23	2	0
29	8	180	0	116	17	0
29	9	273	0	184	14	0
29	a	272	0	181	0	0
29	b	292	0	206	0	0
29	c	274	0	178	0	0
30	1	42	0	56	3	0
30	2	42	0	56	8	0
30	3	42	0	56	12	0
30	4	42	0	56	7	0
30	5	42	0	56	2	0
30	6	42	0	56	6	0
30	7	42	0	56	14	0
30	8	42	0	56	5	0
30	9	84	0	112	9	0
30	a	84	0	112	0	0
30	b	84	0	112	0	0
30	c	84	0	112	0	0
31	1	44	0	56	3	0
31	2	44	0	56	2	0
31	3	44	0	56	4	0
31	4	44	0	56	4	0
31	5	44	0	56	7	0
31	6	44	0	56	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	7	44	0	56	5	0
31	8	44	0	56	5	0
31	9	44	0	56	2	0
31	a	44	0	56	0	0
31	c	44	0	56	0	0
32	9	44	0	56	3	0
32	b	44	0	56	0	0
32	c	44	0	56	0	0
All	All	56417	0	54439	1134	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 12.

All (1134) 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)
21:3:409:CLA:C4	30:3:416:LUT:H28	1.47	1.43
21:A:852:CLA:O1D	21:B:801:CLA:H61	1.31	1.22
21:K:203:CLA:HMC1	24:K:205:BCR:H312	1.28	1.15
21:2:609:CLA:H43	30:2:616:LUT:H7	1.25	1.13
21:2:609:CLA:HBC2	21:2:609:CLA:HHD	1.30	1.10
21:K:203:CLA:CMC	24:K:205:BCR:H312	1.82	1.09
18:8:224:LYS:HG3	21:8:609:CLA:HMD3	1.18	1.08
21:3:409:CLA:H43	30:3:416:LUT:H28	1.15	1.06
21:2:609:CLA:CHB	21:2:609:CLA:H11	1.85	1.06
21:3:409:CLA:C4	30:3:416:LUT:C28	2.32	1.06
24:A:854:BCR:H353	24:K:205:BCR:H323	1.38	1.01
18:8:224:LYS:HG3	21:8:609:CLA:CMD	1.90	1.01
16:2:196:TYR:HD1	21:2:609:CLA:O1D	1.45	1.00
21:4:609:CLA:H41	30:4:615:LUT:H28	1.39	0.99
2:B:411:MET:HE2	24:B:844:BCR:H403	1.43	0.98
21:K:203:CLA:HMC1	24:K:205:BCR:C31	1.93	0.97
21:3:409:CLA:H43	30:3:416:LUT:C28	1.94	0.97
24:6:618:BCR:H312	21:8:609:CLA:HBB2	1.46	0.97
17:7:299:LEU:HD21	30:7:415:LUT:H163	1.44	0.96
21:A:802:CLA:HBB1	21:A:852:CLA:C4B	1.97	0.95
21:4:609:CLA:C4	30:4:615:LUT:H28	1.97	0.94
21:A:842:CLA:HMD2	24:B:846:BCR:H383	1.52	0.91
18:8:224:LYS:CG	21:8:609:CLA:HMD3	2.02	0.90
21:1:309:CLA:HHC	21:1:309:CLA:CBB	1.99	0.90
2:B:411:MET:CE	24:B:844:BCR:H403	2.03	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:K:203:CLA:CMC	24:K:205:BCR:C31	2.49	0.88
24:A:854:BCR:H353	24:K:205:BCR:C32	2.03	0.88
21:2:609:CLA:C4	30:2:616:LUT:H7	2.04	0.88
1:A:390:HIS:HE1	21:A:828:CLA:ND	1.71	0.87
1:A:311:THR:HG22	1:A:312:ASN:H	1.40	0.86
21:2:609:CLA:H41	30:2:616:LUT:H10	1.56	0.85
21:1:309:CLA:HHC	21:1:309:CLA:HBB1	1.56	0.85
21:A:852:CLA:O1D	21:B:801:CLA:C6	2.24	0.84
16:2:196:TYR:CD1	21:2:609:CLA:O1D	2.31	0.83
17:7:212:GLU:HG3	21:7:407:CLA:C3B	2.08	0.83
24:6:618:BCR:C31	21:8:609:CLA:HBB2	2.09	0.82
18:4:227:ARG:HB3	21:4:602:CLA:HBC3	1.59	0.82
21:2:609:CLA:HHD	21:2:609:CLA:CBC	2.10	0.82
21:3:409:CLA:CHB	21:3:409:CLA:H11	2.10	0.81
21:7:401:CLA:HMB1	21:7:402:CLA:H3A	1.60	0.81
21:2:609:CLA:CHB	21:2:609:CLA:C1	2.59	0.81
24:6:618:BCR:HC22	21:8:609:CLA:HAB	1.63	0.81
15:1:148:ILE:HG21	21:1:309:CLA:HMC3	1.62	0.81
17:7:212:GLU:HG3	21:7:407:CLA:C2B	2.11	0.80
17:7:212:GLU:HG3	21:7:407:CLA:C4B	2.13	0.79
24:A:854:BCR:C13	24:K:205:BCR:H321	2.14	0.78
21:7:402:CLA:HBC1	21:7:407:CLA:HAC1	1.67	0.77
24:A:854:BCR:C12	24:K:205:BCR:H321	2.14	0.77
21:H:201:CLA:HBB2	24:L:306:BCR:H392	1.67	0.77
16:6:219:LEU:HA	16:6:222:LYS:HE3	1.67	0.76
21:1:309:CLA:HBB1	21:1:309:CLA:CHC	2.11	0.76
21:3:409:CLA:H42	30:3:416:LUT:H28	1.63	0.76
18:8:224:LYS:HD3	21:8:609:CLA:C3D	2.16	0.76
21:2:609:CLA:C4	30:2:616:LUT:H10	2.15	0.75
24:6:618:BCR:H312	21:8:609:CLA:CBB	2.15	0.75
19:9:303:GLN:HB2	21:9:613:CLA:HED2	1.69	0.75
2:B:142:LEU:HD11	24:B:843:BCR:C40	2.16	0.74
2:B:142:LEU:HD11	24:B:843:BCR:H403	1.69	0.74
15:5:194:ARG:HB3	21:5:602:CLA:HBC3	1.68	0.74
17:7:281:VAL:HG11	31:7:416:XAT:H12	1.67	0.74
17:7:311:VAL:HG13	17:7:312:LEU:H	1.52	0.74
21:7:402:CLA:CBC	21:7:407:CLA:HAC1	2.16	0.74
30:8:614:LUT:H30	21:8:618:CLA:HAB	1.69	0.74
1:A:175:TRP:HB2	21:A:812:CLA:HMC3	1.68	0.74
21:A:842:CLA:CMD	24:B:846:BCR:H383	2.17	0.73
21:3:409:CLA:H41	30:3:416:LUT:C28	2.14	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:31:ARG:HD3	24:J:101:BCR:H312	1.70	0.73
16:6:201:TRP:HH2	29:6:614:CHL:NB	1.85	0.73
21:B:807:CLA:H72	24:B:846:BCR:H321	1.71	0.73
15:1:194:ARG:HB3	21:1:303:CLA:HBC2	1.71	0.73
18:8:224:LYS:CG	21:8:609:CLA:CMD	2.62	0.73
19:9:236:GLU:OE1	19:9:239:ARG:NH1	2.22	0.73
24:2:618:BCR:HC42	23:4:618:LHG:HC81	1.71	0.72
10:J:5:LYS:HD3	16:2:99:LEU:HD11	1.70	0.72
21:A:805:CLA:HMC3	21:A:807:CLA:HED3	1.71	0.71
18:8:227:ARG:HB3	21:8:602:CLA:HBC2	1.71	0.71
18:4:233:VAL:HG11	31:4:616:XAT:H12	1.70	0.71
1:A:455:HIS:HE1	21:A:834:CLA:NA	1.86	0.71
2:B:257:PHE:HE2	2:B:493:TRP:HE3	1.39	0.71
2:B:712:HIS:HE1	21:B:839:CLA:ND	1.88	0.71
21:3:409:CLA:H11	21:3:409:CLA:C1B	2.21	0.71
2:B:26:ALA:HB2	27:B:847:DGD:HA42	1.71	0.71
18:8:111:CYS:HB2	18:8:226:GLY:HA3	1.73	0.71
21:9:602:CLA:H52	30:9:615:LUT:H28	1.73	0.71
21:K:203:CLA:HMC2	24:K:205:BCR:H312	1.72	0.70
18:8:113:TRP:CE2	29:8:607:CHL:HED2	2.26	0.70
21:B:822:CLA:HBB1	21:B:837:CLA:H152	1.72	0.70
21:6:604:CLA:NC	24:6:618:BCR:H272	2.04	0.70
5:E:84:ARG:HH21	6:F:244:SER:H	1.40	0.70
21:A:818:CLA:HHC	21:A:818:CLA:HBB1	1.71	0.70
1:A:294:HIS:HB2	21:A:818:CLA:C1B	2.22	0.69
15:5:197:LEU:HD23	21:5:602:CLA:HMC3	1.72	0.69
29:5:606:CHL:HAB	31:5:616:XAT:H7	1.74	0.69
18:4:196:TYR:HD1	21:4:609:CLA:O1D	1.75	0.69
15:1:126:THR:H	15:1:131:PRO:HA	1.57	0.69
5:E:84:ARG:HG3	6:F:243:VAL:HG22	1.75	0.69
15:5:137:LEU:O	15:5:141:LEU:HB2	1.92	0.69
15:5:225:ASP:OD1	15:5:228:HIS:ND1	2.26	0.69
15:5:137:LEU:HA	15:5:141:LEU:HD23	1.74	0.69
17:7:117:GLY:HA3	17:7:271:VAL:HG11	1.74	0.69
21:5:602:CLA:HAB	31:5:616:XAT:H32	1.75	0.69
21:A:840:CLA:H2	21:B:831:CLA:H42	1.76	0.68
1:A:403:ALA:HB2	24:A:849:BCR:H323	1.76	0.68
1:A:117:PRO:HB3	1:A:122:LYS:HD2	1.73	0.68
18:8:221:LYS:HG2	21:8:609:CLA:OBD	1.92	0.68
1:A:683:MET:HB2	21:A:802:CLA:C1C	2.23	0.68
17:7:305:ASP:HB3	17:7:308:HIS:HB2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:3:187:PRO:HG3	21:3:401:CLA:HMD2	1.74	0.68
15:5:121:PRO:HA	15:5:137:LEU:HD21	1.75	0.68
2:B:257:PHE:CE2	2:B:493:TRP:HE3	2.10	0.67
2:B:439:HIS:HE1	21:B:832:CLA:NA	1.88	0.67
16:6:236:GLY:O	16:6:240:GLN:HG3	1.95	0.67
1:A:50:HIS:HE1	21:A:804:CLA:ND	1.93	0.67
15:5:126:THR:HG22	15:5:131:PRO:HB3	1.76	0.67
16:6:197:PRO:HG2	16:6:202:PHE:HD2	1.59	0.67
17:7:212:GLU:HG3	21:7:407:CLA:C1B	2.23	0.67
1:A:118:ILE:HG23	1:A:119:VAL:HG22	1.77	0.67
21:1:310:CLA:HAB	30:1:317:LUT:H32	1.77	0.67
16:6:156:ILE:HG12	21:8:612:CLA:HAA2	1.77	0.67
21:B:820:CLA:HMD2	24:G:201:BCR:HC7	1.77	0.67
4:D:152:ARG:NH2	4:D:182:GLU:OE2	2.28	0.67
12:L:164:LYS:NZ	12:L:167:GLU:OE1	2.28	0.67
1:A:703:HIS:HE1	21:A:840:CLA:ND	1.92	0.66
2:B:455:ILE:CD1	24:J:104:BCR:C32	2.74	0.66
21:B:837:CLA:H141	24:B:844:BCR:H15C	1.78	0.66
6:F:227:GLY:O	18:4:99:ARG:NH2	2.29	0.66
11:K:117:VAL:HG22	24:K:205:BCR:H333	1.76	0.66
14:O:75:LEU:HD22	14:O:86:ASN:HD22	1.59	0.66
24:6:618:BCR:HC22	21:8:609:CLA:CAB	2.25	0.66
21:7:402:CLA:HMD2	21:7:407:CLA:ND	2.11	0.66
18:8:239:GLN:NE2	21:8:611:CLA:O1D	2.29	0.66
2:B:174:ARG:HB2	21:B:812:CLA:HBC2	1.78	0.65
17:7:164:VAL:HG21	24:7:418:BCR:H291	1.78	0.65
21:2:609:CLA:H43	30:2:616:LUT:C7	2.17	0.65
17:7:299:LEU:HD11	30:7:415:LUT:H172	1.77	0.65
24:A:854:BCR:C11	24:K:205:BCR:C32	2.73	0.65
2:B:275:HIS:HE1	21:B:815:CLA:C4D	2.10	0.65
3:C:62:PHE:HD2	4:D:198:ILE:HG21	1.62	0.65
18:8:153:LEU:O	18:8:157:GLU:HG2	1.97	0.65
19:9:299:VAL:HG22	19:9:300:SER:H	1.61	0.65
6:F:182:ILE:HG12	21:F:304:CLA:ND	2.12	0.65
2:B:159:PRO:HA	2:B:162:LYS:HE2	1.79	0.65
2:B:542:ARG:NH2	4:D:203:ASN:OD1	2.30	0.65
16:2:234:VAL:HG11	31:2:617:XAT:H12	1.78	0.65
2:B:389:HIS:HE1	21:B:828:CLA:NA	1.93	0.65
16:6:235:LEU:HD21	21:6:603:CLA:HAB	1.77	0.65
17:3:132:ALA:HB1	17:3:138:PRO:HD3	1.77	0.64
21:3:409:CLA:H41	30:3:416:LUT:H30	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:813:CLA:HBA1	24:B:843:BCR:H393	1.79	0.64
15:5:48:LEU:HD11	29:5:601:CHL:HED3	1.78	0.64
19:9:188:PRO:O	19:9:200:GLN:NE2	2.28	0.64
18:8:67:LEU:HD11	18:8:74:ALA:HB2	1.79	0.64
29:8:605:CHL:C4A	24:8:616:BCR:H383	2.22	0.64
21:7:402:CLA:HMD2	21:7:407:CLA:C1D	2.27	0.64
17:3:281:VAL:HG11	31:3:417:XAT:H12	1.79	0.64
24:6:618:BCR:C31	21:8:609:CLA:CBB	2.75	0.64
2:B:256:THR:H	2:B:271:THR:HB	1.63	0.64
21:K:203:CLA:HMC2	24:K:205:BCR:C31	2.26	0.64
17:3:256:PHE:HB2	21:3:409:CLA:HBA1	1.80	0.64
4:D:174:HIS:HB3	4:D:175:PRO:HD3	1.78	0.64
8:H:46:LYS:NZ	12:L:71:ASN:O	2.31	0.64
21:6:610:CLA:HAB	24:7:417:BCR:H313	1.79	0.64
18:8:204:PRO:HD2	30:8:614:LUT:H23	1.80	0.64
21:A:810:CLA:HAB	21:B:832:CLA:HMD2	1.79	0.63
21:B:827:CLA:H101	24:B:842:BCR:H19C	1.80	0.63
19:9:302:LEU:O	19:9:303:GLN:HG2	1.98	0.63
6:F:182:ILE:HG12	21:F:304:CLA:C4D	2.28	0.63
21:6:604:CLA:C1B	24:6:618:BCR:H282	2.29	0.63
21:A:822:CLA:HMB2	21:A:823:CLA:H2	1.79	0.63
15:1:230:THR:HG23	15:1:232:ALA:H	1.63	0.63
16:6:229:LEU:HD22	30:6:616:LUT:H402	1.81	0.63
21:8:611:CLA:H92	21:8:611:CLA:HMC2	1.80	0.63
2:B:142:LEU:CD1	24:B:843:BCR:H403	2.29	0.62
14:O:81:PRO:HB2	14:O:84:ASN:HB2	1.81	0.62
1:A:455:HIS:HE1	21:A:834:CLA:C1A	2.11	0.62
24:A:854:BCR:C11	24:K:205:BCR:H322	2.29	0.62
16:2:112:ARG:NH1	29:2:607:CHL:OBD	2.31	0.62
21:K:202:CLA:HBA1	21:K:202:CLA:HBD	1.80	0.62
14:O:67:ILE:HG23	21:O:202:CLA:HBB2	1.82	0.62
1:A:419:GLN:HG3	1:A:422:ASN:HD21	1.63	0.62
24:B:844:BCR:H291	24:B:845:BCR:H383	1.81	0.62
21:2:604:CLA:HBA2	24:2:618:BCR:H292	1.81	0.62
19:9:120:LYS:HB2	19:9:124:THR:HA	1.80	0.62
17:3:184:VAL:HG11	31:3:417:XAT:H172	1.81	0.62
21:2:609:CLA:H11	21:2:609:CLA:C4A	2.29	0.62
18:8:161:MET:HG2	21:8:608:CLA:HMC3	1.82	0.62
22:B:841:PQN:H301	24:L:305:BCR:H343	1.80	0.62
16:2:165:GLU:HG3	21:2:608:CLA:C4B	2.30	0.62
16:2:198:GLY:HA2	21:2:609:CLA:HED3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:5:97:ILE:HG13	15:5:203:PHE:HE2	1.64	0.61
16:6:183:VAL:HG22	21:8:609:CLA:CBB	2.29	0.61
16:6:234:VAL:HG21	31:6:617:XAT:H14	1.81	0.61
21:8:603:CLA:HMC2	31:8:615:XAT:H203	1.81	0.61
21:B:824:CLA:HMB2	21:B:837:CLA:HBA1	1.81	0.61
1:A:390:HIS:HE1	21:A:828:CLA:C1D	2.13	0.61
2:B:65:LEU:HD11	24:B:843:BCR:C40	2.30	0.61
2:B:303:GLU:HG3	7:G:91:GLN:HA	1.83	0.61
17:7:281:VAL:HG12	17:7:285:PHE:HE2	1.65	0.61
17:7:212:GLU:CG	21:7:407:CLA:C1B	2.78	0.61
23:9:618:LHG:H272	23:9:618:LHG:H102	1.83	0.61
1:A:588:ASP:OD2	1:A:723:ARG:NH1	2.34	0.61
18:4:90:PRO:HB3	23:4:619:LHG:HC61	1.82	0.61
1:A:50:HIS:HE1	21:A:804:CLA:C4D	2.13	0.61
17:7:280:ALA:HB1	30:7:415:LUT:H8	1.83	0.61
21:9:612:CLA:HHC	21:9:612:CLA:HBB1	1.82	0.61
21:K:201:CLA:NA	24:K:205:BCR:C40	2.63	0.61
15:1:167:PRO:HG3	21:1:308:CLA:HMD2	1.83	0.61
18:8:201:TRP:HH2	29:8:613:CHL:NB	1.98	0.61
14:O:61:ARG:O	14:O:136:LYS:NZ	2.34	0.60
15:5:90:ALA:HA	15:5:197:LEU:HD13	1.82	0.60
21:A:803:CLA:C4B	21:B:802:CLA:HBB1	2.22	0.60
15:5:81:ARG:NH1	21:5:603:CLA:O1A	2.31	0.60
16:6:244:THR:HG22	16:6:267:LEU:HG	1.81	0.60
17:7:277:ALA:HB2	30:7:415:LUT:H202	1.81	0.60
15:1:149:ALA:CA	21:1:309:CLA:HAB	2.31	0.60
23:5:617:LHG:HC92	24:8:616:BCR:H313	1.83	0.60
1:A:317:HIS:HB3	1:A:322:ILE:HD11	1.82	0.60
18:4:198:GLY:CA	21:4:609:CLA:HED3	2.31	0.60
17:7:111:LEU:HD13	17:7:118:ASP:OD1	2.01	0.60
2:B:65:LEU:HD11	24:B:843:BCR:H402	1.83	0.60
29:2:601:CHL:H2	21:3:415:CLA:HMA2	1.84	0.60
17:3:188:VAL:HG13	26:3:420:LMU:H5'	1.82	0.60
2:B:279:ALA:HA	21:B:815:CLA:HMC3	1.82	0.60
18:8:224:LYS:CD	21:8:609:CLA:CMD	2.79	0.60
21:3:409:CLA:C4	30:3:416:LUT:H30	2.32	0.59
17:7:120:GLY:N	21:7:401:CLA:OBD	2.35	0.59
3:C:2:ALA:N	3:C:71:ALA:O	2.35	0.59
21:3:409:CLA:H41	30:3:416:LUT:C30	2.33	0.59
21:A:805:CLA:H2	21:A:812:CLA:H92	1.83	0.59
21:A:832:CLA:HMB1	21:A:832:CLA:HBB1	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:95:ASN:HB3	21:L:302:CLA:HAC1	1.84	0.59
17:7:280:ALA:CB	30:7:415:LUT:H8	2.32	0.59
19:9:302:LEU:HD22	19:9:306:HIS:HB2	1.85	0.59
21:1:304:CLA:HMD2	21:1:309:CLA:C1D	2.33	0.59
16:6:86:PHE:HB2	29:6:602:CHL:HMD1	1.85	0.59
17:7:140:TRP:HZ3	21:7:402:CLA:HBA1	1.68	0.59
16:6:67:LEU:HD11	16:6:74:ALA:HB2	1.84	0.59
19:9:285:MET:HG3	23:9:618:LHG:H281	1.84	0.59
21:9:602:CLA:H61	30:9:615:LUT:H371	1.83	0.59
21:B:831:CLA:HHC	21:B:831:CLA:HBB1	1.84	0.59
1:A:729:HIS:HE1	21:A:841:CLA:ND	2.00	0.59
1:A:293:HIS:HE1	21:A:817:CLA:C4D	2.16	0.58
17:3:261:LYS:O	17:3:265:GLU:HG2	2.03	0.58
2:B:299:HIS:HB3	2:B:304:ILE:HD11	1.85	0.58
29:2:601:CHL:HHC	29:2:601:CHL:HBB1	1.85	0.58
29:8:605:CHL:NB	24:8:616:BCR:H382	2.13	0.58
5:E:76:GLY:HA2	5:E:94:LYS:NZ	2.17	0.58
17:7:258:LYS:HD2	17:7:259:ASN:HB2	1.83	0.58
6:F:128:ASN:O	6:F:132:GLU:HG2	2.03	0.58
18:4:198:GLY:HA2	21:4:609:CLA:HED3	1.86	0.58
1:A:335:HIS:CD2	21:A:824:CLA:ND	2.72	0.58
1:A:353:ASN:ND2	21:A:806:CLA:OBD	2.33	0.58
12:L:125:VAL:HG22	12:L:140:GLY:HA3	1.84	0.58
21:5:609:CLA:HAB	30:5:615:LUT:H32	1.85	0.58
17:7:111:LEU:HD11	17:7:120:GLY:HA2	1.85	0.58
1:A:379:THR:HG21	1:A:515:VAL:HB	1.86	0.58
21:2:609:CLA:C1	21:2:609:CLA:C1B	2.81	0.58
18:4:262:THR:HG23	18:4:264:LEU:H	1.69	0.58
16:6:232:LEU:HD11	23:6:619:LHG:H272	1.86	0.58
18:4:221:LYS:HD3	21:4:611:CLA:HBA1	1.84	0.58
17:7:286:THR:HG21	21:7:411:CLA:HAC2	1.84	0.58
21:B:836:CLA:H112	21:B:836:CLA:HMC2	1.86	0.58
24:7:417:BCR:H403	24:7:418:BCR:H351	1.85	0.58
2:B:142:LEU:CD1	24:B:843:BCR:C40	2.82	0.58
2:B:275:HIS:HE1	21:B:815:CLA:ND	1.98	0.58
19:9:297:THR:HG22	19:9:298:GLY:H	1.69	0.58
2:B:292:ARG:NH1	7:G:92:GLY:O	2.37	0.57
2:B:657:TRP:CE3	21:B:801:CLA:HMA1	2.39	0.57
24:F:303:BCR:H24C	21:F:305:CLA:HMB2	1.86	0.57
21:A:803:CLA:HMB1	21:A:803:CLA:HBB1	1.86	0.57
23:A:855:LHG:H251	23:A:855:LHG:HC92	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:838:CLA:HBB1	21:A:838:CLA:HMB1	1.86	0.57
7:G:155:PHE:HB2	15:1:119:ALA:HB1	1.86	0.57
19:9:90:ILE:HG13	19:9:260:LEU:HD23	1.86	0.57
16:6:207:TRP:HE3	30:6:616:LUT:H22	1.69	0.57
2:B:133:GLN:HE21	13:M:2:THR:HB	1.70	0.57
7:G:144:LEU:O	7:G:148:ASN:ND2	2.36	0.57
29:6:602:CHL:HBA1	31:6:617:XAT:H241	1.86	0.57
2:B:442:VAL:HG21	21:B:832:CLA:HAC2	1.85	0.57
18:8:183:ILE:HG13	24:8:616:BCR:H332	1.86	0.57
18:8:218:ILE:O	18:8:222:GLU:HG2	2.05	0.57
19:9:168:TRP:CD1	29:9:609:CHL:HMD3	2.40	0.57
1:A:198:HIS:CD2	21:A:814:CLA:NB	2.72	0.57
21:A:821:CLA:HMB2	21:A:825:CLA:HMA3	1.86	0.57
21:B:827:CLA:H43	24:B:842:BCR:H393	1.85	0.57
21:B:835:CLA:HMB1	21:B:835:CLA:HBB1	1.86	0.57
16:2:154:PHE:HB2	29:2:606:CHL:HBC1	1.85	0.57
21:2:609:CLA:CGA	30:2:616:LUT:H41	2.34	0.57
15:5:89:HIS:CD2	21:5:603:CLA:NB	2.73	0.57
1:A:294:HIS:NE2	21:A:818:CLA:NC	2.52	0.57
21:A:819:CLA:H92	21:A:829:CLA:H91	1.87	0.57
29:5:601:CHL:HHC	29:5:601:CHL:HBB1	1.86	0.57
21:7:404:CLA:HAA1	24:7:417:BCR:H21C	1.86	0.57
18:8:112:ARG:NH1	29:8:607:CHL:OBD	2.34	0.57
1:A:683:MET:HB2	21:A:802:CLA:NC	2.19	0.57
21:A:810:CLA:HBB1	24:J:103:BCR:H23C	1.86	0.57
24:A:846:BCR:H362	24:A:847:BCR:H21C	1.87	0.57
28:G:206:LMG:H301	29:1:307:CHL:H11	1.87	0.57
21:K:201:CLA:HED1	24:K:205:BCR:C38	2.35	0.57
29:1:302:CHL:HHC	29:1:302:CHL:HBB1	1.87	0.57
18:8:224:LYS:HD3	21:8:609:CLA:C2D	2.34	0.57
1:A:199:LEU:HD12	1:A:203:LEU:HD12	1.87	0.56
1:A:405:HIS:HE1	21:A:830:CLA:NA	2.01	0.56
2:B:65:LEU:CD1	24:B:843:BCR:H401	2.35	0.56
18:4:189:LEU:HD22	18:4:199:GLY:HA3	1.87	0.56
21:A:806:CLA:H61	24:A:847:BCR:HC8	1.86	0.56
18:8:224:LYS:HD3	21:8:609:CLA:CAD	2.35	0.56
21:A:827:CLA:HBB1	21:A:827:CLA:HMB1	1.87	0.56
2:B:36:ASP:O	2:B:41:ARG:NH1	2.39	0.56
16:6:84:GLY:HA3	16:6:224:ILE:HD11	1.87	0.56
16:2:252:LEU:HD13	21:2:613:CLA:HBC2	1.87	0.56
7:G:85:ARG:NH2	7:G:123:GLY:O	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:4:196:TYR:CD1	21:4:609:CLA:O1D	2.56	0.56
16:6:235:LEU:HD13	31:6:617:XAT:H401	1.87	0.56
21:7:407:CLA:HMB1	21:7:407:CLA:HBB1	1.88	0.56
1:A:91:HIS:HE1	21:A:808:CLA:NA	1.99	0.56
1:A:360:LEU:HD11	21:A:819:CLA:H71	1.87	0.56
21:B:834:CLA:HMB1	21:B:834:CLA:HBB1	1.86	0.56
2:B:439:HIS:HE1	21:B:832:CLA:C1A	2.19	0.56
21:2:610:CLA:HBC3	23:2:619:LHG:H242	1.88	0.56
16:6:97:PRO:HA	16:6:100:LEU:HD13	1.88	0.56
2:B:455:ILE:CD1	24:J:104:BCR:H321	2.36	0.55
21:B:836:CLA:HBB1	21:B:836:CLA:HMB1	1.87	0.55
6:F:202:LYS:NZ	6:F:207:ASP:OD2	2.38	0.55
21:9:604:CLA:HBB1	21:9:604:CLA:HMB1	1.88	0.55
32:9:617:NEX:H192	32:9:617:NEX:H183	1.89	0.55
21:A:852:CLA:HHB	21:B:801:CLA:H202	1.87	0.55
24:A:854:BCR:C12	24:K:205:BCR:C32	2.85	0.55
15:1:149:ALA:HB2	21:1:309:CLA:HAB	1.88	0.55
1:A:54:HIS:HE1	21:A:805:CLA:C1C	2.19	0.55
17:3:245:TYR:HD1	21:3:409:CLA:O1D	1.90	0.55
18:4:204:PRO:HD2	30:4:615:LUT:H23	1.88	0.55
15:5:85:SER:OG	21:5:603:CLA:HAA1	2.07	0.55
2:B:600:THR:HG21	2:B:609:PHE:HB2	1.87	0.55
18:8:221:LYS:HD3	21:8:610:CLA:HBA2	1.88	0.55
29:3:407:CHL:HHC	29:3:407:CHL:HBB1	1.88	0.55
29:8:605:CHL:HMB2	24:8:616:BCR:H373	1.89	0.55
21:9:611:CLA:HBC1	23:9:618:LHG:H292	1.88	0.55
30:5:615:LUT:H12	30:5:615:LUT:H191	1.88	0.54
17:7:151:PHE:CD1	21:7:407:CLA:HBC3	2.41	0.54
21:A:816:CLA:HBB1	21:A:816:CLA:HMB1	1.90	0.54
21:3:409:CLA:H41	30:3:416:LUT:H28	1.62	0.54
15:5:112:VAL:HG21	15:5:212:GLY:H	1.71	0.54
21:7:404:CLA:HBB1	21:7:407:CLA:HMC1	1.89	0.54
1:A:302:PHE:HE1	21:A:821:CLA:HAB	1.72	0.54
1:A:703:HIS:HE1	21:A:840:CLA:C4D	2.20	0.54
21:A:840:CLA:H92	21:B:831:CLA:H43	1.90	0.54
24:A:854:BCR:C35	24:K:205:BCR:C32	2.80	0.54
21:B:822:CLA:HAB	21:B:829:CLA:HMD2	1.88	0.54
21:B:832:CLA:HMB1	21:B:832:CLA:HBB1	1.89	0.54
24:K:205:BCR:H391	21:9:611:CLA:H43	1.89	0.54
1:A:31:HIS:NE2	21:A:812:CLA:O1A	2.41	0.54
21:A:801:CLA:HMB3	21:A:852:CLA:OBD	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:819:CLA:HAB	21:A:819:CLA:H8	1.89	0.54
2:B:524:ALA:HB2	21:B:836:CLA:HMA1	1.90	0.54
15:5:158:GLU:HB2	15:5:164:ARG:HD3	1.89	0.54
19:9:265:ASP:HB3	19:9:268:ILE:HG12	1.88	0.54
19:9:300:SER:HB2	19:9:301:PRO:HD3	1.90	0.54
2:B:721:TYR:HB2	21:B:801:CLA:HED2	1.89	0.54
28:6:615:LMG:HC3	19:9:147:LYS:HE2	1.90	0.54
18:8:224:LYS:HA	18:8:227:ARG:HD2	1.90	0.54
1:A:532:LEU:O	1:A:536:ILE:HG12	2.08	0.53
1:A:538:ALA:HB2	21:A:838:CLA:HMA1	1.91	0.53
17:7:212:GLU:CG	21:7:407:CLA:C2B	2.86	0.53
1:A:530:ASP:HA	1:A:533:VAL:HG12	1.90	0.53
17:7:121:PHE:N	21:7:401:CLA:OBD	2.41	0.53
19:9:168:TRP:CE2	29:9:608:CHL:HED2	2.43	0.53
1:A:534:HIS:HD2	21:A:837:CLA:C1B	2.21	0.53
21:A:825:CLA:HBA1	21:A:829:CLA:H203	1.90	0.53
2:B:516:ASP:OD1	2:B:593:TYR:OH	2.21	0.53
21:5:605:CLA:HBC3	29:5:606:CHL:HBC2	1.89	0.53
21:7:402:CLA:HBC1	21:7:407:CLA:CAC	2.37	0.53
18:8:138:TRP:CH2	18:8:247:PRO:HD3	2.43	0.53
2:B:180:SER:HB3	21:B:819:CLA:HAC2	1.90	0.53
14:O:92:PHE:HE1	14:O:116:TRP:HD1	1.55	0.53
23:4:618:LHG:O4	23:4:618:LHG:O2	2.23	0.53
2:B:455:ILE:HD12	24:J:104:BCR:C32	2.37	0.53
21:O:203:CLA:H3A	21:O:203:CLA:H11	1.89	0.53
29:4:614:CHL:HHC	29:4:614:CHL:HBB1	1.90	0.53
19:9:174:THR:HG23	21:9:604:CLA:HMC3	1.91	0.53
16:6:167:ARG:HH11	16:6:178:VAL:HB	1.74	0.53
7:G:149:ASN:ND2	21:G:202:CLA:OBD	2.41	0.53
21:2:604:CLA:C1C	24:2:618:BCR:H272	2.38	0.53
15:5:72:LEU:HD22	21:5:602:CLA:H42	1.90	0.53
17:7:155:GLY:HA2	31:7:416:XAT:H181	1.91	0.53
17:7:209:GLY:O	17:7:213:HIS:ND1	2.41	0.53
21:1:312:CLA:HHC	21:1:312:CLA:HBB1	1.91	0.53
15:5:111:TRP:CH2	15:5:203:PHE:HB3	2.44	0.53
19:9:179:PRO:HA	19:9:182:ILE:HG12	1.90	0.53
2:B:414:HIS:CD2	21:B:829:CLA:NA	2.77	0.52
21:B:806:CLA:HMB1	21:B:806:CLA:HBB1	1.90	0.52
3:C:24:ASP:OD2	3:C:44:ARG:NH2	2.36	0.52
15:1:149:ALA:HA	21:1:309:CLA:HAB	1.90	0.52
18:4:69:LEU:HD13	21:4:601:CLA:HMA3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:7:402:CLA:HBC2	21:7:407:CLA:HAC1	1.90	0.52
29:9:607:CHL:HHC	29:9:607:CHL:HBB1	1.91	0.52
21:F:302:CLA:O1D	21:F:302:CLA:H2A	2.09	0.52
21:K:201:CLA:HED1	24:K:205:BCR:H383	1.92	0.52
16:2:165:GLU:HG3	21:2:608:CLA:NB	2.24	0.52
29:2:614:CHL:HHC	29:2:614:CHL:HBB1	1.90	0.52
15:5:228:HIS:NE2	18:8:147:PHE:O	2.41	0.52
1:A:293:HIS:HE1	21:A:817:CLA:ND	2.05	0.52
2:B:65:LEU:CD1	24:B:843:BCR:C40	2.88	0.52
2:B:707:LEU:HD22	27:B:847:DGD:HB22	1.91	0.52
15:5:98:PRO:HA	15:5:101:LEU:HG	1.90	0.52
16:6:116:LEU:HB3	21:6:604:CLA:HBB2	1.91	0.52
2:B:26:ALA:HA	21:B:828:CLA:H43	1.92	0.52
2:B:58:PHE:HD1	2:B:142:LEU:HD22	1.75	0.52
2:B:142:LEU:CG	24:B:843:BCR:H403	2.39	0.52
2:B:351:HIS:CD2	21:B:825:CLA:NC	2.77	0.52
1:A:54:HIS:HE1	21:A:805:CLA:NC	2.05	0.52
1:A:91:HIS:HE1	21:A:808:CLA:C1A	2.23	0.52
21:2:609:CLA:C1B	21:2:609:CLA:H12	2.40	0.52
18:8:224:LYS:HD3	21:8:609:CLA:CMD	2.39	0.52
17:7:269:LYS:HD3	21:7:410:CLA:HAA2	1.92	0.52
24:G:201:BCR:H362	24:G:205:BCR:H312	1.91	0.52
10:J:12:PRO:HB2	24:J:101:BCR:H391	1.92	0.52
16:6:197:PRO:HB3	29:6:607:CHL:HBC2	1.92	0.52
15:5:231:ILE:HG22	15:5:235:LEU:HG	1.91	0.52
19:9:243:VAL:HG12	19:9:245:GLU:H	1.73	0.52
1:A:179:HIS:HE1	21:A:812:CLA:NA	2.08	0.52
16:2:197:PRO:HD2	21:2:609:CLA:OBD	2.10	0.52
29:2:601:CHL:HMD2	24:3:418:BCR:H323	1.91	0.52
21:2:604:CLA:NC	24:2:618:BCR:H272	2.24	0.52
17:3:112:ASP:OD1	17:3:113:GLY:N	2.43	0.52
19:9:215:PHE:O	19:9:217:ASN:N	2.43	0.52
21:A:841:CLA:HBA1	21:A:841:CLA:HBD	1.93	0.51
18:4:167:ARG:HD3	29:4:607:CHL:HBB1	1.92	0.51
15:5:102:ILE:HD12	21:5:604:CLA:HAC2	1.93	0.51
19:9:287:MET:HG3	30:9:615:LUT:H12	1.92	0.51
1:A:118:ILE:HD13	24:J:101:BCR:H313	1.93	0.51
9:I:29:TYR:HH	13:M:31:TYR:HH	1.56	0.51
2:B:69:ALA:HB2	2:B:135:LEU:HB2	1.92	0.51
16:6:104:VAL:HA	16:6:107:GLU:HG2	1.92	0.51
29:8:605:CHL:H3A	24:8:616:BCR:C21	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:L:304:CLA:HMB1	21:L:304:CLA:HBB1	1.92	0.51
15:1:97:ILE:HD11	30:1:317:LUT:H15	1.92	0.51
18:8:138:TRP:HH2	18:8:247:PRO:HD3	1.75	0.51
18:8:215:LEU:HD13	18:8:219:ARG:HE	1.76	0.51
21:A:827:CLA:C4D	21:A:835:CLA:HMB1	2.40	0.51
21:B:814:CLA:H121	24:G:201:BCR:H21C	1.93	0.51
21:B:825:CLA:HMB1	21:B:825:CLA:HBB1	1.93	0.51
29:1:307:CHL:HHC	29:1:307:CHL:HBB1	1.92	0.51
2:B:436:LEU:CD1	24:J:104:BCR:H311	2.40	0.51
2:B:515:GLY:O	2:B:519:VAL:HG23	2.10	0.51
11:K:116:HIS:CD2	21:K:203:CLA:NC	2.78	0.51
21:3:404:CLA:C4B	24:3:418:BCR:H281	2.30	0.51
17:7:266:LEU:O	17:7:270:GLU:HG2	2.11	0.51
21:9:610:CLA:HBB1	21:9:610:CLA:HMB1	1.92	0.51
15:1:208:VAL:HG23	21:1:315:CLA:HBC3	1.92	0.51
16:6:122:PHE:CE2	30:6:616:LUT:H28	2.46	0.51
21:A:809:CLA:HMC3	21:A:810:CLA:HMD2	1.92	0.51
21:A:827:CLA:C4A	21:A:835:CLA:HMB2	2.33	0.51
24:J:103:BCR:H12C	24:J:103:BCR:H341	1.91	0.51
15:5:80:GLU:HA	15:5:83:LYS:HE3	1.92	0.51
1:A:503:THR:HG21	21:A:827:CLA:HAB	1.92	0.50
21:3:408:CLA:HMB2	21:3:415:CLA:C4B	2.41	0.50
19:9:259:PRO:HD2	30:9:614:LUT:H23	1.91	0.50
1:A:582:CYS:HB2	2:B:667:TRP:HB3	1.94	0.50
8:H:93:THR:O	12:L:193:ALA:HB1	2.11	0.50
21:3:404:CLA:C4A	24:3:418:BCR:H271	2.41	0.50
2:B:411:MET:CE	24:B:844:BCR:C40	2.86	0.50
16:6:201:TRP:CE2	29:6:614:CHL:ND	2.79	0.50
18:8:108:LEU:HD21	18:8:196:TYR:CZ	2.47	0.50
23:8:617:LHG:H302	23:8:617:LHG:H141	1.93	0.50
19:9:307:ASP:OD2	19:9:308:TRP:N	2.44	0.50
1:A:448:HIS:HE1	21:A:833:CLA:C1A	2.25	0.50
21:B:824:CLA:HMA1	24:B:845:BCR:H14C	1.94	0.50
4:D:161:PHE:CE2	4:D:174:HIS:HB2	2.46	0.50
15:5:95:LEU:HB3	21:5:604:CLA:HBB2	1.93	0.50
16:6:255:HIS:CD2	21:6:613:CLA:NC	2.79	0.50
29:9:605:CHL:HHC	29:9:605:CHL:HBB1	1.94	0.50
2:B:142:LEU:HD11	24:B:843:BCR:H402	1.94	0.50
16:6:227:GLY:O	16:6:231:MET:HG3	2.12	0.50
21:6:604:CLA:HBA2	24:6:618:BCR:H292	1.93	0.50
2:B:436:LEU:HD11	24:J:104:BCR:H311	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:818:CLA:HMB2	21:B:823:CLA:HMA3	1.92	0.50
18:4:113:TRP:CE2	29:4:607:CHL:HED2	2.47	0.50
21:5:605:CLA:HMC2	31:5:616:XAT:H183	1.92	0.50
16:6:110:HIS:CE1	21:6:603:CLA:NA	2.80	0.50
1:A:534:HIS:HD2	21:A:837:CLA:NB	2.05	0.50
1:A:559:ARG:O	4:D:140:ARG:NH1	2.45	0.50
2:B:92:TRP:CZ3	2:B:94:PRO:HG3	2.47	0.50
2:B:667:TRP:O	2:B:671:TRP:HD1	1.95	0.50
21:B:827:CLA:H161	24:B:843:BCR:H361	1.93	0.50
29:9:601:CHL:HED1	30:9:615:LUT:H362	1.92	0.50
24:L:305:BCR:H403	24:L:305:BCR:H23C	1.93	0.50
21:3:404:CLA:NA	24:3:418:BCR:H271	2.27	0.50
18:4:198:GLY:HA2	21:4:609:CLA:CED	2.42	0.50
21:8:604:CLA:HMB3	31:8:615:XAT:H22	1.93	0.50
19:9:209:TYR:CD1	19:9:210:LEU:HD23	2.47	0.50
15:1:75:VAL:HB	15:1:78:ASN:HB2	1.94	0.49
21:3:402:CLA:HAB	31:3:417:XAT:H32	1.92	0.49
16:6:162:ALA:HA	21:6:608:CLA:HBB1	1.94	0.49
29:6:606:CHL:HHC	29:6:606:CHL:HBB1	1.94	0.49
26:A:856:LMU:H3B	26:3:420:LMU:H4'	1.94	0.49
2:B:319:HIS:CD2	21:B:822:CLA:ND	2.80	0.49
5:E:82:LEU:HD11	5:E:131:GLU:HG3	1.94	0.49
12:L:62:GLU:N	14:O:140:ASP:O	2.45	0.49
1:A:582:CYS:HB3	2:B:667:TRP:HE3	1.77	0.49
21:B:823:CLA:HMC1	21:B:823:CLA:HBC2	1.94	0.49
15:1:149:ALA:CB	21:1:309:CLA:HAB	2.43	0.49
29:2:606:CHL:HHC	29:2:606:CHL:HBB1	1.93	0.49
19:9:135:GLY:O	19:9:136:GLU:HG2	2.11	0.49
21:A:830:CLA:HMB1	21:A:830:CLA:HBB1	1.94	0.49
2:B:528:HIS:CD2	21:B:837:CLA:NB	2.79	0.49
21:B:827:CLA:H142	24:B:843:BCR:C37	2.42	0.49
17:7:230:PHE:HD2	17:7:233:LEU:HB2	1.77	0.49
21:B:813:CLA:HBA1	24:B:843:BCR:C39	2.41	0.49
1:A:264:LEU:HD21	11:K:120:VAL:HG22	1.94	0.49
21:4:602:CLA:CHB	21:4:602:CLA:H11	2.42	0.49
21:6:610:CLA:HMB1	17:7:231:LEU:HD11	1.95	0.49
15:1:222:HIS:CD2	21:1:314:CLA:NC	2.80	0.49
21:5:603:CLA:HMD2	21:5:608:CLA:C1D	2.43	0.49
16:6:69:PHE:CE1	21:7:414:CLA:HMD3	2.48	0.49
16:6:113:TRP:CE2	29:6:607:CHL:HED2	2.47	0.49
16:6:163:TRP:HE1	16:6:167:ARG:HH21	1.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:840:CLA:HMB1	21:B:840:CLA:HBB1	1.94	0.49
29:6:614:CHL:HHC	29:6:614:CHL:HBB1	1.95	0.49
21:A:840:CLA:HAB	21:A:840:CLA:H93	1.94	0.49
4:D:140:ARG:NH2	4:D:142:GLU:OE1	2.46	0.49
21:9:611:CLA:H41	21:9:611:CLA:H61	1.55	0.49
1:A:559:ARG:NH2	4:D:94:THR:O	2.45	0.49
16:2:272:GLY:HA2	17:3:186:PRO:HG2	1.93	0.49
29:6:605:CHL:HHC	29:6:605:CHL:HBB1	1.95	0.49
1:A:317:HIS:HE1	21:A:822:CLA:C4A	2.25	0.48
24:A:854:BCR:C13	24:K:205:BCR:C32	2.89	0.48
2:B:624:LEU:HD22	21:B:801:CLA:CMD	2.43	0.48
21:4:601:CLA:HBB1	23:4:618:LHG:H262	1.94	0.48
16:6:122:PHE:CZ	30:6:616:LUT:H28	2.48	0.48
23:6:619:LHG:HC81	24:7:417:BCR:H333	1.94	0.48
1:A:393:TRP:HB3	21:A:828:CLA:HMC3	1.95	0.48
21:3:401:CLA:HMB1	21:3:401:CLA:HBB1	1.94	0.48
21:A:826:CLA:HAA2	21:A:827:CLA:OBD	2.13	0.48
18:4:254:HIS:CD2	21:4:613:CLA:NC	2.81	0.48
16:6:187:ASN:HB3	29:6:614:CHL:C2D	2.43	0.48
21:6:604:CLA:C1C	24:6:618:BCR:H272	2.43	0.48
18:8:225:ASN:OD1	30:8:614:LUT:H201	2.14	0.48
1:A:216:HIS:HE1	21:A:816:CLA:C4D	2.27	0.48
1:A:262:PHE:HA	21:K:203:CLA:HBC3	1.94	0.48
24:A:854:BCR:H23C	11:K:114:LEU:HD13	1.95	0.48
21:B:831:CLA:HBC3	21:B:831:CLA:HHD	1.95	0.48
16:6:212:ASP:OD1	16:6:216:LEU:N	2.46	0.48
17:7:132:ALA:HA	17:7:136:ILE:HD12	1.95	0.48
18:8:215:LEU:HB2	18:8:219:ARG:HE	1.78	0.48
2:B:411:MET:HE3	24:B:844:BCR:H403	1.92	0.48
21:4:602:CLA:HBC1	23:4:618:LHG:H252	1.96	0.48
21:4:609:CLA:HBB1	21:4:609:CLA:HMB1	1.95	0.48
15:5:136:ASN:O	15:5:140:ILE:HG12	2.13	0.48
16:6:112:ARG:HB3	29:6:607:CHL:HED1	1.95	0.48
17:7:260:GLU:O	17:7:264:GLN:HG2	2.13	0.48
17:7:281:VAL:HG12	17:7:285:PHE:CE2	2.46	0.48
18:8:224:LYS:CG	21:8:609:CLA:HMD1	2.44	0.48
21:8:602:CLA:H93	21:8:603:CLA:HMB3	1.96	0.48
1:A:450:PHE:HD2	21:B:802:CLA:H61	1.79	0.48
1:A:657:ILE:HD12	2:B:621:ARG:HG3	1.94	0.48
2:B:29:HIS:HE1	21:B:803:CLA:C4B	2.27	0.48
24:J:104:BCR:HC8	24:J:104:BCR:H331	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:8:94:ALA:HB2	21:8:602:CLA:HBA1	1.95	0.48
18:8:149:ASP:HB3	18:8:152:THR:HG23	1.96	0.48
1:A:311:THR:HG22	1:A:312:ASN:N	2.19	0.48
2:B:441:ASP:OD1	2:B:615:TYR:HB2	2.14	0.48
21:2:609:CLA:CBC	21:2:609:CLA:CHD	2.78	0.48
1:A:118:ILE:HG13	1:A:119:VAL:HG13	1.94	0.48
2:B:173:SER:O	2:B:177:HIS:HD2	1.97	0.48
2:B:323:TYR:CE1	21:B:823:CLA:HBC1	2.49	0.48
3:C:60:THR:O	3:C:61:ASP:C	2.51	0.48
2:B:411:MET:HE2	24:B:844:BCR:C40	2.28	0.48
29:2:602:CHL:HBB1	29:2:602:CHL:HHC	1.96	0.48
21:5:602:CLA:HAB	31:5:616:XAT:C32	2.44	0.48
17:7:245:TYR:OH	21:7:408:CLA:H2A	2.13	0.48
19:9:297:THR:HG22	19:9:298:GLY:N	2.29	0.48
21:A:818:CLA:H62	21:A:818:CLA:H41	1.62	0.47
21:B:839:CLA:H192	12:L:157:ILE:HD13	1.96	0.47
5:E:101:ALA:HB3	5:E:104:VAL:HG23	1.95	0.47
21:2:609:CLA:C4B	21:2:609:CLA:H42	2.44	0.47
18:4:202:PHE:HB3	21:4:609:CLA:HMD1	1.94	0.47
1:A:380:ASP:OD2	1:A:383:THR:OG1	2.32	0.47
21:A:840:CLA:H92	21:B:831:CLA:H11	1.95	0.47
2:B:276:HIS:HB2	21:B:816:CLA:C1B	2.44	0.47
21:3:408:CLA:HBB1	21:3:408:CLA:HHC	1.96	0.47
19:9:118:LEU:HB3	19:9:124:THR:HG21	1.96	0.47
1:A:511:ASP:OD1	1:A:511:ASP:N	2.47	0.47
16:2:156:ILE:HG12	21:4:613:CLA:HAA2	1.96	0.47
21:2:609:CLA:HMB1	21:2:609:CLA:HBB1	1.96	0.47
21:3:409:CLA:HBB1	21:3:409:CLA:HMB1	1.96	0.47
17:7:117:GLY:HA2	17:7:268:VAL:HG23	1.95	0.47
2:B:192:GLY:O	2:B:196:HIS:HB2	2.13	0.47
3:C:61:ASP:HB2	5:E:123:ASN:ND2	2.29	0.47
17:3:302:HIS:CD2	21:3:413:CLA:NC	2.81	0.47
21:B:809:CLA:HBA1	21:B:809:CLA:H3A	1.68	0.47
21:3:404:CLA:CHC	24:3:418:BCR:H393	2.45	0.47
17:7:143:TYR:O	17:7:147:ILE:HG12	2.14	0.47
18:8:224:LYS:CD	21:8:609:CLA:C2D	2.93	0.47
21:1:304:CLA:HMB1	21:1:304:CLA:HBB1	1.97	0.47
16:6:183:VAL:HG22	21:8:609:CLA:HBB1	1.94	0.47
21:6:603:CLA:HMD2	21:6:608:CLA:C1D	2.44	0.47
1:A:50:HIS:CE1	21:A:804:CLA:C4D	2.97	0.47
1:A:133:GLN:OE1	6:F:113:ARG:NH2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:842:CLA:HMC2	21:B:838:CLA:H11	1.97	0.47
21:A:852:CLA:HMB1	21:A:852:CLA:HBB1	1.97	0.47
26:A:856:LMU:O4'	26:3:420:LMU:O6'	2.27	0.47
2:B:287:ALA:HB2	21:B:818:CLA:HBC2	1.97	0.47
21:B:807:CLA:H11	21:B:826:CLA:HBA2	1.96	0.47
21:B:813:CLA:H3A	24:B:843:BCR:H393	1.96	0.47
21:4:609:CLA:H12	21:4:609:CLA:CHB	2.45	0.47
21:7:413:CLA:HBB1	21:7:413:CLA:HMB1	1.97	0.47
18:8:80:GLY:HA2	18:8:85:ASP:HB3	1.95	0.47
31:9:616:XAT:H11	31:9:616:XAT:H191	1.76	0.47
21:A:820:CLA:HBB1	24:A:854:BCR:H14C	1.97	0.47
21:8:609:CLA:HBB1	21:8:609:CLA:HMB1	1.96	0.47
2:B:662:MET:HB2	21:B:802:CLA:C1C	2.45	0.47
16:6:117:GLY:HA3	31:6:617:XAT:H10	1.96	0.47
21:6:604:CLA:HMA1	31:6:617:XAT:H41	1.97	0.47
18:8:197:PRO:HB3	29:8:607:CHL:HBC2	1.97	0.47
30:8:614:LUT:H30	21:8:618:CLA:CAB	2.41	0.47
1:A:25:LYS:HB2	21:A:812:CLA:HAA2	1.97	0.47
21:A:801:CLA:C1A	21:B:801:CLA:HAB	2.45	0.47
2:B:498:LEU:HA	2:B:501:ILE:HG22	1.96	0.47
21:B:804:CLA:H3A	21:B:804:CLA:HBA1	1.31	0.47
3:C:47:ASP:OD2	4:D:141:LYS:NZ	2.44	0.47
29:2:614:CHL:HBB2	24:2:618:BCR:H321	1.96	0.47
15:5:154:GLN:HE22	21:5:607:CLA:C4C	2.28	0.47
17:7:284:TYR:HE1	30:7:415:LUT:H21	1.78	0.47
18:8:99:ARG:O	18:8:103:MET:HG2	2.14	0.47
1:A:294:HIS:CD2	1:A:298:ILE:HG12	2.50	0.46
21:A:825:CLA:H143	21:A:825:CLA:H161	1.76	0.46
2:B:459:PHE:CD1	21:F:305:CLA:HMC2	2.50	0.46
29:2:602:CHL:H3A	29:2:602:CHL:HBA2	1.60	0.46
29:4:606:CHL:HHC	29:4:606:CHL:HBB1	1.97	0.46
24:A:854:BCR:H402	11:K:114:LEU:HD22	1.97	0.46
21:B:809:CLA:H92	12:L:143:ALA:HA	1.97	0.46
21:B:812:CLA:H151	21:B:827:CLA:HMD2	1.96	0.46
28:G:206:LMG:H122	29:1:307:CHL:H12	1.97	0.46
11:K:72:PHE:O	11:K:74:LEU:N	2.45	0.46
16:6:219:LEU:HB3	21:6:609:CLA:HMA1	1.96	0.46
21:6:609:CLA:HBB1	21:6:611:CLA:H3A	1.96	0.46
18:8:224:LYS:HE2	21:8:609:CLA:C2D	2.45	0.46
18:8:254:HIS:CD2	21:8:612:CLA:NC	2.82	0.46
16:2:263:THR:HG23	16:2:265:PHE:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:3:269:LYS:HD3	21:3:411:CLA:HAA2	1.97	0.46
21:3:412:CLA:H2	21:3:412:CLA:H61	1.67	0.46
18:8:201:TRP:CE2	29:8:613:CHL:ND	2.83	0.46
29:9:606:CHL:HBB1	30:9:615:LUT:H161	1.96	0.46
23:9:618:LHG:HC62	23:9:618:LHG:H242	1.62	0.46
1:A:287:TRP:HB2	1:A:290:ASP:OD2	2.15	0.46
21:A:821:CLA:H52	21:A:824:CLA:H2	1.96	0.46
15:1:128:LEU:O	15:1:128:LEU:HD23	2.15	0.46
15:1:141:LEU:HD13	29:1:307:CHL:HBC1	1.96	0.46
29:2:607:CHL:HHC	29:2:607:CHL:HBB1	1.96	0.46
21:4:609:CLA:H41	21:4:609:CLA:H62	1.45	0.46
29:6:601:CHL:OBD	17:7:214:ARG:NH1	2.48	0.46
1:A:498:ASN:HB2	21:A:836:CLA:HED2	1.98	0.46
2:B:89:HIS:CD2	21:B:807:CLA:NA	2.83	0.46
2:B:209:TRP:CH2	24:B:843:BCR:H351	2.51	0.46
17:3:256:PHE:CB	21:3:409:CLA:HBA1	2.44	0.46
29:7:406:CHL:HMA1	24:7:417:BCR:H361	1.97	0.46
1:A:360:LEU:O	1:A:364:VAL:HG23	2.15	0.46
21:A:840:CLA:HED2	2:B:420:SER:HB3	1.97	0.46
3:C:32:ASP:OD1	3:C:32:ASP:N	2.48	0.46
6:F:158:VAL:HG12	6:F:168:PHE:HB2	1.97	0.46
14:O:96:ILE:HG22	14:O:104:PRO:HG2	1.96	0.46
21:O:201:CLA:HMB1	21:O:201:CLA:HBB1	1.98	0.46
17:3:247:GLY:HA2	21:3:409:CLA:HED3	1.97	0.46
17:7:212:GLU:CD	21:7:407:CLA:C1B	2.84	0.46
18:8:224:LYS:CE	21:8:609:CLA:C2D	2.93	0.46
1:A:197:HIS:HE1	21:A:813:CLA:NA	2.12	0.46
16:2:113:TRP:CE2	29:2:607:CHL:HED2	2.51	0.46
1:A:328:GLY:N	23:A:845:LHG:HC32	2.31	0.46
21:3:403:CLA:HMD2	21:3:408:CLA:C1D	2.46	0.46
18:4:196:TYR:HB3	21:4:609:CLA:O1D	2.15	0.46
21:6:609:CLA:O1D	21:6:609:CLA:H2A	2.16	0.46
1:A:291:THR:HG23	21:A:819:CLA:HMA3	1.97	0.46
1:A:578:ARG:HG2	3:C:78:GLY:HA3	1.98	0.46
2:B:47:PHE:CE2	2:B:51:PHE:HE2	2.34	0.46
21:B:805:CLA:HMA2	21:B:805:CLA:H42	1.98	0.46
21:B:814:CLA:H91	21:B:814:CLA:H112	1.72	0.46
21:5:607:CLA:HBA2	21:5:607:CLA:H3A	1.52	0.46
17:7:311:VAL:HG13	17:7:312:LEU:N	2.26	0.46
21:9:610:CLA:H2	30:9:614:LUT:H28	1.96	0.46
1:A:432:ASP:OD1	4:D:94:THR:OG1	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:95:HIS:HE1	21:B:809:CLA:NB	2.05	0.46
24:K:205:BCR:H361	24:K:205:BCR:H20C	1.75	0.46
18:4:115:MET:SD	21:4:609:CLA:HAB	2.56	0.46
15:5:183:GLU:OE1	15:5:183:GLU:N	2.49	0.46
17:7:312:LEU:HG	17:7:314:ASN:H	1.81	0.46
18:8:254:HIS:HB2	21:8:611:CLA:HAA2	1.98	0.46
29:8:607:CHL:HHC	29:8:607:CHL:HBB1	1.97	0.46
1:A:366:HIS:HA	1:A:369:TYR:CE1	2.51	0.45
2:B:33:SER:HB3	27:B:847:DGD:HE62	1.98	0.45
2:B:142:LEU:HD21	24:B:843:BCR:H23C	1.97	0.45
7:G:149:ASN:OD1	7:G:150:GLY:N	2.50	0.45
16:2:112:ARG:HB3	21:2:609:CLA:HAC2	1.98	0.45
18:4:154:PHE:O	18:4:157:GLU:HG2	2.16	0.45
16:6:255:HIS:CE1	16:6:259:PRO:HB3	2.51	0.45
19:9:224:VAL:O	19:9:228:GLN:HG2	2.16	0.45
21:B:817:CLA:H112	21:B:817:CLA:H72	1.53	0.45
21:1:312:CLA:HMC2	30:1:317:LUT:C11	2.46	0.45
15:5:67:PHE:HB3	21:5:602:CLA:CAD	2.46	0.45
15:5:111:TRP:HZ3	15:5:215:PRO:HD3	1.81	0.45
17:7:306:PRO:O	21:7:412:CLA:HMA3	2.17	0.45
1:A:729:HIS:HE1	21:A:841:CLA:C4D	2.29	0.45
21:A:808:CLA:HBB1	21:A:808:CLA:HMB1	1.97	0.45
2:B:191:THR:HG21	2:B:278:LEU:HB2	1.96	0.45
12:L:97:PRO:O	12:L:108:ARG:HD2	2.17	0.45
29:2:602:CHL:HBB1	31:2:617:XAT:H32	1.97	0.45
17:3:108:LEU:HB3	17:3:110:TYR:CE2	2.51	0.45
17:7:140:TRP:CZ3	21:7:402:CLA:HBA1	2.48	0.45
17:7:302:HIS:CG	21:7:411:CLA:HAA2	2.51	0.45
21:8:611:CLA:H51	21:8:611:CLA:H8	1.53	0.45
19:9:308:TRP:NE1	21:9:613:CLA:HBA1	2.31	0.45
1:A:275:PHE:HE2	1:A:499:ALA:HB2	1.81	0.45
1:A:393:TRP:CD1	21:A:828:CLA:HAB	2.51	0.45
2:B:156:HIS:HE1	21:B:810:CLA:C1A	2.29	0.45
21:B:827:CLA:H142	21:B:827:CLA:H112	1.80	0.45
21:B:834:CLA:HMB2	28:G:206:LMG:H232	1.97	0.45
17:3:208:MET:HB2	21:3:408:CLA:HBB1	1.98	0.45
17:7:201:PHE:O	17:7:204:GLU:HG3	2.16	0.45
21:G:202:CLA:CGA	21:G:202:CLA:H3A	2.42	0.45
9:I:19:PRO:HA	9:I:22:THR:HG22	1.98	0.45
29:1:302:CHL:HBA1	29:1:302:CHL:H3A	1.78	0.45
21:5:602:CLA:O1A	31:5:616:XAT:H241	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:K:201:CLA:NA	24:K:205:BCR:H402	2.32	0.45
16:6:239:VAL:HG11	21:6:612:CLA:HAC2	1.98	0.45
18:8:113:TRP:CZ2	29:8:607:CHL:HED2	2.51	0.45
1:A:642:ASN:HB2	2:B:651:LEU:HD11	1.99	0.45
23:A:855:LHG:HC61	23:A:855:LHG:H241	1.58	0.45
15:5:148:ILE:HA	15:5:151:VAL:HG22	1.99	0.45
18:8:146:TYR:CE1	21:8:604:CLA:HAA2	2.52	0.45
29:8:605:CHL:C1B	24:8:616:BCR:H383	2.47	0.45
19:9:236:GLU:HG3	29:9:609:CHL:C4B	2.47	0.45
21:B:814:CLA:H112	24:G:201:BCR:H23C	1.99	0.45
18:4:137:SER:HB3	18:4:140:LYS:HG2	1.99	0.45
29:5:601:CHL:OBD	18:8:167:ARG:NH1	2.50	0.45
30:7:415:LUT:H15	30:7:415:LUT:H201	1.80	0.45
19:9:273:LYS:O	19:9:277:ILE:HG12	2.17	0.45
31:9:616:XAT:H391	31:9:616:XAT:H31	1.66	0.45
21:B:801:CLA:HBA2	21:B:801:CLA:H3A	1.66	0.45
24:J:103:BCR:H341	24:J:103:BCR:C12	2.46	0.45
18:4:181:ASP:HB3	18:4:184:PHE:O	2.17	0.45
17:7:230:PHE:CD2	17:7:233:LEU:HB2	2.52	0.45
1:A:294:HIS:HD2	1:A:294:HIS:O	2.00	0.45
21:A:813:CLA:HMB1	21:A:813:CLA:HBB1	1.98	0.45
21:1:306:CLA:HED2	21:1:306:CLA:HBD	1.82	0.45
1:A:713:GLN:NE2	5:E:114:LYS:HB2	2.32	0.44
4:D:161:PHE:CZ	4:D:174:HIS:HB2	2.52	0.44
21:3:405:CLA:HMB1	21:3:408:CLA:HBC2	1.99	0.44
16:6:113:TRP:CD1	21:6:608:CLA:HMD3	2.52	0.44
24:7:418:BCR:H361	24:7:418:BCR:H20C	1.85	0.44
19:9:141:TYR:HD2	29:9:601:CHL:HMD2	1.82	0.44
2:B:180:SER:OG	2:B:288:GLY:HA3	2.18	0.44
15:1:184:GLU:HG2	15:1:188:LYS:HE3	1.98	0.44
21:1:304:CLA:H51	21:1:304:CLA:H11	1.72	0.44
21:1:306:CLA:HMC2	31:1:318:XAT:H163	1.98	0.44
15:5:151:VAL:O	15:5:154:GLN:HG3	2.17	0.44
18:8:167:ARG:HH21	18:8:178:VAL:HB	1.83	0.44
21:A:826:CLA:HAB	24:A:849:BCR:H311	2.00	0.44
15:5:120:THR:OG1	15:5:121:PRO:HD3	2.17	0.44
16:6:234:VAL:HG23	16:6:235:LEU:HD12	2.00	0.44
21:6:612:CLA:C1B	21:6:613:CLA:HMD3	2.47	0.44
21:8:609:CLA:C1B	23:8:617:LHG:HC32	2.47	0.44
21:A:830:CLA:CAD	23:A:844:LHG:H252	2.48	0.44
21:B:827:CLA:H161	24:B:843:BCR:C36	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:836:CLA:H143	21:B:836:CLA:H161	1.81	0.44
6:F:146:LEU:HD21	10:J:38:VAL:HG11	1.99	0.44
12:L:165:GLU:N	12:L:165:GLU:OE1	2.50	0.44
21:3:409:CLA:H3A	21:3:409:CLA:HBA2	1.42	0.44
18:4:231:LEU:HD23	18:4:231:LEU:HA	1.87	0.44
21:6:610:CLA:HMC3	24:7:417:BCR:H312	1.99	0.44
21:A:802:CLA:CGA	21:A:802:CLA:H3A	2.48	0.44
21:A:832:CLA:HBB1	21:A:842:CLA:HAA2	1.98	0.44
21:A:842:CLA:H152	21:A:842:CLA:H112	1.75	0.44
24:I:101:BCR:H11C	24:I:101:BCR:H341	1.86	0.44
21:4:602:CLA:O1A	31:4:616:XAT:H241	2.17	0.44
15:5:73:GLY:HA3	15:5:79:LEU:HD13	2.00	0.44
17:7:165:LEU:HD23	17:7:165:LEU:HA	1.87	0.44
17:7:204:GLU:HA	21:7:404:CLA:HMA3	1.98	0.44
17:7:214:ARG:HH11	17:7:225:MET:HE3	1.82	0.44
19:9:237:TYR:CE1	19:9:241:LYS:HG3	2.53	0.44
29:9:601:CHL:HHC	29:9:601:CHL:HBB1	2.00	0.44
2:B:593:TYR:CZ	21:B:835:CLA:HBC3	2.53	0.44
21:B:823:CLA:H111	21:B:823:CLA:H91	1.62	0.44
5:E:76:GLY:HA2	5:E:94:LYS:HZ3	1.80	0.44
21:3:409:CLA:H41	30:3:416:LUT:C29	2.48	0.44
21:4:609:CLA:H43	30:4:615:LUT:H26	1.99	0.44
16:6:111:CYS:HB2	16:6:227:GLY:HA3	2.00	0.44
17:7:208:MET:HB3	21:7:407:CLA:HAB	2.00	0.44
7:G:83:PHE:O	7:G:87:ASN:ND2	2.25	0.44
31:1:318:XAT:H35	31:1:318:XAT:H401	1.89	0.44
30:7:415:LUT:H191	30:7:415:LUT:H12	2.00	0.44
16:2:201:TRP:HH2	29:2:614:CHL:NB	2.14	0.44
30:4:615:LUT:H11	30:4:615:LUT:H191	1.87	0.44
29:6:607:CHL:HMA1	24:6:618:BCR:H362	1.99	0.44
1:A:480:PHE:HB3	21:A:837:CLA:H12	2.00	0.44
2:B:359:ALA:O	2:B:360:PHE:HB2	2.18	0.44
2:B:395:ILE:HD12	2:B:555:TYR:HD1	1.83	0.44
2:B:519:VAL:HG11	2:B:593:TYR:CG	2.52	0.44
21:B:817:CLA:H143	21:B:817:CLA:H161	1.80	0.44
11:K:88:LEU:HD12	21:K:204:CLA:HED3	2.00	0.44
21:1:306:CLA:HBB2	29:1:307:CHL:CBB	2.48	0.44
15:5:162:GLU:HG2	15:5:165:LYS:HZ1	1.82	0.44
19:9:92:GLU:HA	19:9:95:LYS:HB3	1.99	0.44
1:A:302:PHE:CE1	21:A:821:CLA:HAB	2.52	0.43
21:B:807:CLA:H8	21:B:807:CLA:HBB1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:69:THR:HA	7:G:136:GLY:HA3	2.00	0.43
15:1:151:VAL:HG13	21:1:308:CLA:C1B	2.48	0.43
16:2:198:GLY:HA2	21:2:609:CLA:CED	2.48	0.43
16:2:223:GLU:HG3	21:2:609:CLA:C4B	2.48	0.43
17:3:303:LEU:HD21	21:3:413:CLA:HMC3	2.00	0.43
16:6:230:ALA:O	16:6:234:VAL:HG22	2.18	0.43
21:7:401:CLA:HBB2	31:7:416:XAT:H34	1.98	0.43
29:9:605:CHL:HBA1	29:9:605:CHL:H3A	1.80	0.43
2:B:62:SER:HB2	2:B:142:LEU:HB2	2.01	0.43
21:B:806:CLA:H93	21:B:806:CLA:H61	1.70	0.43
24:L:306:BCR:H20C	24:L:306:BCR:H361	1.86	0.43
15:1:199:ALA:HA	21:1:313:CLA:HBB1	2.00	0.43
21:1:309:CLA:HMC1	21:1:309:CLA:HBC3	1.99	0.43
16:2:187:ASN:HB3	29:2:614:CHL:C2D	2.47	0.43
16:2:255:HIS:CD2	21:2:613:CLA:NC	2.86	0.43
17:3:216:ALA:HB2	21:3:408:CLA:HMA1	1.99	0.43
21:3:408:CLA:H62	21:3:408:CLA:H41	1.53	0.43
24:3:418:BCR:H11C	24:3:418:BCR:H341	1.88	0.43
29:5:606:CHL:HBB1	29:5:606:CHL:HHC	2.00	0.43
21:8:611:CLA:HED2	21:8:611:CLA:HBD	1.81	0.43
1:A:305:ALA:HB2	21:A:821:CLA:HBC2	1.99	0.43
24:A:849:BCR:H15C	24:A:849:BCR:H351	1.90	0.43
2:B:196:HIS:HE1	21:B:814:CLA:C1A	2.30	0.43
21:B:839:CLA:HBA1	21:B:839:CLA:HBD	2.01	0.43
8:H:102:LEU:HD11	12:L:152:THR:HG22	1.98	0.43
21:1:304:CLA:HED2	21:1:304:CLA:H43	2.00	0.43
18:4:167:ARG:NE	29:4:607:CHL:OMC	2.39	0.43
15:5:142:ALA:O	15:5:146:ILE:HG12	2.18	0.43
21:5:610:CLA:C1D	21:5:611:CLA:HMD2	2.48	0.43
29:6:607:CHL:HHC	29:6:607:CHL:HBB1	2.00	0.43
21:7:410:CLA:HAB	30:7:415:LUT:C14	2.48	0.43
2:B:388:ALA:O	2:B:392:ILE:HG13	2.19	0.43
21:B:805:CLA:H151	21:B:827:CLA:HBB2	2.00	0.43
17:3:245:TYR:CD1	21:3:409:CLA:O1D	2.71	0.43
21:6:603:CLA:HMC2	31:6:617:XAT:H203	2.00	0.43
29:7:406:CHL:HHC	29:7:406:CHL:HBB1	2.01	0.43
18:8:193:ASP:OD1	18:8:193:ASP:N	2.52	0.43
4:D:130:ARG:NH2	8:H:51:SER:OG	2.52	0.43
16:2:114:ALA:CB	16:2:231:MET:HG2	2.49	0.43
15:5:194:ARG:O	15:5:198:VAL:HG22	2.18	0.43
16:6:234:VAL:CG2	31:6:617:XAT:H14	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:9:187:THR:HB	19:9:190:PHE:HB2	2.00	0.43
1:A:367:HIS:ND1	21:A:818:CLA:OBD	2.49	0.43
1:A:545:VAL:HG21	21:A:839:CLA:HMA1	1.99	0.43
2:B:142:LEU:HG	24:B:843:BCR:H403	2.00	0.43
4:D:120:GLU:O	4:D:150:ARG:NH1	2.51	0.43
7:G:121:PRO:HG2	21:G:204:CLA:HBC2	2.00	0.43
9:I:5:TYR:O	9:I:8:SER:OG	2.32	0.43
24:L:301:BCR:H352	21:L:303:CLA:HAB	2.00	0.43
15:5:72:LEU:HB3	15:5:82:PHE:HE2	1.84	0.43
16:6:129:LYS:HE2	16:6:253:LEU:HD11	2.01	0.43
16:6:136:PRO:HD2	21:6:604:CLA:HED2	2.01	0.43
17:7:172:PRO:O	17:7:175:THR:OG1	2.31	0.43
21:A:821:CLA:H101	24:A:849:BCR:H10C	2.00	0.43
21:B:808:CLA:H13	27:B:847:DGD:HAW2	2.01	0.43
21:B:811:CLA:H3A	21:B:811:CLA:HBA2	1.63	0.43
21:B:830:CLA:H3A	21:B:830:CLA:HBA2	1.58	0.43
24:M:101:BCR:H15C	24:M:101:BCR:H351	1.86	0.43
24:2:618:BCR:H15C	24:2:618:BCR:H351	1.89	0.43
16:6:67:LEU:O	17:7:229:TYR:OH	2.25	0.43
17:7:146:ILE:HD11	17:7:244:ALA:HB1	2.01	0.43
19:9:236:GLU:HG3	29:9:609:CHL:NB	2.33	0.43
1:A:588:ASP:HA	1:A:591:PHE:HB3	2.01	0.43
1:A:672:LEU:HD11	2:B:617:MET:HB2	2.00	0.43
21:A:833:CLA:H143	22:B:841:PQN:H191	2.00	0.43
4:D:113:SER:OG	4:D:115:LYS:O	2.37	0.43
6:F:151:ASP:N	6:F:151:ASP:OD1	2.52	0.43
6:F:175:PHE:HB2	24:F:301:BCR:H321	2.00	0.43
1:A:669:LEU:HD22	21:A:852:CLA:C7	2.49	0.43
21:B:839:CLA:O1D	21:B:839:CLA:H2A	2.19	0.43
15:1:84:GLU:O	15:1:88:ILE:HG12	2.19	0.43
29:1:307:CHL:HBA1	21:1:315:CLA:HMC2	2.01	0.43
21:4:611:CLA:HMB1	21:4:611:CLA:HBB1	2.01	0.43
16:6:108:LEU:O	16:6:112:ARG:HD3	2.19	0.43
16:2:116:LEU:HD23	16:2:116:LEU:HA	1.89	0.43
17:7:275:ARG:HG2	21:7:401:CLA:C4C	2.49	0.43
18:8:239:GLN:HA	18:8:242:VAL:HG12	2.01	0.43
19:9:281:ARG:O	19:9:285:MET:HG2	2.19	0.43
21:A:838:CLA:H61	21:A:838:CLA:H41	1.82	0.42
12:L:218:ASN:O	12:L:224:LYS:NZ	2.48	0.42
16:2:256:LEU:HD23	16:2:256:LEU:HA	1.89	0.42
18:4:224:LYS:HD2	23:4:618:LHG:HC61	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:7:108:LEU:HB2	17:7:110:TYR:CD1	2.54	0.42
18:8:79:ASP:N	18:8:79:ASP:OD1	2.52	0.42
30:9:615:LUT:H31	30:9:615:LUT:H391	1.91	0.42
1:A:535:HIS:HE1	21:A:838:CLA:ND	2.18	0.42
21:A:817:CLA:H62	21:A:817:CLA:H41	1.37	0.42
2:B:707:LEU:HD23	27:B:847:DGD:HA21	2.01	0.42
21:B:805:CLA:H172	21:B:827:CLA:HBB2	2.01	0.42
30:7:415:LUT:H30	30:7:415:LUT:H27	1.79	0.42
23:8:617:LHG:H241	23:8:617:LHG:HC62	1.61	0.42
19:9:157:ARG:HG2	19:9:161:GLN:HE22	1.84	0.42
21:A:819:CLA:H3A	21:A:819:CLA:HBA2	1.47	0.42
21:A:833:CLA:C3B	21:A:834:CLA:HMB2	2.49	0.42
2:B:177:HIS:CG	21:B:812:CLA:HMC2	2.54	0.42
2:B:432:HIS:HE1	21:B:831:CLA:C4D	2.32	0.42
21:4:609:CLA:H43	30:4:615:LUT:H28	1.91	0.42
15:5:111:TRP:CZ2	15:5:203:PHE:HB3	2.54	0.42
16:6:168:ARG:O	16:6:172:ILE:HG12	2.19	0.42
29:9:607:CHL:HAB	29:9:607:CHL:HMB1	1.92	0.42
1:A:441:VAL:HG21	21:A:839:CLA:HMC3	2.01	0.42
23:A:855:LHG:H141	10:J:4:VAL:HG21	2.01	0.42
21:K:201:CLA:HED1	24:K:205:BCR:H381	2.01	0.42
15:5:53:ARG:HH22	15:5:65:PHE:HA	1.84	0.42
16:6:168:ARG:HA	16:6:171:ASP:OD2	2.19	0.42
24:6:618:BCR:H24C	24:6:618:BCR:H371	1.88	0.42
24:7:417:BCR:H351	24:7:417:BCR:H15C	1.87	0.42
18:8:262:THR:OG1	18:8:263:ILE:N	2.53	0.42
21:A:833:CLA:HAA2	24:L:301:BCR:C14	2.49	0.42
2:B:365:PHE:HB3	2:B:602:TRP:CZ3	2.54	0.42
2:B:494:LEU:HD23	2:B:494:LEU:HA	1.86	0.42
24:G:201:BCR:H15C	24:G:201:BCR:H351	1.91	0.42
14:O:102:HIS:O	14:O:104:PRO:HD3	2.19	0.42
14:O:135:PHE:C	14:O:137:GLY:H	2.23	0.42
15:1:110:ASN:C	15:1:112:VAL:H	2.23	0.42
31:1:318:XAT:H31	31:1:318:XAT:H391	1.90	0.42
15:5:178:LYS:H	15:5:178:LYS:HG2	1.67	0.42
16:6:263:THR:OG1	16:6:264:ILE:N	2.51	0.42
29:6:601:CHL:C1C	23:6:619:LHG:HC82	2.50	0.42
17:7:133:GLY:H	17:7:136:ILE:HB	1.84	0.42
1:A:356:MET:HG3	21:A:825:CLA:HBB	2.02	0.42
21:A:803:CLA:H2	2:B:655:LEU:HD22	2.02	0.42
21:A:819:CLA:H161	21:A:819:CLA:H122	1.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:828:CLA:HBB1	21:A:828:CLA:HMB1	2.01	0.42
23:A:855:LHG:HC82	16:2:95:SER:OG	2.19	0.42
21:2:610:CLA:C1D	21:2:611:CLA:HMD2	2.49	0.42
17:3:167:ARG:HD2	17:3:167:ARG:HA	1.76	0.42
21:8:602:CLA:H43	31:8:615:XAT:O24	2.20	0.42
21:9:603:CLA:HMD2	29:9:609:CHL:C1D	2.49	0.42
21:B:824:CLA:HBA2	21:B:824:CLA:H3A	1.72	0.42
24:O:205:BCR:H11C	24:O:205:BCR:H341	1.85	0.42
16:2:177:CYS:SG	16:2:178:VAL:HG13	2.59	0.42
21:2:609:CLA:HBA2	21:2:609:CLA:H3A	1.45	0.42
30:2:616:LUT:H15	30:2:616:LUT:H201	1.81	0.42
21:4:602:CLA:HBA2	21:4:602:CLA:H3A	1.25	0.42
16:6:104:VAL:O	16:6:108:LEU:HG	2.19	0.42
17:7:149:GLY:O	17:7:153:MET:HG2	2.19	0.42
19:9:234:LEU:HD23	32:9:617:NEX:H203	2.00	0.42
1:A:317:HIS:HE1	21:A:822:CLA:NA	2.08	0.42
1:A:405:HIS:HA	1:A:408:ILE:HD12	2.02	0.42
9:I:1:MET:HB3	9:I:4:SER:HB3	2.02	0.42
21:L:302:CLA:HBA1	24:L:306:BCR:H363	2.02	0.42
15:1:110:ASN:O	15:1:111:TRP:CD1	2.73	0.42
17:3:106:GLN:HG2	17:3:107:SER:N	2.35	0.42
15:5:223:LEU:HD21	21:5:613:CLA:HMC3	2.01	0.42
15:5:230:THR:HA	21:5:612:CLA:HAA1	2.01	0.42
21:8:609:CLA:CHA	21:8:609:CLA:HBA1	2.37	0.42
1:A:235:PRO:HG2	1:A:240:PHE:CZ	2.55	0.42
2:B:154:TRP:HD1	13:M:29:SER:HG	1.67	0.42
8:H:46:LYS:HB2	8:H:61:ASN:HB3	2.02	0.42
21:5:602:CLA:HMC2	31:5:616:XAT:H31	2.02	0.42
24:6:618:BCR:H15C	24:6:618:BCR:H351	1.88	0.42
19:9:280:GLY:O	19:9:284:MET:HG3	2.20	0.42
1:A:197:HIS:CG	21:A:814:CLA:HMC2	2.55	0.42
2:B:273:MET:CE	21:B:817:CLA:H2A	2.50	0.42
5:E:76:GLY:HA2	5:E:94:LYS:HZ1	1.83	0.42
24:F:301:BCR:H11C	24:F:301:BCR:H341	1.95	0.42
13:M:6:ASP:O	13:M:10:ILE:HG12	2.20	0.42
16:2:225:LYS:HB2	16:2:225:LYS:HE2	1.73	0.42
30:2:616:LUT:H191	30:2:616:LUT:H11	1.79	0.42
21:3:408:CLA:H12	21:3:415:CLA:HBB2	2.01	0.42
21:6:604:CLA:HMB3	31:6:617:XAT:O4	2.19	0.42
17:7:212:GLU:OE1	21:7:407:CLA:C4A	2.68	0.42
18:8:234:LEU:HB2	31:8:615:XAT:H35	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:9:260:LEU:HD13	30:9:614:LUT:H221	2.01	0.42
2:B:53:GLN:HB2	21:B:804:CLA:HMB2	2.02	0.41
21:B:827:CLA:HBB1	21:B:827:CLA:HMB1	2.02	0.41
21:B:830:CLA:H41	21:B:830:CLA:H62	1.45	0.41
21:B:836:CLA:H93	21:B:837:CLA:HBC1	2.01	0.41
24:B:846:BCR:H15C	24:B:846:BCR:H351	1.85	0.41
14:O:78:SER:O	14:O:85:GLY:HA3	2.19	0.41
18:4:214:LYS:O	18:4:214:LYS:NZ	2.32	0.41
18:8:102:TRP:CZ2	21:8:608:CLA:HAA2	2.55	0.41
18:8:235:GLY:O	18:8:239:GLN:HG2	2.20	0.41
1:A:423:LEU:HD13	21:A:824:CLA:C1C	2.50	0.41
1:A:676:PHE:CD2	24:A:850:BCR:H363	2.56	0.41
21:A:834:CLA:H51	24:L:301:BCR:H363	2.02	0.41
2:B:95:HIS:HE1	21:B:809:CLA:C4B	2.32	0.41
2:B:270:LEU:HD23	2:B:270:LEU:HA	1.89	0.41
2:B:357:PRO:HG3	21:B:817:CLA:HBA1	2.02	0.41
21:B:807:CLA:H202	21:B:807:CLA:H161	1.83	0.41
21:B:817:CLA:H3A	21:B:817:CLA:HBA2	1.40	0.41
15:1:149:ALA:HA	21:1:309:CLA:CAB	2.50	0.41
18:4:212:GLU:O	18:4:213:ASP:HB2	2.21	0.41
18:4:234:LEU:HG	21:4:612:CLA:HBC2	2.02	0.41
15:5:86:GLU:HB2	21:5:602:CLA:C1B	2.50	0.41
15:5:89:HIS:CE1	21:5:608:CLA:HMD1	2.55	0.41
30:8:614:LUT:H31	30:8:614:LUT:H391	1.95	0.41
19:9:240:ILE:HD13	29:9:609:CHL:HMA1	2.02	0.41
2:B:389:HIS:HE1	21:B:828:CLA:C4A	2.33	0.41
24:B:844:BCR:H15C	24:B:844:BCR:H351	1.89	0.41
21:3:409:CLA:HED2	21:3:409:CLA:HBD	1.91	0.41
31:3:417:XAT:H31	31:3:417:XAT:H391	1.94	0.41
21:B:805:CLA:H92	21:B:805:CLA:H61	1.78	0.41
21:1:303:CLA:H3A	21:1:303:CLA:HBA2	1.27	0.41
24:3:419:BCR:H11C	24:3:419:BCR:H341	1.81	0.41
15:5:48:LEU:HD12	15:5:48:LEU:HA	1.84	0.41
15:5:90:ALA:O	15:5:94:MET:HG3	2.19	0.41
15:5:214:GLY:O	15:5:217:GLU:HG3	2.19	0.41
21:5:602:CLA:H93	21:5:602:CLA:H61	1.77	0.41
24:7:418:BCR:H341	24:7:418:BCR:H11C	1.84	0.41
18:8:154:PHE:HD1	29:8:606:CHL:HMC	1.85	0.41
24:8:616:BCR:H20C	24:8:616:BCR:H361	1.97	0.41
1:A:72:SER:OG	1:A:178:TYR:HB2	2.20	0.41
1:A:297:ALA:HA	21:A:817:CLA:HMC3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:576:PHE:O	2:B:580:VAL:HG23	2.21	0.41
4:D:177:ASP:OD1	4:D:177:ASP:N	2.48	0.41
24:M:101:BCR:H20C	24:M:101:BCR:H361	1.89	0.41
16:2:201:TRP:CE2	29:2:614:CHL:ND	2.88	0.41
21:4:609:CLA:ND	30:4:615:LUT:H382	2.36	0.41
16:6:122:PHE:CE2	30:6:616:LUT:H30	2.55	0.41
17:7:275:ARG:HG2	21:7:401:CLA:C3C	2.50	0.41
17:7:293:VAL:HG21	17:7:297:GLN:OE1	2.21	0.41
21:B:816:CLA:HMD3	21:B:817:CLA:H141	2.02	0.41
8:H:81:GLN:HG2	21:H:201:CLA:NC	2.34	0.41
15:1:124:GLN:HG2	15:1:136:ASN:HA	2.03	0.41
21:2:603:CLA:HED2	21:2:603:CLA:HBD	1.75	0.41
17:3:235:LYS:NZ	15:5:77:GLU:HG3	2.36	0.41
15:5:235:LEU:HD12	18:8:155:ILE:HD11	2.03	0.41
16:6:198:GLY:HA2	16:6:203:ASP:OD2	2.20	0.41
21:6:604:CLA:CHB	24:6:618:BCR:H392	2.51	0.41
21:7:404:CLA:H3A	24:7:417:BCR:C21	2.50	0.41
21:7:408:CLA:HMC2	30:7:415:LUT:C32	2.50	0.41
18:8:112:ARG:O	18:8:115:MET:HG2	2.20	0.41
18:8:189:LEU:HD11	29:8:613:CHL:HBC1	2.03	0.41
1:A:294:HIS:CD2	1:A:294:HIS:O	2.74	0.41
21:A:827:CLA:H152	21:A:827:CLA:H111	1.61	0.41
21:A:831:CLA:H2A	21:A:831:CLA:O2D	2.20	0.41
2:B:308:HIS:HE1	21:B:821:CLA:NC	2.19	0.41
2:B:395:ILE:HD13	2:B:555:TYR:HA	2.03	0.41
2:B:421:HIS:CD2	21:B:830:CLA:NC	2.89	0.41
21:B:826:CLA:HBB1	21:B:826:CLA:HMB1	2.02	0.41
24:B:845:BCR:H11C	24:B:845:BCR:H341	1.90	0.41
15:1:113:SER:HA	15:1:116:LYS:HB2	2.02	0.41
18:8:197:PRO:HD3	29:8:607:CHL:HMD2	2.03	0.41
21:8:604:CLA:HBA2	21:8:604:CLA:H3A	1.55	0.41
21:A:827:CLA:O1D	21:A:835:CLA:HAB	2.21	0.41
21:A:834:CLA:H141	21:A:834:CLA:H161	1.78	0.41
21:A:841:CLA:H142	21:A:841:CLA:H112	1.69	0.41
21:B:803:CLA:HHC	21:B:805:CLA:OBD	2.21	0.41
21:B:808:CLA:H111	27:B:847:DGD:HAH2	2.03	0.41
24:B:842:BCR:H15C	24:B:842:BCR:H351	1.92	0.41
27:B:847:DGD:HB72	27:B:847:DGD:HB41	1.83	0.41
24:J:101:BCR:H333	21:J:102:CLA:HMD3	2.03	0.41
29:6:602:CHL:HBB1	31:6:617:XAT:H30	2.02	0.41
17:7:309:ASN:OD1	17:7:310:ASN:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:TRP:CD2	21:A:810:CLA:HED3	2.56	0.41
1:A:669:LEU:HD21	2:B:445:ALA:HB2	2.03	0.41
21:A:806:CLA:H111	21:A:806:CLA:H91	1.71	0.41
21:A:852:CLA:H41	21:A:852:CLA:H61	1.70	0.41
2:B:15:ASP:OD2	2:B:17:THR:OG1	2.36	0.41
2:B:432:HIS:CD2	24:J:104:BCR:H333	2.56	0.41
2:B:656:VAL:HG22	21:B:839:CLA:HMB3	2.02	0.41
2:B:667:TRP:O	2:B:671:TRP:CD1	2.73	0.41
21:B:807:CLA:HMC3	21:B:808:CLA:C3D	2.51	0.41
3:C:29:VAL:HG22	4:D:188:ARG:HB3	2.03	0.41
3:C:35:LYS:HE3	3:C:35:LYS:HB2	1.89	0.41
7:G:149:ASN:ND2	7:G:151:TYR:H	2.18	0.41
24:J:104:BCR:H24C	24:J:104:BCR:H21C	1.82	0.41
24:M:101:BCR:H11C	24:M:101:BCR:H341	1.84	0.41
16:2:115:MET:HG3	16:2:227:GLY:HA2	2.03	0.41
16:2:156:ILE:O	16:2:160:LEU:HG	2.21	0.41
21:3:406:CLA:HMC1	26:3:420:LMU:H112	2.03	0.41
21:3:409:CLA:H43	30:3:416:LUT:H26	2.03	0.41
31:4:616:XAT:H15	31:4:616:XAT:H201	1.93	0.41
15:5:105:ALA:HA	15:5:216:LEU:HD22	2.03	0.41
15:5:145:PHE:HA	15:5:148:ILE:HG22	2.03	0.41
15:5:167:PRO:HG3	21:5:607:CLA:HMD2	2.02	0.41
21:5:602:CLA:HMC2	31:5:616:XAT:C31	2.51	0.41
16:6:69:PHE:CD1	29:6:601:CHL:HMA3	2.56	0.41
16:6:197:PRO:HG2	16:6:202:PHE:CD2	2.45	0.41
21:7:408:CLA:C1B	30:7:415:LUT:H373	2.50	0.41
21:9:611:CLA:H91	21:9:611:CLA:H111	1.63	0.41
2:B:519:VAL:HG11	2:B:593:TYR:HB2	2.03	0.41
6:F:103:GLU:O	6:F:107:ILE:HG12	2.20	0.41
18:4:188:LYS:NZ	18:4:189:LEU:O	2.49	0.41
24:8:616:BCR:H11C	24:8:616:BCR:H341	1.87	0.41
1:A:294:HIS:HD2	1:A:298:ILE:HG12	1.85	0.40
1:A:448:HIS:HE1	21:A:833:CLA:C4D	2.34	0.40
1:A:521:LEU:HD23	1:A:521:LEU:HA	1.96	0.40
1:A:570:ARG:NH1	23:A:844:LHG:O10	2.54	0.40
21:A:805:CLA:HMA2	21:A:812:CLA:HMD2	2.03	0.40
24:A:847:BCR:H11C	24:A:847:BCR:H341	1.91	0.40
7:G:149:ASN:CG	7:G:151:TYR:H	2.23	0.40
21:5:602:CLA:H111	21:5:602:CLA:H91	1.79	0.40
21:5:614:CLA:H3A	21:5:614:CLA:HBA1	1.84	0.40
16:6:240:GLN:HG2	21:6:612:CLA:C1D	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:9:617:NEX:H35	32:9:617:NEX:H401	1.91	0.40
21:A:840:CLA:H111	21:A:840:CLA:HMC2	2.02	0.40
21:B:816:CLA:HBA2	21:B:825:CLA:HBB2	2.02	0.40
3:C:73:THR:H	3:C:76:SER:HB2	1.86	0.40
8:H:73:ASP:HB3	12:L:100:ARG:HH22	1.86	0.40
17:7:270:GLU:OE2	21:7:408:CLA:HMB3	2.21	0.40
24:J:101:BCR:H24C	24:J:101:BCR:H371	1.98	0.40
12:L:126:LEU:HD12	21:L:304:CLA:HMB2	2.03	0.40
16:2:113:TRP:CD1	21:2:608:CLA:HMD3	2.56	0.40
21:2:603:CLA:HMD2	21:2:608:CLA:C1D	2.52	0.40
29:3:407:CHL:HAB	29:3:407:CHL:HMB1	1.91	0.40
21:4:603:CLA:HMD2	21:4:608:CLA:CHD	2.51	0.40
29:4:607:CHL:HBB1	29:4:607:CHL:HHC	2.02	0.40
30:6:616:LUT:H15	30:6:616:LUT:H201	1.82	0.40
21:7:408:CLA:HMC2	30:7:415:LUT:H32	2.03	0.40
31:7:416:XAT:H35	31:7:416:XAT:H401	1.90	0.40
18:8:154:PHE:CD1	29:8:606:CHL:HAC2	2.57	0.40
21:8:604:CLA:HMB1	21:8:604:CLA:HBB1	2.02	0.40
19:9:232:MET:O	19:9:236:GLU:HG2	2.22	0.40
1:A:448:HIS:HE1	21:A:833:CLA:CHA	2.34	0.40
21:A:807:CLA:HED2	21:A:807:CLA:HBD	1.92	0.40
21:A:842:CLA:HHB	24:B:846:BCR:C38	2.52	0.40
2:B:418:ILE:HG23	21:B:837:CLA:HBB2	2.03	0.40
2:B:697:PRO:O	3:C:81:TYR:OH	2.30	0.40
21:B:838:CLA:HBB2	22:B:841:PQN:H141	2.04	0.40
24:G:205:BCR:H15C	24:G:205:BCR:H351	1.93	0.40
21:2:610:CLA:CAB	24:3:418:BCR:H312	2.51	0.40
18:4:154:PHE:O	18:4:158:LEU:HG	2.21	0.40
18:4:255:LEU:HD21	21:4:613:CLA:HMC3	2.02	0.40
17:7:278:MET:HE3	21:7:401:CLA:HMC3	2.03	0.40
21:9:611:CLA:H62	21:9:611:CLA:H92	1.79	0.40
1:A:294:HIS:HB2	21:A:818:CLA:C2B	2.51	0.40
24:A:854:BCR:H20C	24:A:854:BCR:H361	1.89	0.40
21:B:817:CLA:HMD2	21:B:827:CLA:H93	2.03	0.40
21:B:827:CLA:H142	24:B:843:BCR:H372	2.04	0.40
14:O:74:TRP:CD1	14:O:124:LEU:HB2	2.56	0.40
15:1:225:ASP:OD1	15:1:228:HIS:ND1	2.55	0.40
16:2:236:GLY:O	16:2:240:GLN:HG3	2.21	0.40
31:4:616:XAT:H31	31:4:616:XAT:H391	1.91	0.40
30:7:415:LUT:H35	30:7:415:LUT:H401	1.94	0.40
31:7:416:XAT:H15	31:7:416:XAT:H201	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:8:613:CHL:HHC	29:8:613:CHL:HBB1	2.04	0.40
31:8:615:XAT:H191	31:8:615:XAT:H11	1.88	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	740/742 (100%)	715 (97%)	25 (3%)	0	100	100
2	B	731/733 (100%)	701 (96%)	30 (4%)	0	100	100
3	C	78/80 (98%)	72 (92%)	6 (8%)	0	100	100
4	D	139/141 (99%)	132 (95%)	7 (5%)	0	100	100
5	E	60/62 (97%)	60 (100%)	0	0	100	100
6	F	157/159 (99%)	154 (98%)	3 (2%)	0	100	100
7	G	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
8	H	93/95 (98%)	90 (97%)	3 (3%)	0	100	100
9	I	32/34 (94%)	29 (91%)	3 (9%)	0	100	100
10	J	39/41 (95%)	39 (100%)	0	0	100	100
11	K	79/81 (98%)	76 (96%)	3 (4%)	0	100	100
12	L	161/163 (99%)	153 (95%)	8 (5%)	0	100	100
13	M	30/32 (94%)	29 (97%)	0	1 (3%)	3	6
14	O	87/89 (98%)	79 (91%)	8 (9%)	0	100	100
15	1	190/192 (99%)	183 (96%)	7 (4%)	0	100	100
15	5	190/192 (99%)	176 (93%)	12 (6%)	2 (1%)	12	27
16	2	209/211 (99%)	201 (96%)	8 (4%)	0	100	100
16	6	203/211 (96%)	199 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	3	214/216 (99%)	203 (95%)	11 (5%)	0	100	100
17	7	211/216 (98%)	198 (94%)	12 (6%)	1 (0%)	25	46
18	4	203/205 (99%)	193 (95%)	10 (5%)	0	100	100
18	8	202/205 (98%)	192 (95%)	10 (5%)	0	100	100
19	9	223/225 (99%)	201 (90%)	22 (10%)	0	100	100
20	a	216/227 (95%)	208 (96%)	7 (3%)	1 (0%)	25	46
20	b	216/227 (95%)	208 (96%)	7 (3%)	1 (0%)	25	46
20	c	224/227 (99%)	215 (96%)	8 (4%)	1 (0%)	30	52
All	All	5023/5104 (98%)	4800 (96%)	216 (4%)	7 (0%)	50	71

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	5	170	PRO
20	b	152	VAL
20	c	152	VAL
20	a	152	VAL
13	M	4	ILE
15	5	168	GLY
17	7	311	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	603/603 (100%)	601 (100%)	2 (0%)	91	97
2	B	595/595 (100%)	593 (100%)	2 (0%)	91	97
3	C	67/67 (100%)	67 (100%)	0	100	100
4	D	115/115 (100%)	115 (100%)	0	100	100
5	E	52/52 (100%)	52 (100%)	0	100	100
6	F	129/129 (100%)	129 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	78/78 (100%)	77 (99%)	1 (1%)	65	84
8	H	77/77 (100%)	77 (100%)	0	100	100
9	I	30/30 (100%)	30 (100%)	0	100	100
10	J	35/35 (100%)	35 (100%)	0	100	100
11	K	58/58 (100%)	58 (100%)	0	100	100
12	L	126/126 (100%)	126 (100%)	0	100	100
13	M	27/27 (100%)	27 (100%)	0	100	100
14	O	73/73 (100%)	73 (100%)	0	100	100
15	1	151/151 (100%)	151 (100%)	0	100	100
15	5	150/151 (99%)	149 (99%)	1 (1%)	81	92
16	2	168/168 (100%)	167 (99%)	1 (1%)	84	93
16	6	163/168 (97%)	163 (100%)	0	100	100
17	3	169/169 (100%)	169 (100%)	0	100	100
17	7	166/169 (98%)	164 (99%)	2 (1%)	67	85
18	4	164/164 (100%)	164 (100%)	0	100	100
18	8	163/164 (99%)	162 (99%)	1 (1%)	84	93
19	9	179/179 (100%)	178 (99%)	1 (1%)	84	93
20	a	165/173 (95%)	165 (100%)	0	100	100
20	b	165/173 (95%)	164 (99%)	1 (1%)	84	93
20	c	173/173 (100%)	172 (99%)	1 (1%)	84	93
All	All	4041/4067 (99%)	4028 (100%)	13 (0%)	90	97

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

Mol	Chain	Res	Type
1	A	439	ASN
1	A	585	SER
2	B	106	ARG
2	B	571	SER
7	G	117	LYS
16	2	273	LYS
15	5	171	PHE
17	7	258	LYS
17	7	302	HIS
18	8	174	ARG

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Mol	Chain	Res	Type
19	9	157	ARG
20	b	68	TYR
20	c	42	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	GLN
1	A	294	HIS
2	B	177	HIS
15	5	154	GLN
15	5	206	GLN
16	6	240	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
20	TPO	c	40	20	8,10,11	1.58	1 (12%)	10,14,16	1.77	1 (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
20	TPO	c	40	20	-	2/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	c	40	TPO	P-O1P	3.35	1.61	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	c	40	TPO	P-OG1-CB	-4.89	108.44	123.21

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	c	40	TPO	CB-OG1-P-O2P
20	c	40	TPO	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

364 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	$\# Z > 2$
29	CHL	8	606	-	46,54,74	2.39	16 (34%)	49,90,114	3.48	24 (48%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	XAT	4	616	-	39,47,47	1.65	8 (20%)	54,74,74	1.62	11 (20%)
21	CLA	A	824	-	55,63,73	1.60	6 (10%)	64,101,113	1.44	8 (12%)
21	CLA	B	817	-	65,73,73	1.47	7 (10%)	76,113,113	1.39	8 (10%)
24	BCR	A	854	-	41,41,41	1.69	8 (19%)	56,56,56	1.44	8 (14%)
24	BCR	A	847	-	41,41,41	1.69	8 (19%)	56,56,56	1.39	9 (16%)
24	BCR	F	301	-	41,41,41	1.67	8 (19%)	56,56,56	1.56	9 (16%)
21	CLA	L	303	-	45,53,73	1.74	6 (13%)	52,89,113	1.62	9 (17%)
30	LUT	c	616	-	42,43,43	1.63	8 (19%)	51,60,60	1.57	11 (21%)
26	LMU	A	853	-	36,36,36	0.39	0	47,47,47	0.80	1 (2%)
21	CLA	8	608	18	43,51,73	1.93	7 (16%)	47,86,113	1.55	5 (10%)
29	CHL	5	601	15	46,54,74	2.30	14 (30%)	49,90,114	3.51	24 (48%)
29	CHL	2	614	-	46,54,74	2.31	16 (34%)	49,90,114	3.49	25 (51%)
30	LUT	9	615	-	42,43,43	1.63	8 (19%)	51,60,60	1.59	11 (21%)
29	CHL	b	306	20	46,54,74	2.36	16 (34%)	49,90,114	3.48	24 (48%)
21	CLA	A	839	-	45,53,73	1.81	6 (13%)	52,89,113	1.62	6 (11%)
21	CLA	1	304	-	55,63,73	1.61	6 (10%)	64,101,113	1.50	7 (10%)
21	CLA	G	204	7	43,52,73	1.83	5 (11%)	49,88,113	1.58	6 (12%)
21	CLA	4	602	18	57,66,73	1.56	6 (10%)	65,104,113	1.47	9 (13%)
21	CLA	8	602	18	57,66,73	1.58	5 (8%)	65,104,113	1.44	9 (13%)
21	CLA	G	203	-	50,58,73	1.70	6 (12%)	58,95,113	1.50	8 (13%)
23	LHG	A	855	-	48,48,48	0.27	0	51,54,54	0.37	0
29	CHL	2	605	-	46,54,74	2.31	14 (30%)	49,90,114	3.56	24 (48%)
29	CHL	a	605	20	44,53,74	2.42	16 (36%)	46,89,114	3.56	23 (50%)
29	CHL	6	605	-	46,54,74	2.34	16 (34%)	49,90,114	3.54	24 (48%)
21	CLA	7	401	17	45,53,73	1.79	6 (13%)	52,89,113	1.58	7 (13%)
21	CLA	7	414	-	39,48,73	1.89	6 (15%)	44,83,113	1.70	7 (15%)
29	CHL	1	302	15	51,59,74	2.20	14 (27%)	55,96,114	3.41	27 (49%)
21	CLA	F	304	-	45,53,73	1.80	6 (13%)	52,89,113	1.56	9 (17%)
29	CHL	4	614	18	42,50,74	2.41	14 (33%)	44,85,114	3.72	23 (52%)
24	BCR	3	419	-	41,41,41	1.73	8 (19%)	56,56,56	1.90	12 (21%)
24	BCR	J	103	-	41,41,41	1.76	8 (19%)	56,56,56	1.58	11 (19%)
21	CLA	5	604	-	49,57,73	1.72	5 (10%)	55,93,113	1.53	7 (12%)
21	CLA	7	411	-	53,62,73	1.67	5 (9%)	61,100,113	1.42	9 (14%)
29	CHL	6	602	-	53,61,74	2.15	14 (26%)	57,98,114	3.36	29 (50%)
21	CLA	4	601	18	45,53,73	1.78	6 (13%)	52,89,113	1.59	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CHL	b	302	20	46,54,74	2.36	16 (34%)	49,90,114	3.50	23 (46%)
21	CLA	A	808	-	45,53,73	1.75	6 (13%)	52,89,113	1.65	7 (13%)
21	CLA	6	604	-	45,53,73	1.82	5 (11%)	52,89,113	1.56	6 (11%)
21	CLA	5	613	-	37,46,73	2.00	6 (16%)	46,81,113	1.71	9 (19%)
21	CLA	B	805	-	65,73,73	1.45	6 (9%)	76,113,113	1.40	7 (9%)
21	CLA	4	608	18	43,51,73	1.88	7 (16%)	47,86,113	1.59	5 (10%)
21	CLA	a	610	20	45,53,73	1.78	5 (11%)	52,89,113	1.58	6 (11%)
21	CLA	5	608	15	40,48,73	1.91	6 (15%)	50,83,113	1.71	9 (18%)
21	CLA	B	836	-	65,73,73	1.45	7 (10%)	76,113,113	1.48	7 (9%)
21	CLA	3	409	17	52,60,73	1.52	7 (13%)	60,97,113	2.27	20 (33%)
29	CHL	9	606	19	46,54,74	2.31	16 (34%)	49,90,114	3.55	23 (46%)
29	CHL	b	308	-	53,61,74	2.16	14 (26%)	57,98,114	3.40	28 (49%)
29	CHL	7	406	-	39,48,74	2.57	16 (41%)	44,83,114	3.86	25 (56%)
21	CLA	B	834	-	45,53,73	1.74	6 (13%)	52,89,113	1.68	8 (15%)
21	CLA	A	829	-	65,73,73	1.47	6 (9%)	76,113,113	1.32	7 (9%)
21	CLA	B	833	-	45,53,73	1.76	6 (13%)	52,89,113	1.58	7 (13%)
21	CLA	B	812	-	65,73,73	1.47	7 (10%)	76,113,113	1.38	8 (10%)
21	CLA	9	602	19	53,61,73	1.65	7 (13%)	61,98,113	1.51	9 (14%)
21	CLA	c	613	-	65,73,73	1.47	6 (9%)	76,113,113	1.40	6 (7%)
21	CLA	7	405	17	39,48,73	1.95	6 (15%)	48,83,113	1.69	8 (16%)
21	CLA	3	413	-	39,48,73	1.90	6 (15%)	44,83,113	1.62	7 (15%)
21	CLA	6	608	16	45,53,73	1.81	5 (11%)	52,89,113	1.52	6 (11%)
31	XAT	6	617	-	39,47,47	1.73	8 (20%)	54,74,74	1.79	12 (22%)
21	CLA	3	401	-	39,48,73	1.83	6 (15%)	44,83,113	1.80	8 (18%)
21	CLA	B	830	-	56,64,73	1.57	6 (10%)	65,102,113	1.43	7 (10%)
21	CLA	B	832	-	56,64,73	1.57	7 (12%)	65,102,113	1.56	8 (12%)
29	CHL	c	601	20	49,57,74	2.22	13 (26%)	52,93,114	3.44	24 (46%)
21	CLA	8	609	23	45,53,73	1.93	7 (15%)	52,89,113	2.06	11 (21%)
29	CHL	9	609	-	46,54,74	2.32	15 (32%)	49,90,114	3.56	25 (51%)
21	CLA	L	304	-	42,50,73	1.76	6 (14%)	48,85,113	1.64	6 (12%)
21	CLA	B	838	-	65,73,73	1.47	6 (9%)	76,113,113	1.34	7 (9%)
21	CLA	1	309	15	41,49,73	1.90	8 (19%)	47,84,113	2.29	17 (36%)
21	CLA	B	826	-	52,60,73	1.62	6 (11%)	60,97,113	1.54	8 (13%)
24	BCR	A	849	-	41,41,41	1.70	8 (19%)	56,56,56	1.71	12 (21%)
21	CLA	4	609	18	52,60,73	1.60	8 (15%)	60,97,113	2.33	19 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	BCR	B	843	-	41,41,41	0.76	0	56,56,56	2.53	24 (42%)
21	CLA	8	618	-	41,49,73	1.83	7 (17%)	47,84,113	1.63	9 (19%)
31	XAT	2	617	-	39,47,47	1.65	8 (20%)	54,74,74	1.60	11 (20%)
21	CLA	c	612	20	44,52,73	1.81	6 (13%)	49,87,113	1.55	6 (12%)
21	CLA	1	312	15	45,53,73	1.81	6 (13%)	52,89,113	1.53	6 (11%)
21	CLA	4	604	-	43,51,73	1.78	6 (13%)	48,86,113	1.59	7 (14%)
21	CLA	b	313	20	45,53,73	1.80	6 (13%)	52,89,113	1.53	7 (13%)
31	XAT	a	618	-	39,47,47	1.68	8 (20%)	54,74,74	1.77	11 (20%)
24	BCR	J	101	-	41,41,41	1.75	8 (19%)	56,56,56	1.87	10 (17%)
21	CLA	3	408	17	59,67,73	1.58	7 (11%)	68,105,113	1.42	9 (13%)
30	LUT	8	614	-	42,43,43	1.67	8 (19%)	51,60,60	1.68	9 (17%)
21	CLA	A	828	-	60,68,73	1.52	6 (10%)	70,107,113	1.38	9 (12%)
21	CLA	1	303	15	61,69,73	1.51	6 (9%)	71,108,113	1.44	8 (11%)
29	CHL	5	606	-	46,54,74	2.37	16 (34%)	49,90,114	3.48	24 (48%)
21	CLA	1	311	23	37,46,73	1.97	7 (18%)	46,81,113	1.73	10 (21%)
21	CLA	A	831	-	55,63,73	1.60	6 (10%)	64,101,113	1.53	8 (12%)
21	CLA	B	801	-	65,73,73	2.06	16 (24%)	76,113,113	2.75	29 (38%)
21	CLA	A	825	-	65,73,73	1.45	6 (9%)	76,113,113	1.41	7 (9%)
23	LHG	A	844	-	48,48,48	0.27	0	51,54,54	0.35	0
30	LUT	7	415	-	42,43,43	1.68	8 (19%)	51,60,60	1.77	13 (25%)
21	CLA	A	836	1	45,53,73	1.79	6 (13%)	52,89,113	1.54	7 (13%)
23	LHG	1	319	21	27,27,48	0.35	0	30,33,54	0.47	0
21	CLA	B	803	-	55,63,73	1.60	6 (10%)	64,101,113	1.47	7 (10%)
29	CHL	2	606	-	46,54,74	2.28	14 (30%)	49,90,114	3.53	24 (48%)
29	CHL	a	606	-	46,54,74	2.35	15 (32%)	49,90,114	3.55	25 (51%)
29	CHL	6	606	-	46,54,74	2.33	15 (32%)	49,90,114	3.52	24 (48%)
21	CLA	B	835	-	65,73,73	1.44	6 (9%)	76,113,113	1.41	8 (10%)
29	CHL	4	605	-	41,49,74	2.20	13 (31%)	48,84,114	3.79	27 (56%)
21	CLA	A	834	-	65,73,73	1.47	6 (9%)	76,113,113	1.37	8 (10%)
29	CHL	9	601	19	43,51,74	2.34	15 (34%)	45,86,114	3.67	24 (53%)
21	CLA	1	305	-	49,57,73	1.69	6 (12%)	55,93,113	1.54	8 (14%)
21	CLA	2	603	-	45,53,73	1.83	7 (15%)	52,89,113	1.51	6 (11%)
21	CLA	7	409	-	39,48,73	1.90	5 (12%)	44,83,113	1.67	7 (15%)
21	CLA	6	603	-	45,53,73	1.84	6 (13%)	52,89,113	1.59	7 (13%)
21	CLA	B	806	-	63,71,73	1.48	6 (9%)	73,110,113	1.44	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CHL	9	608	-	46,54,74	2.30	15 (32%)	49,90,114	3.52	23 (46%)
21	CLA	K	204	11	45,53,73	1.78	6 (13%)	52,89,113	1.57	6 (11%)
21	CLA	K	201	11	46,54,73	1.73	6 (13%)	53,90,113	1.56	6 (11%)
21	CLA	1	314	-	37,46,73	2.00	7 (18%)	46,81,113	1.69	11 (23%)
26	LMU	3	420	-	36,36,36	0.40	0	47,47,47	0.72	1 (2%)
24	BCR	L	301	-	41,41,41	1.69	8 (19%)	56,56,56	1.43	9 (16%)
29	CHL	c	606	20	46,54,74	2.35	16 (34%)	49,90,114	3.49	24 (48%)
21	CLA	A	809	1	59,67,73	1.53	6 (10%)	68,105,113	1.48	9 (13%)
21	CLA	3	411	17	43,51,73	1.82	6 (13%)	49,86,113	1.57	6 (12%)
21	CLA	A	841	-	65,73,73	1.48	6 (9%)	76,113,113	1.42	7 (9%)
21	CLA	B	810	-	54,62,73	1.67	7 (12%)	67,100,113	1.50	10 (14%)
21	CLA	c	602	20	60,68,73	1.54	7 (11%)	70,107,113	1.39	8 (11%)
21	CLA	A	804	-	65,73,73	1.47	6 (9%)	76,113,113	1.44	8 (10%)
24	BCR	7	417	-	41,41,41	1.73	8 (19%)	56,56,56	1.52	9 (16%)
30	LUT	9	614	-	42,43,43	1.63	8 (19%)	51,60,60	1.56	12 (23%)
21	CLA	3	405	-	40,49,73	1.85	7 (17%)	45,84,113	1.65	6 (13%)
24	BCR	B	845	-	41,41,41	1.71	8 (19%)	56,56,56	1.48	8 (14%)
21	CLA	O	204	-	39,48,73	1.91	6 (15%)	44,83,113	1.59	7 (15%)
21	CLA	B	837	-	63,72,73	1.49	6 (9%)	73,112,113	1.41	7 (9%)
21	CLA	8	603	-	43,52,73	1.84	5 (11%)	49,88,113	1.55	7 (14%)
23	LHG	c	619	21	48,48,48	0.26	0	51,54,54	0.31	0
21	CLA	A	801	-	52,60,73	1.97	6 (11%)	60,97,113	2.24	17 (28%)
21	CLA	B	815	-	53,62,73	1.65	7 (13%)	61,100,113	1.43	8 (13%)
21	CLA	B	821	-	55,63,73	1.63	6 (10%)	64,101,113	1.51	8 (12%)
21	CLA	B	816	-	52,60,73	1.65	7 (13%)	60,97,113	1.56	8 (13%)
21	CLA	5	611	15	45,53,73	1.79	6 (13%)	52,89,113	1.61	6 (11%)
21	CLA	1	316	15	43,51,73	1.89	8 (18%)	54,87,113	1.65	8 (14%)
21	CLA	A	832	-	45,53,73	1.74	6 (13%)	52,89,113	1.60	7 (13%)
29	CHL	b	309	-	49,57,74	2.22	13 (26%)	52,93,114	3.45	25 (48%)
29	CHL	a	607	-	43,51,74	2.31	14 (32%)	45,86,114	3.67	24 (53%)
21	CLA	3	410	-	39,48,73	1.91	5 (12%)	44,83,113	1.63	7 (15%)
21	CLA	B	813	-	43,52,73	1.77	6 (13%)	49,88,113	1.62	7 (14%)
21	CLA	F	305	6	41,49,73	1.80	6 (14%)	47,84,113	1.64	7 (14%)
24	BCR	A	850	-	41,41,41	1.70	8 (19%)	56,56,56	1.78	9 (16%)
21	CLA	b	305	-	45,53,73	1.78	6 (13%)	52,89,113	1.60	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	PQN	B	841	-	34,34,34	0.40	0	42,45,45	0.37	0
30	LUT	1	317	-	42,43,43	1.69	8 (19%)	51,60,60	1.70	9 (17%)
21	CLA	A	817	-	65,73,73	1.44	6 (9%)	76,113,113	1.40	7 (9%)
21	CLA	9	613	-	53,61,73	1.62	5 (9%)	61,98,113	1.52	8 (13%)
29	CHL	2	602	16	53,61,74	2.16	15 (28%)	57,98,114	3.38	28 (49%)
24	BCR	M	101	-	41,41,41	1.77	8 (19%)	56,56,56	1.83	12 (21%)
21	CLA	9	603	19	45,53,73	1.80	6 (13%)	52,89,113	1.61	6 (11%)
29	CHL	3	407	-	39,48,74	2.41	13 (33%)	44,83,114	3.58	24 (54%)
24	BCR	L	306	-	41,41,41	1.72	8 (19%)	56,56,56	1.78	11 (19%)
21	CLA	4	613	-	43,51,73	1.80	6 (13%)	49,86,113	1.56	7 (14%)
21	CLA	b	304	-	45,53,73	1.76	6 (13%)	52,89,113	1.63	7 (13%)
30	LUT	5	615	-	42,43,43	1.67	8 (19%)	51,60,60	1.69	10 (19%)
21	CLA	B	807	-	65,73,73	1.47	7 (10%)	76,113,113	1.39	8 (10%)
21	CLA	A	833	-	65,73,73	1.50	6 (9%)	76,113,113	1.36	7 (9%)
29	CHL	b	310	-	51,60,74	2.19	16 (31%)	54,97,114	3.34	27 (50%)
31	XAT	1	318	-	39,47,47	1.67	8 (20%)	54,74,74	1.62	12 (22%)
21	CLA	a	602	-	60,68,73	1.54	6 (10%)	70,107,113	1.43	7 (10%)
21	CLA	2	609	16	51,59,73	1.70	6 (11%)	58,95,113	2.08	15 (25%)
24	BCR	2	618	-	41,41,41	1.71	8 (19%)	56,56,56	1.55	10 (17%)
24	BCR	6	618	-	41,41,41	1.73	8 (19%)	56,56,56	1.65	10 (17%)
21	CLA	A	806	-	65,73,73	1.46	7 (10%)	76,113,113	1.40	6 (7%)
21	CLA	8	604	-	43,51,73	1.81	6 (13%)	48,86,113	1.64	6 (12%)
22	PQN	A	843	-	34,34,34	0.39	0	42,45,45	0.43	0
26	LMU	b	301	-	36,36,36	0.37	0	47,47,47	0.76	0
23	LHG	2	619	21	34,34,48	0.33	0	37,40,54	0.41	0
21	CLA	c	614	-	45,53,73	1.81	6 (13%)	52,89,113	1.50	6 (11%)
24	BCR	7	418	-	41,41,41	1.73	8 (19%)	56,56,56	1.98	12 (21%)
23	LHG	6	619	-	34,34,48	0.31	0	37,40,54	0.37	0
29	CHL	1	307	-	51,59,74	2.19	14 (27%)	55,96,114	3.43	27 (49%)
21	CLA	A	805	-	55,63,73	1.60	6 (10%)	64,101,113	1.45	7 (10%)
21	CLA	3	402	17	60,68,73	1.52	6 (10%)	70,107,113	1.43	8 (11%)
24	BCR	A	848	-	41,41,41	1.68	8 (19%)	56,56,56	1.36	8 (14%)
21	CLA	2	612	16	45,53,73	1.78	6 (13%)	52,89,113	1.59	7 (13%)
21	CLA	A	802	-	52,60,73	1.66	7 (13%)	60,97,113	1.52	9 (15%)
21	CLA	5	607	-	43,52,73	1.83	5 (11%)	49,88,113	1.57	7 (14%)
21	CLA	4	611	18	44,52,73	1.79	6 (13%)	51,88,113	1.64	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	BCR	B	846	-	41,41,41	0.75	0	56,56,56	1.94	18 (32%)
29	CHL	4	606	-	46,54,74	2.31	14 (30%)	49,90,114	3.55	23 (46%)
21	CLA	6	610	-	41,50,73	1.86	6 (14%)	49,85,113	1.59	6 (12%)
29	CHL	a	608	-	46,54,74	2.30	16 (34%)	49,90,114	3.51	24 (48%)
30	LUT	b	316	-	42,43,43	1.64	8 (19%)	51,60,60	1.59	9 (17%)
21	CLA	B	829	-	45,53,73	1.84	6 (13%)	52,89,113	1.70	7 (13%)
23	LHG	a	617	-	48,48,48	0.26	0	51,54,54	0.35	0
30	LUT	3	416	-	42,43,43	1.64	7 (16%)	51,60,60	1.68	11 (21%)
21	CLA	B	814	-	60,68,73	1.54	6 (10%)	70,107,113	1.47	8 (11%)
24	BCR	G	205	-	41,41,41	1.70	8 (19%)	56,56,56	1.56	10 (17%)
21	CLA	7	412	-	39,48,73	2.01	5 (12%)	44,83,113	1.61	7 (15%)
21	CLA	H	201	8	45,53,73	1.79	6 (13%)	52,89,113	1.55	6 (11%)
23	LHG	5	617	-	27,27,48	0.35	0	30,33,54	0.44	0
23	LHG	4	619	-	48,48,48	0.28	0	51,54,54	0.62	1 (1%)
21	CLA	a	613	-	57,65,73	1.60	5 (8%)	66,103,113	1.44	9 (13%)
21	CLA	5	610	-	37,46,73	1.99	7 (18%)	46,81,113	1.75	9 (19%)
21	CLA	c	610	20	45,53,73	1.76	5 (11%)	52,89,113	1.61	8 (15%)
29	CHL	c	607	-	46,54,74	2.39	16 (34%)	49,90,114	3.50	25 (51%)
21	CLA	A	813	-	54,62,73	1.59	6 (11%)	62,99,113	1.59	7 (11%)
21	CLA	A	840	-	65,73,73	1.45	6 (9%)	76,113,113	1.38	8 (10%)
21	CLA	9	611	23	57,65,73	1.58	6 (10%)	66,103,113	1.44	7 (10%)
21	CLA	7	403	-	41,50,73	1.94	7 (17%)	51,86,113	1.66	8 (15%)
30	LUT	c	615	-	42,43,43	1.64	8 (19%)	51,60,60	1.50	10 (19%)
29	CHL	c	608	-	46,54,74	2.34	15 (32%)	49,90,114	3.53	23 (46%)
21	CLA	A	810	-	45,53,73	1.75	6 (13%)	52,89,113	1.61	7 (13%)
21	CLA	a	603	-	41,49,73	1.85	6 (14%)	47,84,113	1.64	7 (14%)
21	CLA	7	404	-	40,49,73	1.86	6 (15%)	45,84,113	1.63	6 (13%)
21	CLA	A	811	-	45,53,73	1.74	6 (13%)	52,89,113	1.62	8 (15%)
21	CLA	A	823	-	56,64,73	1.62	7 (12%)	65,102,113	1.42	8 (12%)
30	LUT	4	615	-	42,43,43	1.66	8 (19%)	51,60,60	1.75	10 (19%)
21	CLA	3	403	-	55,63,73	1.65	7 (12%)	64,101,113	1.44	6 (9%)
21	CLA	A	826	-	65,73,73	1.46	6 (9%)	76,113,113	1.42	8 (10%)
24	BCR	B	844	-	41,41,41	0.71	0	56,56,56	2.10	22 (39%)
21	CLA	9	604	-	45,53,73	1.75	7 (15%)	52,89,113	1.66	6 (11%)
21	CLA	B	811	-	45,53,73	1.84	7 (15%)	52,89,113	1.69	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	7	410	-	43,51,73	1.82	5 (11%)	49,86,113	1.56	6 (12%)
21	CLA	b	311	20	54,62,73	1.61	6 (11%)	62,99,113	1.51	9 (14%)
21	CLA	a	604	-	46,55,73	1.75	6 (13%)	52,91,113	1.54	7 (13%)
23	LHG	1	301	21	22,22,48	0.34	0	25,28,54	0.67	1 (4%)
21	CLA	7	413	-	37,44,73	1.95	6 (16%)	42,77,113	1.68	7 (16%)
21	CLA	7	408	-	41,49,73	1.88	5 (12%)	47,84,113	1.62	7 (14%)
21	CLA	8	601	18	45,53,73	1.80	5 (11%)	52,89,113	1.55	6 (11%)
29	CHL	a	609	-	46,54,74	2.43	16 (34%)	49,90,114	3.56	24 (48%)
21	CLA	8	611	-	54,62,73	1.65	5 (9%)	62,99,113	1.44	8 (12%)
21	CLA	7	402	-	45,53,73	1.82	6 (13%)	52,89,113	1.58	7 (13%)
21	CLA	A	814	-	65,73,73	1.45	6 (9%)	76,113,113	1.44	8 (10%)
21	CLA	5	612	-	45,53,73	1.81	5 (11%)	52,89,113	1.57	6 (11%)
29	CHL	8	605	18	41,49,74	2.21	14 (34%)	48,84,114	3.76	28 (58%)
23	LHG	b	319	21	48,48,48	0.27	0	51,54,54	0.32	0
24	BCR	4	617	-	41,41,41	1.72	8 (19%)	56,56,56	1.46	9 (16%)
21	CLA	B	822	-	45,53,73	1.76	7 (15%)	52,89,113	1.61	6 (11%)
21	CLA	B	831	-	56,64,73	1.63	7 (12%)	65,102,113	1.42	10 (15%)
21	CLA	O	202	-	36,46,73	1.95	6 (16%)	41,80,113	1.69	8 (19%)
28	LMG	2	615	-	13,13,55	0.19	0	18,18,63	0.34	0
29	CHL	8	613	-	42,50,74	2.46	15 (35%)	44,85,114	3.62	23 (52%)
21	CLA	B	825	-	65,73,73	1.45	7 (10%)	76,113,113	1.42	8 (10%)
24	BCR	O	205	-	41,41,41	1.73	8 (19%)	56,56,56	1.67	11 (19%)
21	CLA	A	827	-	63,72,73	1.48	5 (7%)	73,112,113	1.43	7 (9%)
21	CLA	b	312	23	45,53,73	1.81	5 (11%)	52,89,113	1.54	6 (11%)
25	SF4	A	851	2,1	0,12,12	-	-	-	-	-
30	LUT	2	616	-	42,43,43	1.65	8 (19%)	51,60,60	1.74	12 (23%)
21	CLA	A	837	-	51,59,73	1.70	7 (13%)	59,96,113	1.41	8 (13%)
29	CHL	6	607	-	51,59,74	2.26	16 (31%)	55,96,114	3.35	28 (50%)
32	NEX	9	617	-	38,46,46	1.61	7 (18%)	50,70,70	1.60	8 (16%)
21	CLA	3	415	-	39,48,73	1.88	6 (15%)	44,83,113	1.61	7 (15%)
21	CLA	A	835	-	50,58,73	1.64	5 (10%)	58,95,113	1.55	7 (12%)
21	CLA	b	303	20	59,67,73	1.56	6 (10%)	68,105,113	1.40	7 (10%)
21	CLA	B	819	-	43,51,73	1.77	7 (16%)	49,86,113	1.61	7 (14%)
21	CLA	B	802	-	65,73,73	1.46	7 (10%)	76,113,113	1.41	7 (9%)
21	CLA	1	306	-	39,48,73	1.87	6 (15%)	45,82,113	1.70	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	3	406	17	39,48,73	1.93	7 (17%)	48,83,113	1.68	8 (16%)
21	CLA	B	839	-	65,73,73	1.50	7 (10%)	76,113,113	1.38	8 (10%)
21	CLA	1	313	15	45,53,73	1.78	6 (13%)	52,89,113	1.57	8 (15%)
21	CLA	b	314	-	53,61,73	1.65	7 (13%)	61,98,113	1.51	7 (11%)
21	CLA	B	828	-	52,60,73	1.64	7 (13%)	60,97,113	1.51	7 (11%)
21	CLA	2	604	-	45,53,73	1.76	6 (13%)	52,89,113	1.60	7 (13%)
23	LHG	A	845	21	26,26,48	0.33	0	29,32,54	0.44	0
21	CLA	B	809	-	61,70,73	1.54	6 (9%)	70,109,113	1.35	7 (10%)
21	CLA	5	603	-	45,53,73	1.82	7 (15%)	52,89,113	1.53	7 (13%)
21	CLA	J	102	10	42,50,73	1.80	6 (14%)	48,85,113	1.58	6 (12%)
29	CHL	9	607	-	46,54,74	2.32	15 (32%)	49,90,114	3.52	23 (46%)
28	LMG	J	105	-	30,30,55	0.26	0	38,38,63	0.35	0
26	LMU	A	856	-	36,36,36	0.38	0	47,47,47	0.74	1 (2%)
21	CLA	B	804	-	65,73,73	1.50	7 (10%)	76,113,113	1.40	8 (10%)
21	CLA	3	412	-	53,62,73	1.64	6 (11%)	61,100,113	1.41	7 (11%)
23	LHG	9	618	21	48,48,48	0.27	0	51,54,54	0.33	0
31	XAT	7	416	-	39,47,47	1.70	8 (20%)	54,74,74	1.70	12 (22%)
21	CLA	c	603	-	55,63,73	1.60	6 (10%)	64,101,113	1.42	7 (10%)
29	CHL	9	605	19	46,54,74	2.36	16 (34%)	49,90,114	3.52	23 (46%)
21	CLA	O	201	23	42,50,73	1.77	6 (14%)	48,85,113	1.66	6 (12%)
21	CLA	5	614	15	43,51,73	1.90	6 (13%)	54,87,113	1.62	8 (14%)
28	LMG	G	206	-	55,55,55	0.21	0	63,63,63	0.26	0
21	CLA	G	202	-	45,53,73	1.77	6 (13%)	52,89,113	1.67	7 (13%)
21	CLA	3	404	-	41,50,73	1.90	7 (17%)	51,86,113	1.67	9 (17%)
21	CLA	2	611	-	41,49,73	1.82	6 (14%)	47,84,113	1.69	8 (17%)
21	CLA	A	820	-	44,52,73	1.82	6 (13%)	51,88,113	1.59	6 (11%)
21	CLA	6	611	-	41,49,73	1.86	5 (12%)	47,84,113	1.66	7 (14%)
24	BCR	F	303	-	41,41,41	1.72	8 (19%)	56,56,56	1.50	11 (19%)
21	CLA	B	827	-	65,73,73	1.46	6 (9%)	76,113,113	1.35	7 (9%)
31	XAT	5	616	-	39,47,47	1.65	8 (20%)	54,74,74	1.56	8 (14%)
21	CLA	1	308	-	43,52,73	1.82	6 (13%)	49,88,113	1.59	7 (14%)
29	CHL	c	609	20	43,52,74	2.46	16 (37%)	46,88,114	3.46	22 (47%)
21	CLA	b	315	-	45,53,73	1.80	6 (13%)	52,89,113	1.51	7 (13%)
21	CLA	c	604	-	45,53,73	1.78	7 (15%)	52,89,113	1.63	6 (11%)
21	CLA	9	610	19	54,62,73	1.59	6 (11%)	62,99,113	1.51	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	LUT	a	615	-	42,43,43	1.64	7 (16%)	51,60,60	1.63	10 (19%)
21	CLA	4	603	-	43,52,73	1.84	6 (13%)	49,88,113	1.56	7 (14%)
29	CHL	4	607	-	51,59,74	2.15	14 (27%)	55,96,114	3.39	27 (49%)
32	NEX	c	618	-	38,46,46	1.60	7 (18%)	50,70,70	1.61	9 (18%)
24	BCR	3	418	-	41,41,41	1.69	8 (19%)	56,56,56	1.47	9 (16%)
21	CLA	c	611	23	58,66,73	1.56	6 (10%)	67,104,113	1.43	8 (11%)
24	BCR	K	205	-	41,41,41	0.74	0	56,56,56	2.13	19 (33%)
21	CLA	4	610	23	45,53,73	1.75	6 (13%)	52,89,113	1.60	6 (11%)
21	CLA	5	602	15	61,69,73	1.53	6 (9%)	71,108,113	1.39	8 (11%)
21	CLA	B	820	-	46,54,73	1.77	6 (13%)	53,90,113	1.54	7 (13%)
23	LHG	4	618	21	36,36,48	0.32	0	39,42,54	0.40	0
21	CLA	6	612	-	45,53,73	1.85	5 (11%)	52,89,113	1.60	7 (13%)
21	CLA	2	613	-	42,50,73	1.82	6 (14%)	48,85,113	1.60	7 (14%)
21	CLA	1	310	15	42,51,73	1.81	6 (14%)	48,87,113	1.62	7 (14%)
21	CLA	A	807	1	65,73,73	1.45	6 (9%)	76,113,113	1.41	6 (7%)
21	CLA	6	613	-	42,50,73	1.84	6 (14%)	48,85,113	1.58	7 (14%)
24	BCR	B	842	-	41,41,41	1.71	8 (19%)	56,56,56	1.44	8 (14%)
24	BCR	A	846	-	41,41,41	1.71	8 (19%)	56,56,56	1.63	9 (16%)
21	CLA	2	608	16	55,63,73	1.60	6 (10%)	64,101,113	1.43	8 (12%)
21	CLA	A	838	-	65,73,73	1.44	6 (9%)	76,113,113	1.44	7 (9%)
24	BCR	G	201	-	41,41,41	1.70	8 (19%)	56,56,56	1.53	9 (16%)
26	LMU	O	206	-	36,36,36	0.40	0	47,47,47	0.69	0
21	CLA	A	812	-	65,73,73	1.45	6 (9%)	76,113,113	1.33	8 (10%)
27	DGD	B	847	-	67,67,67	0.83	2 (2%)	81,81,81	0.98	3 (3%)
24	BCR	J	104	-	41,41,41	0.92	1 (2%)	56,56,56	2.29	20 (35%)
32	NEX	b	318	-	38,46,46	1.61	7 (18%)	50,70,70	1.59	8 (16%)
21	CLA	9	612	19	45,53,73	1.80	6 (13%)	52,89,113	1.54	6 (11%)
29	CHL	8	607	-	51,59,74	2.20	16 (31%)	55,96,114	3.35	28 (50%)
21	CLA	K	202	-	50,58,73	1.66	6 (12%)	58,95,113	1.66	11 (18%)
21	CLA	B	824	-	65,73,73	1.45	6 (9%)	76,113,113	1.43	8 (10%)
29	CHL	6	614	-	46,54,74	2.39	16 (34%)	49,90,114	3.46	25 (51%)
29	CHL	2	607	-	51,59,74	2.17	14 (27%)	55,96,114	3.41	27 (49%)
30	LUT	a	616	-	42,43,43	1.66	8 (19%)	51,60,60	1.57	10 (19%)
24	BCR	8	616	-	41,41,41	1.75	8 (19%)	56,56,56	1.49	9 (16%)
24	BCR	I	101	-	41,41,41	1.73	8 (19%)	56,56,56	1.49	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	A	821	-	65,73,73	1.45	6 (9%)	76,113,113	1.42	9 (11%)
21	CLA	8	612	-	43,51,73	1.83	5 (11%)	49,86,113	1.56	7 (14%)
24	BCR	L	305	-	41,41,41	1.71	8 (19%)	56,56,56	1.46	8 (14%)
21	CLA	A	830	-	52,60,73	1.78	7 (13%)	60,97,113	2.10	16 (26%)
25	SF4	C	102	3	0,12,12	-	-	-	-	-
21	CLA	4	612	-	55,63,73	1.62	6 (10%)	64,101,113	1.45	8 (12%)
21	CLA	3	414	-	37,44,73	1.93	7 (18%)	42,77,113	1.64	6 (14%)
21	CLA	7	407	17	43,52,73	2.35	11 (25%)	49,88,113	4.02	23 (46%)
29	CHL	c	605	-	42,51,74	2.39	15 (35%)	46,86,114	3.75	23 (50%)
21	CLA	A	842	-	65,73,73	1.47	7 (10%)	76,113,113	1.37	7 (9%)
29	CHL	b	307	-	46,54,74	2.30	14 (30%)	49,90,114	3.57	23 (46%)
21	CLA	A	852	-	52,60,73	1.65	7 (13%)	60,97,113	1.52	9 (15%)
21	CLA	a	614	-	41,49,73	1.85	6 (14%)	47,84,113	1.60	8 (17%)
28	LMG	6	615	-	13,13,55	0.20	0	18,18,63	0.49	0
21	CLA	A	818	-	52,60,73	1.73	7 (13%)	60,97,113	1.50	8 (13%)
31	XAT	c	617	-	39,47,47	1.67	8 (20%)	54,74,74	1.66	10 (18%)
21	CLA	L	302	12	45,53,73	1.77	6 (13%)	52,89,113	1.63	8 (15%)
21	CLA	A	816	-	42,50,73	1.77	6 (14%)	48,85,113	1.66	7 (14%)
21	CLA	8	610	-	44,52,73	1.82	6 (13%)	51,88,113	1.57	6 (11%)
21	CLA	6	609	-	42,50,73	1.82	6 (14%)	48,85,113	1.72	7 (14%)
21	CLA	2	610	23	41,50,73	1.81	6 (14%)	49,85,113	1.61	6 (12%)
21	CLA	5	605	-	39,48,73	1.90	6 (15%)	45,82,113	1.65	8 (17%)
21	CLA	a	611	-	47,55,73	1.75	5 (10%)	54,91,113	1.53	7 (12%)
21	CLA	B	823	-	65,73,73	1.46	6 (9%)	76,113,113	1.50	9 (11%)
30	LUT	b	317	-	42,43,43	1.62	8 (19%)	51,60,60	1.55	10 (19%)
21	CLA	O	203	-	49,58,73	1.66	6 (12%)	58,94,113	1.52	8 (13%)
25	SF4	C	101	3	0,12,12	-	-	-	-	-
21	CLA	B	808	2	65,73,73	1.46	6 (9%)	76,113,113	1.40	6 (7%)
21	CLA	B	818	-	58,66,73	1.56	7 (12%)	67,104,113	1.42	7 (10%)
29	CHL	a	601	20	46,54,74	2.39	16 (34%)	49,90,114	3.54	24 (48%)
21	CLA	A	803	-	52,60,73	1.62	6 (11%)	60,97,113	1.53	9 (15%)
29	CHL	2	601	16	53,61,74	2.14	15 (28%)	57,98,114	3.36	28 (49%)
29	CHL	6	601	16	44,52,74	2.43	16 (36%)	51,88,114	3.79	26 (50%)
21	CLA	B	840	23	65,73,73	1.43	6 (9%)	76,113,113	1.43	7 (9%)
21	CLA	A	819	-	65,73,73	1.48	6 (9%)	76,113,113	1.38	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	LHG	8	617	21	36,36,48	0.31	0	39,42,54	0.36	0
31	XAT	3	417	-	39,47,47	1.67	8 (20%)	54,74,74	1.60	9 (16%)
21	CLA	A	815	-	45,53,73	1.74	6 (13%)	52,89,113	1.62	7 (13%)
31	XAT	9	616	-	39,47,47	1.73	8 (20%)	54,74,74	2.33	15 (27%)
21	CLA	a	612	-	45,53,73	1.81	5 (11%)	52,89,113	1.56	6 (11%)
31	XAT	8	615	-	39,47,47	1.71	8 (20%)	54,74,74	1.67	9 (16%)
21	CLA	A	822	-	44,52,73	1.80	6 (13%)	51,88,113	1.65	7 (13%)
21	CLA	F	302	-	61,69,73	1.52	6 (9%)	71,108,113	1.43	9 (12%)
30	LUT	6	616	-	42,43,43	1.65	8 (19%)	51,60,60	1.66	12 (23%)
21	CLA	5	609	-	42,51,73	1.84	6 (14%)	48,87,113	1.60	7 (14%)
21	CLA	1	315	-	45,53,73	1.80	6 (13%)	52,89,113	1.57	7 (13%)
21	CLA	K	203	-	44,52,73	1.82	8 (18%)	55,88,113	1.66	8 (14%)

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
29	CHL	8	606	-	3/3/16/26	5/15/113/137	-
31	XAT	4	616	-	-	0/31/93/93	0/4/4/4
21	CLA	A	824	-	1/1/13/20	11/25/103/115	-
21	CLA	B	817	-	1/1/15/20	20/37/115/115	-
24	BCR	A	854	-	-	0/29/63/63	0/2/2/2
24	BCR	A	847	-	-	0/29/63/63	0/2/2/2
24	BCR	F	301	-	-	0/29/63/63	0/2/2/2
21	CLA	L	303	-	1/1/11/20	3/13/91/115	-
30	LUT	c	616	-	-	0/29/67/67	0/2/2/2
26	LMU	A	853	-	-	0/21/61/61	0/2/2/2
21	CLA	8	608	18	1/1/10/20	4/7/87/115	-
29	CHL	5	601	15	3/3/16/26	7/15/113/137	-
29	CHL	2	614	-	3/3/16/26	4/15/113/137	-
30	LUT	9	615	-	-	2/29/67/67	0/2/2/2
29	CHL	b	306	20	3/3/16/26	6/15/113/137	-
21	CLA	A	839	-	1/1/11/20	2/13/91/115	-
21	CLA	1	304	-	1/1/13/20	5/25/103/115	-
21	CLA	G	204	7	1/1/11/20	4/11/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	4	602	18	1/1/13/20	10/28/106/115	-
21	CLA	8	602	18	1/1/13/20	8/28/106/115	-
21	CLA	G	203	-	1/1/12/20	7/19/97/115	-
23	LHG	A	855	-	-	7/53/53/53	-
29	CHL	2	605	-	3/3/16/26	3/15/113/137	-
29	CHL	a	605	20	3/3/16/26	4/13/111/137	-
29	CHL	6	605	-	3/3/16/26	3/15/113/137	-
21	CLA	7	401	17	1/1/11/20	6/13/91/115	-
21	CLA	7	414	-	1/1/10/20	2/6/84/115	-
29	CHL	1	302	15	3/3/17/26	8/21/119/137	-
21	CLA	F	304	-	1/1/11/20	1/13/91/115	-
29	CHL	4	614	18	3/3/15/26	2/10/108/137	-
24	BCR	3	419	-	-	8/29/63/63	0/2/2/2
24	BCR	J	103	-	-	3/29/63/63	0/2/2/2
21	CLA	5	604	-	1/1/11/20	6/18/96/115	-
21	CLA	7	411	-	1/1/13/20	7/23/101/115	-
29	CHL	6	602	-	3/3/17/26	9/24/122/137	-
21	CLA	4	601	18	1/1/11/20	3/13/91/115	-
29	CHL	b	302	20	3/3/16/26	8/15/113/137	-
21	CLA	A	808	-	1/1/11/20	3/13/91/115	-
21	CLA	6	604	-	1/1/11/20	6/13/91/115	-
21	CLA	5	613	-	1/1/10/20	2/4/80/115	-
21	CLA	B	805	-	1/1/15/20	19/37/115/115	-
21	CLA	4	608	18	1/1/10/20	0/7/87/115	-
21	CLA	a	610	20	1/1/11/20	4/13/91/115	-
21	CLA	5	608	15	1/1/10/20	4/8/84/115	-
21	CLA	B	836	-	1/1/15/20	16/37/115/115	-
21	CLA	3	409	17	1/1/12/20	10/22/100/115	-
29	CHL	9	606	19	3/3/16/26	6/15/113/137	-
29	CHL	b	308	-	3/3/17/26	7/24/122/137	-
29	CHL	7	406	-	3/3/15/26	0/6/104/137	-
21	CLA	B	834	-	1/1/11/20	5/13/91/115	-
21	CLA	A	829	-	1/1/15/20	9/37/115/115	-
21	CLA	B	833	-	1/1/11/20	1/13/91/115	-
21	CLA	B	812	-	1/1/15/20	19/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	9	602	19	1/1/12/20	5/23/101/115	-
21	CLA	c	613	-	1/1/15/20	13/37/115/115	-
21	CLA	7	405	17	1/1/10/20	3/8/84/115	-
21	CLA	3	413	-	1/1/10/20	0/6/84/115	-
21	CLA	6	608	16	1/1/11/20	5/13/91/115	-
31	XAT	6	617	-	-	6/31/93/93	0/4/4/4
21	CLA	3	401	-	1/1/10/20	0/6/84/115	-
21	CLA	B	830	-	1/1/13/20	12/27/105/115	-
21	CLA	B	832	-	1/1/13/20	7/27/105/115	-
29	CHL	c	601	20	3/3/16/26	5/19/117/137	-
21	CLA	8	609	23	1/1/11/20	6/13/91/115	-
29	CHL	9	609	-	3/3/16/26	5/15/113/137	-
21	CLA	L	304	-	1/1/10/20	4/10/88/115	-
21	CLA	B	838	-	1/1/15/20	8/37/115/115	-
21	CLA	1	309	15	1/1/10/20	3/8/86/115	-
21	CLA	B	826	-	1/1/12/20	9/22/100/115	-
24	BCR	A	849	-	-	3/29/63/63	0/2/2/2
21	CLA	4	609	18	-	10/22/100/115	-
24	BCR	B	843	-	-	12/29/63/63	0/2/2/2
21	CLA	8	618	-	1/1/10/20	3/8/86/115	-
31	XAT	2	617	-	-	0/31/93/93	0/4/4/4
21	CLA	c	612	20	1/1/10/20	3/11/90/115	-
21	CLA	1	312	15	1/1/11/20	5/13/91/115	-
21	CLA	4	604	-	1/1/10/20	3/9/88/115	-
21	CLA	b	313	20	1/1/11/20	6/13/91/115	-
31	XAT	a	618	-	-	1/31/93/93	0/4/4/4
24	BCR	J	101	-	-	7/29/63/63	0/2/2/2
21	CLA	3	408	17	1/1/13/20	7/30/108/115	-
30	LUT	8	614	-	-	4/29/67/67	0/2/2/2
21	CLA	A	828	-	1/1/14/20	14/31/109/115	-
21	CLA	1	303	15	1/1/14/20	17/33/111/115	-
29	CHL	5	606	-	3/3/16/26	5/15/113/137	-
21	CLA	1	311	23	1/1/10/20	0/4/80/115	-
21	CLA	A	831	-	1/1/13/20	8/25/103/115	-
21	CLA	B	801	-	1/1/15/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	A	825	-	1/1/15/20	11/37/115/115	-
23	LHG	A	844	-	-	10/53/53/53	-
30	LUT	7	415	-	-	6/29/67/67	0/2/2/2
21	CLA	A	836	1	1/1/11/20	4/13/91/115	-
23	LHG	1	319	21	-	7/32/32/53	-
21	CLA	B	803	-	1/1/13/20	7/25/103/115	-
29	CHL	2	606	-	3/3/16/26	2/15/113/137	-
29	CHL	a	606	-	3/3/16/26	5/15/113/137	-
29	CHL	6	606	-	3/3/16/26	5/15/113/137	-
21	CLA	B	835	-	1/1/15/20	8/37/115/115	-
29	CHL	4	605	-	3/3/15/26	2/10/106/137	-
21	CLA	A	834	-	1/1/15/20	10/37/115/115	-
29	CHL	9	601	19	3/3/15/26	2/12/110/137	-
21	CLA	1	305	-	1/1/11/20	7/18/96/115	-
21	CLA	2	603	-	1/1/11/20	6/13/91/115	-
21	CLA	7	409	-	1/1/10/20	1/6/84/115	-
21	CLA	6	603	-	1/1/11/20	6/13/91/115	-
21	CLA	B	806	-	1/1/14/20	13/35/113/115	-
29	CHL	9	608	-	3/3/16/26	5/15/113/137	-
21	CLA	K	204	11	1/1/11/20	5/13/91/115	-
21	CLA	K	201	11	1/1/11/20	4/15/93/115	-
21	CLA	1	314	-	1/1/10/20	2/4/80/115	-
26	LMU	3	420	-	-	3/21/61/61	0/2/2/2
24	BCR	L	301	-	-	4/29/63/63	0/2/2/2
29	CHL	c	606	20	3/3/16/26	4/15/113/137	-
21	CLA	A	809	1	1/1/13/20	5/30/108/115	-
21	CLA	3	411	17	1/1/10/20	3/11/89/115	-
21	CLA	A	841	-	1/1/15/20	18/37/115/115	-
21	CLA	B	810	-	1/1/13/20	3/25/101/115	-
21	CLA	c	602	20	1/1/14/20	5/31/109/115	-
21	CLA	A	804	-	1/1/15/20	9/37/115/115	-
24	BCR	7	417	-	-	2/29/63/63	0/2/2/2
30	LUT	9	614	-	-	2/29/67/67	0/2/2/2
21	CLA	3	405	-	1/1/10/20	3/8/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	B	845	-	-	2/29/63/63	0/2/2/2
21	CLA	O	204	-	1/1/10/20	3/6/84/115	-
21	CLA	B	837	-	1/1/15/20	12/35/113/115	-
21	CLA	8	603	-	1/1/11/20	4/11/89/115	-
23	LHG	c	619	21	-	6/53/53/53	-
21	CLA	A	801	-	-	6/22/100/115	-
21	CLA	B	815	-	1/1/13/20	5/23/101/115	-
21	CLA	B	821	-	1/1/13/20	4/25/103/115	-
21	CLA	B	816	-	1/1/12/20	4/22/100/115	-
21	CLA	5	611	15	1/1/11/20	5/13/91/115	-
21	CLA	1	316	15	1/1/11/20	4/11/87/115	-
21	CLA	A	832	-	1/1/11/20	5/13/91/115	-
29	CHL	b	309	-	3/3/16/26	5/19/117/137	-
29	CHL	a	607	-	3/3/15/26	1/12/110/137	-
21	CLA	3	410	-	1/1/10/20	1/6/84/115	-
21	CLA	B	813	-	1/1/11/20	2/11/89/115	-
21	CLA	F	305	6	1/1/10/20	3/8/86/115	-
24	BCR	A	850	-	-	4/29/63/63	0/2/2/2
21	CLA	b	305	-	1/1/11/20	6/13/91/115	-
22	PQN	B	841	-	-	1/23/43/43	0/2/2/2
30	LUT	1	317	-	-	4/29/67/67	0/2/2/2
21	CLA	A	817	-	1/1/15/20	19/37/115/115	-
21	CLA	9	613	-	1/1/12/20	8/23/101/115	-
29	CHL	2	602	16	3/3/17/26	9/24/122/137	-
24	BCR	M	101	-	-	8/29/63/63	0/2/2/2
21	CLA	9	603	19	1/1/11/20	3/13/91/115	-
29	CHL	3	407	-	3/3/15/26	0/6/104/137	-
24	BCR	L	306	-	-	4/29/63/63	0/2/2/2
21	CLA	4	613	-	1/1/10/20	0/11/89/115	-
21	CLA	b	304	-	1/1/11/20	4/13/91/115	-
30	LUT	5	615	-	-	7/29/67/67	0/2/2/2
21	CLA	B	807	-	1/1/15/20	16/37/115/115	-
21	CLA	A	833	-	1/1/15/20	7/37/115/115	-
29	CHL	b	310	-	3/3/17/26	2/22/120/137	-
31	XAT	1	318	-	-	0/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	a	602	-	1/1/14/20	11/31/109/115	-
21	CLA	2	609	16	1/1/11/20	9/20/98/115	-
24	BCR	2	618	-	-	3/29/63/63	0/2/2/2
24	BCR	6	618	-	-	4/29/63/63	0/2/2/2
21	CLA	A	806	-	1/1/15/20	20/37/115/115	-
21	CLA	8	604	-	1/1/10/20	8/9/88/115	-
22	PQN	A	843	-	-	1/23/43/43	0/2/2/2
26	LMU	b	301	-	-	6/21/61/61	0/2/2/2
23	LHG	2	619	21	-	7/39/39/53	-
21	CLA	c	614	-	1/1/11/20	7/13/91/115	-
24	BCR	7	418	-	-	6/29/63/63	0/2/2/2
23	LHG	6	619	-	-	5/39/39/53	-
29	CHL	1	307	-	3/3/17/26	2/21/119/137	-
21	CLA	A	805	-	1/1/13/20	6/25/103/115	-
21	CLA	3	402	17	1/1/14/20	5/31/109/115	-
24	BCR	A	848	-	-	2/29/63/63	0/2/2/2
21	CLA	2	612	16	1/1/11/20	6/13/91/115	-
21	CLA	A	802	-	1/1/12/20	1/22/100/115	-
21	CLA	5	607	-	1/1/11/20	2/11/89/115	-
21	CLA	4	611	18	1/1/11/20	4/11/89/115	-
24	BCR	B	846	-	-	3/29/63/63	0/2/2/2
29	CHL	4	606	-	3/3/16/26	4/15/113/137	-
21	CLA	6	610	-	1/1/10/20	0/7/85/115	-
29	CHL	a	608	-	3/3/16/26	5/15/113/137	-
30	LUT	b	316	-	-	2/29/67/67	0/2/2/2
21	CLA	B	829	-	1/1/11/20	2/13/91/115	-
23	LHG	a	617	-	-	10/53/53/53	-
30	LUT	3	416	-	-	5/29/67/67	0/2/2/2
21	CLA	B	814	-	1/1/14/20	8/31/109/115	-
24	BCR	G	205	-	-	2/29/63/63	0/2/2/2
21	CLA	7	412	-	1/1/10/20	0/6/84/115	-
21	CLA	H	201	8	1/1/11/20	4/13/91/115	-
23	LHG	5	617	-	-	7/32/32/53	-
23	LHG	4	619	-	-	11/53/53/53	-
21	CLA	a	613	-	1/1/13/20	5/28/106/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	5	610	-	1/1/10/20	0/4/80/115	-
21	CLA	c	610	20	1/1/11/20	7/13/91/115	-
29	CHL	c	607	-	3/3/16/26	3/15/113/137	-
21	CLA	A	813	-	1/1/12/20	4/24/102/115	-
21	CLA	A	840	-	1/1/15/20	14/37/115/115	-
21	CLA	9	611	23	1/1/13/20	7/28/106/115	-
21	CLA	7	403	-	1/1/11/20	2/9/85/115	-
30	LUT	c	615	-	-	1/29/67/67	0/2/2/2
29	CHL	c	608	-	3/3/16/26	7/15/113/137	-
21	CLA	A	810	-	1/1/11/20	4/13/91/115	-
21	CLA	a	603	-	1/1/10/20	0/8/86/115	-
21	CLA	7	404	-	1/1/10/20	3/8/86/115	-
21	CLA	A	811	-	1/1/11/20	3/13/91/115	-
21	CLA	A	823	-	1/1/13/20	7/27/105/115	-
30	LUT	4	615	-	-	4/29/67/67	0/2/2/2
21	CLA	3	403	-	1/1/13/20	6/25/103/115	-
21	CLA	A	826	-	1/1/15/20	9/37/115/115	-
24	BCR	B	844	-	-	11/29/63/63	0/2/2/2
21	CLA	9	604	-	1/1/11/20	7/13/91/115	-
21	CLA	B	811	-	1/1/11/20	3/13/91/115	-
21	CLA	7	410	-	1/1/10/20	3/11/89/115	-
21	CLA	b	311	20	1/1/12/20	9/24/102/115	-
21	CLA	a	604	-	1/1/11/20	8/15/93/115	-
23	LHG	1	301	21	-	7/26/26/53	-
21	CLA	7	413	-	1/1/8/20	0/0/74/115	-
21	CLA	7	408	-	1/1/10/20	2/8/86/115	-
21	CLA	8	601	18	1/1/11/20	9/13/91/115	-
29	CHL	a	609	-	3/3/16/26	5/15/113/137	-
21	CLA	8	611	-	1/1/12/20	13/23/101/115	-
21	CLA	7	402	-	1/1/11/20	9/13/91/115	-
21	CLA	A	814	-	1/1/15/20	10/37/115/115	-
21	CLA	5	612	-	1/1/11/20	5/13/91/115	-
29	CHL	8	605	18	3/3/15/26	4/10/106/137	-
23	LHG	b	319	21	-	8/53/53/53	-
24	BCR	4	617	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	B	822	-	1/1/11/20	6/13/91/115	-
21	CLA	B	831	-	1/1/13/20	9/27/105/115	-
21	CLA	O	202	-	1/1/9/20	2/4/78/115	-
28	LMG	2	615	-	-	1/4/24/70	0/1/1/1
29	CHL	8	613	-	3/3/15/26	4/10/108/137	-
21	CLA	B	825	-	1/1/15/20	12/37/115/115	-
24	BCR	O	205	-	-	8/29/63/63	0/2/2/2
21	CLA	A	827	-	1/1/15/20	17/35/113/115	-
21	CLA	b	312	23	1/1/11/20	2/13/91/115	-
25	SF4	A	851	2,1	-	-	0/6/5/5
30	LUT	2	616	-	-	4/29/67/67	0/2/2/2
21	CLA	A	837	-	1/1/12/20	7/21/99/115	-
29	CHL	6	607	-	3/3/17/26	5/21/119/137	-
32	NEX	9	617	-	-	2/27/83/83	0/3/3/3
21	CLA	3	415	-	1/1/10/20	1/6/84/115	-
21	CLA	A	835	-	1/1/12/20	2/19/97/115	-
21	CLA	b	303	20	1/1/13/20	12/30/108/115	-
21	CLA	B	819	-	1/1/10/20	4/11/89/115	-
21	CLA	B	802	-	1/1/15/20	19/37/115/115	-
21	CLA	1	306	-	1/1/9/20	4/8/82/115	-
21	CLA	3	406	17	1/1/10/20	0/8/84/115	-
21	CLA	B	839	-	1/1/15/20	10/37/115/115	-
21	CLA	1	313	15	1/1/11/20	4/13/91/115	-
21	CLA	b	314	-	1/1/12/20	9/23/101/115	-
21	CLA	B	828	-	1/1/12/20	6/22/100/115	-
21	CLA	2	604	-	1/1/11/20	4/13/91/115	-
23	LHG	A	845	21	-	6/31/31/53	-
21	CLA	B	809	-	1/1/14/20	11/33/111/115	-
21	CLA	5	603	-	1/1/11/20	3/13/91/115	-
21	CLA	J	102	10	1/1/10/20	8/10/88/115	-
29	CHL	9	607	-	3/3/16/26	7/15/113/137	-
28	LMG	J	105	-	-	5/25/45/70	0/1/1/1
26	LMU	A	856	-	-	3/21/61/61	0/2/2/2
21	CLA	B	804	-	1/1/15/20	12/37/115/115	-
21	CLA	3	412	-	1/1/13/20	9/23/101/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	LHG	9	618	21	-	10/53/53/53	-
31	XAT	7	416	-	-	0/31/93/93	0/4/4/4
21	CLA	c	603	-	1/1/13/20	6/25/103/115	-
29	CHL	9	605	19	3/3/16/26	2/15/113/137	-
21	CLA	O	201	23	1/1/10/20	4/10/88/115	-
21	CLA	5	614	15	1/1/11/20	5/11/87/115	-
28	LMG	G	206	-	-	10/50/70/70	0/1/1/1
21	CLA	G	202	-	1/1/11/20	6/13/91/115	-
21	CLA	3	404	-	1/1/11/20	0/9/85/115	-
21	CLA	2	611	-	1/1/10/20	0/8/86/115	-
21	CLA	A	820	-	1/1/11/20	1/11/89/115	-
21	CLA	6	611	-	1/1/10/20	3/8/86/115	-
24	BCR	F	303	-	-	0/29/63/63	0/2/2/2
21	CLA	B	827	-	1/1/15/20	12/37/115/115	-
31	XAT	5	616	-	-	4/31/93/93	0/4/4/4
21	CLA	1	308	-	1/1/11/20	3/11/89/115	-
29	CHL	c	609	20	3/3/16/26	7/11/109/137	-
21	CLA	b	315	-	1/1/11/20	10/13/91/115	-
21	CLA	c	604	-	1/1/11/20	7/13/91/115	-
21	CLA	9	610	19	1/1/12/20	3/24/102/115	-
30	LUT	a	615	-	-	5/29/67/67	0/2/2/2
21	CLA	4	603	-	1/1/11/20	5/11/89/115	-
29	CHL	4	607	-	3/3/17/26	4/21/119/137	-
32	NEX	c	618	-	-	2/27/83/83	0/3/3/3
24	BCR	3	418	-	-	4/29/63/63	0/2/2/2
21	CLA	c	611	23	1/1/13/20	9/29/107/115	-
24	BCR	K	205	-	-	3/29/63/63	0/2/2/2
21	CLA	4	610	23	1/1/11/20	2/13/91/115	-
21	CLA	5	602	15	1/1/14/20	17/33/111/115	-
21	CLA	B	820	-	1/1/11/20	3/15/93/115	-
23	LHG	4	618	21	-	9/41/41/53	-
21	CLA	6	612	-	1/1/11/20	5/13/91/115	-
21	CLA	2	613	-	1/1/10/20	1/10/88/115	-
21	CLA	1	310	15	1/1/11/20	3/9/87/115	-
21	CLA	A	807	1	1/1/15/20	11/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	6	613	-	1/1/10/20	4/10/88/115	-
24	BCR	B	842	-	-	0/29/63/63	0/2/2/2
24	BCR	A	846	-	-	4/29/63/63	0/2/2/2
21	CLA	2	608	16	1/1/13/20	8/25/103/115	-
21	CLA	A	838	-	1/1/15/20	13/37/115/115	-
24	BCR	G	201	-	-	0/29/63/63	0/2/2/2
26	LMU	O	206	-	-	5/21/61/61	0/2/2/2
21	CLA	A	812	-	1/1/15/20	5/37/115/115	-
27	DGD	B	847	-	-	16/55/95/95	0/2/2/2
24	BCR	J	104	-	-	9/29/63/63	0/2/2/2
32	NEX	b	318	-	-	2/27/83/83	0/3/3/3
21	CLA	9	612	19	1/1/11/20	4/13/91/115	-
29	CHL	8	607	-	3/3/17/26	5/21/119/137	-
21	CLA	K	202	-	1/1/12/20	2/19/97/115	-
21	CLA	B	824	-	1/1/15/20	10/37/115/115	-
29	CHL	6	614	-	3/3/16/26	5/15/113/137	-
29	CHL	2	607	-	3/3/17/26	4/21/119/137	-
30	LUT	a	616	-	-	4/29/67/67	0/2/2/2
24	BCR	8	616	-	-	6/29/63/63	0/2/2/2
24	BCR	I	101	-	-	4/29/63/63	0/2/2/2
21	CLA	A	821	-	1/1/15/20	11/37/115/115	-
21	CLA	8	612	-	1/1/10/20	3/11/89/115	-
24	BCR	L	305	-	-	2/29/63/63	0/2/2/2
21	CLA	A	830	-	1/1/12/20	4/22/100/115	-
25	SF4	C	102	3	-	-	0/6/5/5
21	CLA	4	612	-	1/1/13/20	5/25/103/115	-
21	CLA	3	414	-	1/1/8/20	0/0/74/115	-
21	CLA	7	407	17	-	5/11/89/115	-
29	CHL	c	605	-	3/3/15/26	3/9/107/137	-
21	CLA	A	842	-	1/1/15/20	14/37/115/115	-
29	CHL	b	307	-	3/3/16/26	3/15/113/137	-
21	CLA	A	852	-	1/1/12/20	6/22/100/115	-
21	CLA	a	614	-	1/1/10/20	2/8/86/115	-
28	LMG	6	615	-	-	3/4/24/70	0/1/1/1
21	CLA	A	818	-	1/1/12/20	8/22/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	XAT	c	617	-	-	1/31/93/93	0/4/4/4
21	CLA	L	302	12	1/1/11/20	7/13/91/115	-
21	CLA	A	816	-	1/1/10/20	3/10/88/115	-
21	CLA	8	610	-	1/1/11/20	6/11/89/115	-
21	CLA	6	609	-	1/1/10/20	5/10/88/115	-
21	CLA	2	610	23	1/1/10/20	1/7/85/115	-
21	CLA	5	605	-	1/1/9/20	4/8/82/115	-
21	CLA	a	611	-	1/1/11/20	6/16/94/115	-
21	CLA	B	823	-	1/1/15/20	12/37/115/115	-
30	LUT	b	317	-	-	2/29/67/67	0/2/2/2
21	CLA	O	203	-	1/1/11/20	4/17/95/115	-
25	SF4	C	101	3	-	-	0/6/5/5
21	CLA	B	808	2	1/1/15/20	7/37/115/115	-
21	CLA	B	818	-	1/1/13/20	9/29/107/115	-
29	CHL	a	601	20	3/3/16/26	4/15/113/137	-
21	CLA	A	803	-	1/1/12/20	7/22/100/115	-
29	CHL	2	601	16	3/3/17/26	10/24/122/137	-
29	CHL	6	601	16	3/3/16/26	6/11/109/137	-
21	CLA	B	840	23	1/1/15/20	6/37/115/115	-
21	CLA	A	819	-	1/1/15/20	16/37/115/115	-
23	LHG	8	617	21	-	9/41/41/53	-
31	XAT	3	417	-	-	0/31/93/93	0/4/4/4
21	CLA	A	815	-	1/1/11/20	5/13/91/115	-
31	XAT	9	616	-	-	8/31/93/93	0/4/4/4
21	CLA	a	612	-	1/1/11/20	5/13/91/115	-
31	XAT	8	615	-	-	0/31/93/93	0/4/4/4
21	CLA	A	822	-	1/1/11/20	1/11/89/115	-
21	CLA	F	302	-	1/1/14/20	8/33/111/115	-
30	LUT	6	616	-	-	2/29/67/67	0/2/2/2
21	CLA	5	609	-	1/1/11/20	3/9/87/115	-
21	CLA	1	315	-	1/1/11/20	4/13/91/115	-
21	CLA	K	203	-	1/1/11/20	2/13/89/115	-

All (2580) bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	7	412	CLA	C4B-NB	8.30	1.42	1.35
21	A	818	CLA	C4B-NB	8.22	1.42	1.35
21	7	407	CLA	C1D-ND	8.02	1.47	1.37
21	6	603	CLA	C4B-NB	7.91	1.42	1.35
21	B	811	CLA	C4B-NB	7.88	1.42	1.35
21	6	612	CLA	C4B-NB	7.84	1.42	1.35
21	B	831	CLA	C4B-NB	7.80	1.42	1.35
21	9	612	CLA	C4B-NB	7.76	1.42	1.35
21	1	312	CLA	C4B-NB	7.74	1.42	1.35
21	b	312	CLA	C4B-NB	7.73	1.42	1.35
21	7	408	CLA	C4B-NB	7.73	1.42	1.35
21	6	604	CLA	C4B-NB	7.71	1.42	1.35
21	9	603	CLA	C4B-NB	7.68	1.42	1.35
21	2	603	CLA	C4B-NB	7.67	1.42	1.35
21	A	839	CLA	C4B-NB	7.66	1.42	1.35
21	B	829	CLA	C4B-NB	7.65	1.42	1.35
21	5	603	CLA	C4B-NB	7.65	1.42	1.35
21	3	408	CLA	C4B-NB	7.65	1.42	1.35
21	5	614	CLA	C4B-NB	7.64	1.42	1.35
21	B	815	CLA	C4B-NB	7.62	1.42	1.35
21	8	612	CLA	C4B-NB	7.62	1.42	1.35
21	A	833	CLA	C4B-NB	7.62	1.42	1.35
21	a	612	CLA	C4B-NB	7.61	1.42	1.35
21	4	603	CLA	C4B-NB	7.61	1.42	1.35
21	3	411	CLA	C4B-NB	7.61	1.42	1.35
21	5	612	CLA	C4B-NB	7.61	1.42	1.35
21	7	410	CLA	C4B-NB	7.60	1.42	1.35
21	6	611	CLA	C4B-NB	7.59	1.42	1.35
21	8	603	CLA	C4B-NB	7.59	1.42	1.35
21	c	612	CLA	C4B-NB	7.59	1.42	1.35
21	3	403	CLA	C4B-NB	7.59	1.42	1.35
21	A	823	CLA	C4B-NB	7.58	1.42	1.35
21	F	304	CLA	C4B-NB	7.58	1.42	1.35
21	a	613	CLA	C4B-NB	7.58	1.42	1.35
21	B	821	CLA	C4B-NB	7.57	1.42	1.35
21	7	402	CLA	C4B-NB	7.57	1.42	1.35
21	8	601	CLA	C4B-NB	7.57	1.42	1.35
21	8	611	CLA	C4B-NB	7.57	1.42	1.35
21	3	410	CLA	C4B-NB	7.56	1.42	1.35
21	c	614	CLA	C4B-NB	7.56	1.42	1.35
21	5	611	CLA	C4B-NB	7.55	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	7	411	CLA	C4B-NB	7.55	1.41	1.35
21	B	804	CLA	C4B-NB	7.55	1.41	1.35
21	7	413	CLA	C4B-NB	7.55	1.41	1.35
21	a	611	CLA	C4B-NB	7.55	1.41	1.35
21	b	313	CLA	C4B-NB	7.54	1.41	1.35
21	1	315	CLA	C4B-NB	7.54	1.41	1.35
21	6	608	CLA	C4B-NB	7.53	1.41	1.35
21	A	802	CLA	C4B-NB	7.53	1.41	1.35
21	6	613	CLA	C4B-NB	7.53	1.41	1.35
21	7	409	CLA	C4B-NB	7.53	1.41	1.35
21	B	810	CLA	C4B-NB	7.53	1.41	1.35
21	2	613	CLA	C4B-NB	7.53	1.41	1.35
21	4	612	CLA	C4B-NB	7.53	1.41	1.35
21	a	603	CLA	C4B-NB	7.53	1.41	1.35
21	1	316	CLA	C4B-NB	7.52	1.41	1.35
21	7	414	CLA	C4B-NB	7.52	1.41	1.35
21	a	614	CLA	C4B-NB	7.52	1.41	1.35
21	5	607	CLA	C4B-NB	7.51	1.41	1.35
21	3	413	CLA	C4B-NB	7.51	1.41	1.35
21	G	203	CLA	C4B-NB	7.51	1.41	1.35
21	B	820	CLA	C4B-NB	7.50	1.41	1.35
21	A	841	CLA	C4B-NB	7.50	1.41	1.35
21	1	304	CLA	C4B-NB	7.50	1.41	1.35
21	B	839	CLA	C4B-NB	7.50	1.41	1.35
21	7	401	CLA	C4B-NB	7.50	1.41	1.35
21	8	610	CLA	C4B-NB	7.49	1.41	1.35
21	8	608	CLA	C4B-NB	7.48	1.41	1.35
21	A	820	CLA	C4B-NB	7.48	1.41	1.35
21	7	403	CLA	C4B-NB	7.48	1.41	1.35
21	A	836	CLA	C4B-NB	7.47	1.41	1.35
21	1	308	CLA	C4B-NB	7.47	1.41	1.35
21	4	601	CLA	C4B-NB	7.46	1.41	1.35
21	G	204	CLA	C4B-NB	7.46	1.41	1.35
21	3	414	CLA	C4B-NB	7.45	1.41	1.35
21	O	204	CLA	C4B-NB	7.45	1.41	1.35
21	7	405	CLA	C4B-NB	7.45	1.41	1.35
21	G	202	CLA	C4B-NB	7.45	1.41	1.35
21	b	315	CLA	C4B-NB	7.44	1.41	1.35
21	1	314	CLA	C4B-NB	7.44	1.41	1.35
21	3	412	CLA	C4B-NB	7.44	1.41	1.35
21	b	314	CLA	C4B-NB	7.44	1.41	1.35
21	5	604	CLA	C4B-NB	7.44	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	5	609	CLA	C4B-NB	7.43	1.41	1.35
21	B	809	CLA	C4B-NB	7.43	1.41	1.35
21	5	613	CLA	C4B-NB	7.43	1.41	1.35
21	a	610	CLA	C4B-NB	7.43	1.41	1.35
21	b	305	CLA	C4B-NB	7.43	1.41	1.35
21	6	610	CLA	C4B-NB	7.43	1.41	1.35
21	4	613	CLA	C4B-NB	7.42	1.41	1.35
21	a	602	CLA	C4B-NB	7.42	1.41	1.35
21	5	610	CLA	C4B-NB	7.42	1.41	1.35
21	8	604	CLA	C4B-NB	7.42	1.41	1.35
21	5	608	CLA	C4B-NB	7.42	1.41	1.35
21	A	804	CLA	C4B-NB	7.41	1.41	1.35
21	2	612	CLA	C4B-NB	7.41	1.41	1.35
21	c	603	CLA	C4B-NB	7.41	1.41	1.35
21	A	822	CLA	C4B-NB	7.39	1.41	1.35
21	1	313	CLA	C4B-NB	7.39	1.41	1.35
21	8	602	CLA	C4B-NB	7.39	1.41	1.35
21	c	604	CLA	C4B-NB	7.39	1.41	1.35
21	K	204	CLA	C4B-NB	7.39	1.41	1.35
21	6	609	CLA	C4B-NB	7.38	1.41	1.35
21	A	805	CLA	C4B-NB	7.38	1.41	1.35
21	L	302	CLA	C4B-NB	7.38	1.41	1.35
21	b	303	CLA	C4B-NB	7.38	1.41	1.35
21	7	404	CLA	C4B-NB	7.37	1.41	1.35
21	2	611	CLA	C4B-NB	7.37	1.41	1.35
21	B	803	CLA	C4B-NB	7.36	1.41	1.35
21	B	802	CLA	C4B-NB	7.36	1.41	1.35
21	2	608	CLA	C4B-NB	7.36	1.41	1.35
21	5	605	CLA	C4B-NB	7.35	1.41	1.35
21	9	611	CLA	C4B-NB	7.35	1.41	1.35
21	H	201	CLA	C4B-NB	7.35	1.41	1.35
21	9	602	CLA	C4B-NB	7.35	1.41	1.35
21	A	837	CLA	C4B-NB	7.34	1.41	1.35
21	5	602	CLA	C4B-NB	7.34	1.41	1.35
21	A	852	CLA	C4B-NB	7.32	1.41	1.35
21	3	406	CLA	C4B-NB	7.32	1.41	1.35
21	B	814	CLA	C4B-NB	7.31	1.41	1.35
21	c	611	CLA	C4B-NB	7.31	1.41	1.35
21	A	834	CLA	C4B-NB	7.31	1.41	1.35
21	O	202	CLA	C4B-NB	7.30	1.41	1.35
21	1	306	CLA	C4B-NB	7.30	1.41	1.35
21	A	819	CLA	C4B-NB	7.29	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	a	604	CLA	C4B-NB	7.28	1.41	1.35
21	c	613	CLA	C4B-NB	7.28	1.41	1.35
21	3	415	CLA	C4B-NB	7.28	1.41	1.35
21	B	838	CLA	C4B-NB	7.27	1.41	1.35
21	A	829	CLA	C4B-NB	7.27	1.41	1.35
21	2	604	CLA	C4B-NB	7.27	1.41	1.35
21	A	831	CLA	C4B-NB	7.26	1.41	1.35
21	B	828	CLA	C4B-NB	7.26	1.41	1.35
21	3	405	CLA	C4B-NB	7.26	1.41	1.35
21	4	611	CLA	C4B-NB	7.26	1.41	1.35
21	B	807	CLA	C4B-NB	7.25	1.41	1.35
21	B	806	CLA	C4B-NB	7.24	1.41	1.35
21	B	818	CLA	C4B-NB	7.24	1.41	1.35
21	B	837	CLA	C4B-NB	7.24	1.41	1.35
21	8	618	CLA	C4B-NB	7.24	1.41	1.35
21	b	311	CLA	C4B-NB	7.23	1.41	1.35
21	A	835	CLA	C4B-NB	7.23	1.41	1.35
21	c	610	CLA	C4B-NB	7.23	1.41	1.35
21	c	602	CLA	C4B-NB	7.23	1.41	1.35
21	1	303	CLA	C4B-NB	7.23	1.41	1.35
21	4	604	CLA	C4B-NB	7.22	1.41	1.35
21	3	402	CLA	C4B-NB	7.22	1.41	1.35
21	3	404	CLA	C4B-NB	7.22	1.41	1.35
21	B	817	CLA	C4B-NB	7.22	1.41	1.35
21	9	604	CLA	C4B-NB	7.22	1.41	1.35
21	B	826	CLA	C4B-NB	7.22	1.41	1.35
21	F	302	CLA	C4B-NB	7.21	1.41	1.35
21	B	812	CLA	C4B-NB	7.21	1.41	1.35
21	A	811	CLA	C4B-NB	7.21	1.41	1.35
21	A	824	CLA	C4B-NB	7.21	1.41	1.35
21	9	613	CLA	C4B-NB	7.21	1.41	1.35
21	B	816	CLA	C4B-NB	7.21	1.41	1.35
21	A	806	CLA	C4B-NB	7.20	1.41	1.35
21	A	810	CLA	C4B-NB	7.20	1.41	1.35
21	B	827	CLA	C4B-NB	7.20	1.41	1.35
21	1	305	CLA	C4B-NB	7.20	1.41	1.35
21	b	304	CLA	C4B-NB	7.20	1.41	1.35
21	A	840	CLA	C4B-NB	7.19	1.41	1.35
21	1	311	CLA	C4B-NB	7.19	1.41	1.35
21	A	842	CLA	C4B-NB	7.19	1.41	1.35
21	J	102	CLA	C4B-NB	7.19	1.41	1.35
21	4	608	CLA	C4B-NB	7.19	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	833	CLA	C4B-NB	7.19	1.41	1.35
21	O	203	CLA	C4B-NB	7.18	1.41	1.35
21	A	832	CLA	C4B-NB	7.18	1.41	1.35
21	B	830	CLA	C4B-NB	7.18	1.41	1.35
21	9	610	CLA	C4B-NB	7.18	1.41	1.35
21	A	808	CLA	C4B-NB	7.18	1.41	1.35
21	4	610	CLA	C4B-NB	7.18	1.41	1.35
21	B	832	CLA	C4B-NB	7.17	1.41	1.35
21	4	602	CLA	C4B-NB	7.17	1.41	1.35
21	A	828	CLA	C4B-NB	7.17	1.41	1.35
21	1	309	CLA	C4B-NB	7.17	1.41	1.35
21	A	815	CLA	C4B-NB	7.17	1.41	1.35
21	A	826	CLA	C4B-NB	7.16	1.41	1.35
21	K	201	CLA	C4B-NB	7.16	1.41	1.35
21	B	819	CLA	C4B-NB	7.16	1.41	1.35
21	A	817	CLA	C4B-NB	7.16	1.41	1.35
21	A	830	CLA	C4B-NB	7.15	1.41	1.35
21	A	812	CLA	C4B-NB	7.15	1.41	1.35
21	K	203	CLA	C4B-NB	7.15	1.41	1.35
21	A	809	CLA	C4B-NB	7.14	1.41	1.35
21	K	202	CLA	C4B-NB	7.12	1.41	1.35
21	1	310	CLA	C4B-NB	7.12	1.41	1.35
21	B	823	CLA	C4B-NB	7.12	1.41	1.35
21	B	836	CLA	C4B-NB	7.12	1.41	1.35
21	L	303	CLA	C4B-NB	7.12	1.41	1.35
21	O	201	CLA	C4B-NB	7.12	1.41	1.35
21	8	609	CLA	C4B-NB	7.12	1.41	1.35
21	A	825	CLA	C4B-NB	7.11	1.41	1.35
21	B	805	CLA	C4B-NB	7.11	1.41	1.35
21	B	822	CLA	C4B-NB	7.11	1.41	1.35
21	A	813	CLA	C4B-NB	7.10	1.41	1.35
21	A	816	CLA	C4B-NB	7.10	1.41	1.35
21	B	824	CLA	C4B-NB	7.10	1.41	1.35
21	F	305	CLA	C4B-NB	7.09	1.41	1.35
21	A	814	CLA	C4B-NB	7.09	1.41	1.35
21	A	803	CLA	C4B-NB	7.08	1.41	1.35
21	A	827	CLA	C4B-NB	7.08	1.41	1.35
21	B	834	CLA	C4B-NB	7.08	1.41	1.35
21	A	801	CLA	C4B-NB	7.08	1.41	1.35
21	3	401	CLA	C4B-NB	7.07	1.41	1.35
21	A	838	CLA	C4B-NB	7.07	1.41	1.35
21	A	821	CLA	C4B-NB	7.06	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	808	CLA	C4B-NB	7.06	1.41	1.35
21	2	610	CLA	C4B-NB	7.05	1.41	1.35
21	2	609	CLA	C4B-NB	7.02	1.41	1.35
21	A	807	CLA	C4B-NB	7.02	1.41	1.35
21	B	813	CLA	C4B-NB	7.00	1.41	1.35
21	B	835	CLA	C4B-NB	6.97	1.41	1.35
21	L	304	CLA	C4B-NB	6.95	1.41	1.35
21	B	825	CLA	C4B-NB	6.95	1.41	1.35
21	B	840	CLA	C4B-NB	6.90	1.41	1.35
21	A	801	CLA	C1D-ND	6.31	1.45	1.37
29	3	407	CHL	C3A-C2A	-6.07	1.48	1.54
29	a	605	CHL	C3B-C2B	5.77	1.48	1.40
29	6	601	CHL	C3C-C2C	5.75	1.47	1.36
29	c	609	CHL	C3B-C2B	5.74	1.48	1.40
29	6	614	CHL	C3B-C2B	5.71	1.48	1.40
29	c	605	CHL	C3B-C2B	5.69	1.48	1.40
29	a	609	CHL	C3B-C2B	5.68	1.48	1.40
29	c	607	CHL	C3B-C2B	5.67	1.48	1.40
29	7	406	CHL	C3B-C2B	5.66	1.48	1.40
29	8	606	CHL	C3B-C2B	5.65	1.48	1.40
29	6	607	CHL	C3B-C2B	5.63	1.48	1.40
29	5	606	CHL	C3B-C2B	5.61	1.48	1.40
29	b	302	CHL	C3B-C2B	5.60	1.48	1.40
29	8	613	CHL	C3B-C2B	5.59	1.48	1.40
29	a	601	CHL	C3B-C2B	5.54	1.48	1.40
29	b	306	CHL	C3B-C2B	5.53	1.48	1.40
29	6	601	CHL	C3B-C2B	5.52	1.48	1.40
29	c	606	CHL	C3B-C2B	5.52	1.48	1.40
29	9	605	CHL	C3B-C2B	5.52	1.48	1.40
29	9	601	CHL	C3B-C2B	5.51	1.48	1.40
29	c	608	CHL	C3B-C2B	5.51	1.48	1.40
21	B	801	CLA	C3B-C2B	5.51	1.48	1.40
29	a	608	CHL	C3B-C2B	5.46	1.47	1.40
29	1	302	CHL	C3B-C2B	5.43	1.47	1.40
29	6	606	CHL	C3B-C2B	5.41	1.47	1.40
29	5	601	CHL	C3B-C2B	5.40	1.47	1.40
29	6	605	CHL	C3B-C2B	5.39	1.47	1.40
21	B	801	CLA	C3C-C2C	5.39	1.48	1.36
29	2	614	CHL	C3B-C2B	5.38	1.47	1.40
29	8	607	CHL	C3B-C2B	5.37	1.47	1.40
29	7	406	CHL	C3C-C2C	5.37	1.48	1.36
29	2	601	CHL	C3B-C2B	5.37	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	4	614	CHL	C3B-C2B	5.36	1.47	1.40
29	a	607	CHL	C3B-C2B	5.35	1.47	1.40
29	2	606	CHL	C3B-C2B	5.33	1.47	1.40
29	9	609	CHL	C3B-C2B	5.32	1.47	1.40
29	a	606	CHL	C3B-C2B	5.32	1.47	1.40
29	1	307	CHL	C3B-C2B	5.32	1.47	1.40
29	b	308	CHL	C3B-C2B	5.30	1.47	1.40
29	b	310	CHL	C3B-C2B	5.29	1.47	1.40
29	a	601	CHL	C2C-C3C	5.27	1.48	1.36
29	9	608	CHL	C3B-C2B	5.27	1.47	1.40
29	c	605	CHL	C2C-C3C	5.26	1.48	1.36
21	A	801	CLA	O2D-CGD	5.26	1.46	1.33
29	9	601	CHL	C2C-C3C	5.25	1.48	1.36
29	2	602	CHL	C3B-C2B	5.24	1.47	1.40
29	a	606	CHL	C2C-C3C	5.24	1.48	1.36
29	a	609	CHL	C2C-C3C	5.24	1.48	1.36
29	8	606	CHL	C2C-C3C	5.22	1.47	1.36
21	B	801	CLA	CHC-C1C	5.22	1.48	1.35
29	6	614	CHL	O2D-CGD	5.22	1.45	1.33
29	4	606	CHL	C3B-C2B	5.21	1.47	1.40
29	2	605	CHL	C3B-C2B	5.21	1.47	1.40
29	a	609	CHL	O2D-CGD	5.20	1.45	1.33
29	9	605	CHL	O2D-CGD	5.19	1.45	1.33
29	9	606	CHL	C3B-C2B	5.19	1.47	1.40
29	c	608	CHL	O2D-CGD	5.19	1.45	1.33
29	b	306	CHL	O2D-CGD	5.19	1.45	1.33
29	6	602	CHL	C3B-C2B	5.19	1.47	1.40
29	9	607	CHL	O2D-CGD	5.18	1.45	1.33
29	8	605	CHL	O2D-CGD	5.18	1.45	1.33
29	5	606	CHL	O2D-CGD	5.18	1.45	1.33
29	9	609	CHL	O2D-CGD	5.18	1.45	1.33
29	a	609	CHL	CHC-C1C	5.18	1.48	1.35
29	b	309	CHL	C3B-C2B	5.17	1.47	1.40
29	a	605	CHL	C2C-C3C	5.17	1.47	1.36
29	6	606	CHL	O2D-CGD	5.17	1.45	1.33
29	6	614	CHL	C2C-C3C	5.17	1.47	1.36
29	c	607	CHL	C2C-C3C	5.17	1.47	1.36
29	6	605	CHL	O2D-CGD	5.16	1.45	1.33
29	8	606	CHL	O2D-CGD	5.16	1.45	1.33
29	8	613	CHL	O2D-CGD	5.16	1.45	1.33
29	5	606	CHL	C2C-C3C	5.15	1.47	1.36
29	b	302	CHL	O2D-CGD	5.15	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	c	606	CHL	O2D-CGD	5.15	1.45	1.33
29	9	601	CHL	O2D-CGD	5.13	1.45	1.33
29	c	607	CHL	O2D-CGD	5.13	1.45	1.33
29	6	607	CHL	C2C-C3C	5.13	1.47	1.36
29	c	601	CHL	O2D-CGD	5.13	1.45	1.33
29	a	607	CHL	O2D-CGD	5.13	1.45	1.33
29	6	607	CHL	O2D-CGD	5.13	1.45	1.33
29	b	306	CHL	C2C-C3C	5.13	1.47	1.36
29	3	407	CHL	C3B-C2B	5.13	1.47	1.40
29	9	606	CHL	O2D-CGD	5.12	1.45	1.33
29	8	613	CHL	C2C-C3C	5.12	1.47	1.36
29	b	302	CHL	C2C-C3C	5.12	1.47	1.36
29	2	614	CHL	O2D-CGD	5.12	1.45	1.33
29	4	614	CHL	O2D-CGD	5.12	1.45	1.33
21	B	801	CLA	O2D-CGD	5.12	1.45	1.33
29	c	609	CHL	C2C-C3C	5.12	1.47	1.37
29	6	602	CHL	O2D-CGD	5.11	1.45	1.33
29	2	605	CHL	O2D-CGD	5.10	1.45	1.33
29	4	614	CHL	C3A-C2A	-5.10	1.49	1.54
29	4	606	CHL	O2D-CGD	5.10	1.45	1.33
29	9	607	CHL	C3B-C2B	5.10	1.47	1.40
29	7	406	CHL	CHC-C1C	5.10	1.48	1.35
29	9	609	CHL	C2C-C3C	5.10	1.47	1.36
29	4	607	CHL	O2D-CGD	5.09	1.45	1.33
29	b	307	CHL	O2D-CGD	5.09	1.45	1.33
29	c	606	CHL	C2C-C3C	5.09	1.47	1.36
29	2	607	CHL	C3B-C2B	5.08	1.47	1.40
29	4	605	CHL	O2D-CGD	5.08	1.45	1.33
29	c	608	CHL	C2C-C3C	5.08	1.47	1.36
29	9	608	CHL	O2D-CGD	5.08	1.45	1.33
21	8	609	CLA	O2D-CGD	5.07	1.45	1.33
21	B	801	CLA	C1D-ND	5.07	1.44	1.37
29	c	601	CHL	C3B-C2B	5.07	1.47	1.40
29	2	606	CHL	O2D-CGD	5.07	1.45	1.33
29	4	607	CHL	C3B-C2B	5.07	1.47	1.40
29	b	308	CHL	O2D-CGD	5.07	1.45	1.33
29	a	601	CHL	O2D-CGD	5.07	1.45	1.33
29	b	310	CHL	C2C-C3C	5.07	1.47	1.36
29	b	307	CHL	C3B-C2B	5.06	1.47	1.40
29	1	307	CHL	O2D-CGD	5.06	1.45	1.33
29	a	608	CHL	O2D-CGD	5.06	1.45	1.33
29	b	309	CHL	O2D-CGD	5.06	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	6	606	CHL	C2C-C3C	5.06	1.47	1.36
29	a	607	CHL	C2C-C3C	5.05	1.47	1.36
29	8	606	CHL	CHC-C1C	5.05	1.47	1.35
29	9	605	CHL	C2C-C3C	5.05	1.47	1.36
29	a	609	CHL	CHD-C1D	5.04	1.48	1.38
29	2	602	CHL	O2D-CGD	5.04	1.45	1.33
29	2	607	CHL	O2D-CGD	5.04	1.45	1.33
29	a	606	CHL	O2D-CGD	5.03	1.45	1.33
29	6	614	CHL	CHC-C1C	5.03	1.47	1.35
29	9	608	CHL	C2C-C3C	5.03	1.47	1.36
29	c	605	CHL	CHC-C1C	5.03	1.47	1.35
29	6	605	CHL	C2C-C3C	5.01	1.47	1.36
29	c	609	CHL	CHC-C1C	5.00	1.47	1.35
29	9	607	CHL	C2C-C3C	5.00	1.47	1.36
29	8	607	CHL	O2D-CGD	5.00	1.45	1.33
29	1	302	CHL	C2C-C3C	5.00	1.47	1.36
29	b	308	CHL	C2C-C3C	5.00	1.47	1.36
29	2	607	CHL	C2C-C3C	4.99	1.47	1.36
29	2	601	CHL	O2D-CGD	4.99	1.45	1.33
21	3	409	CLA	O2D-CGD	4.99	1.45	1.33
29	5	601	CHL	O2D-CGD	4.99	1.45	1.33
29	6	602	CHL	C2C-C3C	4.99	1.47	1.36
29	5	606	CHL	CHC-C1C	4.98	1.47	1.35
29	8	613	CHL	CHC-C1C	4.98	1.47	1.35
29	c	607	CHL	CHC-C1C	4.98	1.47	1.35
29	2	602	CHL	C2C-C3C	4.98	1.47	1.36
29	6	601	CHL	CHC-C1C	4.97	1.47	1.35
29	2	606	CHL	C2C-C3C	4.96	1.47	1.36
29	c	601	CHL	C2C-C3C	4.96	1.47	1.36
29	1	302	CHL	O2D-CGD	4.96	1.45	1.33
29	6	601	CHL	O2D-CGD	4.96	1.45	1.33
29	a	605	CHL	CHC-C1C	4.96	1.47	1.35
21	1	309	CLA	O2D-CGD	4.95	1.45	1.33
29	5	601	CHL	C2C-C3C	4.95	1.47	1.36
29	a	608	CHL	C2C-C3C	4.95	1.47	1.36
29	8	605	CHL	C2C-C3C	4.95	1.47	1.37
29	2	614	CHL	C2C-C3C	4.95	1.47	1.36
29	a	606	CHL	CHC-C1C	4.94	1.47	1.35
29	1	307	CHL	C2C-C3C	4.94	1.47	1.36
29	2	605	CHL	C2C-C3C	4.94	1.47	1.36
21	4	609	CLA	O2D-CGD	4.94	1.45	1.33
29	8	607	CHL	C2C-C3C	4.93	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	6	602	CHL	CHC-C1C	4.93	1.47	1.35
29	b	307	CHL	CHC-C1C	4.93	1.47	1.35
29	4	605	CHL	C2C-C3C	4.92	1.47	1.37
29	6	607	CHL	CHC-C1C	4.92	1.47	1.35
21	2	609	CLA	O2D-CGD	4.92	1.45	1.33
29	c	606	CHL	CHC-C1C	4.92	1.47	1.35
29	a	601	CHL	CHC-C1C	4.92	1.47	1.35
29	2	602	CHL	CHC-C1C	4.92	1.47	1.35
29	b	306	CHL	CHC-C1C	4.91	1.47	1.35
29	2	601	CHL	C2C-C3C	4.91	1.47	1.36
29	b	307	CHL	C2C-C3C	4.91	1.47	1.36
29	b	309	CHL	C2C-C3C	4.90	1.47	1.36
29	9	605	CHL	CHC-C1C	4.90	1.47	1.35
29	2	607	CHL	CHC-C1C	4.90	1.47	1.35
29	4	606	CHL	C2C-C3C	4.90	1.47	1.36
29	c	608	CHL	CHC-C1C	4.89	1.47	1.35
29	b	302	CHL	CHC-C1C	4.89	1.47	1.35
29	9	606	CHL	C2C-C3C	4.89	1.47	1.36
29	6	605	CHL	CHC-C1C	4.89	1.47	1.35
29	6	606	CHL	CHC-C1C	4.88	1.47	1.35
29	2	605	CHL	CHC-C1C	4.88	1.47	1.35
29	9	601	CHL	CHC-C1C	4.88	1.47	1.35
29	7	406	CHL	CHD-C1D	4.86	1.47	1.38
29	4	607	CHL	CHC-C1C	4.85	1.47	1.35
29	4	607	CHL	C2C-C3C	4.85	1.47	1.36
29	4	614	CHL	C2C-C3C	4.85	1.47	1.36
29	b	309	CHL	CHC-C1C	4.84	1.47	1.35
29	1	307	CHL	CHC-C1C	4.83	1.47	1.35
29	9	606	CHL	CHC-C1C	4.83	1.47	1.35
29	a	608	CHL	CHC-C1C	4.82	1.47	1.35
29	4	606	CHL	CHC-C1C	4.82	1.47	1.35
29	a	607	CHL	CHC-C1C	4.81	1.47	1.35
29	a	601	CHL	CHD-C1D	4.81	1.47	1.38
29	2	606	CHL	CHC-C1C	4.81	1.47	1.35
29	c	605	CHL	CHD-C1D	4.81	1.47	1.38
29	4	605	CHL	CHC-C1C	4.81	1.47	1.35
29	8	607	CHL	CHC-C1C	4.80	1.47	1.35
29	b	310	CHL	CHC-C1C	4.80	1.47	1.35
21	A	801	CLA	MG-ND	-4.80	1.96	2.05
29	8	605	CHL	CHC-C1C	4.79	1.47	1.35
29	9	609	CHL	CHC-C1C	4.78	1.47	1.35
29	b	308	CHL	CHC-C1C	4.78	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	605	CHL	CHD-C1D	4.77	1.47	1.38
29	1	302	CHL	CHC-C1C	4.77	1.47	1.35
29	c	601	CHL	CHC-C1C	4.75	1.47	1.35
29	8	606	CHL	CHD-C1D	4.75	1.47	1.38
29	2	601	CHL	CHC-C1C	4.75	1.47	1.35
29	5	601	CHL	CHC-C1C	4.75	1.47	1.35
29	9	608	CHL	CHC-C1C	4.75	1.47	1.35
24	J	101	BCR	C21-C22	4.75	1.42	1.35
29	4	614	CHL	CHC-C1C	4.74	1.47	1.35
29	c	607	CHL	CHD-C1D	4.73	1.47	1.38
29	c	609	CHL	CHD-C1D	4.73	1.47	1.38
29	6	614	CHL	CHD-C1D	4.72	1.47	1.38
29	2	614	CHL	CHC-C1C	4.71	1.47	1.35
29	b	302	CHL	CHD-C1D	4.70	1.47	1.38
29	9	607	CHL	CHC-C1C	4.70	1.47	1.35
29	c	609	CHL	O2D-CGD	4.70	1.46	1.30
29	6	607	CHL	CHD-C1D	4.67	1.47	1.38
29	a	605	CHL	O2D-CGD	4.67	1.45	1.30
21	7	407	CLA	O2D-CGD	4.66	1.45	1.30
29	7	406	CHL	O2D-CGD	4.66	1.45	1.30
21	A	830	CLA	O2D-CGD	4.66	1.44	1.33
29	6	605	CHL	CHD-C1D	4.65	1.47	1.38
30	5	615	LUT	C10-C9	4.65	1.42	1.35
29	3	407	CHL	CHC-C1C	4.64	1.46	1.35
29	9	607	CHL	CHD-C1D	4.63	1.47	1.38
29	c	608	CHL	CHD-C1D	4.63	1.47	1.38
29	3	407	CHL	O2D-CGD	4.63	1.45	1.30
29	6	601	CHL	CHD-C1D	4.62	1.47	1.38
29	b	310	CHL	O2D-CGD	4.61	1.45	1.30
29	8	613	CHL	C3A-C2A	-4.60	1.50	1.54
29	b	310	CHL	CHD-C1D	4.60	1.47	1.38
29	9	605	CHL	CHD-C1D	4.59	1.47	1.38
30	7	415	LUT	C10-C9	4.59	1.41	1.35
29	8	607	CHL	CHD-C1D	4.58	1.47	1.38
29	a	607	CHL	CHD-C1D	4.57	1.47	1.38
29	a	606	CHL	CHD-C1D	4.56	1.47	1.38
29	b	306	CHL	O2A-CGA	4.56	1.46	1.30
29	c	606	CHL	CHD-C1D	4.56	1.47	1.38
24	J	103	BCR	C10-C9	4.55	1.41	1.35
29	a	606	CHL	O2A-CGA	4.55	1.46	1.30
29	8	613	CHL	CHD-C1D	4.55	1.47	1.38
29	b	306	CHL	CHD-C1D	4.54	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	5	606	CHL	CHD-C1D	4.54	1.47	1.38
29	b	308	CHL	CHD-C1D	4.54	1.47	1.38
29	2	605	CHL	CHD-C1D	4.53	1.47	1.38
29	a	605	CHL	O2A-CGA	4.52	1.45	1.30
29	9	609	CHL	CHD-C1D	4.52	1.47	1.38
29	4	606	CHL	O2A-CGA	4.51	1.45	1.30
29	c	605	CHL	O2A-CGA	4.51	1.45	1.30
29	6	606	CHL	O2A-CGA	4.51	1.45	1.30
29	5	601	CHL	O2A-CGA	4.50	1.45	1.30
29	9	605	CHL	O2A-CGA	4.50	1.45	1.30
29	2	614	CHL	CHD-C1D	4.50	1.47	1.38
29	a	608	CHL	O2A-CGA	4.50	1.45	1.30
29	9	608	CHL	O2A-CGA	4.50	1.45	1.30
29	8	606	CHL	O2A-CGA	4.50	1.45	1.30
29	6	614	CHL	O2A-CGA	4.49	1.45	1.30
29	c	607	CHL	O2A-CGA	4.49	1.45	1.30
29	9	609	CHL	O2A-CGA	4.49	1.45	1.30
29	5	606	CHL	O2A-CGA	4.49	1.45	1.30
29	6	601	CHL	O2A-CGA	4.49	1.45	1.30
29	b	307	CHL	O2A-CGA	4.49	1.45	1.30
29	a	601	CHL	O2A-CGA	4.49	1.45	1.30
29	6	605	CHL	O2A-CGA	4.49	1.45	1.30
29	9	606	CHL	CHD-C1D	4.49	1.47	1.38
29	c	609	CHL	O2A-CGA	4.48	1.45	1.30
29	8	605	CHL	CHD-C1D	4.48	1.47	1.38
21	8	609	CLA	O2A-CGA	4.48	1.45	1.30
29	c	606	CHL	O2A-CGA	4.48	1.45	1.30
29	9	607	CHL	O2A-CGA	4.48	1.45	1.30
29	a	609	CHL	O2A-CGA	4.48	1.45	1.30
29	2	614	CHL	O2A-CGA	4.48	1.45	1.30
29	c	608	CHL	O2A-CGA	4.48	1.45	1.30
29	2	606	CHL	O2A-CGA	4.47	1.45	1.30
29	2	605	CHL	O2A-CGA	4.47	1.45	1.30
29	a	608	CHL	CHD-C1D	4.47	1.47	1.38
29	5	601	CHL	CHD-C1D	4.46	1.47	1.38
29	9	606	CHL	O2A-CGA	4.46	1.45	1.30
21	7	407	CLA	O2A-CGA	4.46	1.45	1.30
29	6	606	CHL	CHD-C1D	4.46	1.47	1.38
29	4	606	CHL	CHD-C1D	4.46	1.47	1.38
29	9	608	CHL	CHD-C1D	4.45	1.47	1.38
31	6	617	XAT	C34-C33	4.45	1.41	1.35
29	1	307	CHL	CHD-C1D	4.44	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	9	601	CHL	CHD-C1D	4.43	1.47	1.38
29	4	614	CHL	CHD-C1D	4.43	1.47	1.38
29	b	307	CHL	CHD-C1D	4.42	1.47	1.38
29	b	302	CHL	O2A-CGA	4.42	1.45	1.30
29	1	302	CHL	CHD-C1D	4.42	1.47	1.38
29	4	605	CHL	CHD-C1D	4.40	1.46	1.38
29	2	607	CHL	CHD-C1D	4.40	1.46	1.38
29	c	601	CHL	CHD-C1D	4.40	1.46	1.38
29	2	602	CHL	CHD-C1D	4.38	1.46	1.38
31	9	616	XAT	C10-C9	4.37	1.41	1.35
29	6	602	CHL	O2A-CGA	4.36	1.46	1.33
29	3	407	CHL	CHD-C1D	4.36	1.46	1.38
29	c	601	CHL	O2A-CGA	4.33	1.46	1.33
29	2	601	CHL	CHD-C1D	4.32	1.46	1.38
29	b	309	CHL	CHD-C1D	4.31	1.46	1.38
29	7	406	CHL	C3A-C2A	-4.30	1.50	1.54
31	6	617	XAT	C10-C9	4.30	1.41	1.35
29	1	302	CHL	O2A-CGA	4.30	1.45	1.33
29	8	607	CHL	O2A-CGA	4.30	1.45	1.33
29	6	607	CHL	O2A-CGA	4.30	1.45	1.33
30	8	614	LUT	C34-C33	4.30	1.41	1.35
24	M	101	BCR	C21-C22	4.29	1.41	1.35
29	b	308	CHL	O2A-CGA	4.29	1.45	1.33
24	M	101	BCR	C10-C9	4.29	1.41	1.35
30	1	317	LUT	C10-C9	4.28	1.41	1.35
29	b	309	CHL	O2A-CGA	4.28	1.45	1.33
29	b	310	CHL	O2A-CGA	4.28	1.45	1.33
29	1	307	CHL	O2A-CGA	4.28	1.45	1.33
31	9	616	XAT	C14-C13	4.27	1.41	1.35
24	8	616	BCR	C14-C13	4.26	1.41	1.35
21	B	801	CLA	O2A-CGA	4.26	1.45	1.33
29	2	607	CHL	O2A-CGA	4.26	1.45	1.33
24	8	616	BCR	C17-C18	4.26	1.41	1.35
29	6	602	CHL	CHD-C1D	4.25	1.46	1.38
31	8	615	XAT	C10-C9	4.25	1.41	1.35
31	9	616	XAT	C34-C33	4.25	1.41	1.35
29	2	601	CHL	O2A-CGA	4.25	1.45	1.33
31	9	616	XAT	C30-C29	4.24	1.41	1.35
30	8	614	LUT	C14-C13	4.22	1.41	1.35
29	4	607	CHL	O2A-CGA	4.22	1.45	1.33
30	6	616	LUT	C30-C29	4.21	1.41	1.35
30	1	317	LUT	C14-C13	4.21	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	8	608	CLA	O1D-CGD	4.21	1.36	1.19
21	B	801	CLA	CHD-C1D	4.20	1.46	1.38
21	4	609	CLA	O2A-CGA	4.20	1.45	1.33
24	M	101	BCR	C17-C18	4.19	1.41	1.35
29	4	607	CHL	CHD-C1D	4.18	1.46	1.38
31	8	615	XAT	C34-C33	4.18	1.41	1.35
21	4	608	CLA	O1D-CGD	4.18	1.36	1.19
27	B	847	DGD	O1G-C1A	4.17	1.45	1.33
31	6	617	XAT	C14-C13	4.17	1.41	1.35
29	2	606	CHL	CHD-C1D	4.17	1.46	1.38
24	2	618	BCR	C21-C22	4.17	1.41	1.35
30	a	616	LUT	C14-C13	4.17	1.41	1.35
30	1	317	LUT	C30-C29	4.16	1.41	1.35
30	1	317	LUT	C34-C33	4.16	1.41	1.35
24	O	205	BCR	C14-C13	4.16	1.41	1.35
30	4	615	LUT	C10-C9	4.16	1.41	1.35
31	8	615	XAT	C14-C13	4.15	1.41	1.35
24	M	101	BCR	C14-C13	4.15	1.41	1.35
24	7	418	BCR	C21-C22	4.14	1.41	1.35
29	2	602	CHL	O2A-CGA	4.13	1.45	1.33
31	7	416	XAT	C14-C13	4.13	1.41	1.35
24	O	205	BCR	C21-C22	4.12	1.41	1.35
24	J	103	BCR	C21-C22	4.12	1.41	1.35
30	b	316	LUT	C34-C33	4.12	1.41	1.35
31	8	615	XAT	C30-C29	4.12	1.41	1.35
24	8	616	BCR	C21-C22	4.12	1.41	1.35
24	O	205	BCR	C17-C18	4.11	1.41	1.35
31	7	416	XAT	C34-C33	4.11	1.41	1.35
30	8	614	LUT	C30-C29	4.11	1.41	1.35
21	A	801	CLA	O2A-CGA	4.11	1.45	1.33
24	7	417	BCR	C17-C18	4.10	1.41	1.35
21	A	830	CLA	O2A-CGA	4.10	1.45	1.33
30	a	615	LUT	C30-C29	4.10	1.41	1.35
30	a	616	LUT	C30-C29	4.10	1.41	1.35
21	7	407	CLA	CHC-C1C	4.10	1.45	1.35
30	6	616	LUT	C10-C9	4.10	1.41	1.35
24	7	418	BCR	C14-C13	4.10	1.41	1.35
24	7	417	BCR	C21-C22	4.09	1.41	1.35
24	6	618	BCR	C17-C18	4.09	1.41	1.35
30	4	615	LUT	C34-C33	4.09	1.41	1.35
24	8	616	BCR	C10-C9	4.08	1.41	1.35
24	6	618	BCR	C10-C9	4.08	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	F	303	BCR	C17-C18	4.08	1.41	1.35
24	7	417	BCR	C10-C9	4.08	1.41	1.35
30	7	415	LUT	C30-C29	4.08	1.41	1.35
32	c	618	NEX	C30-C29	4.07	1.41	1.35
30	c	616	LUT	C14-C13	4.07	1.41	1.35
21	O	204	CLA	C1D-ND	4.07	1.42	1.37
24	O	205	BCR	C10-C9	4.07	1.41	1.35
24	2	618	BCR	C14-C13	4.06	1.41	1.35
30	a	616	LUT	C34-C33	4.06	1.41	1.35
24	6	618	BCR	C21-C22	4.06	1.41	1.35
32	9	617	NEX	C34-C33	4.06	1.41	1.35
30	a	615	LUT	C10-C9	4.05	1.41	1.35
30	b	316	LUT	C10-C9	4.05	1.41	1.35
21	5	612	CLA	C1D-ND	4.05	1.42	1.37
21	3	409	CLA	C1D-ND	4.05	1.42	1.37
21	4	609	CLA	CHC-C1C	4.05	1.45	1.35
30	9	614	LUT	C34-C33	4.05	1.41	1.35
24	6	618	BCR	C14-C13	4.04	1.41	1.35
32	c	618	NEX	C14-C13	4.04	1.41	1.35
24	3	419	BCR	C14-C13	4.04	1.41	1.35
31	7	416	XAT	C30-C29	4.04	1.41	1.35
30	4	615	LUT	C14-C13	4.04	1.41	1.35
24	I	101	BCR	C17-C18	4.04	1.41	1.35
24	I	101	BCR	C10-C9	4.04	1.41	1.35
30	6	616	LUT	C34-C33	4.04	1.41	1.35
21	8	609	CLA	C1D-ND	4.04	1.42	1.37
31	a	618	XAT	C14-C13	4.03	1.41	1.35
31	a	618	XAT	C30-C29	4.03	1.41	1.35
24	L	306	BCR	C21-C22	4.03	1.41	1.35
32	b	318	NEX	C30-C29	4.03	1.41	1.35
24	7	418	BCR	C10-C9	4.03	1.41	1.35
21	A	830	CLA	C1D-ND	4.03	1.42	1.37
30	2	616	LUT	C14-C13	4.03	1.41	1.35
30	5	615	LUT	C34-C33	4.03	1.41	1.35
21	B	801	CLA	CHD-C4C	4.03	1.48	1.39
27	B	847	DGD	O2G-C1B	4.03	1.45	1.34
21	2	609	CLA	C1D-ND	4.03	1.42	1.37
21	3	409	CLA	O2A-CGA	4.02	1.45	1.33
24	3	419	BCR	C21-C22	4.02	1.41	1.35
30	3	416	LUT	C34-C33	4.02	1.41	1.35
30	a	615	LUT	C34-C33	4.02	1.41	1.35
30	a	616	LUT	C10-C9	4.02	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	L	306	BCR	C10-C9	4.02	1.41	1.35
30	c	615	LUT	C30-C29	4.02	1.41	1.35
24	7	417	BCR	C14-C13	4.02	1.41	1.35
21	3	409	CLA	CHC-C1C	4.01	1.45	1.35
30	2	616	LUT	C10-C9	4.01	1.41	1.35
31	a	618	XAT	C34-C33	4.01	1.41	1.35
30	3	416	LUT	C30-C29	4.01	1.41	1.35
24	J	103	BCR	C14-C13	4.01	1.41	1.35
24	7	418	BCR	C17-C18	4.01	1.41	1.35
24	3	419	BCR	C17-C18	4.01	1.41	1.35
32	c	618	NEX	C34-C33	4.01	1.41	1.35
30	b	316	LUT	C14-C13	4.00	1.41	1.35
24	J	103	BCR	C17-C18	4.00	1.41	1.35
24	B	842	BCR	C14-C13	4.00	1.41	1.35
30	c	615	LUT	C34-C33	4.00	1.41	1.35
30	a	615	LUT	C14-C13	3.99	1.41	1.35
31	7	416	XAT	C10-C9	3.99	1.41	1.35
30	6	616	LUT	C14-C13	3.99	1.41	1.35
30	2	616	LUT	C34-C33	3.99	1.41	1.35
30	5	615	LUT	C30-C29	3.99	1.41	1.35
21	4	609	CLA	C1D-ND	3.99	1.42	1.37
24	F	303	BCR	C21-C22	3.99	1.41	1.35
21	1	309	CLA	C1D-ND	3.99	1.42	1.37
24	4	617	BCR	C14-C13	3.98	1.41	1.35
30	2	616	LUT	C30-C29	3.98	1.41	1.35
30	3	416	LUT	C10-C9	3.98	1.41	1.35
30	4	615	LUT	C30-C29	3.98	1.41	1.35
24	J	101	BCR	C14-C13	3.97	1.41	1.35
32	9	617	NEX	C14-C13	3.97	1.41	1.35
24	G	205	BCR	C17-C18	3.97	1.41	1.35
21	7	402	CLA	C1D-ND	3.97	1.42	1.37
21	6	608	CLA	C1D-ND	3.97	1.42	1.37
24	L	306	BCR	C14-C13	3.96	1.41	1.35
24	I	101	BCR	C14-C13	3.96	1.41	1.35
24	A	846	BCR	C21-C22	3.96	1.41	1.35
21	G	204	CLA	C1D-ND	3.96	1.42	1.37
32	b	318	NEX	C34-C33	3.96	1.41	1.35
31	6	617	XAT	C30-C29	3.95	1.41	1.35
24	4	617	BCR	C17-C18	3.95	1.41	1.35
24	2	618	BCR	C10-C9	3.95	1.41	1.35
21	A	818	CLA	C1D-ND	3.95	1.42	1.37
24	4	617	BCR	C21-C22	3.95	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	F	303	BCR	C14-C13	3.95	1.41	1.35
30	9	614	LUT	C14-C13	3.95	1.41	1.35
30	c	615	LUT	C14-C13	3.95	1.41	1.35
30	5	615	LUT	C14-C13	3.94	1.41	1.35
30	9	615	LUT	C30-C29	3.94	1.41	1.35
30	3	416	LUT	C14-C13	3.94	1.41	1.35
24	B	842	BCR	C10-C9	3.94	1.41	1.35
30	b	316	LUT	C30-C29	3.94	1.41	1.35
24	A	846	BCR	C14-C13	3.94	1.41	1.35
24	3	419	BCR	C10-C9	3.94	1.41	1.35
31	c	617	XAT	C14-C13	3.94	1.41	1.35
24	3	418	BCR	C21-C22	3.93	1.41	1.35
30	9	615	LUT	C34-C33	3.93	1.41	1.35
21	7	413	CLA	C1D-ND	3.93	1.42	1.37
24	G	205	BCR	C14-C13	3.93	1.41	1.35
21	5	604	CLA	C1D-ND	3.93	1.42	1.37
24	4	617	BCR	C10-C9	3.93	1.41	1.35
21	6	612	CLA	C1D-ND	3.93	1.42	1.37
24	L	306	BCR	C17-C18	3.93	1.41	1.35
21	6	604	CLA	C1D-ND	3.92	1.42	1.37
21	A	837	CLA	C1D-ND	3.92	1.42	1.37
21	7	411	CLA	C1D-ND	3.92	1.42	1.37
31	5	616	XAT	C10-C9	3.92	1.41	1.35
32	b	318	NEX	C14-C13	3.92	1.41	1.35
21	7	404	CLA	C1D-ND	3.92	1.42	1.37
30	7	415	LUT	C34-C33	3.92	1.41	1.35
21	7	414	CLA	C1D-ND	3.91	1.42	1.37
29	a	609	CHL	CHD-C4C	3.91	1.48	1.39
31	a	618	XAT	C10-C9	3.91	1.41	1.35
29	3	407	CHL	C3C-C2C	3.91	1.45	1.36
24	I	101	BCR	C21-C22	3.91	1.41	1.35
24	B	845	BCR	C14-C13	3.91	1.41	1.35
30	c	616	LUT	C34-C33	3.91	1.41	1.35
24	B	842	BCR	C17-C18	3.91	1.41	1.35
29	7	406	CHL	CHD-C4C	3.91	1.48	1.39
24	G	201	BCR	C21-C22	3.90	1.41	1.35
30	c	616	LUT	C30-C29	3.90	1.41	1.35
24	J	101	BCR	C17-C18	3.90	1.41	1.35
31	c	617	XAT	C10-C9	3.90	1.41	1.35
31	1	318	XAT	C14-C13	3.90	1.41	1.35
21	A	839	CLA	C1D-ND	3.90	1.42	1.37
24	B	845	BCR	C10-C9	3.90	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	9	615	LUT	C14-C13	3.90	1.40	1.35
31	3	417	XAT	C34-C33	3.90	1.40	1.35
21	a	612	CLA	C1D-ND	3.89	1.42	1.37
24	A	846	BCR	C17-C18	3.89	1.40	1.35
21	b	315	CLA	C1D-ND	3.89	1.42	1.37
21	B	811	CLA	C1D-ND	3.88	1.42	1.37
21	1	316	CLA	C1D-ND	3.88	1.42	1.37
21	a	611	CLA	C1D-ND	3.88	1.42	1.37
21	c	612	CLA	C1D-ND	3.88	1.42	1.37
30	b	317	LUT	C14-C13	3.88	1.40	1.35
21	6	610	CLA	C1D-ND	3.88	1.42	1.37
21	5	613	CLA	C1D-ND	3.88	1.42	1.37
21	5	603	CLA	C1D-ND	3.88	1.42	1.37
21	8	612	CLA	C1D-ND	3.88	1.42	1.37
30	c	615	LUT	C10-C9	3.88	1.40	1.35
31	c	617	XAT	C34-C33	3.88	1.40	1.35
21	7	412	CLA	C1D-ND	3.87	1.42	1.37
21	7	409	CLA	C1D-ND	3.87	1.42	1.37
21	c	604	CLA	C1D-ND	3.87	1.42	1.37
31	5	616	XAT	C34-C33	3.87	1.40	1.35
30	b	317	LUT	C30-C29	3.87	1.40	1.35
21	6	609	CLA	C1D-ND	3.87	1.42	1.37
21	7	407	CLA	CHD-C4C	3.87	1.48	1.39
29	c	605	CHL	CHD-C4C	3.87	1.48	1.39
21	6	613	CLA	C1D-ND	3.87	1.42	1.37
24	3	418	BCR	C10-C9	3.87	1.40	1.35
24	G	205	BCR	C21-C22	3.87	1.40	1.35
29	6	614	CHL	CHD-C4C	3.87	1.48	1.39
21	6	611	CLA	C1D-ND	3.87	1.42	1.37
21	b	304	CLA	C1D-ND	3.86	1.42	1.37
31	c	617	XAT	C30-C29	3.86	1.40	1.35
21	8	618	CLA	C1D-ND	3.86	1.42	1.37
30	9	614	LUT	C10-C9	3.86	1.40	1.35
21	4	611	CLA	C1D-ND	3.86	1.42	1.37
24	G	201	BCR	C14-C13	3.86	1.40	1.35
21	5	614	CLA	C1D-ND	3.86	1.42	1.37
21	8	603	CLA	C1D-ND	3.86	1.42	1.37
24	L	301	BCR	C21-C22	3.85	1.40	1.35
21	8	601	CLA	C1D-ND	3.85	1.42	1.37
30	c	616	LUT	C10-C9	3.85	1.40	1.35
21	1	314	CLA	C1D-ND	3.85	1.42	1.37
21	7	408	CLA	C1D-ND	3.85	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	5	605	CLA	C1D-ND	3.85	1.42	1.37
32	9	617	NEX	C30-C29	3.85	1.40	1.35
21	5	611	CLA	C1D-ND	3.85	1.42	1.37
29	a	601	CHL	CHD-C4C	3.85	1.48	1.39
21	6	603	CLA	C1D-ND	3.85	1.42	1.37
24	A	849	BCR	C21-C22	3.85	1.40	1.35
24	G	201	BCR	C17-C18	3.85	1.40	1.35
21	5	608	CLA	C1D-ND	3.84	1.42	1.37
21	7	410	CLA	C1D-ND	3.84	1.42	1.37
24	B	842	BCR	C21-C22	3.84	1.40	1.35
24	A	849	BCR	C17-C18	3.84	1.40	1.35
21	5	610	CLA	C1D-ND	3.84	1.42	1.37
24	2	618	BCR	C17-C18	3.84	1.40	1.35
31	1	318	XAT	C10-C9	3.83	1.40	1.35
30	8	614	LUT	C10-C9	3.83	1.40	1.35
21	7	405	CLA	C1D-ND	3.83	1.42	1.37
21	a	614	CLA	C1D-ND	3.83	1.42	1.37
24	L	305	BCR	C17-C18	3.83	1.40	1.35
29	a	606	CHL	CHD-C4C	3.83	1.48	1.39
21	B	816	CLA	C1D-ND	3.83	1.42	1.37
24	3	418	BCR	C17-C18	3.83	1.40	1.35
21	8	611	CLA	C1D-ND	3.83	1.42	1.37
29	6	607	CHL	CHD-C4C	3.82	1.48	1.39
21	B	825	CLA	C1D-ND	3.82	1.42	1.37
31	1	318	XAT	C34-C33	3.82	1.40	1.35
31	3	417	XAT	C30-C29	3.82	1.40	1.35
21	A	841	CLA	C1D-ND	3.82	1.42	1.37
30	9	614	LUT	C30-C29	3.82	1.40	1.35
21	3	410	CLA	C1D-ND	3.82	1.42	1.37
24	A	850	BCR	C14-C13	3.82	1.40	1.35
24	L	305	BCR	C14-C13	3.82	1.40	1.35
21	8	608	CLA	C1D-ND	3.81	1.42	1.37
21	A	838	CLA	C1D-ND	3.81	1.42	1.37
21	B	801	CLA	OBD-CAD	3.81	1.29	1.22
29	8	606	CHL	CHD-C4C	3.81	1.47	1.39
21	1	315	CLA	C1D-ND	3.81	1.42	1.37
24	A	846	BCR	C10-C9	3.81	1.40	1.35
21	1	305	CLA	C1D-ND	3.81	1.42	1.37
21	8	604	CLA	C1D-ND	3.81	1.42	1.37
21	B	801	CLA	C3D-C2D	3.81	1.49	1.39
21	b	314	CLA	C1D-ND	3.81	1.42	1.37
21	7	407	CLA	MG-NC	3.81	2.15	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	850	BCR	C10-C9	3.80	1.40	1.35
21	1	308	CLA	C1D-ND	3.80	1.42	1.37
24	3	418	BCR	C14-C13	3.80	1.40	1.35
31	3	417	XAT	C14-C13	3.80	1.40	1.35
29	b	310	CHL	CHD-C4C	3.80	1.47	1.39
29	b	302	CHL	CHD-C4C	3.80	1.47	1.39
30	b	317	LUT	C34-C33	3.80	1.40	1.35
21	B	826	CLA	C1D-ND	3.80	1.42	1.37
29	9	607	CHL	OBD-CAD	3.80	1.29	1.22
21	7	403	CLA	C1D-ND	3.80	1.42	1.37
31	1	318	XAT	C30-C29	3.80	1.40	1.35
21	b	313	CLA	C1D-ND	3.80	1.42	1.37
29	5	606	CHL	CHD-C4C	3.80	1.47	1.39
31	5	616	XAT	C14-C13	3.80	1.40	1.35
29	a	605	CHL	CHD-C4C	3.80	1.47	1.39
21	G	203	CLA	C1D-ND	3.80	1.42	1.37
21	8	610	CLA	C1D-ND	3.79	1.42	1.37
29	c	607	CHL	CHD-C4C	3.79	1.47	1.39
21	B	804	CLA	C1D-ND	3.79	1.42	1.37
21	B	837	CLA	C1D-ND	3.79	1.42	1.37
21	4	601	CLA	C1D-ND	3.79	1.42	1.37
21	F	304	CLA	C1D-ND	3.79	1.42	1.37
21	a	604	CLA	C1D-ND	3.79	1.42	1.37
24	A	847	BCR	C17-C18	3.78	1.40	1.35
21	2	603	CLA	C1D-ND	3.78	1.42	1.37
21	b	312	CLA	C1D-ND	3.78	1.42	1.37
31	2	617	XAT	C14-C13	3.78	1.40	1.35
21	c	610	CLA	C1D-ND	3.78	1.42	1.37
21	F	302	CLA	C1D-ND	3.78	1.42	1.37
21	3	406	CLA	C1D-ND	3.78	1.42	1.37
29	8	607	CHL	OBD-CAD	3.78	1.29	1.22
21	K	201	CLA	C1D-ND	3.78	1.42	1.37
24	B	845	BCR	C17-C18	3.78	1.40	1.35
21	B	839	CLA	C1D-ND	3.78	1.42	1.37
31	4	616	XAT	C10-C9	3.78	1.40	1.35
21	9	613	CLA	C1D-ND	3.77	1.42	1.37
21	a	603	CLA	C1D-ND	3.77	1.42	1.37
21	A	827	CLA	C1D-ND	3.77	1.42	1.37
21	4	603	CLA	C1D-ND	3.77	1.42	1.37
24	A	847	BCR	C14-C13	3.77	1.40	1.35
24	L	305	BCR	C10-C9	3.77	1.40	1.35
29	a	605	CHL	OBD-CAD	3.77	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	305	CLA	C1D-ND	3.77	1.42	1.37
24	G	205	BCR	C10-C9	3.77	1.40	1.35
24	L	305	BCR	C21-C22	3.77	1.40	1.35
21	3	412	CLA	C1D-ND	3.77	1.42	1.37
21	a	613	CLA	C1D-ND	3.77	1.42	1.37
29	9	606	CHL	OBD-CAD	3.77	1.29	1.22
21	7	407	CLA	C3D-C4D	-3.76	1.35	1.44
29	9	607	CHL	CHD-C4C	3.76	1.47	1.39
29	c	608	CHL	CHD-C4C	3.76	1.47	1.39
24	A	847	BCR	C21-C22	3.76	1.40	1.35
24	A	854	BCR	C17-C18	3.76	1.40	1.35
31	2	617	XAT	C10-C9	3.76	1.40	1.35
29	c	606	CHL	CHD-C4C	3.76	1.47	1.39
29	6	601	CHL	OBD-CAD	3.76	1.29	1.22
30	9	615	LUT	C10-C9	3.76	1.40	1.35
24	B	845	BCR	C21-C22	3.76	1.40	1.35
29	8	605	CHL	OBD-CAD	3.75	1.28	1.22
21	5	607	CLA	C1D-ND	3.75	1.42	1.37
21	c	613	CLA	C1D-ND	3.75	1.42	1.37
31	4	616	XAT	C30-C29	3.75	1.40	1.35
31	4	616	XAT	C14-C13	3.75	1.40	1.35
21	a	602	CLA	C1D-ND	3.75	1.42	1.37
29	6	605	CHL	OBD-CAD	3.75	1.28	1.22
29	c	608	CHL	OBD-CAD	3.75	1.28	1.22
29	c	605	CHL	OBD-CAD	3.75	1.28	1.22
21	1	313	CLA	C1D-ND	3.75	1.42	1.37
21	9	603	CLA	C1D-ND	3.75	1.42	1.37
31	2	617	XAT	C34-C33	3.75	1.40	1.35
29	8	613	CHL	CHD-C4C	3.75	1.47	1.39
24	G	201	BCR	C10-C9	3.75	1.40	1.35
24	J	101	BCR	C10-C9	3.75	1.40	1.35
21	B	829	CLA	C1D-ND	3.75	1.42	1.37
21	3	401	CLA	C1D-ND	3.75	1.42	1.37
21	L	302	CLA	C1D-ND	3.74	1.42	1.37
21	a	610	CLA	C1D-ND	3.74	1.42	1.37
21	b	303	CLA	C1D-ND	3.74	1.42	1.37
29	9	605	CHL	CHD-C4C	3.74	1.47	1.39
21	A	802	CLA	C1D-ND	3.74	1.42	1.37
29	8	606	CHL	OBD-CAD	3.74	1.28	1.22
21	2	604	CLA	C1D-ND	3.74	1.42	1.37
29	6	614	CHL	OBD-CAD	3.74	1.28	1.22
21	1	311	CLA	C1D-ND	3.74	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	L	301	BCR	C14-C13	3.74	1.40	1.35
24	A	850	BCR	C17-C18	3.73	1.40	1.35
30	7	415	LUT	C14-C13	3.73	1.40	1.35
21	3	402	CLA	C1D-ND	3.73	1.42	1.37
21	B	823	CLA	C1D-ND	3.73	1.42	1.37
21	1	312	CLA	C1D-ND	3.73	1.42	1.37
30	b	317	LUT	C10-C9	3.73	1.40	1.35
21	K	204	CLA	C1D-ND	3.73	1.42	1.37
21	2	611	CLA	C1D-ND	3.73	1.42	1.37
29	5	601	CHL	OBD-CAD	3.73	1.28	1.22
29	a	601	CHL	OBD-CAD	3.73	1.28	1.22
21	A	828	CLA	C1D-ND	3.73	1.42	1.37
21	B	815	CLA	C1D-ND	3.73	1.42	1.37
21	4	610	CLA	C1D-ND	3.73	1.42	1.37
29	6	601	CHL	CHD-C4C	3.73	1.47	1.39
29	6	606	CHL	OBD-CAD	3.72	1.28	1.22
31	5	616	XAT	C30-C29	3.72	1.40	1.35
24	A	849	BCR	C14-C13	3.72	1.40	1.35
21	G	202	CLA	C1D-ND	3.72	1.42	1.37
21	3	415	CLA	C1D-ND	3.72	1.42	1.37
29	5	606	CHL	OBD-CAD	3.72	1.28	1.22
24	L	301	BCR	C17-C18	3.72	1.40	1.35
29	6	605	CHL	CHD-C4C	3.72	1.47	1.39
21	c	611	CLA	C1D-ND	3.72	1.42	1.37
21	J	102	CLA	C1D-ND	3.72	1.42	1.37
29	b	308	CHL	CHD-C4C	3.71	1.47	1.39
21	8	602	CLA	C1D-ND	3.71	1.42	1.37
29	9	605	CHL	OBD-CAD	3.71	1.28	1.22
21	4	604	CLA	C1D-ND	3.71	1.42	1.37
21	2	612	CLA	C1D-ND	3.71	1.42	1.37
21	B	809	CLA	C1D-ND	3.71	1.42	1.37
21	K	203	CLA	C1D-ND	3.71	1.42	1.37
21	B	819	CLA	C1D-ND	3.71	1.42	1.37
21	B	835	CLA	C1D-ND	3.71	1.42	1.37
29	6	607	CHL	OBD-CAD	3.71	1.28	1.22
29	7	406	CHL	OBD-CAD	3.71	1.28	1.22
29	9	601	CHL	CHD-C4C	3.71	1.47	1.39
21	3	413	CLA	C1D-ND	3.71	1.42	1.37
29	4	606	CHL	OBD-CAD	3.71	1.28	1.22
29	c	607	CHL	OBD-CAD	3.71	1.28	1.22
29	2	614	CHL	OBD-CAD	3.70	1.28	1.22
21	3	404	CLA	C1D-ND	3.70	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	310	CLA	C1D-ND	3.70	1.42	1.37
24	A	854	BCR	C10-C9	3.70	1.40	1.35
21	O	202	CLA	C1D-ND	3.70	1.42	1.37
21	B	820	CLA	C1D-ND	3.70	1.42	1.37
21	B	814	CLA	C1D-ND	3.70	1.42	1.37
31	4	616	XAT	C34-C33	3.70	1.40	1.35
29	a	607	CHL	CHD-C4C	3.70	1.47	1.39
21	O	201	CLA	C1D-ND	3.70	1.42	1.37
31	2	617	XAT	C30-C29	3.70	1.40	1.35
21	4	613	CLA	C1D-ND	3.70	1.42	1.37
21	b	311	CLA	C1D-ND	3.70	1.42	1.37
21	B	830	CLA	C1D-ND	3.69	1.42	1.37
29	8	613	CHL	OBD-CAD	3.69	1.28	1.22
29	9	601	CHL	OBD-CAD	3.69	1.28	1.22
21	A	803	CLA	C1D-ND	3.69	1.42	1.37
21	A	824	CLA	C1D-ND	3.69	1.42	1.37
24	F	303	BCR	C10-C9	3.69	1.40	1.35
29	8	607	CHL	CHD-C4C	3.69	1.47	1.39
29	a	607	CHL	OBD-CAD	3.69	1.28	1.22
29	1	302	CHL	CHD-C4C	3.69	1.47	1.39
29	a	609	CHL	OBD-CAD	3.69	1.28	1.22
29	2	605	CHL	CHD-C4C	3.69	1.47	1.39
21	A	822	CLA	C1D-ND	3.69	1.42	1.37
21	B	822	CLA	C1D-ND	3.69	1.42	1.37
21	A	834	CLA	C1D-ND	3.69	1.42	1.37
21	A	804	CLA	C1D-ND	3.69	1.42	1.37
21	H	201	CLA	C1D-ND	3.69	1.42	1.37
21	3	405	CLA	C1D-ND	3.69	1.42	1.37
21	L	304	CLA	C1D-ND	3.69	1.42	1.37
21	c	603	CLA	C1D-ND	3.68	1.42	1.37
29	1	307	CHL	OBD-CAD	3.68	1.28	1.22
21	B	810	CLA	C1D-ND	3.68	1.42	1.37
21	3	411	CLA	C1D-ND	3.68	1.42	1.37
29	b	306	CHL	OBD-CAD	3.68	1.28	1.22
29	c	606	CHL	OBD-CAD	3.68	1.28	1.22
21	B	803	CLA	C1D-ND	3.68	1.42	1.37
21	3	414	CLA	C1D-ND	3.68	1.42	1.37
21	A	816	CLA	C1D-ND	3.68	1.42	1.37
21	c	614	CLA	C1D-ND	3.68	1.42	1.37
21	7	407	CLA	C4C-C3C	3.68	1.51	1.45
29	6	606	CHL	CHD-C4C	3.68	1.47	1.39
24	A	848	BCR	C14-C13	3.68	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	836	CLA	C1D-ND	3.67	1.42	1.37
21	A	835	CLA	C1D-ND	3.67	1.42	1.37
21	B	805	CLA	C1D-ND	3.67	1.42	1.37
21	2	610	CLA	C1D-ND	3.67	1.42	1.37
29	4	614	CHL	OBD-CAD	3.67	1.28	1.22
29	c	601	CHL	OBD-CAD	3.67	1.28	1.22
21	A	825	CLA	C1D-ND	3.67	1.42	1.37
29	c	609	CHL	CHD-C4C	3.67	1.47	1.39
24	F	301	BCR	C21-C22	3.67	1.40	1.35
21	A	833	CLA	C1D-ND	3.67	1.42	1.37
21	5	602	CLA	C1D-ND	3.67	1.42	1.37
29	8	605	CHL	CHD-C4C	3.67	1.47	1.39
21	2	613	CLA	C1D-ND	3.67	1.42	1.37
21	3	403	CLA	C1D-ND	3.66	1.42	1.37
24	L	301	BCR	C10-C9	3.66	1.40	1.35
21	A	821	CLA	C1D-ND	3.66	1.42	1.37
29	6	602	CHL	OBD-CAD	3.66	1.28	1.22
29	b	309	CHL	OBD-CAD	3.66	1.28	1.22
24	A	854	BCR	C14-C13	3.66	1.40	1.35
21	A	813	CLA	C1D-ND	3.66	1.42	1.37
21	O	203	CLA	C1D-ND	3.66	1.42	1.37
21	1	306	CLA	C1D-ND	3.66	1.42	1.37
29	2	602	CHL	OBD-CAD	3.66	1.28	1.22
29	3	407	CHL	CHD-C4C	3.66	1.47	1.39
21	1	304	CLA	C1D-ND	3.66	1.42	1.37
21	A	808	CLA	C1D-ND	3.66	1.42	1.37
21	9	610	CLA	C1D-ND	3.66	1.42	1.37
21	A	823	CLA	C1D-ND	3.65	1.42	1.37
29	1	307	CHL	CHD-C4C	3.65	1.47	1.39
29	2	601	CHL	CHD-C4C	3.65	1.47	1.39
29	2	602	CHL	CHD-C4C	3.65	1.47	1.39
29	9	609	CHL	CHD-C4C	3.65	1.47	1.39
31	3	417	XAT	C10-C9	3.65	1.40	1.35
21	K	202	CLA	C1D-ND	3.65	1.42	1.37
21	A	852	CLA	C1D-ND	3.65	1.42	1.37
29	4	605	CHL	OBD-CAD	3.65	1.28	1.22
24	A	848	BCR	C21-C22	3.65	1.40	1.35
24	A	854	BCR	C21-C22	3.65	1.40	1.35
29	4	614	CHL	CHD-C4C	3.65	1.47	1.39
21	A	826	CLA	C1D-ND	3.65	1.42	1.37
21	3	408	CLA	C1D-ND	3.65	1.42	1.37
21	4	612	CLA	C1D-ND	3.64	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	9	606	CHL	CHD-C4C	3.64	1.47	1.39
29	b	306	CHL	CHD-C4C	3.64	1.47	1.39
29	2	605	CHL	OBD-CAD	3.64	1.28	1.22
21	A	820	CLA	C1D-ND	3.64	1.42	1.37
21	B	833	CLA	C1D-ND	3.64	1.42	1.37
29	9	609	CHL	OBD-CAD	3.64	1.28	1.22
24	F	301	BCR	C17-C18	3.64	1.40	1.35
21	F	305	CLA	C1D-ND	3.64	1.42	1.37
29	4	606	CHL	CHD-C4C	3.64	1.47	1.39
21	c	602	CLA	C1D-ND	3.64	1.42	1.37
21	A	815	CLA	C1D-ND	3.64	1.42	1.37
21	9	612	CLA	C1D-ND	3.63	1.42	1.37
29	5	601	CHL	CHD-C4C	3.63	1.47	1.39
29	1	302	CHL	OBD-CAD	3.63	1.28	1.22
21	A	809	CLA	C1D-ND	3.63	1.42	1.37
29	9	608	CHL	OBD-CAD	3.63	1.28	1.22
29	4	605	CHL	CHD-C4C	3.63	1.47	1.39
24	A	849	BCR	C10-C9	3.63	1.40	1.35
21	9	611	CLA	C1D-ND	3.63	1.42	1.37
29	b	307	CHL	CHD-C4C	3.62	1.47	1.39
21	9	604	CLA	C1D-ND	3.62	1.42	1.37
21	A	817	CLA	C1D-ND	3.62	1.42	1.37
21	2	608	CLA	C1D-ND	3.62	1.42	1.37
29	b	302	CHL	OBD-CAD	3.62	1.28	1.22
21	7	407	CLA	OBD-CAD	3.62	1.28	1.22
29	2	614	CHL	CHD-C4C	3.62	1.47	1.39
21	A	805	CLA	C1D-ND	3.62	1.42	1.37
21	B	834	CLA	C1D-ND	3.62	1.42	1.37
21	B	812	CLA	C1D-ND	3.62	1.42	1.37
29	b	309	CHL	CHD-C4C	3.61	1.47	1.39
21	B	832	CLA	C1D-ND	3.61	1.42	1.37
29	9	608	CHL	CHD-C4C	3.61	1.47	1.39
21	A	807	CLA	C1D-ND	3.61	1.42	1.37
21	B	817	CLA	C1D-ND	3.61	1.42	1.37
29	a	608	CHL	CHD-C4C	3.61	1.47	1.39
24	A	850	BCR	C21-C22	3.61	1.40	1.35
21	B	807	CLA	C1D-ND	3.61	1.42	1.37
29	2	601	CHL	OBD-CAD	3.61	1.28	1.22
21	A	840	CLA	C1D-ND	3.61	1.42	1.37
21	4	608	CLA	C1D-ND	3.61	1.42	1.37
29	a	608	CHL	OBD-CAD	3.60	1.28	1.22
21	A	819	CLA	C1D-ND	3.60	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	831	CLA	C1D-ND	3.60	1.42	1.37
21	B	838	CLA	C1D-ND	3.60	1.42	1.37
21	3	406	CLA	CAB-C3B	-3.60	1.44	1.51
21	4	602	CLA	C1D-ND	3.59	1.42	1.37
21	1	311	CLA	CAB-C3B	-3.59	1.44	1.51
29	b	308	CHL	OBD-CAD	3.59	1.28	1.22
29	a	606	CHL	OBD-CAD	3.59	1.28	1.22
29	c	601	CHL	CHD-C4C	3.59	1.47	1.39
21	B	840	CLA	C1D-ND	3.59	1.42	1.37
21	B	836	CLA	C1D-ND	3.58	1.42	1.37
21	3	404	CLA	CAB-C3B	-3.58	1.44	1.51
21	B	808	CLA	C1D-ND	3.58	1.42	1.37
21	B	827	CLA	C1D-ND	3.58	1.42	1.37
21	A	842	CLA	C1D-ND	3.58	1.42	1.37
21	9	602	CLA	C1D-ND	3.58	1.42	1.37
21	B	810	CLA	CAB-C3B	-3.58	1.44	1.51
21	1	303	CLA	C1D-ND	3.58	1.42	1.37
21	A	814	CLA	C1D-ND	3.57	1.42	1.37
21	B	806	CLA	C1D-ND	3.57	1.42	1.37
29	6	602	CHL	CHD-C4C	3.57	1.47	1.39
21	A	832	CLA	C1D-ND	3.57	1.42	1.37
21	5	609	CLA	C1D-ND	3.57	1.42	1.37
24	F	301	BCR	C10-C9	3.56	1.40	1.35
29	2	606	CHL	CHD-C4C	3.56	1.47	1.39
21	5	614	CLA	CAB-C3B	-3.56	1.44	1.51
21	A	812	CLA	C1D-ND	3.56	1.42	1.37
21	A	810	CLA	C1D-ND	3.56	1.42	1.37
21	B	813	CLA	C1D-ND	3.56	1.42	1.37
29	4	607	CHL	OBD-CAD	3.56	1.28	1.22
21	7	403	CLA	CAB-C3B	-3.55	1.44	1.51
24	A	847	BCR	C10-C9	3.55	1.40	1.35
29	c	609	CHL	OBD-CAD	3.55	1.28	1.22
29	4	607	CHL	CHD-C4C	3.55	1.47	1.39
24	F	301	BCR	C14-C13	3.55	1.40	1.35
29	b	307	CHL	OBD-CAD	3.54	1.28	1.22
21	1	316	CLA	CAB-C3B	-3.54	1.44	1.51
29	b	310	CHL	OBD-CAD	3.54	1.28	1.22
21	4	609	CLA	OBD-CAD	3.54	1.28	1.22
24	A	848	BCR	C10-C9	3.54	1.40	1.35
21	B	829	CLA	C4D-ND	-3.54	1.32	1.37
21	B	828	CLA	C1D-ND	3.54	1.42	1.37
21	L	303	CLA	C1D-ND	3.54	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	824	CLA	C1D-ND	3.54	1.42	1.37
29	2	607	CHL	OBD-CAD	3.53	1.28	1.22
21	K	203	CLA	CAB-C3B	-3.53	1.44	1.51
29	2	607	CHL	CHD-C4C	3.52	1.47	1.39
21	B	821	CLA	C1D-ND	3.52	1.42	1.37
21	8	609	CLA	C4D-ND	-3.52	1.32	1.37
21	7	401	CLA	C1D-ND	3.51	1.42	1.37
21	5	613	CLA	CAB-C3B	-3.51	1.44	1.51
21	1	314	CLA	CAB-C3B	-3.51	1.44	1.51
21	B	818	CLA	C1D-ND	3.51	1.42	1.37
21	2	609	CLA	C4D-ND	-3.51	1.32	1.37
21	A	806	CLA	C1D-ND	3.51	1.42	1.37
24	A	848	BCR	C17-C18	3.51	1.40	1.35
21	7	405	CLA	CAB-C3B	-3.51	1.44	1.51
21	5	610	CLA	CAB-C3B	-3.50	1.44	1.51
21	A	811	CLA	C1D-ND	3.50	1.42	1.37
21	A	830	CLA	C4D-ND	-3.47	1.32	1.37
21	B	802	CLA	C1D-ND	3.47	1.42	1.37
29	2	606	CHL	OBD-CAD	3.47	1.28	1.22
21	5	608	CLA	CAB-C3B	-3.45	1.44	1.51
21	B	831	CLA	C1D-ND	3.43	1.42	1.37
21	A	829	CLA	C1D-ND	3.41	1.42	1.37
21	O	204	CLA	CHC-C1C	3.39	1.43	1.35
29	6	602	CHL	C1D-ND	-3.39	1.33	1.37
32	9	617	NEX	C10-C9	3.34	1.40	1.35
29	c	609	CHL	C3D-C2D	3.33	1.48	1.39
21	A	835	CLA	CHC-C1C	3.32	1.43	1.35
29	8	613	CHL	C3D-C2D	3.31	1.48	1.39
29	c	607	CHL	C3D-C2D	3.30	1.48	1.39
29	a	609	CHL	C3D-C2D	3.29	1.48	1.39
21	B	811	CLA	C4D-ND	-3.29	1.33	1.37
32	c	618	NEX	C10-C9	3.28	1.40	1.35
29	7	406	CHL	C3D-C2D	3.28	1.48	1.39
29	b	302	CHL	C3D-C2D	3.28	1.48	1.39
29	6	614	CHL	C3D-C2D	3.27	1.48	1.39
29	c	605	CHL	C3D-C2D	3.27	1.48	1.39
29	a	605	CHL	C3D-C2D	3.26	1.48	1.39
29	b	306	CHL	C3D-C2D	3.26	1.48	1.39
29	8	606	CHL	C3D-C2D	3.26	1.48	1.39
21	8	602	CLA	CHC-C1C	3.25	1.43	1.35
29	a	601	CHL	C3D-C2D	3.25	1.48	1.39
29	2	614	CHL	C3D-C2D	3.25	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	7	412	CLA	CHC-C1C	3.25	1.43	1.35
21	A	827	CLA	C4D-ND	-3.24	1.33	1.37
29	9	601	CHL	C3D-C2D	3.23	1.48	1.39
21	5	602	CLA	CHC-C1C	3.23	1.43	1.35
29	2	606	CHL	C1D-ND	-3.23	1.33	1.37
29	2	602	CHL	C3D-C2D	3.23	1.47	1.39
29	2	602	CHL	C1D-ND	-3.23	1.33	1.37
29	9	607	CHL	C3D-C2D	3.23	1.47	1.39
21	A	819	CLA	C4D-ND	-3.22	1.33	1.37
29	b	310	CHL	C3D-C2D	3.22	1.47	1.39
21	B	820	CLA	C4D-ND	-3.22	1.33	1.37
29	6	602	CHL	C3D-C2D	3.22	1.47	1.39
21	A	837	CLA	CHC-C1C	3.22	1.43	1.35
21	7	413	CLA	CHC-C1C	3.22	1.43	1.35
21	9	602	CLA	CHC-C1C	3.22	1.43	1.35
29	a	607	CHL	C3D-C2D	3.22	1.47	1.39
21	b	303	CLA	CHC-C1C	3.21	1.43	1.35
21	A	805	CLA	CHC-C1C	3.21	1.43	1.35
21	B	803	CLA	CHC-C1C	3.21	1.43	1.35
29	c	608	CHL	C3D-C2D	3.20	1.47	1.39
29	9	605	CHL	C3D-C2D	3.20	1.47	1.39
21	b	311	CLA	CHC-C1C	3.20	1.43	1.35
21	B	821	CLA	C4D-ND	-3.20	1.33	1.37
21	7	401	CLA	CHC-C1C	3.20	1.43	1.35
21	A	822	CLA	C4D-ND	-3.19	1.33	1.37
29	6	606	CHL	C3D-C2D	3.19	1.47	1.39
29	6	607	CHL	C3D-C2D	3.19	1.47	1.39
21	b	315	CLA	CHC-C1C	3.19	1.43	1.35
29	c	601	CHL	C1D-ND	-3.19	1.33	1.37
21	a	602	CLA	CHC-C1C	3.19	1.43	1.35
21	7	410	CLA	CHC-C1C	3.19	1.43	1.35
21	A	809	CLA	CHC-C1C	3.19	1.43	1.35
21	b	312	CLA	CHC-C1C	3.19	1.43	1.35
29	c	606	CHL	C3D-C2D	3.19	1.47	1.39
21	A	836	CLA	C4D-ND	-3.19	1.33	1.37
21	5	613	CLA	CHC-C1C	3.19	1.43	1.35
29	5	606	CHL	C3D-C2D	3.19	1.47	1.39
21	7	414	CLA	CHC-C1C	3.19	1.43	1.35
21	B	809	CLA	C4D-ND	-3.18	1.33	1.37
29	6	605	CHL	C3D-C2D	3.18	1.47	1.39
21	2	608	CLA	CHC-C1C	3.18	1.43	1.35
21	a	610	CLA	CHC-C1C	3.18	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	5	609	CLA	CHC-C1C	3.18	1.43	1.35
21	a	612	CLA	CHC-C1C	3.18	1.43	1.35
29	1	302	CHL	C3D-C2D	3.18	1.47	1.39
29	6	601	CHL	C3D-C2D	3.18	1.47	1.39
21	4	608	CLA	CHC-C1C	3.18	1.43	1.35
21	A	852	CLA	CHC-C1C	3.18	1.43	1.35
21	6	608	CLA	CHC-C1C	3.18	1.43	1.35
21	9	610	CLA	CHC-C1C	3.18	1.43	1.35
29	4	607	CHL	C1D-ND	-3.17	1.33	1.37
21	A	802	CLA	CHC-C1C	3.17	1.43	1.35
21	B	824	CLA	C4D-ND	-3.17	1.33	1.37
29	9	606	CHL	C3D-C2D	3.17	1.47	1.39
21	a	613	CLA	CHC-C1C	3.17	1.43	1.35
21	b	314	CLA	CHC-C1C	3.17	1.43	1.35
29	c	609	CHL	MG-NA	-3.17	1.98	2.06
21	5	607	CLA	CHC-C1C	3.17	1.43	1.35
21	5	611	CLA	CHC-C1C	3.17	1.43	1.35
21	7	409	CLA	CHC-C1C	3.17	1.43	1.35
21	O	202	CLA	CHC-C1C	3.16	1.43	1.35
21	6	610	CLA	CHC-C1C	3.16	1.43	1.35
29	4	606	CHL	C3D-C2D	3.16	1.47	1.39
21	B	815	CLA	CHC-C1C	3.16	1.43	1.35
21	B	833	CLA	CHC-C1C	3.16	1.43	1.35
21	6	613	CLA	CHC-C1C	3.16	1.43	1.35
21	A	836	CLA	CHC-C1C	3.16	1.43	1.35
29	b	308	CHL	C3D-C2D	3.16	1.47	1.39
29	5	601	CHL	C3D-C2D	3.16	1.47	1.39
21	a	604	CLA	CHC-C1C	3.16	1.43	1.35
21	B	814	CLA	C4D-ND	-3.16	1.33	1.37
21	A	823	CLA	CHC-C1C	3.16	1.43	1.35
29	8	607	CHL	C3D-C2D	3.16	1.47	1.39
29	9	608	CHL	C3D-C2D	3.15	1.47	1.39
21	B	812	CLA	CHC-C1C	3.15	1.43	1.35
21	8	611	CLA	CHC-C1C	3.15	1.43	1.35
29	8	605	CHL	C3D-C2D	3.15	1.47	1.39
21	A	818	CLA	CHC-C1C	3.15	1.43	1.35
21	A	826	CLA	CHC-C1C	3.15	1.43	1.35
21	A	832	CLA	CHC-C1C	3.15	1.43	1.35
21	3	415	CLA	CHC-C1C	3.15	1.43	1.35
21	8	604	CLA	CHC-C1C	3.15	1.43	1.35
29	2	601	CHL	C1D-ND	-3.15	1.33	1.37
21	6	611	CLA	CHC-C1C	3.15	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	7	405	CLA	CHC-C1C	3.15	1.43	1.35
32	b	318	NEX	C10-C9	3.15	1.40	1.35
21	B	807	CLA	C4D-ND	-3.15	1.33	1.37
21	c	604	CLA	CHC-C1C	3.15	1.43	1.35
21	3	403	CLA	C4D-ND	-3.15	1.33	1.37
21	B	804	CLA	CHC-C1C	3.15	1.43	1.35
21	8	601	CLA	CHC-C1C	3.14	1.43	1.35
21	8	603	CLA	CHC-C1C	3.14	1.43	1.35
21	4	602	CLA	CHC-C1C	3.14	1.43	1.35
21	1	305	CLA	CHC-C1C	3.14	1.43	1.35
21	A	812	CLA	C4D-ND	-3.14	1.33	1.37
29	2	607	CHL	C1D-ND	-3.14	1.33	1.37
21	L	303	CLA	CHC-C1C	3.14	1.43	1.35
21	A	807	CLA	C4D-ND	-3.14	1.33	1.37
21	8	612	CLA	CHC-C1C	3.14	1.43	1.35
29	2	605	CHL	C3D-C2D	3.14	1.47	1.39
29	3	407	CHL	C3D-C2D	3.14	1.47	1.39
21	2	604	CLA	CHC-C1C	3.14	1.43	1.35
21	5	610	CLA	CHC-C1C	3.14	1.43	1.35
21	5	614	CLA	CHC-C1C	3.14	1.43	1.35
29	4	605	CHL	C3D-C2D	3.14	1.47	1.39
29	c	601	CHL	C3D-C2D	3.14	1.47	1.39
21	L	303	CLA	C4D-ND	-3.14	1.33	1.37
29	2	601	CHL	C3D-C2D	3.14	1.47	1.39
21	A	839	CLA	C4D-ND	-3.13	1.33	1.37
21	B	831	CLA	C4D-ND	-3.13	1.33	1.37
21	A	815	CLA	CHC-C1C	3.13	1.43	1.35
21	6	612	CLA	CHC-C1C	3.13	1.43	1.35
21	7	403	CLA	CHC-C1C	3.13	1.43	1.35
21	7	411	CLA	CHC-C1C	3.13	1.43	1.35
21	c	612	CLA	CHC-C1C	3.13	1.43	1.35
21	B	825	CLA	C4D-ND	-3.13	1.33	1.37
21	6	604	CLA	CHC-C1C	3.13	1.43	1.35
29	4	614	CHL	C3D-C2D	3.13	1.47	1.39
21	B	828	CLA	C4D-ND	-3.13	1.33	1.37
21	B	838	CLA	C4D-ND	-3.13	1.33	1.37
21	1	316	CLA	CHC-C1C	3.13	1.43	1.35
29	b	309	CHL	C1D-ND	-3.13	1.33	1.37
21	2	613	CLA	CHC-C1C	3.13	1.43	1.35
21	F	302	CLA	CHC-C1C	3.12	1.43	1.35
21	2	603	CLA	CHC-C1C	3.12	1.43	1.35
21	B	802	CLA	CHC-C1C	3.12	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	8	610	CLA	CHC-C1C	3.12	1.43	1.35
21	A	831	CLA	C4D-ND	-3.12	1.33	1.37
21	1	306	CLA	CHC-C1C	3.12	1.43	1.35
21	G	204	CLA	CHC-C1C	3.12	1.43	1.35
21	A	829	CLA	CHC-C1C	3.12	1.43	1.35
21	6	609	CLA	CHC-C1C	3.12	1.43	1.35
21	7	408	CLA	CHC-C1C	3.12	1.43	1.35
21	b	305	CLA	CHC-C1C	3.12	1.43	1.35
21	5	608	CLA	CHC-C1C	3.12	1.43	1.35
21	a	603	CLA	CHC-C1C	3.12	1.43	1.35
21	a	611	CLA	CHC-C1C	3.12	1.43	1.35
21	B	817	CLA	C4D-ND	-3.12	1.33	1.37
21	3	406	CLA	CHC-C1C	3.12	1.43	1.35
21	A	808	CLA	CHC-C1C	3.12	1.43	1.35
29	9	601	CHL	C1D-ND	-3.12	1.34	1.37
21	2	611	CLA	CHC-C1C	3.12	1.43	1.35
21	7	404	CLA	CHC-C1C	3.12	1.43	1.35
21	A	824	CLA	C4D-ND	-3.12	1.33	1.37
21	B	820	CLA	CHC-C1C	3.12	1.43	1.35
21	B	831	CLA	CHC-C1C	3.12	1.43	1.35
21	4	611	CLA	CHC-C1C	3.12	1.43	1.35
21	A	823	CLA	C4D-ND	-3.11	1.33	1.37
21	A	806	CLA	CHC-C1C	3.11	1.42	1.35
21	G	202	CLA	CHC-C1C	3.11	1.42	1.35
21	B	827	CLA	C4D-ND	-3.11	1.33	1.37
21	9	602	CLA	C4D-ND	-3.11	1.33	1.37
21	F	304	CLA	CHC-C1C	3.11	1.42	1.35
21	c	610	CLA	CHC-C1C	3.11	1.42	1.35
21	B	824	CLA	CHC-C1C	3.11	1.42	1.35
21	1	314	CLA	CHC-C1C	3.11	1.42	1.35
21	3	404	CLA	CHC-C1C	3.11	1.42	1.35
21	A	812	CLA	CHC-C1C	3.11	1.42	1.35
21	1	313	CLA	CHC-C1C	3.11	1.42	1.35
21	c	614	CLA	CHC-C1C	3.11	1.42	1.35
21	B	836	CLA	C4D-ND	-3.11	1.33	1.37
21	3	405	CLA	C4D-ND	-3.11	1.33	1.37
29	1	302	CHL	C1D-ND	-3.11	1.34	1.37
21	1	303	CLA	CHC-C1C	3.11	1.42	1.35
21	3	408	CLA	CHC-C1C	3.11	1.42	1.35
21	A	808	CLA	C4D-ND	-3.11	1.33	1.37
21	1	310	CLA	CHC-C1C	3.11	1.42	1.35
21	3	402	CLA	CHC-C1C	3.11	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	9	609	CHL	C3D-C2D	3.11	1.47	1.39
29	b	309	CHL	C3D-C2D	3.11	1.47	1.39
21	A	811	CLA	CHC-C1C	3.11	1.42	1.35
21	A	804	CLA	CHC-C1C	3.11	1.42	1.35
21	4	613	CLA	CHC-C1C	3.11	1.42	1.35
21	c	603	CLA	CHC-C1C	3.10	1.42	1.35
21	B	806	CLA	C4D-ND	-3.10	1.33	1.37
21	6	603	CLA	CHC-C1C	3.10	1.42	1.35
21	c	613	CLA	CHC-C1C	3.10	1.42	1.35
21	5	612	CLA	CHC-C1C	3.10	1.42	1.35
21	A	809	CLA	C4D-ND	-3.10	1.33	1.37
21	B	818	CLA	C4D-ND	-3.10	1.33	1.37
21	3	414	CLA	CHC-C1C	3.10	1.42	1.35
21	1	305	CLA	C4D-ND	-3.10	1.33	1.37
21	1	311	CLA	CHC-C1C	3.10	1.42	1.35
21	4	610	CLA	CHC-C1C	3.10	1.42	1.35
21	A	827	CLA	CHC-C1C	3.10	1.42	1.35
21	c	602	CLA	CHC-C1C	3.10	1.42	1.35
21	A	826	CLA	C4D-ND	-3.10	1.33	1.37
29	a	608	CHL	C3D-C2D	3.10	1.47	1.39
21	L	302	CLA	CHC-C1C	3.10	1.42	1.35
21	A	820	CLA	CHC-C1C	3.09	1.42	1.35
21	8	608	CLA	CHC-C1C	3.09	1.42	1.35
21	a	614	CLA	CHC-C1C	3.09	1.42	1.35
21	G	203	CLA	CHC-C1C	3.09	1.42	1.35
21	B	822	CLA	C4D-ND	-3.09	1.33	1.37
21	9	611	CLA	CHC-C1C	3.09	1.42	1.35
21	J	102	CLA	CHC-C1C	3.09	1.42	1.35
21	A	806	CLA	C4D-ND	-3.09	1.33	1.37
21	K	203	CLA	C4D-ND	-3.09	1.33	1.37
21	4	604	CLA	CHC-C1C	3.09	1.42	1.35
21	1	315	CLA	CHC-C1C	3.09	1.42	1.35
29	b	302	CHL	MG-NA	-3.09	1.98	2.06
29	7	406	CHL	MG-NA	-3.09	1.98	2.06
21	B	821	CLA	CHC-C1C	3.09	1.42	1.35
21	A	819	CLA	CHC-C1C	3.08	1.42	1.35
21	A	824	CLA	CHC-C1C	3.08	1.42	1.35
21	A	838	CLA	C4D-ND	-3.08	1.33	1.37
29	b	307	CHL	C3D-C2D	3.08	1.47	1.39
21	O	203	CLA	C4D-ND	-3.08	1.33	1.37
21	A	815	CLA	C4D-ND	-3.08	1.33	1.37
21	A	801	CLA	CHC-C1C	3.08	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	821	CLA	CHC-C1C	3.08	1.42	1.35
21	4	612	CLA	C4D-ND	-3.08	1.33	1.37
21	B	834	CLA	CHC-C1C	3.08	1.42	1.35
29	2	606	CHL	C3D-C2D	3.08	1.47	1.39
21	B	813	CLA	CHC-C1C	3.08	1.42	1.35
21	A	803	CLA	C4D-ND	-3.08	1.33	1.37
21	B	836	CLA	CHC-C1C	3.08	1.42	1.35
21	5	605	CLA	CHC-C1C	3.08	1.42	1.35
29	2	607	CHL	C3D-C2D	3.08	1.47	1.39
21	B	834	CLA	C4D-ND	-3.08	1.33	1.37
21	3	413	CLA	CHC-C1C	3.08	1.42	1.35
21	A	825	CLA	CHC-C1C	3.07	1.42	1.35
21	B	810	CLA	CHC-C1C	3.07	1.42	1.35
21	4	601	CLA	CHC-C1C	3.07	1.42	1.35
21	A	828	CLA	CHC-C1C	3.07	1.42	1.35
29	a	606	CHL	C1D-ND	-3.07	1.34	1.37
21	B	818	CLA	CHC-C1C	3.07	1.42	1.35
21	L	304	CLA	CHC-C1C	3.07	1.42	1.35
29	1	307	CHL	C3D-C2D	3.07	1.47	1.39
21	9	604	CLA	CHC-C1C	3.07	1.42	1.35
21	3	410	CLA	CHC-C1C	3.07	1.42	1.35
21	5	604	CLA	CHC-C1C	3.07	1.42	1.35
29	9	606	CHL	C1D-ND	-3.06	1.34	1.37
21	c	611	CLA	CHC-C1C	3.06	1.42	1.35
21	A	820	CLA	C4D-ND	-3.06	1.33	1.37
21	A	821	CLA	C4D-ND	-3.06	1.33	1.37
21	B	839	CLA	C4D-ND	-3.06	1.33	1.37
21	8	618	CLA	CHC-C1C	3.06	1.42	1.35
21	B	813	CLA	C4D-ND	-3.06	1.33	1.37
21	A	840	CLA	CHC-C1C	3.06	1.42	1.35
21	A	816	CLA	CHC-C1C	3.06	1.42	1.35
21	H	201	CLA	CHC-C1C	3.06	1.42	1.35
21	4	612	CLA	CHC-C1C	3.06	1.42	1.35
21	K	202	CLA	CHC-C1C	3.06	1.42	1.35
21	B	822	CLA	CHC-C1C	3.06	1.42	1.35
21	B	832	CLA	CHC-C1C	3.06	1.42	1.35
21	A	810	CLA	CHC-C1C	3.06	1.42	1.35
21	K	204	CLA	CHC-C1C	3.06	1.42	1.35
29	3	407	CHL	C1D-ND	-3.06	1.34	1.37
29	4	606	CHL	C1D-ND	-3.06	1.34	1.37
21	9	612	CLA	CHC-C1C	3.06	1.42	1.35
29	b	307	CHL	C1D-ND	-3.05	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	830	CLA	CHC-C1C	3.05	1.42	1.35
21	L	304	CLA	C4D-ND	-3.05	1.33	1.37
21	1	312	CLA	C4D-ND	-3.05	1.33	1.37
21	1	312	CLA	CHC-C1C	3.05	1.42	1.35
21	O	203	CLA	CHC-C1C	3.05	1.42	1.35
21	b	313	CLA	CHC-C1C	3.05	1.42	1.35
21	A	822	CLA	CHC-C1C	3.05	1.42	1.35
21	B	840	CLA	C4D-ND	-3.05	1.33	1.37
21	7	402	CLA	CHC-C1C	3.05	1.42	1.35
21	B	835	CLA	CHC-C1C	3.05	1.42	1.35
29	b	310	CHL	C1D-ND	-3.05	1.34	1.37
21	A	816	CLA	C4D-ND	-3.05	1.33	1.37
21	B	812	CLA	C4D-ND	-3.05	1.33	1.37
21	A	842	CLA	CHC-C1C	3.05	1.42	1.35
21	B	805	CLA	C4D-ND	-3.05	1.33	1.37
21	B	826	CLA	CHC-C1C	3.05	1.42	1.35
21	B	838	CLA	CHC-C1C	3.05	1.42	1.35
21	B	840	CLA	CHC-C1C	3.05	1.42	1.35
21	F	305	CLA	CHC-C1C	3.05	1.42	1.35
21	B	828	CLA	CHC-C1C	3.05	1.42	1.35
21	B	808	CLA	C4D-ND	-3.05	1.33	1.37
21	B	808	CLA	CHC-C1C	3.05	1.42	1.35
21	3	412	CLA	CHC-C1C	3.05	1.42	1.35
21	L	302	CLA	C4D-ND	-3.05	1.33	1.37
29	4	607	CHL	C3D-C2D	3.05	1.47	1.39
21	9	603	CLA	CHC-C1C	3.05	1.42	1.35
21	O	201	CLA	CHC-C1C	3.04	1.42	1.35
21	B	811	CLA	CHC-C1C	3.04	1.42	1.35
21	A	803	CLA	CHC-C1C	3.04	1.42	1.35
21	B	825	CLA	CHC-C1C	3.04	1.42	1.35
29	2	614	CHL	C1D-ND	-3.04	1.34	1.37
21	9	613	CLA	CHC-C1C	3.04	1.42	1.35
21	B	804	CLA	C4D-ND	-3.04	1.33	1.37
29	4	605	CHL	C1D-ND	-3.04	1.34	1.37
21	c	602	CLA	C4D-ND	-3.04	1.33	1.37
29	b	308	CHL	C1D-ND	-3.04	1.34	1.37
29	c	605	CHL	MG-NA	-3.04	1.99	2.06
21	5	603	CLA	CHC-C1C	3.04	1.42	1.35
29	a	609	CHL	MG-NA	-3.04	1.99	2.06
21	A	831	CLA	CHC-C1C	3.04	1.42	1.35
21	B	837	CLA	CHC-C1C	3.04	1.42	1.35
21	4	604	CLA	C4D-ND	-3.04	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	817	CLA	CHC-C1C	3.04	1.42	1.35
21	B	816	CLA	CHC-C1C	3.04	1.42	1.35
21	K	202	CLA	C4D-ND	-3.04	1.33	1.37
21	A	818	CLA	C4D-ND	-3.03	1.33	1.37
21	B	830	CLA	C4D-ND	-3.03	1.33	1.37
29	4	614	CHL	C1D-ND	-3.03	1.34	1.37
21	B	819	CLA	C4D-ND	-3.03	1.33	1.37
21	B	835	CLA	C4D-ND	-3.03	1.33	1.37
21	1	313	CLA	C4D-ND	-3.03	1.33	1.37
21	A	807	CLA	CHC-C1C	3.03	1.42	1.35
21	A	832	CLA	C4D-ND	-3.03	1.33	1.37
21	B	823	CLA	CHC-C1C	3.03	1.42	1.35
21	3	411	CLA	CHC-C1C	3.03	1.42	1.35
21	3	411	CLA	C4D-ND	-3.03	1.33	1.37
21	3	412	CLA	C4D-ND	-3.03	1.33	1.37
29	8	606	CHL	MG-NA	-3.03	1.99	2.06
21	A	805	CLA	C4D-ND	-3.03	1.33	1.37
21	1	303	CLA	C4D-ND	-3.03	1.33	1.37
21	2	612	CLA	C4D-ND	-3.03	1.33	1.37
21	3	410	CLA	C4D-ND	-3.03	1.33	1.37
29	b	306	CHL	C1D-ND	-3.03	1.34	1.37
21	B	805	CLA	CHC-C1C	3.03	1.42	1.35
29	2	605	CHL	C1D-ND	-3.03	1.34	1.37
21	B	819	CLA	CHC-C1C	3.02	1.42	1.35
21	A	833	CLA	CHC-C1C	3.02	1.42	1.35
21	A	838	CLA	CHC-C1C	3.02	1.42	1.35
21	B	807	CLA	CHC-C1C	3.02	1.42	1.35
21	B	814	CLA	CHC-C1C	3.02	1.42	1.35
21	1	306	CLA	C4D-ND	-3.02	1.33	1.37
21	1	304	CLA	CHC-C1C	3.02	1.42	1.35
29	a	606	CHL	C3D-C2D	3.02	1.47	1.39
21	A	811	CLA	C4D-ND	-3.02	1.33	1.37
21	A	814	CLA	C4D-ND	-3.02	1.33	1.37
21	3	408	CLA	C4D-ND	-3.02	1.33	1.37
21	A	814	CLA	CHC-C1C	3.02	1.42	1.35
21	K	203	CLA	CHC-C1C	3.02	1.42	1.35
21	6	612	CLA	C4D-ND	-3.01	1.33	1.37
21	A	841	CLA	CHC-C1C	3.01	1.42	1.35
21	8	609	CLA	CHC-C1C	3.01	1.42	1.35
21	B	809	CLA	CHC-C1C	3.01	1.42	1.35
21	2	612	CLA	CHC-C1C	3.01	1.42	1.35
21	K	201	CLA	CHC-C1C	3.01	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	F	305	CLA	C4D-ND	-3.01	1.33	1.37
21	2	611	CLA	C4D-ND	-3.01	1.33	1.37
21	9	611	CLA	C4D-ND	-3.01	1.33	1.37
21	3	403	CLA	CHC-C1C	3.01	1.42	1.35
21	b	303	CLA	C4D-ND	-3.01	1.33	1.37
21	1	308	CLA	CHC-C1C	3.01	1.42	1.35
21	A	842	CLA	C4D-ND	-3.01	1.33	1.37
29	9	608	CHL	C1D-ND	-3.01	1.34	1.37
21	3	414	CLA	C4D-ND	-3.00	1.33	1.37
21	B	806	CLA	CHC-C1C	3.00	1.42	1.35
21	4	608	CLA	C4D-ND	-3.00	1.33	1.37
21	a	602	CLA	C4D-ND	-3.00	1.33	1.37
29	9	605	CHL	C1D-ND	-3.00	1.34	1.37
21	A	810	CLA	C4D-ND	-3.00	1.33	1.37
24	A	850	BCR	C23-C22	-3.00	1.39	1.45
21	2	610	CLA	C4D-ND	-3.00	1.33	1.37
24	A	848	BCR	C23-C22	-3.00	1.39	1.45
29	8	613	CHL	C1D-ND	-3.00	1.34	1.37
21	A	813	CLA	CHC-C1C	3.00	1.42	1.35
29	1	307	CHL	C1D-ND	-3.00	1.34	1.37
21	A	829	CLA	C4D-ND	-3.00	1.33	1.37
21	A	839	CLA	CHC-C1C	2.99	1.42	1.35
21	A	830	CLA	CHC-C1C	2.99	1.42	1.35
21	A	834	CLA	C4D-ND	-2.99	1.33	1.37
21	8	602	CLA	C4D-ND	-2.99	1.33	1.37
21	3	402	CLA	C4D-ND	-2.99	1.33	1.37
21	A	834	CLA	CHC-C1C	2.99	1.42	1.35
21	B	823	CLA	C4D-ND	-2.99	1.33	1.37
21	B	832	CLA	C4D-ND	-2.99	1.33	1.37
21	2	603	CLA	C4D-ND	-2.99	1.33	1.37
21	A	828	CLA	C4D-ND	-2.99	1.33	1.37
21	4	603	CLA	C4D-ND	-2.99	1.33	1.37
24	F	301	BCR	C8-C9	-2.98	1.39	1.45
21	A	835	CLA	C4D-ND	-2.98	1.33	1.37
21	O	201	CLA	C4D-ND	-2.98	1.33	1.37
21	O	202	CLA	C4D-ND	-2.98	1.33	1.37
21	3	405	CLA	CHC-C1C	2.98	1.42	1.35
21	B	803	CLA	C4D-ND	-2.98	1.33	1.37
21	7	401	CLA	C4D-ND	-2.98	1.33	1.37
21	B	810	CLA	C4D-ND	-2.98	1.33	1.37
21	3	413	CLA	C4D-ND	-2.98	1.33	1.37
29	c	609	CHL	C1D-ND	-2.98	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	310	CLA	C4D-ND	-2.98	1.33	1.37
29	a	608	CHL	C1D-ND	-2.98	1.34	1.37
21	F	304	CLA	C4D-ND	-2.97	1.33	1.37
24	A	848	BCR	C8-C9	-2.97	1.39	1.45
21	A	825	CLA	C4D-ND	-2.97	1.33	1.37
21	B	816	CLA	C4D-ND	-2.97	1.33	1.37
24	A	849	BCR	C8-C9	-2.97	1.39	1.45
21	8	601	CLA	C4D-ND	-2.97	1.33	1.37
21	1	309	CLA	CHC-C1C	2.97	1.42	1.35
29	5	601	CHL	C1D-ND	-2.97	1.34	1.37
21	3	406	CLA	C4D-ND	-2.97	1.33	1.37
29	9	609	CHL	C1D-ND	-2.97	1.34	1.37
21	3	401	CLA	CHC-C1C	2.97	1.42	1.35
21	2	610	CLA	CHC-C1C	2.97	1.42	1.35
21	9	612	CLA	C4D-ND	-2.97	1.33	1.37
21	b	304	CLA	C4D-ND	-2.97	1.33	1.37
24	A	850	BCR	C8-C9	-2.96	1.39	1.45
21	B	827	CLA	CHC-C1C	2.96	1.42	1.35
21	c	613	CLA	C4D-ND	-2.96	1.33	1.37
30	7	415	LUT	C8-C9	-2.96	1.39	1.45
21	b	304	CLA	CHC-C1C	2.96	1.42	1.35
21	4	601	CLA	C4D-ND	-2.96	1.33	1.37
21	7	409	CLA	C4D-ND	-2.96	1.33	1.37
21	A	817	CLA	C4D-ND	-2.96	1.33	1.37
21	B	833	CLA	C4D-ND	-2.96	1.33	1.37
21	2	604	CLA	C4D-ND	-2.96	1.33	1.37
21	B	829	CLA	CHC-C1C	2.96	1.42	1.35
21	A	833	CLA	C4D-ND	-2.96	1.33	1.37
21	2	609	CLA	CHC-C1C	2.96	1.42	1.35
21	K	201	CLA	C4D-ND	-2.96	1.33	1.37
21	A	840	CLA	C4D-ND	-2.96	1.33	1.37
21	4	611	CLA	C4D-ND	-2.96	1.33	1.37
21	3	415	CLA	C4D-ND	-2.96	1.33	1.37
21	7	403	CLA	C4D-ND	-2.95	1.33	1.37
29	a	601	CHL	MG-NA	-2.95	1.99	2.06
21	A	841	CLA	C4D-ND	-2.95	1.33	1.37
29	a	605	CHL	MG-NA	-2.95	1.99	2.06
21	5	602	CLA	C4D-ND	-2.95	1.33	1.37
21	b	305	CLA	C4D-ND	-2.95	1.33	1.37
21	4	603	CLA	CHC-C1C	2.95	1.42	1.35
29	6	606	CHL	C1D-ND	-2.95	1.34	1.37
21	1	311	CLA	C4D-ND	-2.95	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	813	CLA	C4D-ND	-2.95	1.33	1.37
21	9	613	CLA	C4D-ND	-2.95	1.33	1.37
21	a	613	CLA	C4D-ND	-2.95	1.33	1.37
21	B	839	CLA	CHC-C1C	2.94	1.42	1.35
21	A	817	CLA	CHC-C1C	2.94	1.42	1.35
21	2	613	CLA	C4D-ND	-2.94	1.33	1.37
21	9	604	CLA	C4D-ND	-2.94	1.33	1.37
21	B	802	CLA	C4D-ND	-2.94	1.33	1.37
21	B	837	CLA	C4D-ND	-2.93	1.33	1.37
21	9	610	CLA	C4D-ND	-2.93	1.33	1.37
21	6	610	CLA	C4D-ND	-2.93	1.33	1.37
21	1	308	CLA	C4D-ND	-2.93	1.33	1.37
24	A	854	BCR	C23-C22	-2.93	1.39	1.45
29	5	606	CHL	C1D-ND	-2.93	1.34	1.37
24	J	101	BCR	C8-C9	-2.93	1.39	1.45
21	4	610	CLA	C4D-ND	-2.92	1.33	1.37
24	A	847	BCR	C23-C22	-2.92	1.39	1.45
21	8	618	CLA	C4D-ND	-2.92	1.33	1.37
21	A	802	CLA	C4D-ND	-2.92	1.33	1.37
21	7	405	CLA	C4D-ND	-2.92	1.33	1.37
21	c	604	CLA	C4D-ND	-2.92	1.33	1.37
21	5	609	CLA	C4D-ND	-2.92	1.33	1.37
21	A	852	CLA	C4D-ND	-2.92	1.33	1.37
24	F	303	BCR	C8-C9	-2.92	1.39	1.45
29	6	605	CHL	C1D-ND	-2.92	1.34	1.37
21	1	304	CLA	C4D-ND	-2.92	1.33	1.37
21	B	826	CLA	C4D-ND	-2.91	1.33	1.37
29	a	607	CHL	C1D-ND	-2.91	1.34	1.37
30	b	317	LUT	C8-C9	-2.91	1.39	1.45
21	b	314	CLA	C4D-ND	-2.91	1.33	1.37
21	K	204	CLA	C4D-ND	-2.91	1.33	1.37
24	A	854	BCR	C8-C9	-2.91	1.39	1.45
21	4	602	CLA	C4D-ND	-2.91	1.33	1.37
21	8	608	CLA	C4D-ND	-2.91	1.33	1.37
21	c	611	CLA	C4D-ND	-2.91	1.33	1.37
29	a	606	CHL	MG-NA	-2.91	1.99	2.06
29	6	607	CHL	C1D-ND	-2.91	1.34	1.37
29	8	605	CHL	C1D-ND	-2.91	1.34	1.37
21	A	837	CLA	C4D-ND	-2.91	1.33	1.37
21	8	610	CLA	C4D-ND	-2.91	1.33	1.37
24	A	847	BCR	C8-C9	-2.91	1.39	1.45
24	A	849	BCR	C23-C22	-2.91	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	a	610	CLA	C4D-ND	-2.91	1.33	1.37
21	5	613	CLA	C4D-ND	-2.90	1.33	1.37
24	L	305	BCR	C23-C22	-2.90	1.39	1.45
21	J	102	CLA	C4D-ND	-2.90	1.33	1.37
29	9	607	CHL	C1D-ND	-2.90	1.34	1.37
21	5	610	CLA	C4D-ND	-2.90	1.33	1.37
21	c	614	CLA	C4D-ND	-2.90	1.33	1.37
21	4	613	CLA	C4D-ND	-2.90	1.33	1.37
21	c	610	CLA	C4D-ND	-2.90	1.33	1.37
29	6	614	CHL	MG-NA	-2.90	1.99	2.06
21	b	312	CLA	C4D-ND	-2.89	1.33	1.37
21	H	201	CLA	C4D-ND	-2.89	1.33	1.37
24	L	301	BCR	C8-C9	-2.89	1.39	1.45
21	1	316	CLA	C4D-ND	-2.89	1.33	1.37
24	3	419	BCR	C8-C9	-2.89	1.39	1.45
21	b	311	CLA	C4D-ND	-2.89	1.33	1.37
24	B	845	BCR	C8-C9	-2.89	1.39	1.45
24	M	101	BCR	C8-C9	-2.89	1.39	1.45
21	c	612	CLA	C4D-ND	-2.89	1.33	1.37
21	3	401	CLA	C4D-ND	-2.89	1.33	1.37
29	c	607	CHL	MG-NA	-2.89	1.99	2.06
21	G	203	CLA	C4D-ND	-2.88	1.33	1.37
21	5	605	CLA	C4D-ND	-2.88	1.33	1.37
21	F	302	CLA	C4D-ND	-2.88	1.33	1.37
21	1	309	CLA	C3A-C2A	-2.88	1.51	1.54
24	I	101	BCR	C23-C22	-2.88	1.39	1.45
24	B	845	BCR	C23-C22	-2.88	1.39	1.45
29	8	607	CHL	C1D-ND	-2.87	1.34	1.37
30	9	615	LUT	C8-C9	-2.87	1.39	1.45
29	c	606	CHL	C1D-ND	-2.87	1.34	1.37
24	L	305	BCR	C8-C9	-2.87	1.39	1.45
21	5	612	CLA	C4D-ND	-2.87	1.33	1.37
21	8	603	CLA	C4D-ND	-2.87	1.33	1.37
21	2	608	CLA	C4D-ND	-2.87	1.33	1.37
29	a	605	CHL	C1D-ND	-2.87	1.34	1.37
24	L	301	BCR	C23-C22	-2.87	1.39	1.45
21	5	604	CLA	C4D-ND	-2.86	1.33	1.37
21	G	204	CLA	C4D-ND	-2.86	1.33	1.37
29	6	601	CHL	C1D-ND	-2.86	1.34	1.37
21	8	604	CLA	C4D-ND	-2.86	1.33	1.37
29	5	606	CHL	MG-NA	-2.86	1.99	2.06
21	6	611	CLA	C4D-ND	-2.86	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	6	604	CLA	C4D-ND	-2.86	1.33	1.37
21	5	608	CLA	C4D-ND	-2.86	1.33	1.37
29	b	302	CHL	C1D-ND	-2.86	1.34	1.37
29	c	607	CHL	C1D-ND	-2.86	1.34	1.37
24	B	842	BCR	C23-C22	-2.86	1.39	1.45
30	8	614	LUT	C8-C9	-2.85	1.39	1.45
29	a	606	CHL	C4D-CHA	2.85	1.48	1.38
21	6	603	CLA	C4D-ND	-2.85	1.33	1.37
21	5	614	CLA	C4D-ND	-2.85	1.33	1.37
21	G	202	CLA	C4D-ND	-2.85	1.33	1.37
21	1	315	CLA	C4D-ND	-2.85	1.33	1.37
21	7	411	CLA	C4D-ND	-2.85	1.33	1.37
21	9	603	CLA	C4D-ND	-2.85	1.33	1.37
21	7	412	CLA	C4D-ND	-2.85	1.33	1.37
21	6	608	CLA	C4D-ND	-2.85	1.33	1.37
29	c	608	CHL	C1D-ND	-2.85	1.34	1.37
21	8	611	CLA	C4D-ND	-2.85	1.33	1.37
21	A	804	CLA	C4D-ND	-2.84	1.33	1.37
21	c	603	CLA	C4D-ND	-2.84	1.33	1.37
21	b	315	CLA	C4D-ND	-2.84	1.33	1.37
29	a	605	CHL	C4D-CHA	2.84	1.48	1.38
24	A	846	BCR	C8-C9	-2.84	1.39	1.45
24	F	301	BCR	C23-C22	-2.84	1.39	1.45
21	6	613	CLA	C4D-ND	-2.84	1.33	1.37
21	7	413	CLA	C4D-ND	-2.84	1.33	1.37
24	3	418	BCR	C8-C9	-2.83	1.39	1.45
21	a	604	CLA	C4D-ND	-2.83	1.33	1.37
29	8	606	CHL	C1D-ND	-2.83	1.34	1.37
29	9	601	CHL	MG-NA	-2.83	1.99	2.06
24	2	618	BCR	C8-C9	-2.83	1.39	1.45
29	8	613	CHL	MG-NA	-2.83	1.99	2.06
24	I	101	BCR	C8-C9	-2.83	1.39	1.45
21	a	612	CLA	C4D-ND	-2.82	1.33	1.37
29	c	605	CHL	C1D-ND	-2.82	1.34	1.37
24	G	205	BCR	C8-C9	-2.82	1.39	1.45
30	c	615	LUT	C8-C9	-2.82	1.39	1.45
21	7	410	CLA	C4D-ND	-2.82	1.33	1.37
21	1	314	CLA	C4D-ND	-2.82	1.33	1.37
29	1	302	CHL	MG-NA	-2.82	1.99	2.06
21	B	815	CLA	C4D-ND	-2.82	1.33	1.37
21	a	611	CLA	C4D-ND	-2.82	1.33	1.37
21	7	404	CLA	C4D-ND	-2.82	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	a	603	CLA	C4D-ND	-2.81	1.33	1.37
21	a	614	CLA	C4D-ND	-2.81	1.33	1.37
21	5	607	CLA	C4D-ND	-2.81	1.33	1.37
21	7	402	CLA	C4D-ND	-2.81	1.33	1.37
24	4	617	BCR	C8-C9	-2.81	1.39	1.45
21	3	404	CLA	C4D-ND	-2.81	1.33	1.37
29	7	406	CHL	C1D-ND	-2.80	1.34	1.37
24	B	842	BCR	C8-C9	-2.80	1.39	1.45
21	8	612	CLA	C4D-ND	-2.80	1.33	1.37
24	G	201	BCR	C8-C9	-2.80	1.39	1.45
29	b	306	CHL	MG-NA	-2.80	1.99	2.06
29	c	606	CHL	MG-NA	-2.80	1.99	2.06
29	a	601	CHL	C1D-ND	-2.79	1.34	1.37
21	5	611	CLA	C4D-ND	-2.79	1.33	1.37
29	6	601	CHL	MG-NA	-2.79	1.99	2.06
29	6	607	CHL	MG-NA	-2.79	1.99	2.06
24	A	846	BCR	C23-C22	-2.78	1.40	1.45
21	7	414	CLA	C4D-ND	-2.78	1.33	1.37
29	9	601	CHL	C4D-CHA	2.78	1.48	1.38
29	a	601	CHL	C4D-CHA	2.78	1.48	1.38
30	9	614	LUT	C8-C9	-2.78	1.40	1.45
24	L	306	BCR	C8-C9	-2.77	1.40	1.45
24	3	419	BCR	C23-C22	-2.77	1.40	1.45
30	2	616	LUT	C8-C9	-2.77	1.40	1.45
24	F	303	BCR	C23-C22	-2.77	1.40	1.45
24	6	618	BCR	C23-C22	-2.77	1.40	1.45
30	4	615	LUT	C8-C9	-2.77	1.40	1.45
24	G	205	BCR	C23-C22	-2.77	1.40	1.45
29	c	609	CHL	C4D-CHA	2.76	1.48	1.38
29	6	614	CHL	C1D-ND	-2.76	1.34	1.37
24	7	418	BCR	C23-C22	-2.76	1.40	1.45
24	G	201	BCR	C23-C22	-2.76	1.40	1.45
21	7	408	CLA	C4D-ND	-2.76	1.33	1.37
30	6	616	LUT	C8-C9	-2.76	1.40	1.45
30	5	615	LUT	C8-C9	-2.76	1.40	1.45
30	c	616	LUT	C8-C9	-2.75	1.40	1.45
24	J	103	BCR	C8-C9	-2.75	1.40	1.45
21	b	313	CLA	C4D-ND	-2.75	1.33	1.37
21	B	808	CLA	CMB-C2B	-2.75	1.45	1.51
24	4	617	BCR	C23-C22	-2.75	1.40	1.45
29	b	302	CHL	C4D-CHA	2.74	1.48	1.38
21	B	828	CLA	CMB-C2B	-2.73	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	M	101	BCR	C23-C22	-2.73	1.40	1.45
24	J	103	BCR	C23-C22	-2.72	1.40	1.45
24	7	417	BCR	C8-C9	-2.72	1.40	1.45
24	L	306	BCR	C23-C22	-2.72	1.40	1.45
29	c	608	CHL	C4D-CHA	2.72	1.48	1.38
21	5	603	CLA	C4D-ND	-2.72	1.34	1.37
29	b	310	CHL	MG-NA	-2.72	1.99	2.06
29	2	602	CHL	MG-NA	-2.71	1.99	2.06
29	9	605	CHL	MG-NA	-2.71	1.99	2.06
24	J	101	BCR	C23-C22	-2.71	1.40	1.45
24	6	618	BCR	C8-C9	-2.71	1.40	1.45
24	7	417	BCR	C23-C22	-2.71	1.40	1.45
29	4	606	CHL	MG-NA	-2.71	1.99	2.06
29	8	606	CHL	C4D-CHA	2.70	1.48	1.38
30	a	615	LUT	C8-C9	-2.70	1.40	1.45
29	c	605	CHL	C4D-CHA	2.70	1.48	1.38
24	7	418	BCR	C8-C9	-2.69	1.40	1.45
21	B	816	CLA	CMB-C2B	-2.69	1.46	1.51
29	7	406	CHL	C4D-CHA	2.69	1.48	1.38
30	a	616	LUT	C8-C9	-2.69	1.40	1.45
24	O	205	BCR	C23-C22	-2.69	1.40	1.45
29	6	601	CHL	C4D-CHA	2.69	1.48	1.38
29	b	308	CHL	MG-NA	-2.68	1.99	2.06
21	6	609	CLA	C4D-ND	-2.68	1.34	1.37
29	a	609	CHL	C1D-ND	-2.68	1.34	1.37
24	8	616	BCR	C8-C9	-2.68	1.40	1.45
29	c	607	CHL	C4D-CHA	2.68	1.47	1.38
21	O	204	CLA	C4D-ND	-2.68	1.34	1.37
29	2	601	CHL	MG-NA	-2.68	1.99	2.06
29	9	607	CHL	C4D-CHA	2.67	1.47	1.38
29	9	607	CHL	MG-NA	-2.67	1.99	2.06
24	3	418	BCR	C23-C22	-2.67	1.40	1.45
29	b	307	CHL	MG-NA	-2.67	1.99	2.06
29	c	606	CHL	C4D-CHA	2.67	1.47	1.38
29	4	614	CHL	MG-NA	-2.67	1.99	2.06
29	5	606	CHL	C4D-CHA	2.66	1.47	1.38
30	1	317	LUT	C8-C9	-2.66	1.40	1.45
29	2	605	CHL	MG-NA	-2.66	2.00	2.06
21	3	408	CLA	CMB-C2B	-2.66	1.46	1.51
30	b	316	LUT	C8-C9	-2.66	1.40	1.45
29	6	614	CHL	C4D-CHA	2.65	1.47	1.38
29	b	309	CHL	MG-NA	-2.65	2.00	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	8	607	CHL	MG-NA	-2.65	2.00	2.06
21	B	807	CLA	CMB-C2B	-2.65	1.46	1.51
21	B	839	CLA	CMB-C2B	-2.65	1.46	1.51
21	3	404	CLA	CMB-C2B	-2.65	1.46	1.51
29	a	609	CHL	C4D-CHA	2.65	1.47	1.38
29	b	308	CHL	C4D-CHA	2.64	1.47	1.38
29	6	602	CHL	MG-NA	-2.64	2.00	2.06
29	9	606	CHL	MG-NA	-2.64	2.00	2.06
29	6	606	CHL	C4D-CHA	2.63	1.47	1.38
29	5	601	CHL	MG-NA	-2.63	2.00	2.06
29	2	614	CHL	MG-NA	-2.63	2.00	2.06
29	9	608	CHL	MG-NA	-2.63	2.00	2.06
24	O	205	BCR	C8-C9	-2.63	1.40	1.45
29	9	606	CHL	C4D-CHA	2.62	1.47	1.38
29	9	605	CHL	C4D-CHA	2.62	1.47	1.38
30	3	416	LUT	C8-C9	-2.62	1.40	1.45
29	6	607	CHL	C4D-CHA	2.62	1.47	1.38
29	3	407	CHL	MG-NA	-2.61	2.00	2.06
21	B	832	CLA	CMB-C2B	-2.61	1.46	1.51
29	2	607	CHL	MG-NA	-2.61	2.00	2.06
29	1	307	CHL	MG-NA	-2.61	2.00	2.06
24	A	850	BCR	C19-C18	-2.61	1.40	1.45
21	B	818	CLA	CMB-C2B	-2.61	1.46	1.51
29	b	309	CHL	C4D-CHA	2.61	1.47	1.38
21	A	842	CLA	CMB-C2B	-2.61	1.46	1.51
29	c	601	CHL	MG-NA	-2.61	2.00	2.06
29	6	602	CHL	C4D-CHA	2.61	1.47	1.38
29	b	306	CHL	C4D-CHA	2.60	1.47	1.38
29	2	606	CHL	MG-NA	-2.60	2.00	2.06
29	1	307	CHL	C4D-CHA	2.60	1.47	1.38
29	a	608	CHL	C4D-CHA	2.60	1.47	1.38
24	2	618	BCR	C23-C22	-2.60	1.40	1.45
29	9	608	CHL	C4D-CHA	2.60	1.47	1.38
29	c	608	CHL	MG-NA	-2.60	2.00	2.06
21	7	407	CLA	CMD-C2D	-2.60	1.45	1.50
29	a	607	CHL	C4D-CHA	2.59	1.47	1.38
29	6	606	CHL	MG-NA	-2.59	2.00	2.06
29	9	609	CHL	MG-NA	-2.59	2.00	2.06
29	2	606	CHL	C4D-CHA	2.59	1.47	1.38
29	9	609	CHL	C4D-CHA	2.59	1.47	1.38
29	c	601	CHL	C4D-CHA	2.58	1.47	1.38
29	b	310	CHL	C4D-CHA	2.58	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	9	604	CLA	CMB-C2B	-2.58	1.46	1.51
29	8	605	CHL	C4D-CHA	2.58	1.47	1.38
29	6	605	CHL	MG-NA	-2.58	2.00	2.06
29	8	607	CHL	C4D-CHA	2.58	1.47	1.38
29	4	606	CHL	C4D-CHA	2.58	1.47	1.38
21	H	201	CLA	CMB-C2B	-2.58	1.46	1.51
29	1	302	CHL	C4D-CHA	2.57	1.47	1.38
24	A	848	BCR	C19-C18	-2.57	1.40	1.45
21	5	609	CLA	CMB-C2B	-2.57	1.46	1.51
21	c	602	CLA	CMB-C2B	-2.57	1.46	1.51
21	A	819	CLA	CMB-C2B	-2.56	1.46	1.51
29	4	614	CHL	C4D-CHA	2.56	1.47	1.38
29	5	601	CHL	C4D-CHA	2.56	1.47	1.38
29	4	607	CHL	MG-NA	-2.56	2.00	2.06
29	8	605	CHL	MG-NA	-2.56	2.00	2.06
29	4	605	CHL	C4D-CHA	2.56	1.47	1.38
21	B	821	CLA	CMB-C2B	-2.56	1.46	1.51
29	4	607	CHL	C4D-CHA	2.56	1.47	1.38
29	2	605	CHL	C4D-CHA	2.56	1.47	1.38
21	B	829	CLA	CMB-C2B	-2.56	1.46	1.51
24	8	616	BCR	C23-C22	-2.56	1.40	1.45
24	F	301	BCR	C12-C13	-2.56	1.40	1.45
21	A	812	CLA	CMB-C2B	-2.55	1.46	1.51
21	B	801	CLA	C1C-C2C	2.55	1.49	1.44
21	A	833	CLA	CMB-C2B	-2.55	1.46	1.51
21	B	827	CLA	CMB-C2B	-2.55	1.46	1.51
29	8	613	CHL	C4D-CHA	2.55	1.47	1.38
29	6	605	CHL	C4D-CHA	2.55	1.47	1.38
21	A	839	CLA	CMB-C2B	-2.54	1.46	1.51
29	3	407	CHL	C4D-CHA	2.54	1.47	1.38
24	A	848	BCR	C12-C13	-2.54	1.40	1.45
29	2	602	CHL	C4D-CHA	2.54	1.47	1.38
21	4	603	CLA	CMB-C2B	-2.54	1.46	1.51
21	A	802	CLA	CMB-C2B	-2.54	1.46	1.51
21	A	831	CLA	CMB-C2B	-2.54	1.46	1.51
21	9	602	CLA	CMB-C2B	-2.53	1.46	1.51
29	b	307	CHL	C4D-CHA	2.53	1.47	1.38
21	B	809	CLA	CMB-C2B	-2.53	1.46	1.51
21	1	314	CLA	CMB-C2B	-2.53	1.46	1.51
21	2	603	CLA	CMB-C2B	-2.53	1.46	1.51
29	2	607	CHL	C4D-CHA	2.53	1.47	1.38
24	A	849	BCR	C12-C13	-2.52	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	4	605	CHL	MG-NA	-2.52	2.00	2.06
21	B	817	CLA	CMB-C2B	-2.52	1.46	1.51
29	a	607	CHL	MG-NA	-2.52	2.00	2.06
21	4	601	CLA	CMB-C2B	-2.52	1.46	1.51
21	9	610	CLA	CMB-C2B	-2.52	1.46	1.51
21	6	609	CLA	CMB-C2B	-2.52	1.46	1.51
21	4	612	CLA	CMB-C2B	-2.52	1.46	1.51
29	2	614	CHL	C4D-CHA	2.52	1.47	1.38
21	A	820	CLA	CMB-C2B	-2.52	1.46	1.51
21	9	611	CLA	CMB-C2B	-2.52	1.46	1.51
21	A	818	CLA	CMB-C2B	-2.51	1.46	1.51
21	3	410	CLA	CMB-C2B	-2.51	1.46	1.51
21	K	203	CLA	CMB-C2B	-2.51	1.46	1.51
21	3	401	CLA	CMB-C2B	-2.51	1.46	1.51
21	A	841	CLA	CMB-C2B	-2.51	1.46	1.51
21	3	403	CLA	CMB-C2B	-2.51	1.46	1.51
21	7	401	CLA	CMB-C2B	-2.51	1.46	1.51
21	B	804	CLA	CMB-C2B	-2.51	1.46	1.51
21	3	406	CLA	CMB-C2B	-2.51	1.46	1.51
29	2	601	CHL	C4D-CHA	2.51	1.47	1.38
21	3	411	CLA	CMB-C2B	-2.51	1.46	1.51
21	F	302	CLA	CMB-C2B	-2.50	1.46	1.51
21	A	834	CLA	CMB-C2B	-2.50	1.46	1.51
21	A	803	CLA	CMB-C2B	-2.50	1.46	1.51
21	4	613	CLA	CMB-C2B	-2.50	1.46	1.51
21	c	614	CLA	CMB-C2B	-2.50	1.46	1.51
31	2	617	XAT	C32-C33	-2.49	1.40	1.45
21	O	201	CLA	CMB-C2B	-2.49	1.46	1.51
21	B	833	CLA	CMB-C2B	-2.49	1.46	1.51
24	J	104	BCR	C10-C9	-2.49	1.32	1.35
21	1	310	CLA	CMB-C2B	-2.49	1.46	1.51
21	A	828	CLA	CMB-C2B	-2.49	1.46	1.51
24	A	854	BCR	C19-C18	-2.49	1.40	1.45
21	3	414	CLA	CMB-C2B	-2.49	1.46	1.51
21	5	603	CLA	CMB-C2B	-2.49	1.46	1.51
21	A	810	CLA	CMB-C2B	-2.49	1.46	1.51
21	A	824	CLA	CMB-C2B	-2.49	1.46	1.51
21	7	402	CLA	CMB-C2B	-2.49	1.46	1.51
21	B	823	CLA	CMB-C2B	-2.49	1.46	1.51
21	2	604	CLA	CMB-C2B	-2.49	1.46	1.51
21	A	817	CLA	CMB-C2B	-2.49	1.46	1.51
21	B	819	CLA	CMB-C2B	-2.49	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	801	CLA	C4D-CHA	2.48	1.47	1.38
21	3	412	CLA	CMB-C2B	-2.48	1.46	1.51
29	a	608	CHL	MG-NA	-2.48	2.00	2.06
21	B	805	CLA	CMB-C2B	-2.48	1.46	1.51
21	2	612	CLA	CMB-C2B	-2.48	1.46	1.51
21	A	837	CLA	CMB-C2B	-2.48	1.46	1.51
21	B	810	CLA	CMB-C2B	-2.48	1.46	1.51
21	A	840	CLA	CMB-C2B	-2.48	1.46	1.51
21	F	304	CLA	CMB-C2B	-2.48	1.46	1.51
21	a	610	CLA	CMB-C2B	-2.48	1.46	1.51
21	B	822	CLA	CMB-C2B	-2.48	1.46	1.51
21	9	612	CLA	CMB-C2B	-2.48	1.46	1.51
21	b	305	CLA	CMB-C2B	-2.48	1.46	1.51
21	B	831	CLA	CMB-C2B	-2.48	1.46	1.51
30	b	317	LUT	C12-C13	-2.48	1.40	1.45
31	4	616	XAT	C28-C29	-2.48	1.40	1.45
21	B	812	CLA	CMB-C2B	-2.48	1.46	1.51
21	1	308	CLA	CMB-C2B	-2.48	1.46	1.51
21	8	603	CLA	CMB-C2B	-2.47	1.46	1.51
21	B	836	CLA	CMB-C2B	-2.47	1.46	1.51
21	2	613	CLA	CMB-C2B	-2.47	1.46	1.51
21	B	838	CLA	CMB-C2B	-2.47	1.46	1.51
21	L	302	CLA	CMB-C2B	-2.47	1.46	1.51
21	B	825	CLA	CMB-C2B	-2.47	1.46	1.51
21	B	803	CLA	CMB-C2B	-2.47	1.46	1.51
21	9	603	CLA	CMB-C2B	-2.47	1.46	1.51
21	1	315	CLA	CMB-C2B	-2.47	1.46	1.51
24	A	854	BCR	C12-C13	-2.47	1.40	1.45
21	A	823	CLA	CMB-C2B	-2.47	1.46	1.51
21	1	312	CLA	CMB-C2B	-2.46	1.46	1.51
21	1	305	CLA	CMB-C2B	-2.46	1.46	1.51
21	A	822	CLA	CMB-C2B	-2.46	1.46	1.51
21	A	825	CLA	CMB-C2B	-2.46	1.46	1.51
21	B	802	CLA	CMB-C2B	-2.46	1.46	1.51
21	J	102	CLA	CMB-C2B	-2.46	1.46	1.51
21	B	811	CLA	CMB-C2B	-2.46	1.46	1.51
31	3	417	XAT	C28-C29	-2.46	1.40	1.45
24	F	303	BCR	C12-C13	-2.46	1.40	1.45
21	B	826	CLA	CMB-C2B	-2.46	1.46	1.51
21	b	304	CLA	CMB-C2B	-2.46	1.46	1.51
29	a	609	CHL	C4B-CHC	2.46	1.47	1.41
21	B	815	CLA	CMB-C2B	-2.46	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	3	405	CLA	CMB-C2B	-2.46	1.46	1.51
21	8	608	CLA	CMB-C2B	-2.46	1.46	1.51
24	L	305	BCR	C12-C13	-2.46	1.40	1.45
21	G	203	CLA	CMB-C2B	-2.46	1.46	1.51
21	b	313	CLA	CMB-C2B	-2.46	1.46	1.51
21	A	806	CLA	CMB-C2B	-2.46	1.46	1.51
21	A	811	CLA	CMB-C2B	-2.46	1.46	1.51
21	A	813	CLA	CMB-C2B	-2.46	1.46	1.51
21	a	603	CLA	CMB-C2B	-2.45	1.46	1.51
21	c	611	CLA	CMB-C2B	-2.45	1.46	1.51
21	A	821	CLA	CMB-C2B	-2.45	1.46	1.51
21	B	830	CLA	CMB-C2B	-2.45	1.46	1.51
21	A	836	CLA	CMB-C2B	-2.45	1.46	1.51
21	B	824	CLA	CMB-C2B	-2.45	1.46	1.51
21	K	204	CLA	CMB-C2B	-2.45	1.46	1.51
21	1	313	CLA	CMB-C2B	-2.45	1.46	1.51
21	A	807	CLA	CMB-C2B	-2.45	1.46	1.51
21	1	304	CLA	CMB-C2B	-2.45	1.46	1.51
21	B	820	CLA	CMB-C2B	-2.45	1.46	1.51
21	F	305	CLA	CMB-C2B	-2.45	1.46	1.51
21	L	304	CLA	CMB-C2B	-2.45	1.46	1.51
21	O	202	CLA	CMB-C2B	-2.45	1.46	1.51
21	2	610	CLA	CMB-C2B	-2.45	1.46	1.51
21	9	613	CLA	CMB-C2B	-2.45	1.46	1.51
21	1	303	CLA	CMB-C2B	-2.45	1.46	1.51
21	3	402	CLA	CMB-C2B	-2.45	1.46	1.51
24	L	305	BCR	C19-C18	-2.45	1.40	1.45
21	5	612	CLA	CMB-C2B	-2.45	1.46	1.51
21	5	605	CLA	CMB-C2B	-2.45	1.46	1.51
31	6	617	XAT	C32-C33	-2.44	1.40	1.45
21	A	805	CLA	CMB-C2B	-2.44	1.46	1.51
21	A	809	CLA	CMB-C2B	-2.44	1.46	1.51
21	B	814	CLA	CMB-C2B	-2.44	1.46	1.51
21	A	814	CLA	CMB-C2B	-2.44	1.46	1.51
21	a	614	CLA	CMB-C2B	-2.44	1.46	1.51
21	7	405	CLA	CMB-C2B	-2.44	1.46	1.51
21	5	607	CLA	CMB-C2B	-2.44	1.46	1.51
21	A	832	CLA	CMB-C2B	-2.44	1.46	1.51
21	2	608	CLA	CMB-C2B	-2.44	1.46	1.51
21	4	611	CLA	CMB-C2B	-2.44	1.46	1.51
21	8	604	CLA	CMB-C2B	-2.44	1.46	1.51
21	a	613	CLA	CMB-C2B	-2.44	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	311	CLA	CMB-C2B	-2.44	1.46	1.51
21	B	806	CLA	CMB-C2B	-2.44	1.46	1.51
21	B	834	CLA	CMB-C2B	-2.44	1.46	1.51
21	K	201	CLA	CMB-C2B	-2.44	1.46	1.51
30	7	415	LUT	C12-C13	-2.44	1.40	1.45
21	7	403	CLA	CMB-C2B	-2.44	1.46	1.51
21	K	202	CLA	CMB-C2B	-2.44	1.46	1.51
21	1	311	CLA	CMB-C2B	-2.44	1.46	1.51
21	c	610	CLA	CMB-C2B	-2.43	1.46	1.51
24	L	301	BCR	C12-C13	-2.43	1.40	1.45
31	3	417	XAT	C12-C13	-2.43	1.40	1.45
21	A	852	CLA	CMB-C2B	-2.43	1.46	1.51
30	3	416	LUT	C28-C29	-2.43	1.40	1.45
21	1	306	CLA	CMB-C2B	-2.43	1.46	1.51
21	c	612	CLA	CMB-C2B	-2.43	1.46	1.51
21	4	602	CLA	CMB-C2B	-2.43	1.46	1.51
21	5	614	CLA	CMB-C2B	-2.43	1.46	1.51
21	b	315	CLA	CMB-C2B	-2.43	1.46	1.51
21	O	203	CLA	CMB-C2B	-2.43	1.46	1.51
21	A	829	CLA	CMB-C2B	-2.43	1.46	1.51
21	L	303	CLA	CMB-C2B	-2.43	1.46	1.51
30	b	317	LUT	C32-C33	-2.43	1.40	1.45
21	3	413	CLA	CMB-C2B	-2.43	1.46	1.51
21	6	608	CLA	CMB-C2B	-2.43	1.46	1.51
21	3	415	CLA	CMB-C2B	-2.43	1.46	1.51
21	6	610	CLA	CMB-C2B	-2.43	1.46	1.51
24	B	845	BCR	C19-C18	-2.43	1.40	1.45
30	c	615	LUT	C12-C13	-2.43	1.40	1.45
21	B	840	CLA	CMB-C2B	-2.43	1.46	1.51
21	5	608	CLA	CMB-C2B	-2.43	1.46	1.51
21	c	613	CLA	CMB-C2B	-2.43	1.46	1.51
24	A	847	BCR	C19-C18	-2.43	1.40	1.45
21	8	611	CLA	CMB-C2B	-2.43	1.46	1.51
31	4	616	XAT	C32-C33	-2.43	1.40	1.45
24	L	301	BCR	C19-C18	-2.43	1.40	1.45
24	F	301	BCR	C19-C18	-2.42	1.40	1.45
21	4	608	CLA	CMB-C2B	-2.42	1.46	1.51
21	B	837	CLA	CMB-C2B	-2.42	1.46	1.51
21	c	603	CLA	CMB-C2B	-2.42	1.46	1.51
21	A	815	CLA	CMB-C2B	-2.42	1.46	1.51
29	7	406	CHL	C4B-CHC	2.42	1.47	1.41
21	b	303	CLA	CMB-C2B	-2.42	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	804	CLA	CMB-C2B	-2.42	1.46	1.51
31	c	617	XAT	C12-C13	-2.42	1.40	1.45
31	1	318	XAT	C12-C13	-2.42	1.40	1.45
21	a	612	CLA	CMB-C2B	-2.42	1.46	1.51
21	G	204	CLA	CMB-C2B	-2.42	1.46	1.51
31	3	417	XAT	C32-C33	-2.42	1.40	1.45
21	7	411	CLA	CMB-C2B	-2.42	1.46	1.51
21	A	816	CLA	CMB-C2B	-2.42	1.46	1.51
21	G	202	CLA	CMB-C2B	-2.42	1.46	1.51
29	7	406	CHL	C1C-C2C	2.42	1.49	1.44
21	A	808	CLA	CMB-C2B	-2.42	1.46	1.51
21	1	316	CLA	CMB-C2B	-2.42	1.46	1.51
21	B	801	CLA	C4B-CHC	2.41	1.47	1.41
30	9	614	LUT	C32-C33	-2.41	1.40	1.45
21	A	826	CLA	CMB-C2B	-2.41	1.46	1.51
24	A	847	BCR	C12-C13	-2.41	1.40	1.45
21	6	613	CLA	CMB-C2B	-2.41	1.46	1.51
21	5	610	CLA	CMB-C2B	-2.41	1.46	1.51
21	7	412	CLA	CMB-C2B	-2.41	1.46	1.51
21	A	838	CLA	CMB-C2B	-2.41	1.46	1.51
21	8	601	CLA	CMB-C2B	-2.41	1.46	1.51
21	A	827	CLA	CMB-C2B	-2.41	1.46	1.51
21	B	835	CLA	CMB-C2B	-2.41	1.46	1.51
21	7	408	CLA	CMB-C2B	-2.41	1.46	1.51
21	b	314	CLA	CMB-C2B	-2.41	1.46	1.51
31	4	616	XAT	C12-C13	-2.41	1.40	1.45
31	5	616	XAT	C32-C33	-2.41	1.40	1.45
29	c	609	CHL	C2C-C1C	2.40	1.49	1.44
31	1	318	XAT	C28-C29	-2.40	1.40	1.45
21	4	604	CLA	CMB-C2B	-2.40	1.46	1.51
21	7	409	CLA	CMB-C2B	-2.40	1.46	1.51
21	c	604	CLA	CMB-C2B	-2.40	1.46	1.51
21	6	612	CLA	CMB-C2B	-2.40	1.46	1.51
24	G	201	BCR	C19-C18	-2.40	1.40	1.45
24	J	101	BCR	C12-C13	-2.40	1.40	1.45
21	6	604	CLA	CMB-C2B	-2.40	1.46	1.51
29	b	307	CHL	C2C-C1C	2.40	1.49	1.44
21	6	611	CLA	CMB-C2B	-2.39	1.46	1.51
21	5	604	CLA	CMB-C2B	-2.39	1.46	1.51
24	G	201	BCR	C12-C13	-2.39	1.40	1.45
29	6	601	CHL	C1C-C2C	2.39	1.49	1.44
21	5	611	CLA	CMB-C2B	-2.39	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	c	609	CHL	C4B-CHC	2.39	1.47	1.41
21	4	610	CLA	CMB-C2B	-2.39	1.46	1.51
21	5	602	CLA	CMB-C2B	-2.39	1.46	1.51
24	G	205	BCR	C12-C13	-2.39	1.40	1.45
21	a	611	CLA	CMB-C2B	-2.39	1.46	1.51
31	1	318	XAT	C32-C33	-2.39	1.40	1.45
21	2	611	CLA	CMB-C2B	-2.39	1.46	1.51
21	1	309	CLA	C3D-C4D	-2.39	1.38	1.44
30	9	614	LUT	C12-C13	-2.38	1.40	1.45
21	7	410	CLA	CMB-C2B	-2.38	1.46	1.51
30	8	614	LUT	C12-C13	-2.38	1.40	1.45
21	O	204	CLA	CMB-C2B	-2.38	1.46	1.51
21	8	612	CLA	CMB-C2B	-2.38	1.46	1.51
21	a	602	CLA	CMB-C2B	-2.38	1.46	1.51
24	A	846	BCR	C19-C18	-2.38	1.40	1.45
30	3	416	LUT	C32-C33	-2.38	1.40	1.45
32	9	617	NEX	C28-C29	-2.38	1.40	1.45
21	a	604	CLA	CMB-C2B	-2.38	1.46	1.51
31	2	617	XAT	C8-C9	-2.38	1.40	1.45
24	B	845	BCR	C12-C13	-2.37	1.40	1.45
21	5	613	CLA	CMB-C2B	-2.37	1.46	1.51
21	8	610	CLA	CMB-C2B	-2.37	1.46	1.51
31	5	616	XAT	C28-C29	-2.37	1.40	1.45
24	A	850	BCR	C12-C13	-2.37	1.40	1.45
30	2	616	LUT	C32-C33	-2.37	1.40	1.45
30	9	615	LUT	C12-C13	-2.37	1.40	1.45
24	A	846	BCR	C12-C13	-2.37	1.40	1.45
31	2	617	XAT	C12-C13	-2.37	1.40	1.45
21	B	813	CLA	CMB-C2B	-2.37	1.46	1.51
29	c	605	CHL	C4B-CHC	2.37	1.47	1.41
31	2	617	XAT	C28-C29	-2.37	1.40	1.45
29	6	614	CHL	C4B-CHC	2.37	1.47	1.41
31	4	616	XAT	C8-C9	-2.36	1.40	1.45
30	9	615	LUT	C32-C33	-2.36	1.40	1.45
21	7	404	CLA	CMB-C2B	-2.36	1.46	1.51
30	4	615	LUT	C32-C33	-2.36	1.40	1.45
29	6	607	CHL	C4B-CHC	2.36	1.47	1.41
30	9	615	LUT	C28-C29	-2.36	1.40	1.45
31	5	616	XAT	C12-C13	-2.36	1.40	1.45
30	4	615	LUT	C28-C29	-2.35	1.40	1.45
24	G	205	BCR	C19-C18	-2.35	1.40	1.45
21	8	602	CLA	CMB-C2B	-2.35	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	c	617	XAT	C8-C9	-2.35	1.40	1.45
30	c	616	LUT	C12-C13	-2.35	1.40	1.45
31	6	617	XAT	C28-C29	-2.35	1.40	1.45
21	b	312	CLA	CMB-C2B	-2.34	1.46	1.51
24	3	418	BCR	C12-C13	-2.34	1.40	1.45
24	B	842	BCR	C19-C18	-2.34	1.40	1.45
31	3	417	XAT	C8-C9	-2.34	1.40	1.45
24	B	842	BCR	C12-C13	-2.34	1.40	1.45
32	b	318	NEX	C12-C13	-2.34	1.40	1.45
29	8	613	CHL	C4B-CHC	2.34	1.47	1.41
31	a	618	XAT	C12-C13	-2.33	1.40	1.45
21	7	414	CLA	CMB-C2B	-2.33	1.46	1.51
31	c	617	XAT	C28-C29	-2.33	1.40	1.45
21	7	413	CLA	CMB-C2B	-2.33	1.46	1.51
30	c	616	LUT	C32-C33	-2.33	1.40	1.45
31	1	318	XAT	C8-C9	-2.33	1.40	1.45
29	c	606	CHL	C4B-CHC	2.33	1.47	1.41
29	6	601	CHL	C4B-CHC	2.32	1.47	1.41
21	3	409	CLA	C4D-CHA	2.32	1.46	1.38
29	8	606	CHL	C4B-CHC	2.32	1.47	1.41
30	2	616	LUT	C28-C29	-2.32	1.41	1.45
32	b	318	NEX	C28-C29	-2.32	1.41	1.45
24	3	418	BCR	C19-C18	-2.32	1.41	1.45
29	c	607	CHL	C4B-CHC	2.32	1.47	1.41
29	c	606	CHL	C2C-C1C	2.31	1.49	1.44
30	1	317	LUT	C28-C29	-2.31	1.41	1.45
30	1	317	LUT	C32-C33	-2.31	1.41	1.45
21	6	603	CLA	CMB-C2B	-2.31	1.46	1.51
21	8	618	CLA	CMB-C2B	-2.31	1.46	1.51
32	b	318	NEX	C32-C33	-2.31	1.41	1.45
31	7	416	XAT	C12-C13	-2.30	1.41	1.45
30	b	317	LUT	C28-C29	-2.30	1.41	1.45
24	4	617	BCR	C12-C13	-2.30	1.41	1.45
29	a	605	CHL	C4B-CHC	2.30	1.47	1.41
31	c	617	XAT	C32-C33	-2.30	1.41	1.45
24	A	849	BCR	C19-C18	-2.30	1.41	1.45
31	a	618	XAT	C8-C9	-2.30	1.41	1.45
24	2	618	BCR	C12-C13	-2.30	1.41	1.45
30	a	616	LUT	C32-C33	-2.30	1.41	1.45
29	a	606	CHL	C4C-C3C	2.29	1.49	1.45
30	5	615	LUT	C32-C33	-2.29	1.41	1.45
29	b	307	CHL	C4B-CHC	2.29	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	I	101	BCR	C19-C18	-2.29	1.41	1.45
30	7	415	LUT	C28-C29	-2.29	1.41	1.45
31	7	416	XAT	C8-C9	-2.29	1.41	1.45
30	9	614	LUT	C28-C29	-2.29	1.41	1.45
29	a	606	CHL	C4B-CHC	2.29	1.47	1.41
32	9	617	NEX	C32-C33	-2.29	1.41	1.45
29	8	613	CHL	C2C-C1C	2.29	1.49	1.44
29	6	602	CHL	C4B-CHC	2.29	1.47	1.41
30	a	616	LUT	C12-C13	-2.28	1.41	1.45
31	7	416	XAT	C32-C33	-2.28	1.41	1.45
30	2	616	LUT	C12-C13	-2.28	1.41	1.45
30	c	615	LUT	C28-C29	-2.28	1.41	1.45
29	6	605	CHL	C4B-CHC	2.28	1.47	1.41
24	J	101	BCR	C19-C18	-2.28	1.41	1.45
29	b	306	CHL	C2C-C1C	2.28	1.49	1.44
21	1	309	CLA	C4D-CHA	2.27	1.46	1.38
29	9	601	CHL	C4B-CHC	2.27	1.47	1.41
21	3	409	CLA	C3D-C4D	-2.27	1.39	1.44
29	a	601	CHL	C4C-C3C	2.27	1.49	1.45
21	B	801	CLA	C4C-C3C	2.27	1.48	1.45
29	a	609	CHL	C4C-C3C	2.27	1.48	1.45
29	5	606	CHL	C4B-CHC	2.27	1.47	1.41
24	4	617	BCR	C19-C18	-2.27	1.41	1.45
21	A	829	CLA	CMD-C2D	-2.26	1.46	1.50
21	9	602	CLA	CMD-C2D	-2.26	1.46	1.50
29	2	602	CHL	C4B-CHC	2.26	1.47	1.41
29	b	302	CHL	C4B-CHC	2.26	1.47	1.41
29	9	605	CHL	C4B-CHC	2.26	1.47	1.41
29	2	605	CHL	C4B-CHC	2.26	1.47	1.41
29	a	609	CHL	C1B-CHB	2.26	1.47	1.41
21	B	802	CLA	CMC-C2C	-2.26	1.46	1.50
29	6	606	CHL	C2C-C1C	2.25	1.49	1.44
30	b	316	LUT	C32-C33	-2.25	1.41	1.45
30	c	615	LUT	C32-C33	-2.25	1.41	1.45
30	5	615	LUT	C12-C13	-2.25	1.41	1.45
30	1	317	LUT	C12-C13	-2.25	1.41	1.45
29	6	614	CHL	C4C-C3C	2.25	1.48	1.45
29	7	406	CHL	C1B-CHB	2.25	1.47	1.41
24	L	306	BCR	C12-C13	-2.25	1.41	1.45
29	c	609	CHL	C1B-CHB	2.25	1.47	1.41
30	c	616	LUT	C28-C29	-2.25	1.41	1.45
29	6	602	CHL	C2C-C1C	2.25	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	a	618	XAT	C32-C33	-2.25	1.41	1.45
30	b	316	LUT	C28-C29	-2.25	1.41	1.45
29	6	606	CHL	C4B-CHC	2.25	1.47	1.41
24	6	618	BCR	C19-C18	-2.25	1.41	1.45
30	4	615	LUT	C12-C13	-2.25	1.41	1.45
30	a	615	LUT	C32-C33	-2.24	1.41	1.45
29	2	607	CHL	C4B-CHC	2.24	1.47	1.41
29	2	614	CHL	C4B-CHC	2.24	1.47	1.41
29	5	606	CHL	C2C-C1C	2.24	1.49	1.44
30	a	615	LUT	C12-C13	-2.24	1.41	1.45
31	5	616	XAT	C8-C9	-2.24	1.41	1.45
21	3	403	CLA	C3B-C2B	-2.24	1.37	1.40
30	8	614	LUT	C32-C33	-2.24	1.41	1.45
29	a	601	CHL	C4B-CHC	2.24	1.47	1.41
30	a	616	LUT	C28-C29	-2.23	1.41	1.45
21	B	822	CLA	CMD-C2D	-2.23	1.46	1.50
29	c	605	CHL	C4C-C3C	2.23	1.48	1.45
24	J	103	BCR	C12-C13	-2.23	1.41	1.45
24	F	303	BCR	C19-C18	-2.23	1.41	1.45
29	6	614	CHL	C2C-C1C	2.23	1.49	1.44
32	c	618	NEX	C12-C13	-2.23	1.41	1.45
24	3	419	BCR	C12-C13	-2.23	1.41	1.45
21	B	801	CLA	C1B-CHB	2.22	1.47	1.41
29	b	306	CHL	C4B-CHC	2.22	1.47	1.41
30	6	616	LUT	C12-C13	-2.22	1.41	1.45
24	7	418	BCR	C12-C13	-2.22	1.41	1.45
24	I	101	BCR	C12-C13	-2.22	1.41	1.45
31	8	615	XAT	C12-C13	-2.21	1.41	1.45
30	7	415	LUT	C32-C33	-2.21	1.41	1.45
29	1	307	CHL	C4B-CHC	2.21	1.47	1.41
29	9	605	CHL	C2C-C1C	2.21	1.49	1.44
21	A	818	CLA	CMC-C2C	-2.21	1.46	1.50
29	a	607	CHL	C4B-CHC	2.21	1.47	1.41
21	B	831	CLA	C3B-C2B	-2.21	1.37	1.40
29	4	607	CHL	C4B-CHC	2.21	1.47	1.41
30	8	614	LUT	C28-C29	-2.21	1.41	1.45
29	4	605	CHL	C2C-C1C	2.20	1.49	1.44
31	a	618	XAT	C28-C29	-2.20	1.41	1.45
29	9	606	CHL	C4B-CHC	2.20	1.47	1.41
29	a	608	CHL	C2C-C1C	2.20	1.49	1.44
29	c	608	CHL	C4B-CHC	2.20	1.47	1.41
24	L	306	BCR	C19-C18	-2.20	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	6	618	BCR	C12-C13	-2.20	1.41	1.45
30	5	615	LUT	C28-C29	-2.20	1.41	1.45
21	A	818	CLA	CMD-C2D	-2.20	1.46	1.50
31	7	416	XAT	C28-C29	-2.20	1.41	1.45
29	9	607	CHL	C4C-C3C	2.20	1.48	1.45
24	O	205	BCR	C12-C13	-2.20	1.41	1.45
30	b	316	LUT	C12-C13	-2.20	1.41	1.45
29	a	608	CHL	C4B-CHC	2.19	1.47	1.41
24	J	103	BCR	C19-C18	-2.19	1.41	1.45
24	2	618	BCR	C19-C18	-2.19	1.41	1.45
29	4	605	CHL	C4B-CHC	2.19	1.47	1.41
32	9	617	NEX	C12-C13	-2.19	1.41	1.45
21	7	407	CLA	CHD-C1D	2.19	1.42	1.38
29	9	606	CHL	C2C-C1C	2.19	1.49	1.44
29	c	607	CHL	C1B-CHB	2.19	1.47	1.41
29	b	302	CHL	C1B-CHB	2.19	1.47	1.41
24	7	417	BCR	C19-C18	-2.19	1.41	1.45
29	9	601	CHL	C2C-C1C	2.19	1.49	1.44
29	2	605	CHL	C2C-C1C	2.18	1.49	1.44
21	4	609	CLA	C3D-C4D	-2.18	1.39	1.44
24	3	419	BCR	C19-C18	-2.18	1.41	1.45
21	A	831	CLA	CMD-C2D	-2.18	1.46	1.50
21	3	405	CLA	CMC-C2C	-2.18	1.46	1.50
29	a	605	CHL	C1B-CHB	2.18	1.47	1.41
29	b	308	CHL	C4C-C3C	2.18	1.48	1.45
29	b	309	CHL	C4B-CHC	2.18	1.47	1.41
30	6	616	LUT	C28-C29	-2.18	1.41	1.45
29	4	607	CHL	C2C-C1C	2.18	1.49	1.44
21	B	807	CLA	CMD-C2D	-2.18	1.46	1.50
29	c	605	CHL	C1B-CHB	2.18	1.47	1.41
32	c	618	NEX	C32-C33	-2.17	1.41	1.45
29	6	605	CHL	C2C-C1C	2.17	1.49	1.44
29	c	607	CHL	C2C-C1C	2.17	1.49	1.44
29	a	607	CHL	C4C-C3C	2.17	1.48	1.45
29	6	605	CHL	C4C-C3C	2.17	1.48	1.45
29	4	606	CHL	C4B-CHC	2.17	1.47	1.41
29	6	601	CHL	C1B-CHB	2.17	1.47	1.41
29	c	608	CHL	C4C-C3C	2.17	1.48	1.45
29	2	602	CHL	C2C-C1C	2.17	1.49	1.44
29	2	607	CHL	C2C-C1C	2.17	1.49	1.44
29	8	607	CHL	C4B-CHC	2.17	1.47	1.41
29	5	601	CHL	C4B-CHC	2.17	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	6	607	CHL	C1B-CHB	2.17	1.47	1.41
29	6	614	CHL	C1B-CHB	2.17	1.47	1.41
29	c	605	CHL	C2C-C1C	2.16	1.49	1.44
29	1	302	CHL	C4B-CHC	2.16	1.47	1.41
29	9	608	CHL	C4B-CHC	2.16	1.47	1.41
21	A	810	CLA	CMD-C2D	-2.16	1.46	1.50
24	7	418	BCR	C19-C18	-2.16	1.41	1.45
29	8	606	CHL	C1B-CHB	2.16	1.47	1.41
29	9	605	CHL	C4C-C3C	2.16	1.48	1.45
29	2	606	CHL	C4B-CHC	2.16	1.47	1.41
31	9	616	XAT	C28-C29	-2.16	1.41	1.45
29	9	609	CHL	C4B-CHC	2.16	1.47	1.41
21	B	822	CLA	CMC-C2C	-2.16	1.46	1.50
29	a	605	CHL	C4C-C3C	2.16	1.48	1.45
24	O	205	BCR	C19-C18	-2.16	1.41	1.45
29	4	614	CHL	C4B-CHC	2.16	1.47	1.41
21	4	609	CLA	C4D-CHA	2.16	1.46	1.38
31	8	615	XAT	C28-C29	-2.16	1.41	1.45
29	8	605	CHL	C1B-CHB	2.15	1.47	1.41
29	8	605	CHL	C4B-CHC	2.15	1.47	1.41
21	B	814	CLA	CMD-C2D	-2.15	1.46	1.50
30	6	616	LUT	C32-C33	-2.15	1.41	1.45
21	A	825	CLA	CMD-C2D	-2.15	1.46	1.50
29	a	601	CHL	C1B-CHB	2.15	1.47	1.41
29	b	310	CHL	C4B-CHC	2.15	1.47	1.41
24	8	616	BCR	C12-C13	-2.15	1.41	1.45
29	b	308	CHL	C4B-CHC	2.15	1.47	1.41
21	B	829	CLA	CMD-C2D	-2.14	1.46	1.50
29	7	406	CHL	C4C-C3C	2.14	1.48	1.45
29	6	607	CHL	C4C-C3C	2.14	1.48	1.45
29	8	606	CHL	C4C-C3C	2.14	1.48	1.45
29	c	607	CHL	C4C-C3C	2.14	1.48	1.45
21	A	842	CLA	CMD-C2D	-2.14	1.46	1.50
31	8	615	XAT	C32-C33	-2.14	1.41	1.45
29	a	605	CHL	C2C-C1C	2.14	1.49	1.44
29	8	606	CHL	C2C-C1C	2.14	1.49	1.44
21	6	613	CLA	CMD-C2D	-2.14	1.46	1.50
29	9	601	CHL	C1B-CHB	2.14	1.46	1.41
29	6	607	CHL	C2C-C1C	2.13	1.49	1.44
24	7	417	BCR	C12-C13	-2.13	1.41	1.45
29	8	605	CHL	C4C-C3C	2.13	1.48	1.44
21	A	820	CLA	CMD-C2D	-2.13	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	835	CLA	CMD-C2D	-2.13	1.46	1.50
21	b	304	CLA	CMD-C2D	-2.13	1.46	1.50
21	2	609	CLA	MG-ND	-2.13	2.01	2.05
21	A	837	CLA	C3B-C2B	-2.13	1.37	1.40
29	6	601	CHL	C4C-C3C	2.13	1.48	1.44
21	B	836	CLA	CMC-C2C	-2.13	1.46	1.50
21	B	823	CLA	CMD-C2D	-2.12	1.46	1.50
21	B	812	CLA	CMC-C2C	-2.12	1.46	1.50
29	8	607	CHL	C2C-C1C	2.12	1.49	1.44
29	8	613	CHL	C1B-CHB	2.12	1.46	1.41
21	7	413	CLA	CBD-CAD	2.12	1.56	1.51
21	A	830	CLA	MG-ND	-2.12	2.01	2.05
21	B	816	CLA	CMD-C2D	-2.12	1.46	1.50
21	B	839	CLA	CMD-C2D	-2.12	1.46	1.50
29	5	606	CHL	C4C-C3C	2.12	1.48	1.45
32	c	618	NEX	C28-C29	-2.12	1.41	1.45
29	a	607	CHL	C2C-C1C	2.12	1.49	1.44
21	4	611	CLA	CMD-C2D	-2.12	1.46	1.50
21	A	837	CLA	CMD-C2D	-2.12	1.46	1.50
24	M	101	BCR	C19-C18	-2.12	1.41	1.45
21	9	604	CLA	CMD-C2D	-2.12	1.46	1.50
29	5	606	CHL	C1B-CHB	2.12	1.46	1.41
21	3	401	CLA	CMD-C2D	-2.12	1.46	1.50
21	A	823	CLA	CMD-C2D	-2.12	1.46	1.50
29	2	601	CHL	C4B-CHC	2.11	1.46	1.41
29	b	310	CHL	C4C-C3C	2.11	1.48	1.45
21	B	834	CLA	CMD-C2D	-2.11	1.46	1.50
29	2	606	CHL	C2C-C1C	2.11	1.49	1.44
24	8	616	BCR	C19-C18	-2.11	1.41	1.45
21	4	601	CLA	CMD-C2D	-2.11	1.46	1.50
21	B	830	CLA	CMD-C2D	-2.11	1.46	1.50
21	B	838	CLA	CMD-C2D	-2.11	1.46	1.50
21	A	828	CLA	CMD-C2D	-2.11	1.46	1.50
29	9	609	CHL	C2C-C1C	2.11	1.49	1.44
21	9	612	CLA	CMD-C2D	-2.11	1.46	1.50
29	1	307	CHL	C2C-C1C	2.11	1.49	1.44
29	8	605	CHL	C2C-C1C	2.11	1.49	1.44
29	a	609	CHL	C2C-C1C	2.11	1.49	1.44
21	F	304	CLA	CMD-C2D	-2.10	1.46	1.50
21	K	203	CLA	CMC-C2C	-2.10	1.46	1.50
29	b	306	CHL	C1B-CHB	2.10	1.46	1.41
29	6	606	CHL	C4C-C3C	2.10	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	c	606	CHL	C4C-C3C	2.10	1.48	1.45
21	9	604	CLA	CMC-C2C	-2.10	1.46	1.50
29	9	606	CHL	C4C-C3C	2.10	1.48	1.45
29	9	601	CHL	C4C-C3C	2.10	1.48	1.45
21	B	821	CLA	CMD-C2D	-2.10	1.46	1.50
21	3	408	CLA	CMD-C2D	-2.10	1.46	1.50
21	5	602	CLA	CMD-C2D	-2.10	1.46	1.50
21	L	304	CLA	CMD-C2D	-2.10	1.46	1.50
21	B	828	CLA	CMD-C2D	-2.10	1.46	1.50
21	6	603	CLA	CMD-C2D	-2.10	1.46	1.50
21	B	809	CLA	CMD-C2D	-2.10	1.46	1.50
21	L	303	CLA	CMD-C2D	-2.10	1.46	1.50
29	5	601	CHL	C2C-C1C	2.10	1.49	1.44
21	B	808	CLA	CMD-C2D	-2.10	1.46	1.50
21	9	603	CLA	CMD-C2D	-2.10	1.46	1.50
21	1	309	CLA	MG-ND	-2.10	2.01	2.05
21	A	824	CLA	CMD-C2D	-2.10	1.46	1.50
21	B	827	CLA	CMD-C2D	-2.10	1.46	1.50
21	A	821	CLA	CMD-C2D	-2.10	1.46	1.50
21	8	609	CLA	MG-ND	-2.10	2.01	2.05
21	3	409	CLA	MG-ND	-2.09	2.01	2.05
21	A	842	CLA	CMC-C2C	-2.09	1.46	1.50
21	A	835	CLA	CMD-C2D	-2.09	1.46	1.50
21	c	613	CLA	CMD-C2D	-2.09	1.46	1.50
21	B	833	CLA	CMD-C2D	-2.09	1.46	1.50
21	9	602	CLA	CMC-C2C	-2.09	1.46	1.50
21	B	813	CLA	CMD-C2D	-2.09	1.46	1.50
21	3	405	CLA	CMD-C2D	-2.09	1.46	1.50
21	4	609	CLA	MG-ND	-2.09	2.01	2.05
21	A	822	CLA	CMD-C2D	-2.09	1.46	1.50
21	B	825	CLA	CMC-C2C	-2.09	1.46	1.50
21	A	852	CLA	CMD-C2D	-2.09	1.46	1.50
21	2	603	CLA	CMD-C2D	-2.09	1.46	1.50
21	7	403	CLA	CMD-C2D	-2.09	1.46	1.50
21	a	602	CLA	CMC-C2C	-2.09	1.46	1.50
21	B	840	CLA	CMD-C2D	-2.09	1.46	1.50
21	B	818	CLA	CMD-C2D	-2.09	1.46	1.50
21	4	602	CLA	CMD-C2D	-2.09	1.46	1.50
29	9	605	CHL	C1B-CHB	2.09	1.46	1.41
21	2	610	CLA	CMD-C2D	-2.09	1.46	1.50
21	3	402	CLA	CMD-C2D	-2.08	1.46	1.50
21	O	204	CLA	CMC-C2C	-2.08	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4	603	CLA	CMD-C2D	-2.08	1.46	1.50
21	A	809	CLA	CMD-C2D	-2.08	1.46	1.50
21	2	603	CLA	C3B-C2B	-2.08	1.37	1.40
31	8	615	XAT	C8-C9	-2.08	1.41	1.45
21	L	302	CLA	CMD-C2D	-2.08	1.46	1.50
21	B	824	CLA	CMD-C2D	-2.08	1.46	1.50
21	3	415	CLA	CMD-C2D	-2.08	1.46	1.50
21	1	313	CLA	CMD-C2D	-2.08	1.46	1.50
31	9	616	XAT	C8-C9	-2.08	1.41	1.45
21	K	203	CLA	CMD-C2D	-2.08	1.46	1.50
21	B	812	CLA	CMD-C2D	-2.07	1.46	1.50
21	c	602	CLA	CMD-C2D	-2.07	1.46	1.50
21	3	412	CLA	CMD-C2D	-2.07	1.46	1.50
21	A	806	CLA	CMD-C2D	-2.07	1.46	1.50
29	a	608	CHL	C1B-CHB	2.07	1.46	1.41
21	4	608	CLA	CMD-C2D	-2.07	1.46	1.50
21	A	804	CLA	CMD-C2D	-2.07	1.46	1.50
29	9	606	CHL	C1B-CHB	2.07	1.46	1.41
21	A	817	CLA	CMD-C2D	-2.07	1.46	1.50
21	B	815	CLA	CMD-C2D	-2.07	1.46	1.50
21	2	612	CLA	CMD-C2D	-2.07	1.46	1.50
21	3	414	CLA	CMD-C2D	-2.07	1.46	1.50
21	c	614	CLA	CMD-C2D	-2.07	1.46	1.50
21	A	802	CLA	CMC-C2C	-2.07	1.46	1.50
21	A	806	CLA	CMC-C2C	-2.07	1.46	1.50
21	B	836	CLA	CMD-C2D	-2.07	1.46	1.50
21	B	826	CLA	CMD-C2D	-2.07	1.46	1.50
21	B	819	CLA	CMD-C2D	-2.07	1.46	1.50
21	B	825	CLA	CMD-C2D	-2.07	1.46	1.50
21	c	603	CLA	CMD-C2D	-2.07	1.46	1.50
29	c	609	CHL	C4C-C3C	2.07	1.48	1.44
29	3	407	CHL	C4B-CHC	2.07	1.46	1.41
21	B	805	CLA	CMD-C2D	-2.07	1.46	1.50
21	c	612	CLA	CMD-C2D	-2.07	1.46	1.50
29	a	601	CHL	C2C-C1C	2.07	1.49	1.44
29	c	601	CHL	C4B-CHC	2.06	1.46	1.41
21	J	102	CLA	CMD-C2D	-2.06	1.46	1.50
21	A	841	CLA	CMD-C2D	-2.06	1.46	1.50
29	9	607	CHL	C1B-CHB	2.06	1.46	1.41
29	8	607	CHL	C4C-C3C	2.06	1.48	1.45
21	F	302	CLA	CMD-C2D	-2.06	1.46	1.50
21	7	402	CLA	CMD-C2D	-2.06	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	c	604	CLA	CMD-C2D	-2.06	1.46	1.50
21	B	801	CLA	C3D-C4D	-2.06	1.39	1.44
29	9	608	CHL	C2C-C1C	2.06	1.49	1.44
21	A	811	CLA	CMD-C2D	-2.06	1.46	1.50
29	b	302	CHL	C2C-C1C	2.06	1.49	1.44
29	1	302	CHL	C1B-CHB	2.06	1.46	1.41
29	c	606	CHL	C1B-CHB	2.06	1.46	1.41
21	A	803	CLA	CMD-C2D	-2.06	1.46	1.50
21	B	810	CLA	CMD-C2D	-2.06	1.46	1.50
21	4	610	CLA	CMD-C2D	-2.06	1.46	1.50
21	b	303	CLA	CMD-C2D	-2.06	1.46	1.50
21	F	305	CLA	CMD-C2D	-2.06	1.46	1.50
21	1	304	CLA	CMD-C2D	-2.06	1.46	1.50
21	1	312	CLA	CMD-C2D	-2.06	1.46	1.50
21	B	806	CLA	CMD-C2D	-2.06	1.46	1.50
21	K	201	CLA	CMD-C2D	-2.06	1.46	1.50
21	3	406	CLA	CMD-C2D	-2.06	1.46	1.50
21	A	808	CLA	CMD-C2D	-2.06	1.46	1.50
21	B	820	CLA	CMD-C2D	-2.06	1.46	1.50
21	A	836	CLA	CMD-C2D	-2.06	1.46	1.50
21	7	401	CLA	CMD-C2D	-2.06	1.46	1.50
24	M	101	BCR	C12-C13	-2.05	1.41	1.45
21	5	610	CLA	CMD-C2D	-2.05	1.46	1.50
29	2	601	CHL	C1B-CHB	2.05	1.46	1.41
21	A	802	CLA	CMD-C2D	-2.05	1.46	1.50
21	B	804	CLA	CMD-C2D	-2.05	1.46	1.50
21	9	610	CLA	CMD-C2D	-2.05	1.46	1.50
21	B	832	CLA	CMC-C2C	-2.05	1.46	1.50
21	1	303	CLA	CMD-C2D	-2.05	1.46	1.50
29	b	302	CHL	C4C-C3C	2.05	1.48	1.45
21	A	813	CLA	CMD-C2D	-2.05	1.46	1.50
21	B	837	CLA	CMD-C2D	-2.05	1.46	1.50
29	c	608	CHL	C2C-C1C	2.05	1.49	1.44
21	5	609	CLA	CMD-C2D	-2.05	1.46	1.50
21	A	815	CLA	CMD-C2D	-2.05	1.46	1.50
21	B	802	CLA	CMD-C2D	-2.05	1.46	1.50
21	K	202	CLA	CMD-C2D	-2.05	1.46	1.50
21	5	603	CLA	CMD-C2D	-2.05	1.46	1.50
21	8	604	CLA	CMD-C2D	-2.05	1.46	1.50
21	O	202	CLA	CMD-C2D	-2.05	1.46	1.50
21	c	602	CLA	CMC-C2C	-2.05	1.46	1.50
29	3	407	CHL	C1B-NB	-2.05	1.33	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	608	CLA	CMD-C2D	-2.05	1.46	1.50
21	b	313	CLA	CMD-C2D	-2.05	1.46	1.50
21	9	611	CLA	CMD-C2D	-2.04	1.46	1.50
21	A	832	CLA	CMD-C2D	-2.04	1.46	1.50
21	1	310	CLA	CMD-C2D	-2.04	1.46	1.50
21	3	411	CLA	CMD-C2D	-2.04	1.46	1.50
21	c	611	CLA	CMD-C2D	-2.04	1.46	1.50
21	O	201	CLA	CMD-C2D	-2.04	1.46	1.50
21	8	608	CLA	CMD-C2D	-2.04	1.46	1.50
21	B	804	CLA	C3B-C2B	-2.04	1.37	1.40
21	A	839	CLA	CMD-C2D	-2.04	1.46	1.50
21	4	612	CLA	CMD-C2D	-2.04	1.46	1.50
29	2	614	CHL	C4C-C3C	2.04	1.48	1.45
21	1	316	CLA	CMD-C2D	-2.04	1.46	1.50
21	1	308	CLA	CMD-C2D	-2.04	1.46	1.50
21	2	611	CLA	CMD-C2D	-2.04	1.46	1.50
21	5	605	CLA	CMD-C2D	-2.04	1.46	1.50
21	A	834	CLA	CMD-C2D	-2.04	1.46	1.50
21	A	838	CLA	CMD-C2D	-2.04	1.46	1.50
21	A	807	CLA	CMD-C2D	-2.04	1.46	1.50
21	b	305	CLA	CMD-C2D	-2.04	1.46	1.50
21	2	613	CLA	CMD-C2D	-2.04	1.46	1.50
21	B	831	CLA	CMD-C2D	-2.04	1.46	1.50
21	3	408	CLA	C3B-C2B	-2.04	1.37	1.40
21	A	816	CLA	CMD-C2D	-2.03	1.46	1.50
21	O	203	CLA	CMD-C2D	-2.03	1.46	1.50
21	1	311	CLA	CMD-C2D	-2.03	1.46	1.50
29	8	607	CHL	C1B-CHB	2.03	1.46	1.41
21	A	826	CLA	CMD-C2D	-2.03	1.46	1.50
29	6	605	CHL	C1B-CHB	2.03	1.46	1.41
21	B	816	CLA	CMC-C2C	-2.03	1.46	1.50
21	1	314	CLA	CMD-C2D	-2.03	1.46	1.50
31	9	616	XAT	C32-C33	-2.03	1.41	1.45
21	G	202	CLA	CMD-C2D	-2.03	1.46	1.50
29	b	306	CHL	C4C-C3C	2.03	1.48	1.45
21	8	618	CLA	CMD-C2D	-2.03	1.46	1.50
29	9	608	CHL	C4C-C3C	2.03	1.48	1.45
29	2	601	CHL	C4C-C3C	2.03	1.48	1.45
29	a	608	CHL	C4C-C3C	2.03	1.48	1.45
21	b	314	CLA	CMC-C2C	-2.03	1.46	1.50
31	9	616	XAT	C12-C13	-2.03	1.41	1.45
21	5	603	CLA	C3B-C2B	-2.03	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	3	403	CLA	CMD-C2D	-2.03	1.46	1.50
21	B	839	CLA	C3B-C2B	-2.03	1.37	1.40
21	7	404	CLA	CMD-C2D	-2.03	1.46	1.50
29	2	614	CHL	C1B-CHB	2.03	1.46	1.41
21	A	805	CLA	CMD-C2D	-2.02	1.46	1.50
21	H	201	CLA	CMD-C2D	-2.02	1.46	1.50
21	5	611	CLA	CMD-C2D	-2.02	1.46	1.50
21	A	840	CLA	CMD-C2D	-2.02	1.46	1.50
29	b	310	CHL	C2C-C1C	2.02	1.48	1.44
21	2	604	CLA	CMD-C2D	-2.02	1.46	1.50
21	B	811	CLA	CMC-C2C	-2.02	1.46	1.50
21	B	832	CLA	CMD-C2D	-2.02	1.46	1.50
21	a	604	CLA	CMD-C2D	-2.02	1.46	1.50
21	b	315	CLA	CMD-C2D	-2.02	1.46	1.50
21	A	812	CLA	CMD-C2D	-2.02	1.46	1.50
21	A	814	CLA	CMD-C2D	-2.02	1.46	1.50
21	4	613	CLA	CMD-C2D	-2.02	1.46	1.50
21	B	811	CLA	CMD-C2D	-2.02	1.46	1.50
29	2	602	CHL	C1B-CHB	2.02	1.46	1.41
21	B	817	CLA	CMC-C2C	-2.02	1.46	1.50
21	b	314	CLA	CMD-C2D	-2.02	1.46	1.50
29	a	606	CHL	C2C-C1C	2.02	1.48	1.44
21	B	817	CLA	CMD-C2D	-2.02	1.46	1.50
21	a	603	CLA	CMD-C2D	-2.02	1.46	1.50
21	6	609	CLA	CMD-C2D	-2.02	1.46	1.50
21	A	823	CLA	CMC-C2C	-2.02	1.46	1.50
21	K	204	CLA	CMD-C2D	-2.02	1.46	1.50
21	3	404	CLA	CMD-C2D	-2.02	1.46	1.50
21	1	315	CLA	CMD-C2D	-2.02	1.46	1.50
21	A	852	CLA	CMC-C2C	-2.02	1.46	1.50
29	4	605	CHL	C4C-C3C	2.02	1.48	1.44
29	4	606	CHL	C4C-C3C	2.02	1.48	1.45
21	3	414	CLA	CBD-CAD	2.01	1.56	1.51
21	1	316	CLA	CMC-C2C	-2.01	1.46	1.50
29	b	310	CHL	C1B-CHB	2.01	1.46	1.41
29	4	614	CHL	C1B-CHB	2.01	1.46	1.41
21	B	807	CLA	CMC-C2C	-2.01	1.46	1.50
21	G	203	CLA	CMD-C2D	-2.01	1.46	1.50
21	4	604	CLA	CMD-C2D	-2.01	1.46	1.50
21	A	819	CLA	CMD-C2D	-2.01	1.46	1.50
21	8	610	CLA	CMD-C2D	-2.01	1.46	1.50
21	b	311	CLA	CMD-C2D	-2.01	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	9	609	CHL	C4C-C3C	2.01	1.48	1.45
21	A	833	CLA	C3B-C2B	-2.01	1.37	1.40
21	B	815	CLA	CMC-C2C	-2.01	1.46	1.50
21	3	413	CLA	CMD-C2D	-2.01	1.46	1.50
21	a	614	CLA	CMD-C2D	-2.01	1.46	1.50
29	9	607	CHL	C4B-CHC	2.01	1.46	1.41
21	1	306	CLA	CMD-C2D	-2.01	1.46	1.50
21	8	618	CLA	CMC-C2C	-2.01	1.46	1.50
31	6	617	XAT	C12-C13	-2.01	1.41	1.45
21	B	818	CLA	CMC-C2C	-2.01	1.46	1.50
21	c	604	CLA	CMC-C2C	-2.01	1.46	1.50
31	6	617	XAT	C8-C9	-2.00	1.41	1.45
21	B	819	CLA	CMC-C2C	-2.00	1.46	1.50
29	2	614	CHL	C2C-C1C	2.00	1.48	1.44
21	1	305	CLA	CMD-C2D	-2.00	1.46	1.50
21	7	414	CLA	CMD-C2D	-2.00	1.46	1.50
21	B	803	CLA	CMC-C2C	-2.00	1.46	1.50
21	B	828	CLA	CMC-C2C	-2.00	1.46	1.50
21	6	610	CLA	CMD-C2D	-2.00	1.46	1.50

All (3657) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	7	407	CLA	CAC-C3C-C4C	16.81	146.62	124.81
21	7	407	CLA	C1D-ND-C4D	-10.68	98.75	106.33
29	a	601	CHL	C1D-ND-C4D	10.07	113.49	106.33
29	9	601	CHL	C1D-ND-C4D	10.04	113.47	106.33
29	c	609	CHL	C1D-ND-C4D	10.00	113.44	106.33
29	a	609	CHL	C1D-ND-C4D	9.96	113.41	106.33
29	a	605	CHL	C1D-ND-C4D	9.95	113.40	106.33
29	a	605	CHL	C4D-CHA-C1A	-9.89	109.21	121.25
29	7	406	CHL	C1D-ND-C4D	9.86	113.34	106.33
21	7	407	CLA	CAC-C3C-C2C	-9.83	110.71	127.53
29	6	601	CHL	CMC-C2C-C1C	9.81	139.98	125.04
29	c	607	CHL	C1D-ND-C4D	9.79	113.29	106.33
29	9	601	CHL	C4D-CHA-C1A	-9.77	109.36	121.25
29	b	302	CHL	C1D-ND-C4D	9.76	113.27	106.33
29	c	605	CHL	C1D-ND-C4D	9.76	113.27	106.33
29	b	302	CHL	C4D-CHA-C1A	-9.71	109.43	121.25
29	7	406	CHL	CMC-C2C-C1C	9.64	139.72	125.04
29	8	606	CHL	C1D-ND-C4D	9.62	113.17	106.33
29	5	606	CHL	C4D-CHA-C1A	-9.59	109.58	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	6	601	CHL	C4D-CHA-C1A	-9.59	109.58	121.25
29	1	302	CHL	C4D-CHA-C1A	-9.53	109.65	121.25
29	6	607	CHL	C1D-ND-C4D	9.52	113.10	106.33
29	9	607	CHL	C1D-ND-C4D	9.52	113.10	106.33
29	c	608	CHL	C1D-ND-C4D	9.50	113.09	106.33
29	6	601	CHL	C1D-ND-C4D	9.47	113.06	106.33
29	c	605	CHL	CBD-CHA-C1A	9.47	142.60	127.43
29	7	406	CHL	C4D-CHA-C1A	-9.44	109.76	121.25
29	b	307	CHL	C4D-CHA-C1A	-9.43	109.77	121.25
29	a	601	CHL	C4D-CHA-C1A	-9.42	109.78	121.25
29	b	308	CHL	C4D-CHA-C1A	-9.40	109.81	121.25
29	2	606	CHL	C4D-CHA-C1A	-9.38	109.84	121.25
29	8	606	CHL	C4D-CHA-C1A	-9.38	109.84	121.25
29	6	606	CHL	C4D-CHA-C1A	-9.37	109.84	121.25
29	b	306	CHL	C4D-CHA-C1A	-9.34	109.88	121.25
29	9	606	CHL	C4D-CHA-C1A	-9.34	109.89	121.25
29	c	606	CHL	C4D-CHA-C1A	-9.34	109.89	121.25
29	b	309	CHL	C4D-CHA-C1A	-9.33	109.89	121.25
29	2	605	CHL	C4D-CHA-C1A	-9.32	109.90	121.25
29	9	605	CHL	C4D-CHA-C1A	-9.32	109.91	121.25
29	6	602	CHL	C4D-CHA-C1A	-9.31	109.92	121.25
21	B	801	CLA	C1D-ND-C4D	-9.31	99.72	106.33
29	1	307	CHL	C4D-CHA-C1A	-9.30	109.93	121.25
29	9	609	CHL	C4D-CHA-C1A	-9.29	109.94	121.25
29	c	607	CHL	C4D-CHA-C1A	-9.27	109.97	121.25
29	b	308	CHL	C1D-ND-C4D	9.27	112.92	106.33
29	6	614	CHL	C4D-CHA-C1A	-9.26	109.98	121.25
29	c	605	CHL	C4D-CHA-C1A	-9.25	109.99	121.25
29	3	407	CHL	C4D-CHA-C1A	-9.25	110.00	121.25
29	b	310	CHL	C4D-CHA-C1A	-9.24	110.00	121.25
29	6	607	CHL	C4D-CHA-C1A	-9.24	110.01	121.25
29	4	607	CHL	C4D-CHA-C1A	-9.24	110.01	121.25
29	4	606	CHL	C4D-CHA-C1A	-9.23	110.01	121.25
29	a	608	CHL	C4D-CHA-C1A	-9.23	110.01	121.25
29	6	614	CHL	C1D-ND-C4D	9.23	112.89	106.33
29	b	310	CHL	C1D-ND-C4D	9.23	112.89	106.33
29	c	601	CHL	C4D-CHA-C1A	-9.22	110.03	121.25
29	4	614	CHL	C4D-CHA-C1A	-9.22	110.03	121.25
29	a	609	CHL	C4D-CHA-C1A	-9.22	110.03	121.25
29	9	609	CHL	C1D-ND-C4D	9.21	112.88	106.33
29	2	602	CHL	C4D-CHA-C1A	-9.20	110.06	121.25
29	5	606	CHL	C1D-ND-C4D	9.20	112.87	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	c	608	CHL	C4D-CHA-C1A	-9.19	110.06	121.25
29	2	601	CHL	C4D-CHA-C1A	-9.19	110.06	121.25
29	1	302	CHL	C1D-ND-C4D	9.18	112.86	106.33
29	b	306	CHL	C1D-ND-C4D	9.18	112.86	106.33
29	8	613	CHL	C4D-CHA-C1A	-9.18	110.08	121.25
29	9	605	CHL	C1D-ND-C4D	9.16	112.84	106.33
29	a	606	CHL	C4D-CHA-C1A	-9.16	110.10	121.25
29	9	608	CHL	C4D-CHA-C1A	-9.16	110.10	121.25
29	c	609	CHL	C4D-CHA-C1A	-9.15	110.11	121.25
29	2	607	CHL	C4D-CHA-C1A	-9.15	110.12	121.25
29	6	605	CHL	C4D-CHA-C1A	-9.14	110.12	121.25
29	4	605	CHL	C4D-CHA-C1A	-9.14	110.13	121.25
29	8	605	CHL	C4D-CHA-C1A	-9.14	110.13	121.25
29	8	613	CHL	C1D-ND-C4D	9.10	112.80	106.33
29	c	601	CHL	C1D-ND-C4D	9.10	112.80	106.33
29	9	607	CHL	C4D-CHA-C1A	-9.09	110.18	121.25
29	a	607	CHL	C4D-CHA-C1A	-9.09	110.19	121.25
29	c	606	CHL	C1D-ND-C4D	9.08	112.79	106.33
29	a	607	CHL	C1D-ND-C4D	9.06	112.77	106.33
29	2	607	CHL	C1D-ND-C4D	9.03	112.75	106.33
29	5	601	CHL	C4D-CHA-C1A	-9.03	110.26	121.25
29	2	605	CHL	C1D-ND-C4D	9.03	112.75	106.33
29	8	607	CHL	C4D-CHA-C1A	-9.03	110.26	121.25
29	8	607	CHL	C1D-ND-C4D	9.03	112.75	106.33
29	9	608	CHL	C1D-ND-C4D	9.01	112.74	106.33
29	a	606	CHL	C1D-ND-C4D	9.00	112.73	106.33
29	1	307	CHL	C1D-ND-C4D	9.00	112.72	106.33
29	2	614	CHL	C1D-ND-C4D	8.97	112.71	106.33
29	6	602	CHL	C1D-ND-C4D	8.97	112.70	106.33
29	9	606	CHL	C1D-ND-C4D	8.93	112.68	106.33
29	4	606	CHL	C1D-ND-C4D	8.92	112.67	106.33
29	4	614	CHL	C1D-ND-C4D	8.85	112.62	106.33
29	b	307	CHL	C1D-ND-C4D	8.84	112.61	106.33
29	2	614	CHL	C4D-CHA-C1A	-8.83	110.51	121.25
29	6	606	CHL	C1D-ND-C4D	8.82	112.60	106.33
29	2	601	CHL	C1D-ND-C4D	8.80	112.59	106.33
29	b	309	CHL	C1D-ND-C4D	8.80	112.59	106.33
24	B	843	BCR	C24-C23-C22	-8.78	112.97	126.23
29	3	407	CHL	C1D-ND-C4D	8.77	112.56	106.33
29	a	608	CHL	C1D-ND-C4D	8.74	112.54	106.33
29	5	601	CHL	C1D-ND-C4D	8.72	112.53	106.33
29	4	605	CHL	C1D-ND-C4D	8.70	112.52	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	2	606	CHL	C1D-ND-C4D	8.69	112.51	106.33
29	2	602	CHL	C1D-ND-C4D	8.67	112.49	106.33
29	4	607	CHL	C1D-ND-C4D	8.66	112.49	106.33
29	6	605	CHL	C1D-ND-C4D	8.61	112.45	106.33
29	8	605	CHL	C1D-ND-C4D	8.49	112.36	106.33
24	J	101	BCR	C15-C16-C17	8.19	140.25	123.47
24	B	843	BCR	C16-C17-C18	-8.17	115.65	127.31
24	7	418	BCR	C15-C16-C17	8.16	140.18	123.47
24	A	850	BCR	C15-C16-C17	8.12	140.10	123.47
21	B	801	CLA	C2D-C1D-ND	7.96	115.97	110.10
29	a	609	CHL	C2D-C1D-ND	-7.91	104.28	110.10
29	a	606	CHL	C1B-CHB-C4A	-7.87	114.53	130.12
21	B	811	CLA	C4A-NA-C1A	7.77	110.20	106.71
29	4	605	CHL	CAB-C3B-C4B	7.67	140.25	128.46
29	a	609	CHL	C1B-CHB-C4A	-7.57	115.13	130.12
29	b	302	CHL	C1B-CHB-C4A	-7.57	115.13	130.12
29	a	605	CHL	C1B-CHB-C4A	-7.47	115.32	130.12
29	7	406	CHL	C2D-C1D-ND	-7.46	104.61	110.10
21	B	829	CLA	C4A-NA-C1A	7.44	110.05	106.71
29	a	601	CHL	C1B-CHB-C4A	-7.44	115.39	130.12
21	G	202	CLA	C4A-NA-C1A	7.35	110.01	106.71
29	c	605	CHL	C2D-C1D-ND	-7.31	104.72	110.10
29	c	605	CHL	C1B-CHB-C4A	-7.27	115.72	130.12
29	c	609	CHL	C2D-C1D-ND	-7.24	104.77	110.10
29	c	607	CHL	C2D-C1D-ND	-7.23	104.78	110.10
29	9	601	CHL	C1B-CHB-C4A	-7.20	115.86	130.12
29	6	607	CHL	C2D-C1D-ND	-7.20	104.80	110.10
21	A	841	CLA	C4A-NA-C1A	7.19	109.94	106.71
29	8	606	CHL	C1B-CHB-C4A	-7.19	115.89	130.12
21	3	405	CLA	C4A-NA-C1A	7.17	109.93	106.71
29	a	601	CHL	C2D-C1D-ND	-7.16	104.83	110.10
21	A	817	CLA	C4A-NA-C1A	7.14	109.92	106.71
21	B	823	CLA	C4A-NA-C1A	7.14	109.91	106.71
29	8	605	CHL	CAB-C3B-C4B	7.13	139.42	128.46
21	B	836	CLA	C4A-NA-C1A	7.12	109.91	106.71
29	8	606	CHL	C2D-C1D-ND	-7.10	104.88	110.10
21	B	802	CLA	C4A-NA-C1A	7.09	109.89	106.71
21	6	612	CLA	C4A-NA-C1A	7.09	109.89	106.71
21	B	821	CLA	C4A-NA-C1A	7.05	109.88	106.71
21	A	827	CLA	C4A-NA-C1A	7.04	109.87	106.71
21	3	401	CLA	C4A-NA-C1A	7.01	109.86	106.71
29	a	605	CHL	C2D-C1D-ND	-7.01	104.94	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	804	CLA	C4A-NA-C1A	7.00	109.85	106.71
21	A	801	CLA	C1D-ND-C4D	-7.00	101.36	106.33
21	A	839	CLA	C4A-NA-C1A	6.96	109.84	106.71
29	c	606	CHL	C1B-CHB-C4A	-6.96	116.33	130.12
29	7	406	CHL	C1B-CHB-C4A	-6.95	116.35	130.12
29	6	614	CHL	C2D-C1D-ND	-6.92	105.01	110.10
21	A	806	CLA	C4A-NA-C1A	6.91	109.81	106.71
21	L	302	CLA	C4A-NA-C1A	6.90	109.81	106.71
21	A	804	CLA	C4A-NA-C1A	6.90	109.81	106.71
29	5	606	CHL	C1B-CHB-C4A	-6.90	116.46	130.12
21	c	613	CLA	C4A-NA-C1A	6.90	109.81	106.71
21	A	813	CLA	C4A-NA-C1A	6.88	109.80	106.71
21	A	838	CLA	C4A-NA-C1A	6.87	109.80	106.71
29	b	310	CHL	C2D-C1D-ND	-6.85	105.05	110.10
21	B	814	CLA	C4A-NA-C1A	6.85	109.78	106.71
21	B	837	CLA	C4A-NA-C1A	6.84	109.78	106.71
29	b	302	CHL	C2D-C1D-ND	-6.84	105.06	110.10
21	9	603	CLA	C4A-NA-C1A	6.83	109.78	106.71
21	9	604	CLA	C4A-NA-C1A	6.82	109.77	106.71
29	c	608	CHL	C1B-CHB-C4A	-6.82	116.61	130.12
29	a	606	CHL	C2D-C1D-ND	-6.82	105.08	110.10
21	9	613	CLA	C4A-NA-C1A	6.82	109.77	106.71
29	6	601	CHL	C1B-CHB-C4A	-6.81	116.63	130.12
29	6	602	CHL	CHB-C4A-NA	6.81	133.93	124.51
29	9	607	CHL	C2D-C1D-ND	-6.80	105.09	110.10
21	5	612	CLA	C4A-NA-C1A	6.80	109.76	106.71
21	B	834	CLA	C4A-NA-C1A	6.79	109.76	106.71
29	9	601	CHL	C2D-C1D-ND	-6.78	105.10	110.10
29	c	609	CHL	C1B-CHB-C4A	-6.78	116.69	130.12
21	7	401	CLA	C4A-NA-C1A	6.77	109.75	106.71
21	7	408	CLA	C4A-NA-C1A	6.77	109.75	106.71
29	b	308	CHL	C1B-CHB-C4A	-6.76	116.72	130.12
29	9	607	CHL	C1B-CHB-C4A	-6.76	116.73	130.12
21	A	840	CLA	C4A-NA-C1A	6.75	109.74	106.71
21	7	407	CLA	C4A-NA-C1A	6.75	109.74	106.71
21	A	822	CLA	C4A-NA-C1A	6.74	109.74	106.71
21	A	810	CLA	C4A-NA-C1A	6.74	109.74	106.71
21	K	204	CLA	C4A-NA-C1A	6.74	109.74	106.71
21	1	309	CLA	C4A-NA-C1A	6.74	109.74	106.71
29	9	609	CHL	C2D-C1D-ND	-6.74	105.14	110.10
29	c	601	CHL	CHB-C4A-NA	6.74	133.83	124.51
21	6	611	CLA	C4A-NA-C1A	6.74	109.73	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	b	304	CLA	C4A-NA-C1A	6.73	109.73	106.71
21	K	201	CLA	C4A-NA-C1A	6.72	109.73	106.71
21	B	803	CLA	C4A-NA-C1A	6.70	109.72	106.71
21	O	201	CLA	C4A-NA-C1A	6.69	109.71	106.71
21	B	805	CLA	C4A-NA-C1A	6.68	109.71	106.71
21	1	308	CLA	C4A-NA-C1A	6.68	109.71	106.71
21	3	409	CLA	C4A-NA-C1A	6.68	109.71	106.71
21	B	806	CLA	C4A-NA-C1A	6.68	109.71	106.71
21	7	404	CLA	C4A-NA-C1A	6.68	109.71	106.71
29	6	601	CHL	C2D-C1D-ND	-6.67	105.19	110.10
29	c	608	CHL	C2D-C1D-ND	-6.66	105.19	110.10
21	G	204	CLA	C4A-NA-C1A	6.66	109.70	106.71
21	A	831	CLA	C4A-NA-C1A	6.66	109.70	106.71
21	8	609	CLA	C4A-NA-C1A	6.66	109.70	106.71
29	4	607	CHL	CHB-C4A-NA	6.65	133.71	124.51
29	6	607	CHL	C1B-CHB-C4A	-6.64	116.97	130.12
29	8	613	CHL	C1B-CHB-C4A	-6.64	116.98	130.12
21	A	830	CLA	C4A-NA-C1A	6.64	109.69	106.71
21	5	604	CLA	C4A-NA-C1A	6.64	109.69	106.71
21	a	613	CLA	C4A-NA-C1A	6.64	109.69	106.71
29	6	614	CHL	C1B-CHB-C4A	-6.62	117.00	130.12
21	2	609	CLA	C4A-NA-C1A	6.62	109.68	106.71
21	B	840	CLA	C4A-NA-C1A	6.61	109.68	106.71
21	7	405	CLA	C4A-NA-C1A	6.61	109.68	106.71
21	6	609	CLA	C4A-NA-C1A	6.61	109.68	106.71
21	A	820	CLA	C4A-NA-C1A	6.60	109.67	106.71
29	2	614	CHL	C2D-C1D-ND	-6.60	105.24	110.10
24	3	419	BCR	C15-C16-C17	6.60	137.00	123.47
29	9	605	CHL	C2D-C1D-ND	-6.60	105.24	110.10
21	4	609	CLA	C4A-NA-C1A	6.60	109.67	106.71
29	b	306	CHL	C2D-C1D-ND	-6.60	105.24	110.10
21	3	406	CLA	C4A-NA-C1A	6.59	109.67	106.71
21	5	610	CLA	C4A-NA-C1A	6.58	109.67	106.71
21	b	305	CLA	C4A-NA-C1A	6.58	109.66	106.71
21	5	607	CLA	C4A-NA-C1A	6.57	109.66	106.71
21	5	614	CLA	C4A-NA-C1A	6.57	109.66	106.71
21	1	316	CLA	C4A-NA-C1A	6.57	109.66	106.71
29	8	607	CHL	C2D-C1D-ND	-6.57	105.26	110.10
21	c	604	CLA	C4A-NA-C1A	6.57	109.66	106.71
21	B	822	CLA	C4A-NA-C1A	6.56	109.66	106.71
21	7	409	CLA	C4A-NA-C1A	6.56	109.66	106.71
21	8	610	CLA	C4A-NA-C1A	6.56	109.66	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	1	307	CHL	C2D-C1D-ND	-6.56	105.27	110.10
21	8	612	CLA	C4A-NA-C1A	6.55	109.65	106.71
21	B	826	CLA	C4A-NA-C1A	6.55	109.65	106.71
21	5	611	CLA	C4A-NA-C1A	6.55	109.65	106.71
21	a	611	CLA	C4A-NA-C1A	6.54	109.65	106.71
21	B	839	CLA	C4A-NA-C1A	6.54	109.65	106.71
29	5	606	CHL	C2D-C1D-ND	-6.54	105.28	110.10
29	2	605	CHL	C1B-CHB-C4A	-6.54	117.17	130.12
21	H	201	CLA	C4A-NA-C1A	6.54	109.65	106.71
21	2	604	CLA	C4A-NA-C1A	6.54	109.65	106.71
21	1	309	CLA	O2D-CGD-CBD	6.54	122.88	111.27
29	a	607	CHL	C2D-C1D-ND	-6.53	105.29	110.10
29	2	605	CHL	C2D-C1D-ND	-6.53	105.29	110.10
29	c	606	CHL	C2D-C1D-ND	-6.53	105.29	110.10
21	2	612	CLA	C4A-NA-C1A	6.53	109.64	106.71
21	3	404	CLA	C4A-NA-C1A	6.53	109.64	106.71
21	4	611	CLA	C4A-NA-C1A	6.53	109.64	106.71
21	a	604	CLA	C4A-NA-C1A	6.53	109.64	106.71
21	2	610	CLA	C4A-NA-C1A	6.52	109.64	106.71
21	1	310	CLA	C4A-NA-C1A	6.52	109.64	106.71
29	8	605	CHL	CHB-C4A-NA	6.52	133.53	124.51
21	6	603	CLA	C4A-NA-C1A	6.52	109.64	106.71
21	7	410	CLA	C4A-NA-C1A	6.52	109.64	106.71
29	b	308	CHL	C2D-C1D-ND	-6.51	105.31	110.10
29	b	310	CHL	C1B-CHB-C4A	-6.51	117.23	130.12
21	B	825	CLA	C4A-NA-C1A	6.51	109.63	106.71
21	c	611	CLA	C4A-NA-C1A	6.51	109.63	106.71
21	A	808	CLA	C4A-NA-C1A	6.50	109.63	106.71
21	L	304	CLA	C4A-NA-C1A	6.50	109.63	106.71
21	K	203	CLA	C4A-NA-C1A	6.50	109.63	106.71
21	L	303	CLA	C4A-NA-C1A	6.50	109.63	106.71
21	B	824	CLA	C4A-NA-C1A	6.50	109.63	106.71
29	c	607	CHL	C1B-CHB-C4A	-6.50	117.25	130.12
21	8	601	CLA	C4A-NA-C1A	6.49	109.62	106.71
21	3	410	CLA	C4A-NA-C1A	6.49	109.62	106.71
21	3	414	CLA	C4A-NA-C1A	6.49	109.62	106.71
21	4	612	CLA	C4A-NA-C1A	6.49	109.62	106.71
21	5	609	CLA	C4A-NA-C1A	6.49	109.62	106.71
29	6	602	CHL	C1B-CHB-C4A	-6.49	117.27	130.12
21	A	825	CLA	C4A-NA-C1A	6.48	109.62	106.71
21	A	842	CLA	C4A-NA-C1A	6.48	109.62	106.71
29	8	613	CHL	C2D-C1D-ND	-6.48	105.33	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	838	CLA	C4A-NA-C1A	6.48	109.62	106.71
21	1	313	CLA	C4A-NA-C1A	6.48	109.62	106.71
21	1	315	CLA	C4A-NA-C1A	6.48	109.62	106.71
21	7	411	CLA	C4A-NA-C1A	6.47	109.62	106.71
21	a	612	CLA	C4A-NA-C1A	6.47	109.62	106.71
21	A	807	CLA	C4A-NA-C1A	6.47	109.61	106.71
29	2	607	CHL	C2D-C1D-ND	-6.46	105.34	110.10
21	6	604	CLA	C4A-NA-C1A	6.46	109.61	106.71
29	b	309	CHL	CHB-C4A-NA	6.46	133.44	124.51
21	4	603	CLA	C4A-NA-C1A	6.46	109.61	106.71
21	F	302	CLA	C4A-NA-C1A	6.45	109.61	106.71
21	F	305	CLA	C4A-NA-C1A	6.45	109.61	106.71
21	6	610	CLA	C4A-NA-C1A	6.45	109.61	106.71
21	a	610	CLA	C4A-NA-C1A	6.44	109.60	106.71
21	A	818	CLA	C4A-NA-C1A	6.44	109.60	106.71
29	9	608	CHL	C2D-C1D-ND	-6.43	105.36	110.10
21	A	816	CLA	C4A-NA-C1A	6.43	109.60	106.71
21	A	823	CLA	C4A-NA-C1A	6.43	109.60	106.71
29	1	302	CHL	C2D-C1D-ND	-6.43	105.36	110.10
29	b	308	CHL	CHB-C4A-NA	6.43	133.40	124.51
29	6	605	CHL	C2D-C1D-ND	-6.43	105.37	110.10
21	A	826	CLA	C4A-NA-C1A	6.43	109.59	106.71
21	O	203	CLA	C4A-NA-C1A	6.43	109.59	106.71
21	A	814	CLA	C4A-NA-C1A	6.42	109.59	106.71
21	1	305	CLA	C4A-NA-C1A	6.42	109.59	106.71
29	8	605	CHL	C1B-CHB-C4A	-6.42	117.41	130.12
29	9	609	CHL	CHB-C4A-NA	6.42	133.39	124.51
21	7	403	CLA	C4A-NA-C1A	6.41	109.59	106.71
21	9	611	CLA	C4A-NA-C1A	6.41	109.59	106.71
21	a	602	CLA	C4A-NA-C1A	6.41	109.59	106.71
21	5	613	CLA	C4A-NA-C1A	6.41	109.59	106.71
21	B	813	CLA	C4A-NA-C1A	6.40	109.58	106.71
24	J	104	BCR	C7-C8-C9	-6.40	116.57	126.23
29	4	606	CHL	C2D-C1D-ND	-6.40	105.39	110.10
21	J	102	CLA	C4A-NA-C1A	6.39	109.58	106.71
21	4	601	CLA	C4A-NA-C1A	6.39	109.58	106.71
21	8	608	CLA	C4A-NA-C1A	6.39	109.58	106.71
21	8	603	CLA	C4A-NA-C1A	6.39	109.58	106.71
29	a	608	CHL	CHB-C4A-NA	6.39	133.35	124.51
29	8	607	CHL	C1B-CHB-C4A	-6.39	117.47	130.12
21	4	610	CLA	C4A-NA-C1A	6.39	109.58	106.71
29	b	309	CHL	C1B-CHB-C4A	-6.39	117.47	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	4	606	CHL	CHB-C4A-NA	6.38	133.34	124.51
21	A	833	CLA	C4A-NA-C1A	6.38	109.58	106.71
21	1	312	CLA	C4A-NA-C1A	6.38	109.58	106.71
29	1	302	CHL	C1B-CHB-C4A	-6.38	117.48	130.12
21	4	613	CLA	C4A-NA-C1A	6.38	109.58	106.71
21	3	402	CLA	C4A-NA-C1A	6.38	109.57	106.71
21	8	604	CLA	C4A-NA-C1A	6.38	109.57	106.71
29	1	307	CHL	CHB-C4A-NA	6.38	133.33	124.51
29	9	605	CHL	C1B-CHB-C4A	-6.38	117.49	130.12
21	3	412	CLA	C4A-NA-C1A	6.37	109.57	106.71
21	8	618	CLA	C4A-NA-C1A	6.37	109.57	106.71
24	L	306	BCR	C15-C16-C17	6.37	136.53	123.47
21	4	604	CLA	C4A-NA-C1A	6.37	109.57	106.71
29	6	606	CHL	CHB-C4A-NA	6.37	133.32	124.51
29	2	601	CHL	C2D-C1D-ND	-6.37	105.41	110.10
21	B	809	CLA	C4A-NA-C1A	6.37	109.57	106.71
29	6	606	CHL	C1B-CHB-C4A	-6.37	117.51	130.12
21	1	303	CLA	C4A-NA-C1A	6.36	109.57	106.71
29	9	606	CHL	C2D-C1D-ND	-6.36	105.42	110.10
21	A	811	CLA	C4A-NA-C1A	6.35	109.56	106.71
21	B	815	CLA	C4A-NA-C1A	6.35	109.56	106.71
29	b	307	CHL	C2D-C1D-ND	-6.35	105.42	110.10
21	2	613	CLA	C4A-NA-C1A	6.35	109.56	106.71
29	3	407	CHL	CHB-C4A-NA	6.34	133.28	124.51
21	A	815	CLA	C4A-NA-C1A	6.34	109.56	106.71
21	7	414	CLA	C4A-NA-C1A	6.34	109.56	106.71
21	B	801	CLA	CMD-C2D-C1D	6.34	135.88	124.71
29	2	606	CHL	CHB-C4A-NA	6.34	133.27	124.51
24	J	104	BCR	C16-C17-C18	-6.33	118.27	127.31
29	4	614	CHL	CHB-C4A-NA	6.33	133.27	124.51
21	B	810	CLA	C4A-NA-C1A	6.33	109.55	106.71
21	1	311	CLA	C4A-NA-C1A	6.32	109.55	106.71
21	4	608	CLA	C4A-NA-C1A	6.31	109.55	106.71
29	9	608	CHL	CHB-C4A-NA	6.31	133.24	124.51
21	A	821	CLA	C4A-NA-C1A	6.31	109.54	106.71
21	c	612	CLA	C4A-NA-C1A	6.31	109.54	106.71
29	b	306	CHL	C1B-CHB-C4A	-6.30	117.63	130.12
21	B	817	CLA	C4A-NA-C1A	6.30	109.54	106.71
29	4	614	CHL	C2D-C1D-ND	-6.30	105.46	110.10
21	5	608	CLA	C4A-NA-C1A	6.29	109.53	106.71
29	c	601	CHL	C2D-C1D-ND	-6.29	105.47	110.10
21	B	816	CLA	C4A-NA-C1A	6.29	109.53	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	820	CLA	C4A-NA-C1A	6.29	109.53	106.71
21	7	413	CLA	C4A-NA-C1A	6.29	109.53	106.71
29	9	606	CHL	C1B-CHB-C4A	-6.29	117.67	130.12
21	B	808	CLA	C4A-NA-C1A	6.28	109.53	106.71
21	6	613	CLA	C4A-NA-C1A	6.28	109.53	106.71
21	A	809	CLA	C4A-NA-C1A	6.27	109.53	106.71
21	1	306	CLA	C4A-NA-C1A	6.26	109.52	106.71
21	3	411	CLA	C4A-NA-C1A	6.26	109.52	106.71
21	b	314	CLA	C4A-NA-C1A	6.26	109.52	106.71
21	B	801	CLA	CHD-C1D-ND	-6.26	118.70	124.45
21	4	602	CLA	C4A-NA-C1A	6.26	109.52	106.71
21	B	819	CLA	C4A-NA-C1A	6.26	109.52	106.71
29	a	607	CHL	CHB-C4A-NA	6.26	133.16	124.51
21	A	834	CLA	C4A-NA-C1A	6.25	109.52	106.71
21	K	202	CLA	C4A-NA-C1A	6.25	109.51	106.71
21	A	802	CLA	C4A-NA-C1A	6.24	109.51	106.71
29	9	609	CHL	C1B-CHB-C4A	-6.23	117.77	130.12
21	c	610	CLA	C4A-NA-C1A	6.23	109.51	106.71
29	4	605	CHL	C2D-C1D-ND	-6.23	105.51	110.10
21	7	412	CLA	C4A-NA-C1A	6.23	109.51	106.71
29	b	307	CHL	C1B-CHB-C4A	-6.23	117.79	130.12
21	B	818	CLA	C4A-NA-C1A	6.23	109.50	106.71
29	2	614	CHL	C1B-CHB-C4A	-6.22	117.79	130.12
29	6	606	CHL	C2D-C1D-ND	-6.22	105.52	110.10
29	3	407	CHL	C2D-C1D-ND	-6.22	105.52	110.10
29	4	606	CHL	C1B-CHB-C4A	-6.22	117.81	130.12
21	O	204	CLA	C4A-NA-C1A	6.21	109.50	106.71
21	A	824	CLA	C4A-NA-C1A	6.21	109.50	106.71
21	G	203	CLA	C4A-NA-C1A	6.21	109.50	106.71
21	b	312	CLA	C4A-NA-C1A	6.20	109.49	106.71
29	5	601	CHL	C1B-CHB-C4A	-6.20	117.84	130.12
29	2	607	CHL	CHB-C4A-NA	6.20	133.09	124.51
29	2	607	CHL	C1B-CHB-C4A	-6.20	117.84	130.12
29	5	601	CHL	C2D-C1D-ND	-6.20	105.53	110.10
29	2	602	CHL	C2D-C1D-ND	-6.20	105.54	110.10
29	9	608	CHL	C1B-CHB-C4A	-6.20	117.84	130.12
21	9	612	CLA	C4A-NA-C1A	6.20	109.49	106.71
29	4	605	CHL	CHB-C4A-NA	6.20	133.08	124.51
21	5	602	CLA	C4A-NA-C1A	6.19	109.49	106.71
21	9	602	CLA	C4A-NA-C1A	6.19	109.49	106.71
29	c	601	CHL	C1B-CHB-C4A	-6.19	117.86	130.12
21	B	812	CLA	C4A-NA-C1A	6.19	109.49	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	607	CHL	C1B-CHB-C4A	-6.18	117.87	130.12
29	a	606	CHL	CHB-C4A-NA	6.18	133.06	124.51
21	B	833	CLA	C4A-NA-C1A	6.18	109.49	106.71
29	6	605	CHL	C1B-CHB-C4A	-6.18	117.87	130.12
29	3	407	CHL	C1B-CHB-C4A	-6.18	117.88	130.12
21	A	836	CLA	C4A-NA-C1A	6.18	109.48	106.71
21	B	807	CLA	C4A-NA-C1A	6.17	109.48	106.71
21	B	827	CLA	C4A-NA-C1A	6.17	109.48	106.71
21	3	413	CLA	C4A-NA-C1A	6.17	109.48	106.71
29	1	307	CHL	C1B-CHB-C4A	-6.16	117.91	130.12
29	2	606	CHL	C1B-CHB-C4A	-6.16	117.91	130.12
29	5	601	CHL	CHB-C4A-NA	6.16	133.03	124.51
24	F	301	BCR	C15-C16-C17	6.15	136.08	123.47
21	6	608	CLA	C4A-NA-C1A	6.15	109.47	106.71
29	9	609	CHL	CMD-C2D-C1D	6.15	135.55	124.71
21	O	202	CLA	C4A-NA-C1A	6.15	109.47	106.71
29	b	309	CHL	C2D-C1D-ND	-6.14	105.58	110.10
29	2	602	CHL	C1B-CHB-C4A	-6.14	117.96	130.12
21	3	408	CLA	C4A-NA-C1A	6.14	109.47	106.71
29	a	608	CHL	C2D-C1D-ND	-6.13	105.58	110.10
31	9	616	XAT	C28-C29-C30	6.13	128.35	118.94
21	8	611	CLA	C4A-NA-C1A	6.12	109.46	106.71
29	4	607	CHL	C1B-CHB-C4A	-6.12	118.00	130.12
21	5	605	CLA	C4A-NA-C1A	6.12	109.46	106.71
21	b	303	CLA	C4A-NA-C1A	6.12	109.46	106.71
21	A	832	CLA	C4A-NA-C1A	6.12	109.46	106.71
21	a	614	CLA	C4A-NA-C1A	6.12	109.46	106.71
21	7	402	CLA	C4A-NA-C1A	6.11	109.45	106.71
21	1	304	CLA	C4A-NA-C1A	6.11	109.45	106.71
21	8	602	CLA	C4A-NA-C1A	6.11	109.45	106.71
29	4	614	CHL	C1B-CHB-C4A	-6.10	118.03	130.12
21	A	805	CLA	C4A-NA-C1A	6.10	109.45	106.71
29	9	607	CHL	CHB-C4A-NA	6.10	132.95	124.51
24	A	846	BCR	C15-C16-C17	6.08	135.93	123.47
21	b	313	CLA	C4A-NA-C1A	6.08	109.44	106.71
29	6	605	CHL	CHB-C4A-NA	6.08	132.92	124.51
29	a	608	CHL	C1B-CHB-C4A	-6.08	118.08	130.12
29	2	614	CHL	CHB-C4A-NA	6.08	132.91	124.51
21	a	603	CLA	C4A-NA-C1A	6.07	109.44	106.71
21	A	801	CLA	CHD-C1D-ND	-6.06	118.88	124.45
21	9	610	CLA	C4A-NA-C1A	6.06	109.43	106.71
21	b	315	CLA	C4A-NA-C1A	6.05	109.43	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	6	601	CHL	CMD-C2D-C1D	6.05	135.38	124.71
29	6	601	CHL	O2D-CGD-CBD	6.05	122.02	111.27
29	8	605	CHL	C2D-C1D-ND	-6.05	105.64	110.10
21	A	801	CLA	C4A-NA-C1A	6.05	109.43	106.71
29	8	607	CHL	CMD-C2D-C1D	6.05	135.37	124.71
29	3	407	CHL	CMD-C2D-C1D	6.03	135.34	124.71
21	b	311	CLA	C4A-NA-C1A	6.02	109.41	106.71
29	b	309	CHL	CMD-C2D-C1D	6.02	135.32	124.71
29	b	307	CHL	CHB-C4A-NA	6.01	132.83	124.51
29	4	605	CHL	C1B-CHB-C4A	-6.01	118.21	130.12
21	4	609	CLA	CMD-C2D-C1D	6.01	135.31	124.71
29	2	601	CHL	C1B-CHB-C4A	-6.01	118.23	130.12
21	A	830	CLA	O2D-CGD-CBD	6.00	121.93	111.27
29	a	609	CHL	CMD-C2D-C1D	6.00	135.29	124.71
29	4	614	CHL	CMD-C2D-C1D	6.00	135.28	124.71
21	2	611	CLA	C4A-NA-C1A	5.99	109.40	106.71
29	b	307	CHL	CMD-C2D-C1D	5.99	135.27	124.71
21	c	602	CLA	C4A-NA-C1A	5.98	109.39	106.71
29	5	601	CHL	CMD-C2D-C1D	5.98	135.25	124.71
21	F	304	CLA	C4A-NA-C1A	5.97	109.39	106.71
29	6	605	CHL	CMD-C2D-C1D	5.97	135.24	124.71
29	c	608	CHL	CMD-C2D-C1D	5.97	135.24	124.71
21	B	832	CLA	C4A-NA-C1A	5.97	109.39	106.71
29	8	607	CHL	CHB-C4A-NA	5.97	132.77	124.51
29	a	608	CHL	CMD-C2D-C1D	5.97	135.23	124.71
29	1	307	CHL	CMD-C2D-C1D	5.96	135.22	124.71
29	5	606	CHL	CMD-C2D-C1D	5.96	135.22	124.71
21	A	835	CLA	C4A-NA-C1A	5.96	109.39	106.71
29	1	302	CHL	O2D-CGD-CBD	5.96	121.86	111.27
29	4	607	CHL	CMD-C2D-C1D	5.96	135.21	124.71
29	2	601	CHL	CHB-C4A-NA	5.95	132.74	124.51
29	6	606	CHL	CMD-C2D-C1D	5.95	135.20	124.71
29	c	606	CHL	CMD-C2D-C1D	5.95	135.20	124.71
21	A	812	CLA	C4A-NA-C1A	5.95	109.38	106.71
29	2	605	CHL	CMD-C2D-C1D	5.94	135.18	124.71
29	a	606	CHL	CMD-C2D-C1D	5.93	135.17	124.71
21	A	819	CLA	C4A-NA-C1A	5.93	109.37	106.71
29	8	605	CHL	CMD-C2D-C1D	5.93	135.16	124.71
29	6	602	CHL	C2D-C1D-ND	-5.93	105.73	110.10
29	4	605	CHL	CMD-C2D-C1D	5.92	135.15	124.71
21	A	803	CLA	C4A-NA-C1A	5.92	109.37	106.71
29	b	308	CHL	CMD-C2D-C1D	5.92	135.14	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	2	607	CHL	CMD-C2D-C1D	5.92	135.14	124.71
21	B	801	CLA	CHD-C4C-C3C	-5.92	116.14	124.84
29	2	602	CHL	CHB-C4A-NA	5.90	132.67	124.51
29	c	608	CHL	CHB-C4A-NA	5.89	132.66	124.51
29	a	605	CHL	CMD-C2D-C1D	5.89	135.09	124.71
29	2	601	CHL	CMD-C2D-C1D	5.88	135.08	124.71
29	4	607	CHL	C2D-C1D-ND	-5.88	105.77	110.10
21	B	828	CLA	C4A-NA-C1A	5.88	109.35	106.71
29	9	606	CHL	CHB-C4A-NA	5.87	132.63	124.51
29	c	605	CHL	CMD-C2D-C1D	5.87	135.06	124.71
29	2	605	CHL	CHB-C4A-NA	5.87	132.63	124.51
29	6	614	CHL	CMD-C2D-C1D	5.87	135.06	124.71
29	a	601	CHL	CMD-C2D-C1D	5.87	135.05	124.71
21	5	603	CLA	C4A-NA-C1A	5.86	109.34	106.71
29	9	605	CHL	CMD-C2D-C1D	5.86	135.04	124.71
29	6	607	CHL	CMD-C2D-C1D	5.85	135.03	124.71
21	3	403	CLA	C4A-NA-C1A	5.85	109.34	106.71
29	b	302	CHL	CMD-C2D-C1D	5.84	135.01	124.71
29	b	310	CHL	CHB-C4A-NA	5.84	132.59	124.51
29	7	406	CHL	CMD-C2D-C1D	5.84	135.01	124.71
29	2	606	CHL	CMD-C2D-C1D	5.84	135.00	124.71
21	B	830	CLA	C4A-NA-C1A	5.84	109.33	106.71
29	9	608	CHL	CMD-C2D-C1D	5.83	134.99	124.71
29	a	601	CHL	O2D-CGD-CBD	5.83	121.63	111.27
29	4	606	CHL	CMD-C2D-C1D	5.83	134.98	124.71
29	1	302	CHL	CHB-C4A-NA	5.82	132.57	124.51
29	9	606	CHL	CMD-C2D-C1D	5.80	134.94	124.71
29	8	606	CHL	CMD-C2D-C1D	5.80	134.94	124.71
29	c	601	CHL	CMD-C2D-C1D	5.79	134.93	124.71
29	1	302	CHL	CMD-C2D-C1D	5.79	134.92	124.71
29	a	607	CHL	CMD-C2D-C1D	5.78	134.90	124.71
21	B	835	CLA	C4A-NA-C1A	5.77	109.30	106.71
29	2	606	CHL	C2D-C1D-ND	-5.77	105.85	110.10
29	8	613	CHL	CMD-C2D-C1D	5.77	134.88	124.71
29	9	605	CHL	CHB-C4A-NA	5.76	132.48	124.51
21	2	608	CLA	C4A-NA-C1A	5.73	109.28	106.71
29	b	306	CHL	CMD-C2D-C1D	5.73	134.81	124.71
29	2	614	CHL	CMD-C2D-C1D	5.73	134.81	124.71
29	c	607	CHL	CMD-C2D-C1D	5.72	134.80	124.71
21	c	614	CLA	C4A-NA-C1A	5.72	109.28	106.71
29	2	602	CHL	C4A-NA-C1A	-5.72	104.14	106.71
21	1	314	CLA	C4A-NA-C1A	5.71	109.27	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	b	306	CHL	CHB-C4A-NA	5.70	132.40	124.51
21	A	830	CLA	CMD-C2D-C1D	5.70	134.75	124.71
21	3	409	CLA	CMD-C2D-C1D	5.69	134.75	124.71
21	2	609	CLA	CMD-C2D-C1D	5.69	134.75	124.71
29	c	606	CHL	CHB-C4A-NA	5.68	132.37	124.51
21	B	831	CLA	C4A-NA-C1A	5.67	109.26	106.71
29	b	310	CHL	CMD-C2D-C1D	5.67	134.71	124.71
29	9	607	CHL	CMD-C2D-C1D	5.66	134.69	124.71
24	M	101	BCR	C15-C16-C17	5.64	135.03	123.47
21	A	852	CLA	C4A-NA-C1A	5.63	109.24	106.71
21	8	609	CLA	CMD-C2D-C1D	5.63	134.63	124.71
29	2	602	CHL	CMD-C2D-C1D	5.62	134.62	124.71
21	7	407	CLA	CMC-C2C-C1C	-5.60	116.52	125.04
29	a	606	CHL	O2D-CGD-CBD	5.59	121.19	111.27
29	4	607	CHL	CHD-C4C-C3C	-5.57	116.65	124.84
21	2	603	CLA	C4A-NA-C1A	5.57	109.21	106.71
29	4	607	CHL	C1C-C2C-C3C	-5.56	102.70	107.11
29	6	605	CHL	C2A-C1A-CHA	-5.56	114.14	123.86
29	b	307	CHL	C2A-C1A-CHA	-5.56	114.14	123.86
29	a	607	CHL	O2D-CGD-CBD	5.54	121.11	111.27
21	8	609	CLA	O2D-CGD-CBD	5.53	121.09	111.27
29	4	605	CHL	C2A-C1A-CHA	-5.52	114.21	123.86
29	2	601	CHL	C2A-C1A-CHA	-5.52	114.21	123.86
21	c	603	CLA	C4A-NA-C1A	5.51	109.18	106.71
29	9	601	CHL	CMD-C2D-C1D	5.50	134.40	124.71
29	8	607	CHL	C1C-C2C-C3C	-5.50	102.75	107.11
21	B	801	CLA	C4A-NA-C1A	-5.49	104.24	106.71
29	8	605	CHL	C2A-C1A-CHA	-5.49	114.27	123.86
29	b	307	CHL	C1C-C2C-C3C	-5.47	102.77	107.11
29	6	601	CHL	CHB-C4A-NA	5.45	132.05	124.51
29	6	602	CHL	CHD-C4C-C3C	-5.45	116.83	124.84
29	8	613	CHL	C1C-C2C-C3C	-5.44	102.79	107.11
29	2	606	CHL	O2D-CGD-CBD	5.44	120.93	111.27
29	2	605	CHL	C1C-C2C-C3C	-5.43	102.80	107.11
21	4	609	CLA	C1D-ND-C4D	-5.43	102.48	106.33
29	2	601	CHL	O2D-CGD-CBD	5.42	120.90	111.27
24	G	205	BCR	C15-C16-C17	5.41	134.56	123.47
24	K	205	BCR	C20-C21-C22	-5.39	119.62	127.31
21	A	829	CLA	C4A-NA-C1A	5.38	109.12	106.71
29	5	601	CHL	O2D-CGD-CBD	5.37	120.82	111.27
29	1	307	CHL	O2D-CGD-CBD	5.37	120.80	111.27
29	9	601	CHL	CHB-C4A-NA	5.37	131.93	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	5	601	CHL	C1C-C2C-C3C	-5.37	102.86	107.11
29	2	607	CHL	C2A-C1A-CHA	-5.36	114.48	123.86
29	2	614	CHL	C2A-C1A-CHA	-5.36	114.49	123.86
29	a	608	CHL	C2A-C1A-CHA	-5.36	114.49	123.86
29	9	608	CHL	C2A-C1A-CHA	-5.35	114.50	123.86
29	2	606	CHL	CHD-C4C-C3C	-5.35	116.97	124.84
29	a	607	CHL	C2A-C1A-CHA	-5.34	114.52	123.86
29	c	609	CHL	C1C-C2C-C3C	-5.34	102.87	107.11
29	2	606	CHL	C2A-C1A-CHA	-5.33	114.53	123.86
21	A	801	CLA	CMD-C2D-C1D	5.33	134.10	124.71
29	c	609	CHL	CMD-C2D-C1D	5.32	134.09	124.71
29	4	605	CHL	C1C-C2C-C3C	-5.32	102.89	107.11
29	1	307	CHL	C2A-C1A-CHA	-5.31	114.57	123.86
29	2	614	CHL	C1C-C2C-C3C	-5.31	102.90	107.11
29	4	605	CHL	O2D-CGD-CBD	5.30	120.68	111.27
29	a	608	CHL	C1C-C2C-C3C	-5.29	102.91	107.11
29	6	602	CHL	O2D-CGD-CBD	5.29	120.66	111.27
29	2	607	CHL	CHD-C4C-C3C	-5.29	117.07	124.84
24	B	846	BCR	C16-C17-C18	-5.28	119.77	127.31
29	9	609	CHL	C2A-C1A-CHA	-5.27	114.64	123.86
29	b	309	CHL	C2A-C1A-CHA	-5.27	114.65	123.86
29	6	606	CHL	C1C-C2C-C3C	-5.27	102.93	107.11
24	A	849	BCR	C15-C16-C17	5.27	134.26	123.47
29	4	614	CHL	C2A-C1A-CHA	-5.24	114.71	123.85
29	c	609	CHL	CHB-C4A-NA	5.23	131.75	124.51
29	8	613	CHL	CHB-C4A-NA	5.23	131.75	124.51
29	5	601	CHL	C2A-C1A-CHA	-5.23	114.71	123.86
29	b	302	CHL	C1C-C2C-C3C	-5.23	102.97	107.11
29	2	605	CHL	C2A-C1A-CHA	-5.22	114.73	123.86
29	6	602	CHL	CMD-C2D-C1D	5.22	133.92	124.71
29	2	602	CHL	C2A-C1A-CHA	-5.22	114.73	123.86
29	4	606	CHL	C2A-C1A-CHA	-5.22	114.73	123.86
29	9	605	CHL	O2D-CGD-CBD	5.22	120.54	111.27
29	c	607	CHL	O2D-CGD-CBD	5.22	120.54	111.27
24	6	618	BCR	C15-C16-C17	-5.22	112.79	123.47
29	6	606	CHL	C2A-C1A-CHA	-5.20	114.76	123.86
21	A	828	CLA	C4A-NA-C1A	5.18	109.03	106.71
29	b	310	CHL	C2A-C1A-CHA	-5.18	114.81	123.86
29	b	307	CHL	CHD-C4C-C3C	-5.17	117.24	124.84
29	4	607	CHL	C2A-C1A-CHA	-5.17	114.82	123.86
29	6	614	CHL	CHB-C4A-NA	5.16	131.65	124.51
29	2	605	CHL	O2D-CGD-CBD	5.16	120.44	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	2	616	LUT	C35-C15-C14	5.16	134.04	123.47
31	a	618	XAT	C35-C15-C14	5.16	134.04	123.47
21	3	415	CLA	C4A-NA-C1A	5.15	109.02	106.71
29	b	310	CHL	C1C-C2C-C3C	-5.15	103.03	107.11
29	a	608	CHL	CHD-C4C-C3C	-5.15	117.27	124.84
29	9	606	CHL	C4A-NA-C1A	-5.15	104.39	106.71
21	7	407	CLA	CHD-C1D-ND	-5.15	119.72	124.45
29	b	306	CHL	C1C-C2C-C3C	-5.14	103.03	107.11
29	2	602	CHL	CHD-C4C-C3C	-5.12	117.32	124.84
29	9	606	CHL	C2A-C1A-CHA	-5.11	114.92	123.86
29	c	606	CHL	C1C-C2C-C3C	-5.11	103.06	107.11
29	6	607	CHL	CHB-C4A-NA	5.11	131.57	124.51
29	9	606	CHL	O2D-CGD-CBD	5.11	120.34	111.27
29	1	307	CHL	C1C-C2C-C3C	-5.10	103.07	107.11
29	9	606	CHL	C1C-C2C-C3C	-5.09	103.07	107.11
29	8	605	CHL	O2D-CGD-CBD	5.09	120.32	111.27
29	5	606	CHL	C1C-C2C-C3C	-5.09	103.07	107.11
29	6	605	CHL	O2D-CGD-CBD	5.09	120.31	111.27
31	9	616	XAT	C39-C29-C30	-5.09	115.80	122.92
29	4	606	CHL	O2D-CGD-CBD	5.09	120.30	111.27
29	1	302	CHL	C2A-C1A-CHA	-5.08	114.98	123.86
29	c	601	CHL	C2A-C1A-CHA	-5.08	114.98	123.86
29	a	605	CHL	CHB-C4A-NA	5.07	131.53	124.51
29	5	606	CHL	CHB-C4A-NA	5.07	131.52	124.51
29	c	607	CHL	CHB-C4A-NA	5.06	131.51	124.51
29	a	601	CHL	CHB-C4A-NA	5.06	131.51	124.51
29	9	605	CHL	C1C-C2C-C3C	-5.06	103.10	107.11
29	5	601	CHL	CHD-C4C-C3C	-5.06	117.40	124.84
30	7	415	LUT	C35-C15-C14	5.06	133.84	123.47
29	6	602	CHL	C2A-C1A-CHA	-5.05	115.02	123.86
29	b	306	CHL	C2A-C1A-CHA	-5.05	115.02	123.86
21	B	801	CLA	C2C-C1C-NC	5.05	114.70	109.97
29	b	307	CHL	O2D-CGD-CBD	5.05	120.23	111.27
29	9	605	CHL	C2A-C1A-CHA	-5.04	115.04	123.86
29	3	407	CHL	CHD-C4C-C3C	-5.04	117.43	124.84
29	b	309	CHL	CHD-C4C-C3C	-5.04	117.43	124.84
29	2	606	CHL	C1C-C2C-C3C	-5.03	103.12	107.11
29	c	601	CHL	CHD-C4C-C3C	-5.03	117.44	124.84
29	1	307	CHL	CHD-C4C-C3C	-5.02	117.45	124.84
29	9	608	CHL	CHD-C4C-C3C	-5.02	117.46	124.84
29	b	307	CHL	C4A-NA-C1A	-5.01	104.45	106.71
29	8	607	CHL	C2A-C1A-CHA	-5.01	115.10	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	6	606	CHL	CHD-C4C-C3C	-5.01	117.48	124.84
29	b	302	CHL	CHB-C4A-NA	5.00	131.43	124.51
29	5	606	CHL	O2D-CGD-CBD	5.00	120.16	111.27
29	4	614	CHL	CHD-C4C-C3C	-5.00	117.49	124.84
29	a	609	CHL	CMD-C2D-C3D	-5.00	116.12	127.61
29	b	308	CHL	O2D-CGD-CBD	4.99	120.14	111.27
29	a	607	CHL	C1C-C2C-C3C	-4.99	103.15	107.11
29	2	602	CHL	O2D-CGD-CBD	4.99	120.13	111.27
24	G	201	BCR	C15-C16-C17	4.99	133.69	123.47
29	8	606	CHL	O2D-CGD-CBD	4.97	120.10	111.27
29	6	606	CHL	O2D-CGD-CBD	4.96	120.09	111.27
29	a	609	CHL	O2D-CGD-CBD	4.96	120.08	111.27
29	c	608	CHL	O2D-CGD-CBD	4.96	120.08	111.27
29	c	607	CHL	C1C-C2C-C3C	-4.95	103.18	107.11
29	9	609	CHL	C1C-C2C-C3C	-4.95	103.18	107.11
24	K	205	BCR	C16-C17-C18	-4.93	120.27	127.31
29	4	614	CHL	O2D-CGD-CBD	4.93	120.03	111.27
29	b	302	CHL	O2D-CGD-CBD	4.92	120.02	111.27
29	9	606	CHL	CHD-C4C-C3C	-4.92	117.61	124.84
29	b	306	CHL	O2D-CGD-CBD	4.92	120.00	111.27
31	6	617	XAT	C15-C35-C34	4.91	133.54	123.47
29	2	607	CHL	C1C-C2C-C3C	-4.90	103.23	107.11
29	4	606	CHL	CHD-C4C-C3C	-4.90	117.64	124.84
29	c	601	CHL	C1C-C2C-C3C	-4.89	103.23	107.11
29	8	605	CHL	CHD-C4C-C3C	-4.89	117.34	124.98
29	6	605	CHL	CHD-C4C-C3C	-4.89	117.65	124.84
29	8	613	CHL	O2D-CGD-CBD	4.89	119.95	111.27
30	6	616	LUT	C35-C15-C14	4.89	133.48	123.47
29	6	614	CHL	C2A-C1A-CHA	-4.89	115.32	123.86
29	9	607	CHL	C1C-C2C-C3C	-4.88	103.24	107.11
29	2	605	CHL	CHD-C4C-C3C	-4.88	117.67	124.84
29	a	607	CHL	CHD-C4C-C3C	-4.88	117.67	124.84
29	2	602	CHL	C1C-C2C-C3C	-4.88	103.24	107.11
29	9	609	CHL	CHD-C4C-C3C	-4.87	117.69	124.84
29	4	605	CHL	CHD-C4C-C3C	-4.87	117.38	124.98
21	3	409	CLA	C1-C2-C3	-4.86	117.64	126.04
29	8	613	CHL	C2A-C1A-CHA	-4.86	115.37	123.85
29	a	605	CHL	C1C-C2C-C3C	-4.86	103.26	107.11
29	9	601	CHL	CHD-C4C-C3C	-4.85	117.70	124.84
29	1	302	CHL	C1C-C2C-C3C	-4.85	103.26	107.11
29	6	601	CHL	CMC-C2C-C3C	-4.85	116.69	126.75
29	a	606	CHL	CMD-C2D-C3D	-4.84	116.47	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	837	CLA	C4A-NA-C1A	4.84	108.88	106.71
29	c	606	CHL	O2D-CGD-CBD	4.84	119.87	111.27
29	6	614	CHL	C1C-C2C-C3C	-4.84	103.27	107.11
29	9	607	CHL	O2D-CGD-CBD	4.84	119.86	111.27
29	a	601	CHL	C1C-C2C-C3C	-4.84	103.28	107.11
29	2	614	CHL	CHD-C4C-C3C	-4.83	117.73	124.84
24	B	844	BCR	C3-C4-C5	-4.83	105.45	114.08
29	b	308	CHL	C2A-C1A-CHA	-4.83	115.41	123.86
29	9	608	CHL	C1C-C2C-C3C	-4.83	103.28	107.11
29	9	609	CHL	CMD-C2D-C3D	-4.82	116.52	127.61
29	3	407	CHL	C2A-C1A-CHA	-4.82	115.44	123.85
29	2	601	CHL	CHD-C4C-C3C	-4.82	117.76	124.84
29	c	605	CHL	C1C-C2C-C3C	-4.81	103.29	107.11
29	c	606	CHL	C2A-C1A-CHA	-4.81	115.45	123.86
30	4	615	LUT	C15-C35-C34	4.81	133.32	123.47
29	6	607	CHL	C2A-C1A-CHA	-4.80	115.46	123.86
29	2	601	CHL	C1C-C2C-C3C	-4.80	103.31	107.11
31	8	615	XAT	C35-C15-C14	4.79	133.29	123.47
29	6	607	CHL	C1C-C2C-C3C	-4.79	103.31	107.11
29	6	602	CHL	C1C-C2C-C3C	-4.78	103.32	107.11
29	c	601	CHL	O2D-CGD-CBD	4.78	119.76	111.27
29	b	308	CHL	CHD-C4C-C3C	-4.78	117.81	124.84
30	3	416	LUT	C15-C35-C34	4.78	133.26	123.47
29	b	306	CHL	CHD-C4C-C3C	-4.77	117.82	124.84
29	9	601	CHL	C1C-C2C-C3C	-4.77	103.33	107.11
29	6	607	CHL	CMD-C2D-C3D	-4.76	116.67	127.61
29	6	614	CHL	O2D-CGD-CBD	4.75	119.71	111.27
29	9	605	CHL	CHD-C4C-C3C	-4.75	117.86	124.84
24	J	104	BCR	C24-C23-C22	-4.75	119.06	126.23
29	7	406	CHL	CMD-C2D-C3D	-4.74	116.71	127.61
29	8	606	CHL	C1C-C2C-C3C	-4.74	103.35	107.11
29	1	302	CHL	CHD-C4C-C3C	-4.73	117.89	124.84
29	8	607	CHL	CMD-C2D-C3D	-4.73	116.74	127.61
29	c	606	CHL	CHD-C4C-C3C	-4.72	117.89	124.84
29	2	614	CHL	O2D-CGD-CBD	4.72	119.66	111.27
29	c	605	CHL	CMD-C2D-C3D	-4.72	116.75	127.61
21	4	609	CLA	O2D-CGD-CBD	4.72	119.65	111.27
24	B	844	BCR	C20-C21-C22	-4.71	120.58	127.31
29	6	605	CHL	C4A-NA-C1A	-4.71	104.59	106.71
29	1	307	CHL	CMD-C2D-C3D	-4.70	116.81	127.61
29	6	605	CHL	CMD-C2D-C3D	-4.70	116.81	127.61
29	c	608	CHL	CHD-C4C-C3C	-4.69	117.94	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	6	614	CHL	CMD-C2D-C3D	-4.69	116.83	127.61
29	6	605	CHL	C1C-C2C-C3C	-4.69	103.39	107.11
29	2	605	CHL	C4A-NA-C1A	-4.68	104.60	106.71
29	b	309	CHL	O2D-CGD-CBD	4.68	119.58	111.27
29	9	608	CHL	O2D-CGD-CBD	4.67	119.57	111.27
29	c	605	CHL	CHB-C4A-NA	4.67	130.97	124.51
29	8	607	CHL	CHD-C4C-C3C	-4.67	117.98	124.84
29	6	601	CHL	CMD-C2D-C3D	-4.67	116.88	127.61
29	a	605	CHL	CHA-C4D-ND	4.66	142.24	132.50
29	4	614	CHL	CMD-C2D-C3D	-4.66	116.90	127.61
29	3	407	CHL	CMD-C2D-C3D	-4.66	116.90	127.61
29	2	605	CHL	CMD-C2D-C3D	-4.65	116.91	127.61
29	a	606	CHL	CHD-C4C-C3C	-4.65	118.00	124.84
21	4	609	CLA	CHD-C1D-ND	-4.65	120.18	124.45
29	5	606	CHL	CMD-C2D-C3D	-4.65	116.92	127.61
21	3	409	CLA	C6-C5-C3	-4.64	107.03	114.62
29	a	601	CHL	CHA-C4D-ND	4.64	142.20	132.50
29	8	613	CHL	CHD-C4C-C3C	-4.64	118.03	124.84
29	c	606	CHL	CMD-C2D-C3D	-4.63	116.95	127.61
29	b	307	CHL	CMD-C2D-C3D	-4.63	116.96	127.61
29	8	606	CHL	CHB-C4A-NA	4.63	130.91	124.51
29	a	601	CHL	CMD-C2D-C3D	-4.62	116.98	127.61
29	8	606	CHL	CMD-C2D-C3D	-4.62	116.98	127.61
29	b	309	CHL	CMD-C2D-C3D	-4.62	116.98	127.61
29	a	605	CHL	CMD-C2D-C3D	-4.62	116.98	127.61
29	c	608	CHL	CMD-C2D-C3D	-4.62	116.99	127.61
24	B	846	BCR	C3-C4-C5	-4.61	105.84	114.08
29	2	601	CHL	CMD-C2D-C3D	-4.61	117.01	127.61
29	9	601	CHL	CHA-C4D-ND	4.61	142.13	132.50
29	2	607	CHL	CMD-C2D-C3D	-4.61	117.02	127.61
29	5	601	CHL	CMD-C2D-C3D	-4.60	117.02	127.61
29	6	601	CHL	CHA-C4D-ND	4.60	142.12	132.50
29	6	606	CHL	CMD-C2D-C3D	-4.59	117.05	127.61
29	c	607	CHL	CMD-C2D-C3D	-4.59	117.05	127.61
29	9	609	CHL	CHA-C4D-ND	4.59	142.10	132.50
29	b	302	CHL	CHA-C4D-ND	4.59	142.10	132.50
29	c	608	CHL	CHA-C4D-ND	4.59	142.10	132.50
21	9	610	CLA	CMB-C2B-C1B	-4.59	121.41	128.46
29	4	607	CHL	O2D-CGD-CBD	4.59	119.42	111.27
29	2	607	CHL	O2D-CGD-CBD	4.59	119.42	111.27
29	a	606	CHL	C1C-C2C-C3C	-4.59	103.47	107.11
29	9	605	CHL	CMD-C2D-C3D	-4.59	117.07	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	608	CHL	CMD-C2D-C3D	-4.58	117.07	127.61
29	5	606	CHL	C2A-C1A-CHA	-4.58	115.84	123.86
31	6	617	XAT	C19-C9-C10	-4.58	116.50	122.92
29	b	308	CHL	CHA-C4D-ND	4.58	142.09	132.50
29	9	609	CHL	O2D-CGD-CBD	4.58	119.41	111.27
29	8	605	CHL	C1C-C2C-C3C	-4.58	103.48	107.11
29	4	605	CHL	CMD-C2D-C3D	-4.58	117.08	127.61
29	b	308	CHL	CMD-C2D-C3D	-4.57	117.10	127.61
29	8	605	CHL	CMD-C2D-C3D	-4.57	117.10	127.61
29	1	307	CHL	CHA-C4D-ND	4.57	142.06	132.50
29	a	609	CHL	CHA-C4D-ND	4.57	142.06	132.50
29	b	307	CHL	CHA-C4D-ND	4.57	142.05	132.50
29	2	614	CHL	CMD-C2D-C3D	-4.56	117.13	127.61
29	a	608	CHL	O2D-CGD-CBD	4.56	119.36	111.27
21	B	832	CLA	CMB-C2B-C1B	-4.55	121.46	128.46
29	b	302	CHL	CMD-C2D-C3D	-4.55	117.15	127.61
29	b	310	CHL	CMD-C2D-C3D	-4.54	117.16	127.61
29	4	606	CHL	CMD-C2D-C3D	-4.54	117.16	127.61
29	2	605	CHL	CHA-C4D-ND	4.54	142.00	132.50
24	B	843	BCR	C15-C14-C13	-4.54	120.83	127.31
29	5	606	CHL	CHD-C4C-C3C	-4.54	118.17	124.84
29	2	606	CHL	CHA-C4D-ND	4.54	141.99	132.50
29	9	608	CHL	CMD-C2D-C3D	-4.53	117.18	127.61
29	6	607	CHL	CHD-C4C-C3C	-4.53	118.18	124.84
29	4	607	CHL	CHA-C4D-ND	4.53	141.98	132.50
29	c	601	CHL	CHA-C4D-ND	4.53	141.97	132.50
29	b	309	CHL	C1C-C2C-C3C	-4.53	103.52	107.11
30	1	317	LUT	C15-C35-C34	4.53	132.75	123.47
29	2	607	CHL	CHA-C4D-ND	4.53	141.97	132.50
29	a	609	CHL	C1C-C2C-C3C	-4.53	103.52	107.11
29	b	308	CHL	C1C-C2C-C3C	-4.53	103.52	107.11
31	9	616	XAT	C19-C9-C10	-4.52	116.58	122.92
29	a	607	CHL	CMD-C2D-C3D	-4.52	117.22	127.61
29	5	606	CHL	CHA-C4D-ND	4.51	141.94	132.50
29	9	606	CHL	CMD-C2D-C3D	-4.51	117.23	127.61
29	1	302	CHL	CHA-C4D-ND	4.51	141.93	132.50
21	A	832	CLA	CMB-C2B-C1B	-4.51	121.53	128.46
29	b	306	CHL	CMD-C2D-C3D	-4.51	117.25	127.61
29	c	607	CHL	CHA-C4D-ND	4.51	141.93	132.50
29	9	605	CHL	CHA-C4D-ND	4.51	141.93	132.50
29	6	601	CHL	C2A-C1A-CHA	-4.51	115.98	123.86
29	4	607	CHL	CMD-C2D-C3D	-4.51	117.25	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	4	614	CHL	C1C-C2C-C3C	-4.51	103.54	107.11
29	b	310	CHL	CHD-C4C-C3C	-4.50	118.22	124.84
29	8	607	CHL	CHA-C4D-ND	4.49	141.90	132.50
24	K	205	BCR	C3-C4-C5	-4.49	106.05	114.08
29	6	606	CHL	CHA-C4D-ND	4.49	141.90	132.50
29	6	607	CHL	CHA-C4D-ND	4.49	141.90	132.50
29	a	608	CHL	CHA-C4D-ND	4.49	141.90	132.50
21	B	801	CLA	C3D-C2D-C1D	-4.49	99.71	105.83
29	c	608	CHL	C2A-C1A-CHA	-4.49	116.02	123.86
29	9	606	CHL	CHA-C4D-ND	4.49	141.88	132.50
29	b	309	CHL	CHA-C4D-ND	4.49	141.88	132.50
29	c	606	CHL	CHA-C4D-ND	4.48	141.88	132.50
24	3	419	BCR	C34-C9-C10	-4.48	116.64	122.92
29	9	607	CHL	C2A-C1A-CHA	-4.48	116.02	123.86
29	9	608	CHL	CHA-C4D-ND	4.48	141.87	132.50
29	8	613	CHL	CMD-C2D-C3D	-4.48	117.31	127.61
29	c	601	CHL	CMD-C2D-C3D	-4.48	117.31	127.61
30	4	615	LUT	C35-C15-C14	4.48	132.65	123.47
29	6	601	CHL	CHD-C4C-C3C	-4.48	117.99	124.98
29	a	607	CHL	CHA-C4D-ND	4.47	141.86	132.50
21	2	609	CLA	O2D-CGD-CBD	4.47	119.22	111.27
30	a	615	LUT	C39-C29-C30	-4.47	116.66	122.92
29	c	605	CHL	CHA-C4D-ND	4.47	141.85	132.50
29	4	605	CHL	CHA-C4D-ND	4.47	141.85	132.50
29	9	607	CHL	CHA-C4D-ND	4.47	141.85	132.50
30	1	317	LUT	C35-C15-C14	4.47	132.63	123.47
29	7	406	CHL	CHA-C4D-ND	4.47	141.84	132.50
29	9	607	CHL	CMD-C2D-C3D	-4.46	117.34	127.61
29	1	302	CHL	CMD-C2D-C3D	-4.46	117.35	127.61
31	9	616	XAT	C35-C15-C14	4.46	132.61	123.47
29	8	606	CHL	CHA-C4D-ND	4.46	141.82	132.50
31	9	616	XAT	C8-C9-C10	4.45	125.77	118.94
29	9	607	CHL	CHD-C4C-C3C	-4.45	118.30	124.84
29	4	606	CHL	CHA-C4D-ND	4.45	141.81	132.50
29	a	609	CHL	C2A-C1A-CHA	-4.45	116.08	123.86
29	4	614	CHL	CHA-C4D-ND	4.44	141.79	132.50
29	b	310	CHL	CHA-C4D-ND	4.44	141.78	132.50
29	b	306	CHL	CHA-C4D-ND	4.43	141.77	132.50
29	3	407	CHL	CHA-C4D-ND	4.43	141.76	132.50
29	5	601	CHL	CHA-C4D-ND	4.43	141.76	132.50
29	9	607	CHL	CHC-C1C-NC	4.42	130.91	124.20
29	6	607	CHL	O2D-CGD-CBD	4.42	119.13	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	2	601	CHL	CHA-C4D-ND	4.42	141.75	132.50
29	6	614	CHL	CHA-C4D-ND	4.41	141.73	132.50
29	4	606	CHL	CHC-C1C-NC	4.41	130.90	124.20
21	9	604	CLA	CMB-C2B-C1B	-4.41	121.69	128.46
29	6	605	CHL	CHA-C4D-ND	4.41	141.72	132.50
21	1	309	CLA	CMD-C2D-C1D	4.40	132.48	124.71
30	2	616	LUT	C19-C9-C10	-4.40	116.75	122.92
29	8	605	CHL	CHA-C4D-ND	4.40	141.71	132.50
24	K	205	BCR	C7-C8-C9	-4.40	119.58	126.23
31	9	616	XAT	C32-C33-C34	4.40	125.69	118.94
21	B	834	CLA	CMB-C2B-C1B	-4.39	121.71	128.46
29	6	602	CHL	CHA-C4D-ND	4.39	141.69	132.50
21	B	828	CLA	CMB-C2B-C1B	-4.39	121.72	128.46
29	2	602	CHL	CMD-C2D-C3D	-4.39	117.52	127.61
29	8	613	CHL	CHA-C4D-ND	4.39	141.68	132.50
29	c	607	CHL	C2A-C1A-CHA	-4.38	116.19	123.86
29	c	609	CHL	CHA-C4D-ND	4.38	141.67	132.50
24	L	306	BCR	C37-C22-C21	-4.38	116.78	122.92
29	2	602	CHL	CHA-C4D-ND	4.38	141.66	132.50
29	6	614	CHL	CHD-C4C-C3C	-4.38	118.40	124.84
30	a	616	LUT	C35-C15-C14	4.37	132.42	123.47
24	A	849	BCR	C37-C22-C21	-4.36	116.81	122.92
29	2	606	CHL	CMD-C2D-C3D	-4.36	117.58	127.61
29	c	608	CHL	C1C-C2C-C3C	-4.36	103.65	107.11
24	B	844	BCR	C11-C10-C9	-4.36	121.09	127.31
29	2	614	CHL	CHA-C4D-ND	4.36	141.62	132.50
21	B	836	CLA	CMB-C2B-C1B	-4.36	121.77	128.46
24	O	205	BCR	C37-C22-C21	-4.35	116.83	122.92
21	b	311	CLA	CMB-C2B-C1B	-4.34	121.79	128.46
21	8	604	CLA	CMB-C2B-C1B	-4.33	121.81	128.46
21	7	407	CLA	C4D-C3D-CAD	4.33	113.20	108.10
21	3	409	CLA	O2D-CGD-CBD	4.33	118.96	111.27
29	8	606	CHL	CHD-C4C-C3C	-4.33	118.48	124.84
21	B	801	CLA	C3D-C4D-ND	4.32	117.23	110.24
29	c	607	CHL	CHD-C4C-C3C	-4.32	118.49	124.84
24	M	101	BCR	C37-C22-C21	-4.32	116.87	122.92
21	A	838	CLA	CMB-C2B-C1B	-4.31	121.83	128.46
21	B	825	CLA	CMB-C2B-C1B	-4.31	121.84	128.46
24	7	418	BCR	C37-C22-C21	-4.31	116.89	122.92
29	7	406	CHL	CHB-C4A-NA	4.31	130.47	124.51
21	A	852	CLA	CMB-C2B-C1B	-4.30	121.85	128.46
29	c	609	CHL	CMD-C2D-C3D	-4.30	117.72	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	7	407	CLA	C3B-C4B-NB	4.30	114.77	109.21
29	8	606	CHL	C2A-C1A-CHA	-4.30	116.34	123.86
29	a	606	CHL	CHA-C4D-ND	4.30	141.49	132.50
29	a	605	CHL	CHD-C4C-C3C	-4.29	118.53	124.84
21	B	835	CLA	CMB-C2B-C1B	-4.29	121.87	128.46
29	9	601	CHL	CMD-C2D-C3D	-4.29	117.75	127.61
29	b	308	CHL	CHC-C1C-NC	4.29	130.71	124.20
31	c	617	XAT	C35-C15-C14	4.28	132.25	123.47
29	4	614	CHL	CHC-C1C-NC	4.28	130.69	124.20
21	A	816	CLA	CMB-C2B-C1B	-4.27	121.91	128.46
21	3	409	CLA	C3B-C4B-NB	4.27	114.72	109.21
29	b	302	CHL	CHD-C4C-C3C	-4.26	118.57	124.84
21	A	827	CLA	CMB-C2B-C1B	-4.26	121.91	128.46
29	c	601	CHL	CHC-C1C-NC	4.26	130.67	124.20
29	b	309	CHL	CHC-C1C-NC	4.26	130.67	124.20
29	c	605	CHL	C2A-C1A-CHA	-4.26	116.41	123.86
32	c	618	NEX	C15-C35-C34	4.26	132.19	123.47
29	2	601	CHL	C4A-NA-C1A	-4.26	104.79	106.71
21	A	808	CLA	CMB-C2B-C1B	-4.26	121.92	128.46
24	7	418	BCR	C34-C9-C10	-4.25	116.97	122.92
24	3	419	BCR	C8-C9-C10	4.25	125.46	118.94
31	9	616	XAT	C30-C31-C32	4.25	136.47	123.22
30	8	614	LUT	C15-C35-C34	4.25	132.17	123.47
21	1	304	CLA	CMB-C2B-C1B	-4.23	121.96	128.46
24	7	417	BCR	C34-C9-C10	-4.23	117.00	122.92
21	3	401	CLA	CMB-C2B-C1B	-4.23	121.97	128.46
31	c	617	XAT	C39-C29-C30	-4.23	117.00	122.92
21	B	840	CLA	CMB-C2B-C1B	-4.23	121.97	128.46
21	7	413	CLA	CMB-C2B-C1B	-4.22	121.97	128.46
21	A	821	CLA	CMB-C2B-C1B	-4.22	121.98	128.46
31	9	616	XAT	C27-C28-C29	4.21	132.07	125.53
30	8	614	LUT	C35-C15-C14	4.21	132.11	123.47
24	A	854	BCR	C37-C22-C21	-4.21	117.02	122.92
21	7	414	CLA	CMB-C2B-C1B	-4.21	121.99	128.46
31	a	618	XAT	C19-C9-C10	-4.20	117.03	122.92
21	4	609	CLA	C3B-C4B-NB	4.20	114.64	109.21
24	O	205	BCR	C34-C9-C10	-4.20	117.03	122.92
21	A	815	CLA	CMB-C2B-C1B	-4.20	122.01	128.46
30	6	616	LUT	C19-C9-C10	-4.20	117.04	122.92
29	3	407	CHL	CHC-C1C-NC	4.20	130.57	124.20
29	2	614	CHL	C4A-NA-C1A	-4.19	104.82	106.71
29	6	602	CHL	C1D-CHD-C4C	-4.18	117.03	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	618	XAT	C39-C29-C30	-4.18	117.06	122.92
29	c	605	CHL	CHD-C4C-C3C	-4.18	118.69	124.84
24	3	419	BCR	C37-C22-C21	-4.18	117.07	122.92
21	B	806	CLA	CMB-C2B-C1B	-4.18	122.04	128.46
24	F	303	BCR	C37-C22-C21	-4.18	117.07	122.92
21	6	609	CLA	CMB-C2B-C1B	-4.17	122.05	128.46
29	9	608	CHL	CHC-C1C-NC	4.17	130.52	124.20
29	4	605	CHL	C4B-C3B-C2B	-4.16	103.05	106.92
24	6	618	BCR	C34-C9-C10	-4.16	117.09	122.92
24	A	850	BCR	C34-C9-C10	-4.16	117.09	122.92
24	I	101	BCR	C34-C9-C10	-4.16	117.10	122.92
31	8	615	XAT	C19-C9-C10	-4.16	117.10	122.92
27	B	847	DGD	O2G-C1B-C2B	4.16	120.46	111.50
21	A	813	CLA	CMB-C2B-C1B	-4.15	122.08	128.46
24	M	101	BCR	C34-C9-C10	-4.15	117.11	122.92
30	3	416	LUT	C19-C9-C10	-4.15	117.11	122.92
21	L	304	CLA	CMB-C2B-C1B	-4.15	122.09	128.46
29	9	601	CHL	O2D-CGD-CBD	4.15	118.64	111.27
29	c	608	CHL	CHC-C1C-NC	4.15	130.50	124.20
29	a	601	CHL	CHD-C4C-C3C	-4.14	118.75	124.84
21	B	808	CLA	CMB-C2B-C1B	-4.14	122.10	128.46
29	9	609	CHL	CHC-C1C-NC	4.14	130.48	124.20
21	A	818	CLA	CMB-C2B-C1B	-4.13	122.11	128.46
31	6	617	XAT	C8-C9-C10	4.13	125.28	118.94
21	A	803	CLA	CMB-C2B-C1B	-4.13	122.11	128.46
29	8	607	CHL	O2D-CGD-CBD	4.13	118.60	111.27
24	3	418	BCR	C34-C9-C10	-4.13	117.14	122.92
30	3	416	LUT	C10-C11-C12	4.13	136.10	123.22
21	A	825	CLA	CMB-C2B-C1B	-4.12	122.13	128.46
29	a	606	CHL	CHC-C1C-NC	4.12	130.46	124.20
21	4	611	CLA	CMB-C2B-C1B	-4.12	122.13	128.46
21	A	809	CLA	CMB-C2B-C1B	-4.11	122.14	128.46
29	8	605	CHL	CHC-C1C-NC	4.11	130.44	124.20
24	M	101	BCR	C16-C15-C14	4.11	131.89	123.47
29	4	606	CHL	C4A-NA-C1A	-4.11	104.86	106.71
29	7	406	CHL	CHD-C4C-C3C	-4.10	118.81	124.84
21	8	602	CLA	CMB-C2B-C1B	-4.10	122.16	128.46
21	c	610	CLA	CMB-C2B-C1B	-4.10	122.17	128.46
30	4	615	LUT	C19-C9-C10	-4.10	117.19	122.92
29	1	307	CHL	CHC-C1C-NC	4.09	130.41	124.20
21	A	826	CLA	CMB-C2B-C1B	-4.09	122.17	128.46
31	9	616	XAT	C40-C33-C34	-4.09	117.19	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	2	618	BCR	C37-C22-C21	-4.09	117.19	122.92
24	8	616	BCR	C34-C9-C10	-4.09	117.19	122.92
21	B	824	CLA	CMB-C2B-C1B	-4.09	122.18	128.46
24	7	418	BCR	C16-C15-C14	4.09	131.84	123.47
24	A	848	BCR	C37-C22-C21	-4.08	117.20	122.92
24	G	201	BCR	C34-C9-C10	-4.08	117.20	122.92
24	6	618	BCR	C37-C22-C21	-4.08	117.20	122.92
30	a	616	LUT	C19-C9-C10	-4.08	117.21	122.92
24	B	843	BCR	C28-C27-C26	-4.08	106.79	114.08
24	G	205	BCR	C37-C22-C21	-4.08	117.21	122.92
21	a	602	CLA	CMB-C2B-C1B	-4.08	122.20	128.46
29	4	605	CHL	CAB-C3B-C2B	-4.08	116.70	124.69
32	9	617	NEX	C39-C29-C30	-4.08	117.21	122.92
31	3	417	XAT	C15-C35-C34	4.07	131.81	123.47
24	A	846	BCR	C37-C22-C21	-4.07	117.22	122.92
29	6	601	CHL	C1C-C2C-C3C	-4.07	103.34	107.07
29	6	605	CHL	CHC-C1C-NC	4.07	130.37	124.20
21	B	826	CLA	CMB-C2B-C1B	-4.07	122.22	128.46
31	8	615	XAT	C39-C29-C30	-4.06	117.23	122.92
29	a	609	CHL	CHB-C4A-NA	4.06	130.13	124.51
24	7	417	BCR	C37-C22-C21	-4.06	117.23	122.92
21	4	608	CLA	CMB-C2B-C1B	-4.06	122.22	128.46
24	F	301	BCR	C37-C22-C21	-4.06	117.23	122.92
24	L	306	BCR	C34-C9-C10	-4.06	117.24	122.92
29	4	606	CHL	C1C-C2C-C3C	-4.06	103.89	107.11
21	4	602	CLA	CMB-C2B-C1B	-4.06	122.23	128.46
30	1	317	LUT	C19-C9-C10	-4.06	117.24	122.92
21	O	201	CLA	CMB-C2B-C1B	-4.05	122.24	128.46
24	B	845	BCR	C15-C16-C17	-4.05	115.17	123.47
21	1	310	CLA	CMB-C2B-C1B	-4.05	122.24	128.46
31	c	617	XAT	C19-C9-C10	-4.05	117.25	122.92
21	B	813	CLA	CMB-C2B-C1B	-4.05	122.24	128.46
21	2	611	CLA	CMB-C2B-C1B	-4.05	122.24	128.46
29	1	302	CHL	CHC-C1C-NC	4.05	130.34	124.20
21	A	828	CLA	CMB-C2B-C1B	-4.05	122.24	128.46
21	B	827	CLA	CMB-C2B-C1B	-4.05	122.25	128.46
30	b	316	LUT	C19-C9-C10	-4.04	117.26	122.92
24	O	205	BCR	C15-C16-C17	4.04	131.76	123.47
32	b	318	NEX	C39-C29-C30	-4.03	117.27	122.92
21	A	814	CLA	CMB-C2B-C1B	-4.03	122.27	128.46
21	c	603	CLA	CMB-C2B-C1B	-4.03	122.27	128.46
29	b	310	CHL	C4A-NA-C1A	-4.03	104.89	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	850	BCR	C37-C22-C21	-4.03	117.28	122.92
29	a	607	CHL	CHC-C1C-NC	4.03	130.31	124.20
29	c	609	CHL	CHD-C4C-C3C	-4.03	118.69	124.98
21	B	830	CLA	CMB-C2B-C1B	-4.02	122.28	128.46
30	5	615	LUT	C35-C15-C14	4.02	131.72	123.47
24	3	418	BCR	C37-C22-C21	-4.02	117.29	122.92
31	2	617	XAT	C39-C29-C30	-4.02	117.29	122.92
21	b	314	CLA	CMB-C2B-C1B	-4.02	122.28	128.46
29	8	607	CHL	CHC-C1C-NC	4.02	130.30	124.20
31	5	616	XAT	C19-C9-C10	-4.02	117.29	122.92
24	L	305	BCR	C34-C9-C10	-4.02	117.29	122.92
29	6	602	CHL	CMD-C2D-C3D	-4.02	118.37	127.61
24	2	618	BCR	C34-C9-C10	-4.02	117.30	122.92
32	c	618	NEX	C39-C29-C30	-4.02	117.30	122.92
32	b	318	NEX	C15-C35-C34	4.02	131.70	123.47
24	J	101	BCR	C21-C20-C19	4.01	135.74	123.22
30	5	615	LUT	C39-C29-C30	-4.01	117.31	122.92
30	a	615	LUT	C19-C9-C10	-4.01	117.31	122.92
24	A	847	BCR	C34-C9-C10	-4.00	117.31	122.92
29	4	607	CHL	CHD-C4C-NC	4.00	130.51	124.20
29	b	310	CHL	CHC-C1C-NC	4.00	130.28	124.20
24	A	848	BCR	C34-C9-C10	-4.00	117.32	122.92
29	4	606	CHL	C2C-C3C-C4C	-4.00	103.64	106.49
29	2	601	CHL	CHC-C1C-NC	4.00	130.28	124.20
24	J	103	BCR	C37-C22-C21	-4.00	117.32	122.92
24	B	845	BCR	C34-C9-C10	-4.00	117.32	122.92
30	8	614	LUT	C19-C9-C10	-4.00	117.32	122.92
31	7	416	XAT	C39-C29-C30	-3.99	117.33	122.92
24	4	617	BCR	C37-C22-C21	-3.99	117.33	122.92
29	9	601	CHL	C1D-CHD-C4C	-3.99	117.45	126.06
29	a	609	CHL	CHC-C1C-NC	3.99	130.26	124.20
29	5	601	CHL	CHC-C1C-NC	3.99	130.26	124.20
21	A	805	CLA	CMB-C2B-C1B	-3.99	122.33	128.46
24	A	854	BCR	C34-C9-C10	-3.99	117.34	122.92
31	5	616	XAT	C39-C29-C30	-3.99	117.34	122.92
24	B	842	BCR	C34-C9-C10	-3.99	117.34	122.92
24	L	305	BCR	C37-C22-C21	-3.99	117.34	122.92
31	1	318	XAT	C39-C29-C30	-3.98	117.34	122.92
29	a	608	CHL	CHC-C1C-NC	3.98	130.25	124.20
21	5	611	CLA	CMB-C2B-C1B	-3.98	122.34	128.46
24	L	301	BCR	C34-C9-C10	-3.98	117.34	122.92
24	A	846	BCR	C34-C9-C10	-3.98	117.34	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	2	604	CLA	CMB-C2B-C1B	-3.97	122.36	128.46
24	O	205	BCR	C16-C15-C14	3.97	131.61	123.47
21	7	407	CLA	C3D-C2D-C1D	-3.97	100.41	105.83
24	3	419	BCR	C16-C15-C14	3.97	131.61	123.47
30	b	316	LUT	C15-C35-C34	3.97	131.60	123.47
24	G	201	BCR	C37-C22-C21	-3.97	117.36	122.92
29	4	605	CHL	C4A-NA-C1A	-3.97	104.92	106.71
29	4	605	CHL	CHC-C1C-NC	3.97	130.22	124.20
29	2	606	CHL	CHC-C1C-NC	3.96	130.22	124.20
24	8	616	BCR	C37-C22-C21	-3.96	117.38	122.92
21	B	816	CLA	CMB-C2B-C1B	-3.96	122.38	128.46
29	9	606	CHL	CHC-C1C-NC	3.95	130.20	124.20
21	c	604	CLA	CMB-C2B-C1B	-3.95	122.39	128.46
21	A	819	CLA	CMB-C2B-C1B	-3.95	122.39	128.46
31	4	616	XAT	C39-C29-C30	-3.95	117.39	122.92
24	B	845	BCR	C37-C22-C21	-3.95	117.39	122.92
30	9	615	LUT	C39-C29-C30	-3.94	117.40	122.92
30	c	615	LUT	C19-C9-C10	-3.94	117.40	122.92
30	1	317	LUT	C39-C29-C30	-3.94	117.40	122.92
21	A	802	CLA	CMB-C2B-C1B	-3.94	122.41	128.46
21	2	608	CLA	CMB-C2B-C1B	-3.94	122.41	128.46
21	2	609	CLA	C1-C2-C3	-3.93	119.24	126.04
21	A	835	CLA	CMB-C2B-C1B	-3.93	122.42	128.46
31	9	616	XAT	C12-C13-C14	3.93	124.97	118.94
30	4	615	LUT	C39-C29-C30	-3.93	117.42	122.92
21	2	609	CLA	CMB-C2B-C1B	-3.93	122.43	128.46
30	c	616	LUT	C39-C29-C30	-3.92	117.42	122.92
21	1	303	CLA	CMB-C2B-C1B	-3.92	122.44	128.46
21	3	409	CLA	CMB-C2B-C1B	-3.92	122.44	128.46
29	9	601	CHL	C2A-C1A-CHA	-3.92	117.00	123.86
29	2	607	CHL	C4A-NA-C1A	-3.92	104.94	106.71
24	I	101	BCR	C37-C22-C21	-3.92	117.43	122.92
24	B	844	BCR	C28-C27-C26	-3.92	107.08	114.08
24	J	104	BCR	C11-C12-C13	-3.92	115.41	126.42
32	9	617	NEX	C35-C15-C14	3.92	131.50	123.47
29	8	605	CHL	C4B-C3B-C2B	-3.91	103.28	106.92
31	6	617	XAT	C39-C29-C30	-3.91	117.44	122.92
21	4	609	CLA	CMD-C2D-C3D	-3.91	118.62	127.61
24	A	847	BCR	C37-C22-C21	-3.91	117.45	122.92
29	6	602	CHL	CHC-C1C-NC	3.91	130.13	124.20
21	B	811	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
24	8	616	BCR	C16-C15-C14	3.90	131.47	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	4	617	BCR	C34-C9-C10	-3.90	117.46	122.92
24	J	104	BCR	C38-C26-C25	-3.90	120.15	124.53
29	c	608	CHL	C2C-C3C-C4C	-3.90	103.71	106.49
30	a	615	LUT	C35-C15-C14	3.90	131.46	123.47
29	2	606	CHL	C1D-CHD-C4C	-3.90	117.65	126.06
29	4	607	CHL	C1D-CHD-C4C	-3.90	117.65	126.06
21	A	829	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
30	9	614	LUT	C39-C29-C30	-3.90	117.46	122.92
21	G	202	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
30	8	614	LUT	C39-C29-C30	-3.90	117.47	122.92
24	J	101	BCR	C34-C9-C10	-3.89	117.47	122.92
21	B	801	CLA	C3C-C4C-NC	3.89	114.93	110.57
21	A	811	CLA	CMB-C2B-C1B	-3.89	122.49	128.46
29	a	608	CHL	C1D-CHD-C4C	-3.88	117.69	126.06
24	7	417	BCR	C16-C15-C14	3.88	131.42	123.47
24	B	844	BCR	C15-C14-C13	-3.88	121.78	127.31
24	G	205	BCR	C34-C9-C10	-3.88	117.49	122.92
21	A	835	CLA	CMB-C2B-C3B	3.88	131.93	124.68
21	L	303	CLA	CMB-C2B-C1B	-3.88	122.51	128.46
31	9	616	XAT	C20-C13-C14	-3.88	117.49	122.92
21	A	831	CLA	CMB-C2B-C1B	-3.88	122.51	128.46
21	B	837	CLA	CMB-C2B-C1B	-3.88	122.51	128.46
24	F	301	BCR	C34-C9-C10	-3.87	117.50	122.92
24	B	844	BCR	C7-C8-C9	-3.87	120.38	126.23
29	1	307	CHL	C4A-NA-C1A	-3.87	104.96	106.71
29	8	605	CHL	C1D-CHD-C4C	-3.87	117.70	126.06
29	b	309	CHL	C4A-NA-C1A	-3.87	104.97	106.71
21	B	821	CLA	CMB-C2B-C1B	-3.87	122.51	128.46
24	B	842	BCR	C37-C22-C21	-3.87	117.50	122.92
31	3	417	XAT	C19-C9-C10	-3.87	117.50	122.92
21	A	807	CLA	CMB-C2B-C1B	-3.86	122.52	128.46
30	b	317	LUT	C39-C29-C30	-3.86	117.51	122.92
30	c	615	LUT	C39-C29-C30	-3.86	117.51	122.92
30	c	616	LUT	C19-C9-C10	-3.86	117.51	122.92
29	7	406	CHL	C2A-C1A-CHA	-3.86	117.11	123.85
29	b	308	CHL	C4A-NA-C1A	-3.86	104.97	106.71
21	3	415	CLA	CMB-C2B-C1B	-3.85	122.54	128.46
29	2	607	CHL	CHC-C1C-NC	3.85	130.05	124.20
29	9	605	CHL	CHC-C1C-NC	3.85	130.04	124.20
29	2	607	CHL	C1D-CHD-C4C	-3.85	117.76	126.06
29	a	601	CHL	CHC-C1C-NC	3.84	130.03	124.20
24	J	104	BCR	C20-C21-C22	-3.84	121.83	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	c	609	CHL	C1D-CHD-C4C	-3.84	117.77	126.06
29	2	602	CHL	C1-C2-C3	-3.84	119.40	126.04
21	B	805	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
24	L	301	BCR	C37-C22-C21	-3.84	117.55	122.92
29	6	606	CHL	CHC-C1C-NC	3.84	130.02	124.20
24	L	306	BCR	C16-C15-C14	3.84	131.33	123.47
30	b	316	LUT	C39-C29-C30	-3.83	117.55	122.92
30	b	317	LUT	C19-C9-C10	-3.83	117.55	122.92
21	c	613	CLA	CMB-C2B-C1B	-3.83	122.57	128.46
21	5	610	CLA	CAB-C3B-C4B	-3.83	122.58	128.46
21	A	804	CLA	CMB-C2B-C1B	-3.83	122.58	128.46
21	1	306	CLA	CMB-C2B-C1B	-3.83	122.58	128.46
31	2	617	XAT	C19-C9-C10	-3.83	117.56	122.92
21	O	203	CLA	CMB-C2B-C1B	-3.82	122.59	128.46
21	5	609	CLA	CMB-C2B-C1B	-3.82	122.59	128.46
31	3	417	XAT	C39-C29-C30	-3.82	117.57	122.92
21	7	407	CLA	C3D-C4D-ND	3.82	116.42	110.24
21	B	801	CLA	C1D-CHD-C4C	-3.81	117.83	126.06
29	9	601	CHL	CHC-C1C-NC	3.81	129.99	124.20
21	7	403	CLA	CAB-C3B-C4B	-3.81	122.61	128.46
29	b	308	CHL	C2C-C3C-C4C	-3.81	103.77	106.49
30	9	615	LUT	C19-C9-C10	-3.81	117.59	122.92
29	2	605	CHL	CHC-C1C-NC	3.81	129.98	124.20
29	2	602	CHL	CHC-C1C-NC	3.81	129.98	124.20
21	B	801	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
30	7	415	LUT	C20-C13-C14	-3.81	117.59	122.92
31	4	616	XAT	C19-C9-C10	-3.80	117.60	122.92
21	B	812	CLA	CMB-C2B-C1B	-3.80	122.62	128.46
29	b	302	CHL	CHC-C1C-NC	3.80	129.97	124.20
21	B	817	CLA	CMB-C2B-C1B	-3.80	122.62	128.46
29	4	614	CHL	C1D-CHD-C4C	-3.80	117.86	126.06
21	B	803	CLA	CMB-C2B-C1B	-3.80	122.63	128.46
29	9	608	CHL	C4A-NA-C1A	-3.79	105.00	106.71
29	b	309	CHL	C1D-CHD-C4C	-3.79	117.88	126.06
30	9	615	LUT	C15-C35-C34	3.79	131.24	123.47
21	a	610	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
29	5	601	CHL	C1D-CHD-C4C	-3.79	117.88	126.06
29	6	614	CHL	CHC-C1C-NC	3.79	129.95	124.20
29	a	609	CHL	CHD-C4C-C3C	-3.79	119.28	124.84
24	A	849	BCR	C34-C9-C10	-3.79	117.62	122.92
24	M	101	BCR	C8-C9-C10	3.78	124.75	118.94
21	3	402	CLA	CMB-C2B-C1B	-3.78	122.65	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	b	305	CLA	CMB-C2B-C1B	-3.78	122.65	128.46
29	1	307	CHL	C1D-CHD-C4C	-3.78	117.91	126.06
29	9	608	CHL	C1D-CHD-C4C	-3.78	117.91	126.06
29	9	606	CHL	C1D-CHD-C4C	-3.78	117.91	126.06
29	3	407	CHL	C4A-NA-C1A	-3.78	105.01	106.71
24	J	103	BCR	C16-C15-C14	3.78	131.21	123.47
29	c	601	CHL	C1D-CHD-C4C	-3.78	117.91	126.06
29	4	606	CHL	C1D-CHD-C4C	-3.77	117.92	126.06
29	8	605	CHL	CAB-C3B-C2B	-3.77	117.30	124.69
29	4	614	CHL	C4A-NA-C1A	-3.77	105.01	106.71
29	4	607	CHL	CHC-C1C-NC	3.77	129.92	124.20
24	J	101	BCR	C20-C21-C22	3.77	132.69	127.31
21	G	204	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
29	2	614	CHL	CHC-C1C-NC	3.76	129.91	124.20
21	6	610	CLA	CMB-C2B-C1B	-3.76	122.68	128.46
29	a	605	CHL	CHC-C1C-NC	3.76	129.91	124.20
30	9	614	LUT	C19-C9-C10	-3.76	117.66	122.92
21	B	819	CLA	CMB-C2B-C1B	-3.76	122.69	128.46
21	9	602	CLA	CMB-C2B-C1B	-3.76	122.69	128.46
29	c	608	CHL	C1D-CHD-C4C	-3.75	117.97	126.06
30	3	416	LUT	C39-C29-C30	-3.75	117.67	122.92
29	5	606	CHL	CHC-C1C-NC	3.75	129.89	124.20
29	6	601	CHL	CHC-C1C-NC	3.75	129.89	124.20
21	B	814	CLA	CMB-C2B-C1B	-3.75	122.70	128.46
21	B	823	CLA	CMB-C2B-C1B	-3.75	122.70	128.46
21	9	610	CLA	CMB-C2B-C3B	3.75	131.69	124.68
21	K	202	CLA	CMB-C2B-C1B	-3.74	122.71	128.46
30	7	415	LUT	C12-C13-C14	3.74	124.68	118.94
21	O	204	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
24	F	303	BCR	C34-C9-C10	-3.74	117.69	122.92
21	A	806	CLA	CMB-C2B-C1B	-3.73	122.72	128.46
29	3	407	CHL	CHD-C4C-NC	3.73	130.09	124.20
21	A	832	CLA	CMB-C2B-C3B	3.73	131.66	124.68
21	O	202	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
21	8	609	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
30	7	415	LUT	C39-C29-C30	-3.73	117.70	122.92
31	7	416	XAT	C15-C35-C34	3.73	131.11	123.47
29	2	607	CHL	C1-C2-C3	-3.72	120.73	126.75
29	6	602	CHL	CHD-C4C-NC	3.72	130.07	124.20
21	B	802	CLA	CMB-C2B-C1B	-3.72	122.74	128.46
21	F	302	CLA	O2D-CGD-O1D	-3.72	116.56	123.84
30	b	317	LUT	C15-C35-C34	3.72	131.09	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	616	LUT	C39-C29-C30	-3.72	117.71	122.92
21	A	822	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
29	2	606	CHL	CHD-C4C-NC	3.72	130.06	124.20
31	4	616	XAT	C15-C35-C34	3.72	131.09	123.47
31	1	318	XAT	C19-C9-C10	-3.72	117.72	122.92
29	c	606	CHL	CHC-C1C-NC	3.71	129.84	124.20
21	B	834	CLA	CMB-C2B-C3B	3.71	131.62	124.68
21	B	822	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
29	a	607	CHL	C4A-NA-C1A	-3.71	105.04	106.71
21	4	604	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
29	b	307	CHL	CHD-C4C-NC	3.71	130.05	124.20
30	2	616	LUT	C20-C13-C14	-3.71	117.73	122.92
29	5	601	CHL	CHD-C4C-NC	3.71	130.04	124.20
21	B	801	CLA	O2D-CGD-CBD	3.70	117.85	111.27
21	K	202	CLA	CAA-C2A-C3A	-3.70	102.64	112.78
21	A	852	CLA	CMB-C2B-C3B	3.70	131.59	124.68
21	1	311	CLA	CAB-C3B-C4B	-3.70	122.78	128.46
21	7	407	CLA	C2D-C1D-ND	3.70	112.83	110.10
29	6	606	CHL	C4A-NA-C1A	-3.69	105.05	106.71
29	2	607	CHL	CHD-C4C-NC	3.69	130.02	124.20
29	4	607	CHL	C1-C2-C3	-3.69	120.78	126.75
29	4	605	CHL	C1D-CHD-C4C	-3.69	118.10	126.06
31	a	618	XAT	C20-C13-C14	-3.69	117.76	122.92
30	6	616	LUT	C39-C29-C30	-3.68	117.76	122.92
24	B	846	BCR	C7-C8-C9	-3.68	120.67	126.23
29	8	606	CHL	CHC-C1C-NC	3.68	129.79	124.20
29	c	609	CHL	C2A-C1A-CHA	-3.68	117.43	123.86
29	b	308	CHL	C1D-CHD-C4C	-3.68	118.13	126.06
31	a	618	XAT	C12-C13-C14	3.67	124.58	118.94
21	3	406	CLA	CAB-C3B-C4B	-3.67	122.82	128.46
29	a	607	CHL	C1D-CHD-C4C	-3.67	118.14	126.06
24	6	618	BCR	C16-C15-C14	3.67	130.99	123.47
24	2	618	BCR	C16-C15-C14	3.67	130.99	123.47
21	1	316	CLA	CAB-C3B-C4B	-3.67	122.83	128.46
29	2	602	CHL	C1D-CHD-C4C	-3.66	118.16	126.06
29	b	307	CHL	C1D-CHD-C4C	-3.66	118.16	126.06
21	4	609	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
21	b	303	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
21	K	203	CLA	CAB-C3B-C4B	-3.66	122.84	128.46
29	6	601	CHL	C1D-CHD-C4C	-3.66	118.17	126.06
21	7	404	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
30	6	616	LUT	C20-C13-C14	-3.66	117.80	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	810	CLA	CMB-C2B-C1B	-3.65	122.85	128.46
21	B	836	CLA	CMB-C2B-C3B	3.65	131.51	124.68
21	A	812	CLA	CMB-C2B-C1B	-3.65	122.85	128.46
24	M	101	BCR	C35-C13-C14	-3.65	117.81	122.92
29	6	606	CHL	C1D-CHD-C4C	-3.65	118.18	126.06
24	A	849	BCR	C23-C22-C21	3.65	124.54	118.94
29	9	609	CHL	C1D-CHD-C4C	-3.65	118.19	126.06
21	5	602	CLA	CMB-C2B-C1B	-3.65	122.86	128.46
21	B	835	CLA	CMB-C2B-C3B	3.65	131.50	124.68
29	2	601	CHL	C1D-CHD-C4C	-3.64	118.20	126.06
21	B	832	CLA	CMB-C2B-C3B	3.64	131.50	124.68
29	6	607	CHL	CHC-C1C-NC	3.64	129.73	124.20
24	J	104	BCR	C1-C6-C5	-3.64	117.48	122.61
21	a	604	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
29	1	302	CHL	C1D-CHD-C4C	-3.64	118.20	126.06
21	6	604	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
21	8	611	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
29	2	606	CHL	C4A-NA-C1A	-3.64	105.07	106.71
30	5	615	LUT	C10-C11-C12	3.64	134.57	123.22
21	9	613	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
29	b	306	CHL	CHC-C1C-NC	3.64	129.72	124.20
29	a	608	CHL	CHD-C4C-NC	3.63	129.93	124.20
21	3	408	CLA	CMB-C2B-C1B	-3.63	122.88	128.46
24	2	618	BCR	C36-C18-C17	-3.63	117.83	122.92
21	4	610	CLA	CMB-C2B-C1B	-3.63	122.88	128.46
31	7	416	XAT	C19-C9-C10	-3.63	117.84	122.92
29	c	607	CHL	CHC-C1C-NC	3.63	129.71	124.20
29	3	407	CHL	C1D-CHD-C4C	-3.63	118.23	126.06
21	A	816	CLA	CMB-C2B-C3B	3.63	131.47	124.68
29	b	309	CHL	C2C-C3C-C4C	-3.63	103.90	106.49
21	7	409	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
21	c	612	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
21	7	405	CLA	CAB-C3B-C4B	-3.62	122.89	128.46
21	3	409	CLA	CMD-C2D-C3D	-3.62	119.28	127.61
21	b	311	CLA	CMB-C2B-C3B	3.62	131.46	124.68
21	4	601	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
21	2	613	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
21	A	838	CLA	CMB-C2B-C3B	3.62	131.45	124.68
29	2	602	CHL	CHD-C4C-NC	3.62	129.91	124.20
21	2	609	CLA	CMB-C2B-C3B	3.62	131.45	124.68
30	2	616	LUT	C12-C13-C14	3.62	124.50	118.94
21	9	612	CLA	CMB-C2B-C1B	-3.62	122.91	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	4	605	CHL	CHD-C4C-NC	3.62	129.90	124.20
31	1	318	XAT	C15-C35-C34	3.62	130.88	123.47
29	1	307	CHL	CHD-C4C-NC	3.61	129.90	124.20
29	b	302	CHL	C2A-C1A-CHA	-3.61	117.54	123.86
30	2	616	LUT	C39-C29-C30	-3.61	117.86	122.92
21	3	409	CLA	CMB-C2B-C3B	3.61	131.43	124.68
29	a	606	CHL	C2C-C3C-C4C	-3.61	103.92	106.49
24	B	843	BCR	C7-C8-C9	-3.61	120.78	126.23
21	A	803	CLA	CMB-C2B-C3B	3.61	131.43	124.68
21	B	825	CLA	CMB-C2B-C3B	3.61	131.43	124.68
31	5	616	XAT	C35-C15-C14	3.61	130.86	123.47
21	5	608	CLA	CAB-C3B-C4B	-3.60	122.92	128.46
29	9	607	CHL	C1D-CHD-C4C	-3.60	118.28	126.06
30	c	615	LUT	C35-C15-C14	3.60	130.85	123.47
21	b	304	CLA	CMB-C2B-C1B	-3.60	122.93	128.46
24	J	103	BCR	C10-C11-C12	3.60	134.46	123.22
29	c	601	CHL	CHD-C4C-NC	3.60	129.88	124.20
29	6	607	CHL	C1D-CHD-C4C	-3.60	118.30	126.06
21	A	830	CLA	CMB-C2B-C1B	-3.60	122.94	128.46
21	F	305	CLA	CMB-C2B-C1B	-3.60	122.94	128.46
21	A	817	CLA	CMB-C2B-C1B	-3.60	122.94	128.46
24	7	418	BCR	C36-C18-C17	-3.60	117.89	122.92
21	8	608	CLA	CMB-C2B-C1B	-3.59	122.94	128.46
21	1	305	CLA	CMB-C2B-C1B	-3.59	122.94	128.46
29	9	605	CHL	C1D-CHD-C4C	-3.59	118.31	126.06
21	A	830	CLA	CMD-C2D-C3D	-3.59	119.35	127.61
29	c	606	CHL	C1D-CHD-C4C	-3.59	118.31	126.06
29	4	614	CHL	CHD-C4C-NC	3.59	129.86	124.20
29	b	309	CHL	CHD-C4C-NC	3.59	129.85	124.20
29	c	605	CHL	CHC-C1C-NC	3.58	129.64	124.20
21	5	613	CLA	CAB-C3B-C4B	-3.58	122.95	128.46
21	2	609	CLA	CMD-C2D-C3D	-3.58	119.37	127.61
30	6	616	LUT	C12-C13-C14	3.58	124.44	118.94
21	5	614	CLA	CAB-C3B-C4B	-3.58	122.96	128.46
29	9	601	CHL	C2C-C3C-C4C	-3.58	103.94	106.49
29	7	406	CHL	C1C-C2C-C3C	-3.58	103.19	106.96
21	c	602	CLA	CMB-C2B-C1B	-3.58	122.97	128.46
21	1	304	CLA	CMB-C2B-C3B	3.58	131.37	124.68
21	A	827	CLA	CMB-C2B-C3B	3.57	131.36	124.68
21	A	808	CLA	CMB-C2B-C3B	3.57	131.36	124.68
21	B	818	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
21	7	401	CLA	CMB-C2B-C1B	-3.56	122.98	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	829	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
29	8	607	CHL	C1D-CHD-C4C	-3.56	118.38	126.06
21	2	610	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
29	2	614	CHL	C1D-CHD-C4C	-3.56	118.38	126.06
21	a	612	CLA	CMB-C2B-C1B	-3.56	123.00	128.46
32	c	618	NEX	C40-C33-C34	-3.56	117.94	122.92
21	A	813	CLA	CMB-C2B-C3B	3.56	131.33	124.68
21	A	836	CLA	CMB-C2B-C1B	-3.55	123.00	128.46
21	A	831	CLA	O2D-CGD-O1D	-3.55	116.89	123.84
21	1	314	CLA	CAB-C3B-C4B	-3.55	123.00	128.46
30	9	614	LUT	C15-C35-C34	3.55	130.75	123.47
29	b	307	CHL	CHC-C1C-NC	3.55	129.59	124.20
24	L	306	BCR	C36-C18-C17	-3.55	117.95	122.92
29	4	614	CHL	C2C-C3C-C4C	-3.55	103.96	106.49
21	L	302	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
29	2	605	CHL	CHD-C4C-NC	3.55	129.79	124.20
21	8	609	CLA	CMD-C2D-C3D	-3.54	119.46	127.61
21	3	404	CLA	CAB-C3B-C4B	-3.54	123.02	128.46
29	7	406	CHL	CHC-C1C-NC	3.54	129.57	124.20
21	A	834	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
29	a	605	CHL	C2A-C1A-CHA	-3.54	117.67	123.86
29	c	607	CHL	C1D-CHD-C4C	-3.54	118.42	126.06
24	3	419	BCR	C35-C13-C14	-3.54	117.97	122.92
29	8	613	CHL	CHC-C1C-NC	3.54	129.57	124.20
29	a	608	CHL	C4A-NA-C1A	-3.53	105.12	106.71
21	7	413	CLA	CMB-C2B-C3B	3.53	131.29	124.68
30	4	615	LUT	C20-C13-C14	-3.53	117.97	122.92
21	B	820	CLA	CMB-C2B-C1B	-3.53	123.03	128.46
21	B	826	CLA	CMB-C2B-C3B	3.53	131.29	124.68
24	M	101	BCR	C36-C18-C17	-3.53	117.98	122.92
29	6	602	CHL	C2C-C3C-C4C	-3.53	103.97	106.49
24	7	418	BCR	C35-C13-C14	-3.53	117.98	122.92
21	1	315	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
29	6	605	CHL	C2C-C3C-C4C	-3.53	103.97	106.49
21	B	840	CLA	CMB-C2B-C3B	3.53	131.28	124.68
30	4	615	LUT	C40-C33-C34	-3.52	117.99	122.92
29	2	605	CHL	C1D-CHD-C4C	-3.52	118.46	126.06
29	a	601	CHL	C1D-CHD-C4C	-3.52	118.47	126.06
29	9	608	CHL	CHD-C4C-NC	3.52	129.75	124.20
21	A	830	CLA	C1-C2-C3	-3.52	119.96	126.04
21	8	604	CLA	CMB-C2B-C3B	3.52	131.26	124.68
21	B	810	CLA	CAB-C3B-C4B	-3.52	123.06	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	3	411	CLA	CMB-C2B-C1B	-3.52	123.06	128.46
21	B	806	CLA	CMB-C2B-C3B	3.52	131.25	124.68
24	J	103	BCR	C35-C13-C14	-3.52	118.00	122.92
29	8	605	CHL	CHD-C4C-NC	3.51	129.74	124.20
29	a	606	CHL	C2A-C1A-CHA	-3.51	117.72	123.86
32	b	318	NEX	C40-C33-C34	-3.51	118.00	122.92
29	b	302	CHL	C1D-CHD-C4C	-3.51	118.48	126.06
21	1	309	CLA	C1D-ND-C4D	-3.51	103.84	106.33
29	8	607	CHL	C1-C2-C3	-3.51	121.07	126.75
29	6	606	CHL	CHD-C4C-NC	3.51	129.73	124.20
21	A	840	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
29	8	605	CHL	C2C-C3C-C4C	-3.51	103.88	106.49
21	3	404	CLA	CMB-C2B-C1B	-3.51	123.08	128.46
21	a	613	CLA	CMB-C2B-C1B	-3.51	123.08	128.46
24	A	854	BCR	C36-C18-C17	-3.50	118.02	122.92
29	9	606	CHL	CHD-C4C-NC	3.50	129.72	124.20
21	A	828	CLA	CMB-C2B-C3B	3.50	131.23	124.68
21	B	838	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
24	O	205	BCR	C35-C13-C14	-3.50	118.02	122.92
29	9	608	CHL	C2C-C3C-C4C	-3.50	103.99	106.49
21	6	608	CLA	CMB-C2B-C1B	-3.50	123.09	128.46
24	6	618	BCR	C36-C18-C17	-3.50	118.03	122.92
21	9	604	CLA	CMB-C2B-C3B	3.50	131.22	124.68
21	1	316	CLA	CMB-C2B-C1B	-3.50	123.09	128.46
29	3	407	CHL	CHC-C1C-C2C	-3.49	117.06	126.72
29	b	310	CHL	C1D-CHD-C4C	-3.49	118.52	126.06
21	1	312	CLA	CMB-C2B-C1B	-3.49	123.09	128.46
24	7	417	BCR	C36-C18-C17	-3.49	118.03	122.92
29	a	606	CHL	C1D-CHD-C4C	-3.49	118.53	126.06
21	A	839	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
21	F	302	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
21	A	815	CLA	CMB-C2B-C3B	3.49	131.21	124.68
30	7	415	LUT	C10-C11-C12	3.49	134.10	123.22
30	c	616	LUT	C35-C15-C14	3.49	130.62	123.47
21	B	828	CLA	CMB-C2B-C3B	3.49	131.20	124.68
29	6	605	CHL	C1D-CHD-C4C	-3.48	118.54	126.06
29	8	607	CHL	CHD-C4C-NC	3.48	129.69	124.20
21	7	414	CLA	CMB-C2B-C3B	3.48	131.19	124.68
21	5	603	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
24	7	418	BCR	C23-C22-C21	3.48	124.28	118.94
21	8	602	CLA	CMB-C2B-C3B	3.48	131.19	124.68
24	7	417	BCR	C35-C13-C14	-3.48	118.05	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	2	612	CLA	CMB-C2B-C1B	-3.48	123.12	128.46
24	7	418	BCR	C19-C18-C17	3.48	124.28	118.94
24	O	205	BCR	C36-C18-C17	-3.48	118.05	122.92
21	3	401	CLA	CMB-C2B-C3B	3.48	131.18	124.68
21	4	612	CLA	CMB-C2B-C1B	-3.48	123.12	128.46
29	4	607	CHL	C4A-NA-C1A	-3.47	105.14	106.71
29	a	605	CHL	C1D-CHD-C4C	-3.47	118.56	126.06
21	B	815	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
21	B	801	CLA	C1-C2-C3	-3.47	120.04	126.04
21	B	833	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
29	1	307	CHL	C1-C2-C3	-3.47	121.14	126.75
21	A	842	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
21	A	830	CLA	O2D-CGD-O1D	-3.47	117.06	123.84
21	B	809	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
21	4	609	CLA	C1-C2-C3	-3.47	120.04	126.04
21	B	807	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
21	8	603	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
24	M	101	BCR	C12-C13-C14	3.47	124.26	118.94
21	A	821	CLA	CMB-C2B-C3B	3.47	131.16	124.68
21	B	824	CLA	CMB-C2B-C3B	3.46	131.16	124.68
29	9	605	CHL	C4A-NA-C1A	-3.46	105.15	106.71
21	A	825	CLA	CMB-C2B-C3B	3.46	131.16	124.68
24	3	419	BCR	C36-C18-C17	-3.46	118.07	122.92
21	F	304	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
29	a	609	CHL	CHD-C1D-C2D	3.46	132.74	125.48
24	F	303	BCR	C36-C18-C17	-3.46	118.07	122.92
21	A	809	CLA	CMB-C2B-C3B	3.46	131.15	124.68
21	3	409	CLA	C1D-ND-C4D	-3.46	103.88	106.33
21	2	603	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
21	8	609	CLA	CMB-C2B-C3B	3.46	131.15	124.68
31	8	615	XAT	C20-C13-C14	-3.46	118.08	122.92
29	8	613	CHL	CHD-C4C-NC	3.46	129.65	124.20
24	K	205	BCR	C24-C23-C22	-3.46	121.01	126.23
29	a	601	CHL	C2A-C1A-CHA	-3.46	117.81	123.86
21	6	613	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
30	5	615	LUT	C11-C10-C9	3.45	132.24	127.31
21	A	801	CLA	C6-C5-C3	-3.45	108.97	114.62
21	9	611	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
29	b	306	CHL	C1D-CHD-C4C	-3.45	118.61	126.06
30	1	317	LUT	C40-C33-C34	-3.45	118.09	122.92
29	9	609	CHL	C2C-C3C-C4C	-3.45	104.03	106.49
29	a	607	CHL	C2C-C3C-C4C	-3.45	104.03	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	9	617	NEX	C20-C13-C14	-3.45	118.09	122.92
29	9	601	CHL	CHD-C4C-NC	3.45	129.63	124.20
21	4	608	CLA	CMB-C2B-C3B	3.45	131.13	124.68
29	6	614	CHL	C1D-CHD-C4C	-3.45	118.62	126.06
29	b	306	CHL	C4A-NA-C1A	-3.44	105.16	106.71
24	B	843	BCR	C20-C21-C22	-3.44	122.40	127.31
21	3	410	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
29	4	606	CHL	CHD-C4C-NC	3.44	129.62	124.20
21	7	403	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
29	8	606	CHL	C1D-CHD-C4C	-3.44	118.64	126.06
30	5	615	LUT	C20-C13-C14	-3.44	118.11	122.92
29	2	607	CHL	OBD-CAD-C3D	-3.44	120.25	128.52
21	1	314	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
21	1	313	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
29	2	601	CHL	C2C-C3C-C4C	-3.43	104.04	106.49
30	a	615	LUT	C20-C13-C14	-3.43	118.12	122.92
21	8	612	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
29	a	606	CHL	CHD-C4C-NC	3.43	129.61	124.20
21	3	403	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
30	2	616	LUT	C8-C9-C10	3.43	124.20	118.94
21	8	601	CLA	CMB-C2B-C1B	-3.43	123.20	128.46
21	L	304	CLA	CMB-C2B-C3B	3.43	131.09	124.68
21	8	610	CLA	CMB-C2B-C1B	-3.42	123.20	128.46
24	7	418	BCR	C12-C13-C14	3.42	124.19	118.94
24	K	205	BCR	C15-C14-C13	-3.42	122.42	127.31
21	a	602	CLA	CMB-C2B-C3B	3.42	131.08	124.68
29	2	614	CHL	CHD-C4C-NC	3.42	129.59	124.20
29	6	607	CHL	C2C-C3C-C4C	-3.42	104.05	106.49
24	B	846	BCR	C15-C14-C13	-3.42	122.43	127.31
24	A	849	BCR	C36-C18-C17	-3.42	118.13	122.92
21	J	102	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
21	A	826	CLA	CMB-C2B-C3B	3.42	131.07	124.68
21	c	610	CLA	CMB-C2B-C3B	3.42	131.07	124.68
24	L	306	BCR	C23-C22-C21	3.42	124.18	118.94
24	J	101	BCR	C16-C15-C14	3.42	130.47	123.47
29	5	606	CHL	C1D-CHD-C4C	-3.42	118.69	126.06
21	4	609	CLA	CMB-C2B-C3B	3.42	131.07	124.68
21	3	414	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
29	6	605	CHL	CHD-C4C-NC	3.41	129.58	124.20
21	B	813	CLA	CMB-C2B-C3B	3.41	131.06	124.68
21	7	407	CLA	CMD-C2D-C3D	3.41	135.46	127.61
21	4	611	CLA	CMB-C2B-C3B	3.41	131.06	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	b	313	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
21	A	841	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
21	A	837	CLA	CMB-C2B-C1B	-3.41	123.23	128.46
21	7	412	CLA	CMB-C2B-C1B	-3.41	123.23	128.46
21	c	603	CLA	CMB-C2B-C3B	3.41	131.05	124.68
29	8	613	CHL	C1D-CHD-C4C	-3.41	118.71	126.06
30	a	615	LUT	C39-C29-C28	3.40	123.44	118.08
29	1	302	CHL	CHD-C4C-NC	3.40	129.57	124.20
21	5	608	CLA	CMB-C2B-C1B	-3.40	123.23	128.46
21	B	830	CLA	CMB-C2B-C3B	3.40	131.04	124.68
21	A	809	CLA	O2D-CGD-O1D	-3.40	117.19	123.84
29	2	607	CHL	C2C-C3C-C4C	-3.40	104.06	106.49
24	A	850	BCR	C16-C15-C14	3.40	130.44	123.47
21	3	413	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
21	5	605	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
29	2	601	CHL	CHD-C4C-NC	3.40	129.56	124.20
24	6	618	BCR	C35-C13-C14	-3.40	118.17	122.92
29	9	607	CHL	C2C-C3C-C4C	-3.40	104.07	106.49
21	1	311	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
21	5	610	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
21	a	603	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
21	a	614	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
21	2	611	CLA	CMB-C2B-C3B	3.40	131.03	124.68
21	4	602	CLA	CMB-C2B-C3B	3.40	131.03	124.68
21	6	611	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
29	a	601	CHL	C2C-C3C-C4C	-3.39	104.07	106.49
30	c	616	LUT	C15-C35-C34	3.39	130.42	123.47
24	B	843	BCR	C33-C5-C6	-3.39	120.72	124.53
21	a	611	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
30	1	317	LUT	C20-C13-C14	-3.39	118.18	122.92
21	5	607	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
24	J	104	BCR	C21-C20-C19	-3.38	112.66	123.22
21	A	820	CLA	CMB-C2B-C1B	-3.38	123.26	128.46
21	1	308	CLA	CMB-C2B-C1B	-3.38	123.26	128.46
24	3	419	BCR	C12-C13-C14	3.38	124.13	118.94
21	7	405	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
29	c	605	CHL	C1D-CHD-C4C	-3.38	118.76	126.06
29	6	601	CHL	CHC-C1C-C2C	-3.38	117.37	126.72
21	6	609	CLA	CMB-C2B-C3B	3.38	131.00	124.68
24	I	101	BCR	C16-C15-C14	3.38	130.40	123.47
21	A	801	CLA	C1-C2-C3	-3.38	120.20	126.04
29	a	607	CHL	CHD-C4C-NC	3.38	129.53	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	M	101	BCR	C23-C22-C21	3.38	124.12	118.94
24	L	301	BCR	C16-C15-C14	3.38	130.39	123.47
21	B	823	CLA	O2D-CGD-O1D	-3.38	117.24	123.84
24	L	301	BCR	C36-C18-C17	-3.38	118.19	122.92
24	J	101	BCR	C36-C18-C17	-3.37	118.20	122.92
29	c	606	CHL	CHD-C4C-NC	3.37	129.52	124.20
21	3	406	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
29	9	605	CHL	CHD-C4C-NC	3.37	129.52	124.20
30	8	614	LUT	C40-C33-C34	-3.37	118.20	122.92
31	c	617	XAT	C20-C13-C14	-3.37	118.20	122.92
21	A	814	CLA	CMB-C2B-C3B	3.37	130.99	124.68
24	A	846	BCR	C36-C18-C17	-3.37	118.20	122.92
24	L	306	BCR	C35-C13-C14	-3.37	118.20	122.92
21	b	314	CLA	CMB-C2B-C3B	3.37	130.98	124.68
21	B	807	CLA	O2D-CGD-O1D	-3.37	117.25	123.84
29	1	302	CHL	C1-C2-C3	-3.37	121.30	126.75
21	7	410	CLA	CMB-C2B-C1B	-3.37	123.29	128.46
21	c	604	CLA	CMB-C2B-C3B	3.36	130.97	124.68
24	M	101	BCR	C19-C18-C17	3.36	124.10	118.94
29	1	302	CHL	C2C-C3C-C4C	-3.36	104.09	106.49
29	9	609	CHL	CHD-C4C-NC	3.36	129.50	124.20
21	3	405	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
24	I	101	BCR	C35-C13-C14	-3.36	118.22	122.92
21	B	827	CLA	CMB-C2B-C3B	3.36	130.97	124.68
29	4	607	CHL	OBD-CAD-C3D	-3.36	120.43	128.52
29	5	606	CHL	CHD-C4C-NC	3.36	129.50	124.20
24	B	846	BCR	C24-C23-C22	-3.36	121.16	126.23
21	1	310	CLA	CMB-C2B-C3B	3.36	130.96	124.68
24	B	843	BCR	C3-C4-C5	-3.36	108.08	114.08
30	4	615	LUT	C32-C33-C34	3.35	124.09	118.94
21	B	837	CLA	CMB-C2B-C3B	3.35	130.95	124.68
21	5	611	CLA	CMB-C2B-C3B	3.35	130.95	124.68
24	8	616	BCR	C35-C13-C14	-3.35	118.23	122.92
21	c	611	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
21	4	613	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
30	1	317	LUT	C32-C33-C34	3.35	124.08	118.94
21	K	204	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
24	A	849	BCR	C16-C15-C14	3.35	130.33	123.47
21	A	830	CLA	CMB-C2B-C3B	3.35	130.94	124.68
31	9	616	XAT	C15-C35-C34	3.34	130.32	123.47
29	b	308	CHL	CHD-C4C-NC	3.34	129.47	124.20
31	6	617	XAT	C20-C13-C14	-3.34	118.25	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	b	306	CHL	CHD-C4C-NC	3.34	129.46	124.20
21	b	315	CLA	CMB-C2B-C1B	-3.33	123.34	128.46
24	L	306	BCR	C19-C18-C17	3.33	124.06	118.94
24	3	419	BCR	C19-C18-C17	3.33	124.06	118.94
29	6	602	CHL	C4A-NA-C1A	-3.33	105.21	106.71
21	B	808	CLA	CMB-C2B-C3B	3.33	130.91	124.68
21	O	201	CLA	CMB-C2B-C3B	3.33	130.91	124.68
21	6	612	CLA	CMB-C2B-C1B	-3.33	123.34	128.46
30	9	615	LUT	C40-C33-C34	-3.33	118.26	122.92
29	6	601	CHL	C4C-C3C-C2C	-3.33	104.02	107.07
24	8	616	BCR	C36-C18-C17	-3.33	118.26	122.92
29	7	406	CHL	CMC-C2C-C3C	-3.33	117.09	126.12
21	3	415	CLA	CMB-C2B-C3B	3.32	130.89	124.68
24	2	618	BCR	C35-C13-C14	-3.32	118.27	122.92
21	5	612	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
21	G	203	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
21	A	819	CLA	CMB-C2B-C3B	3.32	130.89	124.68
29	5	601	CHL	C4A-NA-C1A	-3.32	105.21	106.71
21	b	312	CLA	CMB-C2B-C1B	-3.32	123.37	128.46
21	B	801	CLA	C3B-C4B-NB	3.32	113.50	109.21
24	O	205	BCR	C23-C22-C21	3.32	124.03	118.94
29	c	601	CHL	C2C-C3C-C4C	-3.32	104.12	106.49
24	L	301	BCR	C35-C13-C14	-3.32	118.28	122.92
29	2	602	CHL	C6-C5-C3	-3.32	109.20	114.62
29	6	601	CHL	CHD-C4C-NC	3.31	129.43	124.20
21	6	603	CLA	CMB-C2B-C1B	-3.31	123.37	128.46
21	A	829	CLA	CMB-C2B-C3B	3.31	130.88	124.68
29	2	606	CHL	C2C-C3C-C4C	-3.31	104.13	106.49
29	9	609	CHL	C4A-NA-C1A	-3.31	105.22	106.71
32	c	618	NEX	C32-C33-C34	3.31	124.02	118.94
24	J	103	BCR	C34-C9-C10	-3.31	118.29	122.92
24	A	848	BCR	C36-C18-C17	-3.31	118.29	122.92
21	5	604	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
21	3	412	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
21	K	203	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
24	J	103	BCR	C36-C18-C17	-3.30	118.29	122.92
24	F	303	BCR	C19-C18-C17	3.30	124.01	118.94
30	a	616	LUT	C20-C13-C14	-3.30	118.30	122.92
21	A	834	CLA	O2D-CGD-O1D	-3.30	117.38	123.84
24	4	617	BCR	C16-C15-C14	3.30	130.24	123.47
32	b	318	NEX	C35-C15-C14	3.30	130.23	123.47
21	B	804	CLA	CMB-C2B-C1B	-3.30	123.39	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	847	BCR	C36-C18-C17	-3.30	118.30	122.92
32	c	618	NEX	C20-C13-C14	-3.30	118.30	122.92
21	7	411	CLA	CMB-C2B-C1B	-3.30	123.40	128.46
24	O	205	BCR	C12-C13-C14	3.30	124.00	118.94
30	4	615	LUT	C12-C13-C14	3.30	124.00	118.94
24	O	205	BCR	C19-C18-C17	3.29	124.00	118.94
21	5	613	CLA	CMB-C2B-C1B	-3.29	123.40	128.46
24	B	845	BCR	C36-C18-C17	-3.29	118.31	122.92
21	c	614	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
29	8	605	CHL	C4A-NA-C1A	-3.29	105.23	106.71
29	8	607	CHL	C4A-NA-C1A	-3.29	105.23	106.71
29	2	602	CHL	C2C-C3C-C4C	-3.29	104.14	106.49
21	1	303	CLA	CMB-C2B-C3B	3.29	130.83	124.68
29	8	606	CHL	C2C-C3C-C4C	-3.29	104.15	106.49
21	B	831	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
21	A	805	CLA	CMB-C2B-C3B	3.28	130.82	124.68
24	B	844	BCR	C16-C17-C18	-3.28	122.63	127.31
29	c	605	CHL	C2C-C3C-C4C	-3.28	104.15	106.49
24	A	854	BCR	C19-C18-C17	3.28	123.97	118.94
21	9	603	CLA	CMB-C2B-C1B	-3.28	123.43	128.46
31	7	416	XAT	C40-C33-C34	-3.28	118.33	122.92
32	b	318	NEX	C20-C13-C14	-3.27	118.34	122.92
21	A	839	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
29	c	601	CHL	C4A-NA-C1A	-3.27	105.23	106.71
21	2	604	CLA	CMB-C2B-C3B	3.27	130.80	124.68
24	A	846	BCR	C16-C15-C14	3.27	130.17	123.47
29	8	613	CHL	C4A-NA-C1A	-3.27	105.24	106.71
24	B	842	BCR	C16-C15-C14	3.27	130.17	123.47
21	A	807	CLA	O2D-CGD-O1D	-3.27	117.45	123.84
21	5	614	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
29	7	406	CHL	C1D-CHD-C4C	-3.27	119.01	126.06
29	7	406	CHL	C4A-NA-C1A	-3.26	105.24	106.71
21	G	202	CLA	CMB-C2B-C3B	3.26	130.78	124.68
23	4	619	LHG	O7-C7-C8	3.26	118.53	111.50
24	B	842	BCR	C35-C13-C14	-3.26	118.35	122.92
24	3	418	BCR	C36-C18-C17	-3.26	118.36	122.92
21	B	810	CLA	CMB-C2B-C1B	-3.26	123.45	128.46
30	7	415	LUT	C11-C10-C9	3.26	131.96	127.31
24	L	305	BCR	C36-C18-C17	-3.26	118.36	122.92
24	G	205	BCR	C36-C18-C17	-3.26	118.36	122.92
21	A	811	CLA	CMB-C2B-C3B	3.26	130.77	124.68
21	2	608	CLA	CMB-C2B-C3B	3.26	130.77	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	609	CHL	C1D-CHD-C4C	-3.26	119.03	126.06
29	c	608	CHL	CHD-C4C-NC	3.26	129.33	124.20
21	A	824	CLA	CMB-C2B-C1B	-3.26	123.46	128.46
24	3	418	BCR	C16-C15-C14	3.26	130.14	123.47
32	9	617	NEX	C40-C33-C34	-3.25	118.36	122.92
29	b	302	CHL	CHD-C4C-NC	3.25	129.33	124.20
24	I	101	BCR	C36-C18-C17	-3.25	118.37	122.92
24	3	418	BCR	C35-C13-C14	-3.25	118.37	122.92
21	K	201	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
29	b	310	CHL	CHD-C4C-NC	3.25	129.32	124.20
30	3	416	LUT	C40-C33-C34	-3.25	118.37	122.92
21	A	819	CLA	O2D-CGD-O1D	-3.25	117.49	123.84
21	4	603	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
21	2	609	CLA	C6-C5-C3	-3.24	109.31	114.62
29	8	606	CHL	CHD-C4C-NC	3.24	129.31	124.20
29	9	605	CHL	C2C-C3C-C4C	-3.24	104.18	106.49
21	6	609	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
31	7	416	XAT	C35-C15-C14	3.24	130.11	123.47
21	A	823	CLA	CMB-C2B-C1B	-3.24	123.49	128.46
24	J	104	BCR	C11-C10-C9	-3.24	122.69	127.31
24	6	618	BCR	C19-C18-C17	3.24	123.91	118.94
30	8	614	LUT	C12-C13-C14	3.24	123.91	118.94
29	6	614	CHL	C2C-C3C-C4C	-3.23	104.18	106.49
30	b	316	LUT	C40-C33-C34	-3.23	118.39	122.92
21	A	823	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
29	6	607	CHL	CHD-C4C-NC	3.23	129.29	124.20
21	K	202	CLA	O2D-CGD-O1D	-3.23	117.53	123.84
31	a	618	XAT	C40-C33-C34	-3.23	118.40	122.92
21	7	407	CLA	CMC-C2C-C3C	3.23	134.87	126.12
29	b	306	CHL	C2C-C3C-C4C	-3.23	104.19	106.49
21	A	831	CLA	CMB-C2B-C3B	3.23	130.71	124.68
21	B	817	CLA	CMB-C2B-C3B	3.23	130.71	124.68
21	A	818	CLA	O2D-CGD-O1D	-3.22	117.53	123.84
24	G	201	BCR	C36-C18-C17	-3.22	118.41	122.92
24	4	617	BCR	C36-C18-C17	-3.22	118.41	122.92
21	L	303	CLA	CMB-C2B-C3B	3.22	130.70	124.68
31	5	616	XAT	C20-C13-C14	-3.22	118.41	122.92
29	6	614	CHL	CHD-C4C-NC	3.22	129.28	124.20
24	2	618	BCR	C19-C18-C17	3.22	123.88	118.94
32	9	617	NEX	C15-C35-C34	3.22	130.06	123.47
30	8	614	LUT	C20-C13-C14	-3.22	118.42	122.92
21	7	402	CLA	CMB-C2B-C1B	-3.22	123.52	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	3	417	XAT	C40-C33-C34	-3.22	118.42	122.92
24	K	205	BCR	C38-C26-C27	3.21	119.79	113.62
24	A	846	BCR	C35-C13-C14	-3.21	118.42	122.92
21	A	807	CLA	CMB-C2B-C3B	3.21	130.69	124.68
24	3	419	BCR	C7-C8-C9	3.21	131.09	126.23
31	2	617	XAT	C35-C15-C14	3.21	130.05	123.47
29	6	607	CHL	C4A-NA-C1A	-3.21	105.26	106.71
24	B	843	BCR	C33-C5-C4	3.21	119.78	113.62
21	L	302	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
32	b	318	NEX	C32-C33-C34	3.21	123.86	118.94
21	B	816	CLA	CMB-C2B-C3B	3.21	130.68	124.68
29	c	607	CHL	C4A-NA-C1A	-3.21	105.27	106.71
31	4	616	XAT	C40-C33-C34	-3.20	118.43	122.92
24	K	205	BCR	C28-C27-C26	-3.20	108.36	114.08
24	J	103	BCR	C12-C13-C14	3.20	123.86	118.94
21	A	838	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
21	1	306	CLA	CMB-C2B-C3B	3.20	130.67	124.68
21	B	839	CLA	CMB-C2B-C1B	-3.20	123.55	128.46
29	a	605	CHL	C2C-C3C-C4C	-3.20	104.21	106.49
21	O	203	CLA	CMB-C2B-C3B	3.20	130.66	124.68
21	O	204	CLA	CMB-C2B-C3B	3.20	130.66	124.68
24	A	850	BCR	C35-C13-C14	-3.20	118.44	122.92
32	c	618	NEX	C35-C15-C14	3.20	130.02	123.47
29	7	406	CHL	CHD-C4C-NC	3.20	129.24	124.20
24	A	850	BCR	C36-C18-C17	-3.20	118.45	122.92
29	c	607	CHL	C2C-C3C-C4C	-3.20	104.21	106.49
21	B	806	CLA	O2D-CGD-O1D	-3.20	117.59	123.84
30	7	415	LUT	C40-C33-C34	-3.20	118.45	122.92
21	B	828	CLA	O2D-CGD-O1D	-3.19	117.59	123.84
31	2	617	XAT	C15-C35-C34	3.19	130.02	123.47
21	b	305	CLA	CMB-C2B-C3B	3.19	130.65	124.68
21	B	824	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
31	1	318	XAT	C40-C33-C34	-3.19	118.46	122.92
31	5	616	XAT	C15-C35-C34	3.18	130.00	123.47
21	A	801	CLA	CMD-C2D-C3D	-3.18	120.29	127.61
21	B	805	CLA	CMB-C2B-C3B	3.18	130.63	124.68
24	4	617	BCR	C35-C13-C14	-3.18	118.47	122.92
21	c	613	CLA	CMB-C2B-C3B	3.18	130.62	124.68
21	B	811	CLA	CMB-C2B-C3B	3.18	130.62	124.68
21	B	803	CLA	CMB-C2B-C3B	3.17	130.62	124.68
21	B	814	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
24	7	417	BCR	C12-C13-C14	3.17	123.81	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	825	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
29	9	607	CHL	CHD-C4C-NC	3.17	129.19	124.20
29	a	605	CHL	CHD-C4C-NC	3.17	129.19	124.20
21	B	819	CLA	CMB-C2B-C3B	3.17	130.60	124.68
24	G	201	BCR	C35-C13-C14	-3.17	118.49	122.92
21	B	821	CLA	CMB-C2B-C3B	3.16	130.60	124.68
21	L	303	CLA	O2D-CGD-O1D	-3.16	117.65	123.84
21	2	608	CLA	O2D-CGD-O1D	-3.16	117.65	123.84
29	c	607	CHL	CHD-C4C-NC	3.16	129.19	124.20
24	B	845	BCR	C35-C13-C14	-3.16	118.49	122.92
30	c	616	LUT	C40-C33-C34	-3.16	118.49	122.92
21	A	813	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
21	A	841	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
24	A	854	BCR	C35-C13-C14	-3.16	118.50	122.92
21	4	609	CLA	C6-C5-C3	-3.16	109.46	114.62
24	F	301	BCR	C36-C18-C17	-3.16	118.50	122.92
21	A	804	CLA	CMB-C2B-C3B	3.16	130.58	124.68
29	a	609	CHL	C2C-C3C-C4C	-3.16	104.24	106.49
30	b	317	LUT	C40-C33-C34	-3.15	118.50	122.92
24	A	849	BCR	C19-C18-C17	3.15	123.78	118.94
31	2	617	XAT	C40-C33-C34	-3.15	118.50	122.92
30	b	316	LUT	C20-C13-C14	-3.15	118.51	122.92
21	B	812	CLA	CMB-C2B-C3B	3.15	130.57	124.68
29	9	608	CHL	OBD-CAD-C3D	-3.15	120.94	128.52
21	A	805	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
30	c	616	LUT	C20-C13-C14	-3.15	118.52	122.92
21	O	202	CLA	CMB-C2B-C3B	3.15	130.56	124.68
31	c	617	XAT	C40-C33-C34	-3.15	118.52	122.92
21	A	826	CLA	O2D-CGD-O1D	-3.14	117.69	123.84
24	J	101	BCR	C35-C13-C14	-3.14	118.52	122.92
21	3	402	CLA	CMB-C2B-C3B	3.14	130.55	124.68
21	B	823	CLA	CMB-C2B-C3B	3.14	130.55	124.68
21	6	610	CLA	CMB-C2B-C3B	3.14	130.55	124.68
24	B	842	BCR	C36-C18-C17	-3.14	118.53	122.92
29	c	601	CHL	OBD-CAD-C3D	-3.14	120.97	128.52
21	B	814	CLA	CMB-C2B-C3B	3.14	130.55	124.68
21	K	202	CLA	CMB-C2B-C3B	3.14	130.54	124.68
30	a	615	LUT	C12-C13-C14	3.13	123.75	118.94
29	7	406	CHL	CHC-C1C-C2C	-3.13	118.05	126.72
29	5	606	CHL	OBD-CAD-C3D	-3.13	120.98	128.52
21	H	201	CLA	CMB-C2B-C1B	-3.13	123.65	128.46
30	6	616	LUT	C40-C33-C34	-3.13	118.54	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	806	CLA	CMB-C2B-C3B	3.13	130.53	124.68
21	a	610	CLA	CMB-C2B-C3B	3.13	130.53	124.68
21	4	610	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
21	A	822	CLA	CMB-C2B-C3B	3.13	130.53	124.68
29	2	601	CHL	C6-C5-C3	-3.13	109.51	114.62
21	B	839	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
21	B	817	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
30	5	615	LUT	C40-C33-C34	-3.12	118.55	122.92
29	8	613	CHL	OBD-CAD-C3D	-3.12	121.01	128.52
29	c	605	CHL	CHD-C4C-NC	3.12	129.12	124.20
21	B	810	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
21	2	609	CLA	C4-C3-C5	3.12	120.52	115.27
21	5	609	CLA	CMB-C2B-C3B	3.12	130.51	124.68
24	L	305	BCR	C16-C15-C14	3.12	129.86	123.47
21	7	408	CLA	CMB-C2B-C1B	-3.11	123.68	128.46
24	7	417	BCR	C19-C18-C17	3.11	123.72	118.94
21	B	802	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
31	9	616	XAT	C10-C11-C12	3.11	132.93	123.22
21	4	610	CLA	CMB-C2B-C3B	3.11	130.50	124.68
21	B	825	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
24	G	205	BCR	C35-C13-C14	-3.11	118.56	122.92
21	A	808	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
21	8	611	CLA	CMB-C2B-C3B	3.11	130.50	124.68
31	7	416	XAT	C7-C8-C9	3.11	130.35	125.53
31	7	416	XAT	C20-C13-C14	-3.11	118.57	122.92
21	A	833	CLA	CMB-C2B-C1B	-3.11	123.69	128.46
21	A	817	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
31	5	616	XAT	C40-C33-C34	-3.11	118.57	122.92
30	a	615	LUT	C40-C33-C34	-3.10	118.57	122.92
32	9	617	NEX	C12-C13-C14	3.10	123.70	118.94
21	B	821	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
24	K	205	BCR	C11-C10-C9	-3.10	122.88	127.31
21	A	824	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
21	B	833	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
29	6	606	CHL	C2C-C3C-C4C	-3.10	104.28	106.49
29	8	605	CHL	C1B-C2B-C3B	-3.10	104.03	106.92
21	7	401	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
30	8	614	LUT	C32-C33-C34	3.10	123.70	118.94
21	A	812	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
29	6	601	CHL	O2D-CGD-O1D	-3.10	117.78	123.84
24	J	104	BCR	C15-C14-C13	-3.10	122.89	127.31
21	B	832	CLA	O2D-CGD-O1D	-3.10	117.78	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	9	606	CHL	C2C-C3C-C4C	-3.09	104.28	106.49
21	B	816	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
21	A	828	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
21	G	204	CLA	CMB-C2B-C3B	3.09	130.46	124.68
21	B	836	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
24	A	854	BCR	C16-C15-C14	3.08	129.79	123.47
31	8	615	XAT	C12-C13-C14	3.08	123.67	118.94
21	2	612	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
29	1	307	CHL	C2C-C3C-C4C	-3.08	104.29	106.49
24	L	306	BCR	C12-C13-C14	3.08	123.67	118.94
21	B	831	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
31	c	617	XAT	C12-C13-C14	3.08	123.67	118.94
24	A	849	BCR	C35-C13-C14	-3.08	118.61	122.92
31	8	615	XAT	C40-C33-C34	-3.08	118.61	122.92
24	K	205	BCR	C33-C5-C6	-3.08	121.07	124.53
24	8	616	BCR	C12-C13-C14	3.08	123.67	118.94
24	L	305	BCR	C35-C13-C14	-3.08	118.61	122.92
24	6	618	BCR	C12-C13-C14	3.08	123.66	118.94
21	B	822	CLA	CMB-C2B-C3B	3.07	130.43	124.68
21	3	402	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
21	A	810	CLA	CMB-C2B-C3B	3.07	130.43	124.68
21	4	604	CLA	CMB-C2B-C3B	3.07	130.42	124.68
21	B	804	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
21	9	602	CLA	C1-C2-C3	-3.07	120.73	126.04
29	b	310	CHL	C2C-C3C-C4C	-3.07	104.30	106.49
21	9	602	CLA	CMB-C2B-C3B	3.07	130.42	124.68
30	9	615	LUT	C35-C15-C14	3.07	129.76	123.47
21	6	604	CLA	CMB-C2B-C3B	3.07	130.41	124.68
30	5	615	LUT	C19-C9-C10	-3.07	118.63	122.92
21	B	819	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
21	4	601	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
21	9	613	CLA	CMB-C2B-C3B	3.06	130.41	124.68
21	a	604	CLA	CMB-C2B-C3B	3.06	130.41	124.68
29	2	601	CHL	C4-C3-C5	3.06	120.42	115.27
21	A	801	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
24	B	844	BCR	C38-C26-C27	3.06	119.49	113.62
21	A	803	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
24	A	846	BCR	C19-C18-C17	3.06	123.63	118.94
21	B	801	CLA	O2A-CGA-CBA	3.06	121.50	111.91
29	a	608	CHL	OBD-CAD-C3D	-3.06	121.16	128.52
32	c	618	NEX	C19-C9-C10	-3.06	118.64	122.92
21	A	812	CLA	CMB-C2B-C3B	3.06	130.39	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	b	309	CHL	OBD-CAD-C3D	-3.05	121.17	128.52
21	6	611	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
29	c	606	CHL	C2C-C3C-C4C	-3.05	104.31	106.49
21	A	806	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
21	2	611	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
29	6	601	CHL	OBD-CAD-C3D	-3.05	121.17	128.52
21	A	820	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
21	8	608	CLA	CMB-C2B-C3B	3.05	130.39	124.68
21	B	812	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
24	K	205	BCR	C30-C25-C26	-3.05	118.32	122.61
21	5	602	CLA	CMB-C2B-C3B	3.05	130.38	124.68
21	1	306	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
24	J	101	BCR	C37-C22-C21	-3.05	118.65	122.92
30	1	317	LUT	C12-C13-C14	3.05	123.62	118.94
29	c	607	CHL	OBD-CAD-C3D	-3.05	121.19	128.52
21	b	303	CLA	CMB-C2B-C3B	3.04	130.38	124.68
21	7	409	CLA	CMB-C2B-C3B	3.04	130.37	124.68
21	A	833	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
21	7	404	CLA	CMB-C2B-C3B	3.04	130.37	124.68
29	a	608	CHL	C2C-C3C-C4C	-3.04	104.32	106.49
21	2	610	CLA	CMB-C2B-C3B	3.04	130.37	124.68
21	A	815	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
21	A	822	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
30	9	614	LUT	C40-C33-C34	-3.04	118.66	122.92
30	b	316	LUT	C35-C15-C14	3.04	129.70	123.47
21	B	826	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
29	b	310	CHL	OBD-CAD-C3D	-3.04	121.20	128.52
21	2	613	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
24	B	844	BCR	C30-C25-C26	-3.04	118.33	122.61
24	B	846	BCR	C16-C15-C14	-3.04	117.25	123.47
21	B	840	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
29	a	601	CHL	CHD-C4C-NC	3.04	128.99	124.20
21	O	201	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
24	G	205	BCR	C16-C15-C14	3.03	129.69	123.47
29	6	602	CHL	OBD-CAD-C3D	-3.03	121.22	128.52
21	3	408	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
29	6	607	CHL	C1-C2-C3	-3.03	121.85	126.75
30	c	615	LUT	C20-C13-C14	-3.03	118.68	122.92
21	4	609	CLA	C4-C3-C5	3.02	120.36	115.27
21	B	835	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
21	1	303	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
21	A	835	CLA	O2D-CGD-O1D	-3.02	117.93	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	1	305	CLA	CMB-C2B-C3B	3.02	130.33	124.68
21	K	204	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
21	1	305	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
21	F	305	CLA	CMB-C2B-C3B	3.02	130.32	124.68
21	5	603	CLA	CMB-C2B-C3B	3.02	130.32	124.68
29	c	608	CHL	OBD-CAD-C3D	-3.02	121.26	128.52
21	2	613	CLA	CMB-C2B-C3B	3.02	130.32	124.68
30	5	615	LUT	C12-C13-C14	3.02	123.57	118.94
31	2	617	XAT	C20-C13-C14	-3.02	118.70	122.92
21	B	805	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
21	A	817	CLA	CMB-C2B-C3B	3.01	130.31	124.68
29	5	606	CHL	C2C-C3C-C4C	-3.01	104.34	106.49
24	G	201	BCR	C16-C15-C14	3.01	129.64	123.47
29	8	607	CHL	OBD-CAD-C3D	-3.01	121.28	128.52
29	3	407	CHL	CBC-CAC-C3C	-3.01	104.13	112.43
21	B	830	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
21	c	614	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
21	K	203	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
30	a	616	LUT	C40-C33-C34	-3.01	118.71	122.92
24	J	103	BCR	C11-C10-C9	3.01	131.60	127.31
29	8	606	CHL	OBD-CAD-C3D	-3.00	121.29	128.52
29	3	407	CHL	CAA-C2A-C3A	-3.00	109.09	116.10
24	J	101	BCR	C19-C18-C17	3.00	123.55	118.94
29	7	406	CHL	CHD-C1D-C2D	3.00	131.77	125.48
21	B	801	CLA	CHD-C4C-NC	3.00	128.92	124.20
30	a	615	LUT	C15-C35-C34	2.99	129.60	123.47
21	8	618	CLA	CMB-C2B-C1B	-2.99	123.86	128.46
24	L	301	BCR	C12-C13-C14	2.99	123.53	118.94
29	b	307	CHL	OBD-CAD-C3D	-2.99	121.33	128.52
29	b	308	CHL	C4-C3-C5	2.99	120.30	115.27
29	a	609	CHL	CHD-C4C-NC	2.99	128.91	124.20
21	c	604	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
21	c	611	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
21	A	852	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
21	c	613	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
21	A	834	CLA	CMB-C2B-C3B	2.98	130.25	124.68
29	c	609	CHL	CHD-C4C-NC	2.98	128.90	124.20
30	b	317	LUT	C20-C13-C14	-2.98	118.75	122.92
21	A	816	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
24	A	850	BCR	C19-C18-C17	2.98	123.51	118.94
31	9	616	XAT	C7-C8-C9	2.98	130.15	125.53
21	A	830	CLA	C4-C3-C5	2.98	120.28	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	8	609	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
29	2	606	CHL	OBD-CAD-C3D	-2.98	121.36	128.52
30	9	615	LUT	C20-C13-C14	-2.98	118.75	122.92
31	6	617	XAT	C40-C33-C34	-2.98	118.75	122.92
24	B	845	BCR	C16-C15-C14	2.98	129.57	123.47
31	6	617	XAT	C32-C33-C34	2.97	123.51	118.94
24	2	618	BCR	C12-C13-C14	2.97	123.50	118.94
21	B	827	CLA	O2D-CGD-O1D	-2.97	118.02	123.84
21	G	202	CLA	O2D-CGD-O1D	-2.97	118.02	123.84
21	4	601	CLA	CMB-C2B-C3B	2.97	130.24	124.68
21	G	203	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
21	4	609	CLA	C4D-CHA-C1A	2.97	124.87	121.25
30	9	615	LUT	C32-C33-C34	2.97	123.50	118.94
21	L	302	CLA	CMB-C2B-C3B	2.97	130.24	124.68
21	1	309	CLA	C4D-CHA-C1A	2.97	124.86	121.25
29	2	602	CHL	OBD-CAD-C3D	-2.97	121.38	128.52
29	1	302	CHL	O2D-CGD-O1D	-2.97	118.03	123.84
24	A	848	BCR	C35-C13-C14	-2.97	118.77	122.92
21	9	611	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
21	b	312	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
30	a	616	LUT	C12-C13-C14	2.97	123.49	118.94
21	c	602	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
21	K	201	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
21	A	840	CLA	CMB-C2B-C3B	2.96	130.22	124.68
29	b	302	CHL	OBD-CAD-C3D	-2.96	121.39	128.52
21	1	304	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
21	b	304	CLA	CMB-C2B-C3B	2.96	130.22	124.68
21	A	804	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
30	5	615	LUT	C15-C35-C34	2.96	129.54	123.47
30	7	415	LUT	C19-C9-C10	-2.96	118.78	122.92
29	6	601	CHL	C2C-C1C-NC	2.96	112.74	109.97
21	A	814	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
29	2	614	CHL	C2C-C3C-C4C	-2.96	104.38	106.49
29	a	605	CHL	OBD-CAD-C3D	-2.96	121.41	128.52
21	B	818	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
21	A	821	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
21	4	611	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
31	7	416	XAT	C6-C7-C8	-2.95	119.75	125.99
24	7	417	BCR	C8-C9-C10	2.95	123.47	118.94
21	3	409	CLA	C4D-CHA-C1A	2.95	124.84	121.25
31	4	616	XAT	C20-C13-C14	-2.95	118.79	122.92
21	6	603	CLA	O2D-CGD-O1D	-2.95	118.07	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	813	CLA	CHB-C4A-NA	2.95	128.59	124.51
21	7	407	CLA	CHD-C4C-C3C	-2.95	120.51	124.84
21	c	602	CLA	CMB-C2B-C3B	2.95	130.19	124.68
29	4	605	CHL	C1B-C2B-C3B	-2.95	104.18	106.92
21	9	610	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
21	A	802	CLA	CMB-C2B-C3B	2.94	130.18	124.68
21	A	829	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
21	1	315	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
29	9	601	CHL	OBD-CAD-C3D	-2.94	121.44	128.52
21	2	603	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
21	2	611	CLA	CAA-C2A-C3A	-2.94	109.24	116.10
24	A	847	BCR	C35-C13-C14	-2.94	118.81	122.92
21	A	801	CLA	O2D-CGD-CBD	2.93	116.48	111.27
24	B	846	BCR	C11-C10-C9	-2.93	123.12	127.31
32	c	618	NEX	C12-C13-C14	2.93	123.44	118.94
24	7	418	BCR	C8-C9-C10	2.93	123.44	118.94
24	I	101	BCR	C12-C13-C14	2.93	123.44	118.94
21	B	801	CLA	CAA-C2A-C3A	-2.93	104.76	112.78
29	1	302	CHL	OBD-CAD-C3D	-2.93	121.47	128.52
29	9	605	CHL	OBD-CAD-C3D	-2.93	121.47	128.52
21	c	612	CLA	CMB-C2B-C3B	2.93	130.15	124.68
31	1	318	XAT	C35-C15-C14	2.92	129.46	123.47
21	a	612	CLA	CMB-C2B-C3B	2.92	130.15	124.68
21	A	842	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
21	7	407	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
21	A	830	CLA	C6-C5-C3	-2.92	109.85	114.62
21	8	612	CLA	CMB-C2B-C3B	2.92	130.13	124.68
21	A	802	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
21	7	401	CLA	CMB-C2B-C3B	2.91	130.13	124.68
24	L	301	BCR	C19-C18-C17	2.91	123.41	118.94
29	9	607	CHL	C4A-NA-C1A	-2.91	105.40	106.71
29	c	608	CHL	OMC-CMC-C2C	-2.91	119.10	125.69
29	4	606	CHL	OBD-CAD-C3D	-2.91	121.52	128.52
30	c	615	LUT	C40-C33-C34	-2.91	118.85	122.92
21	A	840	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
21	H	201	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
21	J	102	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
21	5	602	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
30	3	416	LUT	C20-C13-C14	-2.91	118.85	122.92
32	b	318	NEX	C19-C9-C10	-2.91	118.85	122.92
21	1	309	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
24	8	616	BCR	C19-C18-C17	2.90	123.40	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	1	316	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
21	F	305	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
21	a	603	CLA	CAA-C2A-C3A	-2.90	109.33	116.10
21	A	810	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
31	7	416	XAT	C19-C9-C8	2.90	122.65	118.08
31	4	616	XAT	C35-C15-C14	2.90	129.41	123.47
32	b	318	NEX	C12-C13-C14	2.90	123.39	118.94
21	a	614	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
29	b	306	CHL	OBD-CAD-C3D	-2.90	121.54	128.52
21	7	407	CLA	CMB-C2B-C1B	-2.90	124.01	128.46
21	B	829	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
21	4	612	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
24	B	843	BCR	C27-C26-C25	-2.90	118.53	122.73
21	1	309	CLA	CAC-C3C-C4C	2.90	128.57	124.81
21	A	811	CLA	O2D-CGD-O1D	-2.90	118.18	123.84
24	J	103	BCR	C19-C18-C17	2.90	123.38	118.94
21	4	613	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
30	2	616	LUT	C39-C29-C28	2.89	122.63	118.08
30	3	416	LUT	C32-C33-C34	2.89	123.38	118.94
31	1	318	XAT	C20-C13-C14	-2.89	118.88	122.92
29	2	601	CHL	OBD-CAD-C3D	-2.89	121.58	128.52
24	F	303	BCR	C16-C15-C14	2.88	129.38	123.47
21	5	604	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
30	9	614	LUT	C20-C13-C14	-2.88	118.89	122.92
21	6	604	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
24	B	843	BCR	C8-C7-C6	-2.88	119.11	127.20
29	8	605	CHL	OBD-CAD-C3D	-2.88	121.58	128.52
21	b	304	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
21	B	808	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
21	1	313	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
21	b	313	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
21	9	604	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
21	a	603	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
21	9	603	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
29	c	609	CHL	CHC-C1C-NC	2.87	128.56	124.20
24	B	844	BCR	C33-C5-C4	2.87	119.13	113.62
21	5	605	CLA	CMB-C2B-C3B	2.87	130.05	124.68
27	B	847	DGD	C2G-O2G-C1B	-2.87	110.73	117.79
29	6	607	CHL	OBD-CAD-C3D	-2.87	121.61	128.52
21	9	611	CLA	CMB-C2B-C3B	2.87	130.04	124.68
21	5	608	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
21	b	303	CLA	O2D-CGD-O1D	-2.87	118.23	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	7	402	CLA	CMB-C2B-C3B	2.87	130.04	124.68
21	6	608	CLA	CMB-C2B-C3B	2.87	130.04	124.68
21	A	801	CLA	C4-C3-C5	2.86	120.09	115.27
21	7	402	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
30	9	614	LUT	C35-C15-C14	2.86	129.34	123.47
29	8	605	CHL	OMC-CMC-C2C	-2.86	119.22	125.69
29	7	406	CHL	OBD-CAD-C3D	-2.86	121.63	128.52
21	3	403	CLA	CMB-C2B-C3B	2.86	130.03	124.68
29	c	606	CHL	OBD-CAD-C3D	-2.86	121.64	128.52
21	2	610	CLA	CBD-CHA-C1A	2.86	132.01	127.43
21	5	611	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
29	9	607	CHL	OBD-CAD-C3D	-2.86	121.65	128.52
31	6	617	XAT	C12-C13-C14	2.85	123.32	118.94
30	2	616	LUT	C40-C33-C34	-2.85	118.93	122.92
21	A	832	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
32	9	617	NEX	C32-C33-C34	2.85	123.32	118.94
24	B	842	BCR	C12-C13-C14	2.85	123.32	118.94
21	B	818	CLA	CMB-C2B-C3B	2.85	130.01	124.68
21	5	607	CLA	CMB-C2B-C3B	2.85	130.01	124.68
24	F	301	BCR	C35-C13-C14	-2.85	118.93	122.92
21	5	610	CLA	CAB-C3B-C2B	2.85	130.27	124.69
21	A	818	CLA	CMB-C2B-C3B	2.85	130.01	124.68
29	4	606	CHL	CAC-C3C-C4C	2.85	128.50	124.81
21	a	613	CLA	CMB-C2B-C3B	2.85	130.00	124.68
32	9	617	NEX	C19-C9-C10	-2.85	118.94	122.92
21	4	602	CLA	C1-C2-C3	-2.85	121.12	126.04
29	9	601	CHL	C4A-NA-C1A	-2.84	105.43	106.71
21	2	603	CLA	CMB-C2B-C3B	2.84	130.00	124.68
29	4	614	CHL	OMC-CMC-C2C	-2.84	119.26	125.69
29	c	605	CHL	OBD-CAD-C3D	-2.84	121.68	128.52
21	B	834	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
24	B	846	BCR	C33-C5-C4	2.84	119.08	113.62
29	6	602	CHL	CHD-C1D-ND	2.84	127.07	124.45
21	a	602	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
29	c	609	CHL	C2C-C3C-C4C	-2.84	104.38	106.49
29	2	614	CHL	OBD-CAD-C3D	-2.84	121.68	128.52
21	B	802	CLA	CMB-C2B-C3B	2.84	129.99	124.68
21	b	313	CLA	CMB-C2B-C3B	2.84	129.99	124.68
24	3	418	BCR	C12-C13-C14	2.84	123.30	118.94
29	4	614	CHL	OBD-CAD-C3D	-2.84	121.69	128.52
29	9	607	CHL	CHC-C1C-C2C	-2.84	115.82	126.11
24	A	848	BCR	C19-C18-C17	2.84	123.30	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	838	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
29	1	307	CHL	OBD-CAD-C3D	-2.84	121.69	128.52
21	1	313	CLA	CMB-C2B-C3B	2.84	129.98	124.68
29	5	601	CHL	C2C-C3C-C4C	-2.84	104.47	106.49
21	b	315	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
21	A	837	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
29	a	606	CHL	OBD-CAD-C3D	-2.83	121.70	128.52
21	4	604	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
21	B	803	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
24	B	845	BCR	C19-C18-C17	2.83	123.28	118.94
29	6	602	CHL	C1-C2-C3	-2.83	121.15	126.04
21	A	836	CLA	CMB-C2B-C3B	2.83	129.97	124.68
31	1	318	XAT	C19-C9-C8	2.83	122.53	118.08
21	1	315	CLA	CMB-C2B-C3B	2.83	129.97	124.68
21	7	410	CLA	CMB-C2B-C3B	2.83	129.97	124.68
24	G	205	BCR	C19-C18-C17	2.82	123.28	118.94
21	8	611	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
31	7	416	XAT	C32-C33-C34	2.82	123.27	118.94
29	b	308	CHL	C1-C2-C3	-2.82	121.16	126.04
29	c	609	CHL	C4A-NA-C1A	-2.82	105.44	106.71
24	A	849	BCR	C24-C23-C22	2.82	130.50	126.23
21	B	838	CLA	CMB-C2B-C3B	2.82	129.95	124.68
21	6	613	CLA	CMB-C2B-C3B	2.82	129.95	124.68
21	a	611	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
21	7	410	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
21	8	610	CLA	CMB-C2B-C3B	2.82	129.95	124.68
29	9	607	CHL	C3B-C4B-NB	2.82	112.85	109.21
29	6	606	CHL	OBD-CAD-C3D	-2.82	121.74	128.52
21	3	411	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
29	5	606	CHL	C4A-NA-C1A	-2.82	105.44	106.71
29	6	614	CHL	C4A-NA-C1A	-2.82	105.44	106.71
21	2	612	CLA	CMB-C2B-C3B	2.81	129.94	124.68
29	b	310	CHL	C4-C3-C5	2.81	120.00	115.27
24	L	305	BCR	C19-C18-C17	2.81	123.26	118.94
24	4	617	BCR	C19-C18-C17	2.81	123.26	118.94
29	b	308	CHL	OBD-CAD-C3D	-2.81	121.75	128.52
21	7	403	CLA	CAB-C3B-C2B	2.81	130.19	124.69
21	A	835	CLA	CHB-C4A-NA	2.81	128.40	124.51
21	6	610	CLA	CBD-CHA-C1A	2.81	131.93	127.43
21	3	410	CLA	CMB-C2B-C3B	2.81	129.94	124.68
29	a	609	CHL	OBD-CAD-C3D	-2.81	121.76	128.52
21	B	820	CLA	O2D-CGD-O1D	-2.81	118.34	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	a	611	CLA	CMB-C2B-C3B	2.81	129.93	124.68
21	8	612	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
21	5	605	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
21	B	820	CLA	CMB-C2B-C3B	2.81	129.93	124.68
29	6	614	CHL	OBD-CAD-C3D	-2.81	121.77	128.52
29	4	607	CHL	O2A-CGA-CBA	2.81	120.71	111.91
21	8	604	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
21	7	412	CLA	CAA-C2A-C3A	-2.80	109.56	116.10
21	B	833	CLA	CMB-C2B-C3B	2.80	129.92	124.68
21	c	612	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
21	a	610	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
21	9	612	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
21	4	612	CLA	CMB-C2B-C3B	2.80	129.91	124.68
29	b	302	CHL	C2C-C3C-C4C	-2.80	104.50	106.49
21	B	829	CLA	CMB-C2B-C3B	2.80	129.91	124.68
21	1	309	CLA	CMA-C3A-C2A	-2.80	109.58	116.10
21	B	837	CLA	O2D-CGD-O1D	-2.79	117.74	124.09
21	5	614	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
21	9	612	CLA	CMB-C2B-C3B	2.79	129.90	124.68
21	A	830	CLA	O2A-CGA-CBA	2.79	120.66	111.91
21	4	613	CLA	CMB-C2B-C3B	2.79	129.90	124.68
24	3	419	BCR	C23-C22-C21	2.79	123.22	118.94
24	I	101	BCR	C19-C18-C17	2.79	123.22	118.94
21	6	611	CLA	CMB-C2B-C3B	2.79	129.89	124.68
21	a	614	CLA	CMB-C2B-C3B	2.79	129.89	124.68
21	c	611	CLA	CMB-C2B-C3B	2.79	129.89	124.68
21	B	801	CLA	C4C-C3C-C2C	-2.78	102.84	106.90
21	2	604	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
21	A	842	CLA	CMB-C2B-C3B	2.78	129.89	124.68
21	F	302	CLA	CMB-C2B-C3B	2.78	129.89	124.68
30	b	316	LUT	C32-C33-C34	2.78	123.21	118.94
21	8	603	CLA	CMB-C2B-C3B	2.78	129.88	124.68
21	B	801	CLA	CMA-C3A-C4A	-2.78	104.30	111.77
29	6	605	CHL	OBD-CAD-C3D	-2.78	121.83	128.52
21	9	613	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
21	6	613	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
21	J	102	CLA	CMB-C2B-C3B	2.78	129.87	124.68
21	7	402	CLA	C1B-CHB-C4A	-2.78	124.62	130.12
21	6	609	CLA	CHB-C4A-NA	2.78	128.35	124.51
21	B	807	CLA	CMB-C2B-C3B	2.78	129.87	124.68
21	F	304	CLA	CMB-C2B-C3B	2.78	129.87	124.68
21	A	802	CLA	C1-C2-C3	-2.78	121.24	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	b	309	CHL	O2A-CGA-CBA	2.77	120.61	111.91
21	B	801	CLA	CHC-C1C-C2C	-2.77	119.05	126.72
27	B	847	DGD	O1G-C1A-C2A	2.77	120.61	111.91
21	b	305	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
29	6	602	CHL	OMC-CMC-C2C	-2.77	119.42	125.69
29	a	601	CHL	O2D-CGD-O1D	-2.77	118.42	123.84
21	3	409	CLA	C4-C3-C5	2.77	119.93	115.27
21	8	601	CLA	CMB-C2B-C3B	2.77	129.86	124.68
24	B	844	BCR	C33-C5-C6	-2.77	121.42	124.53
29	c	608	CHL	C4A-NA-C1A	-2.77	105.46	106.71
21	3	413	CLA	CMB-C2B-C3B	2.77	129.86	124.68
21	b	314	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
21	c	603	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
21	1	311	CLA	CAB-C3B-C2B	2.77	130.11	124.69
21	3	405	CLA	CMB-C2B-C3B	2.77	129.86	124.68
21	1	314	CLA	O2D-CGD-O1D	-2.77	117.80	124.09
29	a	609	CHL	C4A-NA-C1A	-2.77	105.46	106.71
29	6	605	CHL	CAC-C3C-C4C	2.77	128.40	124.81
21	K	203	CLA	CAB-C3B-C2B	2.76	130.10	124.69
21	b	311	CLA	O2D-CGD-O1D	-2.76	118.43	123.84
21	b	312	CLA	CMB-C2B-C3B	2.76	129.85	124.68
21	b	315	CLA	CMB-C2B-C3B	2.76	129.85	124.68
21	3	406	CLA	CAB-C3B-C2B	2.76	130.10	124.69
24	K	205	BCR	C27-C26-C25	-2.76	118.72	122.73
21	3	406	CLA	O2D-CGD-O1D	-2.76	117.82	124.09
24	A	847	BCR	C19-C18-C17	2.76	123.18	118.94
29	4	605	CHL	C2C-C3C-C4C	-2.76	104.44	106.49
31	3	417	XAT	C20-C13-C14	-2.76	119.06	122.92
21	A	827	CLA	O2D-CGD-O1D	-2.76	117.83	124.09
21	3	411	CLA	CMB-C2B-C3B	2.76	129.84	124.68
29	2	605	CHL	OBD-CAD-C3D	-2.75	121.89	128.52
21	a	613	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
21	B	823	CLA	CHB-C4A-NA	2.75	128.32	124.51
29	2	601	CHL	O2A-CGA-CBA	2.75	120.54	111.91
21	6	603	CLA	CMB-C2B-C3B	2.75	129.83	124.68
24	J	103	BCR	C8-C9-C10	2.75	123.16	118.94
24	G	201	BCR	C19-C18-C17	2.75	123.16	118.94
21	1	314	CLA	CMB-C2B-C3B	2.75	130.07	124.69
30	a	616	LUT	C15-C35-C34	2.75	129.10	123.47
31	4	616	XAT	C32-C33-C34	2.75	123.16	118.94
21	1	309	CLA	O1D-CGD-CBD	-2.75	118.86	124.48
21	7	407	CLA	C3C-C4C-NC	2.75	113.65	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	L	304	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
21	3	401	CLA	O2D-CGD-O1D	-2.75	117.86	124.09
21	B	809	CLA	CMB-C2B-C3B	2.75	129.81	124.68
21	B	815	CLA	CMB-C2B-C3B	2.74	129.81	124.68
21	a	603	CLA	CMB-C2B-C3B	2.74	129.81	124.68
21	3	415	CLA	O2D-CGD-O1D	-2.74	117.86	124.09
21	A	836	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
24	A	854	BCR	C23-C22-C21	2.74	123.15	118.94
29	9	606	CHL	CAC-C3C-C4C	2.74	128.37	124.81
21	A	819	CLA	C1B-CHB-C4A	-2.74	124.69	130.12
29	6	602	CHL	C6-C5-C3	-2.74	110.14	114.62
29	a	606	CHL	CAC-C3C-C4C	2.74	128.36	124.81
30	b	317	LUT	C35-C15-C14	2.74	129.09	123.47
21	1	316	CLA	CAB-C3B-C2B	2.74	130.05	124.69
21	K	204	CLA	CMB-C2B-C3B	2.74	129.80	124.68
29	2	614	CHL	OMC-CMC-C2C	-2.74	119.50	125.69
21	8	610	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
29	c	609	CHL	CHD-C1D-C2D	2.74	131.22	125.48
21	B	822	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
21	3	404	CLA	O2D-CGD-O1D	-2.73	117.88	124.09
21	c	610	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
21	1	316	CLA	CMB-C2B-C3B	2.73	130.04	124.69
21	7	407	CLA	CBC-CAC-C3C	2.73	119.96	112.43
21	9	602	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
29	a	606	CHL	O2D-CGD-O1D	-2.73	118.50	123.84
21	5	604	CLA	CMB-C2B-C3B	2.73	129.79	124.68
29	c	605	CHL	CHD-C1D-C2D	2.73	131.21	125.48
21	1	312	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
24	B	846	BCR	C38-C26-C25	-2.73	121.46	124.53
21	7	408	CLA	CMB-C2B-C3B	2.73	129.78	124.68
21	B	839	CLA	C1B-CHB-C4A	-2.73	124.72	130.12
21	A	801	CLA	C3A-C2A-C1A	2.73	105.42	101.34
24	G	201	BCR	C12-C13-C14	2.73	123.12	118.94
21	3	404	CLA	CAB-C3B-C2B	2.73	130.03	124.69
21	B	801	CLA	CMC-C2C-C1C	2.73	129.19	125.04
21	7	403	CLA	CMB-C2B-C3B	2.72	130.02	124.69
29	b	307	CHL	C2C-C3C-C4C	-2.72	104.55	106.49
21	A	828	CLA	C1B-CHB-C4A	-2.72	124.72	130.12
24	A	850	BCR	C12-C13-C14	2.72	123.12	118.94
31	a	618	XAT	C32-C33-C34	2.72	123.12	118.94
21	7	412	CLA	CMB-C2B-C3B	2.72	129.77	124.68
21	c	614	CLA	CMB-C2B-C3B	2.72	129.77	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	3	403	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
21	A	839	CLA	CMB-C2B-C3B	2.72	129.76	124.68
21	a	612	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
24	O	205	BCR	C8-C9-C10	2.71	123.11	118.94
24	B	844	BCR	C1-C6-C5	-2.71	118.79	122.61
24	F	303	BCR	C35-C13-C14	-2.71	119.12	122.92
21	8	618	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
21	A	824	CLA	CMB-C2B-C3B	2.71	129.75	124.68
21	7	411	CLA	CMB-C2B-C3B	2.71	129.75	124.68
29	2	602	CHL	O2A-CGA-CBA	2.71	120.42	111.91
29	c	601	CHL	CHC-C1C-C2C	-2.71	116.29	126.11
24	J	101	BCR	C12-C13-C14	2.71	123.10	118.94
21	A	803	CLA	C1B-CHB-C4A	-2.71	124.75	130.12
21	A	820	CLA	CMB-C2B-C3B	2.71	129.75	124.68
31	3	417	XAT	C32-C33-C34	2.71	123.10	118.94
24	K	205	BCR	C38-C26-C25	-2.71	121.49	124.53
29	b	308	CHL	CHC-C1C-C2C	-2.71	116.29	126.11
21	3	412	CLA	O2D-CGD-O1D	-2.71	117.94	124.09
31	4	616	XAT	C19-C9-C8	2.71	122.34	118.08
29	c	601	CHL	OMC-CMC-C2C	-2.71	119.57	125.69
24	B	846	BCR	C21-C20-C19	-2.70	114.78	123.22
21	6	612	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
21	5	610	CLA	CMB-C2B-C3B	2.70	129.98	124.69
21	B	809	CLA	O2D-CGD-O1D	-2.70	117.95	124.09
29	a	607	CHL	OBD-CAD-C3D	-2.70	122.01	128.52
21	F	304	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
21	5	608	CLA	CAB-C3B-C2B	2.70	129.98	124.69
29	1	302	CHL	O2A-CGA-CBA	2.70	120.39	111.91
21	3	414	CLA	CMB-C2B-C3B	2.70	129.73	124.68
24	A	847	BCR	C16-C15-C14	2.70	129.00	123.47
29	2	607	CHL	OMC-CMC-C2C	-2.70	119.59	125.69
30	6	616	LUT	C39-C29-C28	2.70	122.33	118.08
29	c	609	CHL	OBD-CAD-C3D	-2.70	122.03	128.52
21	7	405	CLA	CAB-C3B-C2B	2.70	129.97	124.69
29	b	310	CHL	C6-C5-C3	-2.69	110.21	114.62
21	B	837	CLA	C1B-CHB-C4A	-2.69	124.78	130.12
21	5	613	CLA	CAB-C3B-C2B	2.69	129.96	124.69
24	I	101	BCR	C8-C9-C10	2.69	123.07	118.94
21	5	612	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
24	A	846	BCR	C12-C13-C14	2.69	123.07	118.94
21	7	405	CLA	CMB-C2B-C3B	2.69	129.96	124.69
26	A	853	LMU	C1B-O1B-C4'	-2.69	111.31	117.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	5	608	CLA	CMB-C2B-C3B	2.69	129.95	124.69
21	5	603	CLA	C1B-CHB-C4A	-2.69	124.79	130.12
21	8	601	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
24	F	303	BCR	C34-C9-C8	2.69	122.31	118.08
29	a	608	CHL	CHC-C1C-C2C	-2.69	116.37	126.11
24	B	846	BCR	C20-C21-C22	-2.69	123.48	127.31
31	1	318	XAT	C32-C33-C34	2.69	123.06	118.94
21	B	811	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
29	8	607	CHL	O2A-CGA-CBA	2.69	120.33	111.91
24	B	844	BCR	C23-C24-C25	-2.68	119.67	127.20
29	9	609	CHL	CHC-C1C-C2C	-2.68	116.39	126.11
21	3	413	CLA	O2D-CGD-O1D	-2.68	118.00	124.09
21	5	603	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
21	A	852	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
21	9	603	CLA	CMB-C2B-C3B	2.68	129.69	124.68
21	1	314	CLA	CAB-C3B-C2B	2.68	129.94	124.69
29	a	607	CHL	CHC-C1C-C2C	-2.68	116.40	126.11
29	9	608	CHL	CHC-C1C-C2C	-2.68	116.40	126.11
29	4	614	CHL	CHC-C1C-C2C	-2.68	116.41	126.11
29	9	609	CHL	OBD-CAD-C3D	-2.68	122.08	128.52
21	K	202	CLA	CHB-C4A-NA	2.67	128.21	124.51
21	G	203	CLA	CMB-C2B-C3B	2.67	129.68	124.68
24	4	617	BCR	C12-C13-C14	2.67	123.05	118.94
29	b	309	CHL	CHC-C1C-C2C	-2.67	116.42	126.11
21	7	408	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
24	B	844	BCR	C27-C26-C25	-2.67	118.85	122.73
29	4	606	CHL	OMC-CMC-C2C	-2.67	119.65	125.69
29	c	606	CHL	C4A-NA-C1A	-2.67	105.51	106.71
29	a	601	CHL	OBD-CAD-C3D	-2.67	122.10	128.52
29	5	601	CHL	OMC-CMC-C2C	-2.67	119.66	125.69
31	c	617	XAT	C15-C35-C34	2.67	128.94	123.47
30	6	616	LUT	C8-C9-C10	2.67	123.03	118.94
21	6	608	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
21	B	813	CLA	O2D-CGD-O1D	-2.67	118.03	124.09
29	8	607	CHL	CHC-C1C-C2C	-2.67	116.44	126.11
31	c	617	XAT	C28-C29-C30	2.67	123.03	118.94
21	A	837	CLA	CMB-C2B-C3B	2.67	129.67	124.68
29	2	605	CHL	C2C-C3C-C4C	-2.67	104.59	106.49
24	B	845	BCR	C12-C13-C14	2.66	123.03	118.94
21	3	403	CLA	C1B-CHB-C4A	-2.66	124.84	130.12
24	A	848	BCR	C16-C15-C14	2.66	128.93	123.47
29	8	605	CHL	CHC-C1C-C2C	-2.66	116.45	126.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	J	104	BCR	C30-C25-C24	2.66	123.31	115.78
21	1	312	CLA	CMB-C2B-C3B	2.66	129.66	124.68
21	5	612	CLA	CMB-C2B-C3B	2.66	129.66	124.68
29	1	307	CHL	CHC-C1C-C2C	-2.66	116.46	126.11
29	4	606	CHL	CHC-C1C-C2C	-2.66	116.46	126.11
21	7	409	CLA	CAA-C2A-C3A	-2.66	109.89	116.10
21	1	308	CLA	O2D-CGD-O1D	-2.66	118.05	124.09
21	G	202	CLA	CHB-C4A-NA	2.66	128.19	124.51
21	A	823	CLA	CMB-C2B-C3B	2.66	129.66	124.68
29	6	605	CHL	OMC-CMC-C2C	-2.66	119.67	125.69
29	5	601	CHL	CHC-C1C-C2C	-2.66	116.47	126.11
21	c	614	CLA	C1B-CHB-C4A	-2.66	124.86	130.12
21	B	836	CLA	CHB-C4A-NA	2.66	128.19	124.51
29	4	605	CHL	CHC-C1C-C2C	-2.66	116.48	126.11
30	b	317	LUT	C32-C33-C34	2.65	123.01	118.94
29	4	607	CHL	C2C-C3C-C4C	-2.65	104.60	106.49
21	4	602	CLA	O2D-CGD-O1D	-2.65	118.07	124.09
21	1	308	CLA	CMB-C2B-C3B	2.65	129.64	124.68
26	3	420	LMU	C1B-O1B-C4'	-2.65	111.40	117.96
31	5	616	XAT	C12-C13-C14	2.65	123.01	118.94
21	B	829	CLA	C1B-CHB-C4A	-2.65	124.87	130.12
21	B	829	CLA	CHB-C4A-NA	2.65	128.18	124.51
21	2	611	CLA	CMA-C3A-C2A	-2.65	109.91	116.10
21	A	817	CLA	CHB-C4A-NA	2.65	128.18	124.51
21	5	614	CLA	CAB-C3B-C2B	2.65	129.88	124.69
24	J	104	BCR	C2-C3-C4	-2.65	105.46	111.38
24	F	303	BCR	C23-C22-C21	2.65	123.00	118.94
21	6	612	CLA	CMB-C2B-C3B	2.65	129.63	124.68
21	1	311	CLA	CMB-C2B-C3B	2.64	129.87	124.69
29	6	602	CHL	C4-C3-C5	2.64	119.72	115.27
21	3	406	CLA	CMB-C2B-C3B	2.64	129.86	124.69
21	3	401	CLA	CAA-C2A-C3A	-2.64	109.93	116.10
24	B	842	BCR	C19-C18-C17	2.64	123.00	118.94
29	b	310	CHL	CHC-C1C-C2C	-2.64	116.53	126.11
29	6	614	CHL	CHD-C1D-C2D	2.64	131.02	125.48
30	b	316	LUT	C12-C13-C14	2.64	122.99	118.94
30	5	615	LUT	C32-C33-C34	2.64	122.99	118.94
21	O	203	CLA	CBD-CHA-C1A	2.64	131.65	127.43
21	3	415	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
21	B	810	CLA	CAB-C3B-C2B	2.64	129.85	124.69
21	B	815	CLA	O2D-CGD-O1D	-2.63	118.11	124.09
29	2	606	CHL	O2D-CGD-O1D	-2.63	118.69	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	9	606	CHL	CHC-C1C-C2C	-2.63	116.56	126.11
21	1	311	CLA	O2D-CGD-O1D	-2.63	118.11	124.09
21	B	811	CLA	CHB-C4A-NA	2.63	128.15	124.51
21	K	203	CLA	CHB-C4A-NA	2.63	128.15	124.51
21	6	612	CLA	CHB-C4A-NA	2.63	128.15	124.51
21	A	841	CLA	CHB-C4A-NA	2.63	128.15	124.51
29	5	601	CHL	OBD-CAD-C3D	-2.63	122.19	128.52
21	1	309	CLA	CAA-C2A-C3A	-2.63	109.96	116.10
21	K	201	CLA	CMB-C2B-C3B	2.63	129.60	124.68
31	c	617	XAT	C32-C33-C34	2.63	122.97	118.94
29	2	601	CHL	CHC-C1C-C2C	-2.63	116.59	126.11
30	4	615	LUT	C8-C9-C10	2.63	122.97	118.94
31	6	617	XAT	C35-C15-C14	2.62	128.85	123.47
21	A	841	CLA	CMB-C2B-C3B	2.62	129.59	124.68
29	9	607	CHL	OMC-CMC-C2C	-2.62	119.76	125.69
21	1	308	CLA	CHB-C4A-NA	2.62	128.14	124.51
21	B	804	CLA	CHB-C4A-NA	2.62	128.14	124.51
24	B	843	BCR	C36-C18-C17	-2.62	119.25	122.92
21	B	802	CLA	C1B-CHB-C4A	-2.62	124.93	130.12
29	b	309	CHL	OMC-CMC-C2C	-2.62	119.76	125.69
31	2	617	XAT	C32-C33-C34	2.62	122.96	118.94
21	B	833	CLA	CHB-C4A-NA	2.62	128.13	124.51
21	9	603	CLA	CHB-C4A-NA	2.62	128.13	124.51
21	B	815	CLA	C1-C2-C3	-2.62	121.52	126.04
21	5	605	CLA	C1B-CHB-C4A	-2.61	124.94	130.12
21	B	834	CLA	CHB-C4A-NA	2.61	128.13	124.51
21	B	801	CLA	CBC-CAC-C3C	-2.61	105.23	112.43
21	3	414	CLA	CAA-C2A-C3A	-2.61	110.00	116.10
29	b	308	CHL	OMC-CMC-C2C	-2.61	119.78	125.69
29	6	602	CHL	O2D-CGD-O1D	-2.61	118.74	123.84
24	F	303	BCR	C15-C16-C17	2.61	128.81	123.47
21	K	203	CLA	CMB-C2B-C3B	2.61	129.79	124.69
21	3	405	CLA	O2D-CGD-O1D	-2.61	118.17	124.09
21	5	602	CLA	CHB-C4A-NA	2.61	128.12	124.51
29	2	606	CHL	CHC-C1C-C2C	-2.61	116.67	126.11
30	c	615	LUT	C15-C35-C34	2.61	128.81	123.47
29	6	605	CHL	CHC-C1C-C2C	-2.61	116.67	126.11
21	A	804	CLA	CHB-C4A-NA	2.60	128.11	124.51
21	B	816	CLA	CHB-C4A-NA	2.60	128.11	124.51
21	B	839	CLA	CMB-C2B-C3B	2.60	129.55	124.68
21	3	412	CLA	CMB-C2B-C3B	2.60	129.55	124.68
29	3	407	CHL	C3B-C4B-NB	2.60	112.58	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	854	BCR	C12-C13-C14	2.60	122.94	118.94
21	4	608	CLA	CHB-C4A-NA	2.60	128.11	124.51
29	a	607	CHL	O2D-CGD-O1D	-2.60	118.75	123.84
21	5	611	CLA	CHB-C4A-NA	2.60	128.11	124.51
21	6	604	CLA	C1B-CHB-C4A	-2.60	124.96	130.12
29	6	606	CHL	CHC-C1C-C2C	-2.60	116.68	126.11
24	A	850	BCR	C8-C9-C10	2.60	122.93	118.94
29	3	407	CHL	CMC-C2C-C1C	2.60	129.00	125.04
29	4	614	CHL	CAC-C3C-C4C	2.60	128.18	124.81
21	K	201	CLA	CHB-C4A-NA	2.60	128.10	124.51
29	b	309	CHL	C3B-C4B-NB	2.60	112.57	109.21
29	c	608	CHL	CHC-C1C-C2C	-2.60	116.69	126.11
21	B	825	CLA	CHB-C4A-NA	2.60	128.10	124.51
21	3	401	CLA	CHB-C4A-NA	2.60	128.10	124.51
21	3	408	CLA	CMB-C2B-C3B	2.59	129.53	124.68
29	8	613	CHL	C2C-C3C-C4C	-2.59	104.64	106.49
21	B	806	CLA	C1B-CHB-C4A	-2.59	124.98	130.12
21	8	618	CLA	CMB-C2B-C3B	2.59	129.53	124.68
29	2	614	CHL	CHC-C1C-C2C	-2.59	116.72	126.11
30	2	616	LUT	C10-C11-C12	2.59	131.30	123.22
30	7	415	LUT	C32-C33-C34	2.59	122.92	118.94
21	A	801	CLA	CGD-CBD-CAD	2.59	119.12	110.73
21	5	607	CLA	O2D-CGD-O1D	-2.59	118.21	124.09
21	7	401	CLA	CHB-C4A-NA	2.59	128.09	124.51
21	B	807	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
29	2	602	CHL	O2D-CGD-O1D	-2.59	118.78	123.84
29	2	602	CHL	OMC-CMC-C2C	-2.59	119.84	125.69
21	B	804	CLA	CMB-C2B-C3B	2.59	129.52	124.68
29	1	302	CHL	CHC-C1C-C2C	-2.59	116.73	126.11
21	A	840	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
29	4	606	CHL	C3B-C4B-NB	2.59	112.55	109.21
21	G	204	CLA	O2D-CGD-O1D	-2.59	118.22	124.09
29	8	607	CHL	C2C-C3C-C4C	-2.59	104.65	106.49
29	a	606	CHL	CHC-C1C-C2C	-2.58	116.74	126.11
21	5	613	CLA	CMB-C2B-C3B	2.58	129.75	124.69
29	1	302	CHL	C4A-NA-C1A	-2.58	105.55	106.71
31	8	615	XAT	C15-C35-C34	2.58	128.76	123.47
21	3	404	CLA	CMB-C2B-C3B	2.58	129.74	124.69
21	3	405	CLA	CHB-C4A-NA	2.58	128.08	124.51
24	3	419	BCR	C10-C11-C12	2.58	131.26	123.22
21	7	408	CLA	C1B-CHB-C4A	-2.58	125.01	130.12
21	H	201	CLA	CMB-C2B-C3B	2.58	129.50	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	3	418	BCR	C19-C18-C17	2.58	122.89	118.94
29	a	605	CHL	OMC-CMC-C2C	-2.58	119.86	125.69
21	B	814	CLA	CHB-C4A-NA	2.58	128.07	124.51
21	3	404	CLA	CHB-C4A-NA	2.58	128.07	124.51
21	1	309	CLA	CMD-C2D-C3D	-2.58	121.69	127.61
31	5	616	XAT	C32-C33-C34	2.58	122.89	118.94
21	5	609	CLA	O2D-CGD-O1D	-2.58	118.24	124.09
21	B	831	CLA	C1B-CHB-C4A	-2.57	125.02	130.12
21	4	603	CLA	O2D-CGD-O1D	-2.57	118.24	124.09
21	8	608	CLA	C1B-CHB-C4A	-2.57	125.02	130.12
21	B	810	CLA	CMB-C2B-C3B	2.57	129.73	124.69
29	2	606	CHL	OMC-CMC-C2C	-2.57	119.87	125.69
29	8	606	CHL	OMC-CMC-C2C	-2.57	119.87	125.69
21	B	834	CLA	C1B-CHB-C4A	-2.57	125.02	130.12
30	a	616	LUT	C39-C29-C28	2.57	122.13	118.08
21	2	611	CLA	CHB-C4A-NA	2.57	128.07	124.51
31	8	615	XAT	C32-C33-C34	2.57	122.89	118.94
21	b	311	CLA	C1B-CHB-C4A	-2.57	125.02	130.12
21	7	405	CLA	O2D-CGD-O1D	-2.57	118.25	124.09
21	a	604	CLA	O2D-CGD-O1D	-2.57	118.25	124.09
21	3	410	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
21	B	815	CLA	CHB-C4A-NA	2.57	128.06	124.51
21	b	304	CLA	CHB-C4A-NA	2.57	128.06	124.51
29	4	614	CHL	C3B-C4B-NB	2.57	112.53	109.21
21	1	306	CLA	CBD-CHA-C1A	2.57	131.53	128.50
29	2	607	CHL	C5-C3-C4	2.57	120.27	114.60
21	4	611	CLA	CHB-C4A-NA	2.57	128.06	124.51
21	F	305	CLA	CAA-C2A-C3A	-2.57	110.11	116.10
29	8	606	CHL	C4A-NA-C1A	-2.56	105.55	106.71
29	2	601	CHL	O2D-CGD-O1D	-2.56	118.82	123.84
29	1	307	CHL	O2D-CGD-O1D	-2.56	118.83	123.84
29	3	407	CHL	C2C-C1C-NC	2.56	112.37	109.97
29	8	607	CHL	OMC-CMC-C2C	-2.56	119.89	125.69
29	7	406	CHL	C2C-C1C-NC	2.56	112.37	109.97
21	O	202	CLA	O2D-CGD-O1D	-2.56	118.27	124.09
21	7	404	CLA	O2D-CGD-O1D	-2.56	118.27	124.09
29	c	601	CHL	C3B-C4B-NB	2.56	112.52	109.21
21	B	827	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
29	9	606	CHL	OBD-CAD-C3D	-2.56	122.35	128.52
21	4	602	CLA	CHB-C4A-NA	2.56	128.06	124.51
21	3	411	CLA	CHB-C4A-NA	2.56	128.05	124.51
29	b	302	CHL	OMC-CMC-C2C	-2.56	119.90	125.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	7	409	CLA	O2D-CGD-O1D	-2.56	118.28	124.09
31	6	617	XAT	C7-C8-C9	-2.56	121.56	125.53
24	F	301	BCR	C19-C18-C17	2.56	122.87	118.94
30	c	616	LUT	C32-C33-C34	2.56	122.87	118.94
29	a	608	CHL	C3B-C4B-NB	2.56	112.52	109.21
21	7	414	CLA	O2D-CGD-O1D	-2.56	118.28	124.09
24	B	844	BCR	C38-C26-C25	-2.56	121.66	124.53
21	5	610	CLA	O2D-CGD-O1D	-2.56	118.28	124.09
21	1	314	CLA	C1B-CHB-C4A	-2.56	125.06	130.12
21	1	310	CLA	O2D-CGD-O1D	-2.56	118.29	124.09
29	2	605	CHL	CHC-C1C-C2C	-2.56	116.85	126.11
30	9	615	LUT	C19-C9-C8	2.55	122.10	118.08
30	c	616	LUT	C12-C13-C14	2.55	122.86	118.94
29	4	605	CHL	OBD-CAD-C3D	-2.55	122.37	128.52
21	A	828	CLA	C1-C2-C3	-2.55	121.63	126.04
29	4	607	CHL	CHC-C1C-C2C	-2.55	116.85	126.11
21	7	412	CLA	O2D-CGD-O1D	-2.55	118.29	124.09
30	7	415	LUT	C1-C6-C5	-2.55	119.02	122.61
29	b	308	CHL	O2A-CGA-CBA	2.55	119.91	111.91
21	1	304	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
21	B	828	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
21	L	302	CLA	CHB-C4A-NA	2.55	128.04	124.51
24	A	849	BCR	C12-C13-C14	2.55	122.85	118.94
21	5	609	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
29	9	605	CHL	CHC-C1C-C2C	-2.55	116.87	126.11
24	7	418	BCR	C21-C20-C19	2.55	131.17	123.22
30	3	416	LUT	C8-C9-C10	2.55	122.85	118.94
21	2	603	CLA	C1B-CHB-C4A	-2.55	125.08	130.12
29	8	607	CHL	C3B-C4B-NB	2.55	112.50	109.21
29	8	607	CHL	CAC-C3C-C4C	2.54	128.11	124.81
29	1	307	CHL	O2A-CGA-CBA	2.54	119.89	111.91
29	1	302	CHL	OMC-CMC-C2C	-2.54	119.93	125.69
24	L	305	BCR	C12-C13-C14	2.54	122.85	118.94
21	5	614	CLA	CMB-C2B-C3B	2.54	129.67	124.69
21	B	821	CLA	CHB-C4A-NA	2.54	128.03	124.51
21	7	411	CLA	O2D-CGD-O1D	-2.54	118.32	124.09
29	a	609	CHL	OMC-CMC-C2C	-2.54	119.94	125.69
21	9	613	CLA	CHB-C4A-NA	2.54	128.03	124.51
21	A	812	CLA	C1B-CHB-C4A	-2.54	125.08	130.12
21	B	835	CLA	CHB-C4A-NA	2.54	128.02	124.51
21	F	304	CLA	CHB-C4A-NA	2.54	128.02	124.51
29	b	308	CHL	CAC-C3C-C4C	2.54	128.10	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	846	BCR	C4-C5-C6	-2.54	119.05	122.73
21	1	303	CLA	CHB-C4A-NA	2.54	128.02	124.51
21	A	802	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
21	A	840	CLA	C1-C2-C3	-2.54	121.66	126.04
21	4	603	CLA	CMB-C2B-C3B	2.54	129.42	124.68
21	b	315	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
31	8	615	XAT	C8-C9-C10	2.53	122.83	118.94
29	6	614	CHL	OMC-CMC-C2C	-2.53	119.96	125.69
21	B	817	CLA	CHB-C4A-NA	2.53	128.01	124.51
29	a	607	CHL	C3B-C4B-NB	2.53	112.48	109.21
31	7	416	XAT	C12-C13-C14	2.53	122.83	118.94
21	a	604	CLA	CHB-C4A-NA	2.53	128.01	124.51
29	c	608	CHL	C3B-C4B-NB	2.53	112.48	109.21
29	6	602	CHL	CHC-C1C-C2C	-2.53	116.94	126.11
21	7	403	CLA	O2D-CGD-O1D	-2.53	118.35	124.09
21	c	613	CLA	CHB-C4A-NA	2.53	128.01	124.51
29	6	607	CHL	O2A-CGA-CBA	2.53	119.84	111.91
29	6	606	CHL	C3B-C4B-NB	2.53	112.48	109.21
29	2	601	CHL	OMC-CMC-C2C	-2.53	119.97	125.69
29	2	605	CHL	CAC-C3C-C4C	2.53	128.09	124.81
30	9	614	LUT	C19-C9-C8	2.53	122.06	118.08
21	A	833	CLA	CMB-C2B-C3B	2.52	129.40	124.68
21	8	602	CLA	C1B-CHB-C4A	-2.52	125.12	130.12
29	9	608	CHL	OMC-CMC-C2C	-2.52	119.99	125.69
29	a	601	CHL	OMC-CMC-C2C	-2.52	119.99	125.69
29	1	302	CHL	C3B-C4B-NB	2.52	112.47	109.21
31	2	617	XAT	C19-C9-C8	2.52	122.05	118.08
21	7	404	CLA	CHB-C4A-NA	2.52	128.00	124.51
21	8	610	CLA	CHB-C4A-NA	2.52	128.00	124.51
21	7	407	CLA	O2D-CGD-O1D	-2.52	118.37	124.09
29	2	601	CHL	CAC-C3C-C4C	2.52	128.08	124.81
29	2	607	CHL	CHC-C1C-C2C	-2.52	116.99	126.11
21	B	805	CLA	CHB-C4A-NA	2.52	127.99	124.51
21	B	813	CLA	CHB-C4A-NA	2.52	127.99	124.51
21	A	814	CLA	CHB-C4A-NA	2.51	127.99	124.51
21	7	410	CLA	CHB-C4A-NA	2.51	127.99	124.51
21	B	817	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
29	c	609	CHL	OMC-CMC-C2C	-2.51	120.00	125.69
30	2	616	LUT	C31-C30-C29	2.51	130.90	127.31
21	1	315	CLA	CHB-C4A-NA	2.51	127.99	124.51
21	7	408	CLA	CHB-C4A-NA	2.51	127.99	124.51
21	b	313	CLA	CHB-C4A-NA	2.51	127.99	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	4	607	CHL	C5-C3-C4	2.51	120.16	114.60
24	G	205	BCR	C12-C13-C14	2.51	122.80	118.94
21	A	801	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
21	B	824	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
29	9	605	CHL	C3B-C4B-NB	2.51	112.46	109.21
29	b	308	CHL	C3B-C4B-NB	2.51	112.46	109.21
21	B	831	CLA	CMB-C2B-C3B	2.51	129.38	124.68
21	5	613	CLA	O2D-CGD-O1D	-2.51	118.39	124.09
21	4	601	CLA	CHB-C4A-NA	2.51	127.98	124.51
21	9	612	CLA	CHB-C4A-NA	2.51	127.98	124.51
21	a	612	CLA	CHB-C4A-NA	2.51	127.98	124.51
21	c	611	CLA	CHB-C4A-NA	2.51	127.98	124.51
21	4	608	CLA	C1B-CHB-C4A	-2.51	125.15	130.12
21	1	311	CLA	CAA-C2A-C3A	-2.51	110.24	116.10
29	3	407	CHL	C1C-C2C-C3C	-2.51	104.32	106.96
21	1	305	CLA	CHB-C4A-NA	2.51	127.98	124.51
21	A	801	CLA	O2A-CGA-CBA	2.51	119.78	111.91
29	4	605	CHL	O2D-CGD-O1D	-2.51	118.94	123.84
21	7	414	CLA	CAA-C2A-C3A	-2.51	110.25	116.10
29	2	602	CHL	C4-C3-C5	2.51	119.49	115.27
21	5	605	CLA	CBD-CHA-C1A	2.50	131.45	128.50
21	9	604	CLA	CHB-C4A-NA	2.50	127.97	124.51
21	8	602	CLA	CHB-C4A-NA	2.50	127.97	124.51
21	c	602	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
21	O	202	CLA	CBD-CHA-C1A	2.50	131.45	128.50
21	6	603	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
21	B	832	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
21	H	201	CLA	CHB-C4A-NA	2.50	127.97	124.51
21	A	831	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
21	A	840	CLA	CHB-C4A-NA	2.50	127.97	124.51
21	B	840	CLA	CHB-C4A-NA	2.50	127.97	124.51
21	5	607	CLA	CHB-C4A-NA	2.50	127.97	124.51
21	4	610	CLA	CHB-C4A-NA	2.50	127.97	124.51
29	5	601	CHL	C3B-C4B-NB	2.50	112.44	109.21
29	6	605	CHL	C3B-C4B-NB	2.50	112.44	109.21
29	2	601	CHL	C3B-C4B-NB	2.50	112.44	109.21
29	5	606	CHL	OMC-CMC-C2C	-2.50	120.04	125.69
21	2	608	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
21	9	602	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
21	3	402	CLA	CHB-C4A-NA	2.49	127.96	124.51
30	9	614	LUT	C39-C29-C28	2.49	122.01	118.08
21	A	833	CLA	C1B-CHB-C4A	-2.49	125.18	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	3	414	CLA	CHB-C4A-NA	2.49	127.96	124.51
29	9	601	CHL	CHD-C1D-ND	2.49	126.75	124.45
29	9	606	CHL	OMC-CMC-C2C	-2.49	120.05	125.69
21	7	405	CLA	CHB-C4A-NA	2.49	127.96	124.51
21	c	603	CLA	CHB-C4A-NA	2.49	127.96	124.51
21	1	309	CLA	CHB-C4A-NA	2.49	127.96	124.51
21	A	824	CLA	CHB-C4A-NA	2.49	127.96	124.51
30	6	616	LUT	C15-C35-C34	2.49	128.58	123.47
21	B	819	CLA	CHB-C4A-NA	2.49	127.96	124.51
21	5	613	CLA	CAA-C2A-C3A	-2.49	110.29	116.10
21	B	826	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
21	3	406	CLA	CHB-C4A-NA	2.49	127.95	124.51
21	6	611	CLA	CHB-C4A-NA	2.49	127.95	124.51
21	3	410	CLA	CAA-C2A-C3A	-2.49	110.29	116.10
24	F	303	BCR	C7-C8-C9	2.49	130.00	126.23
29	1	307	CHL	C3B-C4B-NB	2.49	112.43	109.21
29	9	605	CHL	OMC-CMC-C2C	-2.49	120.06	125.69
21	5	612	CLA	CHB-C4A-NA	2.49	127.95	124.51
29	1	307	CHL	OMC-CMC-C2C	-2.49	120.06	125.69
29	9	605	CHL	O2D-CGD-O1D	-2.49	118.97	123.84
21	O	203	CLA	CHB-C4A-NA	2.49	127.95	124.51
21	6	613	CLA	CHB-C4A-NA	2.49	127.95	124.51
21	7	407	CLA	CMB-C2B-C3B	2.49	129.33	124.68
21	c	612	CLA	CHB-C4A-NA	2.49	127.95	124.51
21	8	602	CLA	O2D-CGD-O1D	-2.49	118.45	124.09
21	A	837	CLA	CHB-C4A-NA	2.48	127.95	124.51
29	9	607	CHL	CAC-C3C-C4C	2.48	128.03	124.81
31	1	318	XAT	C7-C8-C9	2.48	129.38	125.53
21	A	816	CLA	CHB-C4A-NA	2.48	127.94	124.51
21	L	303	CLA	CHB-C4A-NA	2.48	127.94	124.51
21	A	829	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
21	A	809	CLA	CHB-C4A-NA	2.48	127.94	124.51
21	7	414	CLA	CHB-C4A-NA	2.48	127.94	124.51
21	a	602	CLA	CHB-C4A-NA	2.48	127.94	124.51
21	8	609	CLA	CHB-C4A-NA	2.48	127.94	124.51
21	7	411	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
29	c	607	CHL	OMC-CMC-C2C	-2.48	120.08	125.69
29	5	601	CHL	O2D-CGD-O1D	-2.48	118.99	123.84
29	9	609	CHL	C3B-C4B-NB	2.48	112.42	109.21
29	c	607	CHL	CHD-C1D-C2D	2.48	130.68	125.48
21	A	811	CLA	CHB-C4A-NA	2.48	127.94	124.51
21	8	601	CLA	CHB-C4A-NA	2.48	127.94	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	K	205	BCR	C23-C24-C25	-2.48	120.24	127.20
21	5	608	CLA	CAA-C2A-C3A	-2.48	110.32	116.10
29	a	606	CHL	OMC-CMC-C2C	-2.48	120.09	125.69
21	6	609	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
21	a	603	CLA	CHB-C4A-NA	2.48	127.94	124.51
21	A	808	CLA	CHB-C4A-NA	2.48	127.94	124.51
21	8	603	CLA	CHB-C4A-NA	2.48	127.94	124.51
29	2	607	CHL	O2A-CGA-CBA	2.47	119.67	111.91
29	a	609	CHL	CAC-C3C-C4C	2.47	128.02	124.81
30	6	616	LUT	C32-C33-C34	2.47	122.73	118.94
21	a	602	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
21	5	608	CLA	CHB-C4A-NA	2.47	127.93	124.51
29	a	601	CHL	CHD-C1D-C2D	2.47	130.66	125.48
29	2	602	CHL	CHC-C1C-C2C	-2.47	117.15	126.11
21	c	610	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
24	A	848	BCR	C34-C9-C8	2.47	121.97	118.08
29	8	607	CHL	C5-C3-C4	2.47	120.06	114.60
29	9	601	CHL	CHC-C1C-C2C	-2.47	117.16	126.11
21	A	821	CLA	CHB-C4A-NA	2.47	127.93	124.51
21	B	833	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
21	B	832	CLA	CHB-C4A-NA	2.47	127.93	124.51
21	2	610	CLA	CHB-C4A-NA	2.47	127.93	124.51
21	7	407	CLA	CHB-C4A-NA	2.47	127.93	124.51
24	B	843	BCR	C38-C26-C27	2.47	118.36	113.62
21	9	611	CLA	CHB-C4A-NA	2.47	127.92	124.51
21	B	814	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
30	9	614	LUT	C32-C33-C34	2.47	122.73	118.94
31	4	616	XAT	C6-C7-C8	-2.47	120.78	125.99
21	B	810	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
21	B	816	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
29	8	606	CHL	CHD-C1D-C2D	2.47	130.65	125.48
21	3	409	CLA	CHB-C4A-NA	2.47	127.92	124.51
21	8	603	CLA	O2D-CGD-O1D	-2.46	118.49	124.09
21	A	816	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
21	O	204	CLA	CHB-C4A-NA	2.46	127.92	124.51
21	2	611	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
21	B	810	CLA	CHB-C4A-NA	2.46	127.92	124.51
21	A	809	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
29	b	310	CHL	O2A-CGA-CBA	2.46	119.64	111.91
29	b	302	CHL	CHC-C1C-C2C	-2.46	117.18	126.11
21	4	609	CLA	CHB-C4A-NA	2.46	127.92	124.51
21	J	102	CLA	CHB-C4A-NA	2.46	127.92	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	1	313	CLA	CHB-C4A-NA	2.46	127.92	124.51
29	9	609	CHL	OMC-CMC-C2C	-2.46	120.12	125.69
29	c	606	CHL	CHC-C1C-C2C	-2.46	117.19	126.11
21	G	203	CLA	CHB-C4A-NA	2.46	127.92	124.51
21	2	608	CLA	CHB-C4A-NA	2.46	127.92	124.51
21	a	613	CLA	CHB-C4A-NA	2.46	127.92	124.51
29	b	306	CHL	OMC-CMC-C2C	-2.46	120.13	125.69
21	B	808	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
21	A	835	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
24	B	843	BCR	C1-C6-C7	2.46	122.73	115.78
21	5	614	CLA	CHB-C4A-NA	2.46	127.91	124.51
30	a	615	LUT	C32-C33-C34	2.46	122.71	118.94
21	5	610	CLA	CHB-C4A-NA	2.46	127.91	124.51
29	6	602	CHL	O2A-CGA-CBA	2.46	119.62	111.91
21	5	610	CLA	CAA-C2A-C3A	-2.46	110.36	116.10
30	c	616	LUT	C19-C9-C8	2.46	121.95	118.08
29	a	601	CHL	CHC-C1C-C2C	-2.46	117.20	126.11
21	1	311	CLA	CHB-C4A-NA	2.46	127.91	124.51
24	B	843	BCR	C11-C12-C13	-2.46	119.52	126.42
21	8	618	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
21	A	806	CLA	CHB-C4A-NA	2.46	127.91	124.51
21	8	604	CLA	CHB-C4A-NA	2.45	127.90	124.51
21	8	612	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
21	B	821	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
21	5	613	CLA	CHB-C4A-NA	2.45	127.90	124.51
21	c	604	CLA	CHB-C4A-NA	2.45	127.90	124.51
24	L	306	BCR	C8-C9-C10	2.45	122.70	118.94
29	4	607	CHL	OMC-CMC-C2C	-2.45	120.15	125.69
21	A	825	CLA	CHB-C4A-NA	2.45	127.90	124.51
21	1	312	CLA	CHB-C4A-NA	2.45	127.90	124.51
21	2	613	CLA	CHB-C4A-NA	2.45	127.90	124.51
21	5	604	CLA	CHB-C4A-NA	2.45	127.90	124.51
21	b	305	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
30	b	317	LUT	C39-C29-C28	2.45	121.93	118.08
21	A	830	CLA	CHB-C4A-NA	2.45	127.90	124.51
21	F	305	CLA	CHB-C4A-NA	2.45	127.90	124.51
21	8	611	CLA	CHB-C4A-NA	2.45	127.89	124.51
30	c	615	LUT	C12-C13-C14	2.45	122.69	118.94
21	A	807	CLA	CHB-C4A-NA	2.45	127.89	124.51
21	3	408	CLA	CHB-C4A-NA	2.45	127.89	124.51
21	1	316	CLA	CHB-C4A-NA	2.44	127.89	124.51
21	A	821	CLA	C1B-CHB-C4A	-2.44	125.28	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	b	305	CLA	CHB-C4A-NA	2.44	127.89	124.51
21	4	612	CLA	CHB-C4A-NA	2.44	127.89	124.51
21	8	608	CLA	CHB-C4A-NA	2.44	127.89	124.51
21	6	611	CLA	CAA-C2A-C3A	-2.44	110.41	116.10
29	6	605	CHL	O2D-CGD-O1D	-2.44	119.07	123.84
29	c	606	CHL	OMC-CMC-C2C	-2.44	120.17	125.69
21	B	818	CLA	CHB-C4A-NA	2.44	127.88	124.51
21	K	204	CLA	CHB-C4A-NA	2.44	127.88	124.51
21	b	314	CLA	CHB-C4A-NA	2.44	127.88	124.51
21	B	815	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
24	J	104	BCR	C16-C15-C14	-2.44	118.48	123.47
21	A	820	CLA	CHB-C4A-NA	2.44	127.88	124.51
21	6	612	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
21	B	832	CLA	CAA-C2A-C3A	-2.43	106.11	112.78
21	a	611	CLA	CHB-C4A-NA	2.43	127.88	124.51
29	6	607	CHL	OMC-CMC-C2C	-2.43	120.18	125.69
29	a	608	CHL	OMC-CMC-C2C	-2.43	120.19	125.69
21	7	409	CLA	CHB-C4A-NA	2.43	127.88	124.51
21	a	610	CLA	CHB-C4A-NA	2.43	127.88	124.51
29	9	606	CHL	C3B-C4B-NB	2.43	112.36	109.21
29	9	608	CHL	C3B-C4B-NB	2.43	112.36	109.21
29	2	601	CHL	C1-C2-C3	-2.43	121.84	126.04
29	b	307	CHL	CHC-C1C-C2C	-2.43	117.29	126.11
21	2	609	CLA	CHB-C4A-NA	2.43	127.88	124.51
21	A	827	CLA	CHB-C4A-NA	2.43	127.87	124.51
29	4	605	CHL	OMC-CMC-C2C	-2.43	120.19	125.69
21	1	310	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
21	B	831	CLA	O2A-CGA-O1A	-2.43	117.46	123.59
21	A	826	CLA	CHB-C4A-NA	2.43	127.87	124.51
29	9	601	CHL	OMC-CMC-C2C	-2.43	120.20	125.69
21	3	409	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
21	A	842	CLA	CHB-C4A-NA	2.43	127.87	124.51
21	B	839	CLA	CHB-C4A-NA	2.43	127.87	124.51
29	2	606	CHL	C3B-C4B-NB	2.42	112.34	109.21
21	B	830	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
31	3	417	XAT	C19-C9-C8	2.42	121.90	118.08
21	B	835	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
21	L	304	CLA	CHB-C4A-NA	2.42	127.86	124.51
21	7	413	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
21	B	822	CLA	CHB-C4A-NA	2.42	127.86	124.51
29	b	306	CHL	CHC-C1C-C2C	-2.42	117.33	126.11
29	8	605	CHL	O2D-CGD-O1D	-2.42	119.10	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	b	308	CHL	O2D-CGD-O1D	-2.42	119.11	123.84
24	A	849	BCR	C34-C9-C8	2.42	121.89	118.08
21	A	838	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
30	b	317	LUT	C19-C9-C8	2.42	121.89	118.08
24	K	205	BCR	C33-C5-C4	2.42	118.26	113.62
21	A	801	CLA	C2A-C1A-CHA	2.42	128.09	123.86
21	A	805	CLA	CHB-C4A-NA	2.42	127.85	124.51
21	A	826	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
21	A	811	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
29	a	607	CHL	OMC-CMC-C2C	-2.42	120.22	125.69
29	5	606	CHL	CHC-C1C-C2C	-2.42	117.35	126.11
29	c	607	CHL	O2D-CGD-O1D	-2.42	119.12	123.84
21	A	819	CLA	CHB-C4A-NA	2.41	127.85	124.51
31	2	617	XAT	C6-C7-C8	-2.41	120.89	125.99
29	6	614	CHL	CHC-C1C-C2C	-2.41	117.36	126.11
21	A	839	CLA	CHB-C4A-NA	2.41	127.85	124.51
21	A	834	CLA	CHB-C4A-NA	2.41	127.85	124.51
21	7	401	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
21	7	405	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
21	3	413	CLA	CAA-C2A-C3A	-2.41	110.47	116.10
21	7	403	CLA	CHB-C4A-NA	2.41	127.84	124.51
21	b	312	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
29	b	307	CHL	O2D-CGD-O1D	-2.41	119.13	123.84
21	A	836	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
21	5	607	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
24	B	843	BCR	C21-C20-C19	-2.41	115.70	123.22
29	a	606	CHL	C3B-C4B-NB	2.41	112.32	109.21
21	9	611	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
21	F	302	CLA	CHB-C4A-NA	2.41	127.84	124.51
21	O	201	CLA	CHB-C4A-NA	2.41	127.84	124.51
21	3	412	CLA	CHB-C4A-NA	2.41	127.84	124.51
29	6	607	CHL	CHC-C1C-C2C	-2.40	117.40	126.11
21	B	826	CLA	CHB-C4A-NA	2.40	127.83	124.51
21	7	413	CLA	CHB-C4A-NA	2.40	127.83	124.51
21	c	602	CLA	CHB-C4A-NA	2.40	127.83	124.51
30	8	614	LUT	C39-C29-C28	2.40	121.86	118.08
21	c	611	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
21	B	804	CLA	O2A-CGA-O1A	-2.40	117.54	123.59
21	9	603	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
21	B	824	CLA	CHB-C4A-NA	2.40	127.83	124.51
21	6	610	CLA	CHB-C4A-NA	2.40	127.83	124.51
30	9	614	LUT	C7-C8-C9	2.40	129.86	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	G	203	CLA	C1-C2-C3	-2.40	122.87	126.75
30	1	317	LUT	C8-C9-C10	2.40	122.62	118.94
21	A	810	CLA	CHB-C4A-NA	2.40	127.83	124.51
29	b	310	CHL	C3B-C4B-NB	2.40	112.31	109.21
21	B	803	CLA	CHB-C4A-NA	2.40	127.82	124.51
21	b	312	CLA	CHB-C4A-NA	2.40	127.82	124.51
29	5	606	CHL	O2D-CGD-O1D	-2.39	119.16	123.84
21	a	604	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
21	O	202	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
21	8	611	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
21	B	831	CLA	CHB-C4A-NA	2.39	127.82	124.51
21	4	609	CLA	O2A-CGA-CBA	2.39	119.42	111.91
29	a	605	CHL	CHC-C1C-C2C	-2.39	117.44	126.11
29	c	605	CHL	OMC-CMC-C2C	-2.39	120.28	125.69
21	4	613	CLA	CHB-C4A-NA	2.39	127.82	124.51
29	2	602	CHL	C3B-C4B-NB	2.39	112.30	109.21
21	B	809	CLA	CHB-C4A-NA	2.39	127.82	124.51
21	A	815	CLA	CHB-C4A-NA	2.39	127.82	124.51
21	B	838	CLA	CHB-C4A-NA	2.39	127.82	124.51
21	7	411	CLA	CHB-C4A-NA	2.39	127.82	124.51
30	c	615	LUT	C39-C29-C28	2.39	121.84	118.08
21	1	310	CLA	CHB-C4A-NA	2.39	127.81	124.51
29	b	310	CHL	OMC-CMC-C2C	-2.39	120.29	125.69
21	3	415	CLA	CAA-C2A-C3A	-2.39	110.53	116.10
30	a	616	LUT	C32-C33-C34	2.39	122.60	118.94
24	J	104	BCR	C34-C9-C8	2.39	121.83	118.08
29	a	607	CHL	CAC-C3C-C4C	2.38	127.90	124.81
21	3	411	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
21	B	820	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
21	5	611	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
21	7	403	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
21	a	603	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
21	B	823	CLA	O2D-CGD-CBD	2.38	115.50	111.27
26	A	856	LMU	C1B-O1B-C4'	-2.38	112.07	117.96
21	A	813	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
21	1	304	CLA	CHB-C4A-NA	2.38	127.80	124.51
21	A	838	CLA	CHB-C4A-NA	2.38	127.80	124.51
21	2	612	CLA	CHB-C4A-NA	2.38	127.80	124.51
21	A	828	CLA	O2A-CGA-O1A	-2.38	117.59	123.59
21	c	604	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
21	4	609	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
21	A	831	CLA	O2D-CGD-CBD	2.38	115.49	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	c	607	CHL	CHC-C1C-C2C	-2.38	117.49	126.11
21	B	832	CLA	O2A-CGA-O1A	-2.38	117.59	123.59
21	A	804	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
21	A	822	CLA	CHB-C4A-NA	2.38	127.80	124.51
21	a	614	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
24	B	843	BCR	C30-C25-C26	-2.38	119.27	122.61
24	B	846	BCR	C33-C5-C6	-2.38	121.86	124.53
21	a	614	CLA	CHB-C4A-NA	2.38	127.80	124.51
29	2	614	CHL	CAC-C3C-C4C	2.38	127.89	124.81
21	3	415	CLA	CHB-C4A-NA	2.37	127.80	124.51
21	A	839	CLA	C1B-CHB-C4A	-2.37	125.41	130.12
29	4	606	CHL	O2D-CGD-O1D	-2.37	119.20	123.84
29	2	605	CHL	C3B-C4B-NB	2.37	112.28	109.21
21	G	204	CLA	CHB-C4A-NA	2.37	127.79	124.51
21	3	413	CLA	CHB-C4A-NA	2.37	127.79	124.51
29	b	309	CHL	CAC-C3C-C4C	2.37	127.89	124.81
21	3	404	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
21	7	402	CLA	C2A-C1A-CHA	2.37	128.01	123.86
29	b	302	CHL	O2D-CGD-O1D	-2.37	119.20	123.84
29	b	310	CHL	CAC-C3C-C4C	2.37	127.89	124.81
21	1	314	CLA	CAA-C2A-C3A	-2.37	110.57	116.10
29	6	607	CHL	CAC-C3C-C4C	2.37	127.89	124.81
29	9	606	CHL	O2D-CGD-O1D	-2.37	119.20	123.84
29	3	407	CHL	O2D-CGD-O1D	-2.37	118.71	124.09
24	B	843	BCR	C34-C9-C8	2.37	121.81	118.08
21	A	833	CLA	CHB-C4A-NA	2.37	127.79	124.51
21	c	610	CLA	CHB-C4A-NA	2.37	127.79	124.51
21	A	821	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
29	2	605	CHL	O2D-CGD-O1D	-2.37	119.21	123.84
21	5	602	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
21	1	308	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
21	2	610	CLA	C1B-CHB-C4A	-2.36	125.43	130.12
21	b	313	CLA	C1B-CHB-C4A	-2.36	125.43	130.12
29	8	613	CHL	CHC-C1C-C2C	-2.36	117.54	126.11
21	5	609	CLA	CHB-C4A-NA	2.36	127.78	124.51
21	3	408	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
21	A	822	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
21	3	413	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
29	c	608	CHL	CAC-C3C-C4C	2.36	127.87	124.81
31	4	616	XAT	C7-C8-C9	2.36	129.19	125.53
21	4	603	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
24	B	843	BCR	C1-C6-C5	-2.36	119.29	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	9	610	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
21	B	802	CLA	CHB-C4A-NA	2.36	127.77	124.51
21	4	612	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
21	5	608	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
29	a	605	CHL	C3B-C4B-NB	2.36	112.26	109.21
24	J	104	BCR	C28-C27-C26	-2.36	109.87	114.08
21	A	823	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
21	A	817	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
21	1	313	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
21	6	610	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
21	b	303	CLA	CHB-C4A-NA	2.36	127.77	124.51
21	b	311	CLA	CHB-C4A-NA	2.36	127.77	124.51
21	1	303	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
21	7	402	CLA	CHB-C4A-NA	2.35	127.77	124.51
21	9	602	CLA	CHB-C4A-NA	2.35	127.77	124.51
24	6	618	BCR	C23-C22-C21	2.35	122.55	118.94
21	6	608	CLA	CHB-C4A-NA	2.35	127.77	124.51
21	b	314	CLA	C1B-CHB-C4A	-2.35	125.45	130.12
29	8	613	CHL	OMC-CMC-C2C	-2.35	120.36	125.69
21	B	806	CLA	CHB-C4A-NA	2.35	127.77	124.51
29	a	608	CHL	CAC-C3C-C4C	2.35	127.86	124.81
29	c	601	CHL	O2A-CGA-CBA	2.35	119.29	111.91
21	4	613	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
21	2	609	CLA	CHD-C1D-ND	-2.35	122.29	124.45
30	3	416	LUT	C11-C12-C13	2.35	133.02	126.42
21	B	807	CLA	CHB-C4A-NA	2.35	127.76	124.51
21	B	812	CLA	CHB-C4A-NA	2.35	127.76	124.51
21	7	410	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
21	B	815	CLA	O2A-CGA-O1A	-2.35	117.66	123.59
21	a	610	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
21	1	309	CLA	C3D-C4D-ND	2.35	114.04	110.24
21	1	309	CLA	C2A-C3A-C4A	2.35	104.78	101.78
21	5	604	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
21	3	409	CLA	CHD-C1D-ND	-2.35	122.30	124.45
21	c	603	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
29	6	606	CHL	OMC-CMC-C2C	-2.35	120.38	125.69
21	A	831	CLA	CHB-C4A-NA	2.35	127.76	124.51
29	a	609	CHL	CHC-C1C-C2C	-2.35	117.61	126.11
24	A	849	BCR	C21-C20-C19	2.34	130.53	123.22
21	A	805	CLA	C1B-CHB-C4A	-2.34	125.47	130.12
21	K	202	CLA	C1-C2-C3	-2.34	122.96	126.75
21	A	802	CLA	CHB-C4A-NA	2.34	127.75	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	818	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
21	8	604	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
21	7	413	CLA	CAA-C2A-C3A	-2.34	110.64	116.10
21	A	832	CLA	CHB-C4A-NA	2.34	127.75	124.51
21	A	823	CLA	O2D-CGD-CBD	2.34	115.42	111.27
21	K	203	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
21	8	618	CLA	CAA-C2A-C3A	-2.34	110.64	116.10
30	9	615	LUT	C12-C13-C14	2.34	122.53	118.94
21	4	602	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
21	B	813	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
21	F	302	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
21	a	611	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
21	a	614	CLA	CAA-C2A-C3A	-2.33	110.65	116.10
21	A	836	CLA	CHB-C4A-NA	2.33	127.74	124.51
21	O	202	CLA	CHB-C4A-NA	2.33	127.74	124.51
21	2	604	CLA	CHB-C4A-NA	2.33	127.74	124.51
21	K	204	CLA	C1B-CHB-C4A	-2.33	125.49	130.12
21	A	824	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
21	B	818	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
21	J	102	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
29	4	607	CHL	C3B-C4B-NB	2.33	112.22	109.21
21	A	826	CLA	CHD-C1D-ND	-2.33	122.31	124.45
29	2	614	CHL	C3B-C4B-NB	2.33	112.22	109.21
29	8	613	CHL	CHD-C1D-C2D	2.33	130.37	125.48
21	G	203	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
21	B	812	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
21	B	836	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
21	1	316	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
21	2	613	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
21	b	303	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
29	c	606	CHL	CAC-C3C-C4C	2.33	127.83	124.81
24	4	617	BCR	C34-C9-C8	2.32	121.74	118.08
21	B	803	CLA	C1B-CHB-C4A	-2.32	125.51	130.12
21	F	304	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
21	A	823	CLA	CHB-C4A-NA	2.32	127.72	124.51
21	1	306	CLA	CHB-C4A-NA	2.32	127.72	124.51
31	2	617	XAT	C12-C13-C14	2.32	122.50	118.94
21	b	304	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
21	4	603	CLA	CHB-C4A-NA	2.32	127.72	124.51
24	B	846	BCR	C10-C11-C12	-2.32	115.97	123.22
29	1	302	CHL	C5-C3-C4	2.32	119.73	114.60
29	c	608	CHL	O2D-CGD-O1D	-2.32	119.30	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	8	606	CHL	CHC-C1C-C2C	-2.32	117.70	126.11
21	8	618	CLA	CHB-C4A-NA	2.32	127.72	124.51
29	6	602	CHL	C3B-C4B-NB	2.32	112.21	109.21
21	A	837	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
21	8	612	CLA	CHB-C4A-NA	2.32	127.72	124.51
21	B	819	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
21	6	613	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
21	A	830	CLA	CHD-C1D-ND	-2.32	122.32	124.45
21	b	311	CLA	C1-C2-C3	-2.32	122.03	126.04
21	A	834	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
23	1	301	LHG	O7-C7-C8	2.31	116.49	111.50
24	A	848	BCR	C12-C13-C14	2.31	122.49	118.94
29	2	607	CHL	C3B-C4B-NB	2.31	112.20	109.21
29	6	606	CHL	O2D-CGD-O1D	-2.31	119.32	123.84
21	8	610	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
21	A	814	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
24	L	306	BCR	C21-C20-C19	2.31	130.43	123.22
21	4	604	CLA	CHB-C4A-NA	2.31	127.71	124.51
24	L	305	BCR	C34-C9-C8	2.31	121.72	118.08
24	G	201	BCR	C8-C9-C10	2.31	122.48	118.94
21	2	609	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
29	8	606	CHL	O2D-CGD-O1D	-2.31	119.32	123.84
21	3	410	CLA	CHB-C4A-NA	2.31	127.70	124.51
21	O	203	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
21	A	814	CLA	C1-C2-C3	-2.31	122.05	126.04
31	c	617	XAT	C36-C21-C22	-2.31	104.97	108.98
21	1	311	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
21	B	838	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
29	9	607	CHL	O2D-CGD-O1D	-2.31	119.33	123.84
29	5	606	CHL	CAC-C3C-C4C	2.31	127.80	124.81
29	9	605	CHL	CAC-C3C-C4C	2.31	127.80	124.81
21	A	841	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
21	3	409	CLA	C2D-C1D-ND	-2.31	108.41	110.10
30	9	615	LUT	C7-C8-C9	2.31	129.72	126.23
24	4	617	BCR	C7-C8-C9	2.30	129.72	126.23
21	9	612	CLA	C1B-CHB-C4A	-2.30	125.55	130.12
21	1	309	CLA	CHD-C1D-ND	-2.30	122.34	124.45
29	b	307	CHL	CAC-C3C-C4C	2.30	127.80	124.81
21	2	603	CLA	CHB-C4A-NA	2.30	127.69	124.51
21	8	609	CLA	CHD-C1D-ND	-2.30	122.34	124.45
21	8	603	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
24	J	104	BCR	C3-C2-C1	-2.30	106.38	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	9	608	CHL	O2D-CGD-O1D	-2.30	119.34	123.84
21	A	827	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
30	b	317	LUT	C12-C13-C14	2.30	122.47	118.94
21	5	613	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
21	B	840	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
21	7	412	CLA	CHB-C4A-NA	2.30	127.69	124.51
29	c	605	CHL	CHC-C1C-C2C	-2.30	117.78	126.11
21	B	822	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
21	1	305	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
21	B	811	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
21	7	408	CLA	CAA-C2A-C3A	-2.30	110.74	116.10
21	5	610	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
21	3	410	CLA	O2D-CGD-O1D	-2.29	118.88	124.09
21	9	610	CLA	CHB-C4A-NA	2.29	127.69	124.51
21	A	832	CLA	C1B-CHB-C4A	-2.29	125.57	130.12
21	B	801	CLA	CMA-C3A-C2A	-2.29	104.57	113.83
21	8	601	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
21	K	202	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
21	B	820	CLA	CHB-C4A-NA	2.29	127.68	124.51
29	2	605	CHL	OMC-CMC-C2C	-2.29	120.50	125.69
21	O	204	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
21	3	406	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
21	6	608	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
29	b	302	CHL	C3B-C4B-NB	2.29	112.17	109.21
29	1	307	CHL	C5-C3-C4	2.29	119.66	114.60
21	L	303	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
24	B	846	BCR	C23-C24-C25	-2.29	120.77	127.20
21	b	311	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
29	9	601	CHL	C3B-C4B-NB	2.29	112.17	109.21
21	4	601	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
21	7	404	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
24	B	844	BCR	C24-C23-C22	-2.29	122.78	126.23
29	6	614	CHL	C3B-C4B-NB	2.29	112.17	109.21
21	B	820	CLA	CHD-C1D-ND	-2.29	122.35	124.45
21	b	311	CLA	CHD-C1D-ND	-2.29	122.35	124.45
21	3	402	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
29	a	609	CHL	O2D-CGD-O1D	-2.29	119.36	123.84
29	c	605	CHL	C4A-NA-C1A	-2.29	105.68	106.71
24	6	618	BCR	C8-C9-C10	2.29	122.45	118.94
21	3	403	CLA	CHB-C4A-NA	2.29	127.68	124.51
29	8	606	CHL	CAC-C3C-C4C	2.29	127.78	124.81
21	F	302	CLA	O1D-CGD-CBD	2.29	129.16	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	805	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
29	c	601	CHL	O2D-CGD-O1D	-2.29	119.37	123.84
24	F	301	BCR	C16-C15-C14	2.29	128.16	123.47
21	L	302	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
21	9	613	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
29	2	602	CHL	CAC-C3C-C4C	2.29	127.78	124.81
21	3	412	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
29	5	606	CHL	C3B-C4B-NB	2.28	112.16	109.21
21	4	611	CLA	C1B-CHB-C4A	-2.28	125.59	130.12
24	A	847	BCR	C12-C13-C14	2.28	122.44	118.94
21	a	613	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
29	b	302	CHL	CHD-C1D-C2D	2.28	130.26	125.48
29	b	308	CHL	C6-C5-C3	-2.28	110.89	114.62
21	A	825	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
21	A	808	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
21	a	612	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
21	B	808	CLA	CHB-C4A-NA	2.28	127.66	124.51
21	A	838	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
21	A	806	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
21	A	818	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
21	4	610	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
21	H	201	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
21	9	604	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
29	8	613	CHL	O2D-CGD-O1D	-2.28	119.39	123.84
21	B	827	CLA	CHB-C4A-NA	2.28	127.66	124.51
21	K	202	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
21	A	809	CLA	CHD-C1D-ND	-2.28	122.36	124.45
29	c	606	CHL	O2D-CGD-O1D	-2.28	119.39	123.84
21	A	842	CLA	C1B-CHB-C4A	-2.27	125.61	130.12
21	A	840	CLA	O2A-CGA-O1A	-2.27	117.85	123.59
21	F	305	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
29	6	606	CHL	CAC-C3C-C4C	2.27	127.76	124.81
24	B	844	BCR	C4-C5-C6	-2.27	119.43	122.73
21	B	833	CLA	CHD-C1D-ND	-2.27	122.37	124.45
21	6	611	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
21	3	405	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
21	B	813	CLA	CHD-C1D-ND	-2.27	122.37	124.45
21	7	409	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
21	A	831	CLA	C1-C2-C3	-2.27	122.12	126.04
21	c	613	CLA	C1B-CHB-C4A	-2.26	125.63	130.12
21	a	613	CLA	C1-C2-C3	-2.26	122.13	126.04
24	B	843	BCR	C10-C11-C12	-2.26	116.15	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	K	205	BCR	C20-C19-C18	-2.26	120.06	126.42
21	A	817	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
29	9	609	CHL	CAC-C3C-C4C	2.26	127.75	124.81
24	A	847	BCR	C34-C9-C8	2.26	121.64	118.08
24	O	205	BCR	C21-C20-C19	2.26	130.28	123.22
29	b	306	CHL	O2D-CGD-O1D	-2.26	119.42	123.84
21	3	404	CLA	CHD-C1D-ND	-2.26	122.38	124.45
29	a	605	CHL	CAC-C3C-C4C	2.26	127.74	124.81
24	F	301	BCR	C34-C9-C8	2.26	121.64	118.08
24	J	104	BCR	C37-C22-C23	2.26	121.64	118.08
29	9	601	CHL	O2D-CGD-O1D	-2.26	119.42	123.84
21	3	409	CLA	C3D-C4D-ND	2.26	113.89	110.24
21	1	306	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
21	A	820	CLA	C1B-CHB-C4A	-2.26	125.65	130.12
21	K	201	CLA	C1B-CHB-C4A	-2.26	125.65	130.12
21	A	830	CLA	CAA-CBA-CGA	-2.26	106.66	113.25
21	A	801	CLA	CED-O2D-CGD	2.26	121.04	115.94
21	B	814	CLA	C1-C2-C3	-2.26	122.14	126.04
29	6	602	CHL	C3C-C4C-NC	2.26	113.10	110.57
21	1	314	CLA	CHB-C4A-NA	2.25	127.63	124.51
21	6	604	CLA	CHB-C4A-NA	2.25	127.63	124.51
21	O	203	CLA	O2A-CGA-O1A	-2.25	117.90	123.59
21	3	408	CLA	C1-C2-C3	-2.25	122.14	126.04
29	b	307	CHL	C3B-C4B-NB	2.25	112.12	109.21
30	3	416	LUT	C39-C29-C28	2.25	121.63	118.08
29	6	614	CHL	CAC-C3C-C4C	2.25	127.73	124.81
21	B	823	CLA	C1B-CHB-C4A	-2.25	125.65	130.12
21	2	612	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
21	B	829	CLA	C2D-C1D-ND	-2.25	108.44	110.10
21	B	835	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
21	9	610	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
30	6	616	LUT	C10-C11-C12	2.25	130.24	123.22
29	a	601	CHL	C3B-C4B-NB	2.25	112.12	109.21
21	B	830	CLA	CHB-C4A-NA	2.25	127.62	124.51
29	a	608	CHL	O2D-CGD-O1D	-2.25	119.44	123.84
29	b	306	CHL	C3B-C4B-NB	2.25	112.12	109.21
21	1	315	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
21	B	828	CLA	CHB-C4A-NA	2.25	127.62	124.51
21	B	801	CLA	CAC-C3C-C4C	2.25	127.73	124.81
21	B	804	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
21	b	315	CLA	CHB-C4A-NA	2.25	127.62	124.51
29	c	607	CHL	CAC-C3C-C4C	2.25	127.72	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	3	416	LUT	C15-C14-C13	2.25	130.51	127.31
21	A	815	CLA	C1B-CHB-C4A	-2.24	125.67	130.12
29	4	614	CHL	O2D-CGD-O1D	-2.24	119.45	123.84
31	6	617	XAT	C6-C7-C8	2.24	130.74	125.99
21	c	612	CLA	C1B-CHB-C4A	-2.24	125.67	130.12
24	B	844	BCR	C30-C25-C24	2.24	122.12	115.78
21	c	614	CLA	CHB-C4A-NA	2.24	127.61	124.51
21	O	204	CLA	O2D-CGD-O1D	-2.24	119.01	124.09
21	B	812	CLA	C1-C2-C3	-2.24	122.17	126.04
21	3	414	CLA	C1B-CHB-C4A	-2.23	125.69	130.12
21	O	201	CLA	C1B-CHB-C4A	-2.23	125.69	130.12
21	5	614	CLA	C1B-CHB-C4A	-2.23	125.69	130.12
24	I	101	BCR	C15-C16-C17	2.23	128.05	123.47
31	4	616	XAT	C12-C13-C14	2.23	122.37	118.94
24	M	101	BCR	C10-C11-C12	2.23	130.18	123.22
31	a	618	XAT	C15-C35-C34	2.23	128.04	123.47
21	6	603	CLA	C2D-C1D-ND	-2.23	108.46	110.10
21	B	802	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
21	5	603	CLA	CHB-C4A-NA	2.23	127.60	124.51
29	8	606	CHL	C3B-C4B-NB	2.23	112.09	109.21
21	B	831	CLA	CHD-C1D-ND	-2.23	122.41	124.45
21	B	826	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
29	6	607	CHL	C5-C3-C4	2.23	119.53	114.60
21	A	835	CLA	CHD-C1D-ND	-2.23	122.41	124.45
21	A	852	CLA	CHD-C1D-ND	-2.23	122.41	124.45
21	B	824	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
21	2	609	CLA	C2D-C1D-ND	-2.23	108.46	110.10
21	L	303	CLA	CHD-C1D-ND	-2.23	122.41	124.45
24	B	843	BCR	C4-C5-C6	-2.23	119.50	122.73
21	B	838	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
21	A	810	CLA	C1B-CHB-C4A	-2.23	125.71	130.12
21	5	612	CLA	C1B-CHB-C4A	-2.23	125.71	130.12
30	c	615	LUT	C32-C33-C34	2.22	122.35	118.94
29	6	607	CHL	C3B-C4B-NB	2.22	112.08	109.21
21	A	834	CLA	O2D-CGD-CBD	2.22	115.22	111.27
21	4	604	CLA	C1B-CHB-C4A	-2.22	125.71	130.12
21	A	812	CLA	CHB-C4A-NA	2.22	127.58	124.51
29	c	606	CHL	C3B-C4B-NB	2.22	112.08	109.21
21	B	839	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
29	b	309	CHL	O2D-CGD-O1D	-2.22	119.50	123.84
21	B	801	CLA	CHB-C4A-NA	2.22	127.58	124.51
21	1	312	CLA	C1B-CHB-C4A	-2.22	125.72	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	816	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
30	6	616	LUT	C31-C30-C29	2.22	130.48	127.31
29	a	601	CHL	O1D-CGD-CBD	-2.22	119.95	124.48
21	B	809	CLA	C1B-CHB-C4A	-2.21	125.73	130.12
21	B	824	CLA	CHD-C1D-ND	-2.21	122.42	124.45
31	1	318	XAT	C6-C7-C8	-2.21	121.31	125.99
21	3	402	CLA	O2A-CGA-O1A	-2.21	118.00	123.59
21	A	841	CLA	CAA-C2A-C3A	-2.21	106.72	112.78
29	a	601	CHL	CAC-C3C-C4C	2.21	127.68	124.81
21	8	618	CLA	CHD-C1D-ND	-2.21	122.42	124.45
21	A	803	CLA	CHD-C1D-ND	-2.21	122.42	124.45
21	2	604	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
21	7	414	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
21	B	825	CLA	C1-C2-C3	-2.21	122.23	126.04
21	A	833	CLA	C1-C2-C3	-2.21	122.23	126.04
21	3	409	CLA	O2A-CGA-CBA	2.21	118.83	111.91
21	8	609	CLA	C2D-C1D-ND	-2.21	108.48	110.10
21	O	204	CLA	CHD-C1D-ND	-2.20	122.43	124.45
21	A	804	CLA	C1-C2-C3	-2.20	122.23	126.04
21	9	613	CLA	C1-C2-C3	-2.20	122.23	126.04
29	6	601	CHL	CHD-C1D-C2D	2.20	130.10	125.48
31	3	417	XAT	C39-C29-C28	2.20	121.55	118.08
21	B	821	CLA	O2D-CGD-CBD	2.20	115.18	111.27
29	2	614	CHL	O2D-CGD-O1D	-2.20	119.54	123.84
21	B	837	CLA	CHB-C4A-NA	2.20	127.55	124.51
24	B	846	BCR	C38-C26-C27	2.20	117.83	113.62
21	B	828	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
24	M	101	BCR	C21-C20-C19	2.19	130.06	123.22
30	7	415	LUT	C15-C35-C34	2.19	127.97	123.47
21	4	613	CLA	CHD-C1D-ND	-2.19	122.44	124.45
29	9	609	CHL	C4D-C3D-CAD	2.19	110.68	108.10
30	c	616	LUT	C7-C8-C9	2.19	129.55	126.23
21	L	304	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
21	A	829	CLA	CHB-C4A-NA	2.19	127.54	124.51
21	B	810	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
21	A	830	CLA	C2D-C1D-ND	-2.19	108.49	110.10
21	5	605	CLA	CHB-C4A-NA	2.19	127.54	124.51
30	7	415	LUT	C39-C29-C28	2.19	121.53	118.08
21	G	204	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
24	J	104	BCR	C15-C16-C17	-2.19	118.99	123.47
21	K	202	CLA	CAA-CBA-CGA	-2.19	106.86	113.25
21	B	831	CLA	CAC-C3C-C4C	2.19	127.65	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	9	602	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
29	5	606	CHL	CHD-C1D-C2D	2.19	130.07	125.48
21	4	602	CLA	CHD-C1D-ND	-2.19	122.44	124.45
24	K	205	BCR	C1-C6-C5	-2.19	119.53	122.61
29	b	306	CHL	CHD-C1D-C2D	2.19	130.06	125.48
21	3	402	CLA	CHD-C1D-ND	-2.19	122.45	124.45
21	B	812	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
21	B	840	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
24	K	205	BCR	C36-C18-C17	-2.18	119.87	122.92
24	B	846	BCR	C8-C7-C6	-2.18	121.08	127.20
24	B	843	BCR	C20-C19-C18	-2.18	120.29	126.42
21	B	825	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
29	a	605	CHL	CHD-C1D-C2D	2.18	130.05	125.48
31	1	318	XAT	C11-C10-C9	2.18	130.42	127.31
21	B	825	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
29	a	605	CHL	O2D-CGD-O1D	-2.18	119.15	124.09
29	c	607	CHL	C3B-C4B-NB	2.18	112.02	109.21
21	A	802	CLA	O1D-CGD-CBD	2.17	128.93	124.48
31	3	417	XAT	C35-C15-C14	2.17	127.93	123.47
21	8	602	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
21	B	839	CLA	CAA-C2A-C3A	-2.17	106.84	112.78
21	1	309	CLA	C2D-C1D-ND	-2.17	108.50	110.10
29	2	607	CHL	O2D-CGD-O1D	-2.17	119.60	123.84
24	7	418	BCR	C24-C23-C22	2.17	129.51	126.23
21	A	811	CLA	CHD-C1D-ND	-2.17	122.46	124.45
21	3	401	CLA	C1B-CHB-C4A	-2.17	125.82	130.12
24	8	616	BCR	C8-C9-C10	2.17	122.27	118.94
29	6	601	CHL	C3B-C4B-NB	2.17	112.01	109.21
24	A	847	BCR	C37-C22-C23	2.17	121.49	118.08
29	1	307	CHL	CAC-C3C-C4C	2.17	127.62	124.81
29	9	608	CHL	CAC-C3C-C4C	2.17	127.62	124.81
21	A	821	CLA	CHD-C1D-ND	-2.17	122.46	124.45
21	1	314	CLA	CMA-C3A-C2A	-2.17	111.05	116.10
21	8	618	CLA	CMA-C3A-C2A	-2.16	111.05	116.10
29	b	307	CHL	OMC-CMC-C2C	-2.16	120.79	125.69
21	4	604	CLA	CHD-C1D-ND	-2.16	122.47	124.45
29	a	606	CHL	CHD-C1D-C2D	2.16	130.01	125.48
31	6	617	XAT	C10-C11-C12	2.16	129.96	123.22
21	A	803	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
21	L	303	CLA	O2D-CGD-CBD	2.16	115.11	111.27
24	3	418	BCR	C37-C22-C23	2.16	121.48	118.08
21	5	602	CLA	O2A-CGA-O1A	-2.16	118.14	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	807	CLA	C1B-CHB-C4A	-2.16	125.84	130.12
21	G	202	CLA	C1B-CHB-C4A	-2.16	125.84	130.12
21	2	608	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
24	2	618	BCR	C15-C16-C17	-2.16	119.06	123.47
24	B	844	BCR	C34-C9-C10	-2.16	119.90	122.92
21	A	852	CLA	C1-C2-C3	-2.15	122.32	126.04
31	1	318	XAT	C12-C13-C14	2.15	122.24	118.94
21	1	303	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
21	a	602	CLA	CHD-C1D-ND	-2.15	122.48	124.45
29	b	310	CHL	O2D-CGD-O1D	-2.15	119.21	124.09
21	A	837	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
21	8	602	CLA	CHD-C1D-ND	-2.15	122.48	124.45
21	7	412	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
30	b	316	LUT	C39-C29-C28	2.15	121.46	118.08
29	8	605	CHL	C3C-C4C-NC	2.15	112.92	110.57
29	b	308	CHL	C1-O2A-CGA	2.15	122.08	116.44
21	O	203	CLA	C1-C2-C3	-2.15	122.33	126.04
21	A	809	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
29	c	605	CHL	CAC-C3C-C4C	2.15	127.59	124.81
21	A	829	CLA	O2A-CGA-O1A	-2.15	118.18	123.59
21	A	826	CLA	O2A-CGA-O1A	-2.14	118.18	123.59
29	6	614	CHL	O2D-CGD-O1D	-2.14	119.65	123.84
21	3	408	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
21	8	602	CLA	C1-C2-C3	-2.14	122.34	126.04
29	6	607	CHL	CHD-C1D-C2D	2.14	129.97	125.48
29	5	601	CHL	CAC-C3C-C4C	2.14	127.59	124.81
29	1	302	CHL	O1D-CGD-CBD	-2.14	120.11	124.48
21	A	852	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
21	B	816	CLA	CHD-C1D-ND	-2.14	122.49	124.45
31	a	618	XAT	C28-C29-C30	2.14	122.22	118.94
30	c	616	LUT	C39-C29-C28	2.14	121.44	118.08
29	2	606	CHL	C3C-C4C-NC	2.14	112.97	110.57
21	O	202	CLA	CHD-C1D-ND	-2.13	122.49	124.45
21	G	202	CLA	CHD-C1D-ND	-2.13	122.49	124.45
21	1	313	CLA	CHD-C1D-ND	-2.13	122.49	124.45
21	A	814	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
21	B	803	CLA	CHD-C1D-ND	-2.13	122.49	124.45
29	b	306	CHL	CAC-C3C-C4C	2.13	127.58	124.81
29	6	607	CHL	O2D-CGD-O1D	-2.13	119.67	123.84
21	B	836	CLA	CHD-C1D-ND	-2.13	122.50	124.45
24	F	303	BCR	C11-C10-C9	2.13	130.35	127.31
21	4	609	CLA	C2A-C1A-CHA	2.13	127.59	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	843	BCR	C8-C9-C10	-2.13	115.67	118.94
24	K	205	BCR	C10-C11-C12	-2.13	116.57	123.22
29	1	302	CHL	CAC-C3C-C4C	2.13	127.57	124.81
21	6	603	CLA	CHB-C4A-NA	2.13	127.45	124.51
24	B	844	BCR	C37-C22-C21	-2.13	119.94	122.92
31	7	416	XAT	C11-C10-C9	2.13	130.35	127.31
29	a	607	CHL	O1D-CGD-CBD	-2.13	120.13	124.48
21	A	802	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
21	B	801	CLA	C4-C3-C5	2.13	118.85	115.27
21	8	611	CLA	CHD-C1D-ND	-2.13	122.50	124.45
21	9	602	CLA	CHD-C1D-ND	-2.13	122.50	124.45
21	B	831	CLA	O2D-CGD-CBD	2.12	115.04	111.27
29	8	613	CHL	C3B-C4B-NB	2.12	111.95	109.21
29	8	607	CHL	CHD-C1D-C2D	2.12	129.93	125.48
24	I	101	BCR	C37-C22-C23	2.12	121.42	118.08
29	7	406	CHL	O2D-CGD-O1D	-2.12	119.28	124.09
21	B	830	CLA	CHD-C1D-ND	-2.12	122.51	124.45
21	A	810	CLA	O2A-CGA-O1A	-2.12	118.02	123.30
24	J	104	BCR	C24-C25-C26	-2.12	116.34	121.46
29	c	605	CHL	C3B-C4B-NB	2.12	111.94	109.21
21	B	817	CLA	CHD-C1D-ND	-2.12	122.51	124.45
24	2	618	BCR	C23-C22-C21	2.12	122.19	118.94
21	6	613	CLA	CHD-C1D-ND	-2.11	122.51	124.45
21	A	812	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
21	B	809	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
30	2	616	LUT	C32-C33-C34	2.11	122.18	118.94
21	b	315	CLA	CHD-C1D-ND	-2.11	122.52	124.45
29	9	609	CHL	O2D-CGD-O1D	-2.11	119.72	123.84
29	4	607	CHL	C4D-C3D-CAD	2.11	110.58	108.10
29	6	606	CHL	C4D-C3D-CAD	2.11	110.58	108.10
24	L	301	BCR	C34-C9-C8	2.11	121.39	118.08
21	3	401	CLA	CHD-C1D-ND	-2.10	122.52	124.45
21	3	412	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
21	b	303	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
21	A	836	CLA	CHD-C1D-ND	-2.10	122.52	124.45
21	B	834	CLA	CHD-C1D-ND	-2.10	122.52	124.45
21	a	614	CLA	CHD-C1D-ND	-2.10	122.53	124.45
21	B	801	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
29	5	601	CHL	O1D-CGD-CBD	-2.10	120.19	124.48
21	B	806	CLA	O2D-CGD-CBD	2.10	114.99	111.27
21	2	608	CLA	CHD-C1D-ND	-2.10	122.53	124.45
21	3	408	CLA	CHD-C1D-ND	-2.10	122.53	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	6	601	CHL	O1D-CGD-CBD	-2.09	120.20	124.48
29	b	302	CHL	CAC-C3C-C4C	2.09	127.53	124.81
29	c	601	CHL	CAC-C3C-C4C	2.09	127.53	124.81
21	B	807	CLA	CAA-C2A-C3A	-2.09	107.05	112.78
24	F	301	BCR	C12-C13-C14	2.09	122.15	118.94
29	c	609	CHL	CAC-C3C-C4C	2.09	128.22	125.04
29	7	406	CHL	CMA-C3A-C2A	-2.09	111.22	116.10
24	B	844	BCR	C21-C20-C19	-2.09	116.69	123.22
24	B	846	BCR	C1-C6-C5	-2.09	119.67	122.61
21	L	302	CLA	O2A-CGA-O1A	-2.09	118.09	123.30
30	2	616	LUT	C15-C35-C34	2.09	127.75	123.47
21	B	818	CLA	CHD-C1D-ND	-2.09	122.53	124.45
30	9	614	LUT	C11-C10-C9	2.09	130.29	127.31
21	2	609	CLA	CBA-CAA-C2A	-2.09	110.53	114.28
29	a	608	CHL	C4D-C3D-CAD	2.09	110.56	108.10
29	2	607	CHL	C3C-C4C-NC	2.09	112.91	110.57
21	A	805	CLA	O2D-CGD-CBD	2.09	114.97	111.27
21	A	823	CLA	CHD-C1D-ND	-2.09	122.54	124.45
21	A	832	CLA	CHD-C1D-ND	-2.09	122.54	124.45
24	B	844	BCR	C15-C16-C17	-2.09	119.20	123.47
29	6	607	CHL	C4D-C3D-CAD	2.09	110.55	108.10
21	7	411	CLA	CHD-C1D-ND	-2.08	122.54	124.45
21	1	305	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
21	5	604	CLA	CHD-C1D-ND	-2.08	122.54	124.45
21	A	824	CLA	CHD-C1D-ND	-2.08	122.54	124.45
21	B	835	CLA	C1-C2-C3	-2.08	122.44	126.04
21	c	610	CLA	CHD-C1D-ND	-2.08	122.54	124.45
21	1	315	CLA	O2A-CGA-O1A	-2.08	118.11	123.30
24	7	417	BCR	C23-C22-C21	2.08	122.13	118.94
21	1	303	CLA	CHD-C1D-ND	-2.08	122.54	124.45
24	8	616	BCR	C37-C22-C23	2.08	121.36	118.08
29	a	605	CHL	C4D-C3D-CAD	2.08	110.55	108.10
21	A	801	CLA	CHB-C4A-NA	2.08	127.39	124.51
21	4	602	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
21	7	407	CLA	C2C-C1C-NC	2.08	111.92	109.97
21	B	805	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
29	8	607	CHL	C4D-C3D-CAD	2.08	110.54	108.10
29	2	614	CHL	CHD-C1D-C2D	2.08	129.84	125.48
29	b	309	CHL	C4D-C3D-CAD	2.07	110.54	108.10
21	G	203	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
32	c	618	NEX	C30-C31-C32	2.07	129.69	123.22
29	8	605	CHL	CAC-C3C-C4C	2.07	128.19	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	c	609	CHL	CHC-C1C-C2C	-2.07	118.60	126.11
21	2	612	CLA	O2A-CGA-O1A	-2.07	118.14	123.30
21	8	612	CLA	CHD-C1D-ND	-2.07	122.55	124.45
30	9	614	LUT	C12-C13-C14	2.07	122.12	118.94
30	a	615	LUT	C8-C9-C10	2.07	122.11	118.94
31	9	616	XAT	C6-C7-C8	-2.07	121.62	125.99
21	B	823	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
21	c	611	CLA	CHD-C1D-ND	-2.07	122.56	124.45
21	4	609	CLA	C3D-C4D-ND	2.06	113.58	110.24
21	B	807	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
29	2	601	CHL	O1D-CGD-CBD	-2.06	120.27	124.48
21	7	401	CLA	O2D-CGD-CBD	2.06	114.93	111.27
24	B	843	BCR	C37-C22-C23	2.06	121.32	118.08
21	B	823	CLA	C1-C2-C3	-2.06	122.48	126.04
24	2	618	BCR	C8-C9-C10	2.06	122.10	118.94
21	A	809	CLA	O2D-CGD-CBD	2.06	114.93	111.27
21	A	803	CLA	CHB-C4A-NA	2.06	127.36	124.51
21	9	613	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
30	9	615	LUT	C39-C29-C28	2.06	121.32	118.08
29	6	602	CHL	CAC-C3C-C4C	2.06	127.48	124.81
29	8	605	CHL	C4D-C3D-CAD	2.06	110.52	108.10
21	K	202	CLA	O2D-CGD-CBD	2.06	114.92	111.27
21	1	310	CLA	O2A-CGA-O1A	-2.06	118.17	123.30
21	7	411	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
21	A	819	CLA	O2D-CGD-CBD	2.06	114.92	111.27
21	A	821	CLA	C1-C2-C3	-2.06	122.49	126.04
21	B	810	CLA	C1-C2-C3	-2.06	122.49	126.04
29	a	606	CHL	O2A-CGA-CBA	2.06	120.63	114.03
21	A	822	CLA	CHD-C1D-ND	-2.05	122.57	124.45
21	4	612	CLA	CHD-C1D-ND	-2.05	122.57	124.45
21	8	603	CLA	CHD-C1D-ND	-2.05	122.57	124.45
29	c	609	CHL	O2D-CGD-O1D	-2.05	119.43	124.09
21	c	602	CLA	CHD-C1D-ND	-2.05	122.57	124.45
21	B	827	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
29	b	310	CHL	CHD-C1D-C2D	2.05	129.79	125.48
21	1	305	CLA	CHD-C1D-ND	-2.05	122.57	124.45
21	5	605	CLA	C2A-C1A-CHA	2.05	125.89	122.71
21	4	609	CLA	C1B-CHB-C4A	-2.05	126.06	130.12
21	B	806	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
29	7	406	CHL	C3B-C4B-NB	2.05	111.86	109.21
21	B	837	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
21	a	613	CLA	O2A-CGA-O1A	-2.05	118.43	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	8	609	CLA	C1B-CHB-C4A	-2.05	126.06	130.12
21	b	314	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
29	4	607	CHL	O2D-CGD-O1D	-2.04	119.84	123.84
21	a	604	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
21	F	304	CLA	C2D-C1D-ND	-2.04	108.60	110.10
21	1	309	CLA	C1B-CHB-C4A	-2.04	126.07	130.12
21	c	603	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
21	A	837	CLA	CHD-C1D-ND	-2.04	122.58	124.45
24	G	205	BCR	C34-C9-C8	2.04	121.29	118.08
21	5	603	CLA	O2A-CGA-O1A	-2.04	118.21	123.30
21	7	413	CLA	CHD-C1D-ND	-2.04	122.58	124.45
21	A	811	CLA	O2A-CGA-O1A	-2.04	118.21	123.30
29	2	607	CHL	C4D-C3D-CAD	2.04	110.50	108.10
29	a	606	CHL	O1D-CGD-CBD	-2.04	120.31	124.48
21	B	804	CLA	CHD-C1D-ND	-2.04	122.58	124.45
29	8	607	CHL	O2D-CGD-O1D	-2.04	119.85	123.84
21	a	613	CLA	CHD-C1D-ND	-2.04	122.58	124.45
21	3	409	CLA	C1B-CHB-C4A	-2.04	126.08	130.12
21	4	603	CLA	O2A-CGA-O1A	-2.04	118.22	123.30
21	5	607	CLA	O2A-CGA-O1A	-2.04	118.22	123.30
21	B	826	CLA	O2D-CGD-CBD	2.04	114.89	111.27
21	b	313	CLA	O2A-CGA-O1A	-2.03	118.23	123.30
30	7	415	LUT	C7-C8-C9	2.03	129.31	126.23
31	a	618	XAT	C8-C9-C10	2.03	122.06	118.94
30	a	616	LUT	C8-C9-C10	2.03	122.06	118.94
21	A	824	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
29	b	310	CHL	C1-C2-C3	-2.03	122.53	126.04
21	5	609	CLA	O2A-CGA-O1A	-2.03	118.23	123.30
29	6	601	CHL	C4D-C3D-CAD	2.03	110.49	108.10
24	L	301	BCR	C37-C22-C23	2.03	121.28	118.08
31	2	617	XAT	C7-C8-C9	2.03	128.68	125.53
29	7	406	CHL	CAC-C3C-C4C	2.03	127.44	124.81
21	F	302	CLA	C1-C2-C3	-2.03	122.53	126.04
21	1	308	CLA	O2A-CGA-O1A	-2.03	118.24	123.30
21	B	801	CLA	C1B-CHB-C4A	-2.03	126.10	130.12
21	7	411	CLA	C1-C2-C3	-2.03	122.53	126.04
29	c	606	CHL	CHD-C1D-C2D	2.03	129.73	125.48
21	B	821	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
21	A	818	CLA	O2D-CGD-CBD	2.03	114.87	111.27
21	2	609	CLA	C1B-CHB-C4A	-2.03	126.10	130.12
21	6	612	CLA	O2A-CGA-O1A	-2.03	118.25	123.30
21	F	302	CLA	O2A-CGA-O1A	-2.03	118.48	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	b	304	CLA	O2A-CGA-O1A	-2.03	118.25	123.30
21	A	827	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
21	B	817	CLA	C1-C2-C3	-2.02	122.54	126.04
29	c	607	CHL	O1D-CGD-CBD	-2.02	120.34	124.48
29	9	601	CHL	CAC-C3C-C4C	2.02	127.44	124.81
21	F	304	CLA	O2A-CGA-O1A	-2.02	118.25	123.30
21	2	604	CLA	CHD-C1D-ND	-2.02	122.59	124.45
29	3	407	CHL	CMA-C3A-C2A	-2.02	111.38	116.10
21	1	313	CLA	O2A-CGA-O1A	-2.02	118.25	123.30
29	4	607	CHL	C3C-C4C-NC	2.02	112.84	110.57
21	A	813	CLA	CHD-C1D-ND	-2.02	122.59	124.45
24	B	842	BCR	C8-C9-C10	2.02	122.05	118.94
21	A	804	CLA	O2D-CGD-CBD	2.02	114.86	111.27
29	2	605	CHL	O1D-CGD-CBD	-2.02	120.35	124.48
21	2	613	CLA	CHD-C1D-ND	-2.02	122.60	124.45
21	7	407	CLA	C1B-CHB-C4A	-2.02	126.11	130.12
24	J	104	BCR	C7-C6-C5	2.02	126.36	121.46
21	c	602	CLA	C1-C2-C3	-2.02	122.55	126.04
30	4	615	LUT	C39-C29-C28	2.02	121.26	118.08
29	a	609	CHL	C3D-C2D-C1D	2.02	108.59	105.83
21	A	815	CLA	O2A-CGA-O1A	-2.02	118.27	123.30
29	2	602	CHL	C1-O2A-CGA	2.02	121.74	116.44
21	c	610	CLA	O2A-CGA-O1A	-2.02	118.27	123.30
21	A	852	CLA	CHB-C4A-NA	2.02	127.30	124.51
21	9	611	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
21	4	612	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
21	6	609	CLA	CAA-C2A-C3A	-2.02	109.22	114.26
24	3	418	BCR	C8-C9-C10	2.01	122.03	118.94
29	1	307	CHL	O1D-CGD-CBD	-2.01	120.36	124.48
21	3	409	CLA	CHA-C4D-ND	-2.01	128.28	132.50
30	c	615	LUT	C19-C9-C8	2.01	121.25	118.08
21	A	818	CLA	CHB-C4A-NA	2.01	127.30	124.51
24	J	103	BCR	C23-C22-C21	2.01	122.03	118.94
21	A	825	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
24	A	846	BCR	C23-C22-C21	2.01	122.03	118.94
29	2	606	CHL	O1D-CGD-CBD	-2.01	120.37	124.48
29	2	614	CHL	O2A-CGA-CBA	2.01	120.49	114.03
21	1	304	CLA	C1-C2-C3	-2.01	122.56	126.04
21	L	303	CLA	O2A-CGA-O1A	-2.01	118.29	123.30
21	A	812	CLA	CHD-C1D-ND	-2.01	122.61	124.45
29	6	605	CHL	C3D-C4D-CHA	-2.01	108.12	112.72
21	B	814	CLA	O2A-CGA-O1A	-2.01	118.52	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	a	611	CLA	CHD-C1D-ND	-2.01	122.61	124.45
21	A	828	CLA	CHB-C4A-NA	2.01	127.29	124.51
21	A	834	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
21	F	304	CLA	CHD-C1D-ND	-2.01	122.61	124.45
21	A	830	CLA	C1B-CHB-C4A	-2.01	126.14	130.12
21	8	611	CLA	C1-C2-C3	-2.01	122.57	126.04
29	4	605	CHL	O1D-CGD-CBD	-2.01	120.38	124.48
21	A	828	CLA	CHD-C1D-ND	-2.01	122.61	124.45
21	1	314	CLA	CHD-C1D-ND	-2.01	122.61	124.45
21	5	602	CLA	CHD-C1D-ND	-2.01	122.61	124.45
24	G	205	BCR	C23-C22-C21	2.01	122.02	118.94
21	A	808	CLA	O2A-CGA-O1A	-2.00	118.30	123.30
21	B	819	CLA	CHD-C1D-ND	-2.00	122.61	124.45
29	3	407	CHL	C4C-C3C-C2C	-2.00	103.98	106.90
21	A	819	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
21	A	816	CLA	CHD-C1D-ND	-2.00	122.61	124.45
21	A	803	CLA	C1-C2-C3	-2.00	122.58	126.04
31	a	618	XAT	O4-C5-C4	-2.00	111.88	113.38
21	B	834	CLA	O2A-CGA-O1A	-2.00	118.31	123.30
21	c	611	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
29	9	609	CHL	C3C-C4C-NC	2.00	112.81	110.57
29	4	605	CHL	C4D-C3D-CAD	2.00	110.45	108.10
29	6	614	CHL	CED-O2D-CGD	2.00	120.46	115.94
21	1	311	CLA	CMA-C3A-C2A	-2.00	111.43	116.10
21	A	842	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
21	L	302	CLA	CHD-C1D-ND	-2.00	122.62	124.45

All (368) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	A	802	CLA	ND
21	A	803	CLA	ND
21	A	804	CLA	ND
21	A	805	CLA	ND
21	A	806	CLA	ND
21	A	807	CLA	ND
21	A	808	CLA	ND
21	A	809	CLA	ND
21	A	810	CLA	ND
21	A	811	CLA	ND
21	A	812	CLA	ND
21	A	813	CLA	ND

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Mol	Chain	Res	Type	Atom
21	A	814	CLA	ND
21	A	815	CLA	ND
21	A	816	CLA	ND
21	A	817	CLA	ND
21	A	818	CLA	ND
21	A	819	CLA	ND
21	A	820	CLA	ND
21	A	821	CLA	ND
21	A	822	CLA	ND
21	A	823	CLA	ND
21	A	824	CLA	ND
21	A	825	CLA	ND
21	A	826	CLA	ND
21	A	827	CLA	ND
21	A	828	CLA	ND
21	A	829	CLA	ND
21	A	830	CLA	ND
21	A	831	CLA	ND
21	A	832	CLA	ND
21	A	833	CLA	ND
21	A	834	CLA	ND
21	A	835	CLA	ND
21	A	836	CLA	ND
21	A	837	CLA	ND
21	A	838	CLA	ND
21	A	839	CLA	ND
21	A	840	CLA	ND
21	A	841	CLA	ND
21	A	842	CLA	ND
21	A	852	CLA	ND
21	B	801	CLA	ND
21	B	802	CLA	ND
21	B	803	CLA	ND
21	B	804	CLA	ND
21	B	805	CLA	ND
21	B	806	CLA	ND
21	B	807	CLA	ND
21	B	808	CLA	ND
21	B	809	CLA	ND
21	B	810	CLA	ND
21	B	811	CLA	ND
21	B	812	CLA	ND

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Mol	Chain	Res	Type	Atom
21	B	813	CLA	ND
21	B	814	CLA	ND
21	B	815	CLA	ND
21	B	816	CLA	ND
21	B	817	CLA	ND
21	B	818	CLA	ND
21	B	819	CLA	ND
21	B	820	CLA	ND
21	B	821	CLA	ND
21	B	822	CLA	ND
21	B	823	CLA	ND
21	B	824	CLA	ND
21	B	825	CLA	ND
21	B	826	CLA	ND
21	B	827	CLA	ND
21	B	828	CLA	ND
21	B	829	CLA	ND
21	B	830	CLA	ND
21	B	831	CLA	ND
21	B	832	CLA	ND
21	B	833	CLA	ND
21	B	834	CLA	ND
21	B	835	CLA	ND
21	B	836	CLA	ND
21	B	837	CLA	ND
21	B	838	CLA	ND
21	B	839	CLA	ND
21	B	840	CLA	ND
21	F	302	CLA	ND
21	F	304	CLA	ND
21	F	305	CLA	ND
21	G	202	CLA	ND
21	G	203	CLA	ND
21	G	204	CLA	ND
21	H	201	CLA	ND
21	J	102	CLA	ND
21	K	201	CLA	ND
21	K	202	CLA	ND
21	K	203	CLA	ND
21	K	204	CLA	ND
21	L	302	CLA	ND
21	L	303	CLA	ND

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Mol	Chain	Res	Type	Atom
21	L	304	CLA	ND
21	O	201	CLA	ND
21	O	202	CLA	ND
21	O	203	CLA	ND
21	O	204	CLA	ND
21	1	303	CLA	ND
21	1	304	CLA	ND
21	1	305	CLA	ND
21	1	306	CLA	ND
21	1	308	CLA	ND
21	1	309	CLA	ND
21	1	310	CLA	ND
21	1	311	CLA	ND
21	1	312	CLA	ND
21	1	313	CLA	ND
21	1	314	CLA	ND
21	1	315	CLA	ND
21	1	316	CLA	ND
21	2	603	CLA	ND
21	2	604	CLA	ND
21	2	608	CLA	ND
21	2	609	CLA	ND
21	2	610	CLA	ND
21	2	611	CLA	ND
21	2	612	CLA	ND
21	2	613	CLA	ND
21	3	401	CLA	ND
21	3	402	CLA	ND
21	3	403	CLA	ND
21	3	404	CLA	ND
21	3	405	CLA	ND
21	3	406	CLA	ND
21	3	408	CLA	ND
21	3	409	CLA	ND
21	3	410	CLA	ND
21	3	411	CLA	ND
21	3	412	CLA	ND
21	3	413	CLA	ND
21	3	414	CLA	ND
21	3	415	CLA	ND
21	4	601	CLA	ND
21	4	602	CLA	ND

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Mol	Chain	Res	Type	Atom
21	4	603	CLA	ND
21	4	604	CLA	ND
21	4	608	CLA	ND
21	4	610	CLA	ND
21	4	611	CLA	ND
21	4	612	CLA	ND
21	4	613	CLA	ND
21	5	602	CLA	ND
21	5	603	CLA	ND
21	5	604	CLA	ND
21	5	605	CLA	ND
21	5	607	CLA	ND
21	5	608	CLA	ND
21	5	609	CLA	ND
21	5	610	CLA	ND
21	5	611	CLA	ND
21	5	612	CLA	ND
21	5	613	CLA	ND
21	5	614	CLA	ND
21	6	603	CLA	ND
21	6	604	CLA	ND
21	6	608	CLA	ND
21	6	609	CLA	ND
21	6	610	CLA	ND
21	6	611	CLA	ND
21	6	612	CLA	ND
21	6	613	CLA	ND
21	7	401	CLA	ND
21	7	402	CLA	ND
21	7	403	CLA	ND
21	7	404	CLA	ND
21	7	405	CLA	ND
21	7	408	CLA	ND
21	7	409	CLA	ND
21	7	410	CLA	ND
21	7	411	CLA	ND
21	7	412	CLA	ND
21	7	413	CLA	ND
21	7	414	CLA	ND
21	8	601	CLA	ND
21	8	602	CLA	ND
21	8	603	CLA	ND

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Mol	Chain	Res	Type	Atom
21	8	604	CLA	ND
21	8	608	CLA	ND
21	8	609	CLA	ND
21	8	610	CLA	ND
21	8	611	CLA	ND
21	8	612	CLA	ND
21	8	618	CLA	ND
21	9	602	CLA	ND
21	9	603	CLA	ND
21	9	604	CLA	ND
21	9	610	CLA	ND
21	9	611	CLA	ND
21	9	612	CLA	ND
21	9	613	CLA	ND
21	a	602	CLA	ND
21	a	603	CLA	ND
21	a	604	CLA	ND
21	a	610	CLA	ND
21	a	611	CLA	ND
21	a	612	CLA	ND
21	a	613	CLA	ND
21	a	614	CLA	ND
21	b	303	CLA	ND
21	b	304	CLA	ND
21	b	305	CLA	ND
21	b	311	CLA	ND
21	b	312	CLA	ND
21	b	313	CLA	ND
21	b	314	CLA	ND
21	b	315	CLA	ND
21	c	602	CLA	ND
21	c	603	CLA	ND
21	c	604	CLA	ND
21	c	610	CLA	ND
21	c	611	CLA	ND
21	c	612	CLA	ND
21	c	613	CLA	ND
21	c	614	CLA	ND
29	1	302	CHL	NC
29	1	302	CHL	NA
29	1	302	CHL	ND
29	1	307	CHL	NC

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Mol	Chain	Res	Type	Atom
29	1	307	CHL	NA
29	1	307	CHL	ND
29	2	601	CHL	NC
29	2	601	CHL	NA
29	2	601	CHL	ND
29	2	602	CHL	NC
29	2	602	CHL	NA
29	2	602	CHL	ND
29	2	605	CHL	NC
29	2	605	CHL	NA
29	2	605	CHL	ND
29	2	606	CHL	NC
29	2	606	CHL	NA
29	2	606	CHL	ND
29	2	607	CHL	NC
29	2	607	CHL	NA
29	2	607	CHL	ND
29	2	614	CHL	NC
29	2	614	CHL	NA
29	2	614	CHL	ND
29	3	407	CHL	NC
29	3	407	CHL	NA
29	3	407	CHL	ND
29	4	605	CHL	NC
29	4	605	CHL	NA
29	4	605	CHL	ND
29	4	606	CHL	NC
29	4	606	CHL	NA
29	4	606	CHL	ND
29	4	607	CHL	NC
29	4	607	CHL	NA
29	4	607	CHL	ND
29	4	614	CHL	NC
29	4	614	CHL	NA
29	4	614	CHL	ND
29	5	601	CHL	NC
29	5	601	CHL	NA
29	5	601	CHL	ND
29	5	606	CHL	NC
29	5	606	CHL	NA
29	5	606	CHL	ND
29	6	601	CHL	NC

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Mol	Chain	Res	Type	Atom
29	6	601	CHL	NA
29	6	601	CHL	ND
29	6	602	CHL	NC
29	6	602	CHL	NA
29	6	602	CHL	ND
29	6	605	CHL	NC
29	6	605	CHL	NA
29	6	605	CHL	ND
29	6	606	CHL	NC
29	6	606	CHL	NA
29	6	606	CHL	ND
29	6	607	CHL	NC
29	6	607	CHL	NA
29	6	607	CHL	ND
29	6	614	CHL	NC
29	6	614	CHL	NA
29	6	614	CHL	ND
29	7	406	CHL	NC
29	7	406	CHL	NA
29	7	406	CHL	ND
29	8	605	CHL	NC
29	8	605	CHL	NA
29	8	605	CHL	ND
29	8	606	CHL	NC
29	8	606	CHL	NA
29	8	606	CHL	ND
29	8	607	CHL	NC
29	8	607	CHL	NA
29	8	607	CHL	ND
29	8	613	CHL	NC
29	8	613	CHL	NA
29	8	613	CHL	ND
29	9	601	CHL	NC
29	9	601	CHL	NA
29	9	601	CHL	ND
29	9	605	CHL	NC
29	9	605	CHL	NA
29	9	605	CHL	ND
29	9	606	CHL	NC
29	9	606	CHL	NA
29	9	606	CHL	ND
29	9	607	CHL	NC

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Mol	Chain	Res	Type	Atom
29	9	607	CHL	NA
29	9	607	CHL	ND
29	9	608	CHL	NC
29	9	608	CHL	NA
29	9	608	CHL	ND
29	9	609	CHL	NC
29	9	609	CHL	NA
29	9	609	CHL	ND
29	a	601	CHL	NC
29	a	601	CHL	NA
29	a	601	CHL	ND
29	a	605	CHL	NC
29	a	605	CHL	NA
29	a	605	CHL	ND
29	a	606	CHL	NC
29	a	606	CHL	NA
29	a	606	CHL	ND
29	a	607	CHL	NC
29	a	607	CHL	NA
29	a	607	CHL	ND
29	a	608	CHL	NC
29	a	608	CHL	NA
29	a	608	CHL	ND
29	a	609	CHL	NC
29	a	609	CHL	NA
29	a	609	CHL	ND
29	b	302	CHL	NC
29	b	302	CHL	NA
29	b	302	CHL	ND
29	b	306	CHL	NC
29	b	306	CHL	NA
29	b	306	CHL	ND
29	b	307	CHL	NC
29	b	307	CHL	NA
29	b	307	CHL	ND
29	b	308	CHL	NC
29	b	308	CHL	NA
29	b	308	CHL	ND
29	b	309	CHL	NC
29	b	309	CHL	NA
29	b	309	CHL	ND
29	b	310	CHL	NC

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Mol	Chain	Res	Type	Atom
29	b	310	CHL	NA
29	b	310	CHL	ND
29	c	601	CHL	NC
29	c	601	CHL	NA
29	c	601	CHL	ND
29	c	605	CHL	NC
29	c	605	CHL	NA
29	c	605	CHL	ND
29	c	606	CHL	NC
29	c	606	CHL	NA
29	c	606	CHL	ND
29	c	607	CHL	NC
29	c	607	CHL	NA
29	c	607	CHL	ND
29	c	608	CHL	NC
29	c	608	CHL	NA
29	c	608	CHL	ND
29	c	609	CHL	NC
29	c	609	CHL	NA
29	c	609	CHL	ND

All (1981) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	A	801	CLA	CBD-CGD-O2D-CED
21	A	804	CLA	C1A-C2A-CAA-CBA
21	A	805	CLA	C3A-C2A-CAA-CBA
21	A	806	CLA	CHA-CBD-CGD-O1D
21	A	806	CLA	CHA-CBD-CGD-O2D
21	A	806	CLA	CAD-CBD-CGD-O1D
21	A	806	CLA	CAD-CBD-CGD-O2D
21	A	807	CLA	C1A-C2A-CAA-CBA
21	A	807	CLA	C3A-C2A-CAA-CBA
21	A	807	CLA	CBD-CGD-O2D-CED
21	A	818	CLA	C3A-C2A-CAA-CBA
21	A	818	CLA	C2-C3-C5-C6
21	A	818	CLA	C4-C3-C5-C6
21	A	819	CLA	C1A-C2A-CAA-CBA
21	A	819	CLA	C3A-C2A-CAA-CBA
21	A	822	CLA	C2A-CAA-CBA-CGA
21	A	824	CLA	CHA-CBD-CGD-O1D
21	A	824	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
21	A	826	CLA	C3A-C2A-CAA-CBA
21	A	827	CLA	C1A-C2A-CAA-CBA
21	A	827	CLA	C3A-C2A-CAA-CBA
21	A	827	CLA	C2A-CAA-CBA-CGA
21	A	827	CLA	CHA-CBD-CGD-O2D
21	A	832	CLA	C1A-C2A-CAA-CBA
21	A	832	CLA	C3A-C2A-CAA-CBA
21	A	834	CLA	CHA-CBD-CGD-O2D
21	A	836	CLA	CHA-CBD-CGD-O1D
21	A	836	CLA	CHA-CBD-CGD-O2D
21	A	837	CLA	C1A-C2A-CAA-CBA
21	A	838	CLA	C2-C3-C5-C6
21	A	838	CLA	C4-C3-C5-C6
21	A	841	CLA	C1A-C2A-CAA-CBA
21	A	842	CLA	C2A-CAA-CBA-CGA
21	A	842	CLA	C2-C1-O2A-CGA
21	A	852	CLA	C2-C3-C5-C6
21	A	852	CLA	C4-C3-C5-C6
21	B	802	CLA	CHA-CBD-CGD-O1D
21	B	802	CLA	CHA-CBD-CGD-O2D
21	B	802	CLA	CBD-CGD-O2D-CED
21	B	804	CLA	C1A-C2A-CAA-CBA
21	B	804	CLA	C3A-C2A-CAA-CBA
21	B	806	CLA	CHA-CBD-CGD-O1D
21	B	807	CLA	C1A-C2A-CAA-CBA
21	B	811	CLA	C1A-C2A-CAA-CBA
21	B	817	CLA	C1A-C2A-CAA-CBA
21	B	817	CLA	C3A-C2A-CAA-CBA
21	B	818	CLA	C1A-C2A-CAA-CBA
21	B	818	CLA	C2A-CAA-CBA-CGA
21	B	818	CLA	CHA-CBD-CGD-O1D
21	B	818	CLA	CHA-CBD-CGD-O2D
21	B	827	CLA	C1A-C2A-CAA-CBA
21	B	827	CLA	C3A-C2A-CAA-CBA
21	B	830	CLA	C1A-C2A-CAA-CBA
21	B	830	CLA	C3A-C2A-CAA-CBA
21	B	832	CLA	C1A-C2A-CAA-CBA
21	B	834	CLA	C1A-C2A-CAA-CBA
21	B	834	CLA	C3A-C2A-CAA-CBA
21	B	836	CLA	C1A-C2A-CAA-CBA
21	B	836	CLA	C3A-C2A-CAA-CBA
21	B	839	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
21	B	839	CLA	CHA-CBD-CGD-O1D
21	B	839	CLA	CAD-CBD-CGD-O1D
21	B	839	CLA	CAD-CBD-CGD-O2D
21	G	202	CLA	C1A-C2A-CAA-CBA
21	G	202	CLA	C3A-C2A-CAA-CBA
21	G	202	CLA	CBD-CGD-O2D-CED
21	G	203	CLA	CBD-CGD-O2D-CED
21	J	102	CLA	C1A-C2A-CAA-CBA
21	J	102	CLA	C3A-C2A-CAA-CBA
21	J	102	CLA	CHA-CBD-CGD-O1D
21	J	102	CLA	CHA-CBD-CGD-O2D
21	J	102	CLA	CAD-CBD-CGD-O1D
21	K	202	CLA	C1A-C2A-CAA-CBA
21	L	302	CLA	C1A-C2A-CAA-CBA
21	O	201	CLA	CHA-CBD-CGD-O1D
21	O	201	CLA	CHA-CBD-CGD-O2D
21	O	201	CLA	CAD-CBD-CGD-O1D
21	O	201	CLA	CAD-CBD-CGD-O2D
21	1	303	CLA	C3A-C2A-CAA-CBA
21	1	305	CLA	C1A-C2A-CAA-CBA
21	1	305	CLA	C3A-C2A-CAA-CBA
21	1	306	CLA	CHA-CBD-CGD-O1D
21	1	306	CLA	CHA-CBD-CGD-O2D
21	1	306	CLA	CBD-CGD-O2D-CED
21	1	312	CLA	CBD-CGD-O2D-CED
21	1	316	CLA	C2A-CAA-CBA-CGA
21	1	316	CLA	CBD-CGD-O2D-CED
21	2	603	CLA	CBD-CGD-O2D-CED
21	2	604	CLA	CHA-CBD-CGD-O1D
21	2	604	CLA	CHA-CBD-CGD-O2D
21	2	608	CLA	C1A-C2A-CAA-CBA
21	2	608	CLA	C3A-C2A-CAA-CBA
21	2	609	CLA	C1A-C2A-CAA-CBA
21	2	609	CLA	C3A-C2A-CAA-CBA
21	2	609	CLA	C4C-C3C-CAC-CBC
21	2	609	CLA	CBD-CGD-O2D-CED
21	2	609	CLA	O1D-CGD-O2D-CED
21	3	408	CLA	C2-C3-C5-C6
21	3	408	CLA	C4-C3-C5-C6
21	3	409	CLA	C1A-C2A-CAA-CBA
21	3	409	CLA	C3A-C2A-CAA-CBA
21	3	409	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	3	411	CLA	CBD-CGD-O2D-CED
21	4	601	CLA	CHA-CBD-CGD-O1D
21	4	602	CLA	C3A-C2A-CAA-CBA
21	4	609	CLA	C3A-C2A-CAA-CBA
21	4	609	CLA	CBD-CGD-O2D-CED
21	5	602	CLA	C3A-C2A-CAA-CBA
21	5	607	CLA	C1A-C2A-CAA-CBA
21	5	607	CLA	C3A-C2A-CAA-CBA
21	5	608	CLA	CHA-CBD-CGD-O1D
21	5	608	CLA	CHA-CBD-CGD-O2D
21	5	608	CLA	CBD-CGD-O2D-CED
21	5	612	CLA	C1A-C2A-CAA-CBA
21	5	612	CLA	C3A-C2A-CAA-CBA
21	5	612	CLA	CBD-CGD-O2D-CED
21	6	603	CLA	CBD-CGD-O2D-CED
21	6	604	CLA	C1A-C2A-CAA-CBA
21	6	604	CLA	C3A-C2A-CAA-CBA
21	6	608	CLA	C3A-C2A-CAA-CBA
21	6	609	CLA	C1A-C2A-CAA-CBA
21	6	609	CLA	C3A-C2A-CAA-CBA
21	6	609	CLA	CBD-CGD-O2D-CED
21	6	613	CLA	CBD-CGD-O2D-CED
21	7	401	CLA	CHA-CBD-CGD-O1D
21	7	401	CLA	CHA-CBD-CGD-O2D
21	7	402	CLA	C1A-C2A-CAA-CBA
21	7	402	CLA	C3A-C2A-CAA-CBA
21	7	402	CLA	CHA-CBD-CGD-O1D
21	7	402	CLA	CHA-CBD-CGD-O2D
21	7	402	CLA	CAD-CBD-CGD-O1D
21	7	405	CLA	C1A-C2A-CAA-CBA
21	7	405	CLA	C3A-C2A-CAA-CBA
21	7	407	CLA	C3A-C2A-CAA-CBA
21	8	601	CLA	CHA-CBD-CGD-O1D
21	8	601	CLA	CHA-CBD-CGD-O2D
21	8	601	CLA	CAD-CBD-CGD-O1D
21	8	601	CLA	CAD-CBD-CGD-O2D
21	8	602	CLA	C1A-C2A-CAA-CBA
21	8	602	CLA	C3A-C2A-CAA-CBA
21	8	604	CLA	C1A-C2A-CAA-CBA
21	8	608	CLA	C1A-C2A-CAA-CBA
21	8	608	CLA	C3A-C2A-CAA-CBA
21	8	609	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
21	8	611	CLA	CBD-CGD-O2D-CED
21	8	612	CLA	CBD-CGD-O2D-CED
21	8	618	CLA	CBD-CGD-O2D-CED
21	9	611	CLA	C2-C3-C5-C6
21	9	611	CLA	C4-C3-C5-C6
21	a	602	CLA	CBD-CGD-O2D-CED
21	a	604	CLA	C1A-C2A-CAA-CBA
21	a	604	CLA	C3A-C2A-CAA-CBA
21	a	611	CLA	CHA-CBD-CGD-O1D
21	a	611	CLA	CHA-CBD-CGD-O2D
21	b	303	CLA	CBD-CGD-O2D-CED
21	b	314	CLA	CHA-CBD-CGD-O1D
21	b	314	CLA	CHA-CBD-CGD-O2D
21	b	314	CLA	CBD-CGD-O2D-CED
21	b	315	CLA	CHA-CBD-CGD-O1D
21	b	315	CLA	CHA-CBD-CGD-O2D
21	c	604	CLA	CAD-CBD-CGD-O1D
21	c	604	CLA	CAD-CBD-CGD-O2D
21	c	610	CLA	CHA-CBD-CGD-O1D
21	c	610	CLA	CHA-CBD-CGD-O2D
21	c	610	CLA	CBD-CGD-O2D-CED
21	c	613	CLA	CHA-CBD-CGD-O1D
21	c	613	CLA	CHA-CBD-CGD-O2D
21	c	614	CLA	CHA-CBD-CGD-O1D
21	c	614	CLA	CHA-CBD-CGD-O2D
21	c	614	CLA	CAD-CBD-CGD-O1D
23	A	844	LHG	C4-O6-P-O5
23	A	855	LHG	O10-C23-O8-C6
23	A	855	LHG	C24-C23-O8-C6
23	1	301	LHG	C4-O6-P-O3
23	1	301	LHG	O9-C7-O7-C5
23	1	301	LHG	C8-C7-O7-C5
23	1	319	LHG	C4-O6-P-O3
23	1	319	LHG	O10-C23-O8-C6
23	1	319	LHG	C24-C23-O8-C6
23	2	619	LHG	C3-O3-P-O5
23	2	619	LHG	C3-O3-P-O6
23	4	618	LHG	C4-O6-P-O5
23	4	618	LHG	O7-C5-C6-O8
23	4	619	LHG	C2-C3-O3-P
23	4	619	LHG	C5-C4-O6-P
23	4	619	LHG	O9-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
23	4	619	LHG	C8-C7-O7-C5
23	4	619	LHG	O10-C23-O8-C6
23	4	619	LHG	C24-C23-O8-C6
23	5	617	LHG	C2-C3-O3-P
23	5	617	LHG	C4-O6-P-O5
23	5	617	LHG	O10-C23-O8-C6
23	5	617	LHG	C24-C23-O8-C6
23	6	619	LHG	C3-O3-P-O5
23	8	617	LHG	C2-C3-O3-P
23	8	617	LHG	C4-O6-P-O4
23	8	617	LHG	C5-C4-O6-P
23	8	617	LHG	O10-C23-O8-C6
23	8	617	LHG	C24-C23-O8-C6
23	9	618	LHG	C3-O3-P-O5
23	9	618	LHG	O10-C23-O8-C6
23	9	618	LHG	C24-C23-O8-C6
23	a	617	LHG	C3-O3-P-O5
23	a	617	LHG	O10-C23-O8-C6
23	a	617	LHG	C24-C23-O8-C6
23	b	319	LHG	C4-O6-P-O5
23	b	319	LHG	O10-C23-O8-C6
23	b	319	LHG	C24-C23-O8-C6
23	c	619	LHG	O10-C23-O8-C6
23	c	619	LHG	C24-C23-O8-C6
24	A	846	BCR	C1-C6-C7-C8
24	B	843	BCR	C7-C8-C9-C34
24	B	843	BCR	C11-C12-C13-C14
24	B	843	BCR	C11-C12-C13-C35
24	B	843	BCR	C36-C18-C19-C20
24	B	843	BCR	C23-C24-C25-C30
24	B	844	BCR	C11-C12-C13-C14
24	B	844	BCR	C11-C12-C13-C35
24	B	846	BCR	C7-C8-C9-C10
24	B	846	BCR	C7-C8-C9-C34
24	I	101	BCR	C7-C8-C9-C10
24	I	101	BCR	C7-C8-C9-C34
24	J	103	BCR	C9-C10-C11-C12
24	J	104	BCR	C11-C12-C13-C14
24	J	104	BCR	C11-C12-C13-C35
24	J	104	BCR	C23-C24-C25-C26
24	J	104	BCR	C23-C24-C25-C30
24	L	306	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
24	L	306	BCR	C37-C22-C23-C24
24	M	101	BCR	C1-C6-C7-C8
24	M	101	BCR	C5-C6-C7-C8
24	M	101	BCR	C7-C8-C9-C10
24	O	205	BCR	C7-C8-C9-C10
24	O	205	BCR	C7-C8-C9-C34
24	O	205	BCR	C21-C22-C23-C24
24	O	205	BCR	C37-C22-C23-C24
24	3	419	BCR	C1-C6-C7-C8
24	3	419	BCR	C21-C22-C23-C24
24	3	419	BCR	C37-C22-C23-C24
24	4	617	BCR	C23-C24-C25-C30
24	6	618	BCR	C5-C6-C7-C8
24	7	418	BCR	C1-C6-C7-C8
24	7	418	BCR	C21-C22-C23-C24
24	7	418	BCR	C37-C22-C23-C24
24	8	616	BCR	C20-C21-C22-C37
24	8	616	BCR	C23-C24-C25-C26
24	8	616	BCR	C23-C24-C25-C30
27	B	847	DGD	O6D-C1D-O3G-C3G
28	J	105	LMG	C2-C1-O1-C7
28	J	105	LMG	O6-C1-O1-C7
28	J	105	LMG	O10-C28-O8-C9
28	J	105	LMG	C29-C28-O8-C9
29	1	302	CHL	C1A-C2A-CAA-CBA
29	2	602	CHL	C3A-C2A-CAA-CBA
29	4	607	CHL	C2A-CAA-CBA-CGA
29	4	607	CHL	CBD-CGD-O2D-CED
29	5	601	CHL	C3C-C2C-CMC-OMC
29	5	601	CHL	CHA-CBD-CGD-O1D
29	5	601	CHL	CHA-CBD-CGD-O2D
29	6	607	CHL	CBD-CGD-O2D-CED
29	9	601	CHL	CBD-CGD-O2D-CED
29	a	608	CHL	CBD-CGD-O2D-CED
29	b	302	CHL	C1A-C2A-CAA-CBA
29	b	308	CHL	C2-C3-C5-C6
29	b	308	CHL	C4-C3-C5-C6
29	c	608	CHL	C1A-C2A-CAA-CBA
29	c	608	CHL	C3A-C2A-CAA-CBA
29	c	609	CHL	C3C-C2C-CMC-OMC
30	2	616	LUT	C7-C8-C9-C10
30	2	616	LUT	C7-C8-C9-C19

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Mol	Chain	Res	Type	Atoms
30	3	416	LUT	C1-C6-C7-C8
30	5	615	LUT	C1-C6-C7-C8
30	7	415	LUT	C9-C10-C11-C12
30	7	415	LUT	C21-C26-C27-C28
30	7	415	LUT	C25-C26-C27-C28
30	7	415	LUT	C27-C28-C29-C30
30	7	415	LUT	C27-C28-C29-C39
30	a	615	LUT	C26-C27-C28-C29
30	a	615	LUT	C27-C28-C29-C39
30	a	616	LUT	C7-C8-C9-C10
30	a	616	LUT	C7-C8-C9-C19
31	5	616	XAT	O4-C6-C7-C8
31	6	617	XAT	C5-C6-C7-C8
31	6	617	XAT	O4-C6-C7-C8
31	6	617	XAT	C11-C12-C13-C20
31	9	616	XAT	C7-C8-C9-C10
31	9	616	XAT	C7-C8-C9-C19
31	9	616	XAT	C25-C26-C27-C28
31	c	617	XAT	O24-C26-C27-C28
21	2	609	CLA	C2C-C3C-CAC-CBC
21	A	801	CLA	O1D-CGD-O2D-CED
21	1	306	CLA	O1D-CGD-O2D-CED
21	3	409	CLA	O1D-CGD-O2D-CED
21	6	603	CLA	O1D-CGD-O2D-CED
21	8	611	CLA	O1D-CGD-O2D-CED
21	b	313	CLA	O1D-CGD-O2D-CED
21	c	610	CLA	O1D-CGD-O2D-CED
21	A	807	CLA	O1D-CGD-O2D-CED
21	G	203	CLA	O1D-CGD-O2D-CED
21	2	603	CLA	O1D-CGD-O2D-CED
21	4	609	CLA	O1D-CGD-O2D-CED
21	5	608	CLA	O1D-CGD-O2D-CED
21	7	408	CLA	O1D-CGD-O2D-CED
21	8	604	CLA	O1D-CGD-O2D-CED
21	8	612	CLA	O1D-CGD-O2D-CED
29	8	607	CHL	O1D-CGD-O2D-CED
21	A	811	CLA	CBD-CGD-O2D-CED
21	B	819	CLA	CBD-CGD-O2D-CED
21	B	834	CLA	CBD-CGD-O2D-CED
21	F	302	CLA	CBD-CGD-O2D-CED
21	1	313	CLA	CBD-CGD-O2D-CED
21	3	403	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	4	604	CLA	CBD-CGD-O2D-CED
21	5	605	CLA	CBD-CGD-O2D-CED
21	5	611	CLA	CBD-CGD-O2D-CED
21	5	614	CLA	CBD-CGD-O2D-CED
21	6	608	CLA	CBD-CGD-O2D-CED
21	6	611	CLA	CBD-CGD-O2D-CED
21	6	612	CLA	CBD-CGD-O2D-CED
21	7	408	CLA	CBD-CGD-O2D-CED
21	7	410	CLA	CBD-CGD-O2D-CED
21	8	604	CLA	CBD-CGD-O2D-CED
21	9	602	CLA	CBD-CGD-O2D-CED
21	9	612	CLA	CBD-CGD-O2D-CED
21	9	613	CLA	CBD-CGD-O2D-CED
21	a	611	CLA	CBD-CGD-O2D-CED
21	a	612	CLA	CBD-CGD-O2D-CED
21	b	313	CLA	CBD-CGD-O2D-CED
21	c	613	CLA	CBD-CGD-O2D-CED
29	2	607	CHL	CBD-CGD-O2D-CED
29	8	607	CHL	CBD-CGD-O2D-CED
29	8	613	CHL	CBD-CGD-O2D-CED
29	9	608	CHL	CBD-CGD-O2D-CED
29	b	309	CHL	CBD-CGD-O2D-CED
21	4	604	CLA	O1D-CGD-O2D-CED
21	5	605	CLA	O1D-CGD-O2D-CED
21	5	614	CLA	O1D-CGD-O2D-CED
21	6	609	CLA	O1D-CGD-O2D-CED
21	7	410	CLA	O1D-CGD-O2D-CED
21	9	613	CLA	O1D-CGD-O2D-CED
21	a	612	CLA	O1D-CGD-O2D-CED
21	B	823	CLA	C4C-C3C-CAC-CBC
21	B	802	CLA	O1D-CGD-O2D-CED
21	1	312	CLA	O1D-CGD-O2D-CED
21	1	316	CLA	O1D-CGD-O2D-CED
21	3	411	CLA	O1D-CGD-O2D-CED
21	5	612	CLA	O1D-CGD-O2D-CED
21	6	611	CLA	O1D-CGD-O2D-CED
21	a	602	CLA	O1D-CGD-O2D-CED
21	b	314	CLA	O1D-CGD-O2D-CED
21	c	613	CLA	O1D-CGD-O2D-CED
29	4	607	CHL	O1D-CGD-O2D-CED
29	6	607	CHL	O1D-CGD-O2D-CED
21	A	816	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	A	821	CLA	CBD-CGD-O2D-CED
21	B	803	CLA	CBD-CGD-O2D-CED
21	B	812	CLA	CBD-CGD-O2D-CED
21	B	818	CLA	CBD-CGD-O2D-CED
21	B	839	CLA	CBD-CGD-O2D-CED
21	1	315	CLA	CBD-CGD-O2D-CED
21	2	612	CLA	CBD-CGD-O2D-CED
21	8	609	CLA	CBD-CGD-O2D-CED
21	a	613	CLA	CBD-CGD-O2D-CED
21	c	612	CLA	CBD-CGD-O2D-CED
21	c	614	CLA	CBD-CGD-O2D-CED
21	A	806	CLA	O1A-CGA-O2A-C1
21	A	821	CLA	O1A-CGA-O2A-C1
21	B	814	CLA	O1A-CGA-O2A-C1
21	B	816	CLA	O1A-CGA-O2A-C1
21	3	403	CLA	O1A-CGA-O2A-C1
21	3	408	CLA	O1A-CGA-O2A-C1
21	4	609	CLA	O1A-CGA-O2A-C1
21	5	604	CLA	O1A-CGA-O2A-C1
21	a	611	CLA	O1A-CGA-O2A-C1
21	c	611	CLA	O1A-CGA-O2A-C1
21	6	613	CLA	O1D-CGD-O2D-CED
21	b	303	CLA	O1D-CGD-O2D-CED
29	9	601	CHL	O1D-CGD-O2D-CED
21	8	618	CLA	O1D-CGD-O2D-CED
29	a	608	CHL	O1D-CGD-O2D-CED
21	A	831	CLA	CBD-CGD-O2D-CED
21	A	833	CLA	CBD-CGD-O2D-CED
21	J	102	CLA	CBD-CGD-O2D-CED
29	9	607	CHL	CBD-CGD-O2D-CED
29	9	609	CHL	CBD-CGD-O2D-CED
29	c	608	CHL	CBD-CGD-O2D-CED
21	G	202	CLA	O1D-CGD-O2D-CED
21	A	817	CLA	C3-C5-C6-C7
21	A	828	CLA	C3-C5-C6-C7
21	B	808	CLA	C3-C5-C6-C7
21	5	602	CLA	C3-C5-C6-C7
21	8	602	CLA	C3-C5-C6-C7
21	8	611	CLA	C3-C5-C6-C7
21	A	828	CLA	CBA-CGA-O2A-C1
21	3	408	CLA	CBA-CGA-O2A-C1
21	5	604	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
21	B	823	CLA	C2C-C3C-CAC-CBC
21	5	611	CLA	O1D-CGD-O2D-CED
29	b	309	CHL	O1D-CGD-O2D-CED
21	A	814	CLA	CBD-CGD-O2D-CED
29	6	605	CHL	CBD-CGD-O2D-CED
29	a	609	CHL	CBD-CGD-O2D-CED
29	2	607	CHL	O1D-CGD-O2D-CED
21	A	852	CLA	C3-C5-C6-C7
21	2	609	CLA	C3-C5-C6-C7
21	4	609	CLA	C3-C5-C6-C7
28	6	615	LMG	O6-C1-O1-C7
21	3	409	CLA	C4-C3-C5-C6
21	A	824	CLA	CBD-CGD-O2D-CED
21	b	311	CLA	CBD-CGD-O2D-CED
21	b	315	CLA	CBD-CGD-O2D-CED
29	8	605	CHL	CBD-CGD-O2D-CED
21	A	832	CLA	C2A-CAA-CBA-CGA
21	B	803	CLA	C2A-CAA-CBA-CGA
21	B	827	CLA	C2A-CAA-CBA-CGA
21	B	838	CLA	C2A-CAA-CBA-CGA
21	G	203	CLA	C2A-CAA-CBA-CGA
21	L	302	CLA	C2A-CAA-CBA-CGA
21	5	611	CLA	C2A-CAA-CBA-CGA
21	7	401	CLA	C2A-CAA-CBA-CGA
21	7	402	CLA	C2A-CAA-CBA-CGA
21	7	407	CLA	C2A-CAA-CBA-CGA
21	8	610	CLA	C2A-CAA-CBA-CGA
21	c	604	CLA	C2A-CAA-CBA-CGA
21	c	611	CLA	C2A-CAA-CBA-CGA
29	2	605	CHL	C2A-CAA-CBA-CGA
29	4	606	CHL	C2A-CAA-CBA-CGA
29	5	601	CHL	C2A-CAA-CBA-CGA
29	6	601	CHL	C2A-CAA-CBA-CGA
29	6	606	CHL	C2A-CAA-CBA-CGA
29	6	614	CHL	C2A-CAA-CBA-CGA
29	8	607	CHL	C2A-CAA-CBA-CGA
29	9	606	CHL	C2A-CAA-CBA-CGA
29	9	608	CHL	C2A-CAA-CBA-CGA
29	c	607	CHL	C2A-CAA-CBA-CGA
29	c	608	CHL	C2A-CAA-CBA-CGA
21	A	842	CLA	C3-C5-C6-C7
21	B	809	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
21	B	814	CLA	C3-C5-C6-C7
21	O	203	CLA	C3-C5-C6-C7
21	A	806	CLA	CBA-CGA-O2A-C1
21	A	821	CLA	CBA-CGA-O2A-C1
21	A	842	CLA	CBA-CGA-O2A-C1
21	B	803	CLA	CBA-CGA-O2A-C1
21	B	814	CLA	CBA-CGA-O2A-C1
21	B	816	CLA	CBA-CGA-O2A-C1
21	B	836	CLA	CBA-CGA-O2A-C1
21	1	303	CLA	CBA-CGA-O2A-C1
21	3	403	CLA	CBA-CGA-O2A-C1
21	4	609	CLA	CBA-CGA-O2A-C1
21	a	611	CLA	CBA-CGA-O2A-C1
21	c	611	CLA	CBA-CGA-O2A-C1
21	B	819	CLA	O1D-CGD-O2D-CED
21	1	313	CLA	O1D-CGD-O2D-CED
21	3	403	CLA	O1D-CGD-O2D-CED
21	A	817	CLA	CBD-CGD-O2D-CED
21	A	811	CLA	O1D-CGD-O2D-CED
21	6	608	CLA	O1D-CGD-O2D-CED
21	6	612	CLA	O1D-CGD-O2D-CED
21	A	828	CLA	O1A-CGA-O2A-C1
21	A	842	CLA	O1A-CGA-O2A-C1
21	B	803	CLA	O1A-CGA-O2A-C1
21	B	817	CLA	O1A-CGA-O2A-C1
21	B	826	CLA	O1A-CGA-O2A-C1
28	6	615	LMG	C2-C1-O1-C7
24	J	101	BCR	C19-C20-C21-C22
30	5	615	LUT	C9-C10-C11-C12
26	b	301	LMU	O5B-C5B-C6B-O6B
21	A	806	CLA	CBD-CGD-O2D-CED
21	A	834	CLA	CBD-CGD-O2D-CED
21	A	841	CLA	CBD-CGD-O2D-CED
21	A	852	CLA	CBD-CGD-O2D-CED
21	B	817	CLA	CBD-CGD-O2D-CED
21	B	822	CLA	CBD-CGD-O2D-CED
21	B	826	CLA	CBD-CGD-O2D-CED
21	B	828	CLA	CBD-CGD-O2D-CED
21	2	604	CLA	CBD-CGD-O2D-CED
21	3	402	CLA	CBD-CGD-O2D-CED
21	5	602	CLA	CBD-CGD-O2D-CED
21	6	604	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	4	614	CHL	CBD-CGD-O2D-CED
29	6	614	CHL	CBD-CGD-O2D-CED
21	B	801	CLA	C3-C5-C6-C7
21	4	602	CLA	C3-C5-C6-C7
21	A	838	CLA	CBA-CGA-O2A-C1
21	B	817	CLA	CBA-CGA-O2A-C1
21	B	826	CLA	CBA-CGA-O2A-C1
29	1	307	CHL	CBA-CGA-O2A-C1
21	F	302	CLA	O1D-CGD-O2D-CED
21	9	612	CLA	O1D-CGD-O2D-CED
29	9	608	CHL	O1D-CGD-O2D-CED
21	B	820	CLA	CBA-CGA-O2A-C1
21	A	819	CLA	CBD-CGD-O2D-CED
21	A	828	CLA	CBD-CGD-O2D-CED
21	A	840	CLA	CBD-CGD-O2D-CED
21	K	203	CLA	CBD-CGD-O2D-CED
21	b	304	CLA	CBD-CGD-O2D-CED
29	c	606	CHL	CBD-CGD-O2D-CED
21	A	838	CLA	O1A-CGA-O2A-C1
21	A	806	CLA	C3-C5-C6-C7
21	B	830	CLA	C3-C5-C6-C7
21	9	602	CLA	O1D-CGD-O2D-CED
21	B	836	CLA	O1A-CGA-O2A-C1
21	1	303	CLA	O1A-CGA-O2A-C1
29	1	307	CHL	O1A-CGA-O2A-C1
21	A	817	CLA	C4-C3-C5-C6
21	B	830	CLA	C4-C3-C5-C6
21	4	609	CLA	C4-C3-C5-C6
21	A	817	CLA	C2-C3-C5-C6
21	B	830	CLA	C2-C3-C5-C6
21	4	609	CLA	C2-C3-C5-C6
29	b	302	CHL	CBD-CGD-O2D-CED
21	A	809	CLA	C2A-CAA-CBA-CGA
21	K	204	CLA	C2A-CAA-CBA-CGA
21	4	609	CLA	C2A-CAA-CBA-CGA
21	9	604	CLA	C2A-CAA-CBA-CGA
29	6	605	CHL	C2A-CAA-CBA-CGA
29	a	605	CHL	C2A-CAA-CBA-CGA
29	b	302	CHL	C2A-CAA-CBA-CGA
21	a	611	CLA	O1D-CGD-O2D-CED
21	A	819	CLA	CBA-CGA-O2A-C1
21	a	604	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	2	607	CHL	CBA-CGA-O2A-C1
29	b	306	CHL	CBD-CGD-O2D-CED
21	B	834	CLA	O1D-CGD-O2D-CED
21	A	816	CLA	O1D-CGD-O2D-CED
29	8	613	CHL	O1D-CGD-O2D-CED
29	2	607	CHL	O1A-CGA-O2A-C1
26	b	301	LMU	C4B-C5B-C6B-O6B
21	A	821	CLA	O1D-CGD-O2D-CED
21	B	839	CLA	O1D-CGD-O2D-CED
21	a	613	CLA	O1D-CGD-O2D-CED
21	c	612	CLA	O1D-CGD-O2D-CED
21	a	604	CLA	O1A-CGA-O2A-C1
21	A	812	CLA	CBA-CGA-O2A-C1
21	A	817	CLA	CBA-CGA-O2A-C1
21	A	823	CLA	CBA-CGA-O2A-C1
21	A	841	CLA	CBA-CGA-O2A-C1
21	B	807	CLA	CBA-CGA-O2A-C1
21	B	825	CLA	CBA-CGA-O2A-C1
21	B	830	CLA	CBA-CGA-O2A-C1
21	G	203	CLA	CBA-CGA-O2A-C1
21	4	602	CLA	CBA-CGA-O2A-C1
29	2	602	CHL	CBA-CGA-O2A-C1
29	6	602	CHL	CBA-CGA-O2A-C1
29	b	308	CHL	CBA-CGA-O2A-C1
24	J	104	BCR	C9-C10-C11-C12
21	B	803	CLA	C5-C6-C7-C8
21	A	818	CLA	C3-C5-C6-C7
21	3	409	CLA	C3-C5-C6-C7
29	b	308	CHL	C3-C5-C6-C7
29	c	601	CHL	O2A-C1-C2-C3
28	G	206	LMG	C2-C1-O1-C7
23	A	844	LHG	O7-C5-C6-O8
21	A	827	CLA	CBA-CGA-O2A-C1
21	A	823	CLA	O1A-CGA-O2A-C1
21	8	611	CLA	C4-C3-C5-C6
21	3	409	CLA	C2-C3-C5-C6
21	A	806	CLA	C11-C10-C8-C9
21	A	809	CLA	C6-C7-C8-C9
21	A	825	CLA	C11-C12-C13-C14
21	A	825	CLA	C14-C13-C15-C16
21	A	826	CLA	C6-C7-C8-C9
21	A	840	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
21	B	802	CLA	C14-C13-C15-C16
21	B	804	CLA	C6-C7-C8-C9
21	B	805	CLA	C6-C7-C8-C9
21	B	812	CLA	C11-C12-C13-C14
21	B	836	CLA	C14-C13-C15-C16
21	B	838	CLA	C6-C7-C8-C9
21	1	303	CLA	C6-C7-C8-C9
21	B	803	CLA	O1D-CGD-O2D-CED
21	B	812	CLA	O1D-CGD-O2D-CED
21	8	609	CLA	O1D-CGD-O2D-CED
29	4	605	CHL	CBD-CGD-O2D-CED
21	A	824	CLA	C2A-CAA-CBA-CGA
21	A	828	CLA	C2A-CAA-CBA-CGA
29	a	608	CHL	C2A-CAA-CBA-CGA
24	A	849	BCR	C37-C22-C23-C24
24	B	844	BCR	C36-C18-C19-C20
24	J	101	BCR	C36-C18-C19-C20
24	J	104	BCR	C37-C22-C23-C24
24	K	205	BCR	C37-C22-C23-C24
24	M	101	BCR	C7-C8-C9-C34
24	M	101	BCR	C37-C22-C23-C24
24	3	419	BCR	C7-C8-C9-C34
24	7	418	BCR	C7-C8-C9-C34
30	5	615	LUT	C11-C12-C13-C20
30	6	616	LUT	C7-C8-C9-C19
31	9	616	XAT	C27-C28-C29-C39
24	A	849	BCR	C21-C22-C23-C24
24	B	843	BCR	C7-C8-C9-C10
24	B	844	BCR	C7-C8-C9-C10
24	J	101	BCR	C17-C18-C19-C20
24	J	104	BCR	C21-C22-C23-C24
24	K	205	BCR	C21-C22-C23-C24
24	M	101	BCR	C21-C22-C23-C24
24	3	419	BCR	C7-C8-C9-C10
24	7	418	BCR	C7-C8-C9-C10
30	5	615	LUT	C11-C12-C13-C14
30	6	616	LUT	C7-C8-C9-C10
31	9	616	XAT	C27-C28-C29-C30
21	A	817	CLA	O1A-CGA-O2A-C1
21	B	825	CLA	O1A-CGA-O2A-C1
21	A	814	CLA	C5-C6-C7-C8
21	A	834	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
21	B	807	CLA	C5-C6-C7-C8
21	B	812	CLA	C10-C11-C12-C13
21	4	612	CLA	C5-C6-C7-C8
21	B	806	CLA	C5-C6-C7-C8
21	B	809	CLA	C5-C6-C7-C8
21	B	823	CLA	C15-C16-C17-C18
23	9	618	LHG	C7-C8-C9-C10
21	B	818	CLA	O1D-CGD-O2D-CED
21	c	614	CLA	O1D-CGD-O2D-CED
21	8	604	CLA	C2A-CAA-CBA-CGA
21	A	807	CLA	C8-C10-C11-C12
21	A	825	CLA	C10-C11-C12-C13
21	B	806	CLA	C8-C10-C11-C12
21	B	809	CLA	C10-C11-C12-C13
21	B	823	CLA	C8-C10-C11-C12
21	B	825	CLA	C13-C15-C16-C17
21	B	836	CLA	C13-C15-C16-C17
21	c	613	CLA	C13-C15-C16-C17
21	B	807	CLA	O1A-CGA-O2A-C1
23	4	618	LHG	C23-C24-C25-C26
21	F	305	CLA	CBD-CGD-O2D-CED
21	1	315	CLA	O1D-CGD-O2D-CED
21	2	612	CLA	O1D-CGD-O2D-CED
21	A	819	CLA	C8-C10-C11-C12
21	A	825	CLA	C13-C15-C16-C17
21	B	812	CLA	C5-C6-C7-C8
21	B	817	CLA	C13-C15-C16-C17
21	A	806	CLA	C2-C1-O2A-CGA
21	B	809	CLA	C8-C10-C11-C12
21	B	817	CLA	C15-C16-C17-C18
23	4	619	LHG	C23-C24-C25-C26
21	9	611	CLA	C8-C10-C11-C12
29	b	309	CHL	O2A-C1-C2-C3
21	A	829	CLA	C5-C6-C7-C8
21	A	819	CLA	C12-C13-C15-C16
21	A	838	CLA	C11-C10-C8-C7
21	B	805	CLA	C11-C12-C13-C15
21	B	818	CLA	C6-C7-C8-C10
21	B	805	CLA	C3-C5-C6-C7
21	A	819	CLA	O1A-CGA-O2A-C1
21	A	841	CLA	O1A-CGA-O2A-C1
21	B	830	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	2	602	CHL	O1A-CGA-O2A-C1
29	6	602	CHL	O1A-CGA-O2A-C1
29	b	308	CHL	O1A-CGA-O2A-C1
24	B	843	BCR	C13-C14-C15-C16
21	6	608	CLA	C2A-CAA-CBA-CGA
21	A	833	CLA	O1D-CGD-O2D-CED
21	J	102	CLA	O1D-CGD-O2D-CED
29	9	609	CHL	O1D-CGD-O2D-CED
29	c	608	CHL	O1D-CGD-O2D-CED
21	A	841	CLA	C10-C11-C12-C13
21	A	841	CLA	C13-C15-C16-C17
21	A	812	CLA	O1A-CGA-O2A-C1
21	G	203	CLA	O1A-CGA-O2A-C1
21	4	602	CLA	O1A-CGA-O2A-C1
21	B	805	CLA	CBD-CGD-O2D-CED
21	B	807	CLA	CBD-CGD-O2D-CED
21	A	840	CLA	C8-C10-C11-C12
21	B	801	CLA	C5-C6-C7-C8
21	B	820	CLA	O1A-CGA-O2A-C1
21	A	817	CLA	C10-C11-C12-C13
21	B	840	CLA	C15-C16-C17-C18
21	5	602	CLA	C5-C6-C7-C8
21	A	807	CLA	CBA-CGA-O2A-C1
21	A	831	CLA	O1D-CGD-O2D-CED
21	A	827	CLA	O1A-CGA-O2A-C1
21	B	807	CLA	C10-C11-C12-C13
21	B	835	CLA	C10-C11-C12-C13
21	A	814	CLA	O1D-CGD-O2D-CED
29	9	607	CHL	O1D-CGD-O2D-CED
21	A	814	CLA	C15-C16-C17-C18
21	A	819	CLA	C13-C15-C16-C17
21	B	804	CLA	C15-C16-C17-C18
21	8	611	CLA	C5-C6-C7-C8
23	A	844	LHG	C4-O6-P-O3
23	4	618	LHG	C4-O6-P-O3
23	8	617	LHG	C4-O6-P-O3
21	B	807	CLA	C3-C5-C6-C7
21	1	305	CLA	CBA-CGA-O2A-C1
21	3	409	CLA	CBA-CGA-O2A-C1
29	2	601	CHL	CBA-CGA-O2A-C1
21	B	817	CLA	C5-C6-C7-C8
29	6	605	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	B	836	CLA	C4-C3-C5-C6
21	A	829	CLA	C15-C16-C17-C18
21	B	807	CLA	C15-C16-C17-C18
21	B	825	CLA	C5-C6-C7-C8
21	B	836	CLA	C5-C6-C7-C8
21	b	311	CLA	O1D-CGD-O2D-CED
21	B	831	CLA	C2C-C3C-CAC-CBC
21	B	826	CLA	C2A-CAA-CBA-CGA
21	8	601	CLA	C2A-CAA-CBA-CGA
29	8	606	CHL	C2A-CAA-CBA-CGA
29	b	306	CHL	C2A-CAA-CBA-CGA
21	9	611	CLA	C3-C5-C6-C7
29	a	609	CHL	O1D-CGD-O2D-CED
21	B	808	CLA	C13-C15-C16-C17
21	8	611	CLA	CAA-CBA-CGA-O2A
21	A	817	CLA	O1D-CGD-O2D-CED
23	8	617	LHG	C23-C24-C25-C26
26	A	856	LMU	C2-C3-C4-C5
21	A	815	CLA	CBD-CGD-O2D-CED
29	5	606	CHL	CBD-CGD-O2D-CED
29	c	601	CHL	CBD-CGD-O2D-CED
27	B	847	DGD	C2B-C1B-O2G-C2G
21	A	829	CLA	C13-C15-C16-C17
21	B	831	CLA	C5-C6-C7-C8
21	8	611	CLA	C2A-CAA-CBA-CGA
21	A	804	CLA	C3-C5-C6-C7
21	3	408	CLA	C3-C5-C6-C7
21	A	824	CLA	O1D-CGD-O2D-CED
29	8	605	CHL	O1D-CGD-O2D-CED
21	B	808	CLA	C16-C17-C18-C19
21	2	608	CLA	C6-C7-C8-C9
21	a	602	CLA	C11-C12-C13-C15
21	c	603	CLA	C6-C7-C8-C10
21	b	315	CLA	O1D-CGD-O2D-CED
29	9	605	CHL	CBD-CGD-O2D-CED
21	A	806	CLA	O1D-CGD-O2D-CED
21	5	602	CLA	O1D-CGD-O2D-CED
23	1	301	LHG	C2-C3-O3-P
23	2	619	LHG	C2-C3-O3-P
23	4	618	LHG	C5-C4-O6-P
21	3	402	CLA	O1D-CGD-O2D-CED
29	4	614	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	2	619	LHG	O2-C2-C3-O3
21	A	831	CLA	C3-C5-C6-C7
29	6	614	CHL	O1D-CGD-O2D-CED
24	8	616	BCR	C20-C21-C22-C23
23	a	617	LHG	O7-C5-C6-O8
21	A	824	CLA	C6-C7-C8-C9
21	A	828	CLA	C11-C12-C13-C15
21	B	808	CLA	C16-C17-C18-C20
21	B	817	CLA	C16-C17-C18-C20
21	A	834	CLA	O1D-CGD-O2D-CED
21	A	852	CLA	O1D-CGD-O2D-CED
21	B	817	CLA	O1D-CGD-O2D-CED
21	6	604	CLA	O1D-CGD-O2D-CED
26	b	301	LMU	C3-C4-C5-C6
21	3	412	CLA	C2-C3-C5-C6
21	A	817	CLA	C6-C7-C8-C9
21	B	837	CLA	C11-C10-C8-C9
21	c	602	CLA	C6-C7-C8-C9
23	a	617	LHG	C23-C24-C25-C26
21	A	852	CLA	C2A-CAA-CBA-CGA
21	B	813	CLA	C2A-CAA-CBA-CGA
21	B	837	CLA	C2A-CAA-CBA-CGA
21	1	303	CLA	C2A-CAA-CBA-CGA
21	2	603	CLA	C2A-CAA-CBA-CGA
29	c	605	CHL	C2A-CAA-CBA-CGA
21	A	807	CLA	O1A-CGA-O2A-C1
29	2	601	CHL	O1A-CGA-O2A-C1
24	B	844	BCR	C7-C8-C9-C34
21	4	612	CLA	C3-C5-C6-C7
21	c	611	CLA	C5-C6-C7-C8
27	B	847	DGD	CAA-CBA-CCA-CDA
21	1	305	CLA	CBD-CGD-O2D-CED
21	2	604	CLA	O1D-CGD-O2D-CED
26	b	301	LMU	C7-C8-C9-C10
27	B	847	DGD	C9A-CAA-CBA-CCA
21	A	821	CLA	C16-C17-C18-C20
21	c	603	CLA	C6-C7-C8-C9
21	A	806	CLA	C10-C11-C12-C13
21	B	826	CLA	O1D-CGD-O2D-CED
29	6	606	CHL	CBD-CGD-O2D-CED
21	b	311	CLA	C5-C6-C7-C8
21	1	305	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
21	3	409	CLA	O1A-CGA-O2A-C1
21	A	801	CLA	CBA-CGA-O2A-C1
21	B	828	CLA	O1D-CGD-O2D-CED
21	A	804	CLA	C3A-C2A-CAA-CBA
21	A	833	CLA	C3A-C2A-CAA-CBA
21	A	837	CLA	C3A-C2A-CAA-CBA
21	A	841	CLA	C3A-C2A-CAA-CBA
21	B	802	CLA	C3A-C2A-CAA-CBA
21	B	807	CLA	C3A-C2A-CAA-CBA
21	3	403	CLA	C3A-C2A-CAA-CBA
21	4	611	CLA	C3A-C2A-CAA-CBA
21	8	604	CLA	C3A-C2A-CAA-CBA
21	8	610	CLA	C3A-C2A-CAA-CBA
21	9	603	CLA	C3A-C2A-CAA-CBA
29	9	606	CHL	C3A-C2A-CAA-CBA
21	A	809	CLA	C5-C6-C7-C8
21	A	841	CLA	C15-C16-C17-C18
21	a	602	CLA	C8-C10-C11-C12
26	O	206	LMU	C2-C1-O1'-C1'
27	B	847	DGD	C4A-C5A-C6A-C7A
21	B	822	CLA	O1D-CGD-O2D-CED
23	2	619	LHG	C4-C5-C6-O8
28	G	206	LMG	C10-C11-C12-C13
21	A	827	CLA	C10-C11-C12-C13
21	B	823	CLA	C10-C11-C12-C13
21	B	825	CLA	C4-C3-C5-C6
21	B	835	CLA	C4-C3-C5-C6
21	B	827	CLA	CBA-CGA-O2A-C1
21	B	825	CLA	C2-C3-C5-C6
21	B	835	CLA	C2-C3-C5-C6
21	7	411	CLA	C2-C3-C5-C6
21	A	803	CLA	C2A-CAA-CBA-CGA
21	6	612	CLA	C2A-CAA-CBA-CGA
23	4	619	LHG	C9-C10-C11-C12
21	2	608	CLA	C6-C7-C8-C10
21	8	611	CLA	C6-C7-C8-C10
21	A	841	CLA	O1D-CGD-O2D-CED
27	B	847	DGD	O1B-C1B-O2G-C2G
21	B	805	CLA	C10-C11-C12-C13
21	B	805	CLA	C15-C16-C17-C18
21	A	824	CLA	C6-C7-C8-C10
21	A	828	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
23	A	844	LHG	C23-C24-C25-C26
29	2	605	CHL	CBD-CGD-O2D-CED
21	c	611	CLA	C3-C5-C6-C7
24	A	846	BCR	C5-C6-C7-C8
24	A	846	BCR	C23-C24-C25-C26
24	A	846	BCR	C23-C24-C25-C30
24	B	843	BCR	C23-C24-C25-C26
24	B	845	BCR	C23-C24-C25-C26
24	B	845	BCR	C23-C24-C25-C30
24	G	205	BCR	C1-C6-C7-C8
24	I	101	BCR	C1-C6-C7-C8
24	I	101	BCR	C5-C6-C7-C8
24	J	101	BCR	C1-C6-C7-C8
24	J	101	BCR	C5-C6-C7-C8
24	J	101	BCR	C23-C24-C25-C26
24	J	101	BCR	C23-C24-C25-C30
24	J	103	BCR	C1-C6-C7-C8
24	J	103	BCR	C5-C6-C7-C8
24	L	306	BCR	C23-C24-C25-C26
24	L	306	BCR	C23-C24-C25-C30
24	M	101	BCR	C23-C24-C25-C26
24	M	101	BCR	C23-C24-C25-C30
24	2	618	BCR	C23-C24-C25-C26
24	2	618	BCR	C23-C24-C25-C30
24	3	418	BCR	C23-C24-C25-C26
24	3	418	BCR	C23-C24-C25-C30
24	3	419	BCR	C5-C6-C7-C8
24	3	419	BCR	C23-C24-C25-C26
24	3	419	BCR	C23-C24-C25-C30
24	4	617	BCR	C23-C24-C25-C26
24	6	618	BCR	C1-C6-C7-C8
24	6	618	BCR	C23-C24-C25-C26
24	6	618	BCR	C23-C24-C25-C30
24	7	418	BCR	C5-C6-C7-C8
30	2	616	LUT	C1-C6-C7-C8
30	2	616	LUT	C5-C6-C7-C8
30	3	416	LUT	C5-C6-C7-C8
30	5	615	LUT	C5-C6-C7-C8
21	c	613	CLA	C15-C16-C17-C18
21	A	830	CLA	C3-C5-C6-C7
21	F	302	CLA	C5-C6-C7-C8
29	c	606	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	3	412	CLA	C4-C3-C5-C6
21	K	203	CLA	O1D-CGD-O2D-CED
21	A	817	CLA	C6-C7-C8-C10
21	A	840	CLA	C11-C12-C13-C15
21	B	802	CLA	C11-C10-C8-C7
21	B	805	CLA	C11-C10-C8-C7
21	B	812	CLA	C11-C12-C13-C15
21	B	812	CLA	C12-C13-C15-C16
21	B	837	CLA	C11-C10-C8-C7
21	a	602	CLA	C6-C7-C8-C10
21	c	602	CLA	C6-C7-C8-C10
21	c	611	CLA	C6-C7-C8-C10
21	A	807	CLA	C3-C5-C6-C7
21	A	801	CLA	O1A-CGA-O2A-C1
24	B	844	BCR	C19-C20-C21-C22
21	L	304	CLA	CBD-CGD-O2D-CED
21	B	817	CLA	C16-C17-C18-C19
21	3	412	CLA	C6-C7-C8-C9
21	A	828	CLA	O1D-CGD-O2D-CED
21	A	830	CLA	CBA-CGA-O2A-C1
21	5	602	CLA	CBA-CGA-O2A-C1
21	7	411	CLA	CBA-CGA-O2A-C1
21	A	823	CLA	C2A-CAA-CBA-CGA
21	B	830	CLA	C2A-CAA-CBA-CGA
21	2	612	CLA	C2A-CAA-CBA-CGA
21	4	602	CLA	C2A-CAA-CBA-CGA
21	9	613	CLA	C2A-CAA-CBA-CGA
29	6	602	CHL	C2A-CAA-CBA-CGA
29	b	308	CHL	C2A-CAA-CBA-CGA
21	A	827	CLA	C8-C10-C11-C12
21	A	819	CLA	O1D-CGD-O2D-CED
21	1	304	CLA	CBD-CGD-O2D-CED
26	A	856	LMU	O1'-C1-C2-C3
21	b	304	CLA	O1D-CGD-O2D-CED
29	b	306	CHL	O1D-CGD-O2D-CED
21	B	817	CLA	C8-C10-C11-C12
21	B	827	CLA	O1A-CGA-O2A-C1
29	8	606	CHL	CBD-CGD-O2D-CED
21	A	840	CLA	C16-C17-C18-C20
21	A	831	CLA	C5-C6-C7-C8
21	A	840	CLA	O1D-CGD-O2D-CED
26	3	420	LMU	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
21	B	802	CLA	C5-C6-C7-C8
21	B	803	CLA	C3-C5-C6-C7
21	B	823	CLA	C3-C5-C6-C7
21	a	602	CLA	C11-C12-C13-C14
23	9	618	LHG	C33-C34-C35-C36
28	J	105	LMG	O6-C5-C6-O5
21	A	828	CLA	C4-C3-C5-C6
21	7	411	CLA	C4-C3-C5-C6
21	B	836	CLA	C2-C3-C5-C6
21	8	611	CLA	C2-C3-C5-C6
21	A	819	CLA	C14-C13-C15-C16
21	A	826	CLA	C14-C13-C15-C16
21	A	838	CLA	C11-C10-C8-C9
21	B	805	CLA	C11-C12-C13-C14
21	B	808	CLA	C11-C10-C8-C9
21	B	812	CLA	C14-C13-C15-C16
21	B	818	CLA	C6-C7-C8-C9
21	1	303	CLA	C11-C10-C8-C9
21	5	602	CLA	C11-C12-C13-C14
21	a	602	CLA	C6-C7-C8-C9
29	2	602	CHL	CBD-CGD-O2D-CED
21	A	818	CLA	C2A-CAA-CBA-CGA
21	A	829	CLA	C2A-CAA-CBA-CGA
21	G	202	CLA	C2A-CAA-CBA-CGA
21	1	313	CLA	C2A-CAA-CBA-CGA
21	3	412	CLA	C2A-CAA-CBA-CGA
21	8	609	CLA	C2A-CAA-CBA-CGA
21	c	602	CLA	C2A-CAA-CBA-CGA
29	2	602	CHL	C2A-CAA-CBA-CGA
29	b	309	CHL	C2A-CAA-CBA-CGA
21	B	805	CLA	C5-C6-C7-C8
23	4	618	LHG	C24-C25-C26-C27
21	A	805	CLA	C1A-C2A-CAA-CBA
21	A	811	CLA	C1A-C2A-CAA-CBA
21	A	818	CLA	C1A-C2A-CAA-CBA
21	A	826	CLA	C1A-C2A-CAA-CBA
21	A	828	CLA	C1A-C2A-CAA-CBA
21	A	830	CLA	C1A-C2A-CAA-CBA
21	A	833	CLA	C1A-C2A-CAA-CBA
21	A	835	CLA	C1A-C2A-CAA-CBA
21	O	203	CLA	C1A-C2A-CAA-CBA
21	1	303	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
21	1	310	CLA	C1A-C2A-CAA-CBA
21	3	403	CLA	C1A-C2A-CAA-CBA
21	4	602	CLA	C1A-C2A-CAA-CBA
21	4	609	CLA	C1A-C2A-CAA-CBA
21	4	610	CLA	C1A-C2A-CAA-CBA
21	4	611	CLA	C1A-C2A-CAA-CBA
21	5	602	CLA	C1A-C2A-CAA-CBA
21	5	609	CLA	C1A-C2A-CAA-CBA
21	6	608	CLA	C1A-C2A-CAA-CBA
21	7	407	CLA	C1A-C2A-CAA-CBA
21	8	610	CLA	C1A-C2A-CAA-CBA
21	9	602	CLA	C1A-C2A-CAA-CBA
21	9	603	CLA	C1A-C2A-CAA-CBA
21	9	604	CLA	C1A-C2A-CAA-CBA
21	a	602	CLA	C1A-C2A-CAA-CBA
21	a	610	CLA	C1A-C2A-CAA-CBA
21	b	311	CLA	C1A-C2A-CAA-CBA
21	c	610	CLA	C1A-C2A-CAA-CBA
21	c	611	CLA	C1A-C2A-CAA-CBA
21	c	614	CLA	C1A-C2A-CAA-CBA
29	2	602	CHL	C1A-C2A-CAA-CBA
29	4	607	CHL	C1A-C2A-CAA-CBA
29	6	601	CHL	C1A-C2A-CAA-CBA
29	8	607	CHL	C1A-C2A-CAA-CBA
29	9	606	CHL	C1A-C2A-CAA-CBA
21	3	412	CLA	C6-C7-C8-C10
21	8	611	CLA	C6-C7-C8-C9
21	B	812	CLA	C2C-C3C-CAC-CBC
21	A	840	CLA	C13-C15-C16-C17
21	B	812	CLA	C8-C10-C11-C12
23	5	617	LHG	C4-O6-P-O3
23	b	319	LHG	C4-O6-P-O3
21	1	309	CLA	C2C-C3C-CAC-CBC
29	b	302	CHL	O1D-CGD-O2D-CED
21	4	612	CLA	C2C-C3C-CAC-CBC
21	A	825	CLA	C8-C10-C11-C12
21	B	802	CLA	C13-C15-C16-C17
28	6	615	LMG	O6-C5-C6-O5
21	O	204	CLA	C3A-C2A-CAA-CBA
21	A	830	CLA	O1A-CGA-O2A-C1
21	B	811	CLA	C2A-CAA-CBA-CGA
21	5	602	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
21	b	305	CLA	C2A-CAA-CBA-CGA
21	c	613	CLA	C16-C17-C18-C20
28	2	615	LMG	O6-C5-C6-O5
23	A	844	LHG	C4-C5-C6-O8
23	1	301	LHG	C4-C5-C6-O8
21	3	408	CLA	C8-C10-C11-C12
29	4	605	CHL	O1D-CGD-O2D-CED
21	A	809	CLA	C11-C12-C13-C14
21	B	821	CLA	C3-C5-C6-C7
21	A	825	CLA	C16-C17-C18-C20
21	a	604	CLA	O2A-C1-C2-C3
28	G	206	LMG	C40-C41-C42-C43
21	5	602	CLA	O1A-CGA-O2A-C1
21	7	411	CLA	O1A-CGA-O2A-C1
23	9	618	LHG	C23-C24-C25-C26
21	2	609	CLA	C2A-CAA-CBA-CGA
30	5	615	LUT	C11-C10-C9-C19
26	O	206	LMU	O5'-C5'-C6'-O6'
21	B	816	CLA	C2A-CAA-CBA-CGA
29	2	614	CHL	C2A-CAA-CBA-CGA
21	A	821	CLA	C13-C15-C16-C17
21	3	412	CLA	C5-C6-C7-C8
21	c	611	CLA	C2-C1-O2A-CGA
21	A	817	CLA	C2C-C3C-CAC-CBC
21	5	605	CLA	C4C-C3C-CAC-CBC
21	O	203	CLA	CBA-CGA-O2A-C1
21	A	840	CLA	C16-C17-C18-C19
21	5	605	CLA	C2C-C3C-CAC-CBC
21	F	305	CLA	O1D-CGD-O2D-CED
21	2	608	CLA	C5-C6-C7-C8
21	A	803	CLA	C4-C3-C5-C6
29	5	606	CHL	O1D-CGD-O2D-CED
21	A	806	CLA	C11-C10-C8-C7
21	A	825	CLA	C12-C13-C15-C16
21	A	826	CLA	C12-C13-C15-C16
21	A	827	CLA	C11-C10-C8-C7
21	A	842	CLA	C6-C7-C8-C10
21	B	802	CLA	C11-C12-C13-C15
21	B	804	CLA	C11-C10-C8-C7
21	B	805	CLA	C12-C13-C15-C16
21	B	807	CLA	C6-C7-C8-C10
21	B	808	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
21	B	817	CLA	C11-C10-C8-C7
21	B	824	CLA	C12-C13-C15-C16
21	B	827	CLA	C11-C10-C8-C7
21	B	830	CLA	C6-C7-C8-C10
21	B	836	CLA	C12-C13-C15-C16
21	1	303	CLA	C11-C10-C8-C7
21	1	303	CLA	C11-C12-C13-C15
21	3	402	CLA	C6-C7-C8-C10
21	5	602	CLA	C11-C12-C13-C15
21	A	812	CLA	C11-C12-C13-C14
21	A	819	CLA	C11-C12-C13-C14
21	A	827	CLA	C11-C10-C8-C9
21	A	828	CLA	C11-C10-C8-C9
21	A	829	CLA	C14-C13-C15-C16
21	B	801	CLA	C6-C7-C8-C9
21	B	802	CLA	C11-C12-C13-C14
21	B	804	CLA	C11-C10-C8-C9
21	B	805	CLA	C14-C13-C15-C16
21	B	806	CLA	C6-C7-C8-C9
21	B	814	CLA	C6-C7-C8-C9
21	B	817	CLA	C6-C7-C8-C9
21	B	805	CLA	O1D-CGD-O2D-CED
29	c	601	CHL	O1D-CGD-O2D-CED
24	B	844	BCR	C37-C22-C23-C24
21	c	613	CLA	C16-C17-C18-C19
24	B	843	BCR	C17-C18-C19-C20
31	6	617	XAT	C11-C12-C13-C14
21	4	612	CLA	C4C-C3C-CAC-CBC
21	a	613	CLA	C3-C5-C6-C7
29	9	605	CHL	O1D-CGD-O2D-CED
21	B	807	CLA	O1D-CGD-O2D-CED
21	A	803	CLA	CBD-CGD-O2D-CED
27	B	847	DGD	C6B-C7B-C8B-C9B
21	A	815	CLA	O1D-CGD-O2D-CED
21	F	302	CLA	C4-C3-C5-C6
21	b	311	CLA	C4-C3-C5-C6
21	A	803	CLA	C2-C3-C5-C6
21	B	831	CLA	C11-C10-C8-C9
21	B	801	CLA	C8-C10-C11-C12
21	A	824	CLA	CBA-CGA-O2A-C1
23	4	618	LHG	C2-C3-O3-P
29	6	606	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	A	842	CLA	C3A-C2A-CAA-CBA
21	B	811	CLA	C3A-C2A-CAA-CBA
21	B	832	CLA	C3A-C2A-CAA-CBA
21	L	302	CLA	C3A-C2A-CAA-CBA
21	L	303	CLA	C3A-C2A-CAA-CBA
21	9	613	CLA	C3A-C2A-CAA-CBA
29	1	302	CHL	C3A-C2A-CAA-CBA
29	6	601	CHL	C3A-C2A-CAA-CBA
29	b	302	CHL	C3A-C2A-CAA-CBA
21	A	842	CLA	C5-C6-C7-C8
26	3	420	LMU	C2-C1-O1'-C1'
21	A	838	CLA	C15-C16-C17-C18
28	G	206	LMG	C32-C33-C34-C35
29	2	601	CHL	C3-C5-C6-C7
23	6	619	LHG	C4-C5-C6-O8
21	A	806	CLA	O2A-C1-C2-C3
21	3	412	CLA	C3-C5-C6-C7
21	b	311	CLA	C3-C5-C6-C7
21	1	305	CLA	O1D-CGD-O2D-CED
21	A	813	CLA	C5-C6-C7-C8
21	a	602	CLA	C10-C11-C12-C13
21	F	302	CLA	C2-C3-C5-C6
29	2	605	CHL	O1D-CGD-O2D-CED
21	B	837	CLA	C13-C15-C16-C17
29	6	602	CHL	C3C-C2C-CMC-OMC
29	9	607	CHL	C3C-C2C-CMC-OMC
21	O	203	CLA	O1A-CGA-O2A-C1
21	b	303	CLA	C11-C12-C13-C14
29	8	606	CHL	O1D-CGD-O2D-CED
21	a	604	CLA	C2A-CAA-CBA-CGA
29	2	601	CHL	C2A-CAA-CBA-CGA
21	B	827	CLA	C10-C11-C12-C13
21	B	809	CLA	CBA-CGA-O2A-C1
21	L	304	CLA	O1D-CGD-O2D-CED
21	B	812	CLA	C16-C17-C18-C19
29	a	601	CHL	CBD-CGD-O2D-CED
21	B	831	CLA	C4C-C3C-CAC-CBC
23	1	301	LHG	O7-C5-C6-O8
23	9	618	LHG	O7-C5-C6-O8
26	A	856	LMU	C1-C2-C3-C4
21	A	817	CLA	C4C-C3C-CAC-CBC
27	B	847	DGD	C7B-C8B-C9B-CAB

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Mol	Chain	Res	Type	Atoms
21	8	601	CLA	CBD-CGD-O2D-CED
21	A	824	CLA	C2-C1-O2A-CGA
21	B	801	CLA	C2-C1-O2A-CGA
21	B	809	CLA	C2-C1-O2A-CGA
21	B	832	CLA	C2-C1-O2A-CGA
21	A	840	CLA	C10-C11-C12-C13
21	A	833	CLA	C11-C10-C8-C9
21	B	806	CLA	C11-C12-C13-C14
21	B	836	CLA	C11-C10-C8-C9
21	3	402	CLA	C6-C7-C8-C9
21	B	824	CLA	CBA-CGA-O2A-C1
21	B	806	CLA	C2A-CAA-CBA-CGA
21	A	821	CLA	C16-C17-C18-C19
21	B	814	CLA	C11-C12-C13-C15
21	B	825	CLA	C16-C17-C18-C19
21	B	836	CLA	C3-C5-C6-C7
24	A	848	BCR	C1-C6-C7-C8
24	L	301	BCR	C1-C6-C7-C8
24	L	301	BCR	C5-C6-C7-C8
24	O	205	BCR	C1-C6-C7-C8
24	O	205	BCR	C5-C6-C7-C8
24	3	418	BCR	C1-C6-C7-C8
24	3	418	BCR	C5-C6-C7-C8
24	7	417	BCR	C1-C6-C7-C8
24	7	417	BCR	C5-C6-C7-C8
24	8	616	BCR	C1-C6-C7-C8
24	8	616	BCR	C5-C6-C7-C8
30	1	317	LUT	C1-C6-C7-C8
30	4	615	LUT	C1-C6-C7-C8
30	4	615	LUT	C5-C6-C7-C8
30	8	614	LUT	C1-C6-C7-C8
30	8	614	LUT	C5-C6-C7-C8
30	9	614	LUT	C1-C6-C7-C8
30	9	614	LUT	C5-C6-C7-C8
30	9	615	LUT	C5-C6-C7-C8
30	b	316	LUT	C1-C6-C7-C8
30	b	316	LUT	C5-C6-C7-C8
30	b	317	LUT	C1-C6-C7-C8
30	b	317	LUT	C5-C6-C7-C8
21	1	309	CLA	C4C-C3C-CAC-CBC
21	1	304	CLA	O1D-CGD-O2D-CED
21	L	304	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
21	2	613	CLA	C1A-C2A-CAA-CBA
21	6	613	CLA	C1A-C2A-CAA-CBA
21	7	404	CLA	C1A-C2A-CAA-CBA
21	A	804	CLA	C13-C15-C16-C17
21	B	802	CLA	C8-C10-C11-C12
27	B	847	DGD	C1A-C2A-C3A-C4A
21	9	610	CLA	C6-C7-C8-C9
21	A	817	CLA	C16-C17-C18-C19
21	A	825	CLA	C16-C17-C18-C19
21	B	812	CLA	C16-C17-C18-C20
21	A	806	CLA	C8-C10-C11-C12
23	8	617	LHG	O6-C4-C5-C6
21	b	314	CLA	C4-C3-C5-C6
21	A	807	CLA	C11-C12-C13-C15
21	A	809	CLA	C6-C7-C8-C10
21	A	812	CLA	C11-C12-C13-C15
21	A	819	CLA	C11-C12-C13-C15
21	A	825	CLA	C11-C12-C13-C15
21	A	826	CLA	C6-C7-C8-C10
21	A	829	CLA	C12-C13-C15-C16
21	A	833	CLA	C11-C10-C8-C7
21	B	801	CLA	C6-C7-C8-C10
21	B	814	CLA	C6-C7-C8-C10
21	B	817	CLA	C6-C7-C8-C10
21	B	823	CLA	C11-C12-C13-C15
21	B	827	CLA	C6-C7-C8-C10
21	B	836	CLA	C6-C7-C8-C10
21	B	836	CLA	C11-C10-C8-C7
21	B	837	CLA	C6-C7-C8-C10
21	4	602	CLA	C11-C10-C8-C7
21	c	613	CLA	C11-C12-C13-C15
24	B	843	BCR	C15-C16-C17-C18
24	B	844	BCR	C9-C10-C11-C12
24	J	104	BCR	C19-C20-C21-C22
21	A	829	CLA	CBA-CGA-O2A-C1
21	B	832	CLA	C2A-CAA-CBA-CGA
29	a	609	CHL	C2A-CAA-CBA-CGA
30	7	415	LUT	C11-C10-C9-C19
31	6	617	XAT	C20-C13-C14-C15
31	a	618	XAT	C11-C10-C9-C19
21	A	821	CLA	C8-C10-C11-C12
21	9	611	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
23	A	844	LHG	C13-C14-C15-C16
23	9	618	LHG	C29-C30-C31-C32
21	A	801	CLA	CAD-CBD-CGD-O2D
21	A	815	CLA	CAD-CBD-CGD-O2D
21	A	833	CLA	CAD-CBD-CGD-O2D
21	B	810	CLA	CAD-CBD-CGD-O2D
21	B	816	CLA	CAD-CBD-CGD-O2D
21	B	823	CLA	CAD-CBD-CGD-O2D
21	B	829	CLA	CAD-CBD-CGD-O2D
21	J	102	CLA	CAD-CBD-CGD-O2D
21	L	304	CLA	CAD-CBD-CGD-O2D
21	2	612	CLA	CAD-CBD-CGD-O2D
21	6	603	CLA	CAD-CBD-CGD-O2D
21	6	613	CLA	CAD-CBD-CGD-O2D
21	7	402	CLA	CAD-CBD-CGD-O2D
21	7	410	CLA	CAD-CBD-CGD-O2D
21	8	612	CLA	CAD-CBD-CGD-O2D
21	8	618	CLA	CAD-CBD-CGD-O2D
21	a	602	CLA	CAD-CBD-CGD-O2D
21	a	614	CLA	CAD-CBD-CGD-O2D
21	b	305	CLA	CAD-CBD-CGD-O2D
21	c	614	CLA	CAD-CBD-CGD-O2D
29	2	614	CHL	CAD-CBD-CGD-O2D
29	6	601	CHL	CAD-CBD-CGD-O2D
29	9	606	CHL	CAD-CBD-CGD-O2D
29	9	609	CHL	CAD-CBD-CGD-O2D
29	a	607	CHL	CAD-CBD-CGD-O2D
29	b	306	CHL	CAD-CBD-CGD-O2D
29	b	308	CHL	CAD-CBD-CGD-O2D
21	B	825	CLA	C10-C11-C12-C13
21	3	412	CLA	CBA-CGA-O2A-C1
23	a	617	LHG	C4-C5-C6-O8
21	A	813	CLA	CBD-CGD-O2D-CED
21	B	824	CLA	O1A-CGA-O2A-C1
28	G	206	LMG	C11-C10-O7-C8
21	B	812	CLA	C15-C16-C17-C18
21	7	403	CLA	C2A-CAA-CBA-CGA
21	a	602	CLA	C2A-CAA-CBA-CGA
21	B	825	CLA	C16-C17-C18-C20
21	A	817	CLA	CHA-CBD-CGD-O1D
21	A	817	CLA	CHA-CBD-CGD-O2D
21	A	831	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
21	A	831	CLA	CHA-CBD-CGD-O2D
21	A	834	CLA	CHA-CBD-CGD-O1D
21	A	839	CLA	CHA-CBD-CGD-O1D
21	A	839	CLA	CHA-CBD-CGD-O2D
21	B	806	CLA	CHA-CBD-CGD-O2D
21	B	812	CLA	CHA-CBD-CGD-O1D
21	B	839	CLA	CHA-CBD-CGD-O2D
21	G	203	CLA	CHA-CBD-CGD-O1D
21	G	203	CLA	CHA-CBD-CGD-O2D
21	K	204	CLA	CHA-CBD-CGD-O1D
21	K	204	CLA	CHA-CBD-CGD-O2D
21	1	303	CLA	CHA-CBD-CGD-O1D
21	1	303	CLA	CHA-CBD-CGD-O2D
21	4	601	CLA	CHA-CBD-CGD-O2D
21	5	602	CLA	CHA-CBD-CGD-O1D
21	5	602	CLA	CHA-CBD-CGD-O2D
21	6	604	CLA	CHA-CBD-CGD-O1D
21	6	604	CLA	CHA-CBD-CGD-O2D
21	8	604	CLA	CHA-CBD-CGD-O1D
21	9	612	CLA	CHA-CBD-CGD-O1D
21	9	612	CLA	CHA-CBD-CGD-O2D
21	b	303	CLA	CHA-CBD-CGD-O1D
21	b	313	CLA	CHA-CBD-CGD-O1D
21	b	313	CLA	CHA-CBD-CGD-O2D
29	1	302	CHL	CHA-CBD-CGD-O1D
29	1	302	CHL	CHA-CBD-CGD-O2D
29	2	601	CHL	CHA-CBD-CGD-O1D
29	2	601	CHL	CHA-CBD-CGD-O2D
29	2	602	CHL	CHA-CBD-CGD-O1D
29	2	602	CHL	CHA-CBD-CGD-O2D
29	8	605	CHL	CHA-CBD-CGD-O1D
29	8	605	CHL	CHA-CBD-CGD-O2D
29	a	601	CHL	CHA-CBD-CGD-O1D
29	a	601	CHL	CHA-CBD-CGD-O2D
21	A	824	CLA	O1A-CGA-O2A-C1
21	B	809	CLA	O1A-CGA-O2A-C1
21	B	812	CLA	C4C-C3C-CAC-CBC
30	5	615	LUT	C11-C10-C9-C8
23	6	619	LHG	O7-C5-C6-O8
21	8	602	CLA	CBA-CGA-O2A-C1
21	B	815	CLA	C6-C7-C8-C10
21	A	838	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
21	A	841	CLA	C14-C13-C15-C16
21	B	801	CLA	C11-C10-C8-C9
21	B	817	CLA	C11-C12-C13-C14
21	B	825	CLA	C11-C12-C13-C14
21	B	835	CLA	C6-C7-C8-C9
21	B	838	CLA	C11-C10-C8-C9
21	4	602	CLA	C11-C10-C8-C9
21	b	303	CLA	C6-C7-C8-C9
29	2	602	CHL	O1D-CGD-O2D-CED
21	A	829	CLA	O1A-CGA-O2A-C1
21	a	610	CLA	C2A-CAA-CBA-CGA
21	4	602	CLA	C2C-C3C-CAC-CBC
24	B	843	BCR	C37-C22-C23-C24
24	B	843	BCR	C21-C22-C23-C24
24	B	844	BCR	C21-C22-C23-C24
21	A	824	CLA	C1A-C2A-CAA-CBA
21	A	842	CLA	C1A-C2A-CAA-CBA
21	B	802	CLA	C1A-C2A-CAA-CBA
21	B	826	CLA	C1A-C2A-CAA-CBA
21	B	831	CLA	C1A-C2A-CAA-CBA
21	B	835	CLA	C1A-C2A-CAA-CBA
21	O	202	CLA	CHA-CBD-CGD-O2D
21	1	308	CLA	CHA-CBD-CGD-O2D
21	3	405	CLA	CHA-CBD-CGD-O2D
21	4	603	CLA	CHA-CBD-CGD-O2D
21	7	407	CLA	CHA-CBD-CGD-O2D
21	8	602	CLA	CHA-CBD-CGD-O2D
29	a	605	CHL	CHA-CBD-CGD-O2D
21	b	314	CLA	CBA-CGA-O2A-C1
24	K	205	BCR	C19-C20-C21-C22
21	A	803	CLA	O1D-CGD-O2D-CED
21	8	601	CLA	O1D-CGD-O2D-CED
29	a	601	CHL	O1D-CGD-O2D-CED
23	4	619	LHG	C4-O6-P-O3
23	6	619	LHG	C3-O3-P-O6
21	B	838	CLA	C3-C5-C6-C7
21	9	611	CLA	O1A-CGA-O2A-C1
23	A	844	LHG	C4-O6-P-O4
23	1	301	LHG	C4-O6-P-O4
23	1	319	LHG	C4-O6-P-O4
23	4	618	LHG	C4-O6-P-O4
23	5	617	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
23	b	319	LHG	C4-O6-P-O4
21	b	311	CLA	CBA-CGA-O2A-C1
29	1	302	CHL	CBA-CGA-O2A-C1
21	A	838	CLA	C10-C11-C12-C13
21	A	817	CLA	C2A-CAA-CBA-CGA
21	3	409	CLA	C2A-CAA-CBA-CGA
29	1	302	CHL	C2A-CAA-CBA-CGA
21	B	815	CLA	C3-C5-C6-C7
21	1	303	CLA	C2C-C3C-CAC-CBC
21	A	804	CLA	C16-C17-C18-C19
21	A	837	CLA	C2-C3-C5-C6
21	F	302	CLA	CAD-CBD-CGD-O1D
21	4	601	CLA	CAD-CBD-CGD-O1D
21	6	611	CLA	CAD-CBD-CGD-O1D
21	b	303	CLA	CAD-CBD-CGD-O1D
21	b	315	CLA	CAD-CBD-CGD-O1D
29	2	601	CHL	CAD-CBD-CGD-O1D
21	3	412	CLA	O1A-CGA-O2A-C1
21	b	303	CLA	C10-C11-C12-C13
21	8	602	CLA	O1A-CGA-O2A-C1
21	A	810	CLA	CBD-CGD-O2D-CED
21	A	815	CLA	C3A-C2A-CAA-CBA
21	A	821	CLA	C11-C10-C8-C7
21	A	834	CLA	C11-C12-C13-C15
21	A	841	CLA	C12-C13-C15-C16
21	B	801	CLA	C11-C10-C8-C7
21	B	802	CLA	C12-C13-C15-C16
21	B	817	CLA	C11-C12-C13-C15
21	B	838	CLA	C11-C10-C8-C7
21	B	840	CLA	C11-C12-C13-C15
21	1	303	CLA	C6-C7-C8-C10
21	7	404	CLA	C3A-C2A-CAA-CBA
21	b	303	CLA	C6-C7-C8-C10
23	8	617	LHG	O6-C4-C5-O7
30	a	615	LUT	C25-C26-C27-C28
21	B	815	CLA	C2A-CAA-CBA-CGA
21	L	303	CLA	C2A-CAA-CBA-CGA
21	4	610	CLA	C2A-CAA-CBA-CGA
29	9	607	CHL	C2A-CAA-CBA-CGA
21	B	814	CLA	C11-C12-C13-C14
21	O	204	CLA	CAD-CBD-CGD-O1D
21	5	613	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
21	7	411	CLA	CAD-CBD-CGD-O1D
21	7	414	CLA	CAD-CBD-CGD-O1D
21	8	603	CLA	CAD-CBD-CGD-O1D
21	a	604	CLA	CAD-CBD-CGD-O1D
23	4	618	LHG	C4-C5-C6-O8
23	4	619	LHG	C28-C29-C30-C31
23	9	618	LHG	C4-C5-C6-O8
29	5	601	CHL	C1C-C2C-CMC-OMC
29	6	602	CHL	C1C-C2C-CMC-OMC
29	9	607	CHL	C1C-C2C-CMC-OMC
29	c	609	CHL	C1C-C2C-CMC-OMC
23	2	619	LHG	O7-C5-C6-O8
23	b	319	LHG	O7-C5-C6-O8
21	A	828	CLA	C10-C11-C12-C13
21	A	817	CLA	C16-C17-C18-C20
21	K	201	CLA	CBA-CGA-O2A-C1
21	b	314	CLA	O1A-CGA-O2A-C1
21	B	802	CLA	CBA-CGA-O2A-C1
21	A	821	CLA	C6-C7-C8-C9
21	A	827	CLA	C6-C7-C8-C9
21	A	842	CLA	C6-C7-C8-C9
21	B	823	CLA	C11-C10-C8-C9
21	B	823	CLA	C11-C12-C13-C14
21	B	824	CLA	C14-C13-C15-C16
21	B	827	CLA	C6-C7-C8-C9
21	B	830	CLA	C6-C7-C8-C9
21	B	836	CLA	C6-C7-C8-C9
21	B	837	CLA	C6-C7-C8-C9
21	c	613	CLA	C11-C12-C13-C14
21	b	311	CLA	O1A-CGA-O2A-C1
29	1	302	CHL	O1A-CGA-O2A-C1
21	H	201	CLA	CBD-CGD-O2D-CED
21	A	827	CLA	C3-C5-C6-C7
21	B	827	CLA	C8-C10-C11-C12
21	B	821	CLA	CBD-CGD-O2D-CED
30	3	416	LUT	C10-C11-C12-C13
21	B	815	CLA	C6-C7-C8-C9
21	B	802	CLA	O1A-CGA-O2A-C1
21	A	828	CLA	C2-C3-C5-C6
21	b	314	CLA	C2-C3-C5-C6
21	A	834	CLA	C13-C15-C16-C17
21	B	838	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
21	1	305	CLA	C1-C2-C3-C4
21	5	604	CLA	C1-C2-C3-C4
21	A	813	CLA	O1D-CGD-O2D-CED
23	a	617	LHG	C14-C15-C16-C17
21	B	809	CLA	C2A-CAA-CBA-CGA
21	4	603	CLA	C2A-CAA-CBA-CGA
21	4	612	CLA	C2A-CAA-CBA-CGA
21	c	613	CLA	C2A-CAA-CBA-CGA
21	A	814	CLA	C2-C1-O2A-CGA
21	A	819	CLA	C2-C1-O2A-CGA
21	B	807	CLA	C2-C1-O2A-CGA
29	1	302	CHL	C2-C1-O2A-CGA
29	b	309	CHL	C2-C1-O2A-CGA
29	b	310	CHL	C2-C1-O2A-CGA
21	A	801	CLA	CAA-CBA-CGA-O2A
21	B	831	CLA	CAA-CBA-CGA-O2A
22	A	843	PQN	C25-C26-C27-C28
21	c	603	CLA	C4-C3-C5-C6
21	7	401	CLA	C2C-C3C-CAC-CBC
24	G	205	BCR	C5-C6-C7-C8
30	1	317	LUT	C5-C6-C7-C8
30	9	615	LUT	C1-C6-C7-C8
23	A	855	LHG	C12-C13-C14-C15
21	A	805	CLA	C6-C7-C8-C10
23	A	844	LHG	C3-O3-P-O6
23	A	845	LHG	C3-O3-P-O6
23	1	319	LHG	C3-O3-P-O6
23	5	617	LHG	C3-O3-P-O6
23	9	618	LHG	C3-O3-P-O6
23	a	617	LHG	C3-O3-P-O6
23	c	619	LHG	C3-O3-P-O6
21	A	810	CLA	O1D-CGD-O2D-CED
23	b	319	LHG	C4-C5-C6-O8
21	A	806	CLA	C4-C3-C5-C6
21	B	806	CLA	C11-C12-C13-C15
21	B	825	CLA	C11-C12-C13-C15
21	B	835	CLA	C6-C7-C8-C10
21	B	840	CLA	C11-C12-C13-C14
21	1	303	CLA	C11-C12-C13-C14
21	9	611	CLA	C11-C10-C8-C9
21	c	611	CLA	C6-C7-C8-C9
21	A	804	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
21	4	602	CLA	C4C-C3C-CAC-CBC
31	5	616	XAT	C11-C12-C13-C20
21	B	831	CLA	C11-C10-C8-C7
26	b	301	LMU	C4-C5-C6-C7
21	b	311	CLA	C2-C3-C5-C6
21	5	603	CLA	CAA-CBA-CGA-O2A
21	2	609	CLA	CAA-CBA-CGA-O2A
21	9	610	CLA	C5-C6-C7-C8
21	A	802	CLA	C2A-CAA-CBA-CGA
21	a	613	CLA	C2A-CAA-CBA-CGA
21	9	604	CLA	CAA-CBA-CGA-O1A
24	B	846	BCR	C9-C10-C11-C12
21	A	819	CLA	C4-C3-C5-C6
21	B	802	CLA	C4-C3-C5-C6
21	B	831	CLA	C4-C3-C5-C6
21	A	819	CLA	C2-C3-C5-C6
21	2	608	CLA	C2-C3-C5-C6
21	c	603	CLA	C2-C3-C5-C6
21	H	201	CLA	O1D-CGD-O2D-CED
21	6	603	CLA	CAA-CBA-CGA-O1A
29	6	602	CHL	C2-C1-O2A-CGA
21	c	604	CLA	CAA-CBA-CGA-O1A
21	A	838	CLA	C2A-CAA-CBA-CGA
21	B	804	CLA	C2A-CAA-CBA-CGA
21	G	204	CLA	C2A-CAA-CBA-CGA
21	7	411	CLA	C2A-CAA-CBA-CGA
21	b	303	CLA	C2A-CAA-CBA-CGA
21	b	315	CLA	C2A-CAA-CBA-CGA
29	5	606	CHL	C2A-CAA-CBA-CGA
21	B	818	CLA	C3A-C2A-CAA-CBA
21	B	835	CLA	C3A-C2A-CAA-CBA
21	B	839	CLA	C3A-C2A-CAA-CBA
21	H	201	CLA	C3A-C2A-CAA-CBA
21	8	601	CLA	C3A-C2A-CAA-CBA
21	b	305	CLA	C3A-C2A-CAA-CBA
21	b	315	CLA	C3A-C2A-CAA-CBA
21	8	608	CLA	CAA-CBA-CGA-O1A
21	A	831	CLA	C6-C7-C8-C10
21	B	801	CLA	CAA-CBA-CGA-O2A
27	B	847	DGD	C2B-C3B-C4B-C5B
29	9	608	CHL	CAA-CBA-CGA-O2A
21	B	801	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
21	2	608	CLA	C4-C3-C5-C6
21	A	823	CLA	C6-C7-C8-C9
21	B	835	CLA	C11-C12-C13-C14
21	B	839	CLA	C14-C13-C15-C16
21	5	602	CLA	C11-C10-C8-C9
21	8	602	CLA	C11-C10-C8-C9
24	A	850	BCR	C11-C10-C9-C34
24	A	850	BCR	C16-C17-C18-C36
24	L	301	BCR	C11-C10-C9-C34
30	1	317	LUT	C20-C13-C14-C15
30	3	416	LUT	C11-C10-C9-C19
30	4	615	LUT	C20-C13-C14-C15
30	8	614	LUT	C20-C13-C14-C15
31	9	616	XAT	C40-C33-C34-C35
32	9	617	NEX	C39-C29-C30-C31
32	b	318	NEX	C39-C29-C30-C31
32	c	618	NEX	C39-C29-C30-C31
21	L	302	CLA	CAA-CBA-CGA-O1A
21	b	315	CLA	CAA-CBA-CGA-O2A
29	4	606	CHL	CAA-CBA-CGA-O1A
21	A	807	CLA	C15-C16-C17-C18
21	A	805	CLA	C6-C7-C8-C9
21	3	402	CLA	C11-C12-C13-C15
21	A	832	CLA	CAA-CBA-CGA-O1A
21	4	603	CLA	CAA-CBA-CGA-O1A
21	6	603	CLA	CAA-CBA-CGA-O2A
29	c	607	CHL	CAA-CBA-CGA-O1A
29	c	607	CHL	CAA-CBA-CGA-O2A
21	A	804	CLA	C15-C16-C17-C18
21	A	842	CLA	C10-C11-C12-C13
21	2	603	CLA	CAA-CBA-CGA-O1A
29	6	606	CHL	CAA-CBA-CGA-O1A
21	A	815	CLA	C1A-C2A-CAA-CBA
21	B	812	CLA	C1A-C2A-CAA-CBA
21	B	828	CLA	C1A-C2A-CAA-CBA
21	F	302	CLA	C1A-C2A-CAA-CBA
21	L	303	CLA	C1A-C2A-CAA-CBA
21	8	601	CLA	C1A-C2A-CAA-CBA
21	9	610	CLA	C1A-C2A-CAA-CBA
21	9	613	CLA	C1A-C2A-CAA-CBA
21	B	837	CLA	C16-C17-C18-C19
28	G	206	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
21	A	804	CLA	C12-C13-C15-C16
21	A	826	CLA	C11-C10-C8-C7
21	B	806	CLA	C12-C13-C15-C16
21	B	823	CLA	C12-C13-C15-C16
21	B	815	CLA	C5-C6-C7-C8
21	b	315	CLA	CAA-CBA-CGA-O1A
21	c	604	CLA	CAA-CBA-CGA-O2A
21	B	834	CLA	C2A-CAA-CBA-CGA
21	B	809	CLA	CAA-CBA-CGA-O2A
21	B	807	CLA	C8-C10-C11-C12
27	B	847	DGD	C4B-C5B-C6B-C7B
21	A	826	CLA	C3-C5-C6-C7
21	5	603	CLA	CAA-CBA-CGA-O1A
21	9	604	CLA	CAA-CBA-CGA-O2A
21	A	827	CLA	C4-C3-C5-C6
21	A	834	CLA	C4-C3-C5-C6
21	B	810	CLA	C4-C3-C5-C6
29	6	614	CHL	CAA-CBA-CGA-O1A
21	A	805	CLA	O1A-CGA-O2A-C1
21	B	826	CLA	C3-C5-C6-C7
24	A	850	BCR	C11-C10-C9-C8
24	A	850	BCR	C16-C17-C18-C19
24	L	301	BCR	C11-C10-C9-C8
30	1	317	LUT	C12-C13-C14-C15
30	3	416	LUT	C11-C10-C9-C8
30	4	615	LUT	C12-C13-C14-C15
30	8	614	LUT	C12-C13-C14-C15
31	9	616	XAT	C32-C33-C34-C35
32	9	617	NEX	C28-C29-C30-C31
32	c	618	NEX	C28-C29-C30-C31
21	2	603	CLA	CAA-CBA-CGA-O2A
21	8	608	CLA	CAA-CBA-CGA-O2A
21	A	810	CLA	CAA-CBA-CGA-O1A
21	A	841	CLA	C8-C10-C11-C12
29	6	606	CHL	CAA-CBA-CGA-O2A
29	6	614	CHL	CAA-CBA-CGA-O2A
29	9	608	CHL	CAA-CBA-CGA-O1A
21	A	828	CLA	C2-C1-O2A-CGA
21	A	841	CLA	C2-C1-O2A-CGA
21	2	608	CLA	C2-C1-O2A-CGA
21	B	801	CLA	C2-C3-C5-C6
21	B	802	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
21	A	832	CLA	CAA-CBA-CGA-O2A
21	8	603	CLA	CAA-CBA-CGA-O1A
21	8	603	CLA	CAA-CBA-CGA-O2A
29	4	606	CHL	CAA-CBA-CGA-O2A
21	A	817	CLA	C14-C13-C15-C16
21	A	821	CLA	C11-C10-C8-C9
21	A	842	CLA	C11-C10-C8-C9
21	B	828	CLA	CBA-CGA-O2A-C1
21	B	821	CLA	O1D-CGD-O2D-CED
21	4	603	CLA	CAA-CBA-CGA-O2A
21	A	837	CLA	C4-C3-C5-C6
21	B	840	CLA	CAA-CBA-CGA-O2A
21	1	303	CLA	C8-C10-C11-C12
21	A	841	CLA	C16-C17-C18-C19
21	B	804	CLA	C16-C17-C18-C19
21	L	302	CLA	CAA-CBA-CGA-O2A
24	A	848	BCR	C5-C6-C7-C8
24	A	849	BCR	C1-C6-C7-C8
24	O	205	BCR	C23-C24-C25-C30
24	2	618	BCR	C1-C6-C7-C8
24	4	617	BCR	C1-C6-C7-C8
24	4	617	BCR	C5-C6-C7-C8
30	a	615	LUT	C1-C6-C7-C8
30	a	616	LUT	C1-C6-C7-C8
30	c	615	LUT	C1-C6-C7-C8
29	6	602	CHL	O1D-CGD-O2D-CED
23	A	855	LHG	C24-C25-C26-C27
21	b	305	CLA	CAA-CBA-CGA-O2A
21	8	611	CLA	CBA-CGA-O2A-C1
24	B	844	BCR	C13-C14-C15-C16
31	5	616	XAT	C9-C10-C11-C12
21	A	805	CLA	CBA-CGA-O2A-C1
21	B	828	CLA	C4-C3-C5-C6
24	B	844	BCR	C17-C18-C19-C20
30	a	615	LUT	C27-C28-C29-C30
21	B	804	CLA	C8-C10-C11-C12
21	A	806	CLA	C2-C3-C5-C6
21	A	840	CLA	C2-C3-C5-C6
21	B	831	CLA	C2-C3-C5-C6
21	G	204	CLA	CAA-CBA-CGA-O2A
21	4	611	CLA	CAA-CBA-CGA-O2A
21	7	401	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
21	7	402	CLA	CAA-CBA-CGA-O2A
29	c	605	CHL	CAA-CBA-CGA-O2A
27	B	847	DGD	C5D-C6D-O5D-C1E
21	A	810	CLA	CAA-CBA-CGA-O2A
21	a	610	CLA	CAA-CBA-CGA-O2A
29	a	606	CHL	CAA-CBA-CGA-O2A
29	a	608	CHL	CAA-CBA-CGA-O2A
23	A	855	LHG	C29-C30-C31-C32
21	b	313	CLA	CAA-CBA-CGA-O2A
29	5	601	CHL	CAA-CBA-CGA-O2A
29	a	606	CHL	CAA-CBA-CGA-O1A
29	a	608	CHL	CAA-CBA-CGA-O1A
29	c	608	CHL	CAA-CBA-CGA-O2A
23	c	619	LHG	C17-C18-C19-C20
21	1	308	CLA	CAA-CBA-CGA-O2A
21	6	612	CLA	CAA-CBA-CGA-O2A
29	8	606	CHL	CAA-CBA-CGA-O2A
21	B	836	CLA	C8-C10-C11-C12
21	B	828	CLA	O1A-CGA-O2A-C1
23	a	617	LHG	C24-C25-C26-C27
21	A	842	CLA	C11-C10-C8-C7
21	B	806	CLA	C6-C7-C8-C10
21	B	837	CLA	C2-C3-C5-C6
21	1	310	CLA	CAA-CBA-CGA-O2A
23	A	845	LHG	O8-C23-C24-C25
31	6	617	XAT	C9-C10-C11-C12
29	9	607	CHL	CAA-CBA-CGA-O2A
21	B	839	CLA	CAA-CBA-CGA-O2A
21	A	837	CLA	C2A-CAA-CBA-CGA
21	9	604	CLA	O1D-CGD-O2D-CED
21	A	831	CLA	C6-C7-C8-C9
21	A	841	CLA	C16-C17-C18-C20
21	1	312	CLA	CAA-CBA-CGA-O2A
21	a	610	CLA	CAA-CBA-CGA-O1A
21	b	312	CLA	CAA-CBA-CGA-O2A
21	c	610	CLA	CAA-CBA-CGA-O2A
29	2	606	CHL	CAA-CBA-CGA-O2A
21	B	821	CLA	C4-C3-C5-C6
29	2	601	CHL	C4-C3-C5-C6
21	B	817	CLA	C10-C11-C12-C13
29	6	601	CHL	CAA-CBA-CGA-O2A
29	c	606	CHL	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
21	A	834	CLA	C2-C3-C5-C6
21	A	807	CLA	C11-C12-C13-C14
21	A	834	CLA	C11-C12-C13-C14
21	B	802	CLA	C11-C10-C8-C9
21	B	805	CLA	C11-C10-C8-C9
21	B	807	CLA	C6-C7-C8-C9
21	B	817	CLA	C11-C10-C8-C9
21	B	822	CLA	CAA-CBA-CGA-O2A
21	b	313	CLA	CAA-CBA-CGA-O1A
21	B	809	CLA	C3A-C2A-CAA-CBA
21	B	812	CLA	C3A-C2A-CAA-CBA
21	B	819	CLA	C3A-C2A-CAA-CBA
21	5	604	CLA	C3A-C2A-CAA-CBA
21	A	818	CLA	CAA-CBA-CGA-O2A
21	K	204	CLA	CAA-CBA-CGA-O2A
21	8	609	CLA	CAA-CBA-CGA-O2A
29	5	606	CHL	CAA-CBA-CGA-O2A
29	8	606	CHL	CAA-CBA-CGA-O1A
29	a	605	CHL	CAA-CBA-CGA-O2A
21	A	803	CLA	CAD-CBD-CGD-O2D
21	A	808	CLA	CAD-CBD-CGD-O2D
21	A	812	CLA	CAD-CBD-CGD-O2D
21	A	818	CLA	CAD-CBD-CGD-O2D
21	A	820	CLA	CAD-CBD-CGD-O2D
21	A	826	CLA	CAD-CBD-CGD-O2D
21	A	841	CLA	CAD-CBD-CGD-O2D
21	B	820	CLA	CAD-CBD-CGD-O2D
21	B	824	CLA	CAD-CBD-CGD-O2D
21	B	833	CLA	CAD-CBD-CGD-O2D
21	B	838	CLA	CAD-CBD-CGD-O2D
21	F	304	CLA	CAD-CBD-CGD-O2D
21	F	305	CLA	CAD-CBD-CGD-O2D
21	G	202	CLA	CAD-CBD-CGD-O2D
21	1	309	CLA	CAD-CBD-CGD-O2D
21	1	313	CLA	CAD-CBD-CGD-O2D
21	1	315	CLA	CAD-CBD-CGD-O2D
21	1	316	CLA	CAD-CBD-CGD-O2D
21	3	411	CLA	CAD-CBD-CGD-O2D
21	4	604	CLA	CAD-CBD-CGD-O2D
21	5	604	CLA	CAD-CBD-CGD-O2D
21	5	612	CLA	CAD-CBD-CGD-O2D
21	8	610	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
21	9	602	CLA	CAD-CBD-CGD-O2D
21	a	612	CLA	CAD-CBD-CGD-O2D
21	a	613	CLA	CAD-CBD-CGD-O2D
21	b	304	CLA	CAD-CBD-CGD-O2D
21	c	612	CLA	CAD-CBD-CGD-O2D
28	G	206	LMG	C7-C8-O7-C10
28	G	206	LMG	C9-C8-O7-C10
29	b	307	CHL	CAD-CBD-CGD-O2D
27	B	847	DGD	C2A-C3A-C4A-C5A
21	A	840	CLA	C2A-CAA-CBA-CGA
29	c	609	CHL	C2A-CAA-CBA-CGA
21	B	825	CLA	C2-C1-O2A-CGA
29	2	601	CHL	C2-C1-O2A-CGA
21	A	836	CLA	CAA-CBA-CGA-O2A
21	5	609	CLA	CAA-CBA-CGA-O2A
21	5	614	CLA	CAA-CBA-CGA-O2A
29	9	609	CHL	CAA-CBA-CGA-O2A
29	c	606	CHL	CAA-CBA-CGA-O1A
29	c	609	CHL	CAA-CBA-CGA-O2A
21	9	604	CLA	CBD-CGD-O2D-CED
21	G	204	CLA	CAA-CBA-CGA-O1A
21	1	308	CLA	CAA-CBA-CGA-O1A
21	5	611	CLA	CAA-CBA-CGA-O2A
21	7	402	CLA	CAA-CBA-CGA-O1A
21	8	610	CLA	CAA-CBA-CGA-O2A
29	5	601	CHL	CAA-CBA-CGA-O1A
29	9	606	CHL	CAA-CBA-CGA-O2A
29	a	609	CHL	CAA-CBA-CGA-O2A
29	c	608	CHL	CAA-CBA-CGA-O1A
21	A	827	CLA	C2-C3-C5-C6
21	B	810	CLA	C2-C3-C5-C6
29	2	601	CHL	C2-C3-C5-C6
21	A	806	CLA	CAA-CBA-CGA-O2A
28	G	206	LMG	C19-C20-C21-C22
31	9	616	XAT	O24-C26-C27-C28
21	4	611	CLA	CAA-CBA-CGA-O1A
21	b	305	CLA	CAA-CBA-CGA-O1A
29	2	614	CHL	CAA-CBA-CGA-O2A
27	B	847	DGD	O6D-C5D-C6D-O5D
21	B	814	CLA	C8-C10-C11-C12
21	A	827	CLA	CAA-CBA-CGA-O2A
21	1	303	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
21	1	312	CLA	CAA-CBA-CGA-O1A
21	8	610	CLA	CAA-CBA-CGA-O1A
29	9	607	CHL	CAA-CBA-CGA-O1A
21	B	805	CLA	O2A-C1-C2-C3
29	6	607	CHL	O2A-C1-C2-C3
29	b	310	CHL	O2A-C1-C2-C3
21	B	805	CLA	O1A-CGA-O2A-C1
21	B	822	CLA	CAA-CBA-CGA-O1A
21	6	612	CLA	CAA-CBA-CGA-O1A
21	7	401	CLA	CAA-CBA-CGA-O1A
21	b	312	CLA	CAA-CBA-CGA-O1A
29	2	606	CHL	CAA-CBA-CGA-O1A
29	b	307	CHL	CAA-CBA-CGA-O2A
29	c	605	CHL	CAA-CBA-CGA-O1A
21	B	808	CLA	C8-C10-C11-C12
23	b	319	LHG	O2-C2-C3-O3
21	A	804	CLA	CHA-CBD-CGD-O1D
21	A	814	CLA	CHA-CBD-CGD-O1D
21	A	819	CLA	CHA-CBD-CGD-O2D
21	A	837	CLA	CHA-CBD-CGD-O1D
21	A	837	CLA	CHA-CBD-CGD-O2D
21	A	838	CLA	CHA-CBD-CGD-O1D
21	A	838	CLA	CHA-CBD-CGD-O2D
21	A	840	CLA	CHA-CBD-CGD-O1D
21	A	840	CLA	CHA-CBD-CGD-O2D
21	B	812	CLA	CHA-CBD-CGD-O2D
21	B	822	CLA	CHA-CBD-CGD-O1D
21	B	822	CLA	CHA-CBD-CGD-O2D
21	B	827	CLA	CHA-CBD-CGD-O2D
21	B	840	CLA	CHA-CBD-CGD-O1D
21	L	302	CLA	CHA-CBD-CGD-O1D
21	L	302	CLA	CHA-CBD-CGD-O2D
21	1	304	CLA	CHA-CBD-CGD-O1D
21	2	603	CLA	CHA-CBD-CGD-O2D
21	5	603	CLA	CHA-CBD-CGD-O1D
21	8	604	CLA	CHA-CBD-CGD-O2D
21	8	611	CLA	CHA-CBD-CGD-O1D
21	8	611	CLA	CHA-CBD-CGD-O2D
21	9	603	CLA	CHA-CBD-CGD-O1D
21	9	604	CLA	CHA-CBD-CGD-O1D
21	a	614	CLA	CHA-CBD-CGD-O2D
21	b	303	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
21	c	604	CLA	CHA-CBD-CGD-O1D
21	c	604	CLA	CHA-CBD-CGD-O2D
24	J	104	BCR	C13-C14-C15-C16
29	8	613	CHL	CHA-CBD-CGD-O1D
29	8	613	CHL	CHA-CBD-CGD-O2D
29	a	606	CHL	CHA-CBD-CGD-O1D
29	a	606	CHL	CHA-CBD-CGD-O2D
29	b	302	CHL	CHA-CBD-CGD-O1D
29	b	302	CHL	CHA-CBD-CGD-O2D
21	1	310	CLA	CAA-CBA-CGA-O1A
21	5	614	CLA	CAA-CBA-CGA-O1A
29	6	601	CHL	CAA-CBA-CGA-O1A
29	a	605	CHL	CAA-CBA-CGA-O1A
21	B	805	CLA	CBA-CGA-O2A-C1
21	B	806	CLA	C2-C3-C5-C6
21	B	824	CLA	C10-C11-C12-C13
32	b	318	NEX	C28-C29-C30-C31
21	c	610	CLA	CAA-CBA-CGA-O1A
29	2	614	CHL	CAA-CBA-CGA-O1A
29	9	609	CHL	CAA-CBA-CGA-O1A
29	c	609	CHL	CAA-CBA-CGA-O1A
21	A	842	CLA	C16-C17-C18-C19
21	c	602	CLA	CAA-CBA-CGA-O2A
23	A	845	LHG	O10-C23-C24-C25
21	A	823	CLA	C5-C6-C7-C8
21	A	836	CLA	CAA-CBA-CGA-O1A
21	5	609	CLA	CAA-CBA-CGA-O1A
21	5	611	CLA	CAA-CBA-CGA-O1A
21	8	609	CLA	CAA-CBA-CGA-O1A
21	K	201	CLA	O1A-CGA-O2A-C1
21	B	837	CLA	CAA-CBA-CGA-O2A
23	A	845	LHG	O7-C7-C8-C9
21	A	814	CLA	C16-C17-C18-C19
21	9	613	CLA	CBA-CGA-O2A-C1
21	c	603	CLA	CBA-CGA-O2A-C1
21	B	832	CLA	CAA-CBA-CGA-O2A
26	3	420	LMU	C4'-C5'-C6'-O6'
21	A	840	CLA	C4-C3-C5-C6
26	O	206	LMU	C5'-C4'-O1B-C1B
21	9	613	CLA	O1A-CGA-O2A-C1
26	b	301	LMU	C6-C7-C8-C9
21	B	804	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
21	B	824	CLA	C6-C7-C8-C10
21	A	814	CLA	C16-C17-C18-C20
21	B	804	CLA	C16-C17-C18-C20
28	G	206	LMG	O6-C1-O1-C7
21	K	204	CLA	CAA-CBA-CGA-O1A
29	9	606	CHL	CAA-CBA-CGA-O1A
21	B	804	CLA	C11-C12-C13-C14
21	B	806	CLA	C14-C13-C15-C16
21	a	612	CLA	CAA-CBA-CGA-O2A
21	B	805	CLA	CAA-CBA-CGA-O2A
21	c	603	CLA	O1A-CGA-O2A-C1
21	A	808	CLA	CAA-CBA-CGA-O2A
21	A	813	CLA	C2A-CAA-CBA-CGA
21	A	814	CLA	C2A-CAA-CBA-CGA
21	B	817	CLA	C2A-CAA-CBA-CGA
21	b	314	CLA	C2A-CAA-CBA-CGA
21	2	612	CLA	CAA-CBA-CGA-O2A
29	5	606	CHL	CAA-CBA-CGA-O1A
21	B	832	CLA	C4-C3-C5-C6
29	b	306	CHL	CAA-CBA-CGA-O2A
21	B	824	CLA	C8-C10-C11-C12
29	4	606	CHL	O1D-CGD-O2D-CED
21	A	803	CLA	C1A-C2A-CAA-CBA
21	A	823	CLA	C1A-C2A-CAA-CBA
21	B	809	CLA	C1A-C2A-CAA-CBA
21	B	813	CLA	CHA-CBD-CGD-O2D
21	B	819	CLA	C1A-C2A-CAA-CBA
21	B	824	CLA	C1A-C2A-CAA-CBA
21	H	201	CLA	C1A-C2A-CAA-CBA
21	1	314	CLA	CHA-CBD-CGD-O2D
21	3	410	CLA	CHA-CBD-CGD-O2D
21	3	415	CLA	CHA-CBD-CGD-O2D
21	5	604	CLA	C1A-C2A-CAA-CBA
21	b	305	CLA	C1A-C2A-CAA-CBA
21	b	315	CLA	C1A-C2A-CAA-CBA
29	c	601	CHL	C1A-C2A-CAA-CBA
29	c	609	CHL	C1A-C2A-CAA-CBA
29	6	607	CHL	CAA-CBA-CGA-O2A
29	b	307	CHL	CAA-CBA-CGA-O1A
29	6	602	CHL	CBD-CGD-O2D-CED
21	9	602	CLA	C2A-CAA-CBA-CGA
21	A	827	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
23	a	617	LHG	C25-C26-C27-C28
21	B	837	CLA	C4-C3-C5-C6
21	b	304	CLA	CAA-CBA-CGA-O2A
29	a	609	CHL	CAA-CBA-CGA-O1A
23	A	844	LHG	C3-O3-P-O5
23	A	845	LHG	C3-O3-P-O5
23	1	319	LHG	C3-O3-P-O5
26	O	206	LMU	C3'-C4'-O1B-C1B
21	A	806	CLA	CAA-CBA-CGA-O1A
23	A	845	LHG	O9-C7-C8-C9
24	L	305	BCR	C23-C24-C25-C26
24	L	305	BCR	C23-C24-C25-C30
24	O	205	BCR	C23-C24-C25-C26
30	a	616	LUT	C5-C6-C7-C8
21	B	801	CLA	C13-C15-C16-C17
21	A	827	CLA	CAA-CBA-CGA-O1A
21	B	805	CLA	CAA-CBA-CGA-O1A
21	K	201	CLA	CAA-CBA-CGA-O2A
29	8	607	CHL	CAA-CBA-CGA-O2A
21	5	614	CLA	C2A-CAA-CBA-CGA
21	c	602	CLA	CAA-CBA-CGA-O1A
29	a	606	CHL	O1D-CGD-O2D-CED
21	1	315	CLA	C4C-C3C-CAC-CBC
26	O	206	LMU	O5B-C1B-O1B-C4'
21	a	612	CLA	CAA-CBA-CGA-O1A
21	1	304	CLA	CAA-CBA-CGA-O2A
21	A	808	CLA	CAA-CBA-CGA-O1A
21	A	814	CLA	CAD-CBD-CGD-O1D
21	A	816	CLA	CAD-CBD-CGD-O1D
21	A	838	CLA	CAD-CBD-CGD-O1D
21	B	812	CLA	CAD-CBD-CGD-O1D
21	B	840	CLA	CAD-CBD-CGD-O1D
21	6	609	CLA	CAD-CBD-CGD-O1D
21	8	604	CLA	CAD-CBD-CGD-O1D
23	A	855	LHG	C4-C5-O7-C7
23	A	855	LHG	C6-C5-O7-C7
29	b	302	CHL	CAD-CBD-CGD-O1D
21	1	303	CLA	CAA-CBA-CGA-O1A
21	B	807	CLA	CAA-CBA-CGA-O2A
21	B	801	CLA	C14-C13-C15-C16
21	B	823	CLA	C14-C13-C15-C16
21	B	824	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
21	B	827	CLA	C11-C10-C8-C9
27	B	847	DGD	C3B-C4B-C5B-C6B
21	B	826	CLA	CAA-CBA-CGA-O2A
29	c	601	CHL	O1A-CGA-O2A-C1
29	6	607	CHL	CAA-CBA-CGA-O1A
21	5	602	CLA	C8-C10-C11-C12
21	A	806	CLA	C2A-CAA-CBA-CGA
21	1	312	CLA	C2A-CAA-CBA-CGA
21	6	603	CLA	C2A-CAA-CBA-CGA
21	A	841	CLA	CAA-CBA-CGA-O2A
21	B	830	CLA	CAA-CBA-CGA-O2A
21	9	613	CLA	CAA-CBA-CGA-O2A
21	b	303	CLA	CAA-CBA-CGA-O2A
21	c	613	CLA	CAA-CBA-CGA-O2A
23	A	844	LHG	O7-C7-C8-C9
21	B	832	CLA	CAA-CBA-CGA-O1A
21	B	806	CLA	C4-C3-C5-C6
21	A	817	CLA	C12-C13-C15-C16
21	B	805	CLA	C6-C7-C8-C10
21	B	838	CLA	C6-C7-C8-C10
21	F	302	CLA	C3A-C2A-CAA-CBA
21	G	204	CLA	CAD-CBD-CGD-O2D
21	K	202	CLA	C3A-C2A-CAA-CBA
21	O	202	CLA	CAD-CBD-CGD-O2D
21	O	204	CLA	CAD-CBD-CGD-O2D
21	1	314	CLA	CHA-CBD-CGD-O1D
21	3	405	CLA	CHA-CBD-CGD-O1D
21	3	405	CLA	CAD-CBD-CGD-O2D
21	4	603	CLA	CHA-CBD-CGD-O1D
21	5	613	CLA	CAD-CBD-CGD-O2D
21	7	403	CLA	CAD-CBD-CGD-O2D
21	7	404	CLA	CAD-CBD-CGD-O2D
21	7	405	CLA	CAD-CBD-CGD-O2D
21	7	407	CLA	CAD-CBD-CGD-O2D
21	7	409	CLA	CAD-CBD-CGD-O2D
21	7	411	CLA	CAD-CBD-CGD-O2D
21	7	414	CLA	CAD-CBD-CGD-O2D
21	8	602	CLA	CAD-CBD-CGD-O2D
21	8	603	CLA	CAD-CBD-CGD-O2D
21	a	604	CLA	CAD-CBD-CGD-O2D
29	c	609	CHL	C3A-C2A-CAA-CBA
21	B	807	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
21	B	837	CLA	CAA-CBA-CGA-O1A
21	B	829	CLA	CAA-CBA-CGA-O2A
23	4	619	LHG	C32-C33-C34-C35
21	A	825	CLA	CAA-CBA-CGA-O2A
21	5	602	CLA	CAA-CBA-CGA-O2A
31	5	616	XAT	C11-C12-C13-C14
21	2	612	CLA	CAA-CBA-CGA-O1A
29	b	306	CHL	CAA-CBA-CGA-O1A
21	B	837	CLA	C16-C17-C18-C20
21	A	823	CLA	CAA-CBA-CGA-O2A
23	c	619	LHG	O8-C23-C24-C25
21	A	829	CLA	C8-C10-C11-C12
21	1	304	CLA	O1A-CGA-O2A-C1
21	A	825	CLA	CAA-CBA-CGA-O1A
21	B	826	CLA	CAA-CBA-CGA-O1A
21	K	201	CLA	CAA-CBA-CGA-O1A
21	5	602	CLA	CAA-CBA-CGA-O1A
21	b	303	CLA	CAA-CBA-CGA-O1A
27	B	847	DGD	C5A-C6A-C7A-C8A
21	2	610	CLA	C2C-C3C-CAC-CBC
21	A	835	CLA	CAA-CBA-CGA-O2A
23	2	619	LHG	O8-C23-C24-C25
23	6	619	LHG	O8-C23-C24-C25
29	6	602	CHL	CAA-CBA-CGA-O2A
21	A	841	CLA	CAA-CBA-CGA-O1A
21	c	613	CLA	CAA-CBA-CGA-O1A
23	c	619	LHG	O10-C23-C24-C25
22	B	841	PQN	C23-C25-C26-C27
21	B	830	CLA	CAA-CBA-CGA-O1A
21	3	408	CLA	CAA-CBA-CGA-O2A
23	1	319	LHG	O8-C23-C24-C25

There are no ring outliers.

277 monomers are involved in 815 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	8	606	CHL	2	0
31	4	616	XAT	4	0
21	A	824	CLA	3	0
21	B	817	CLA	7	0
24	A	854	BCR	13	0
24	A	847	BCR	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	F	301	BCR	2	0
21	L	303	CLA	1	0
21	8	608	CLA	2	0
29	5	601	CHL	3	0
29	2	614	CHL	5	0
30	9	615	LUT	6	0
21	A	839	CLA	2	0
21	1	304	CLA	4	0
21	G	204	CLA	1	0
21	4	602	CLA	5	0
21	8	602	CLA	4	0
23	A	855	LHG	4	0
29	6	605	CHL	1	0
21	7	401	CLA	7	0
21	7	414	CLA	1	0
29	1	302	CHL	2	0
21	F	304	CLA	2	0
29	4	614	CHL	1	0
24	3	419	BCR	1	0
24	J	103	BCR	3	0
21	5	604	CLA	2	0
21	7	411	CLA	2	0
29	6	602	CHL	3	0
21	4	601	CLA	2	0
21	A	808	CLA	3	0
21	6	604	CLA	9	0
21	5	613	CLA	1	0
21	B	805	CLA	5	0
21	4	608	CLA	1	0
21	5	608	CLA	2	0
21	B	836	CLA	5	0
21	3	409	CLA	22	0
29	9	606	CHL	1	0
29	7	406	CHL	2	0
21	B	834	CLA	2	0
21	A	829	CLA	2	0
21	B	812	CLA	3	0
21	9	602	CLA	2	0
21	3	413	CLA	2	0
21	6	608	CLA	3	0
31	6	617	XAT	9	0
21	3	401	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	B	830	CLA	3	0
21	B	832	CLA	5	0
21	8	609	CLA	25	0
29	9	609	CHL	5	0
21	L	304	CLA	2	0
21	B	838	CLA	2	0
21	1	309	CLA	11	0
21	B	826	CLA	2	0
24	A	849	BCR	4	0
21	4	609	CLA	16	0
24	B	843	BCR	20	0
21	8	618	CLA	2	0
31	2	617	XAT	2	0
21	1	312	CLA	2	0
24	J	101	BCR	5	0
21	3	408	CLA	8	0
30	8	614	LUT	5	0
21	A	828	CLA	5	0
21	1	303	CLA	2	0
29	5	606	CHL	3	0
21	A	831	CLA	1	0
21	B	801	CLA	8	0
21	A	825	CLA	4	0
23	A	844	LHG	2	0
30	7	415	LUT	14	0
21	A	836	CLA	1	0
21	B	803	CLA	2	0
29	2	606	CHL	2	0
29	6	606	CHL	1	0
21	B	835	CLA	2	0
21	A	834	CLA	5	0
29	9	601	CHL	3	0
21	2	603	CLA	2	0
21	6	603	CLA	4	0
21	B	806	CLA	2	0
29	9	608	CHL	1	0
21	K	204	CLA	1	0
21	K	201	CLA	5	0
21	1	314	CLA	1	0
26	3	420	LMU	4	0
24	L	301	BCR	3	0
21	A	809	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	3	411	CLA	1	0
21	A	841	CLA	4	0
21	B	810	CLA	1	0
21	A	804	CLA	3	0
24	7	417	BCR	8	0
30	9	614	LUT	3	0
21	3	405	CLA	1	0
24	B	845	BCR	3	0
21	B	837	CLA	6	0
21	8	603	CLA	2	0
21	A	801	CLA	2	0
21	B	815	CLA	3	0
21	B	821	CLA	1	0
21	B	816	CLA	3	0
21	5	611	CLA	1	0
21	A	832	CLA	2	0
21	B	813	CLA	3	0
21	F	305	CLA	2	0
24	A	850	BCR	1	0
22	B	841	PQN	3	0
30	1	317	LUT	3	0
21	A	817	CLA	4	0
21	9	613	CLA	2	0
29	2	602	CHL	3	0
24	M	101	BCR	3	0
21	9	603	CLA	1	0
29	3	407	CHL	2	0
24	L	306	BCR	3	0
21	4	613	CLA	3	0
30	5	615	LUT	2	0
21	B	807	CLA	6	0
21	A	833	CLA	6	0
31	1	318	XAT	3	0
21	2	609	CLA	24	0
24	2	618	BCR	6	0
24	6	618	BCR	14	0
21	A	806	CLA	3	0
21	8	604	CLA	4	0
23	2	619	LHG	1	0
24	7	418	BCR	4	0
23	6	619	LHG	3	0
29	1	307	CHL	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	805	CLA	5	0
21	3	402	CLA	1	0
21	A	802	CLA	4	0
21	5	607	CLA	3	0
21	4	611	CLA	2	0
24	B	846	BCR	5	0
29	4	606	CHL	1	0
21	6	610	CLA	3	0
21	B	829	CLA	2	0
30	3	416	LUT	12	0
21	B	814	CLA	4	0
24	G	205	BCR	2	0
21	7	412	CLA	1	0
21	H	201	CLA	2	0
23	5	617	LHG	1	0
23	4	619	LHG	1	0
21	5	610	CLA	1	0
21	A	813	CLA	2	0
21	A	840	CLA	8	0
21	9	611	CLA	5	0
21	A	810	CLA	4	0
21	7	404	CLA	4	0
21	A	823	CLA	1	0
30	4	615	LUT	7	0
21	3	403	CLA	1	0
21	A	826	CLA	2	0
24	B	844	BCR	8	0
21	9	604	CLA	2	0
21	B	811	CLA	1	0
21	7	410	CLA	2	0
21	7	413	CLA	1	0
21	7	408	CLA	5	0
21	8	611	CLA	5	0
21	7	402	CLA	9	0
21	A	814	CLA	2	0
21	5	612	CLA	1	0
29	8	605	CHL	5	0
21	B	822	CLA	3	0
21	B	831	CLA	6	0
21	O	202	CLA	1	0
29	8	613	CHL	4	0
21	B	825	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	O	205	BCR	1	0
21	A	827	CLA	7	0
30	2	616	LUT	8	0
21	A	837	CLA	3	0
29	6	607	CHL	5	0
32	9	617	NEX	3	0
21	3	415	CLA	3	0
21	A	835	CLA	3	0
21	B	819	CLA	1	0
21	B	802	CLA	3	0
21	1	306	CLA	3	0
21	3	406	CLA	1	0
21	B	839	CLA	5	0
21	1	313	CLA	1	0
21	B	828	CLA	3	0
21	2	604	CLA	3	0
23	A	845	LHG	1	0
21	B	809	CLA	4	0
21	5	603	CLA	4	0
21	J	102	CLA	1	0
29	9	607	CHL	2	0
26	A	856	LMU	2	0
21	B	804	CLA	2	0
21	3	412	CLA	1	0
23	9	618	LHG	4	0
31	7	416	XAT	5	0
29	9	605	CHL	2	0
21	O	201	CLA	1	0
21	5	614	CLA	1	0
28	G	206	LMG	3	0
21	G	202	CLA	2	0
21	3	404	CLA	4	0
21	2	611	CLA	1	0
21	A	820	CLA	1	0
21	6	611	CLA	1	0
24	F	303	BCR	1	0
21	B	827	CLA	12	0
31	5	616	XAT	7	0
21	1	308	CLA	2	0
21	9	610	CLA	2	0
21	4	603	CLA	1	0
29	4	607	CHL	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	3	418	BCR	7	0
24	K	205	BCR	23	0
21	5	602	CLA	12	0
21	B	820	CLA	1	0
23	4	618	LHG	5	0
21	6	612	CLA	3	0
21	2	613	CLA	2	0
21	1	310	CLA	1	0
21	A	807	CLA	2	0
21	6	613	CLA	2	0
24	B	842	BCR	3	0
24	A	846	BCR	1	0
21	2	608	CLA	4	0
21	A	838	CLA	4	0
24	G	201	BCR	5	0
21	A	812	CLA	6	0
27	B	847	DGD	7	0
24	J	104	BCR	8	0
21	9	612	CLA	1	0
29	8	607	CHL	6	0
21	K	202	CLA	1	0
21	B	824	CLA	3	0
29	6	614	CHL	4	0
29	2	607	CHL	3	0
24	8	616	BCR	9	0
24	I	101	BCR	1	0
21	A	821	CLA	6	0
21	8	612	CLA	2	0
24	L	305	BCR	2	0
21	A	830	CLA	3	0
21	4	612	CLA	1	0
21	7	407	CLA	18	0
21	A	842	CLA	6	0
21	A	852	CLA	8	0
28	6	615	LMG	1	0
21	A	818	CLA	6	0
21	L	302	CLA	2	0
21	A	816	CLA	2	0
21	8	610	CLA	1	0
21	6	609	CLA	3	0
21	2	610	CLA	3	0
21	5	605	CLA	2	0

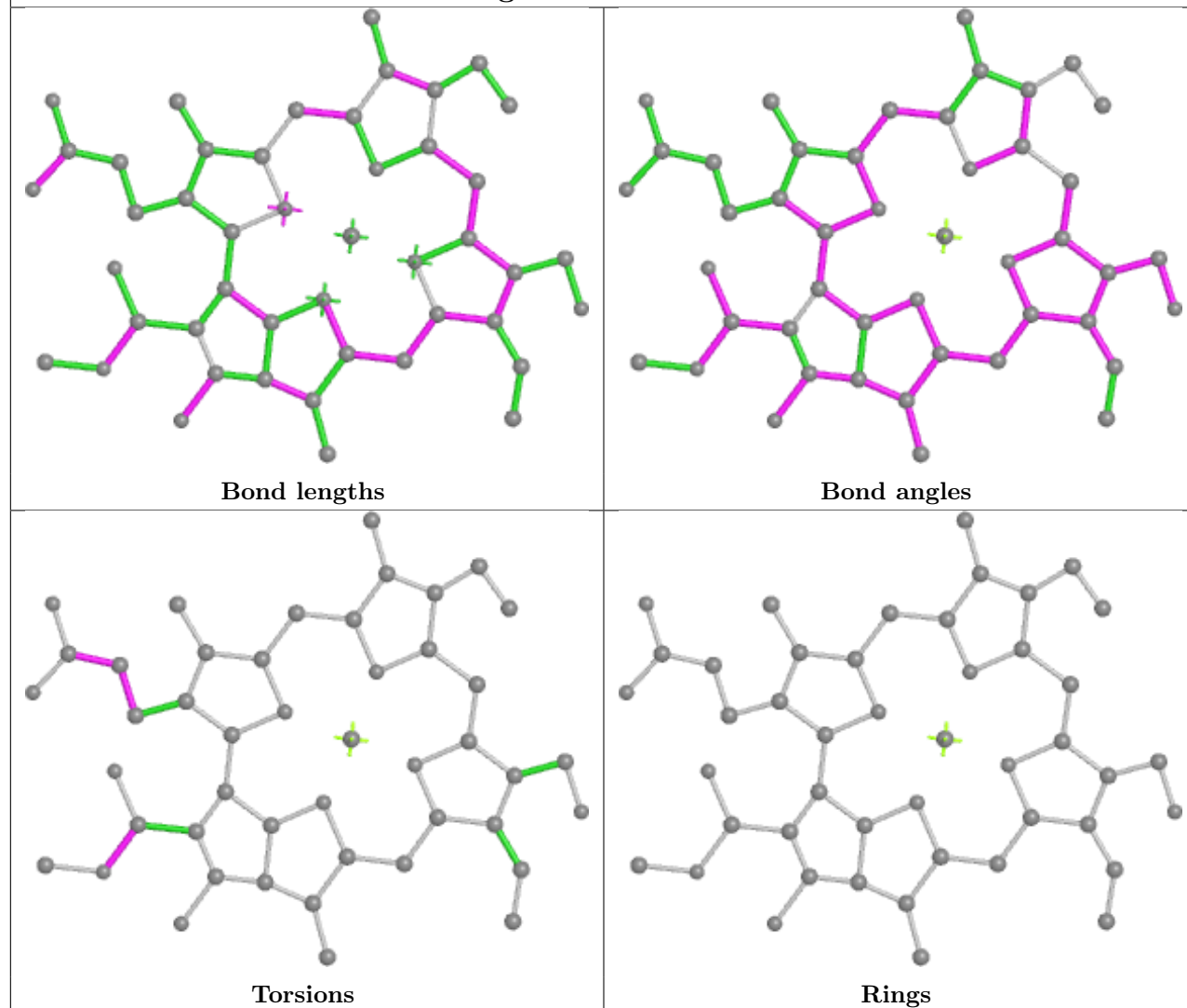
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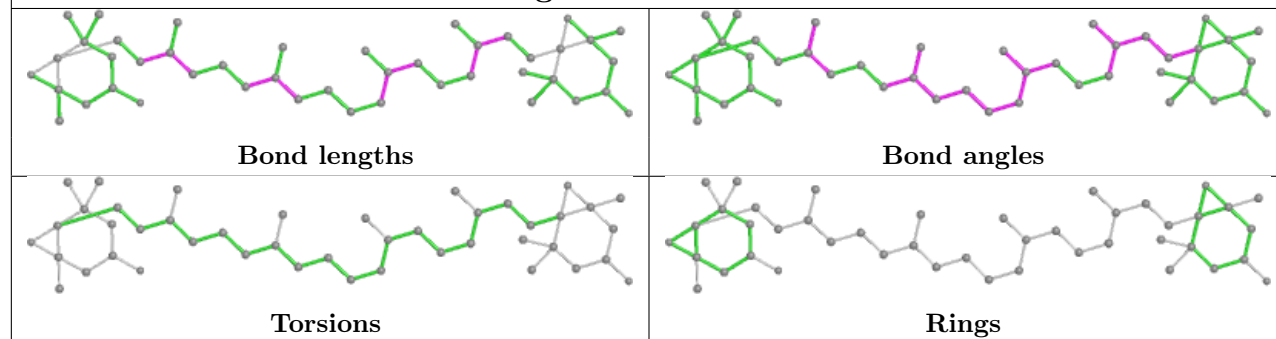
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	B	823	CLA	4	0
21	O	203	CLA	1	0
21	B	808	CLA	3	0
21	B	818	CLA	2	0
21	A	803	CLA	3	0
29	2	601	CHL	3	0
29	6	601	CHL	3	0
21	B	840	CLA	1	0
21	A	819	CLA	6	0
23	8	617	LHG	3	0
31	3	417	XAT	4	0
31	9	616	XAT	2	0
31	8	615	XAT	5	0
21	A	822	CLA	3	0
21	F	302	CLA	1	0
30	6	616	LUT	6	0
21	5	609	CLA	1	0
21	1	315	CLA	2	0
21	K	203	CLA	8	0

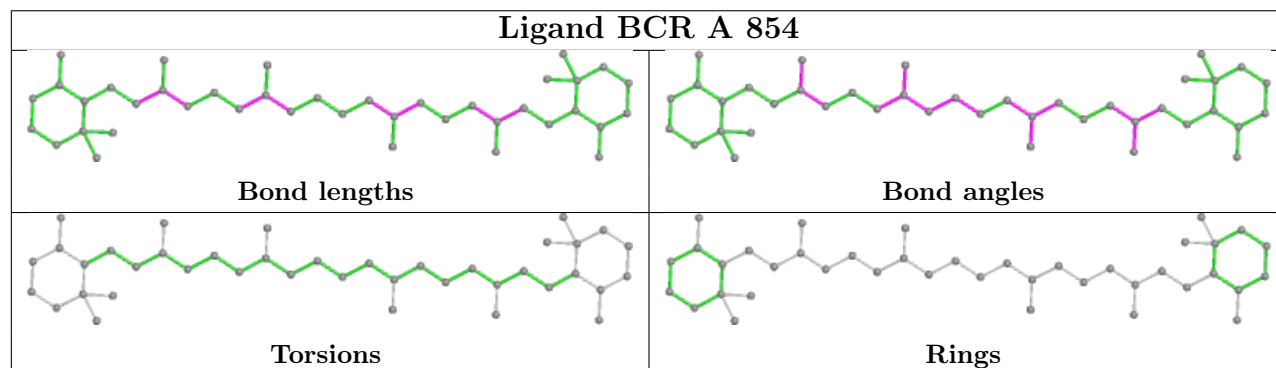
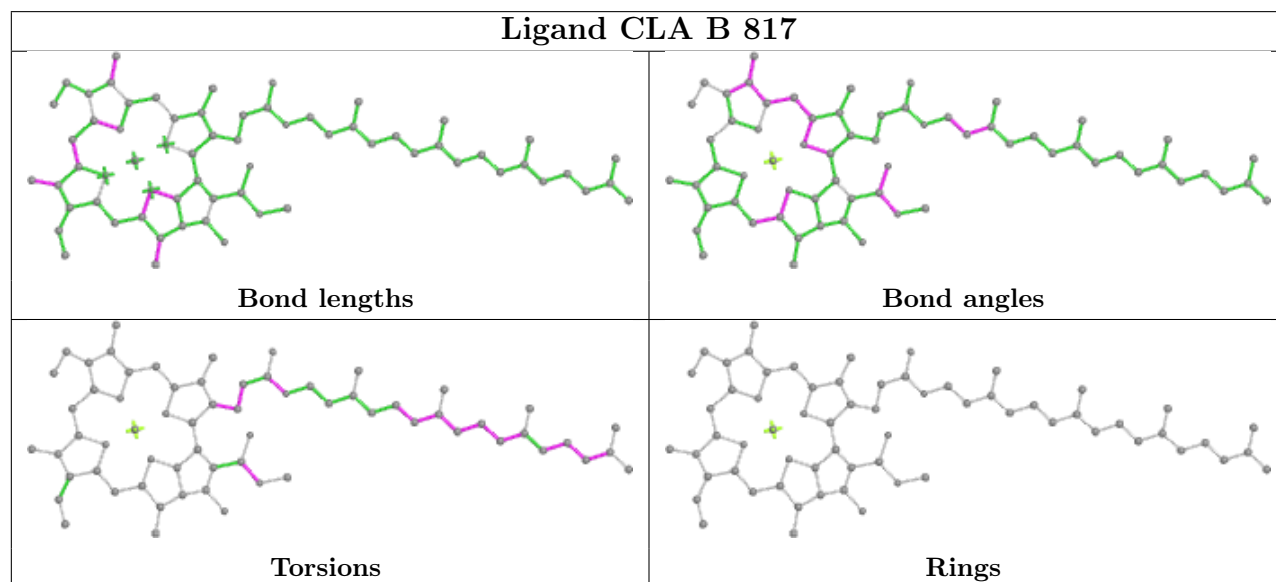
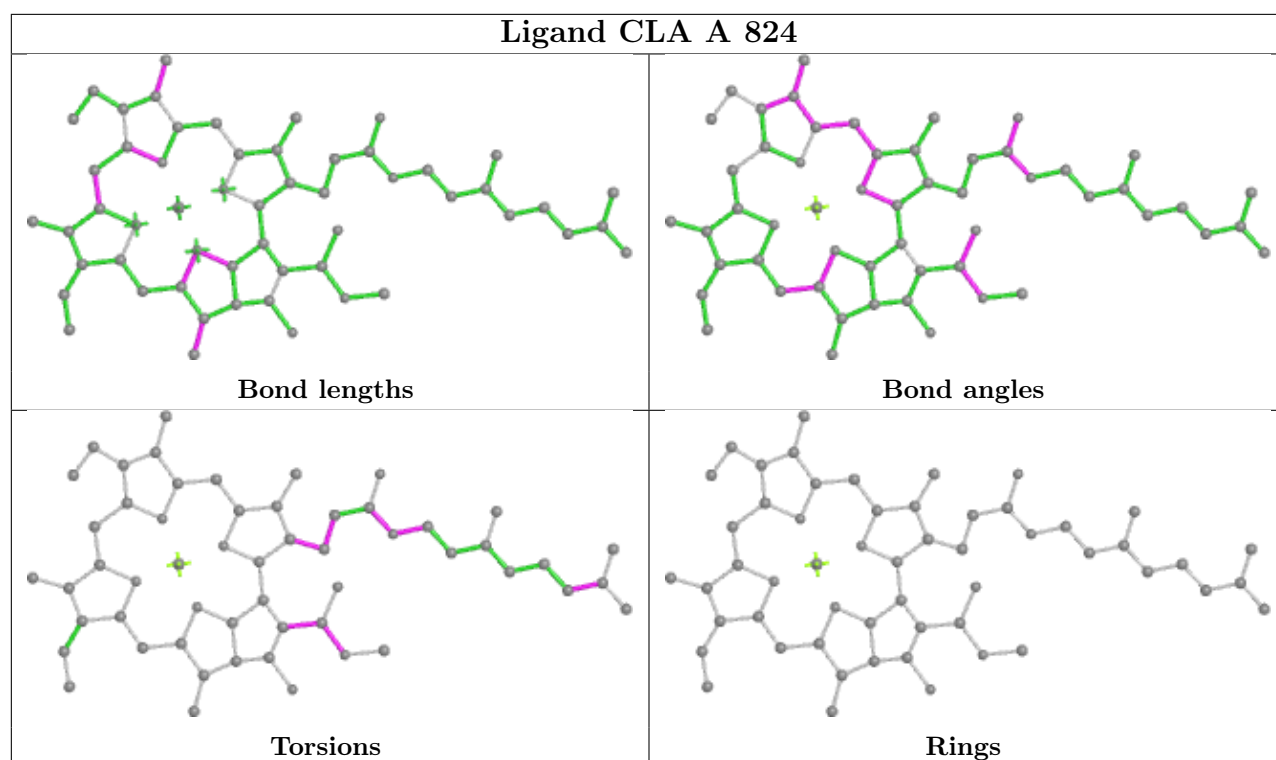
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

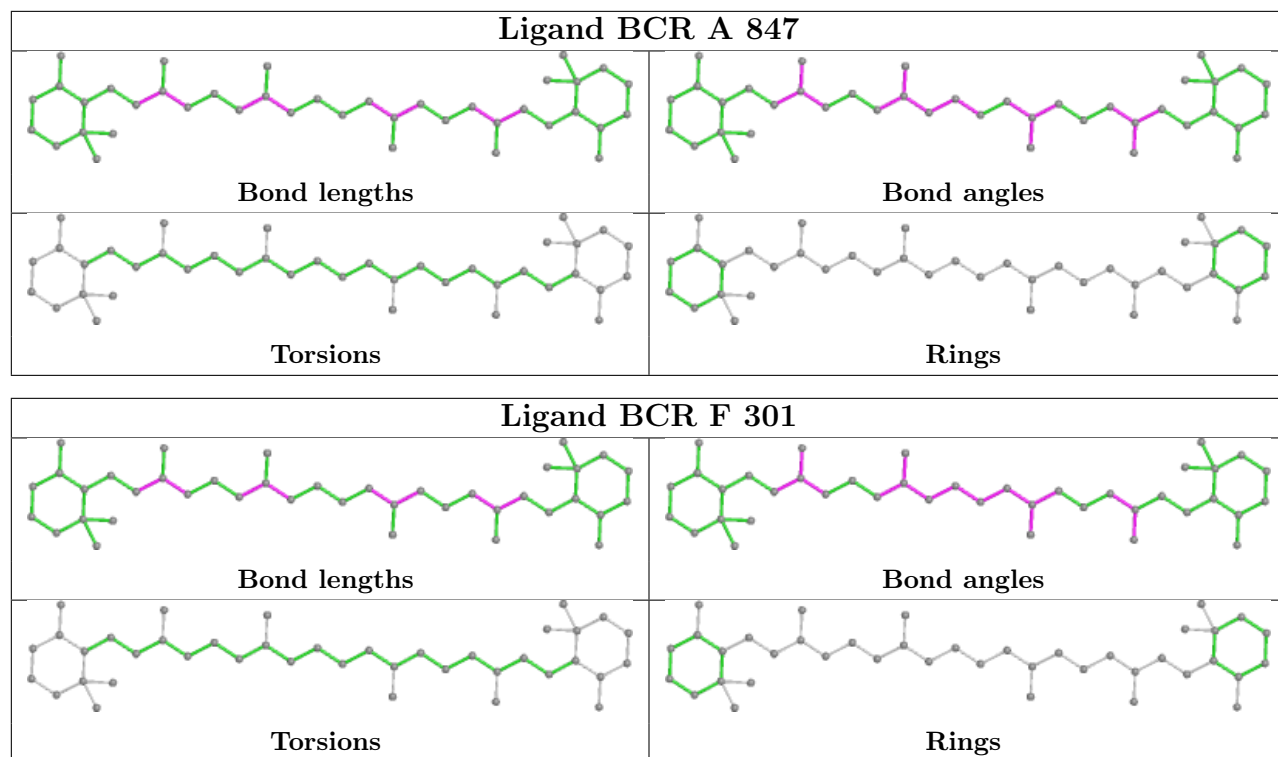
Ligand CHL 8 606



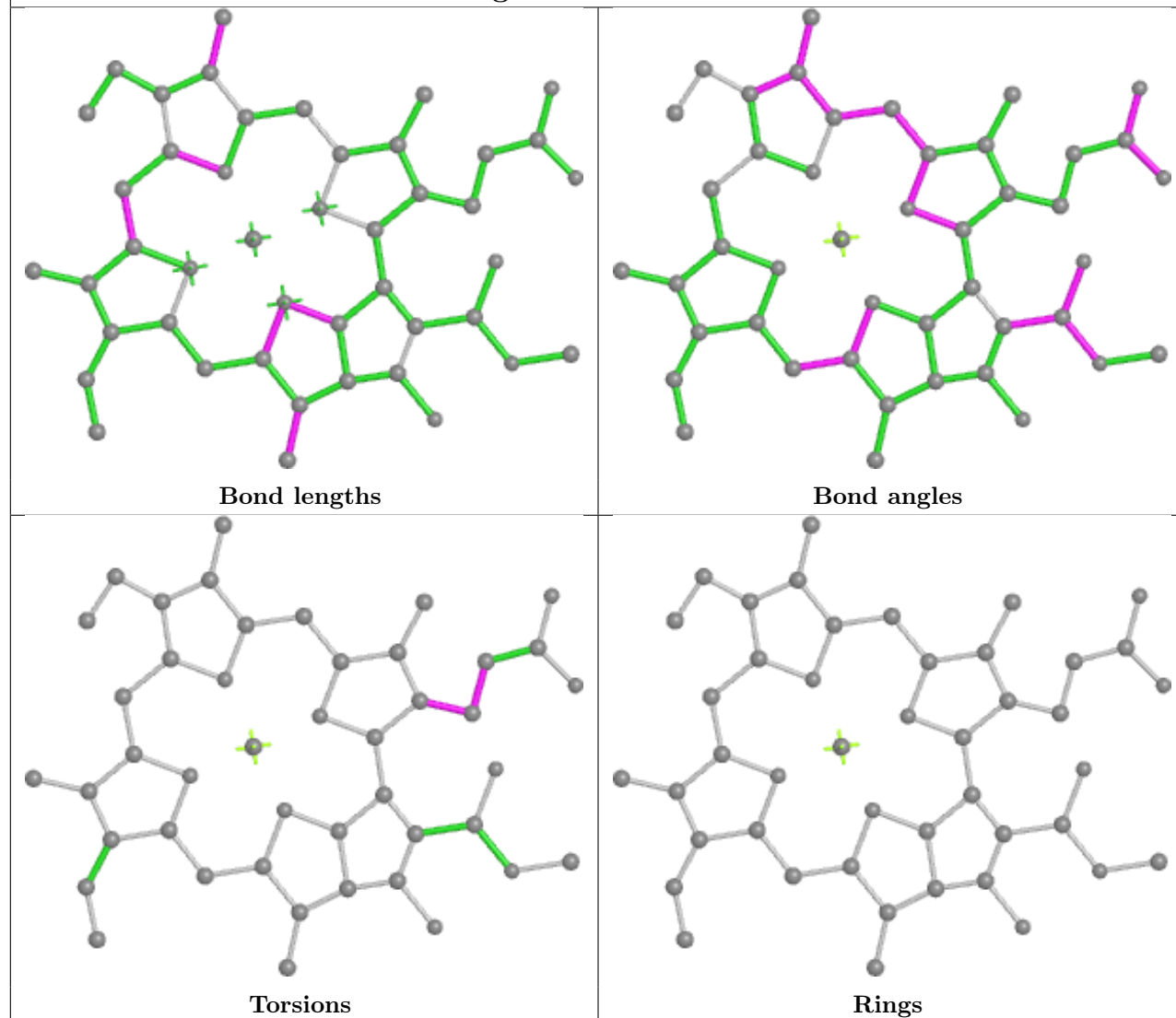
Ligand XAT 4 616



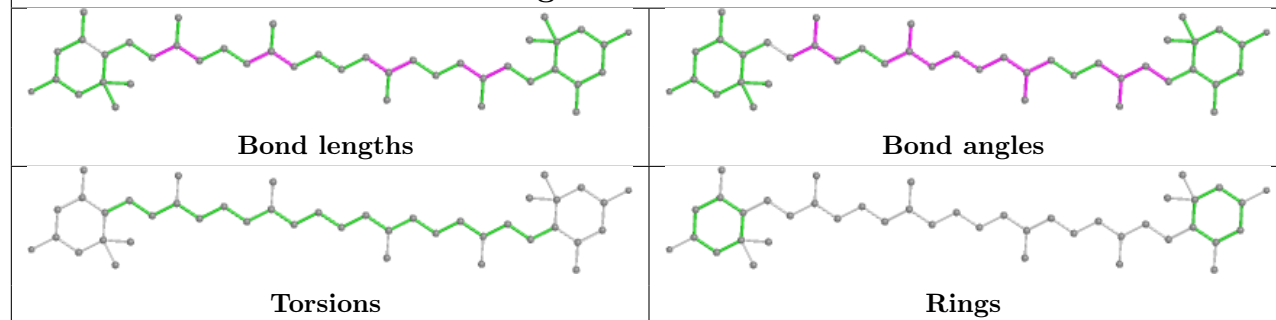


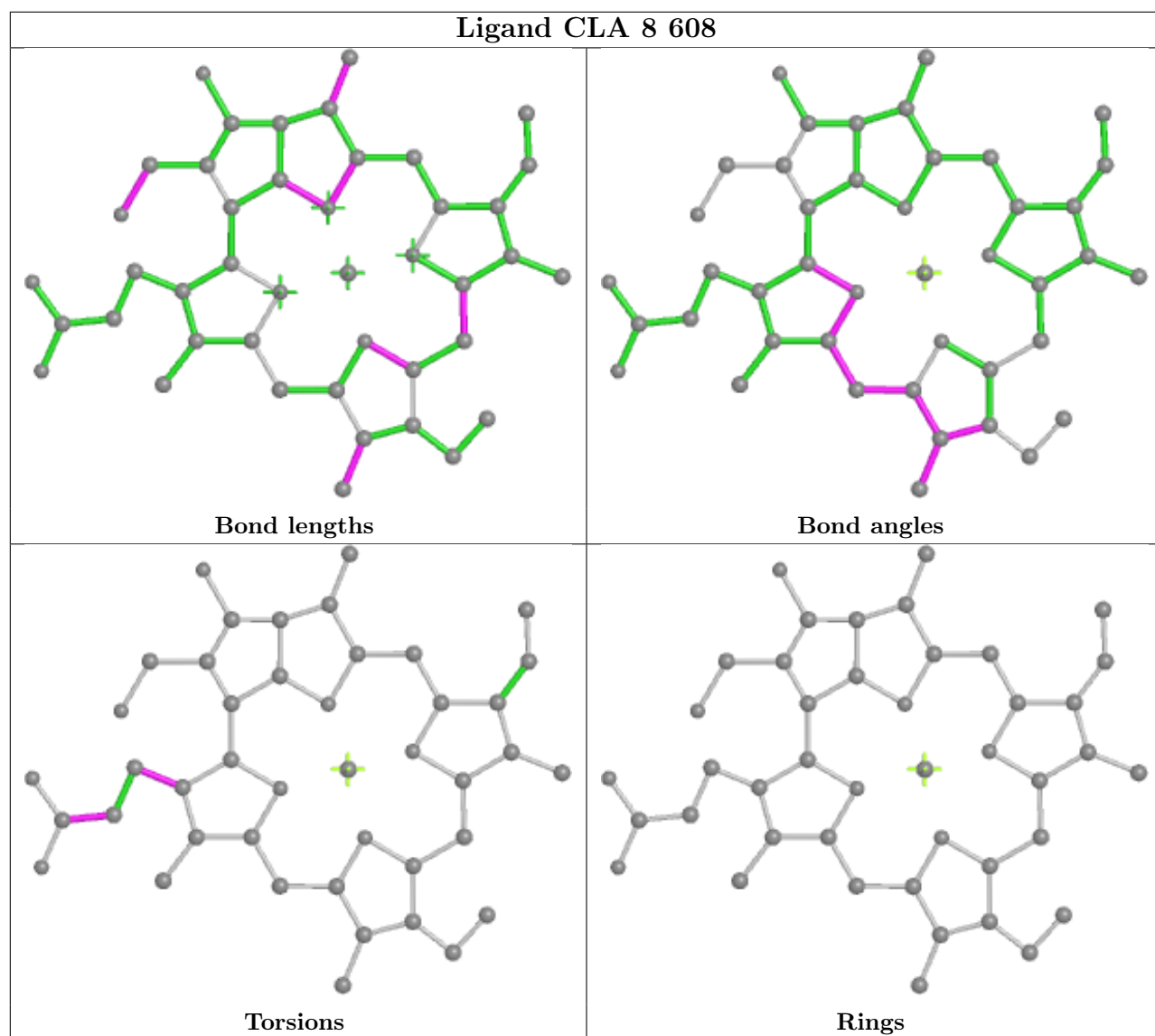
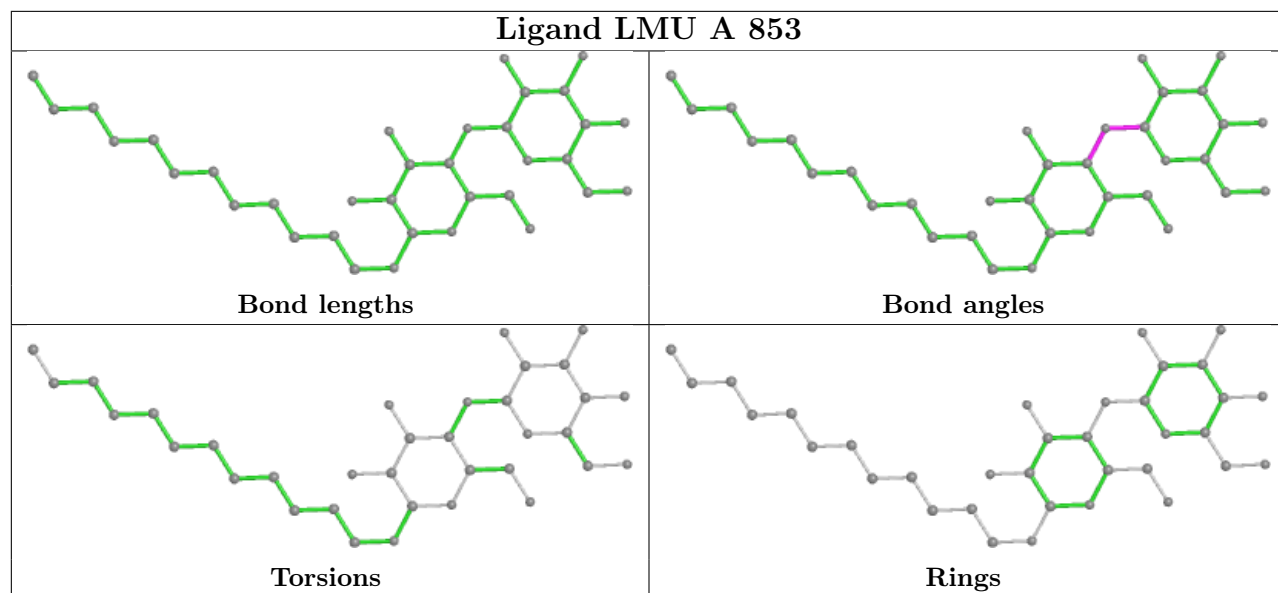


Ligand CLA L 303

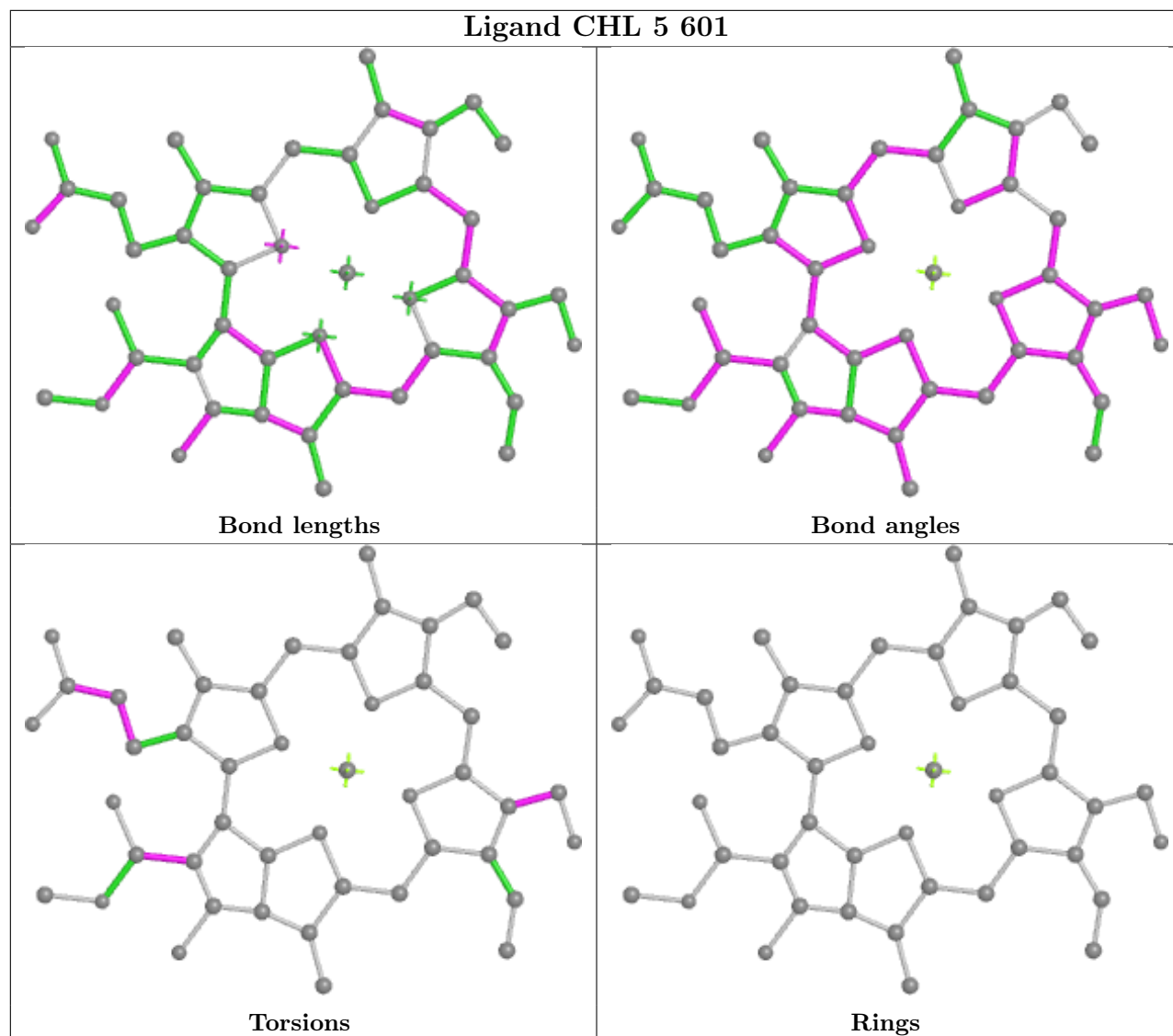


Ligand LUT c 616

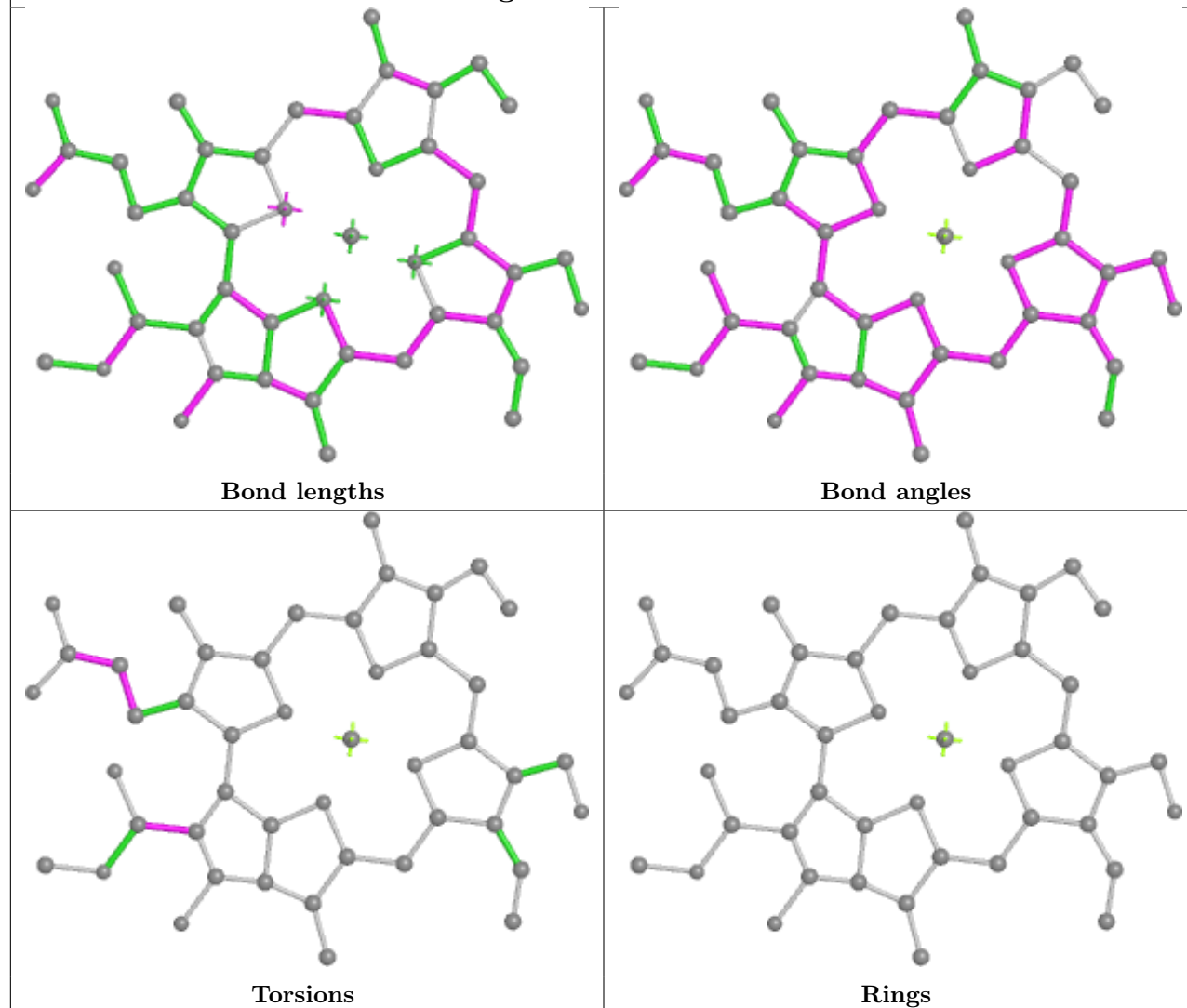




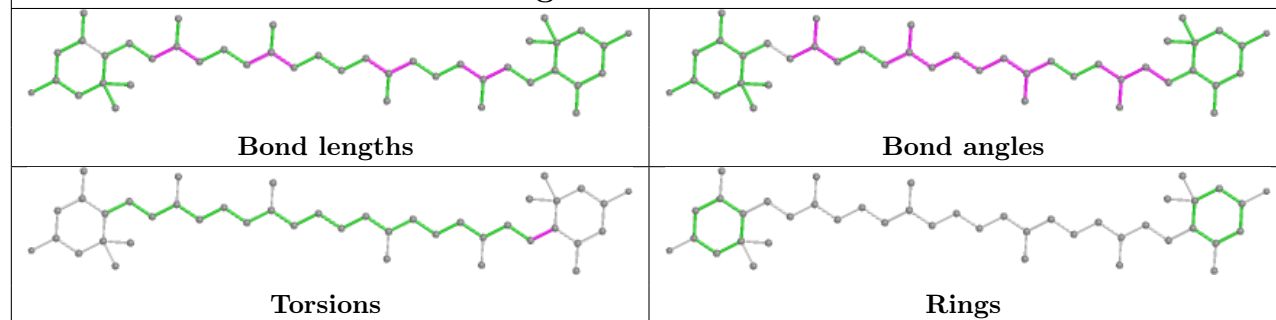
Ligand CHL 5 601



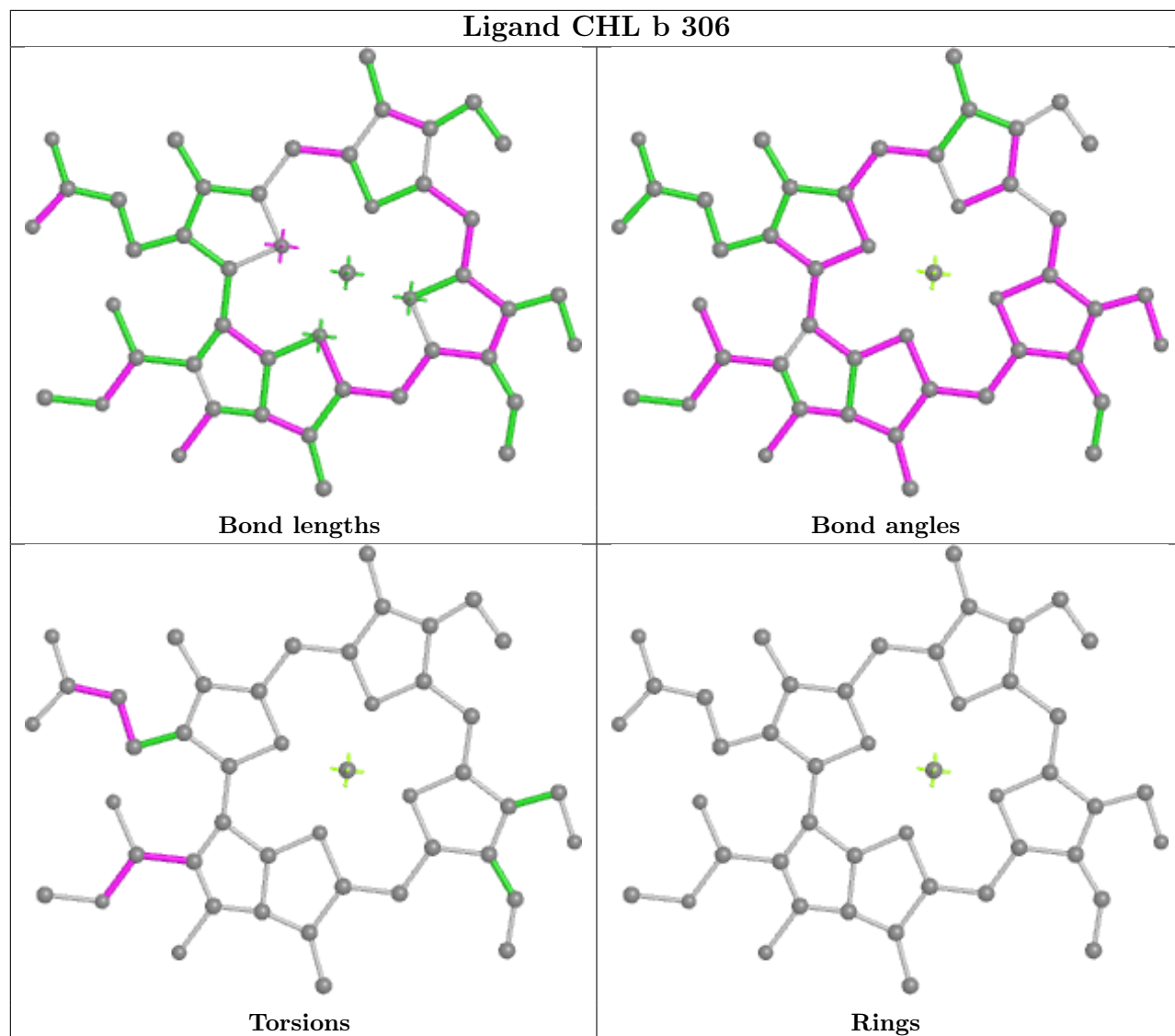
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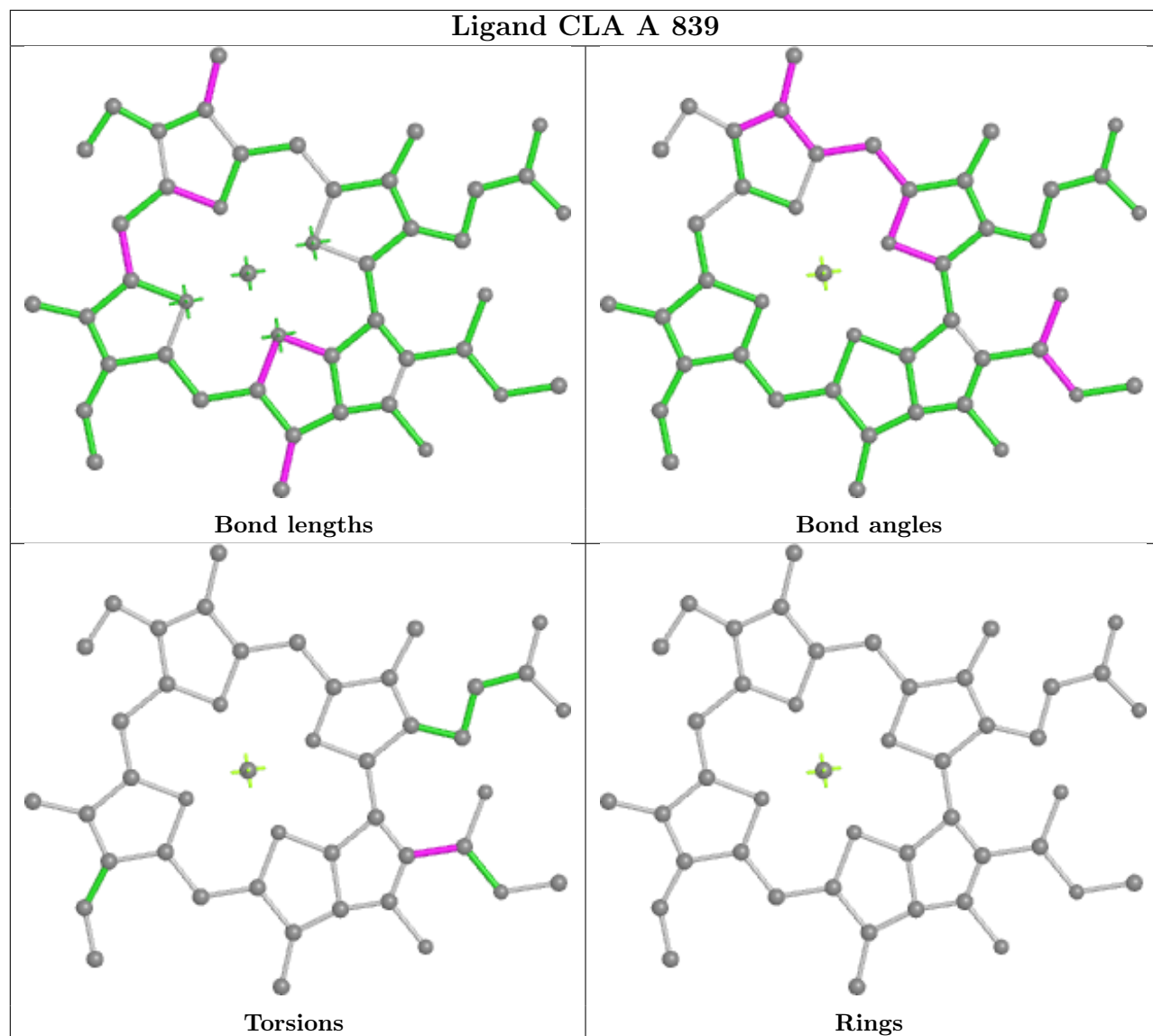
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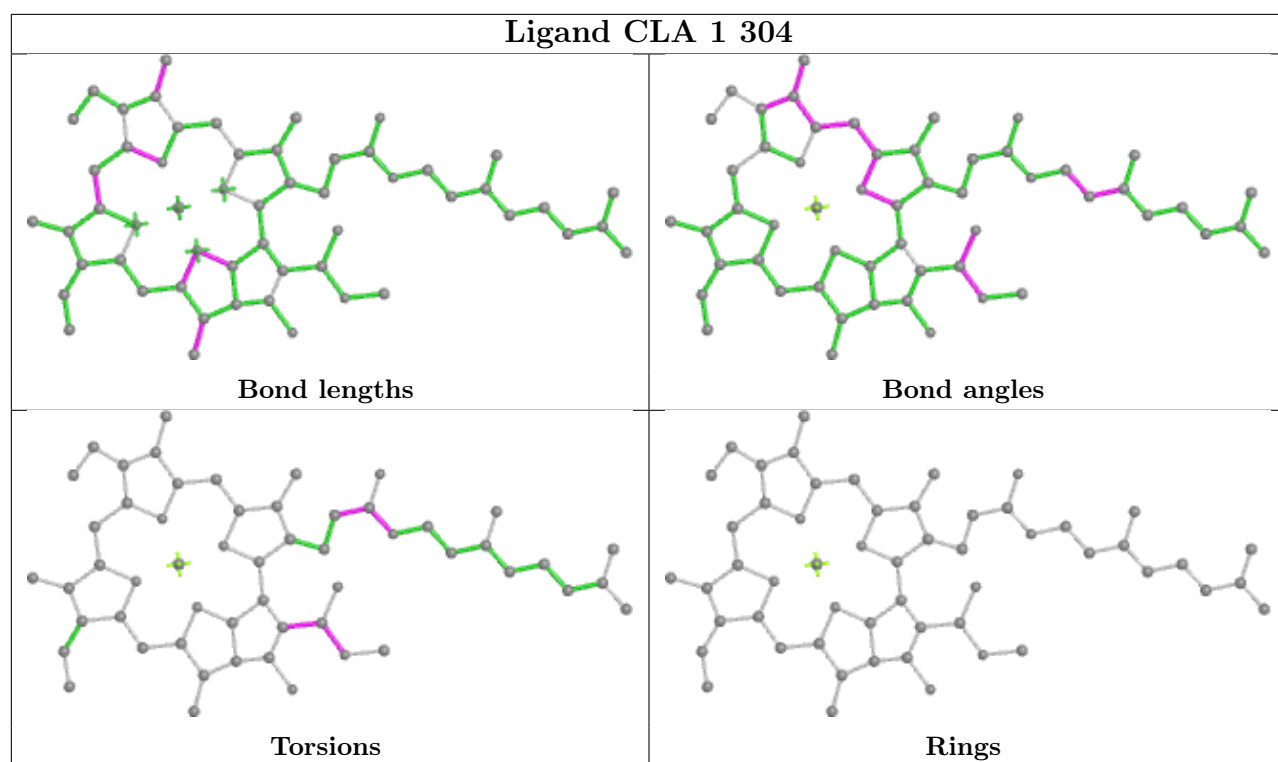


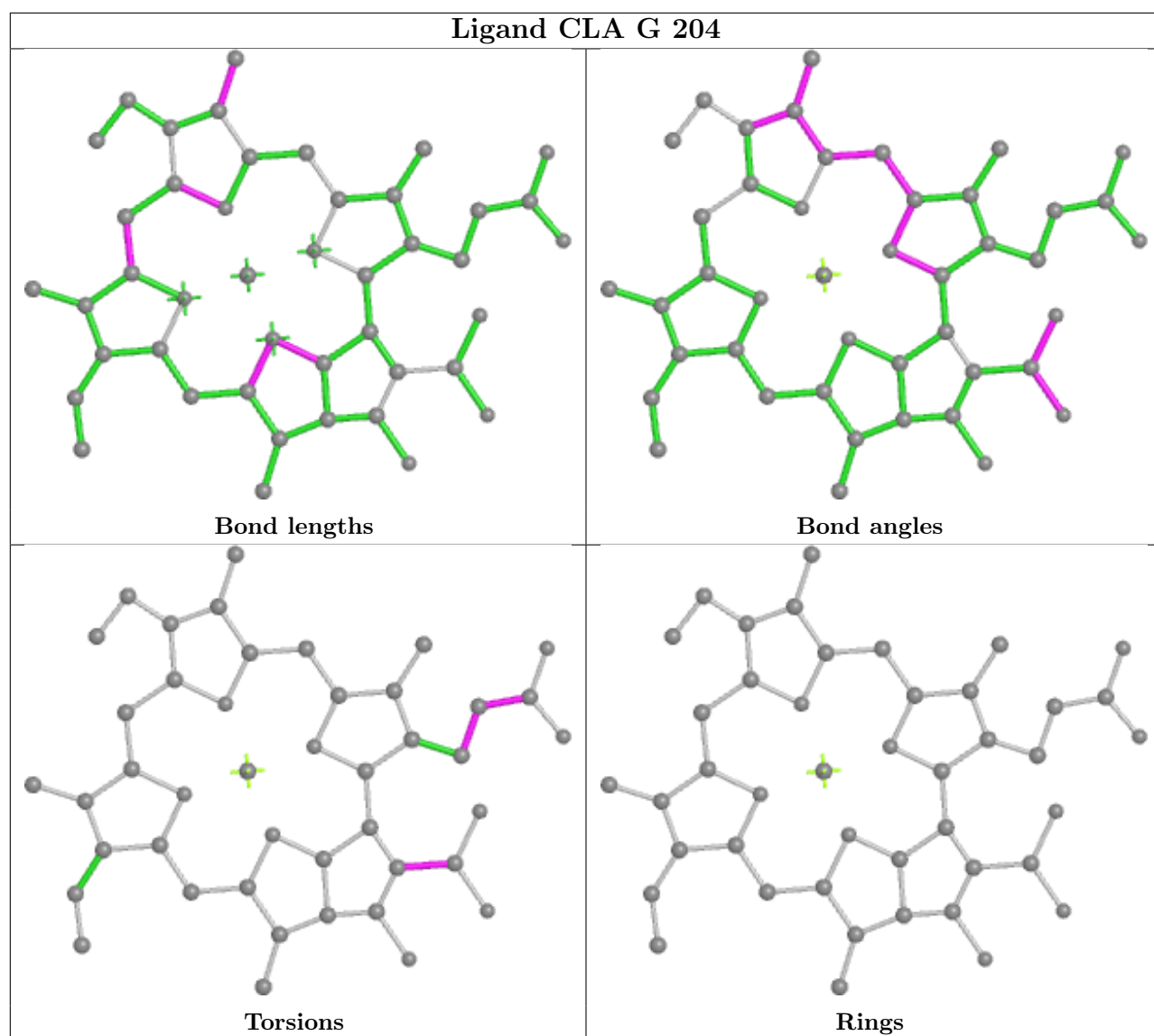
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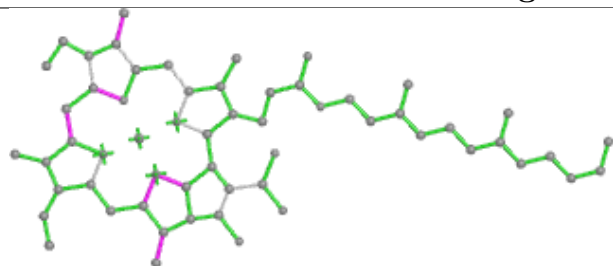


Ligand CLA A 839

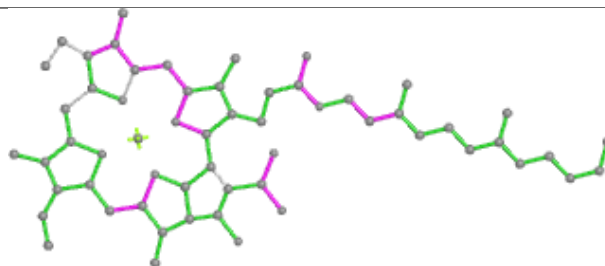




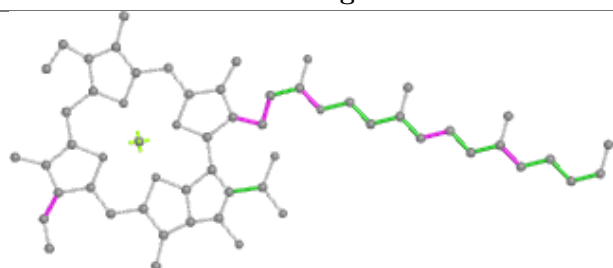


Ligand CLA 4 602

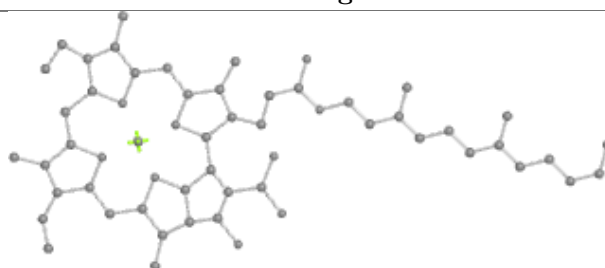
Bond lengths



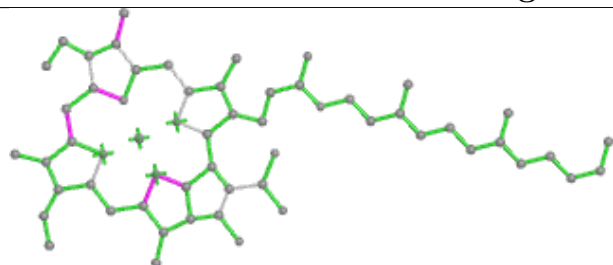
Bond angles



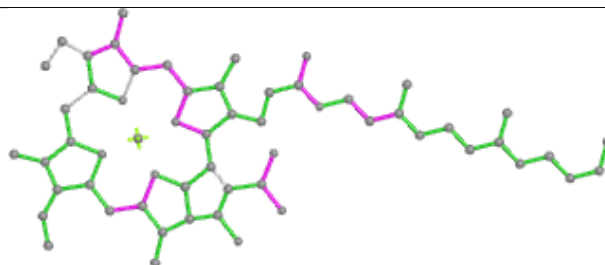
Torsions



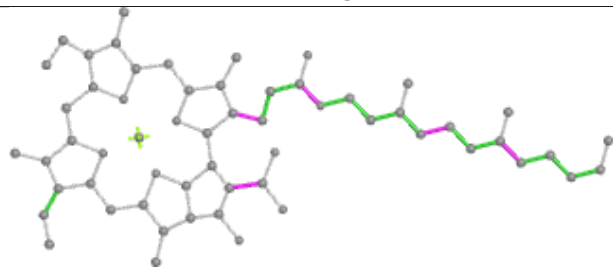
Rings

Ligand CLA 8 602

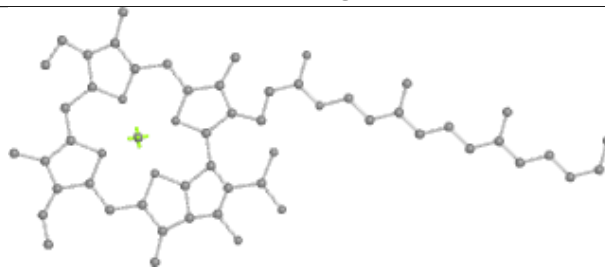
Bond lengths



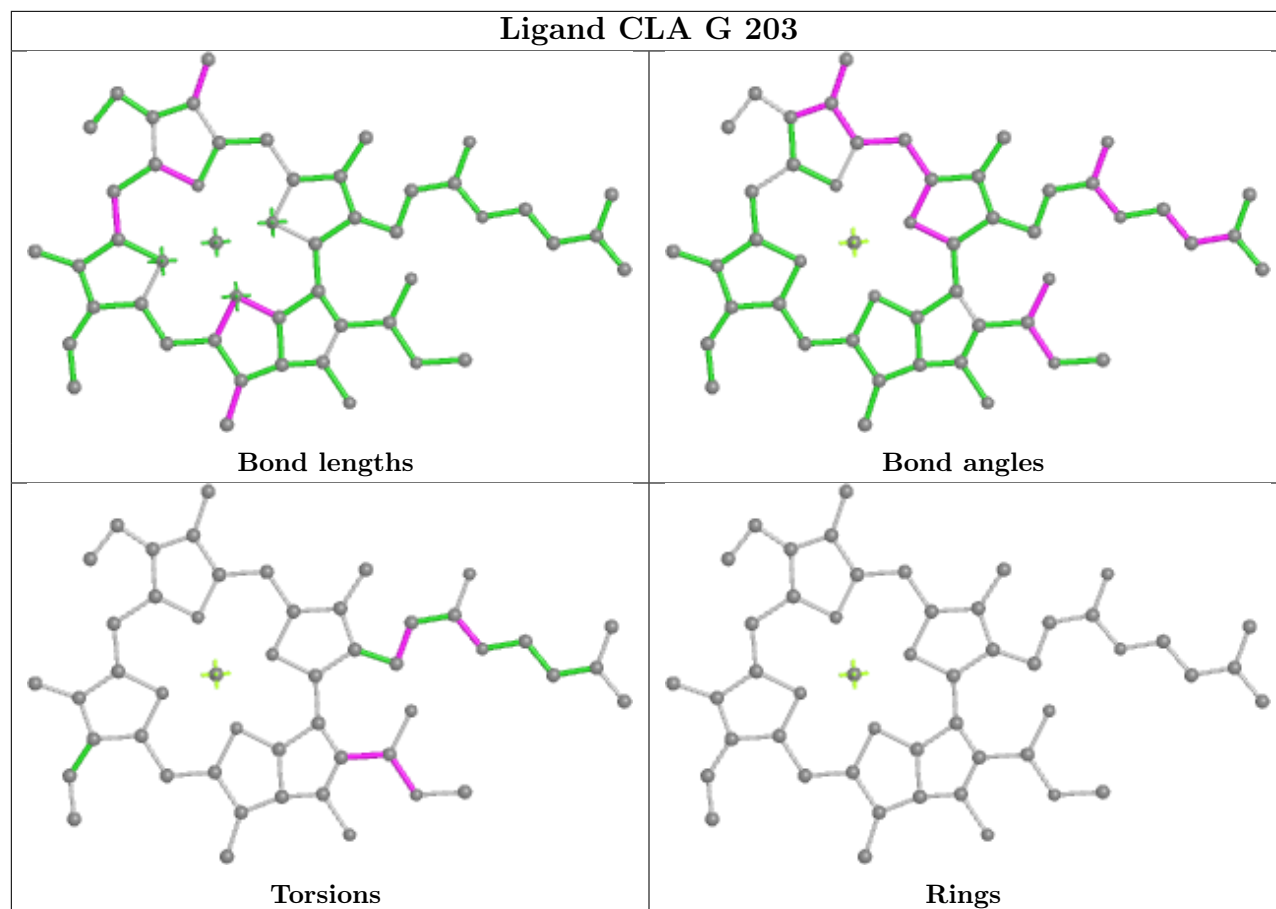
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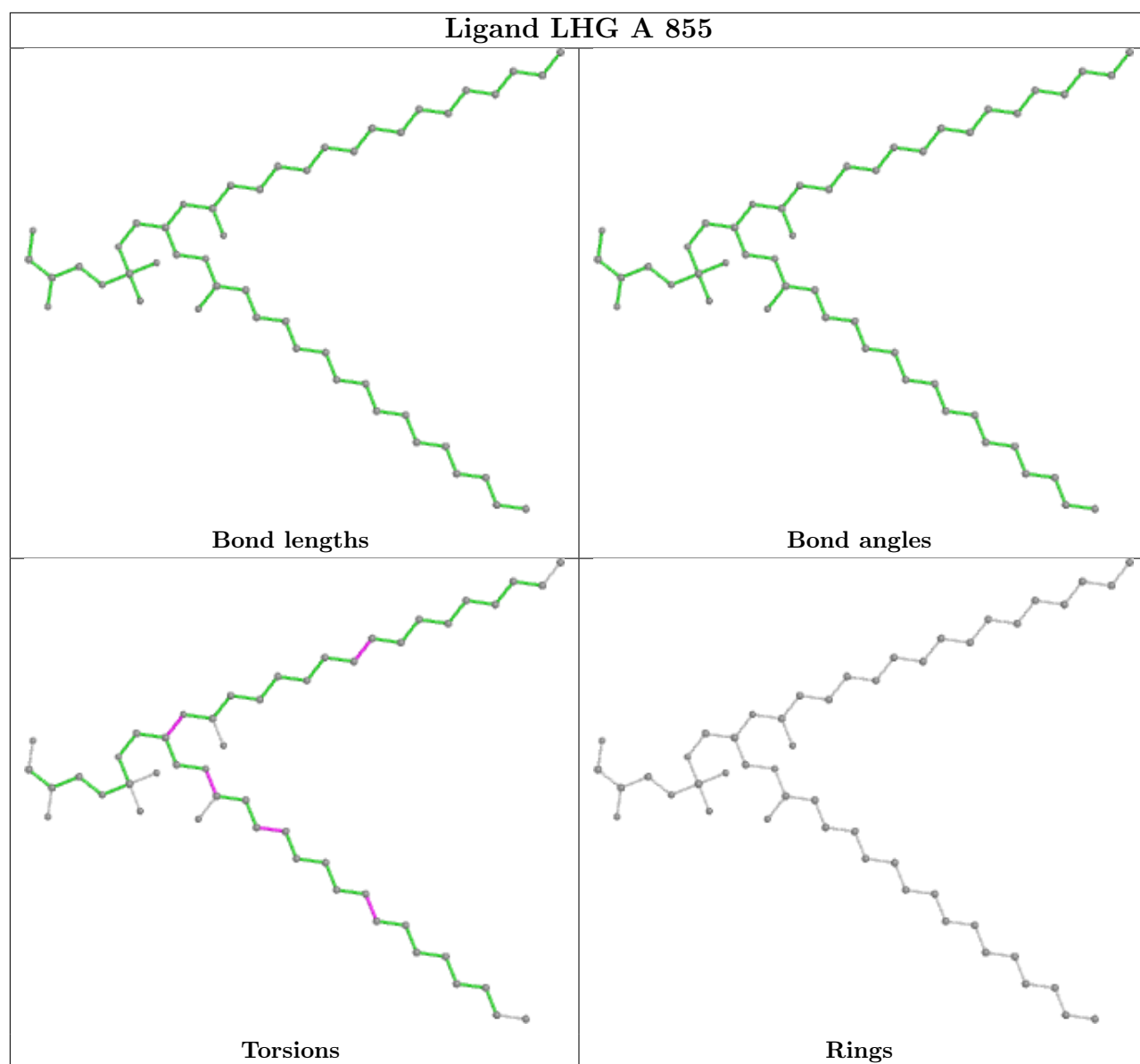


Torsions

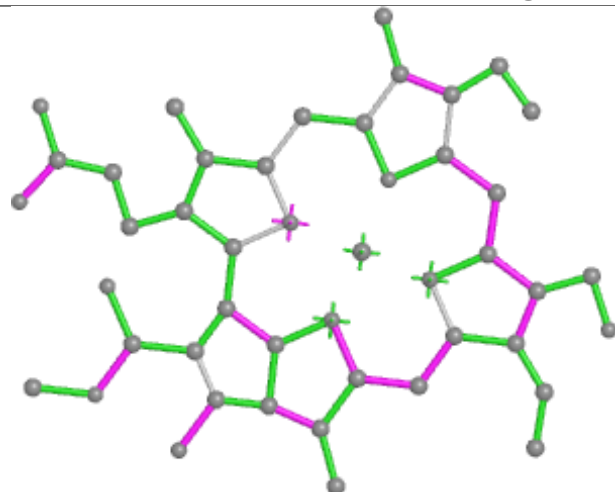


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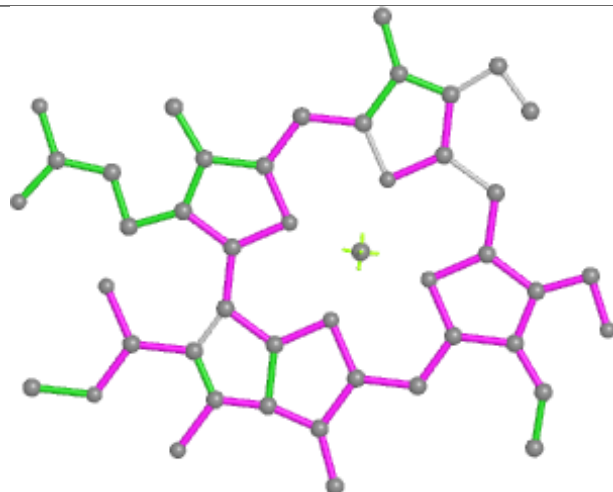




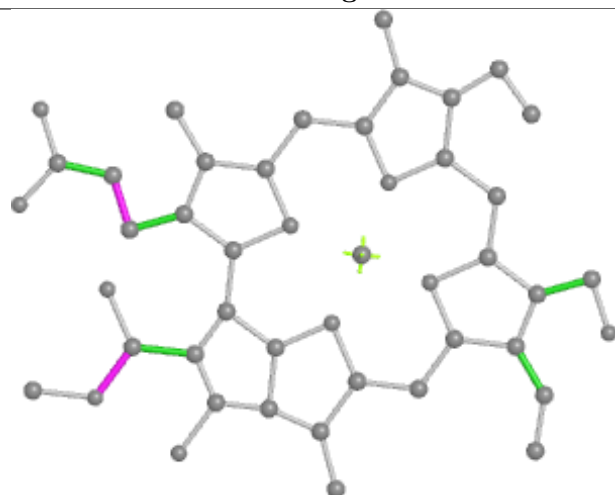
Ligand CHL 2 605



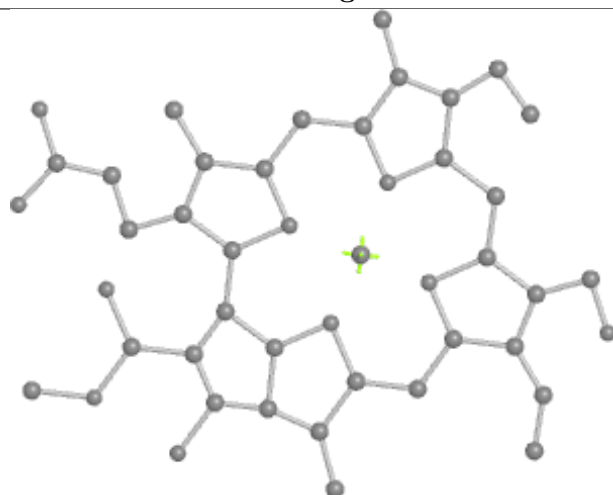
Bond lengths



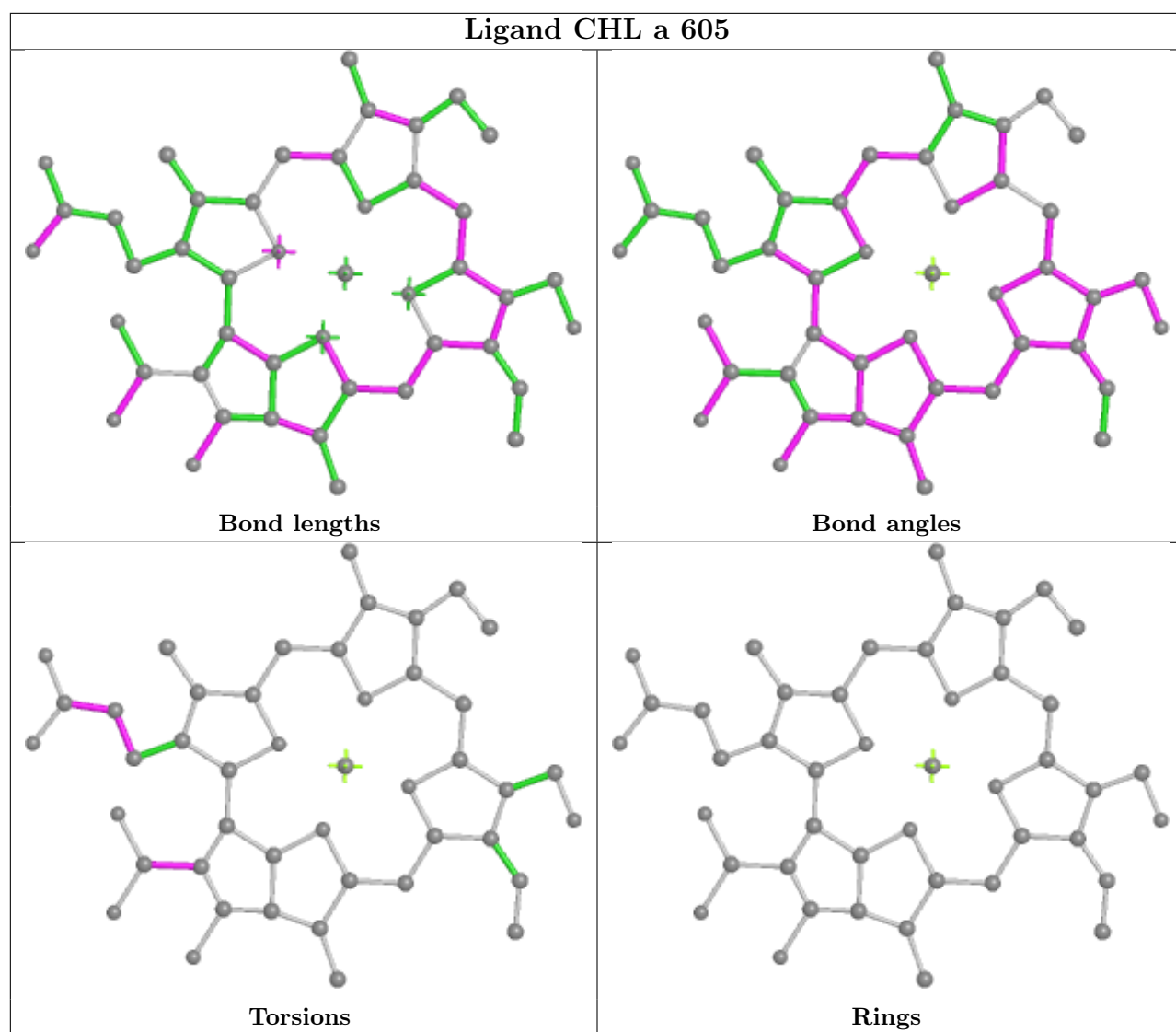
Bond angles



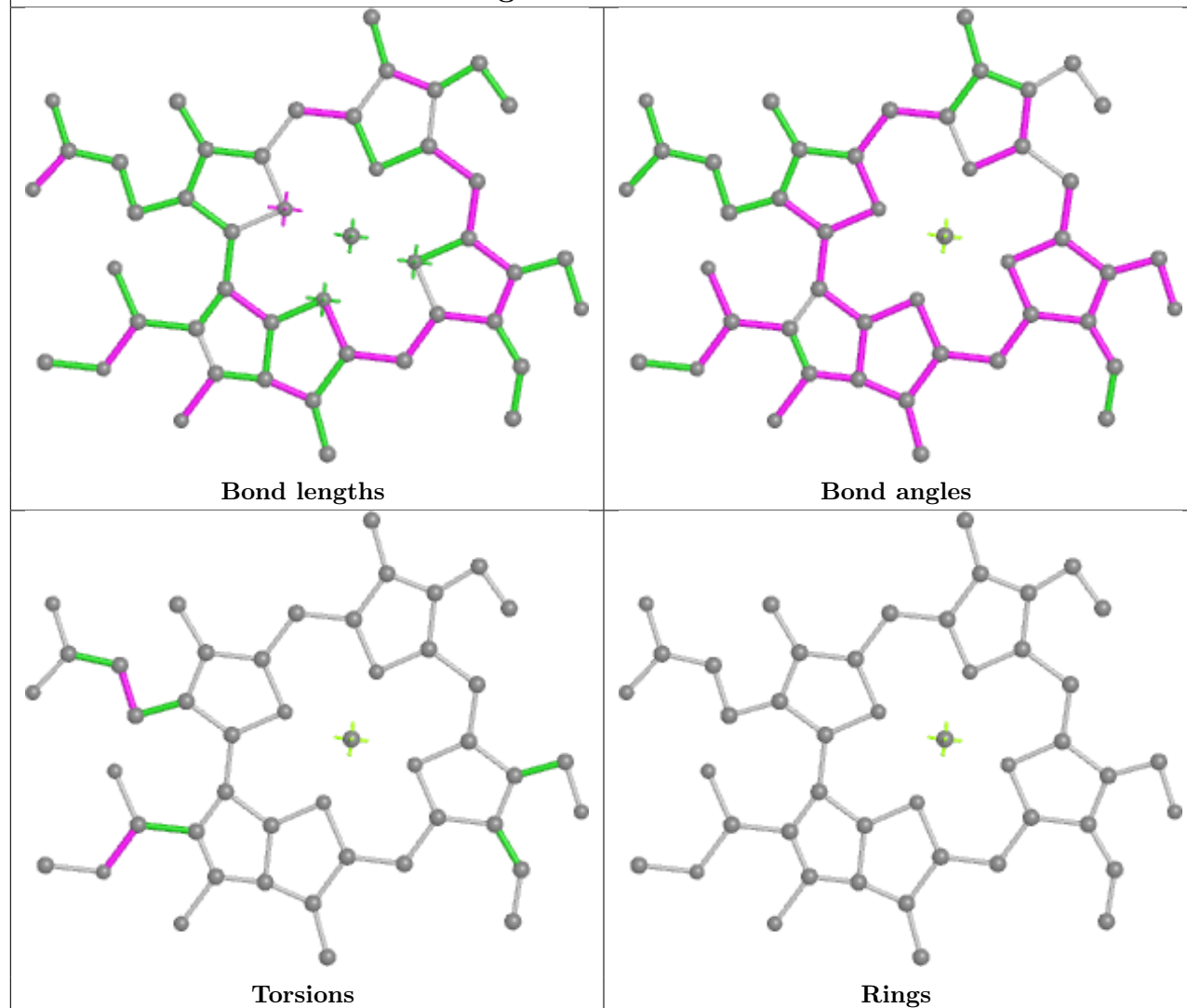
Torsions



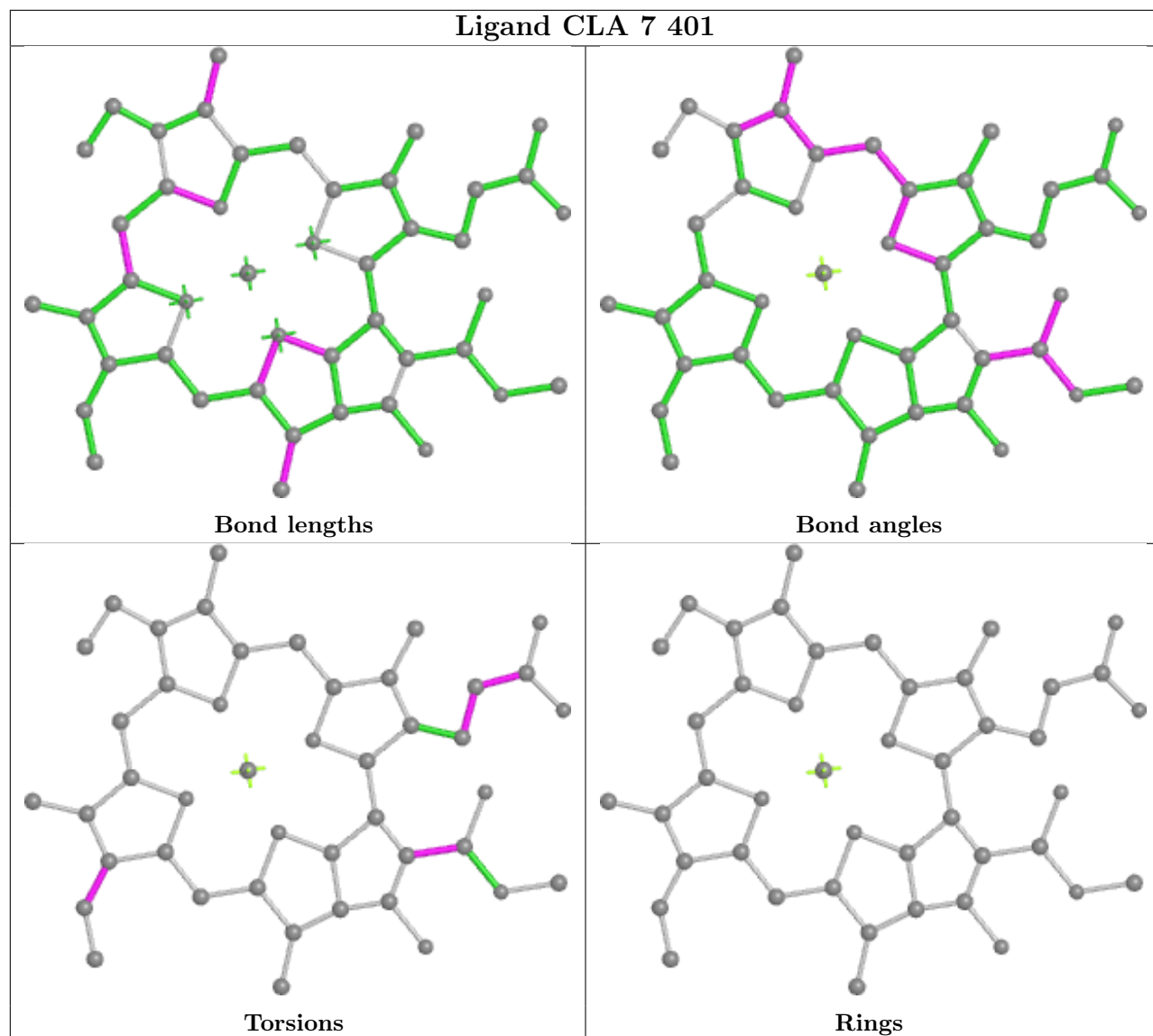
Rings



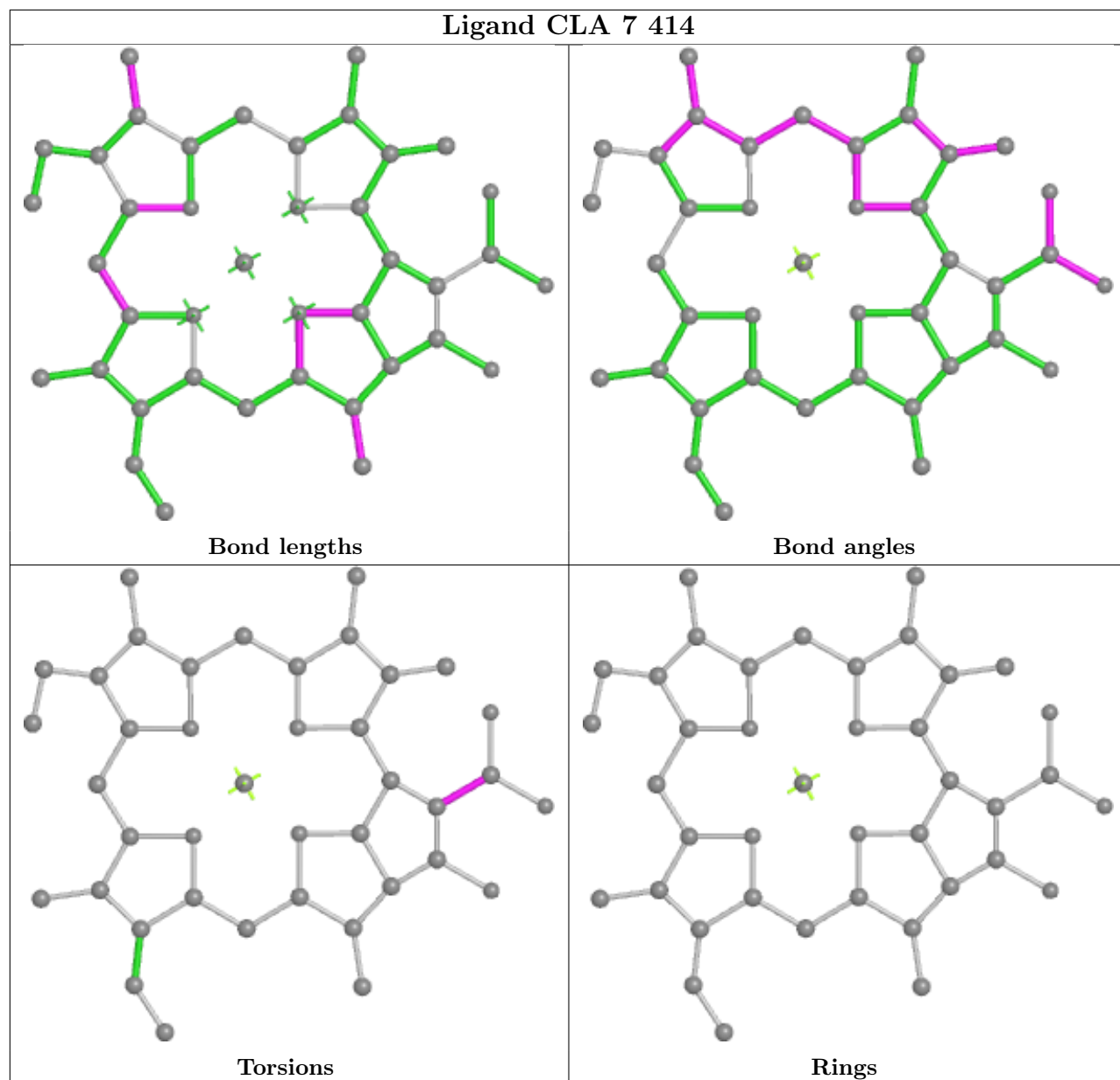
Ligand CHL 6 605

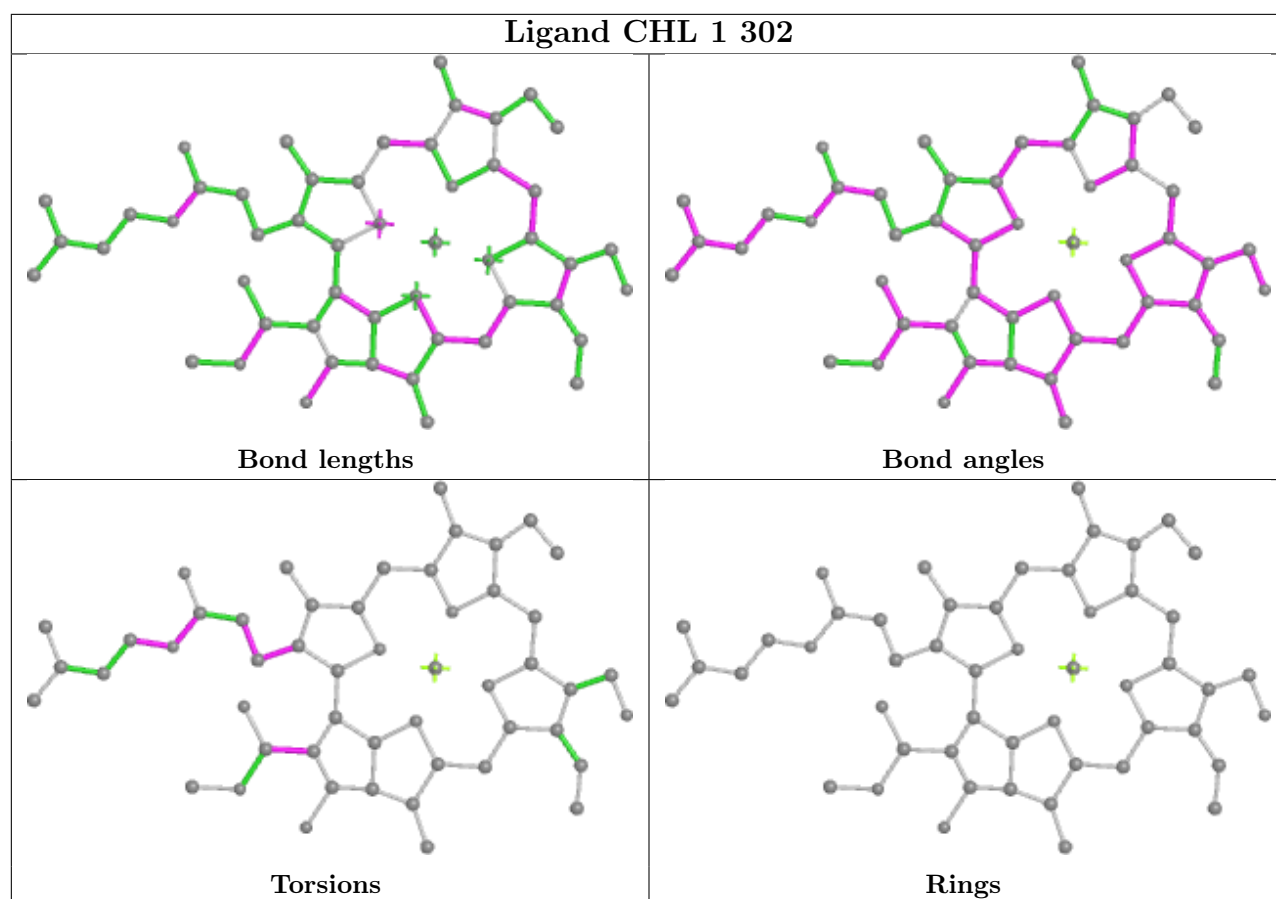


Ligand CLA 7 401

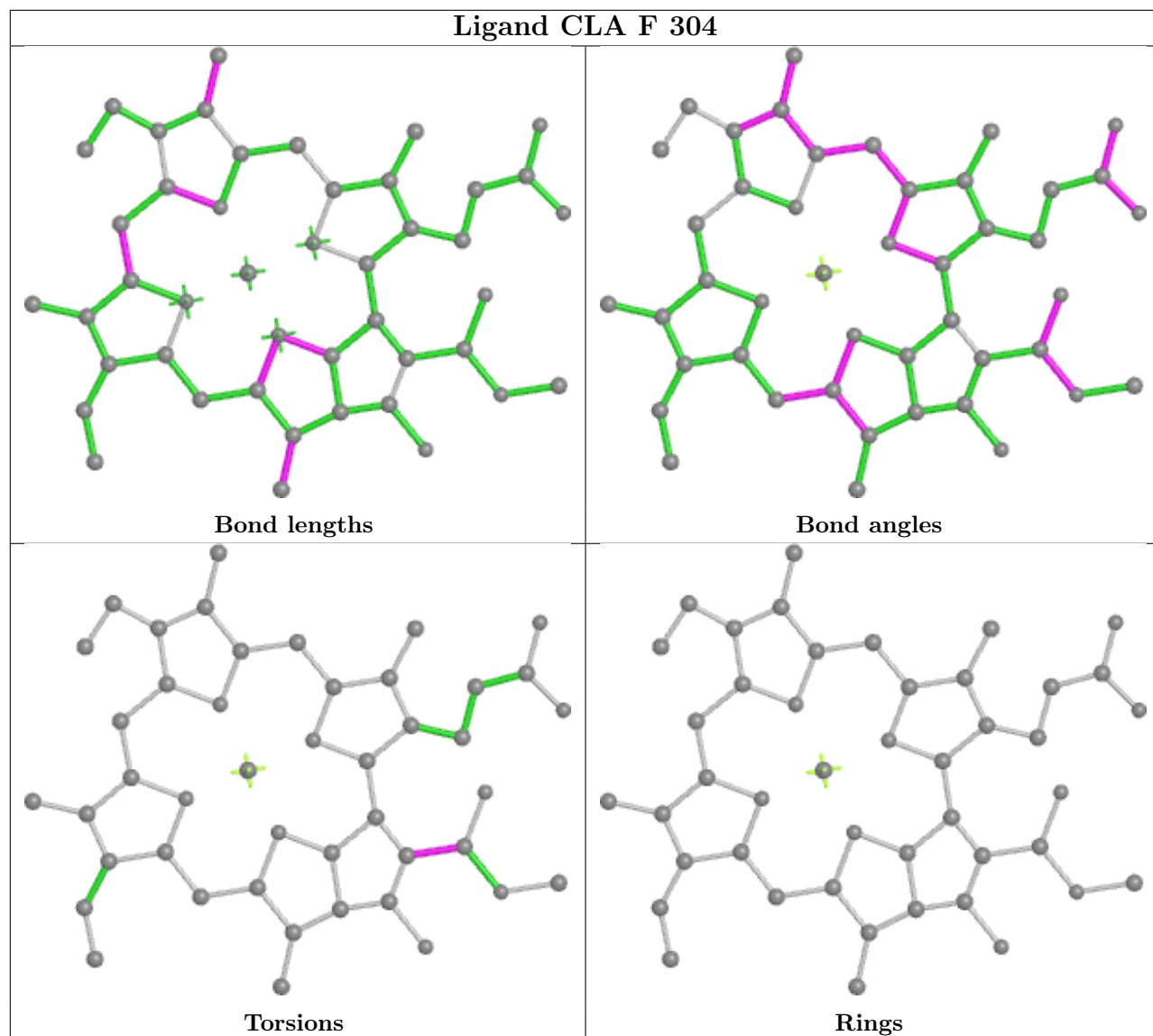


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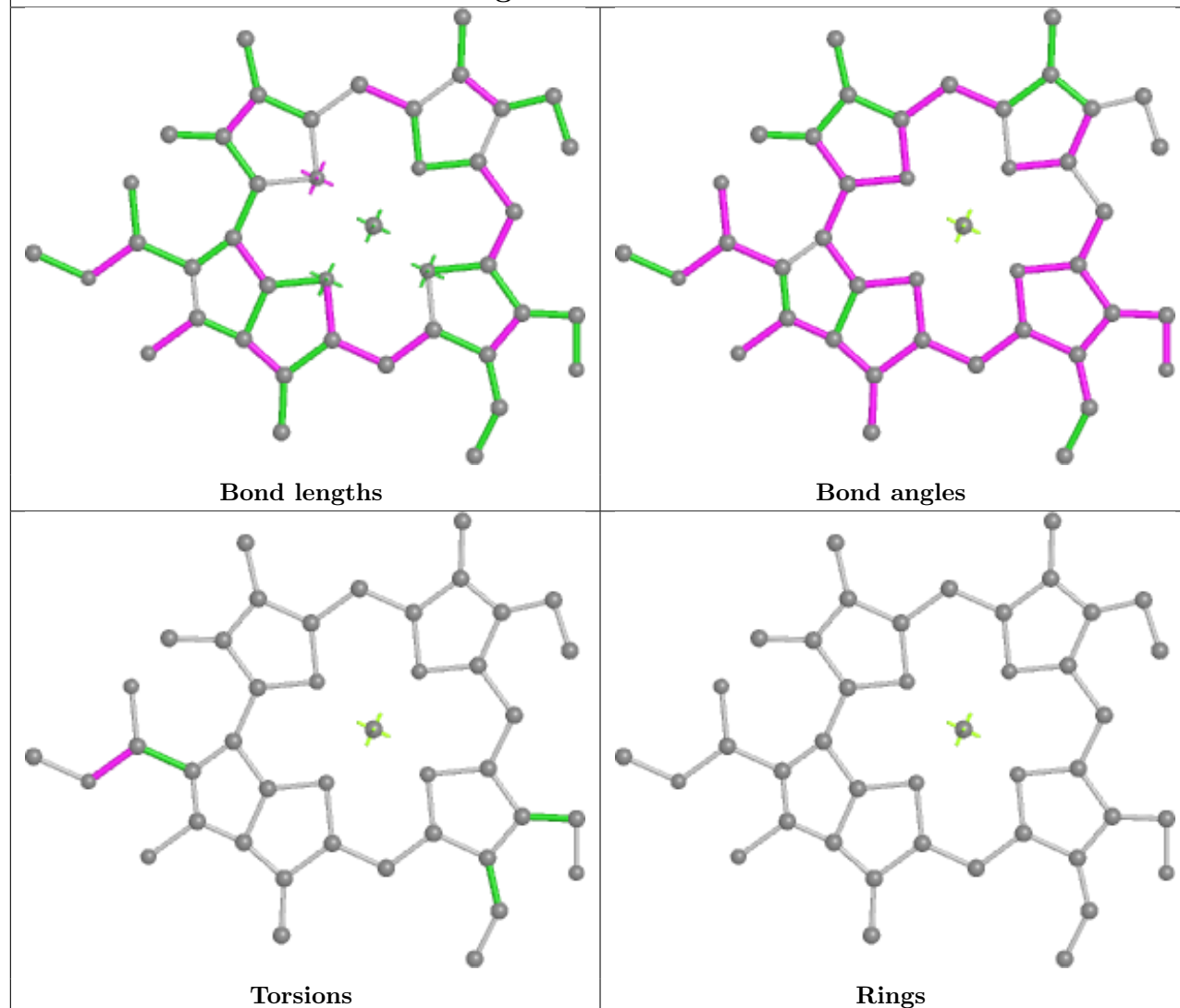




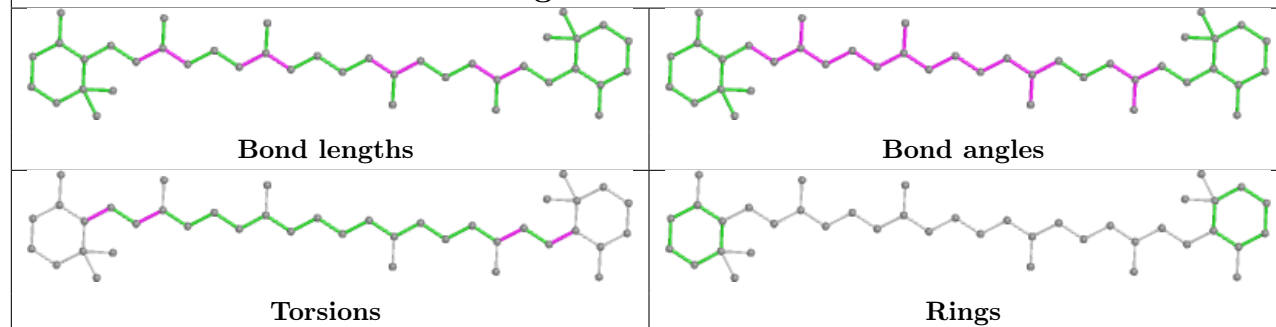
Ligand CLA F 304



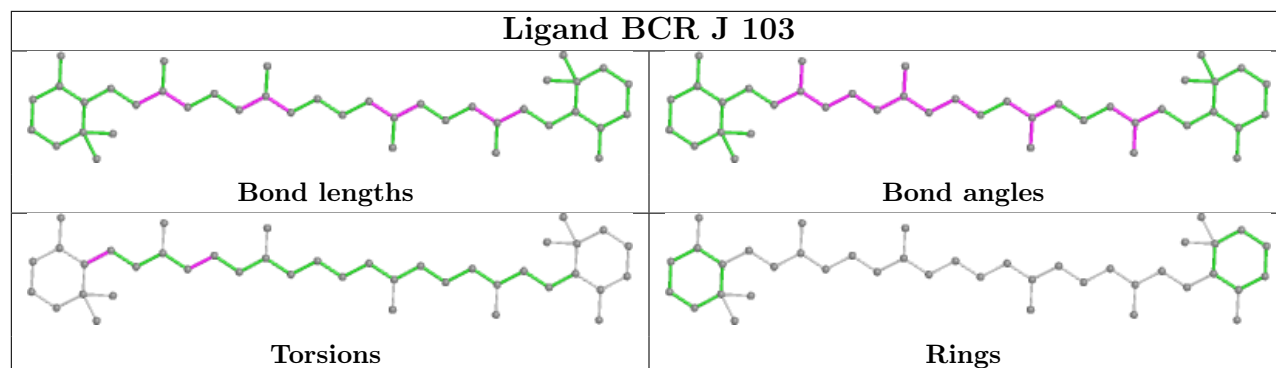
Ligand CHL 4 614



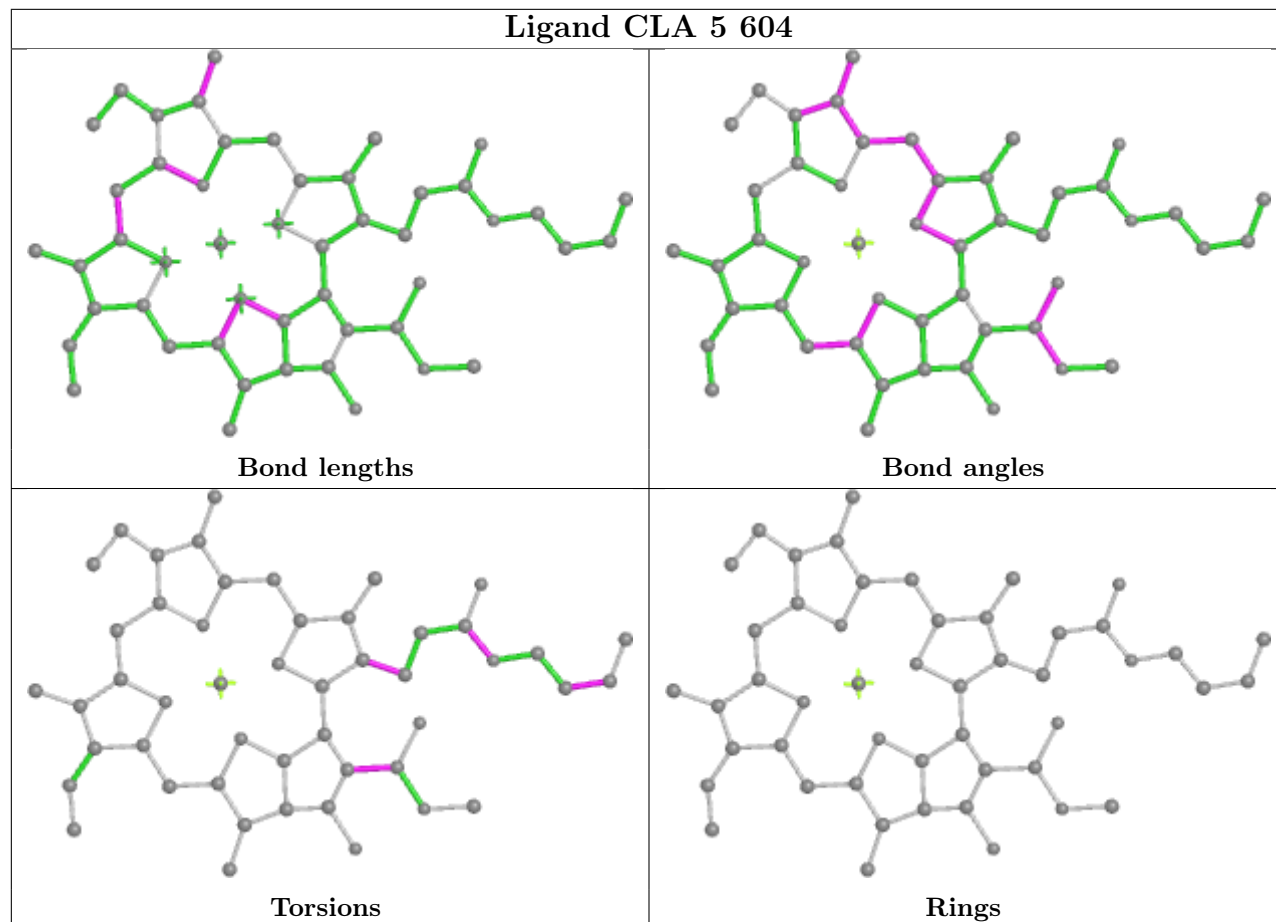
Ligand BCR 3 419



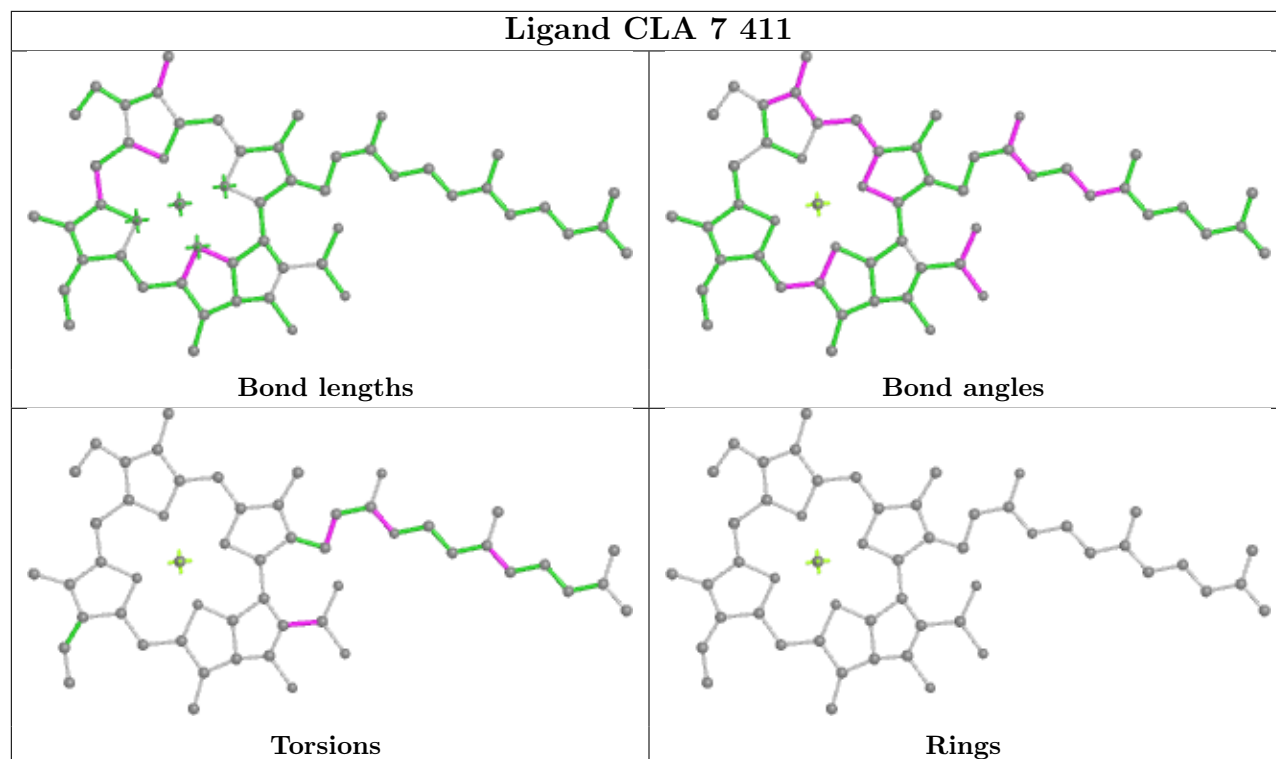
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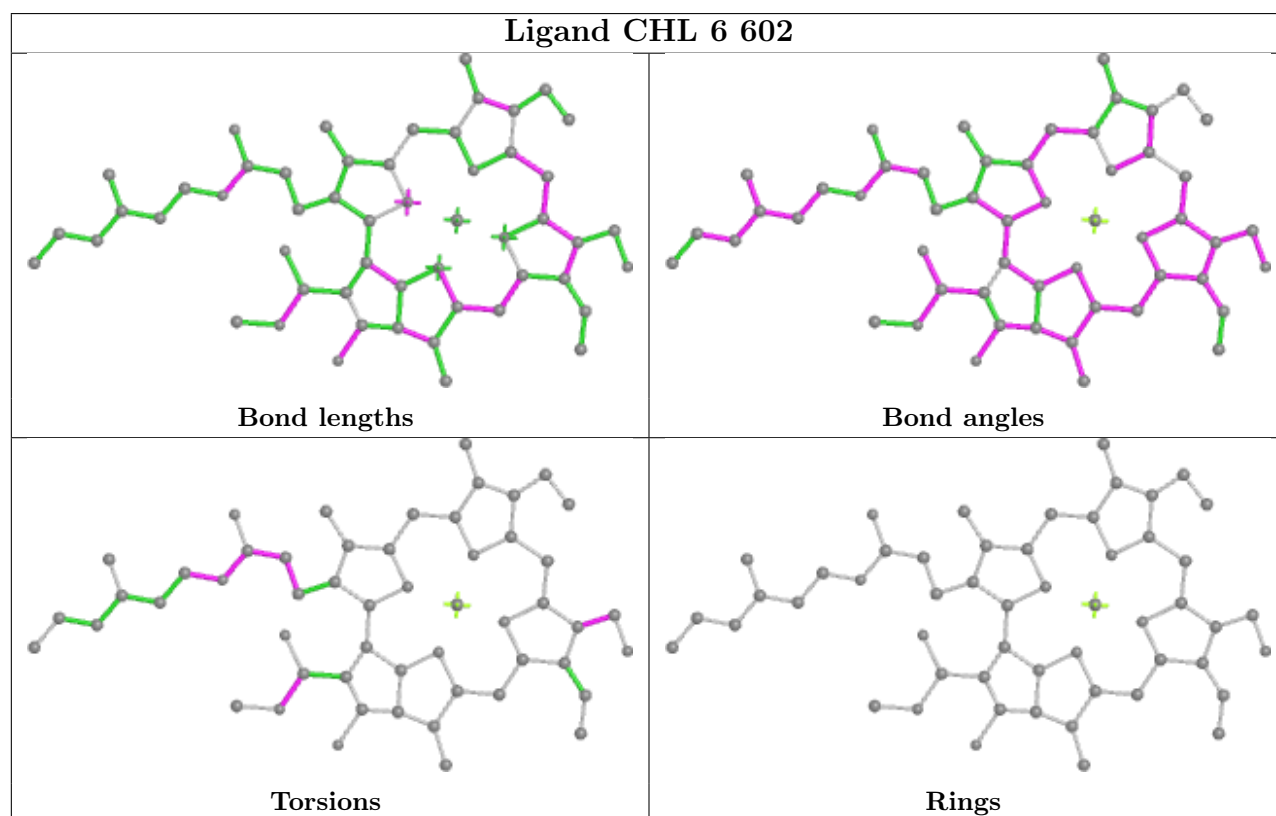
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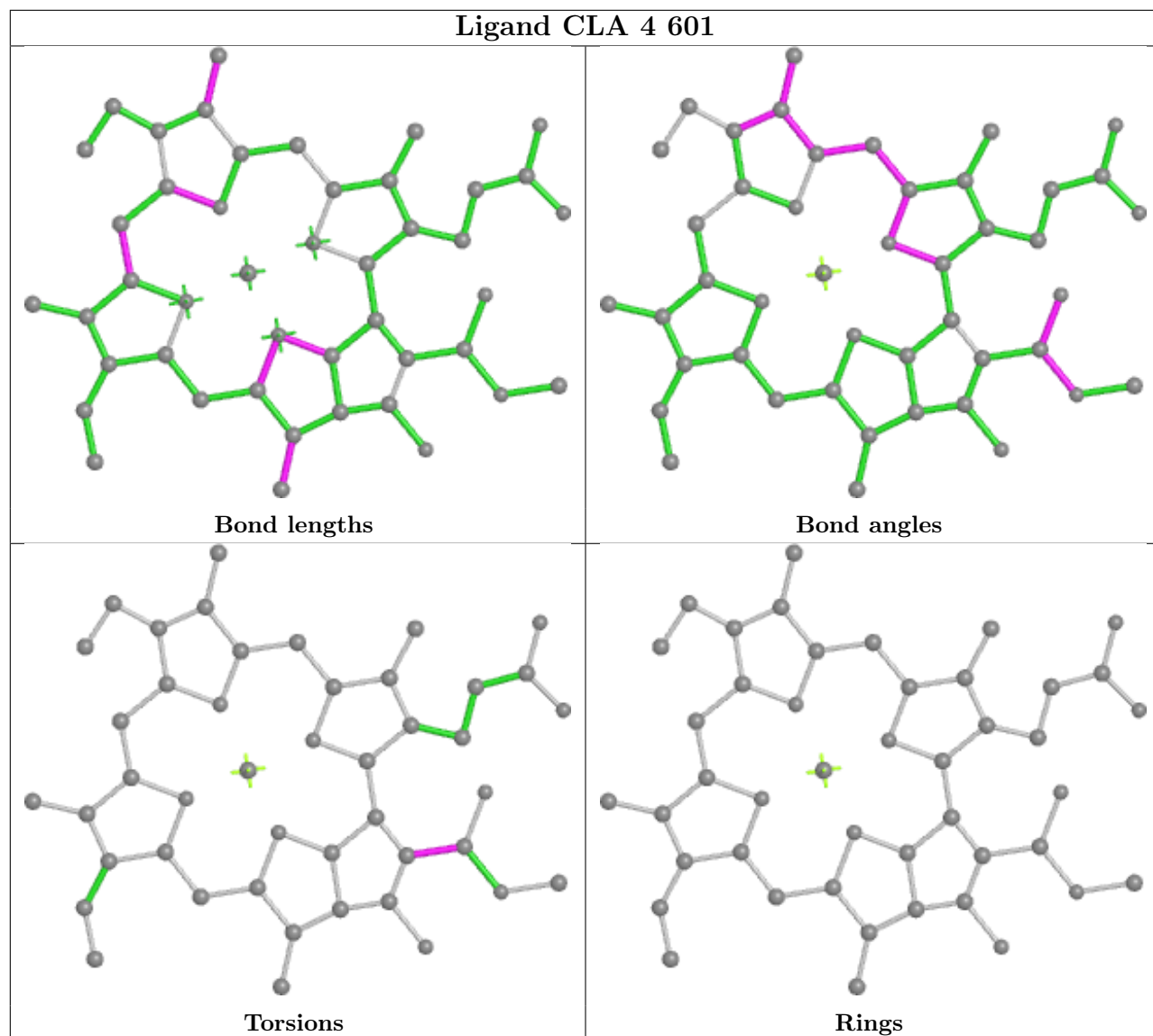
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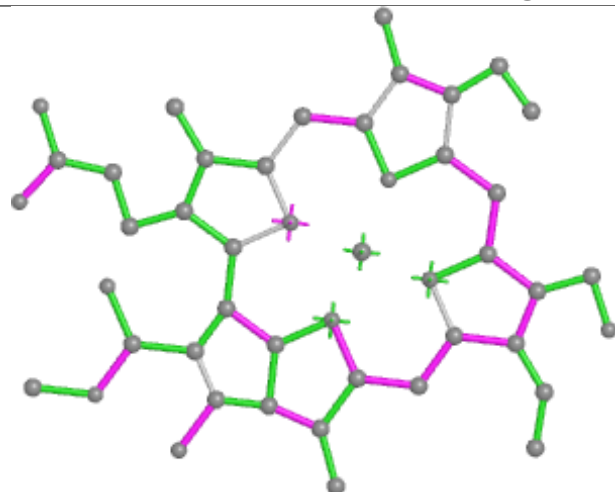
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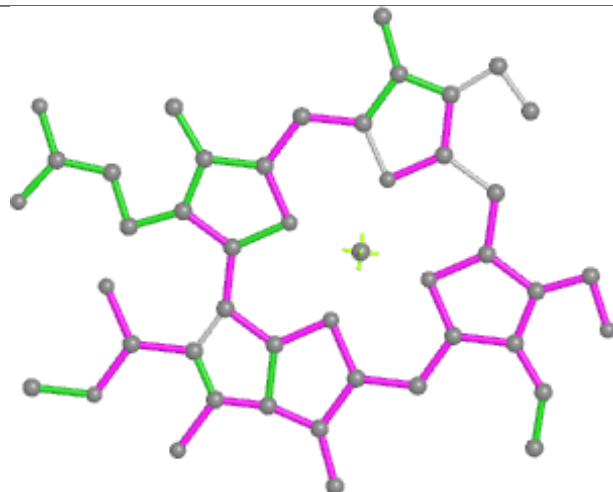
Ligand CLA 4 601



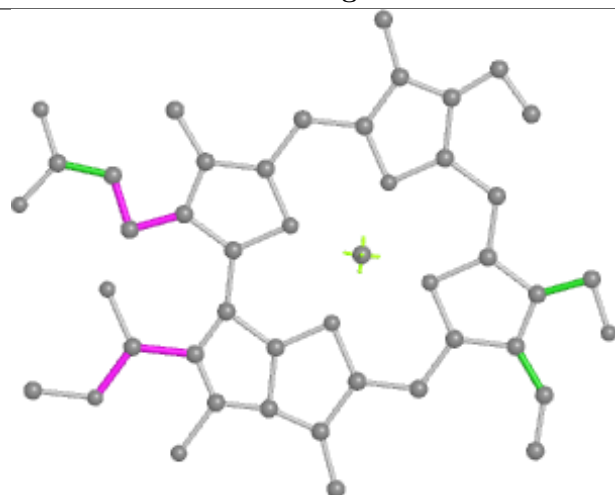
Ligand CHL b 302



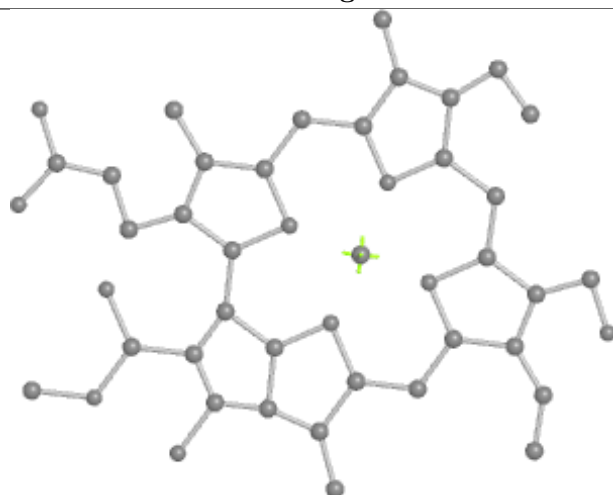
Bond lengths



Bond angles

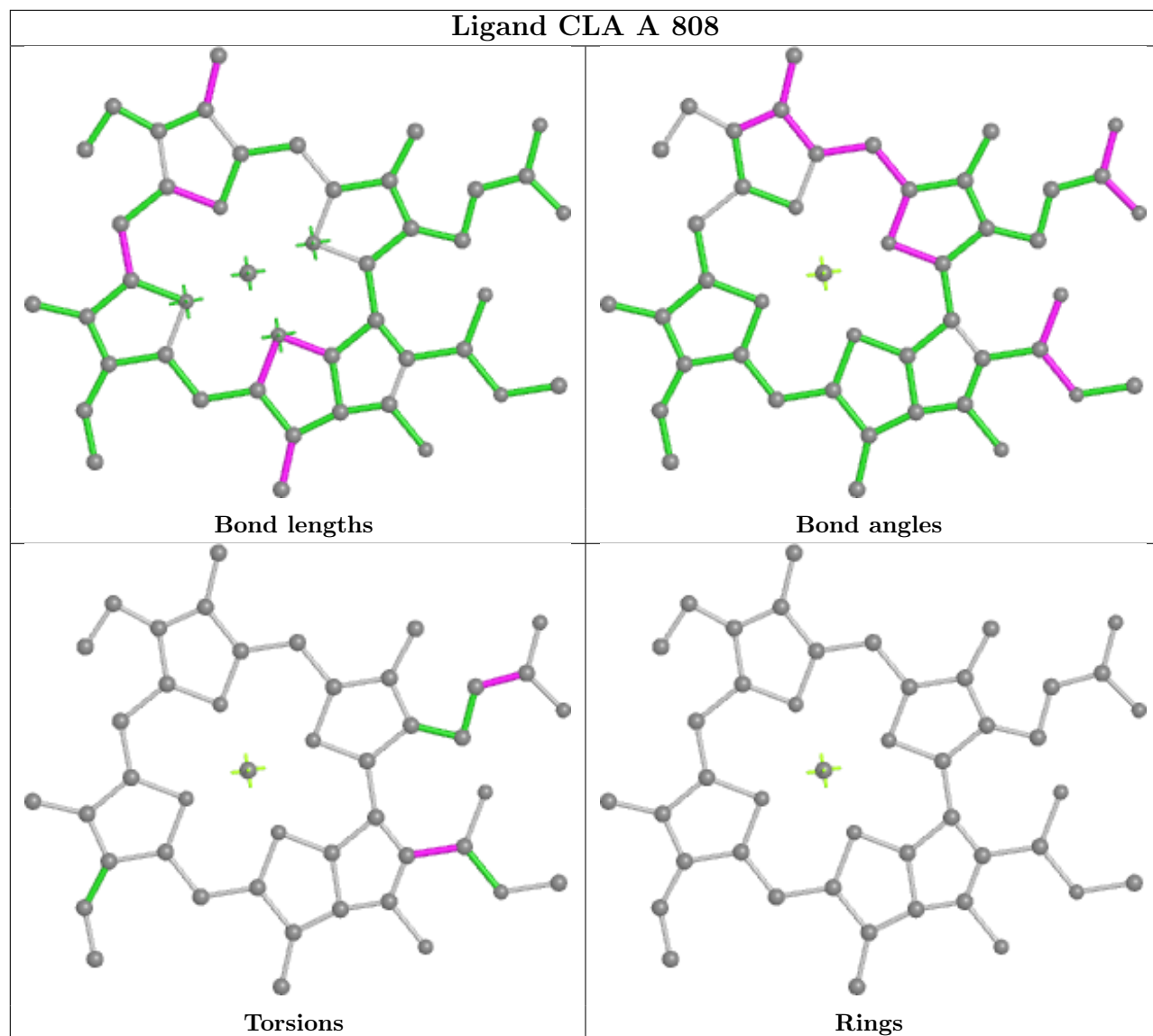


Torsions

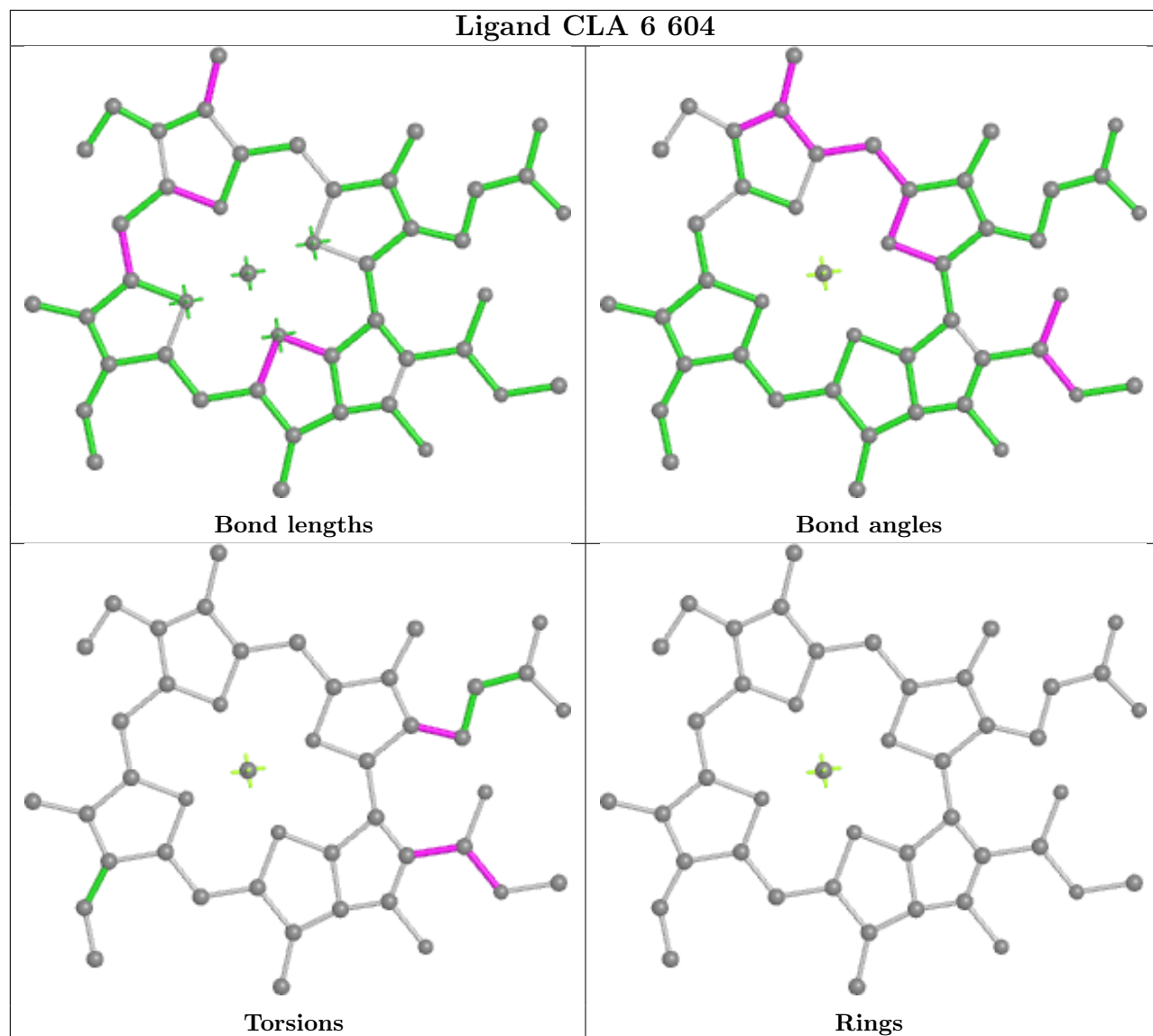


Rings

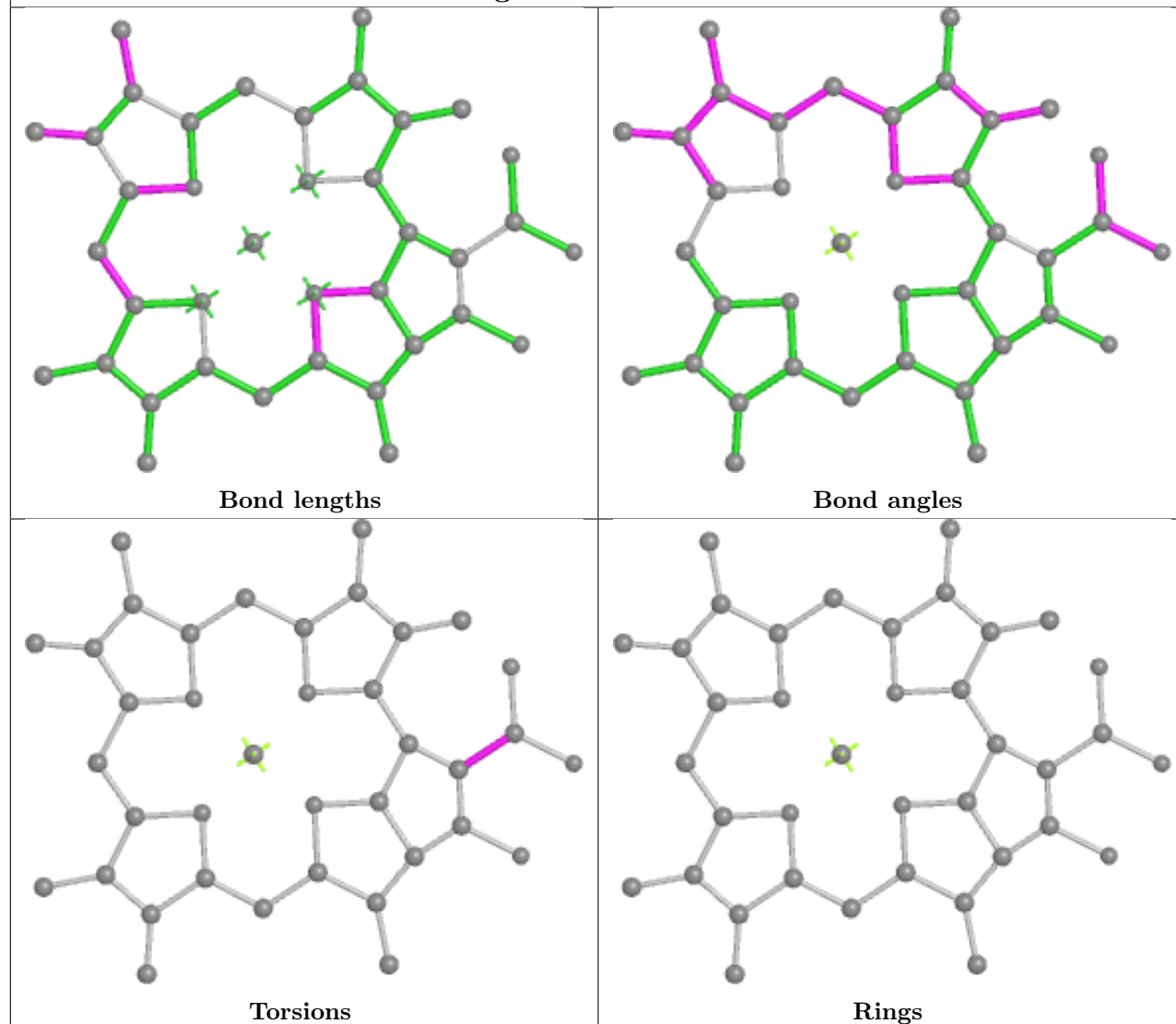
Ligand CLA A 808



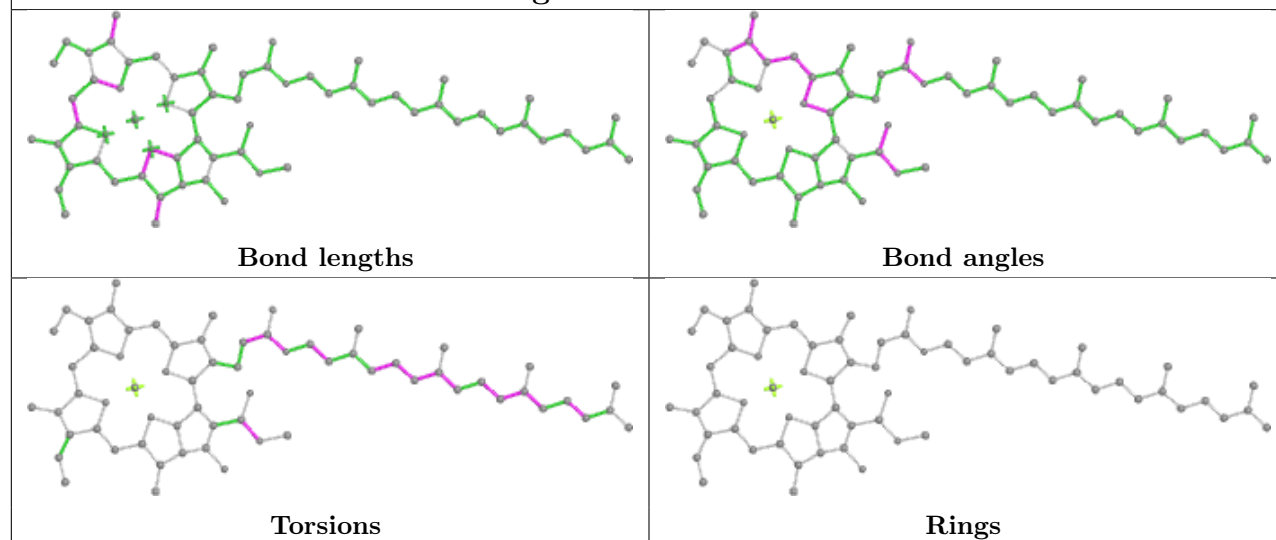
Ligand CLA 6 604



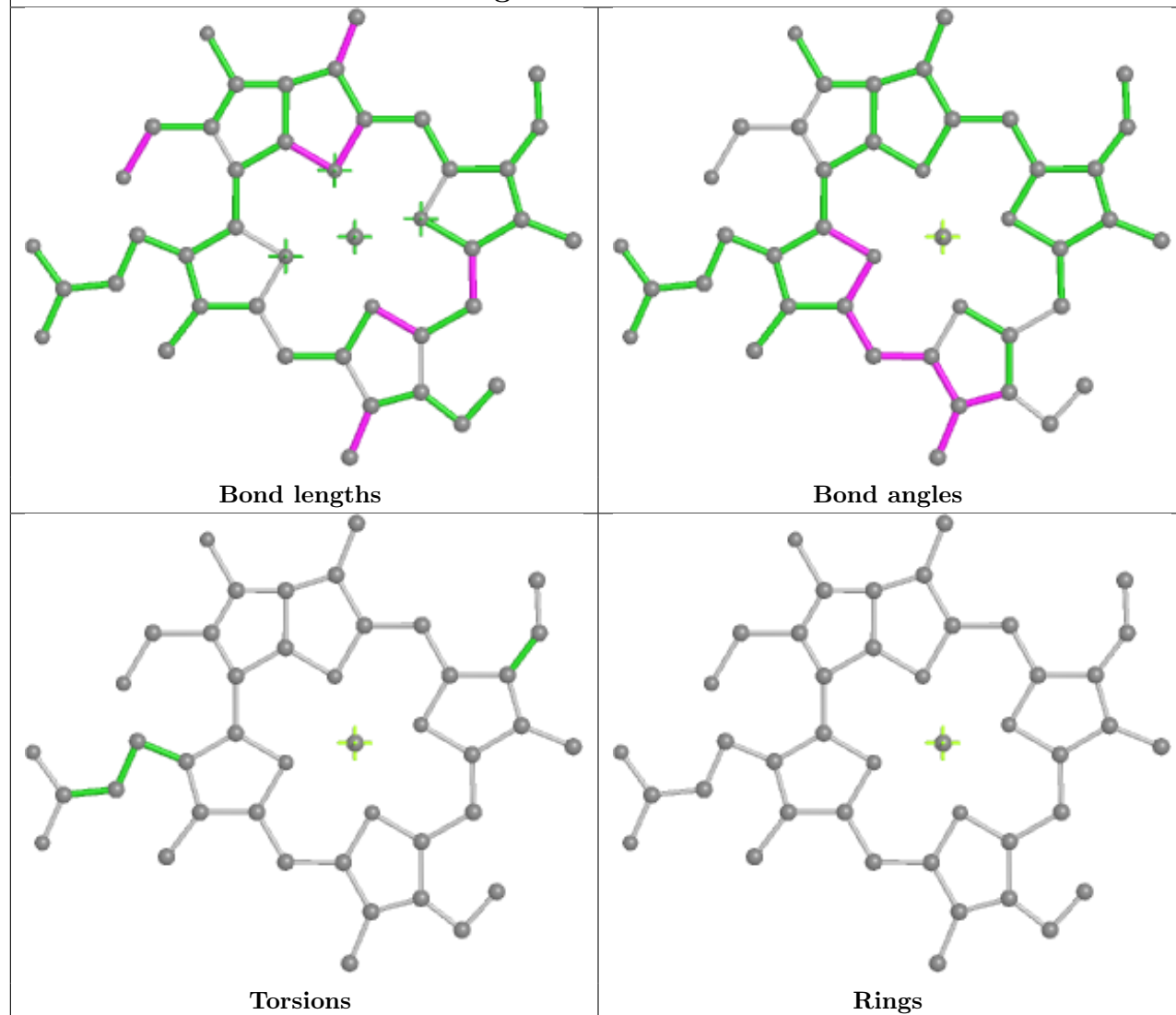
Ligand CLA 5 613



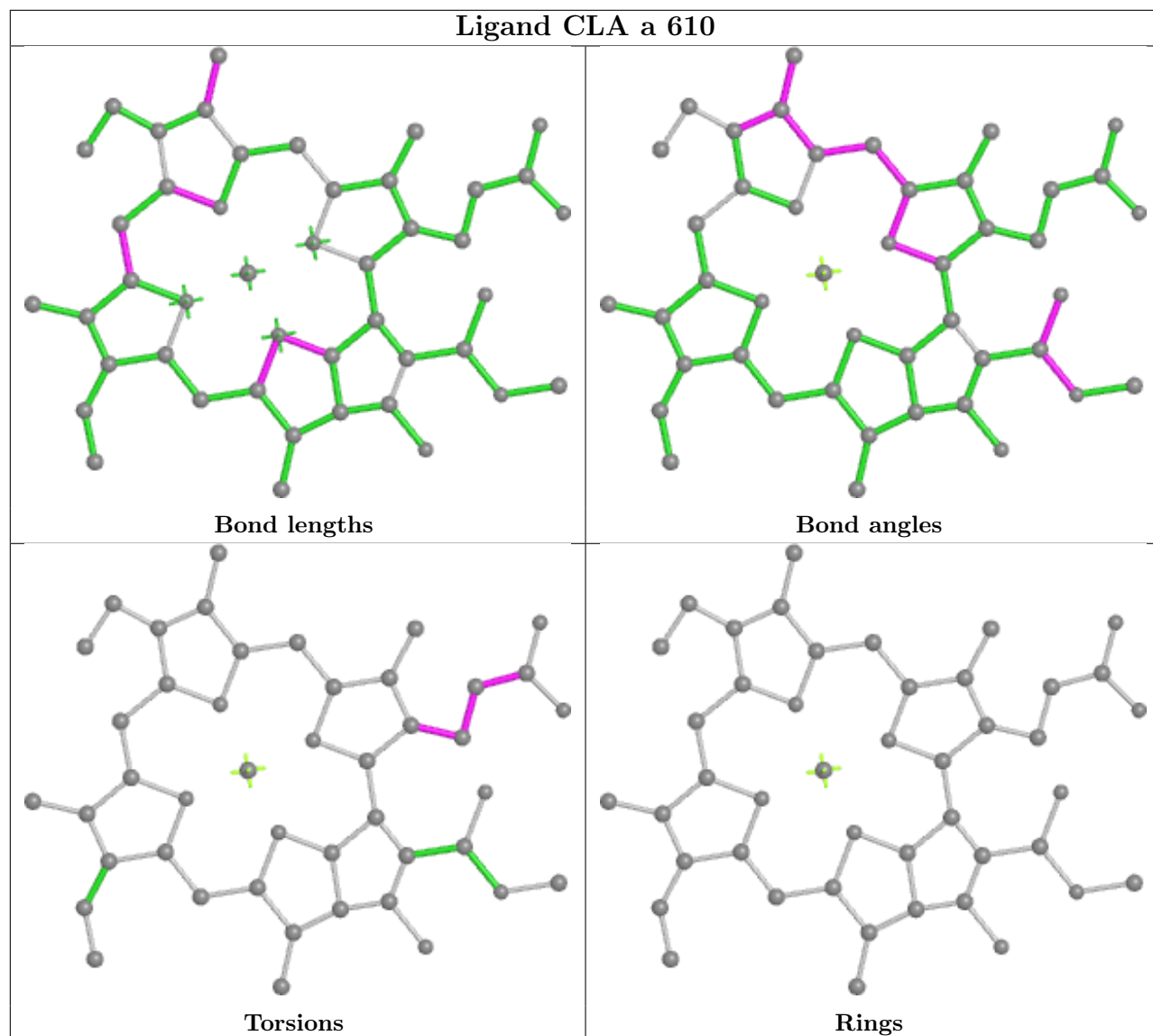
Ligand CLA B 805



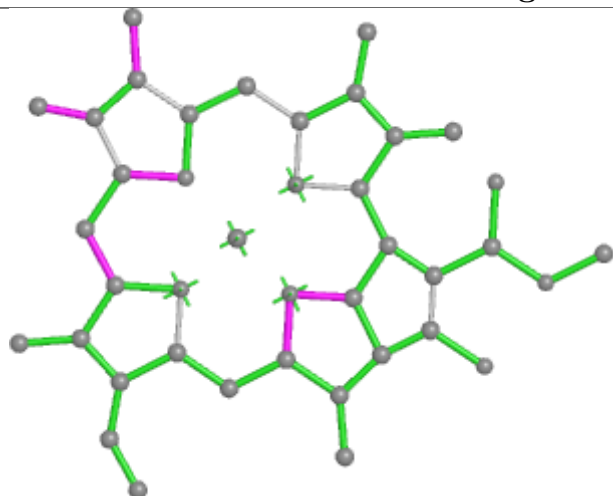
Ligand CLA 4 608



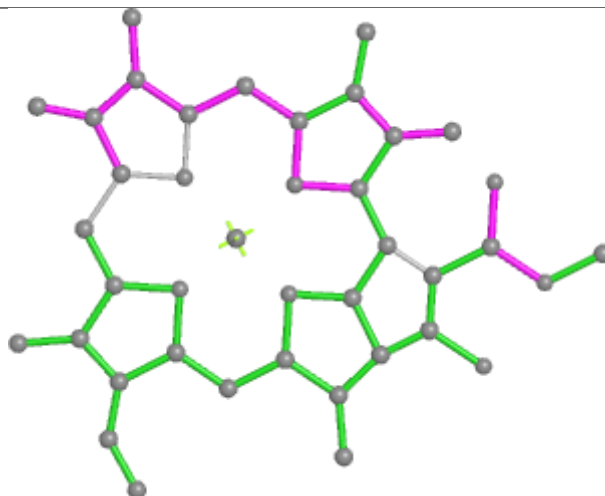
Ligand CLA a 610



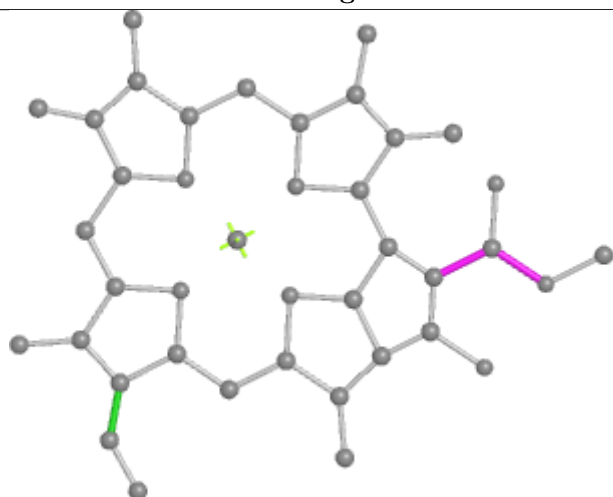
Ligand CLA 5 608



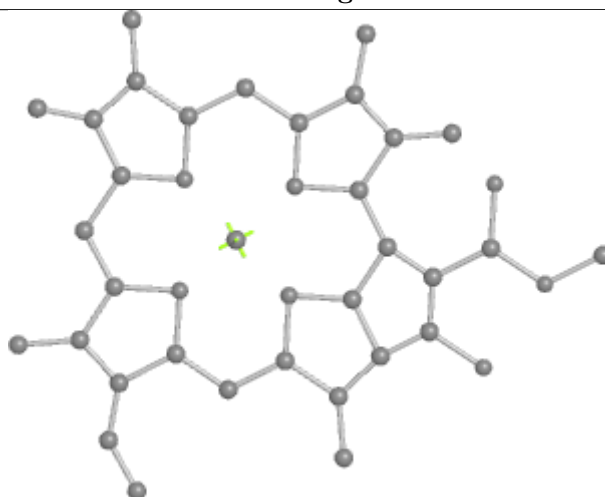
Bond lengths



Bond angles

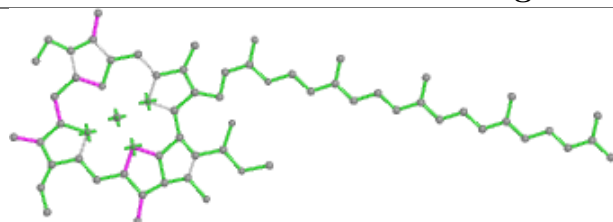


Torsions

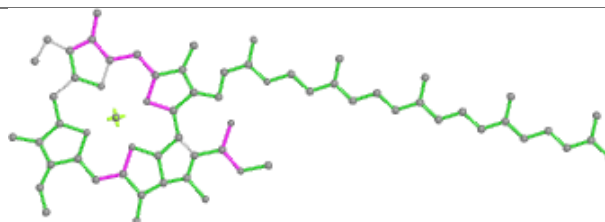


Rings

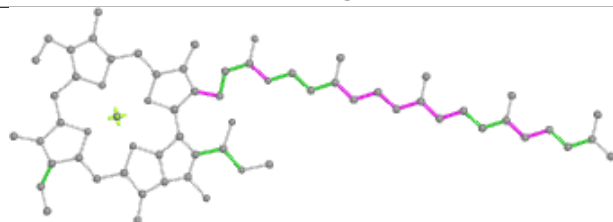
Ligand CLA B 836



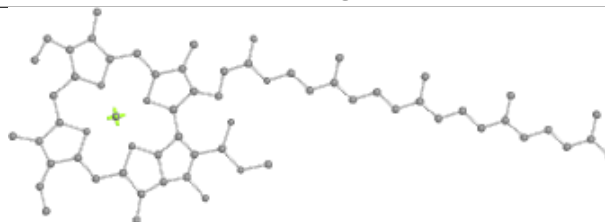
Bond lengths



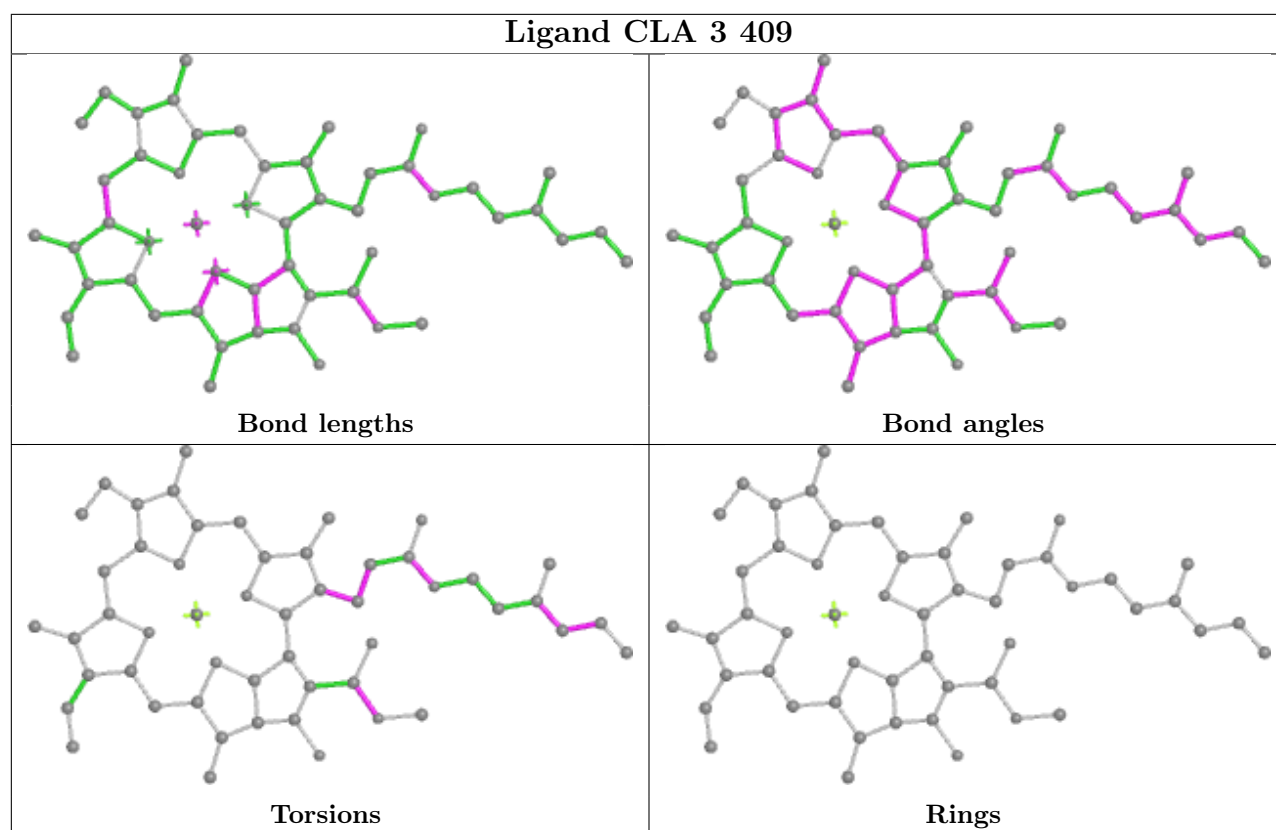
Bond angles



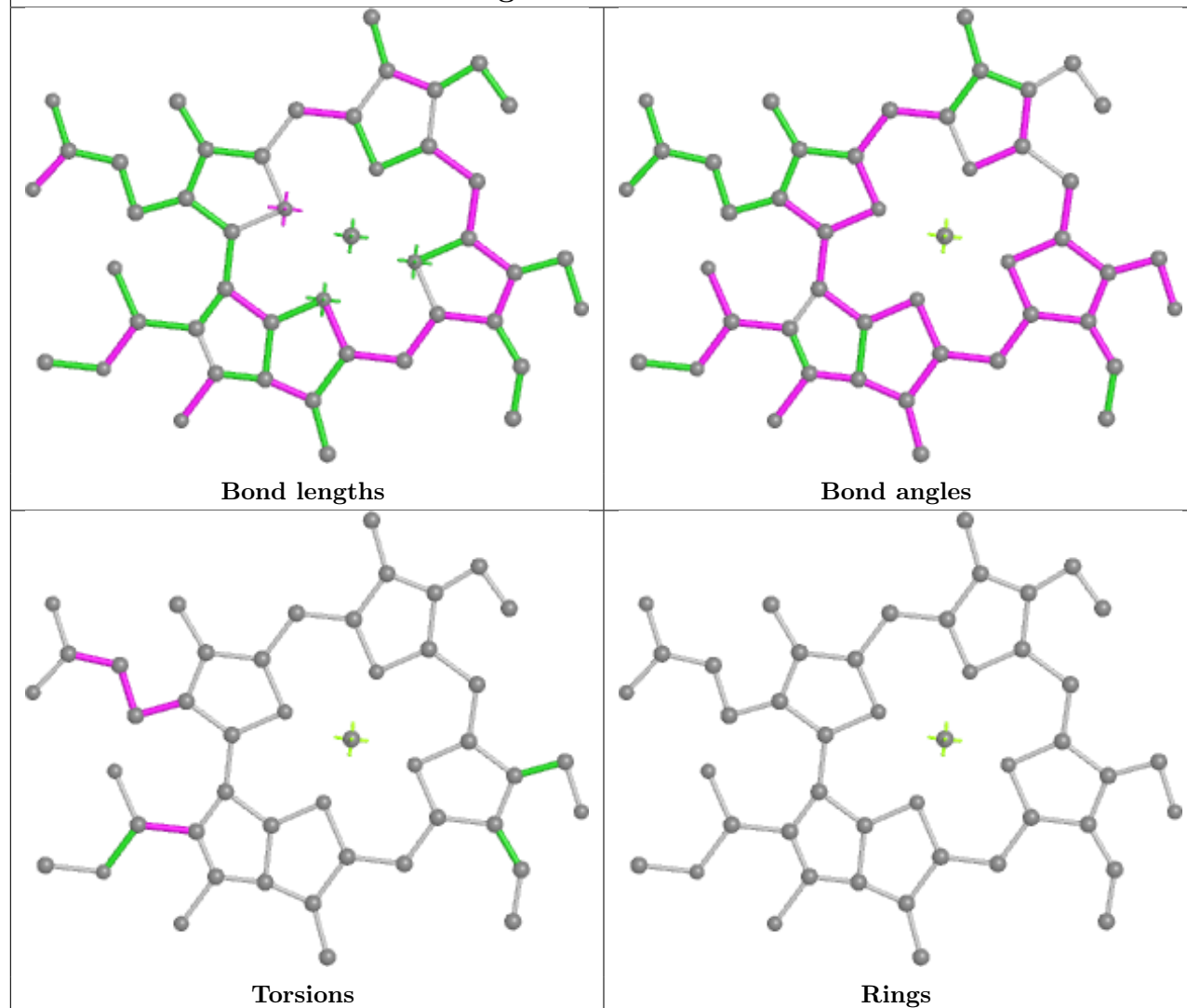
Torsions

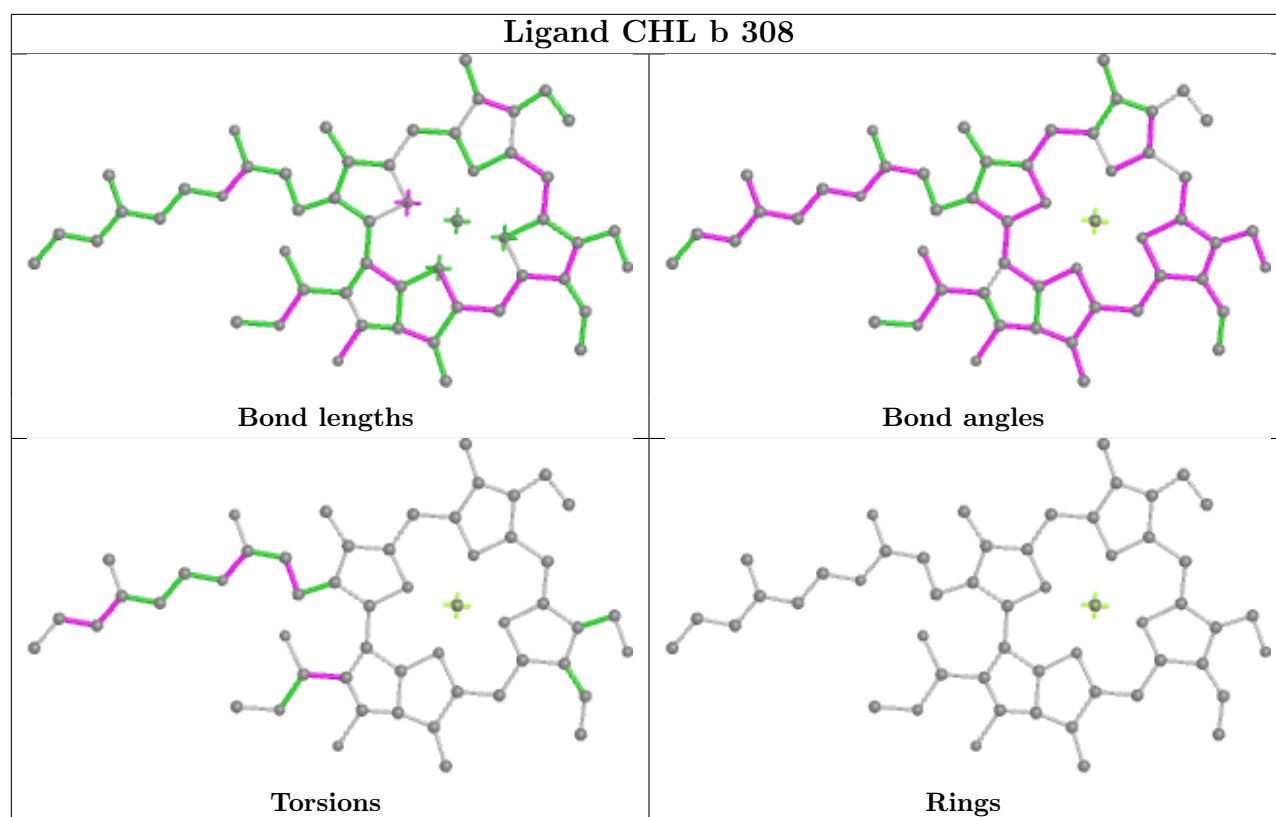


Rings

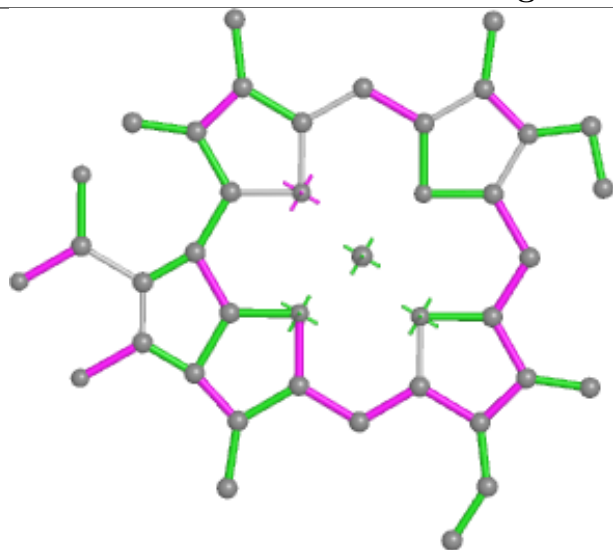


Ligand CHL 9 606

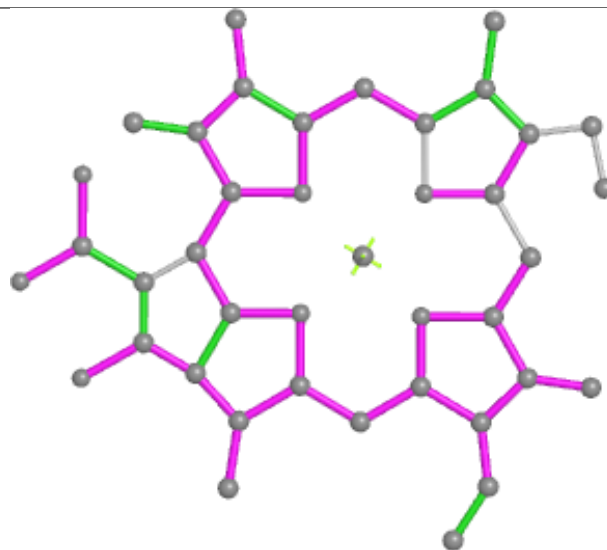




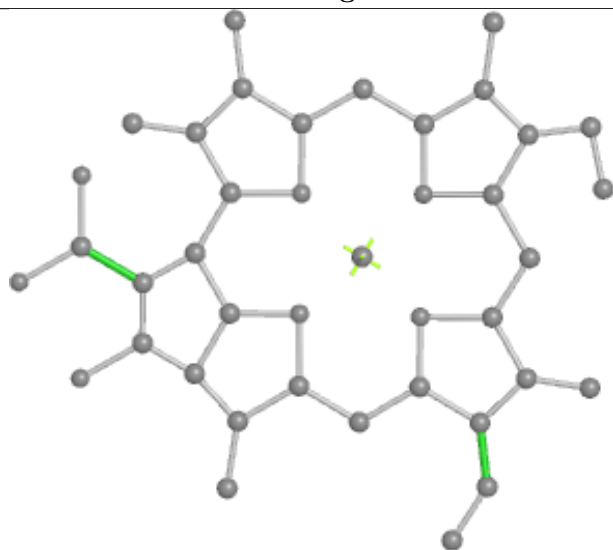
Ligand CHL 7 406



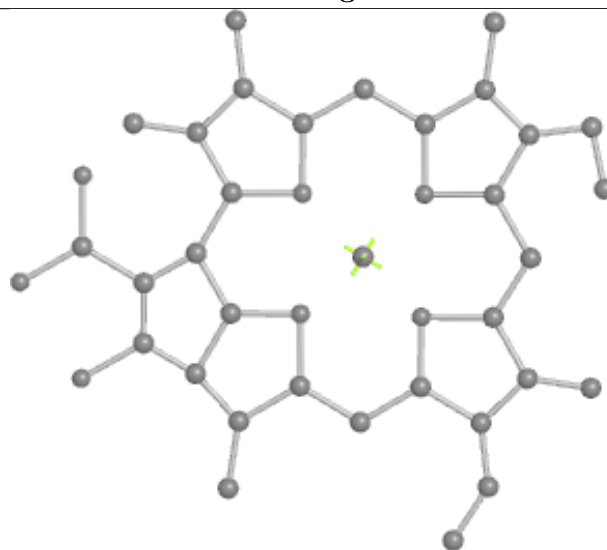
Bond lengths



Bond angles

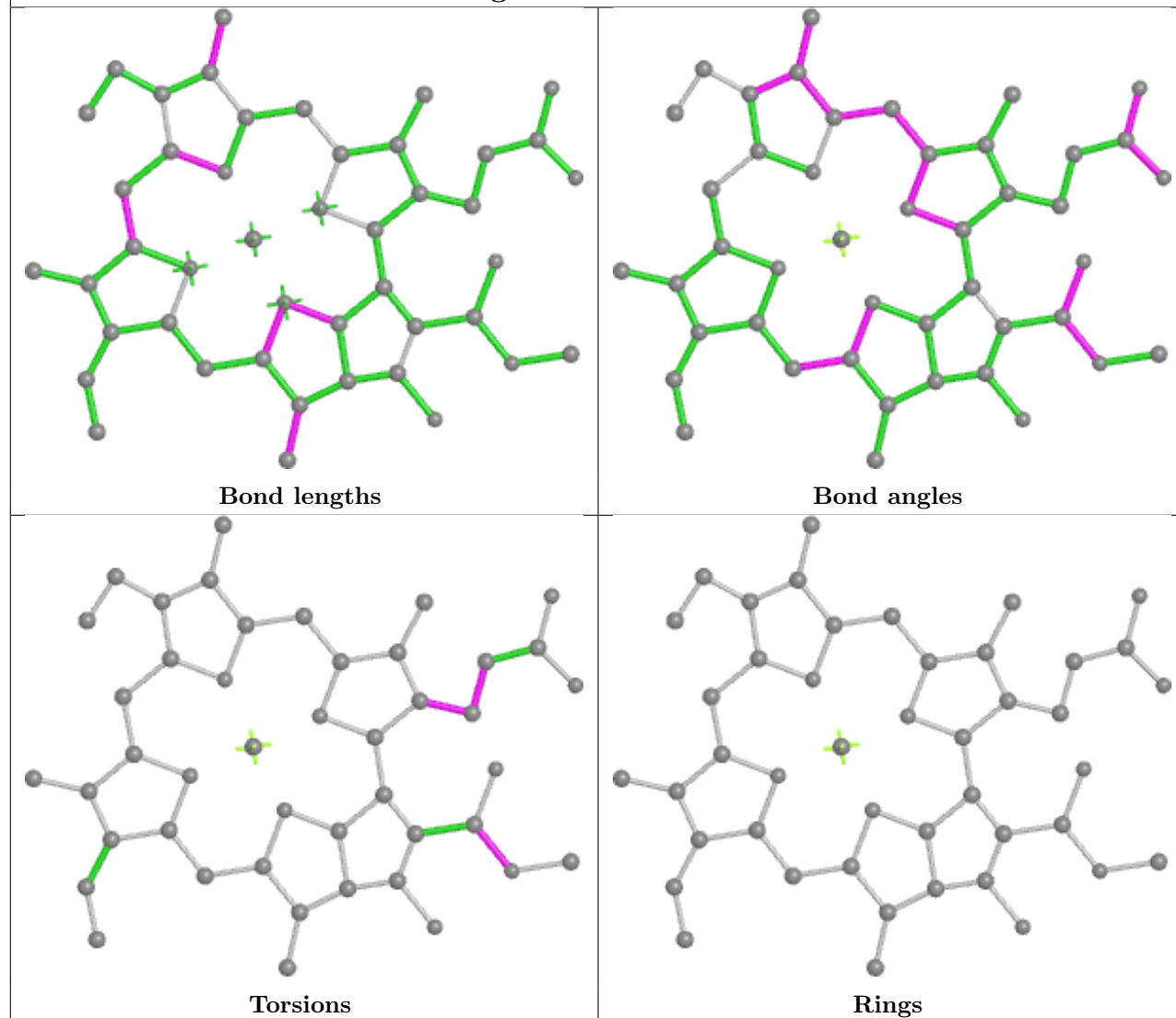


Torsions

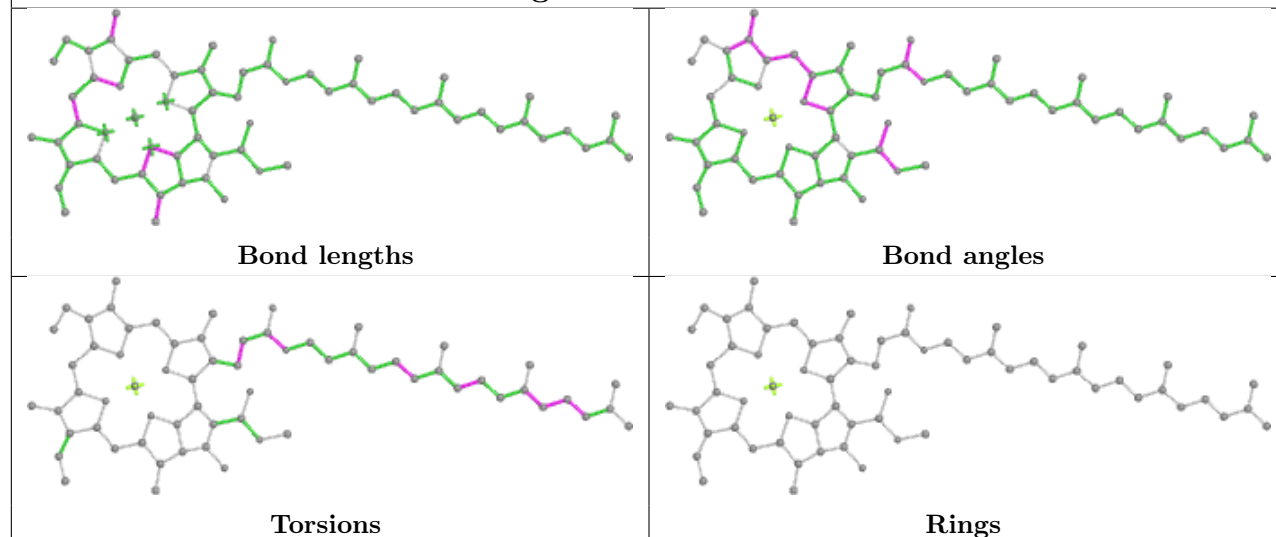


Rings

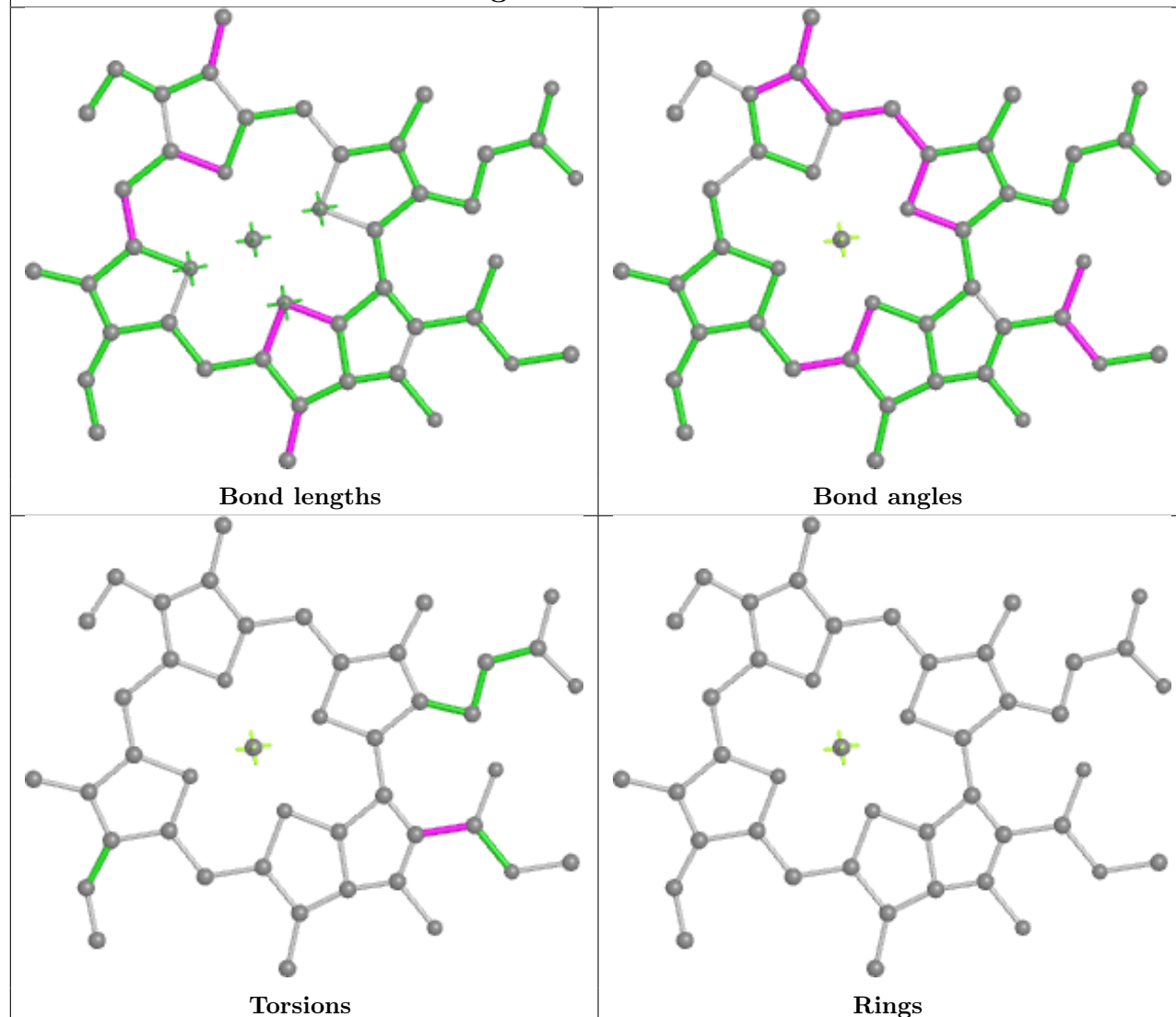
Ligand CLA B 834



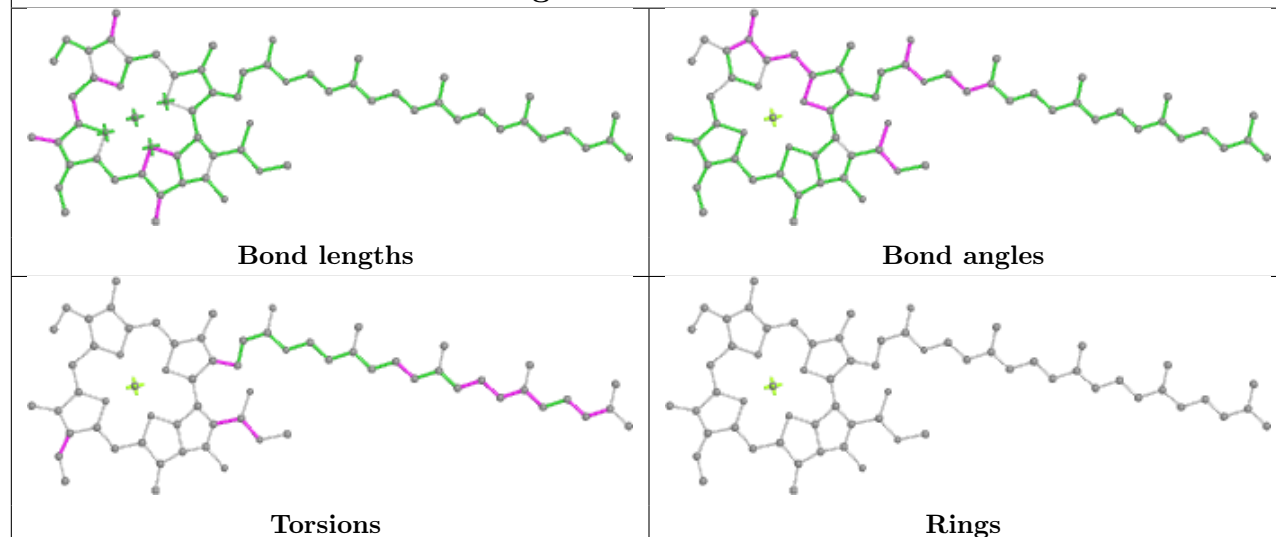
Ligand CLA A 829



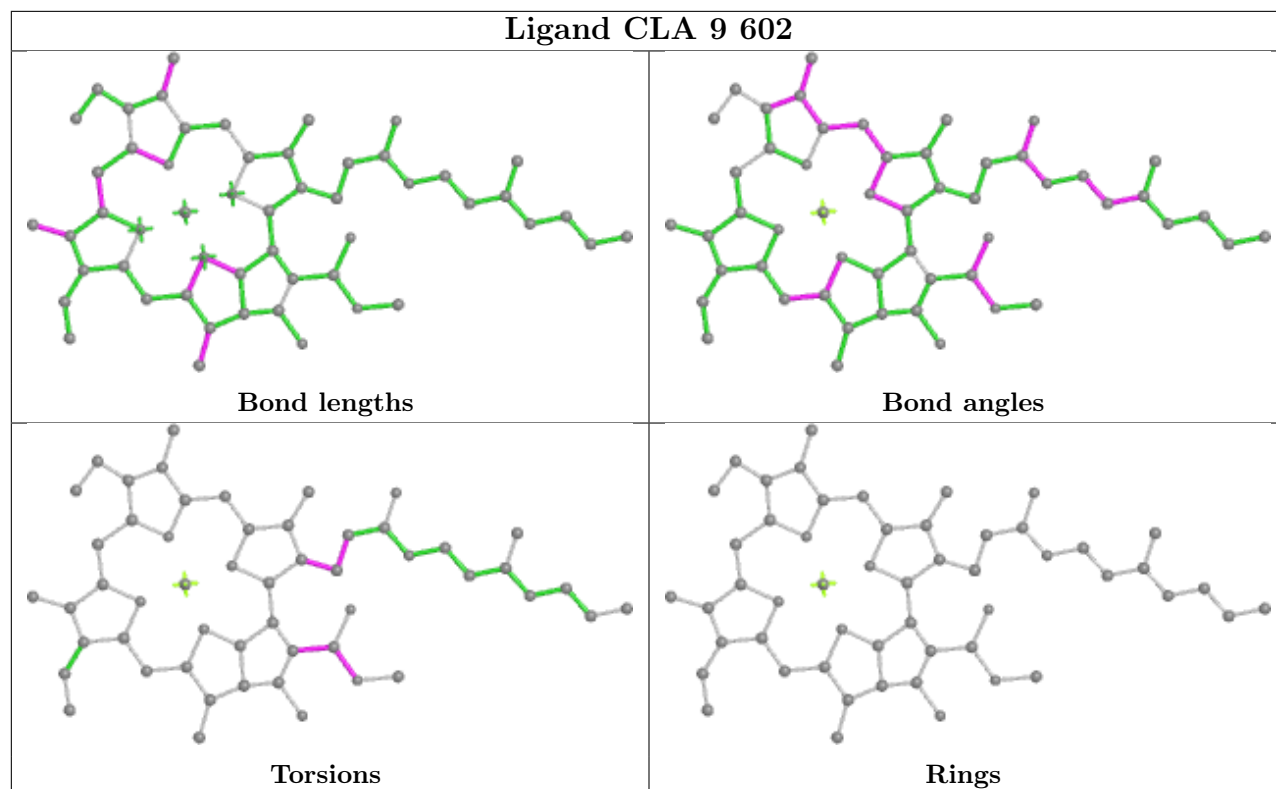
Ligand CLA B 833



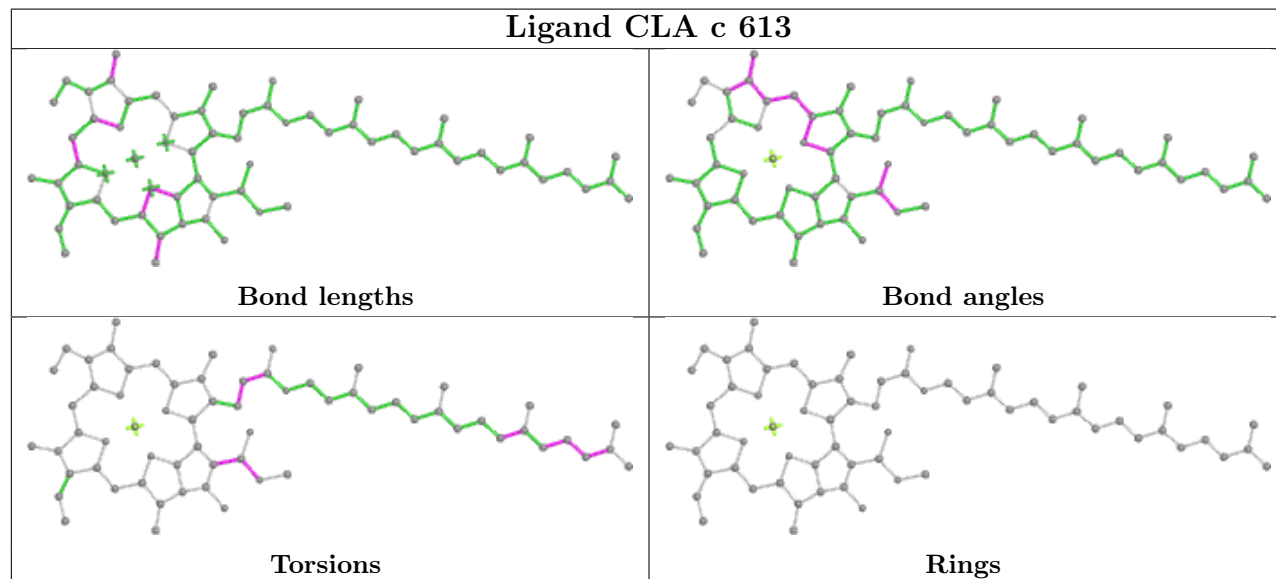
Ligand CLA B 812



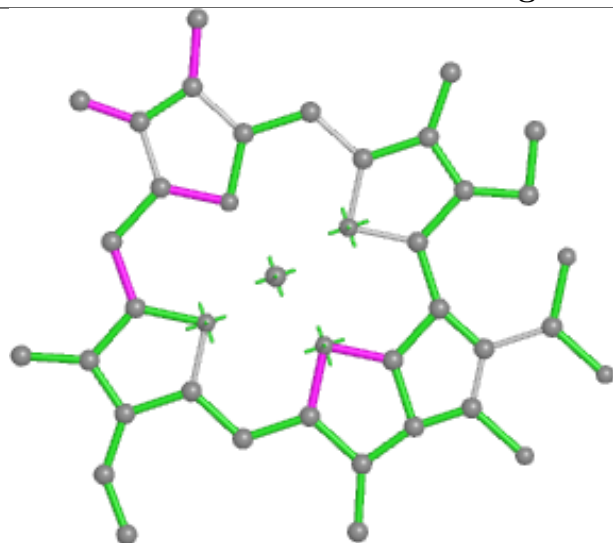
Ligand CLA 9 602



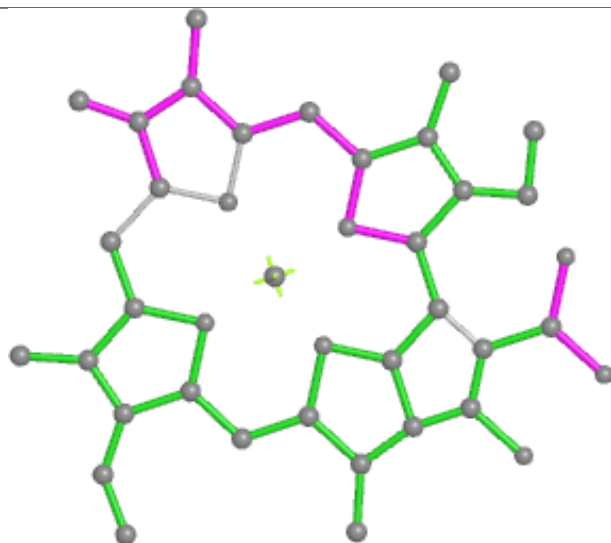
Ligand CLA c 613



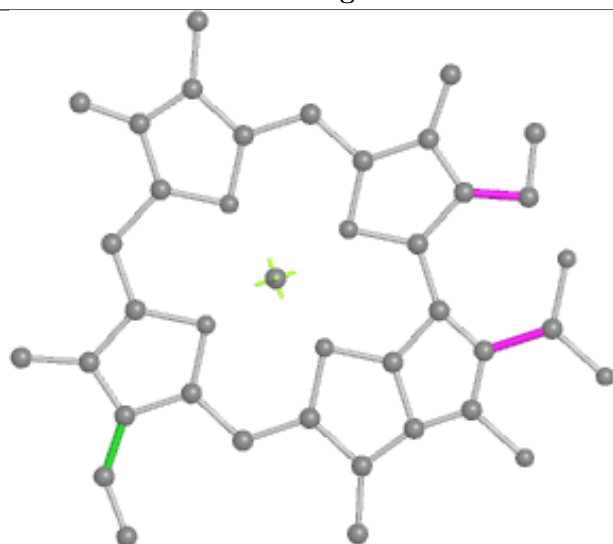
Ligand CLA 7 405



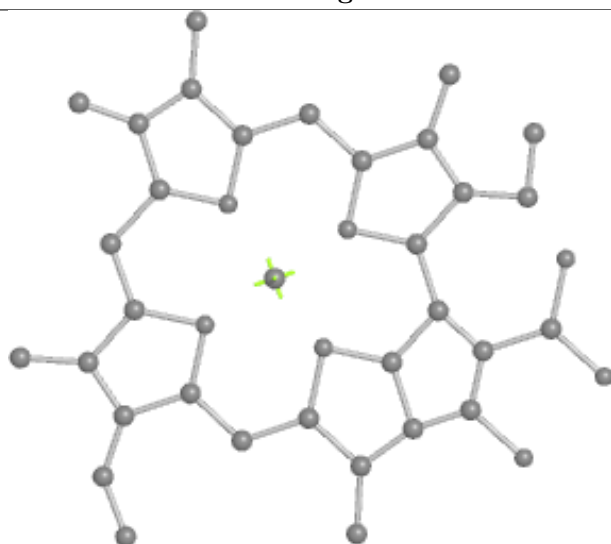
Bond lengths



Bond angles

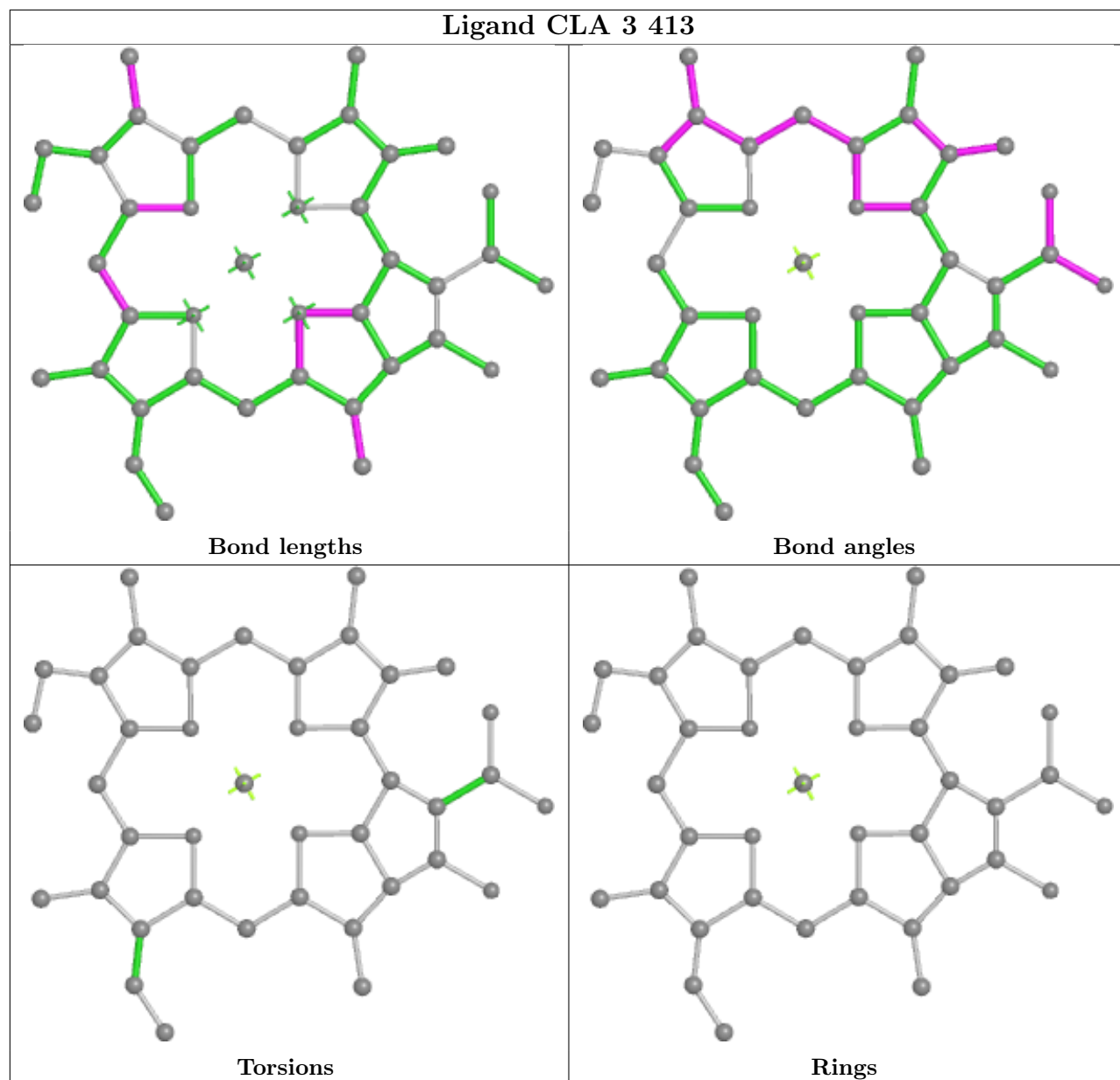


Torsions

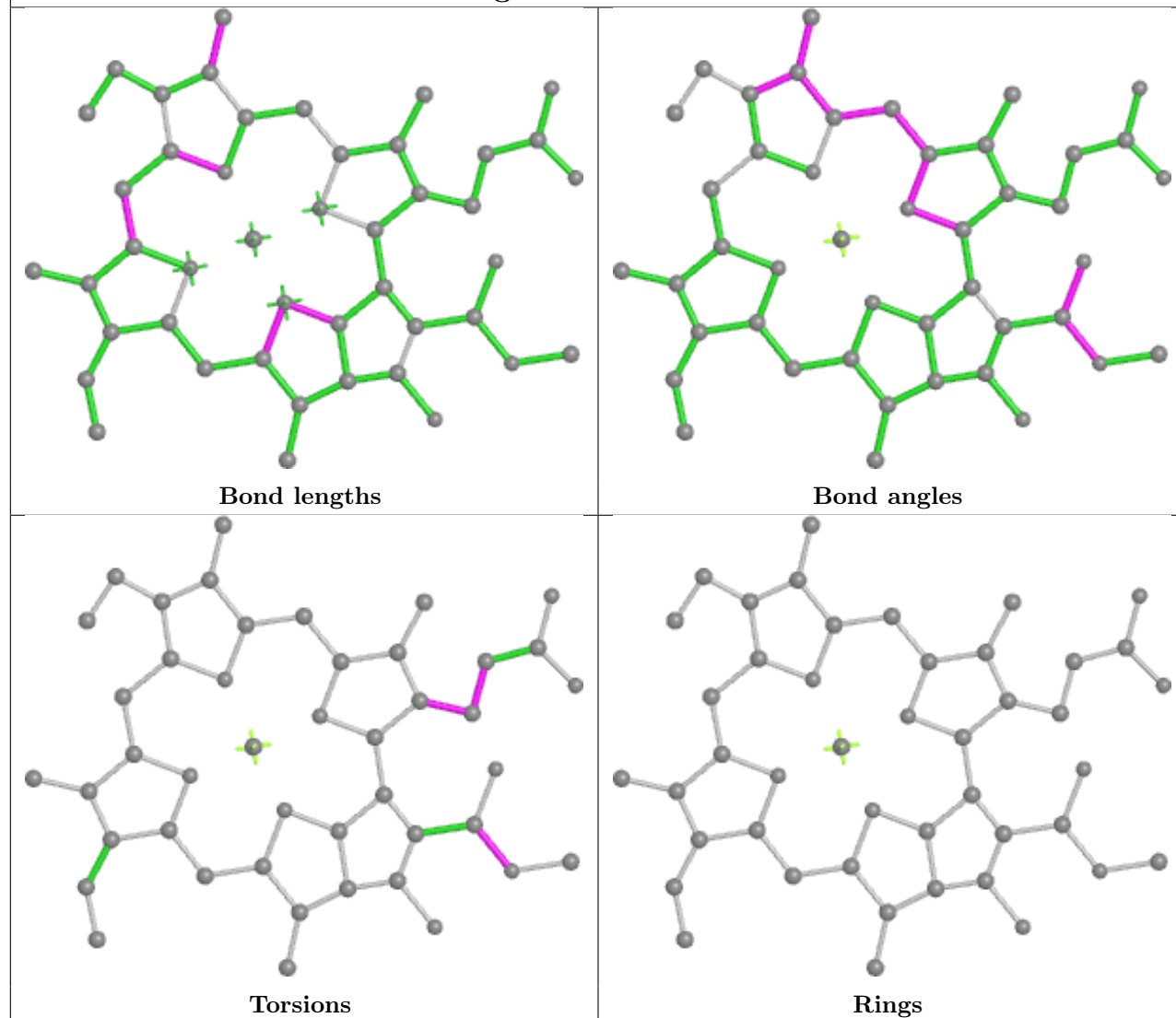


Rings

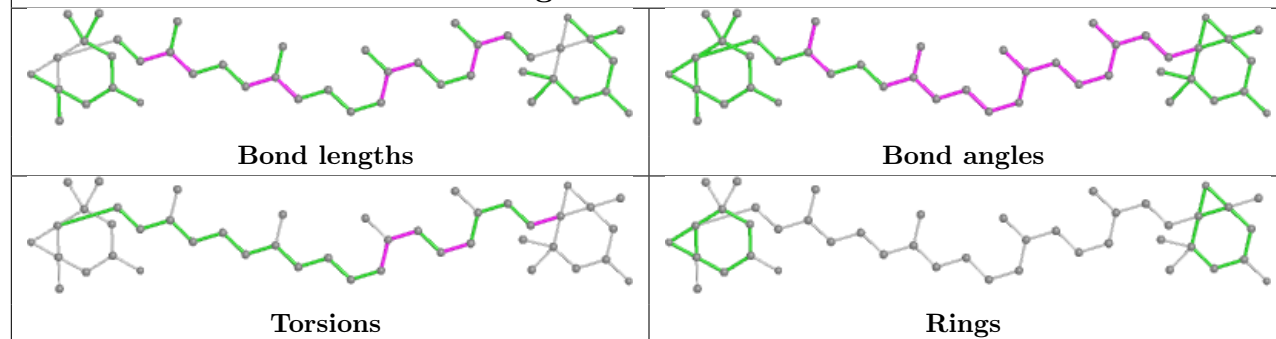
Ligand CLA 3 413



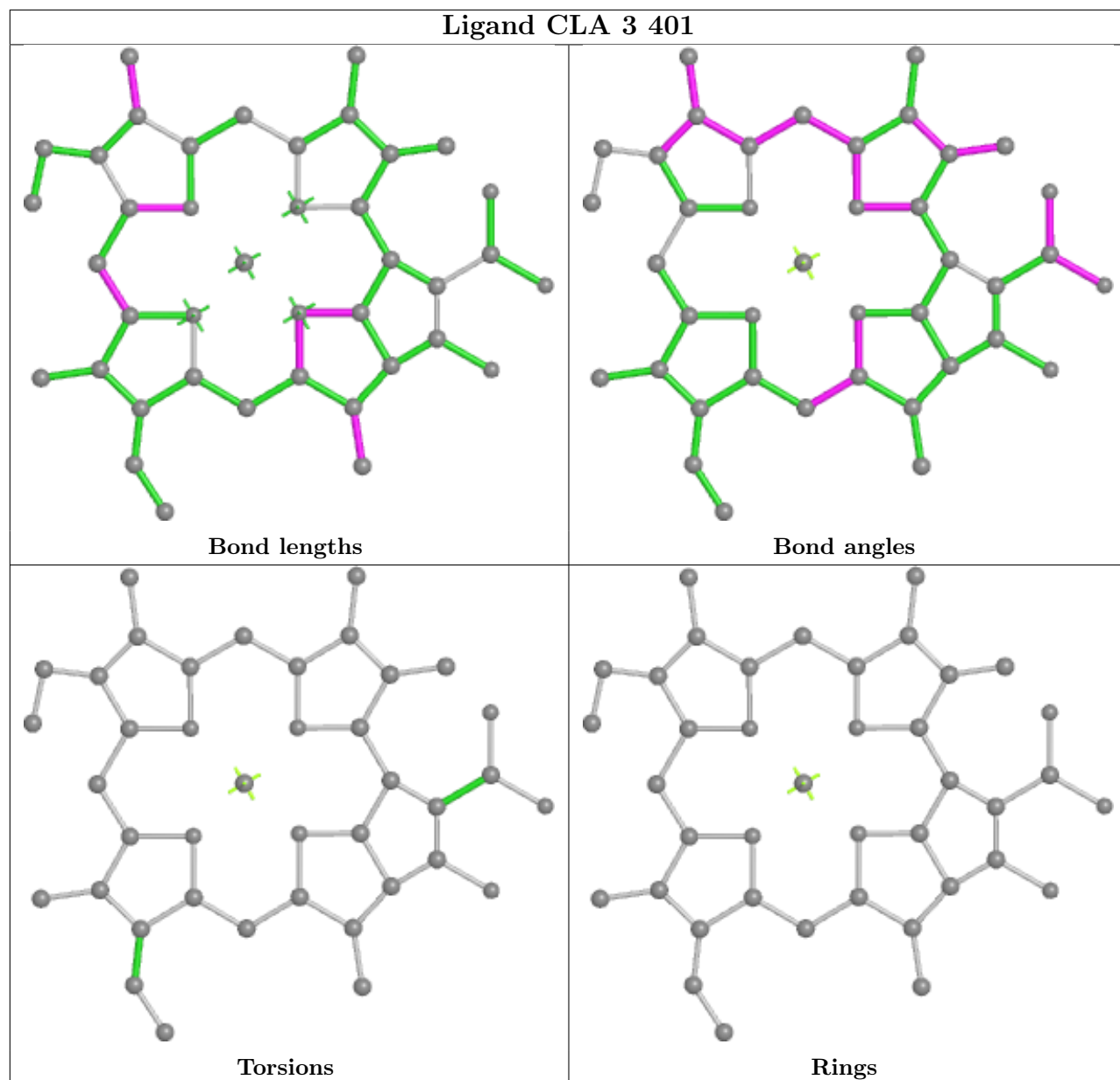
Ligand CLA 6 608



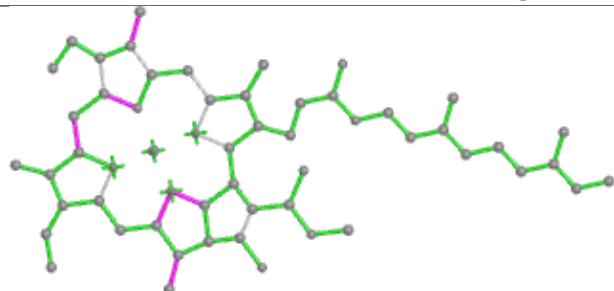
Ligand XAT 6 617



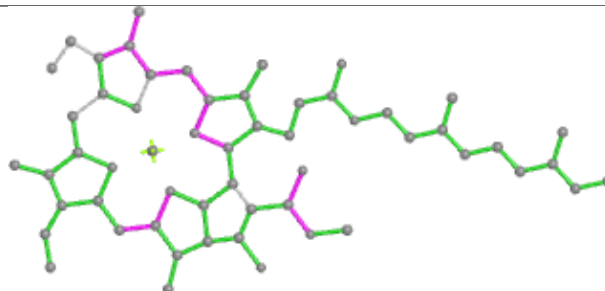
Ligand CLA 3 401



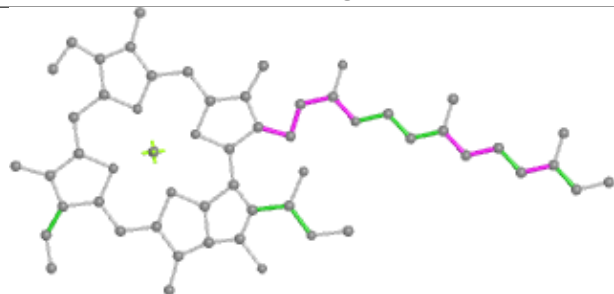
Ligand CLA B 830



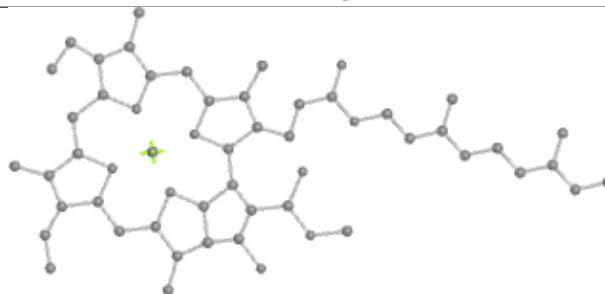
Bond lengths



Bond angles

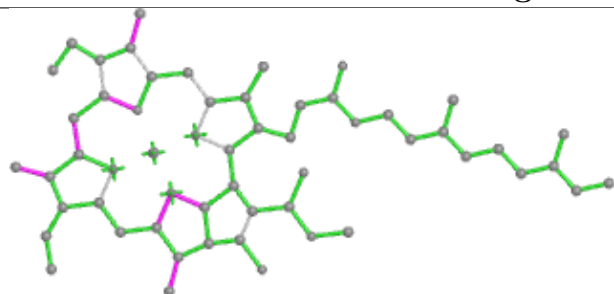


Torsions

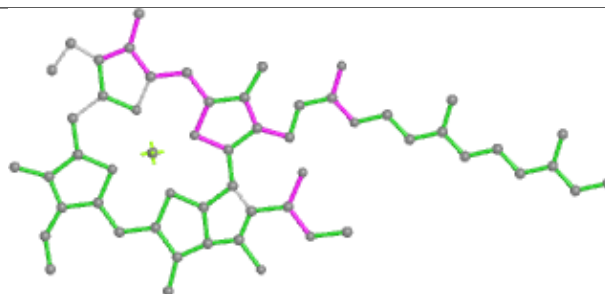


Rings

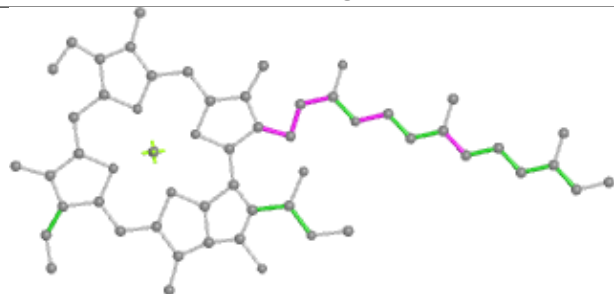
Ligand CLA B 832



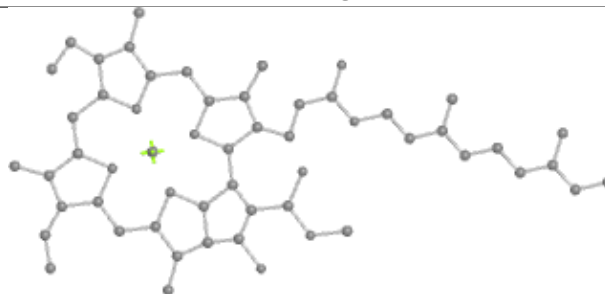
Bond lengths



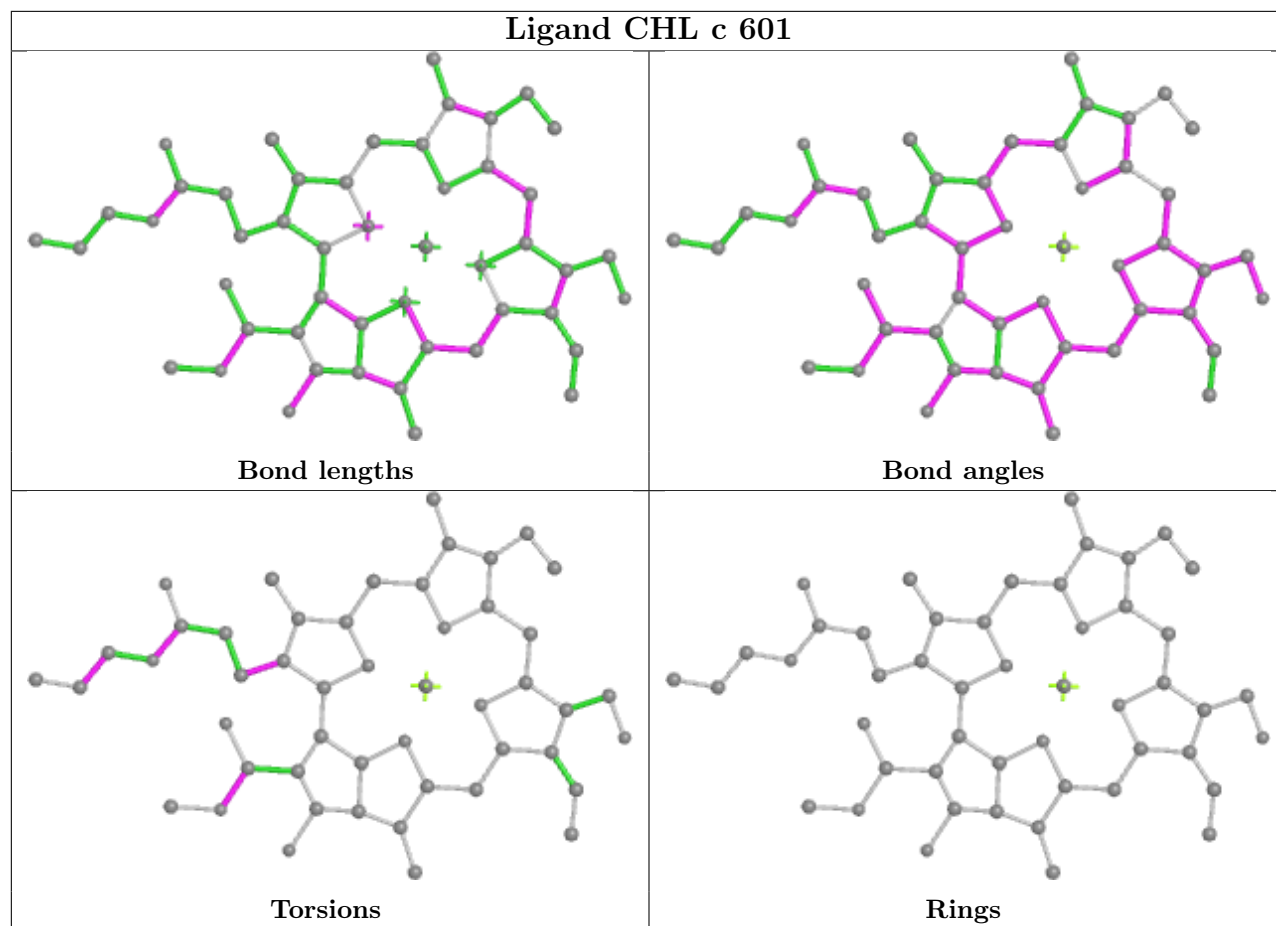
Bond angles



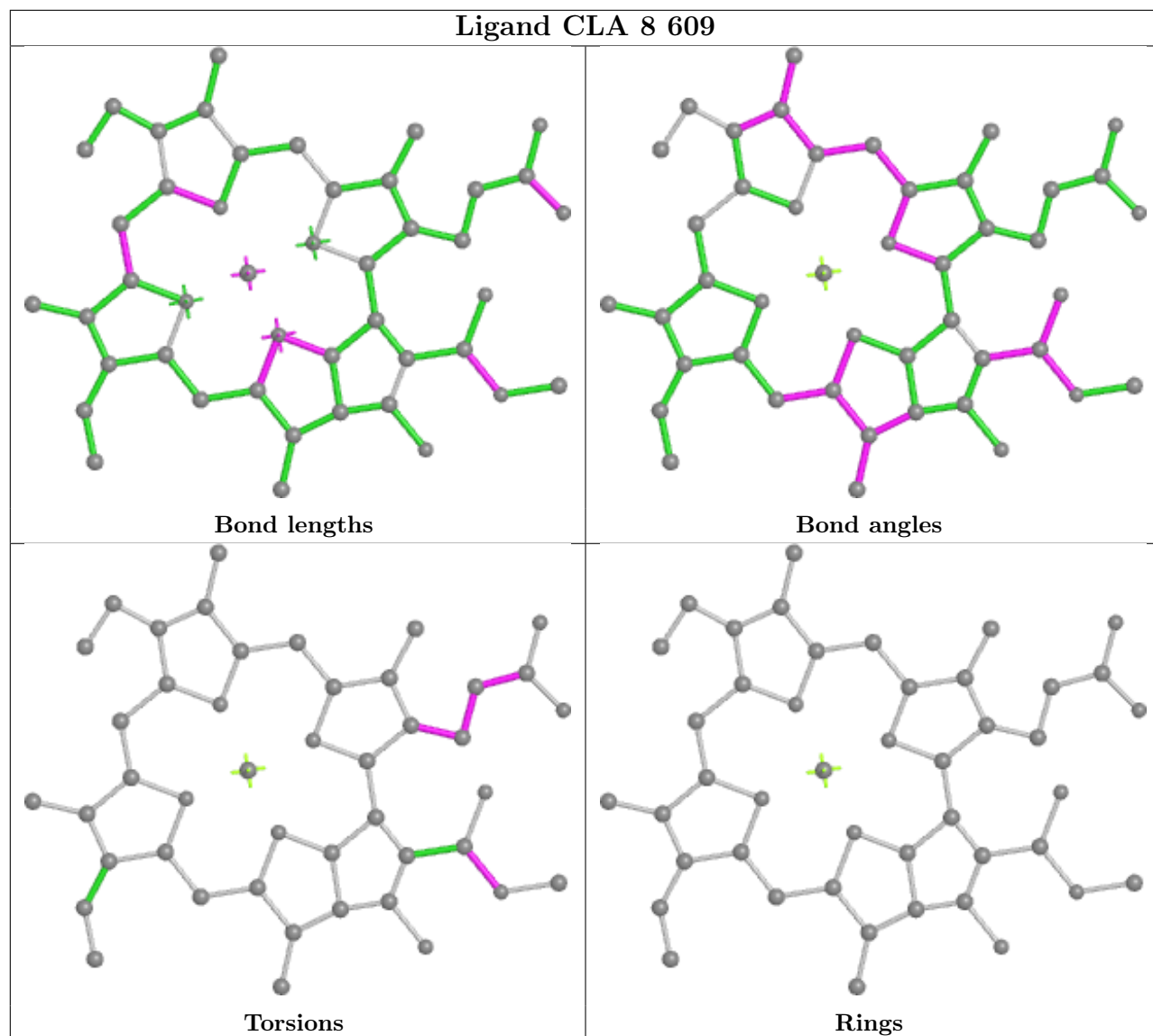
Torsions



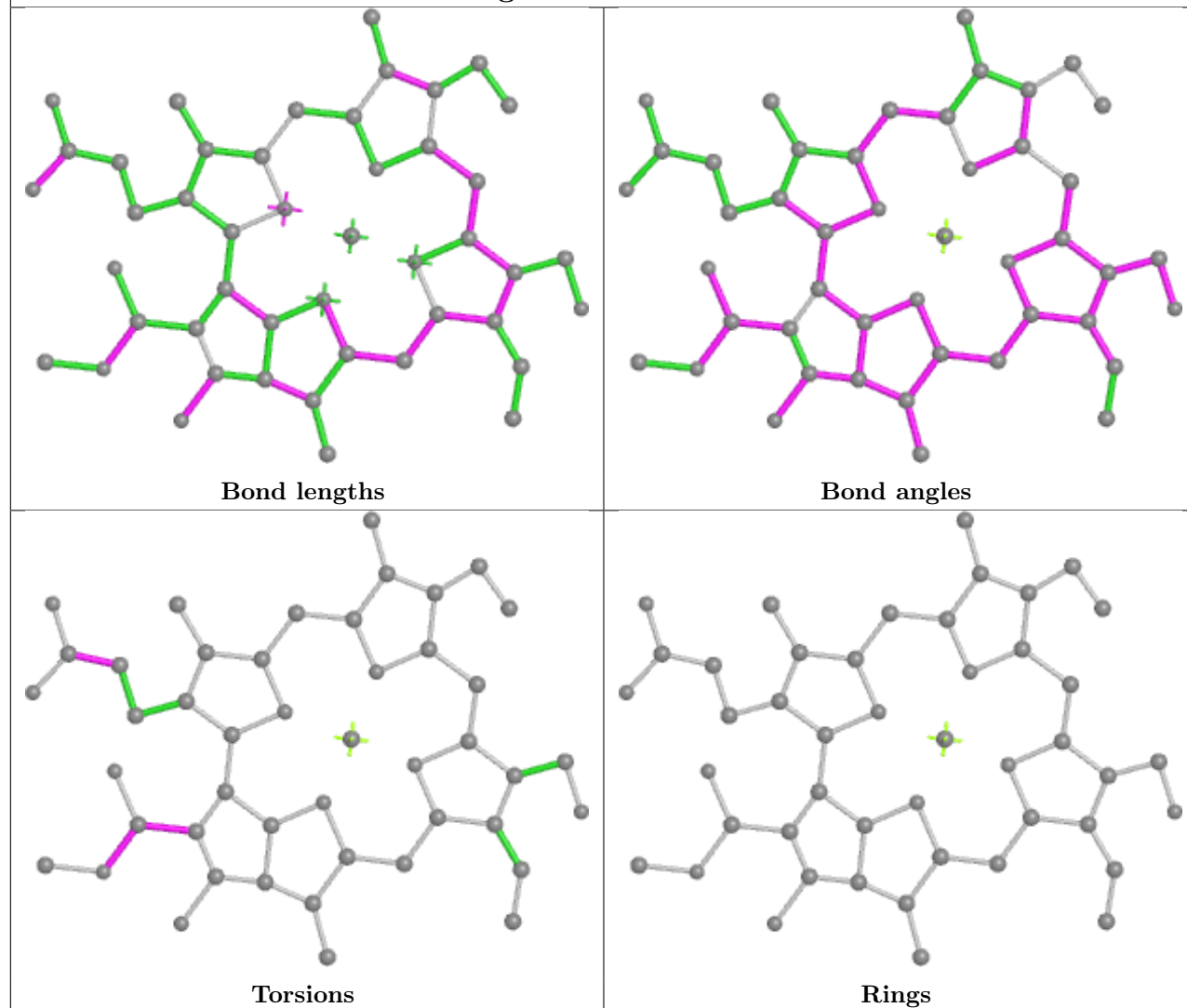
Rings



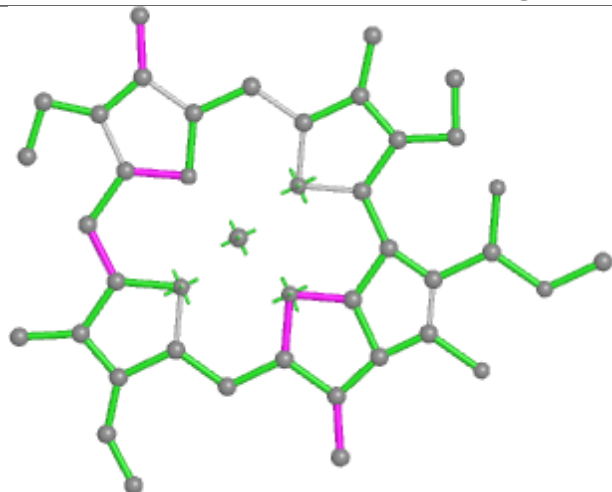
Ligand CLA 8 609



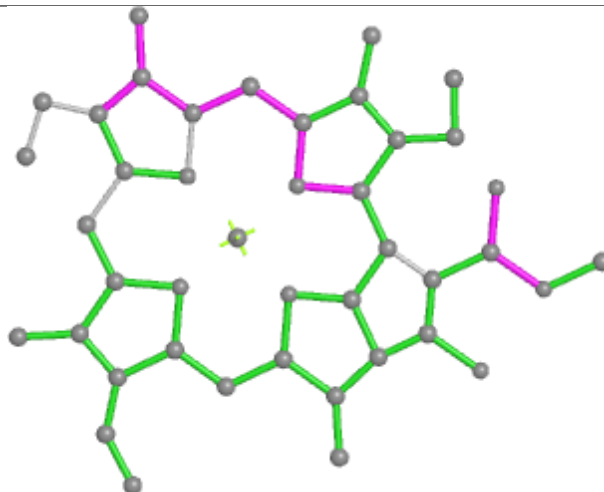
Ligand CHL 9 609



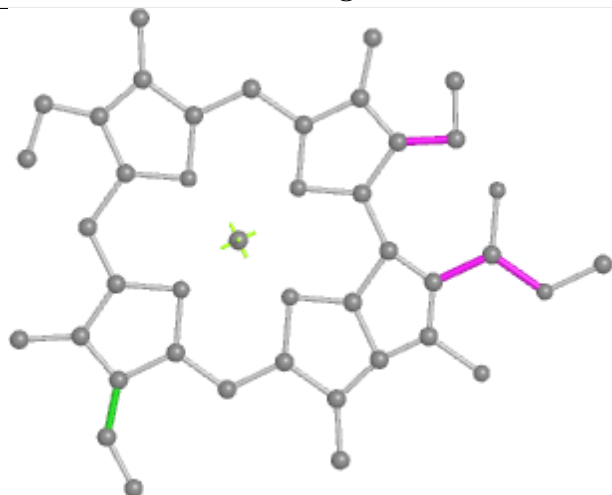
Ligand CLA L 304



Bond lengths



Bond angles

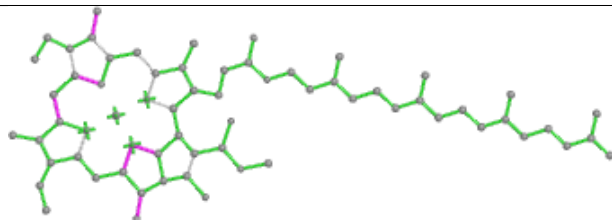


Torsions

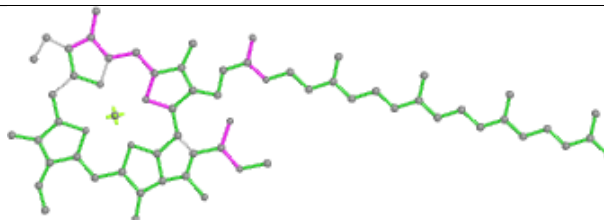


Rings

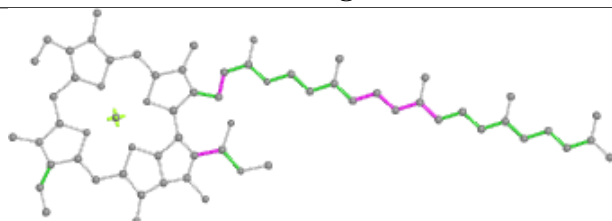
Ligand CLA B 838



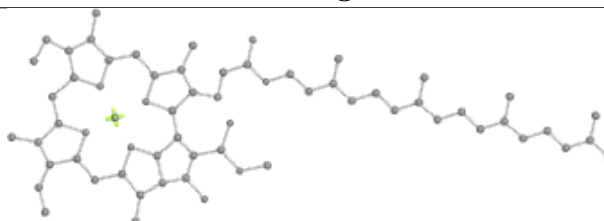
Bond lengths



Bond angles

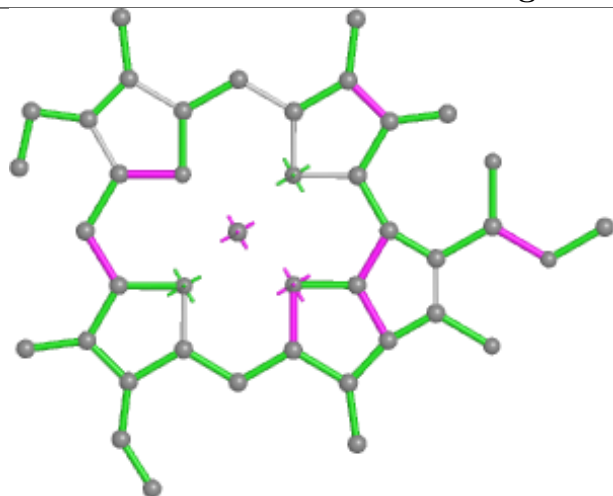


Torsions

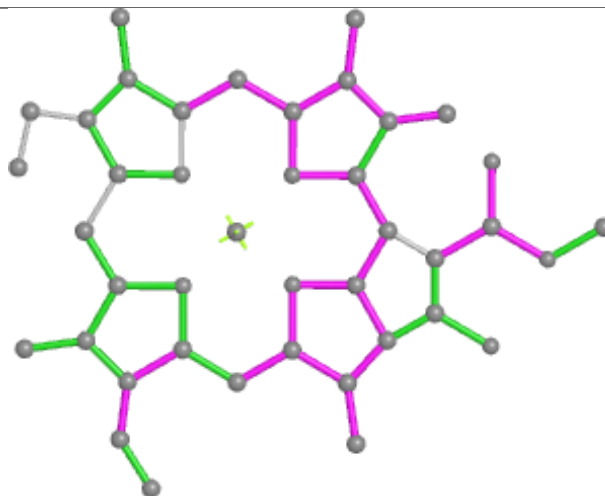


Rings

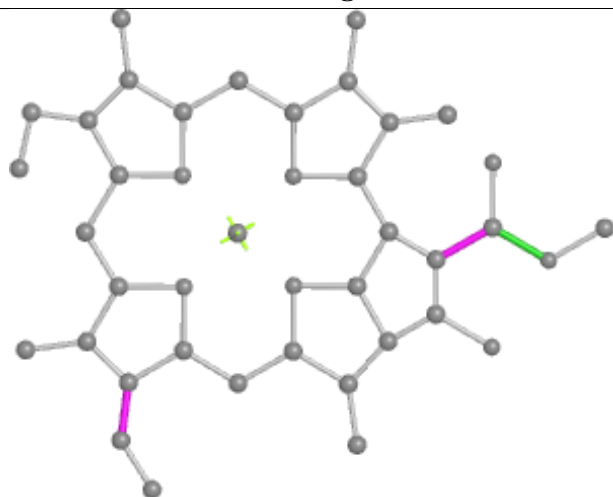
Ligand CLA 1 309



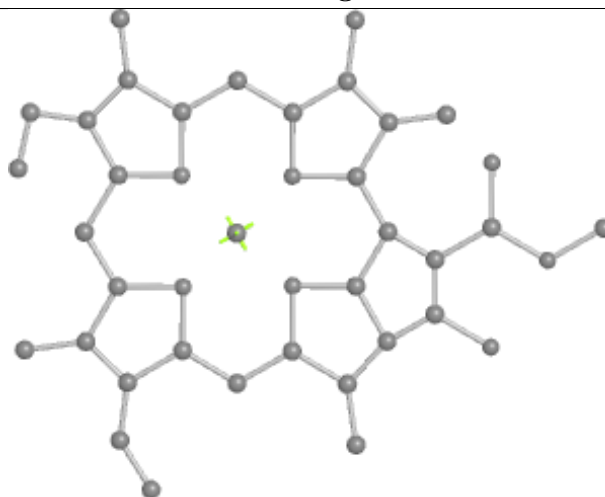
Bond lengths



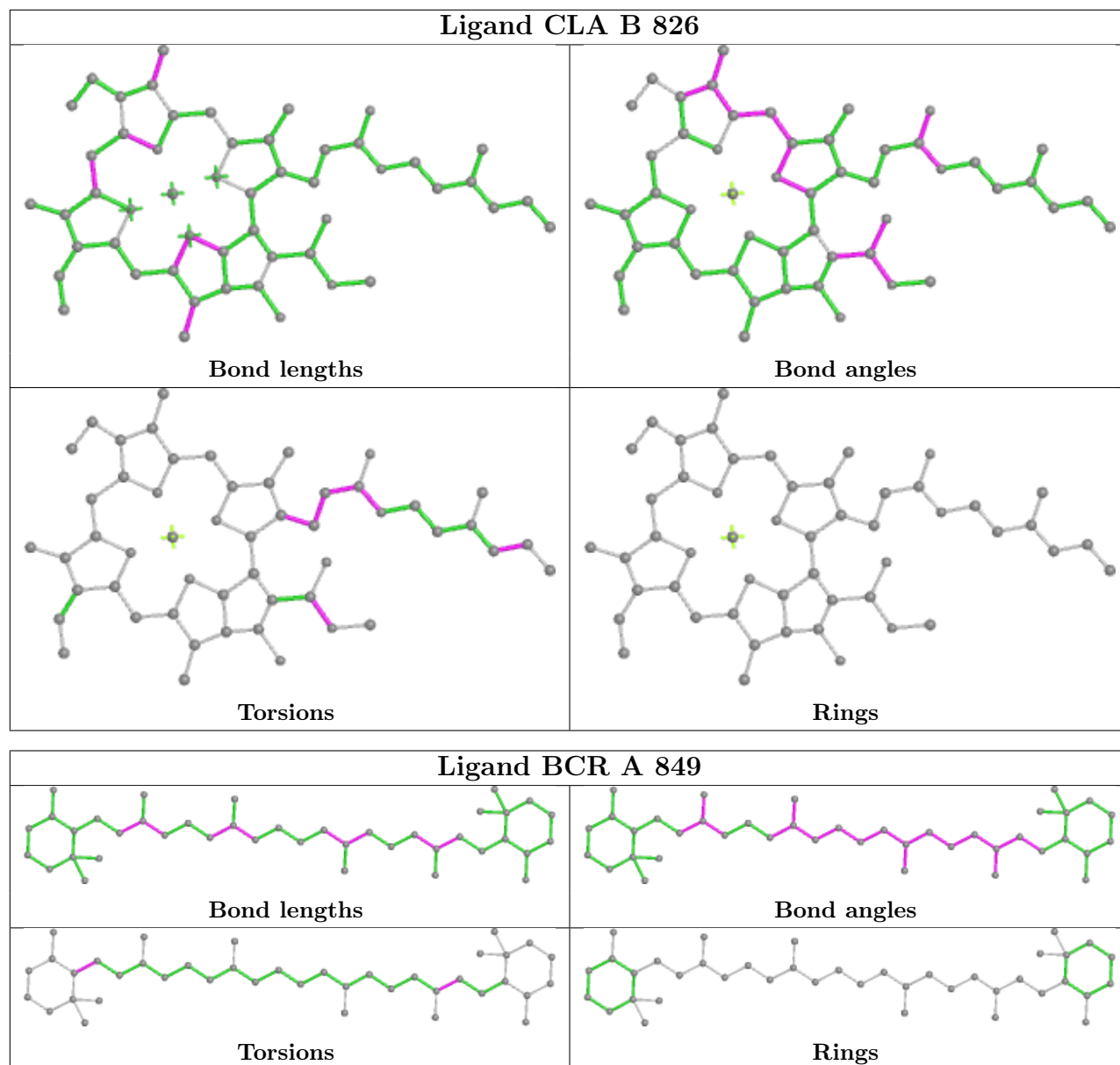
Bond angles

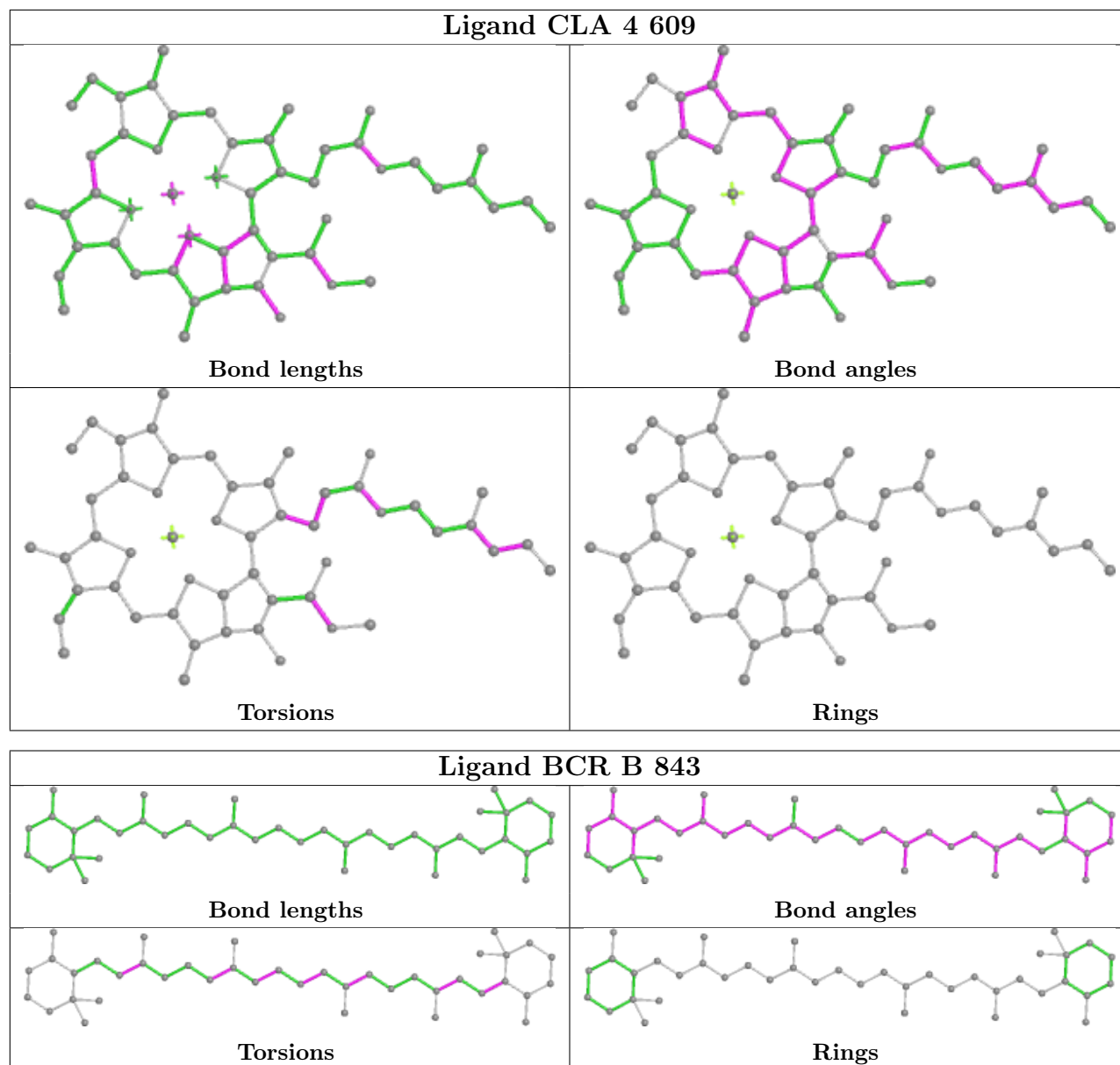


Torsions

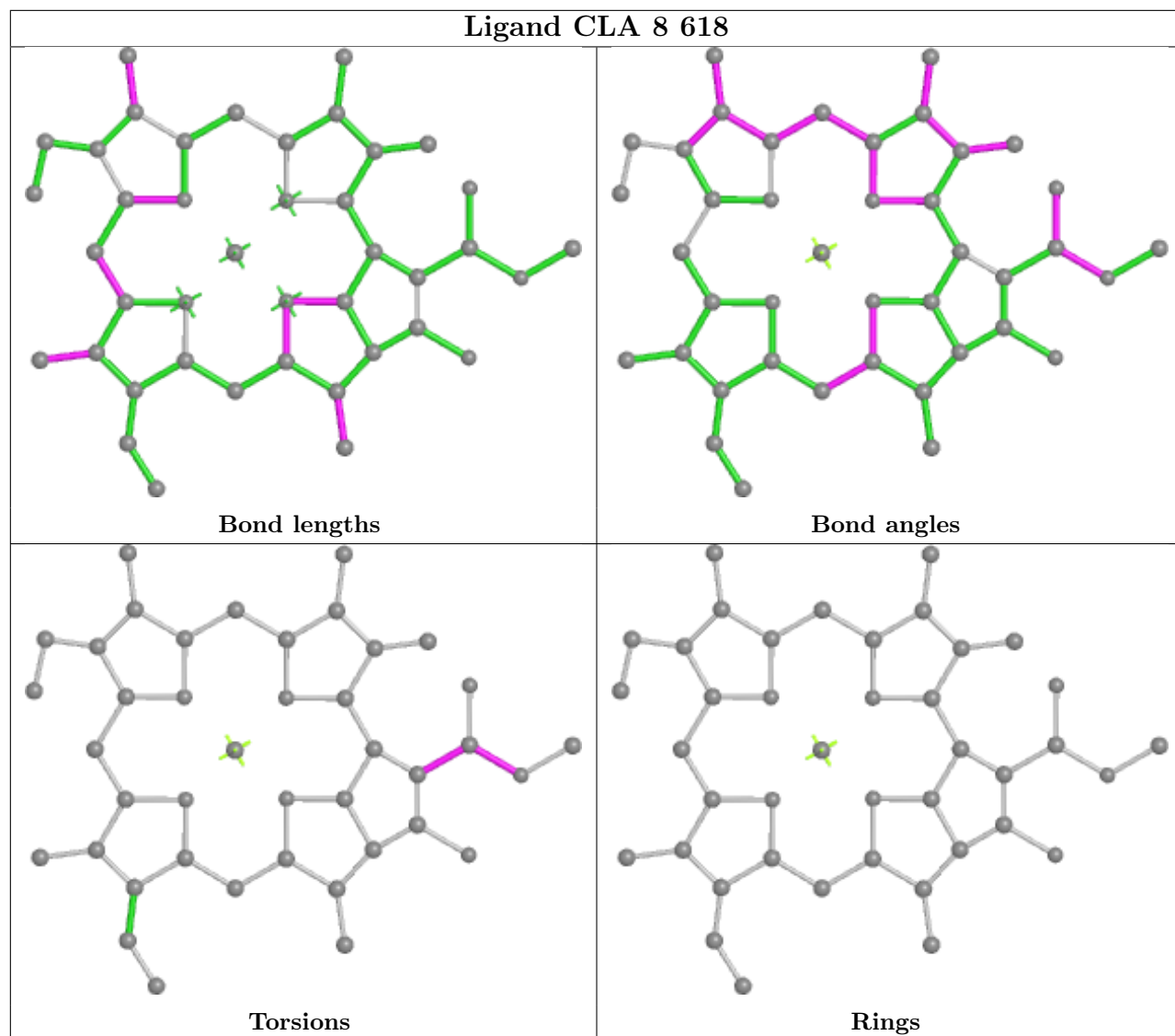


Rings

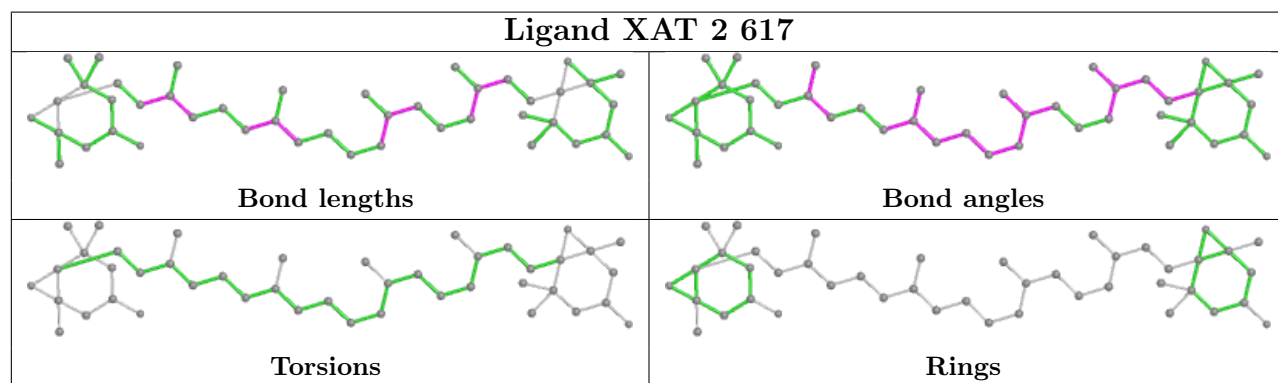




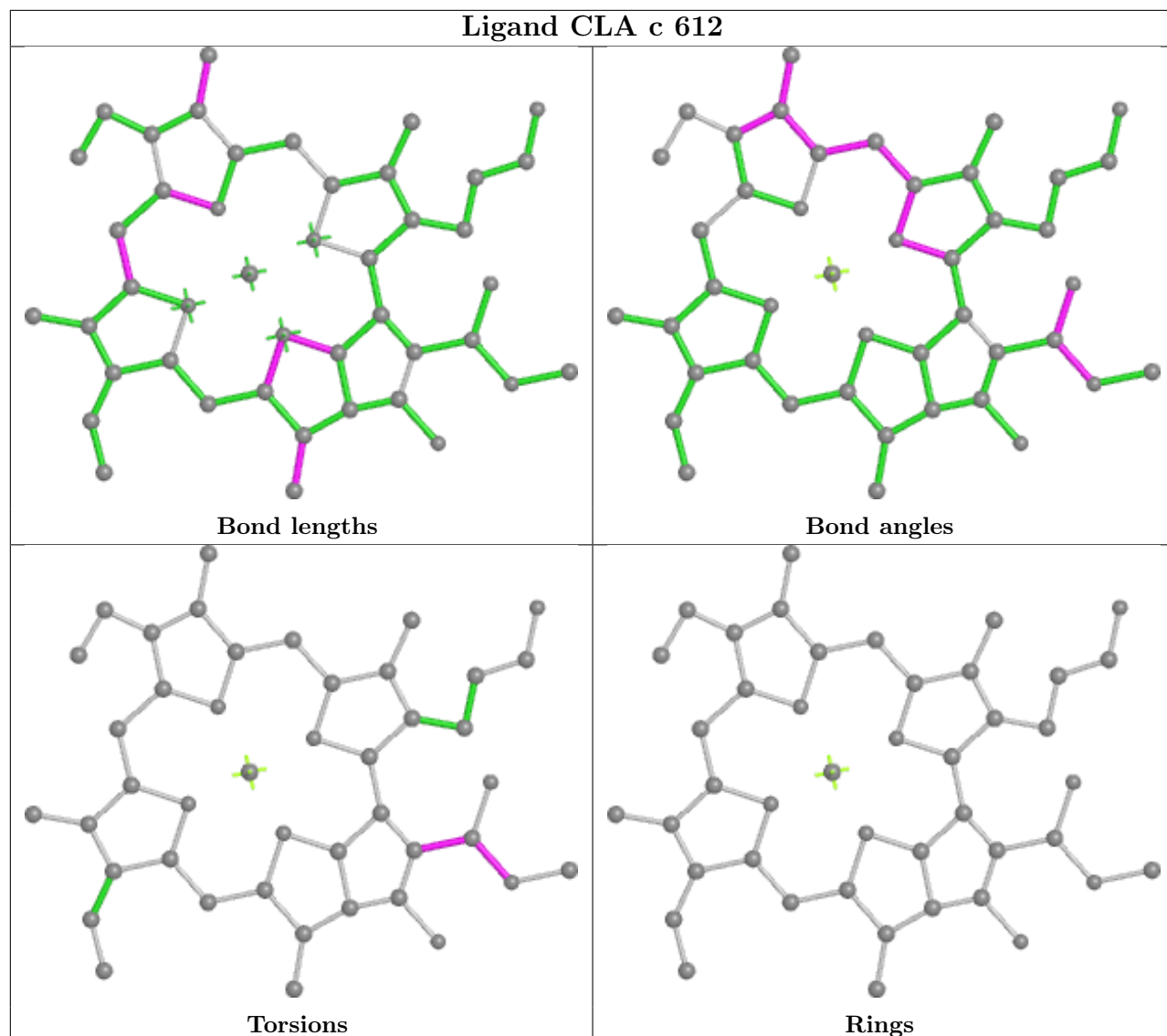
Ligand CLA 8 618



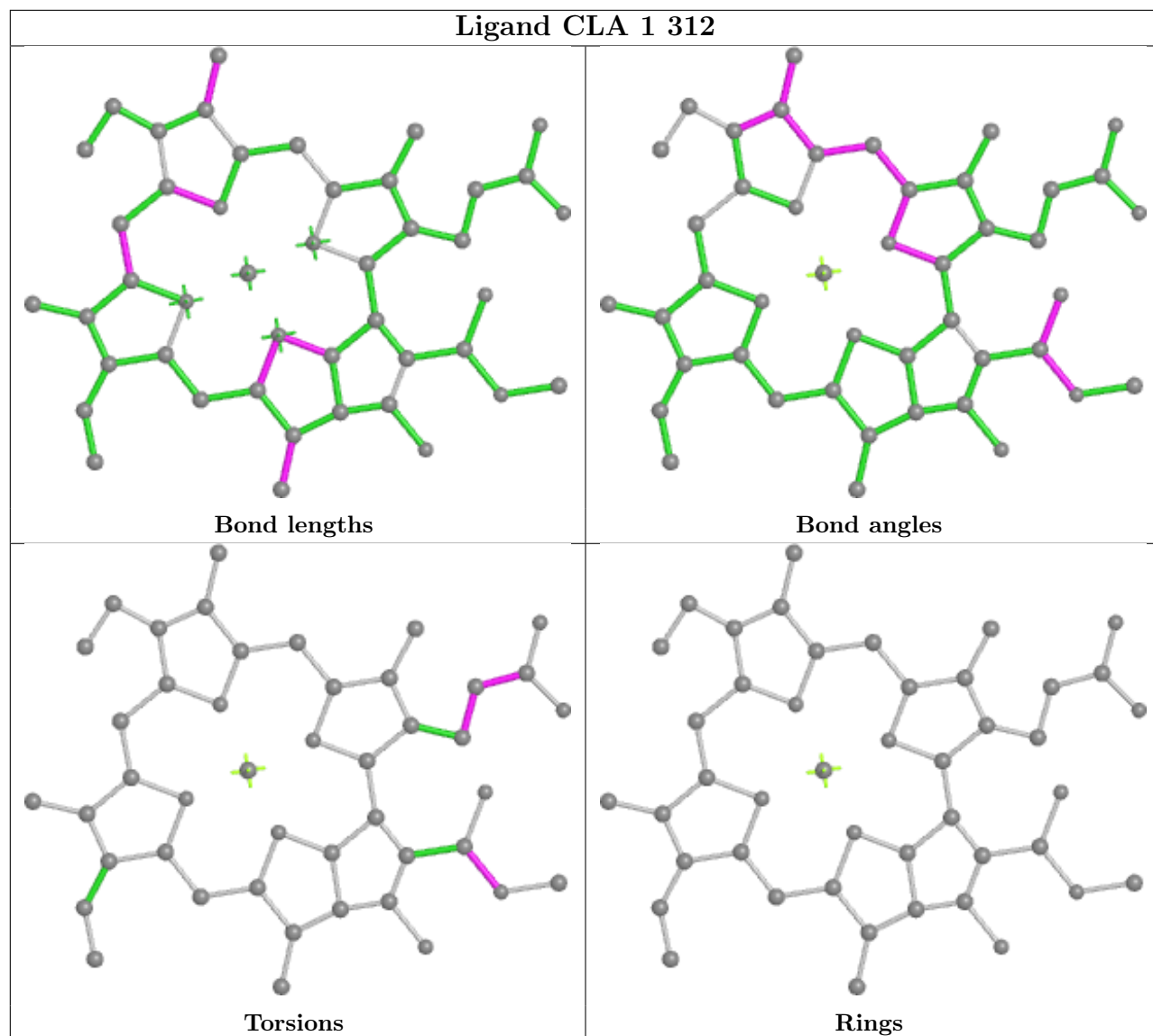
Ligand XAT 2 617



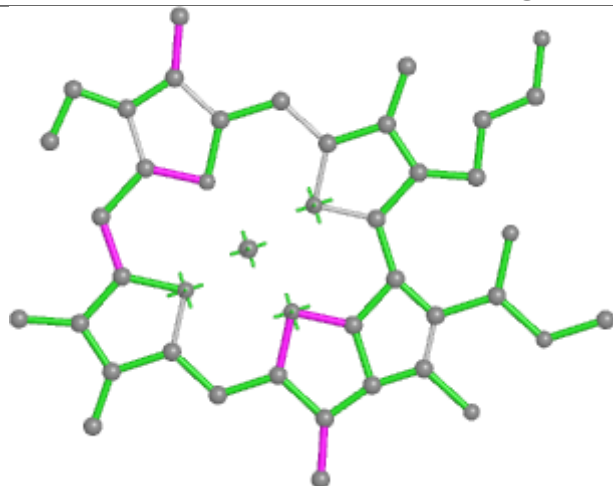
Ligand CLA c 612



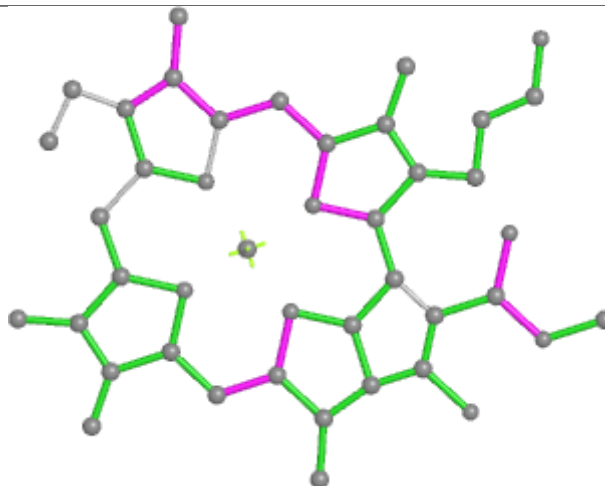
Ligand CLA 1 312



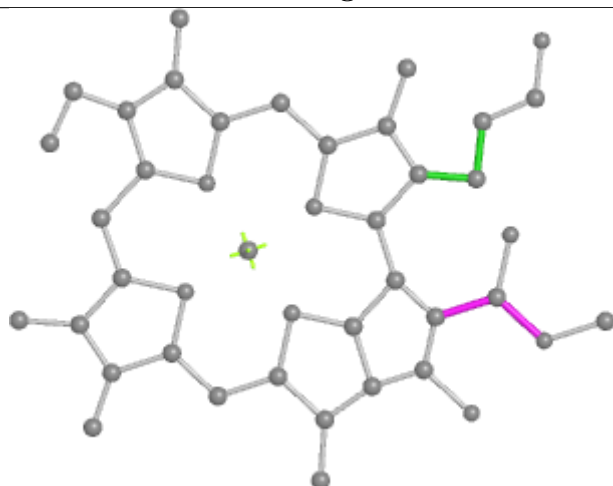
Ligand CLA 4 604



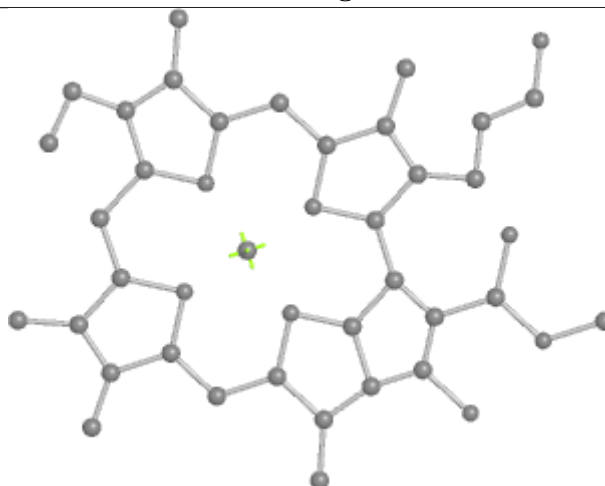
Bond lengths



Bond angles

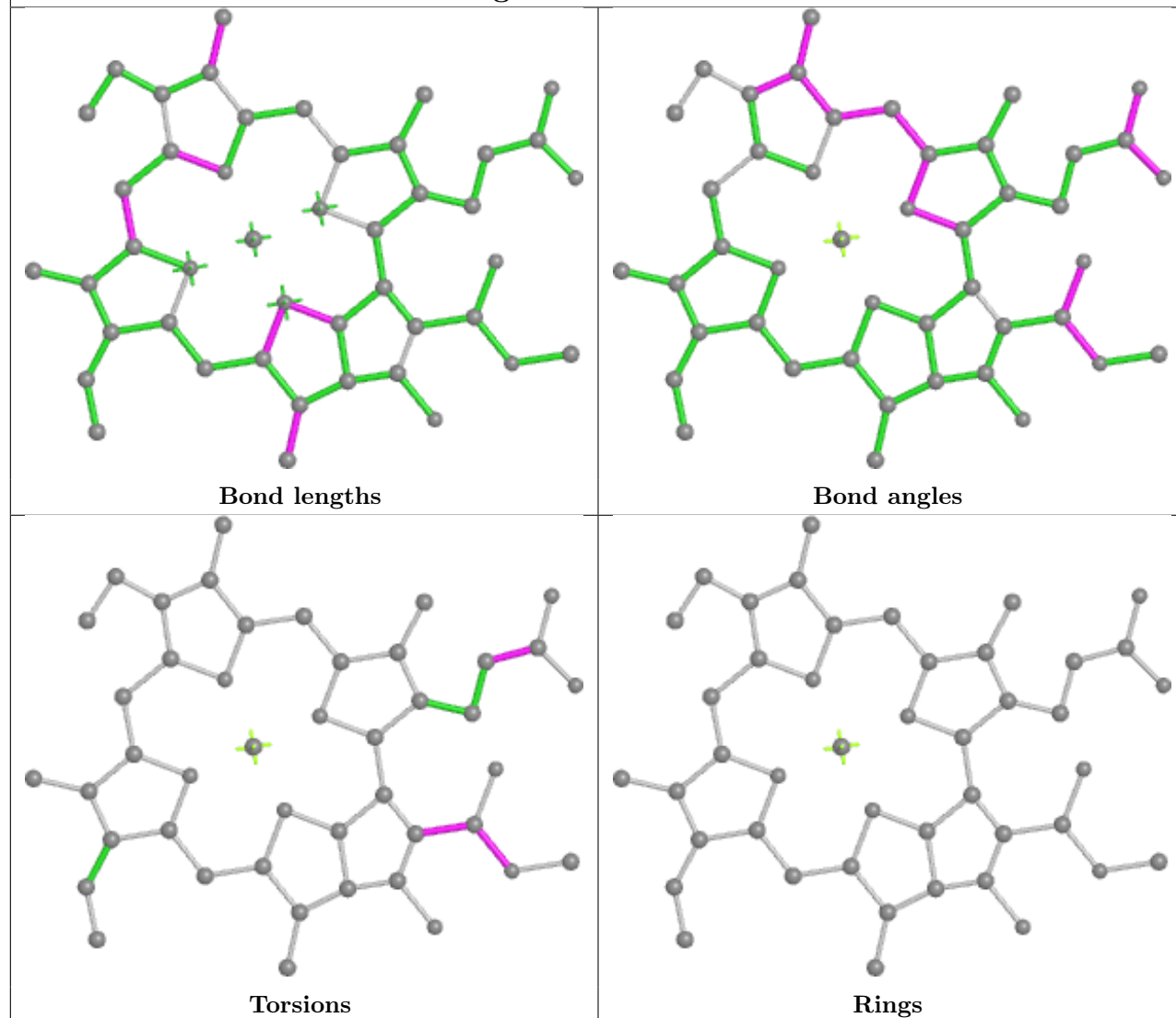


Torsions

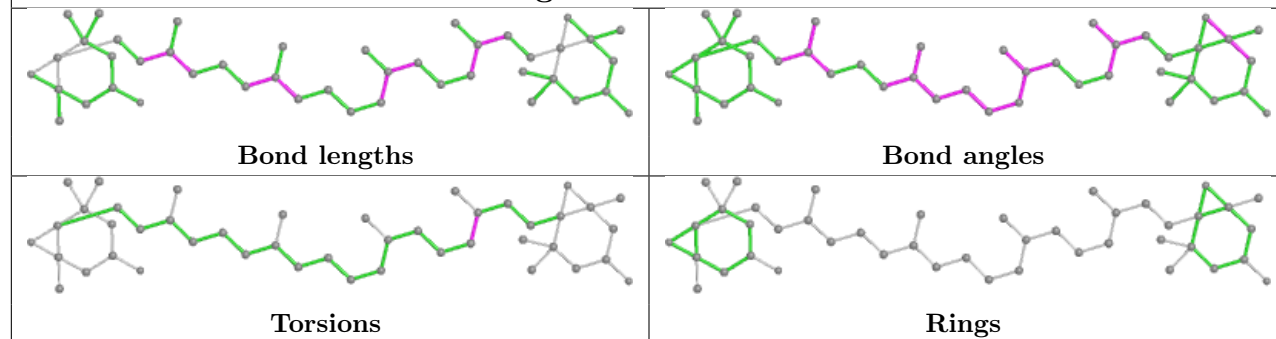


Rings

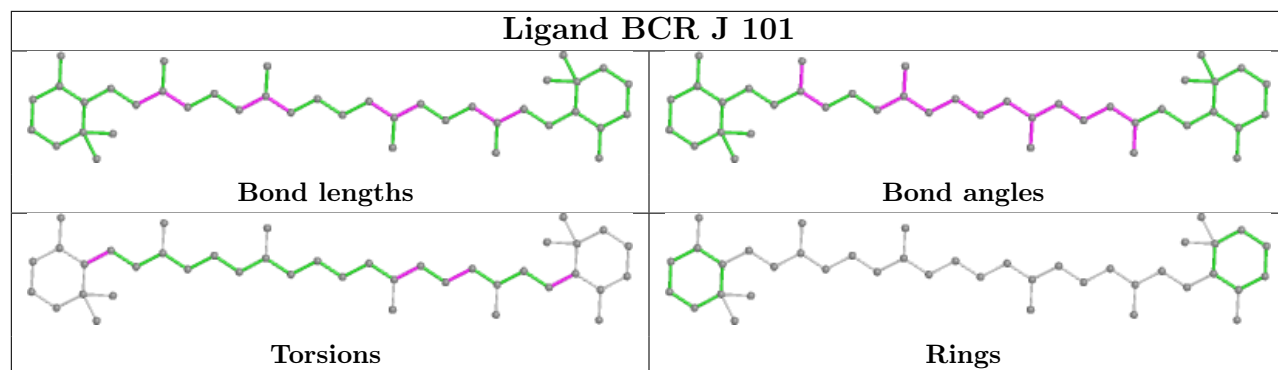
Ligand CLA b 313



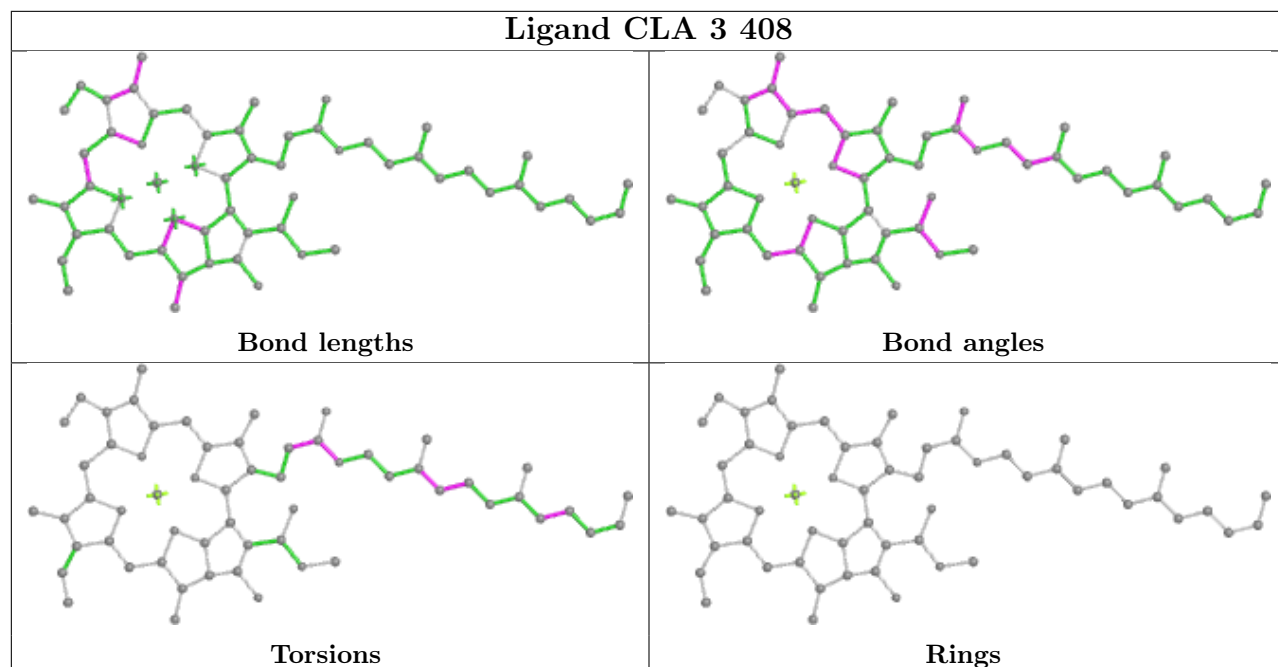
Ligand XAT a 618



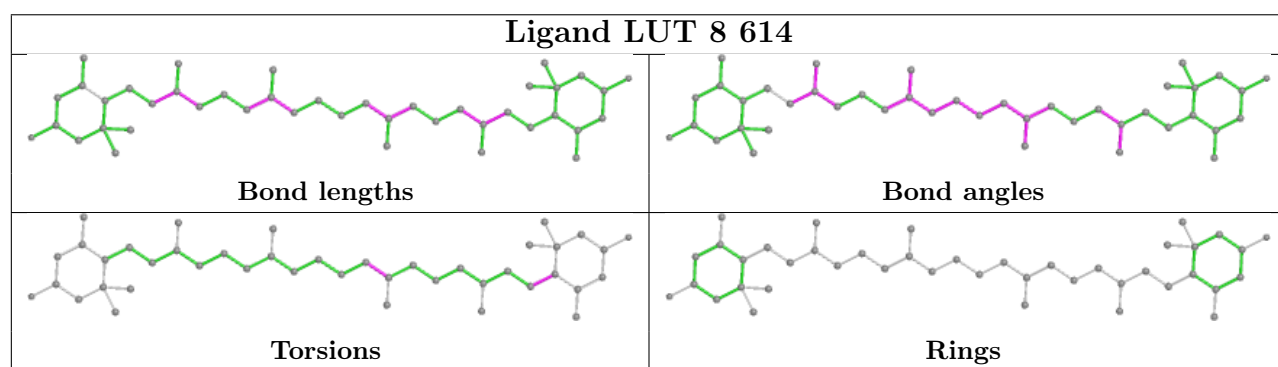
Ligand BCR J 101



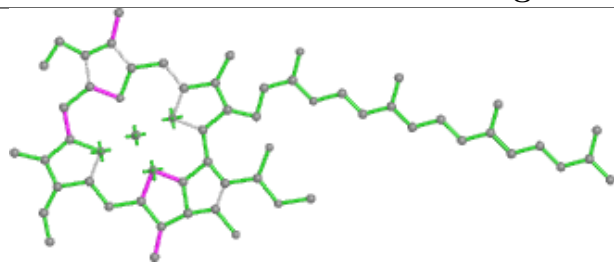
Ligand CLA 3 408



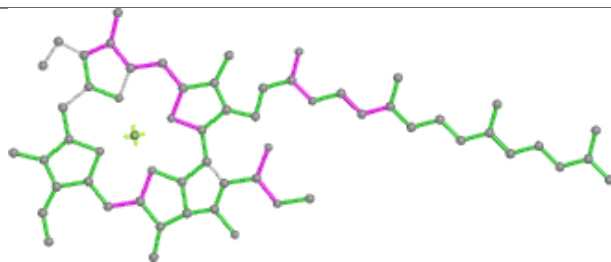
Ligand LUT 8 614



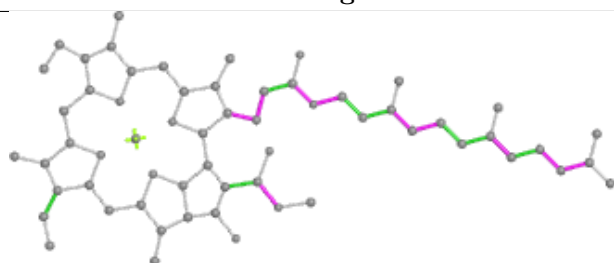
Ligand CLA A 828



Bond lengths



Bond angles

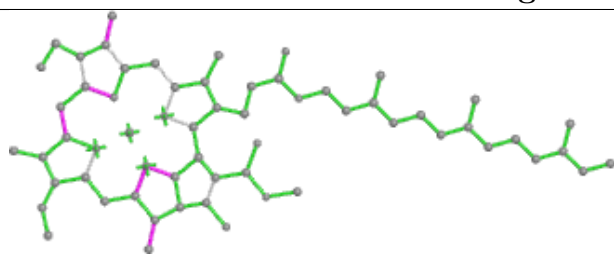


Torsions

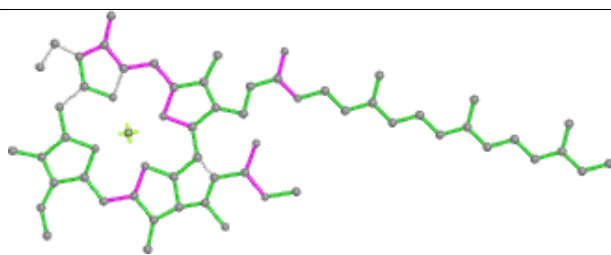


Rings

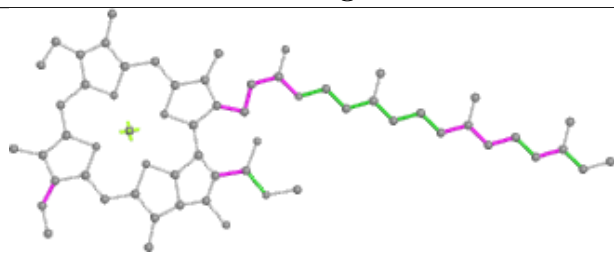
Ligand CLA 1 303



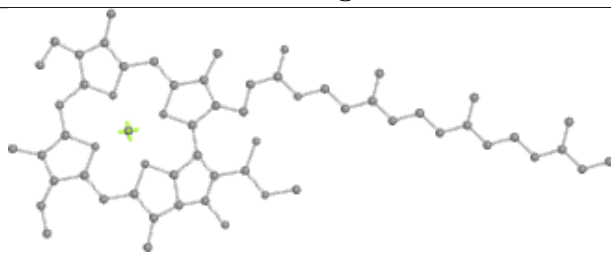
Bond lengths



Bond angles

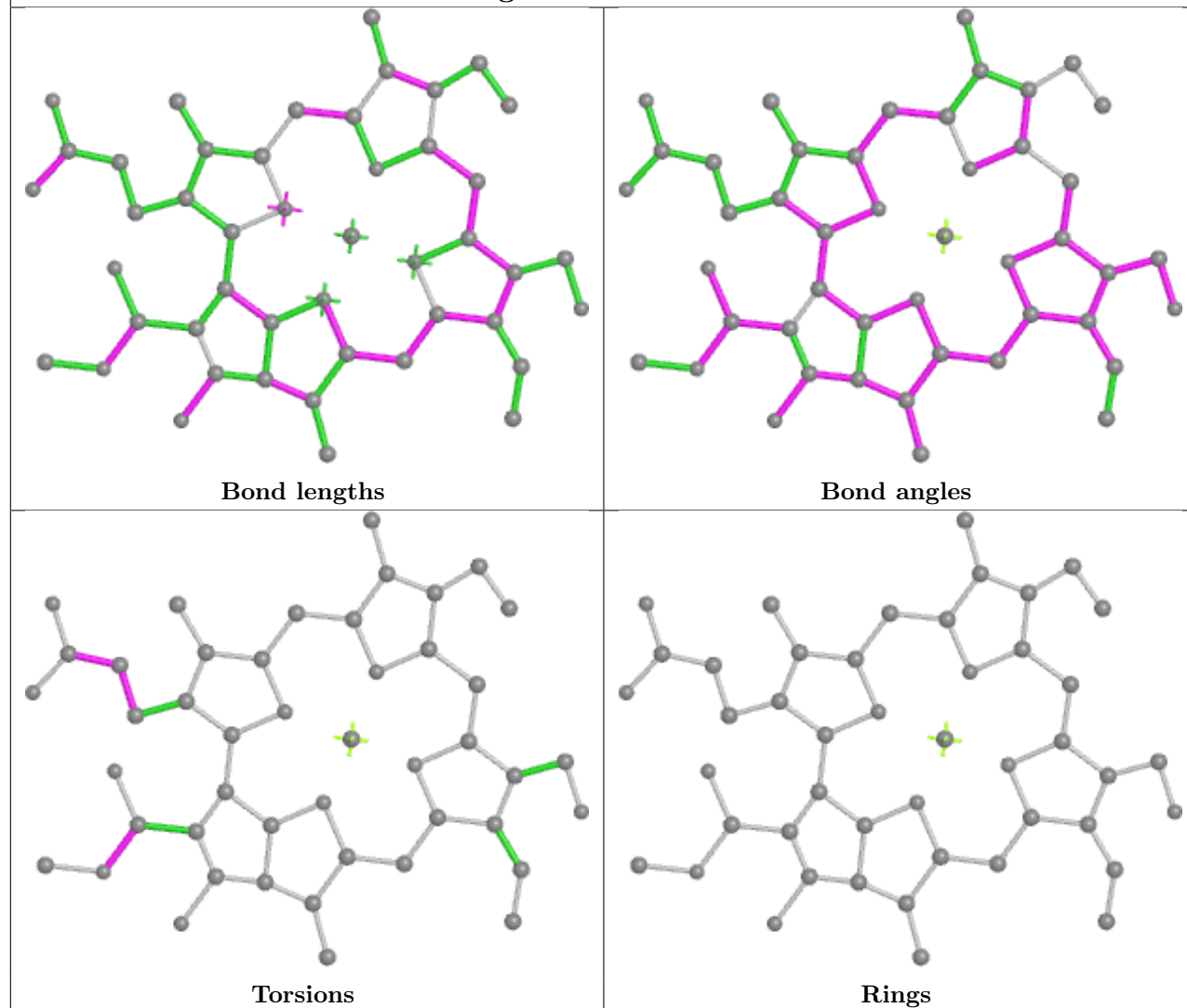


Torsions

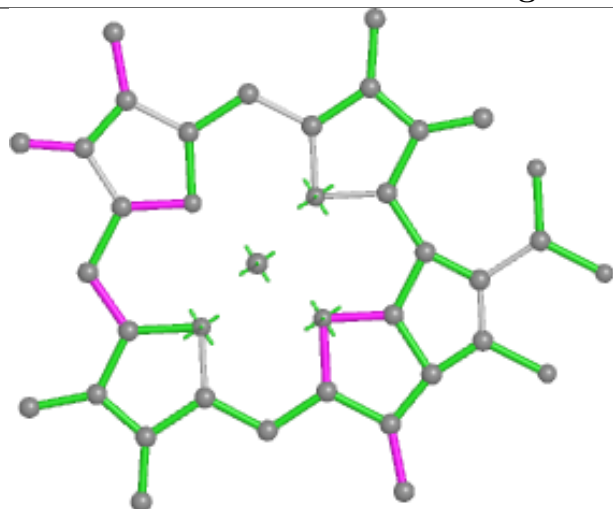


Rings

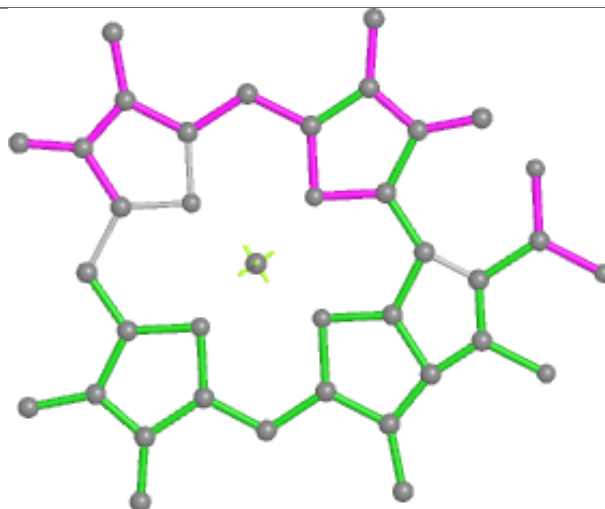
Ligand CHL 5 606



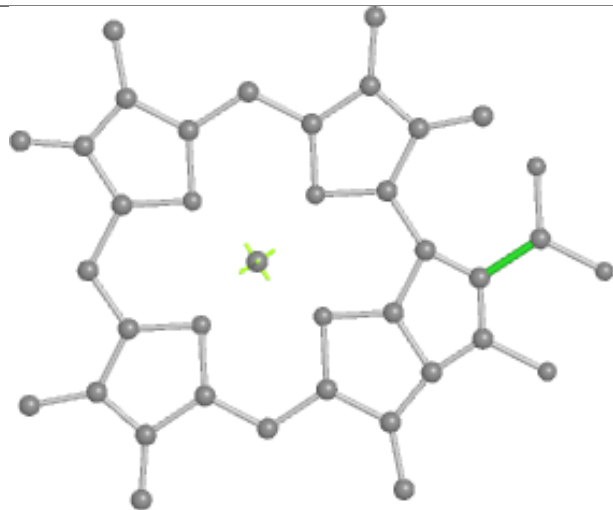
Ligand CLA 1 311



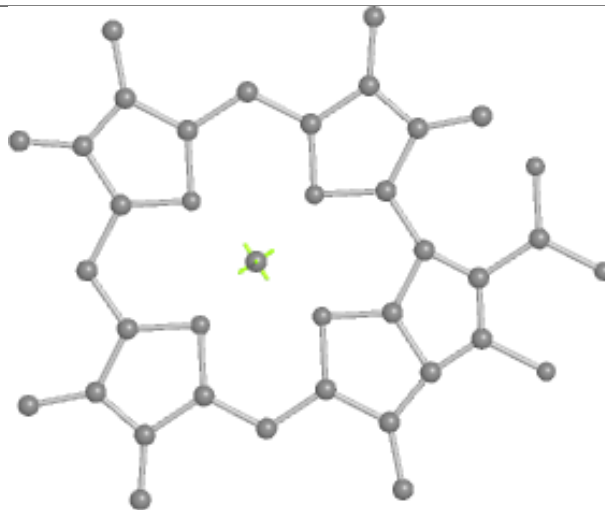
Bond lengths



Bond angles

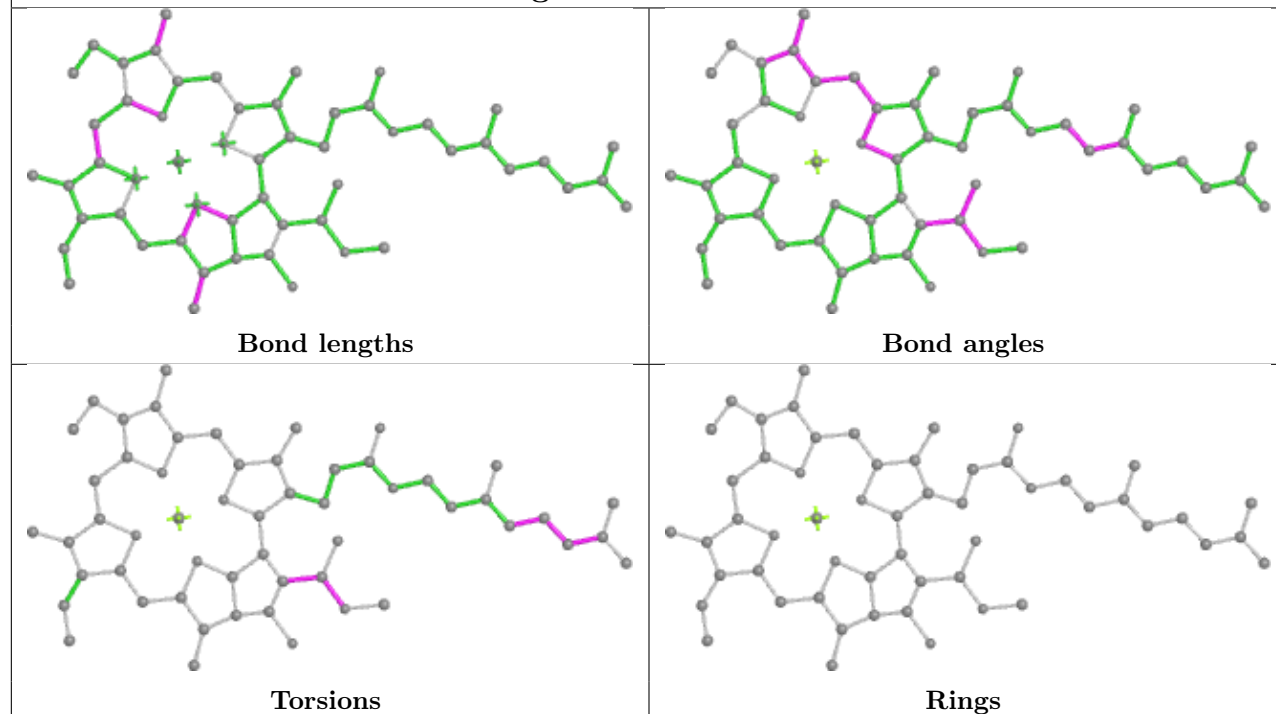


Torsions

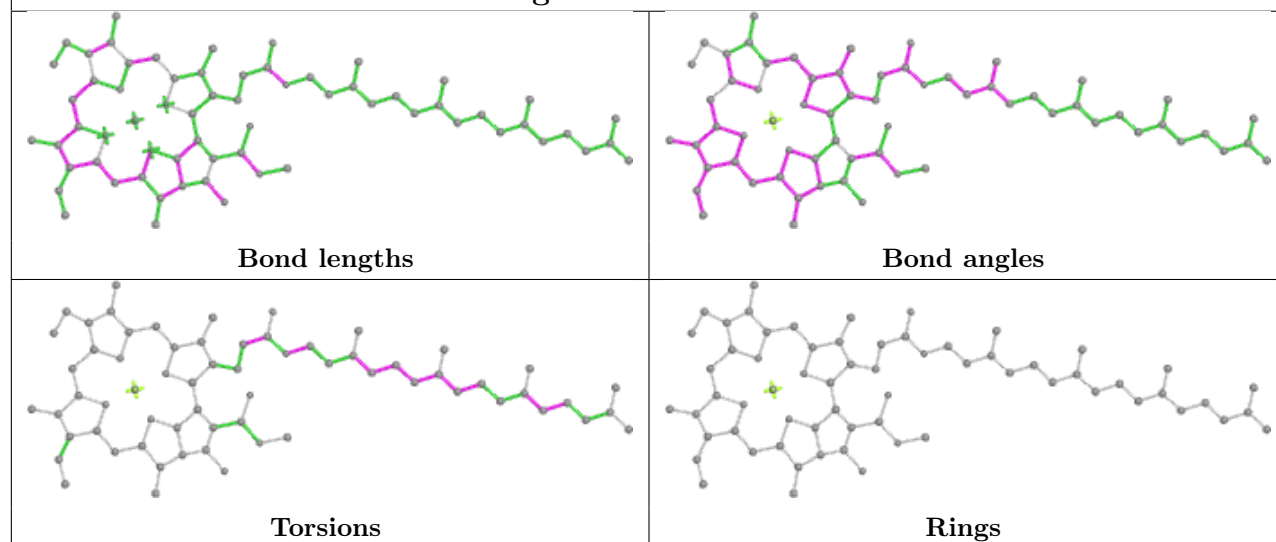


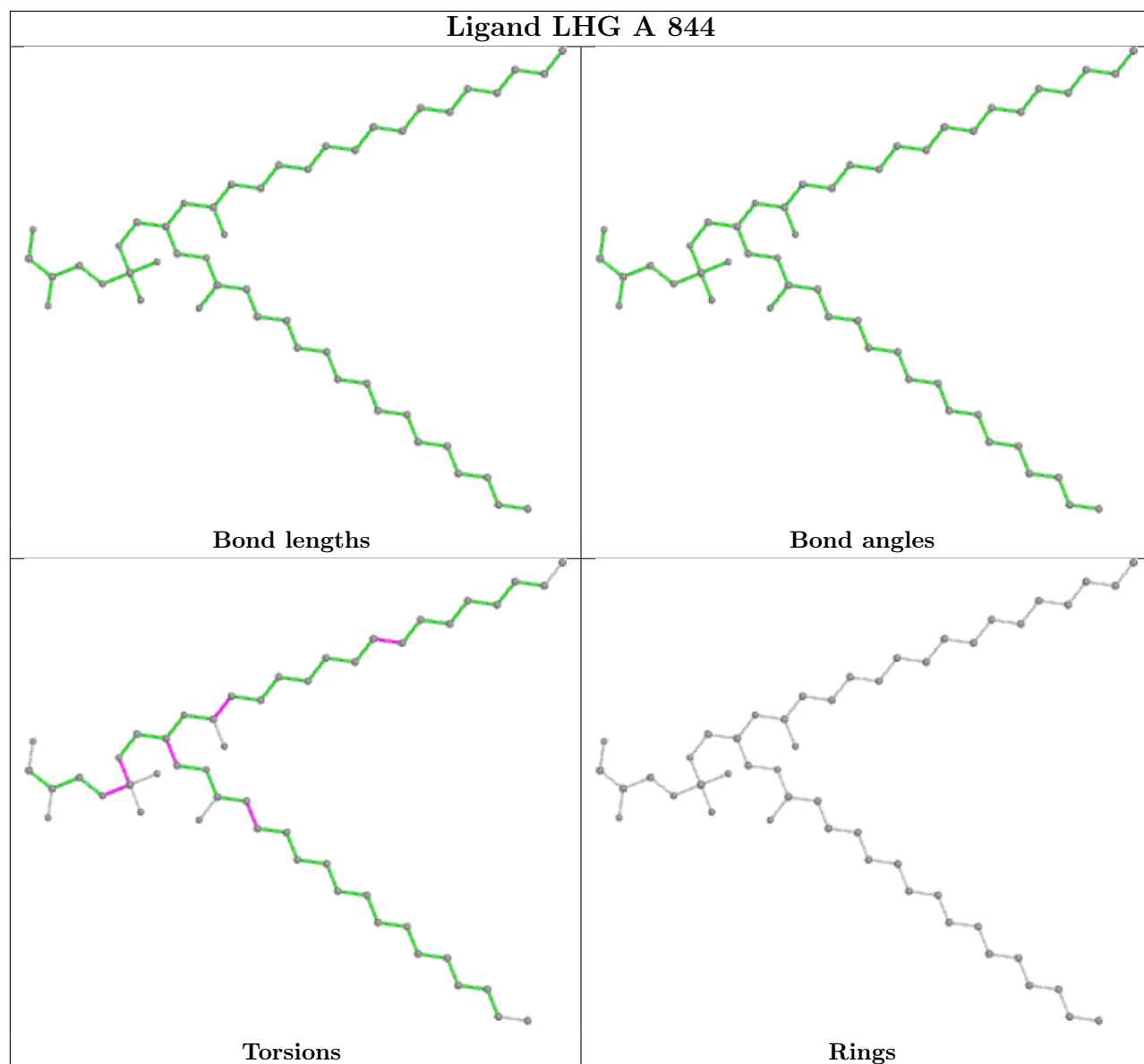
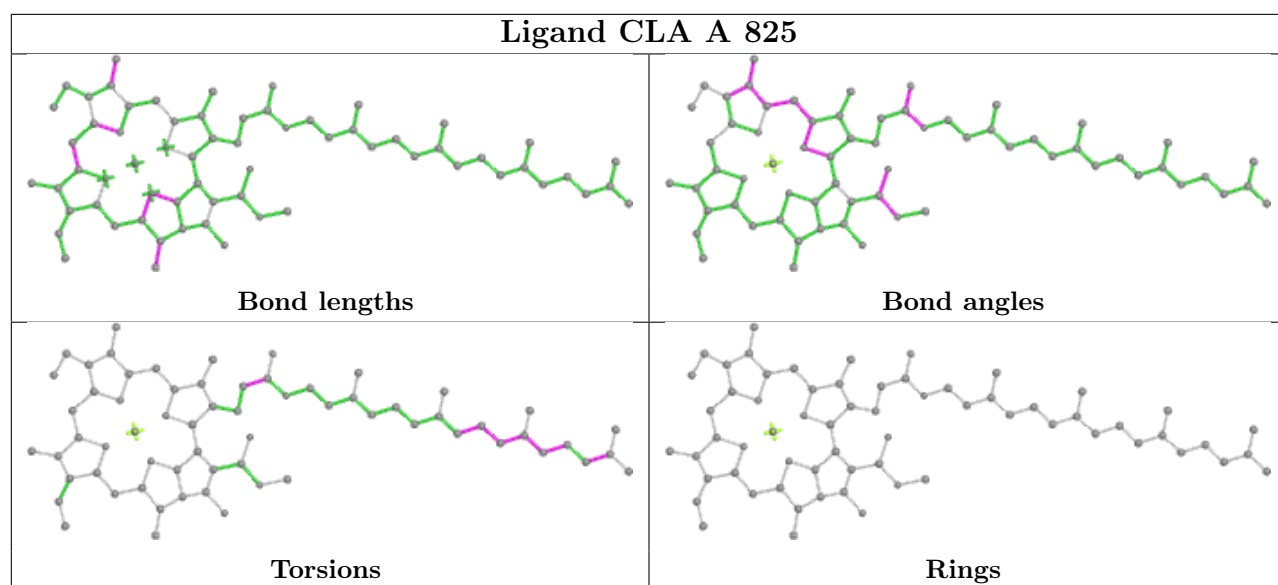
Rings

Ligand CLA A 831

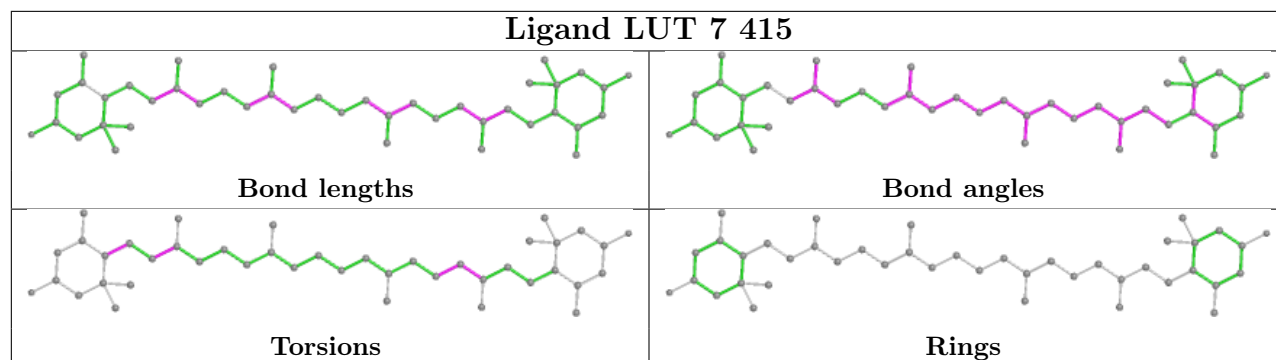


Ligand CLA B 801

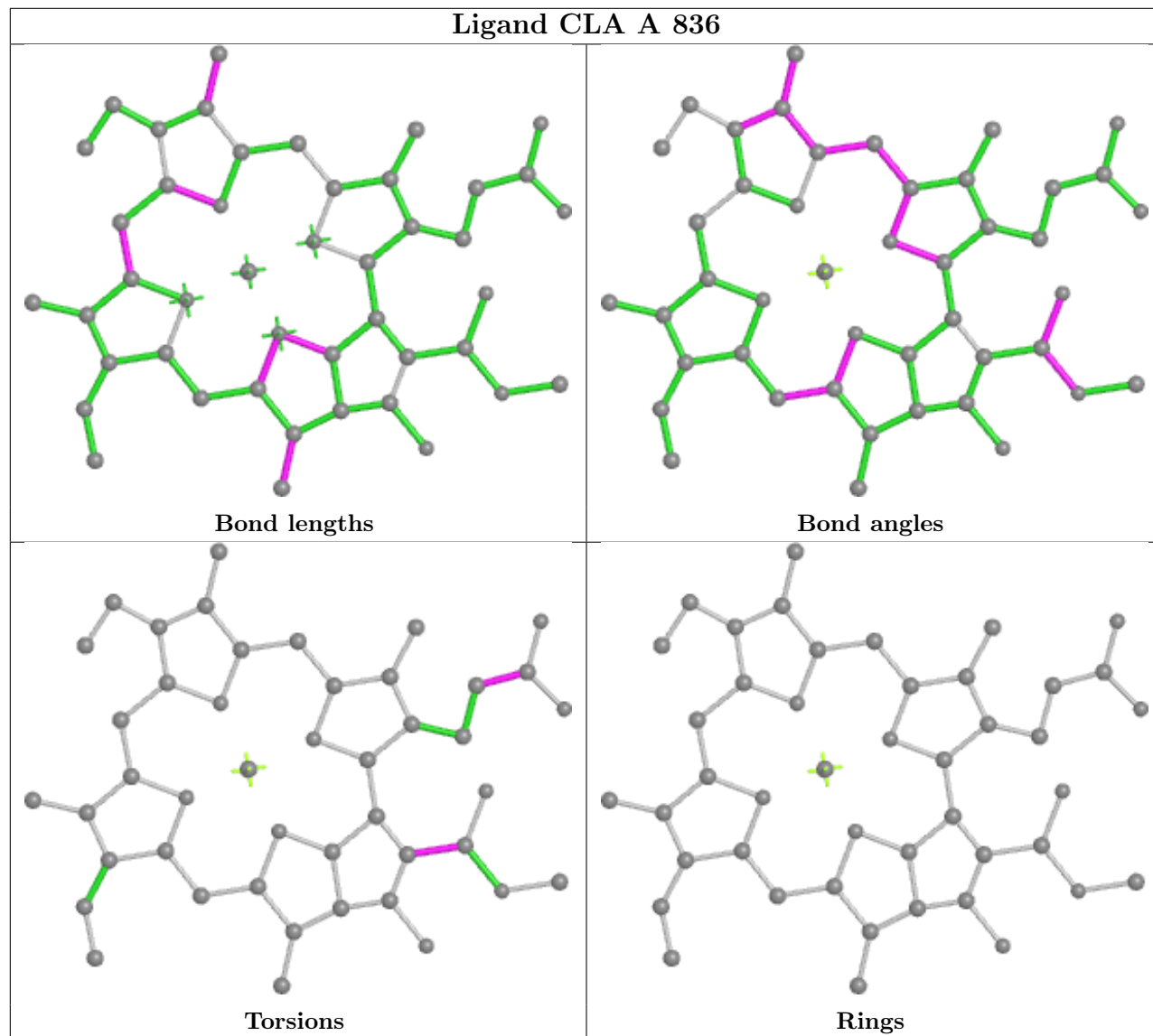




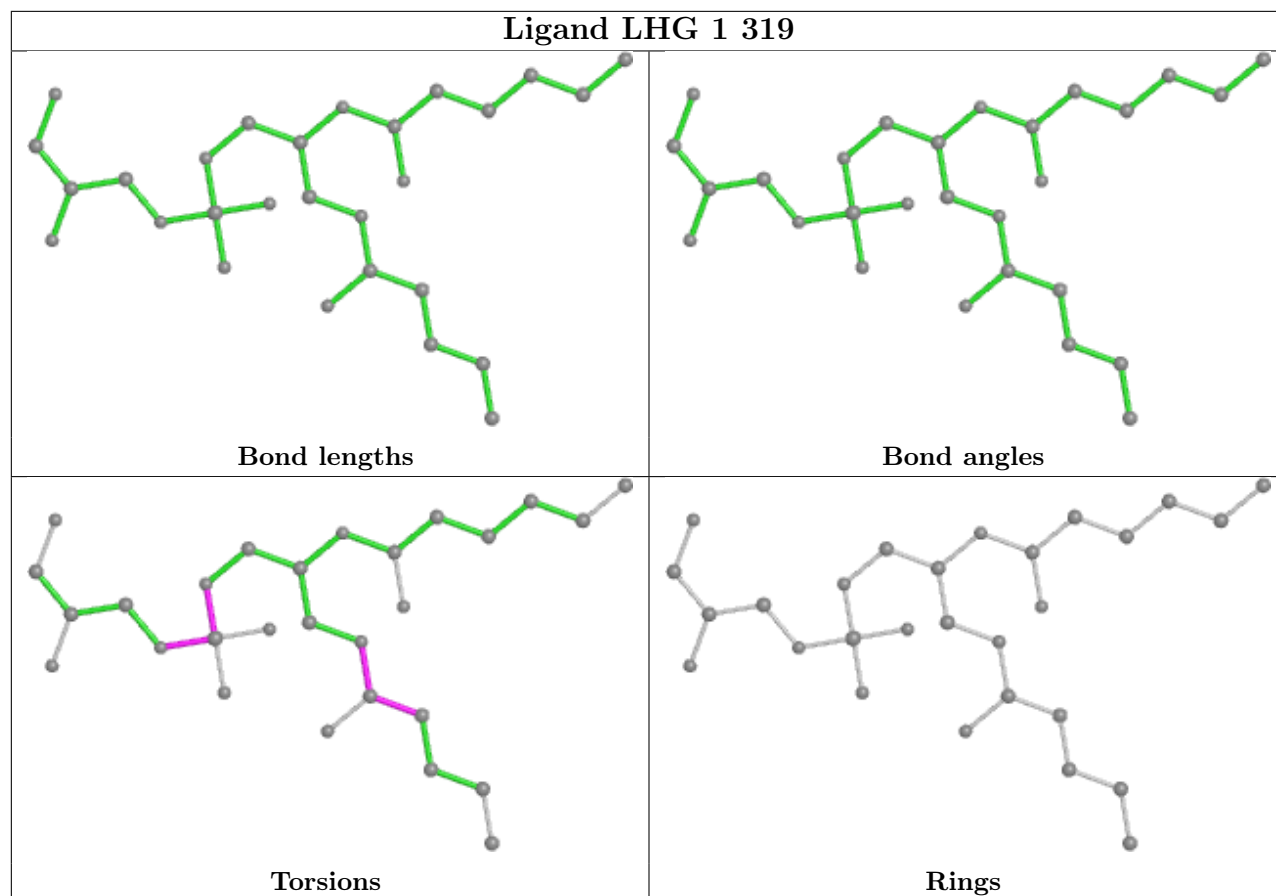
Ligand LUT 7 415



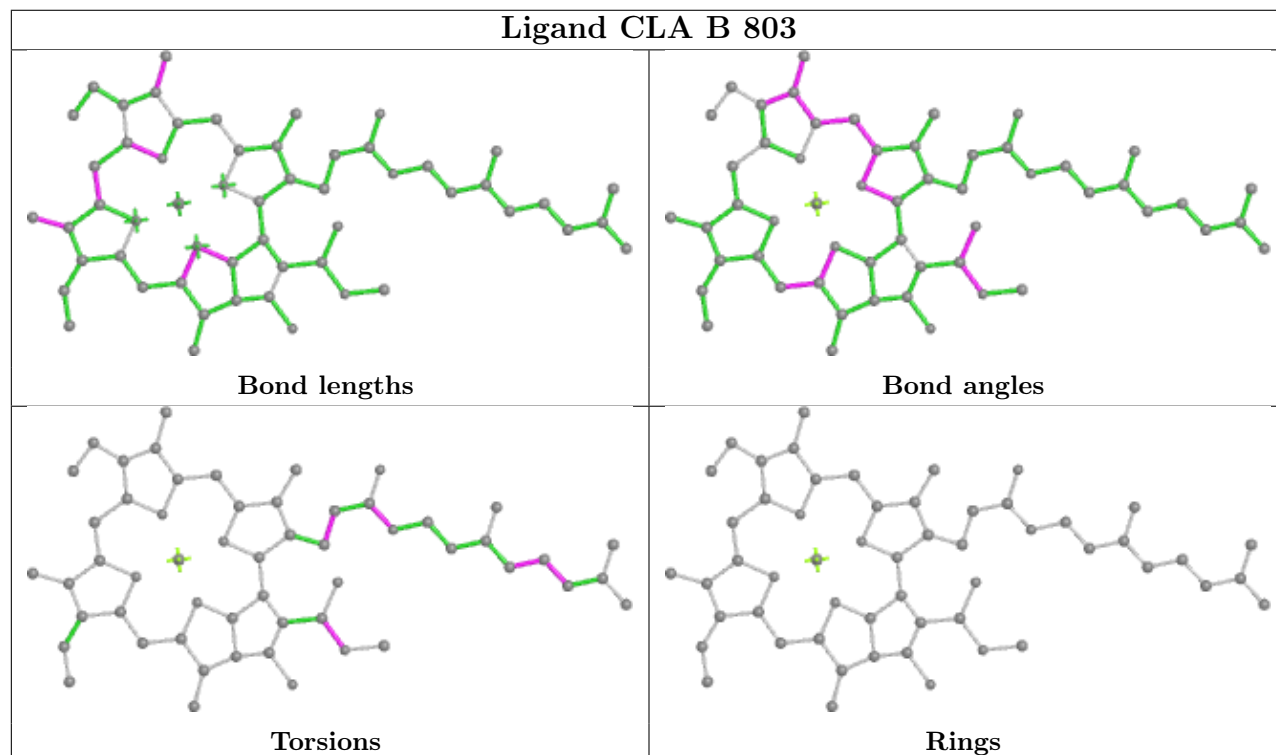
Ligand CLA A 836



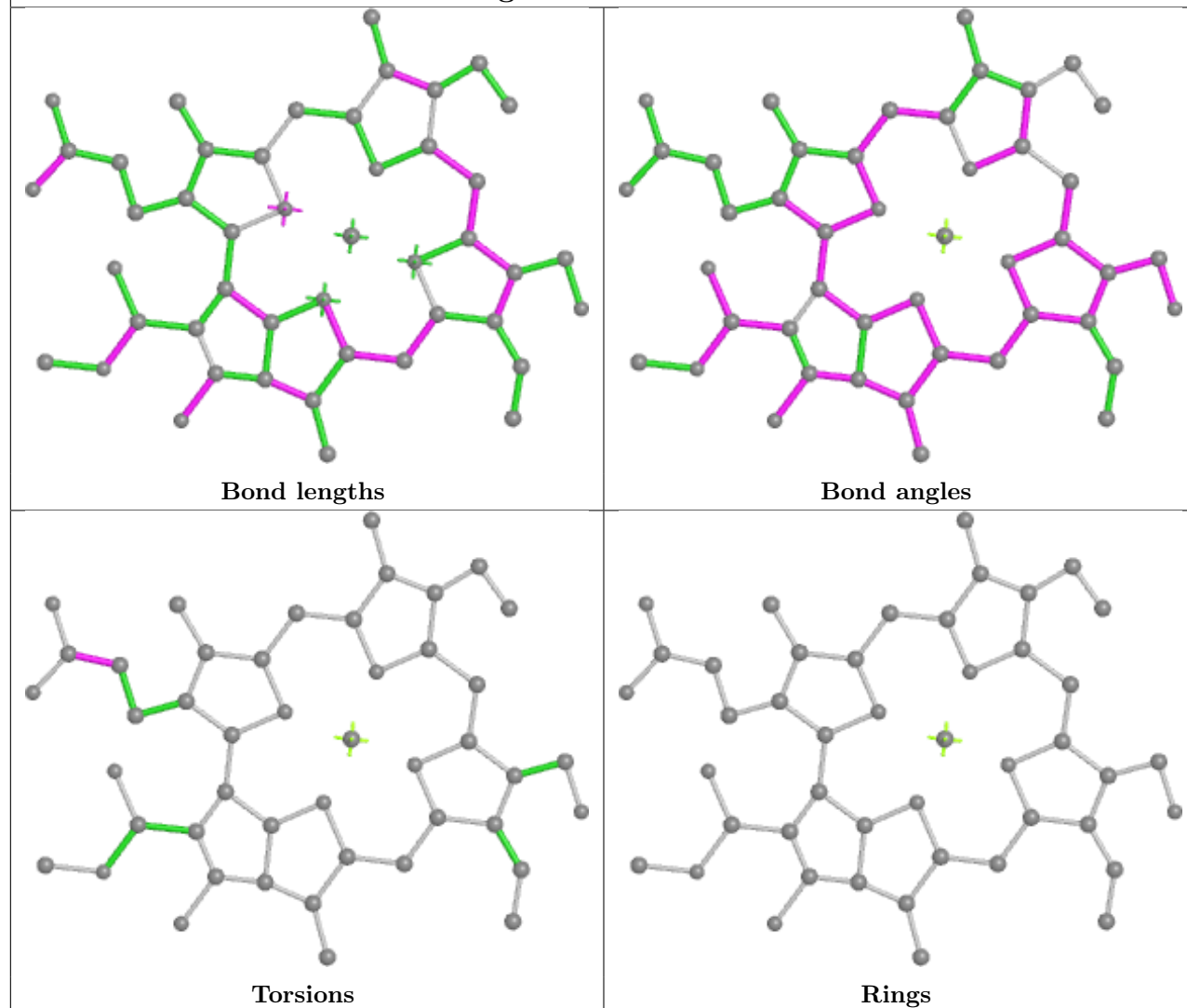
Ligand LHG 1 319



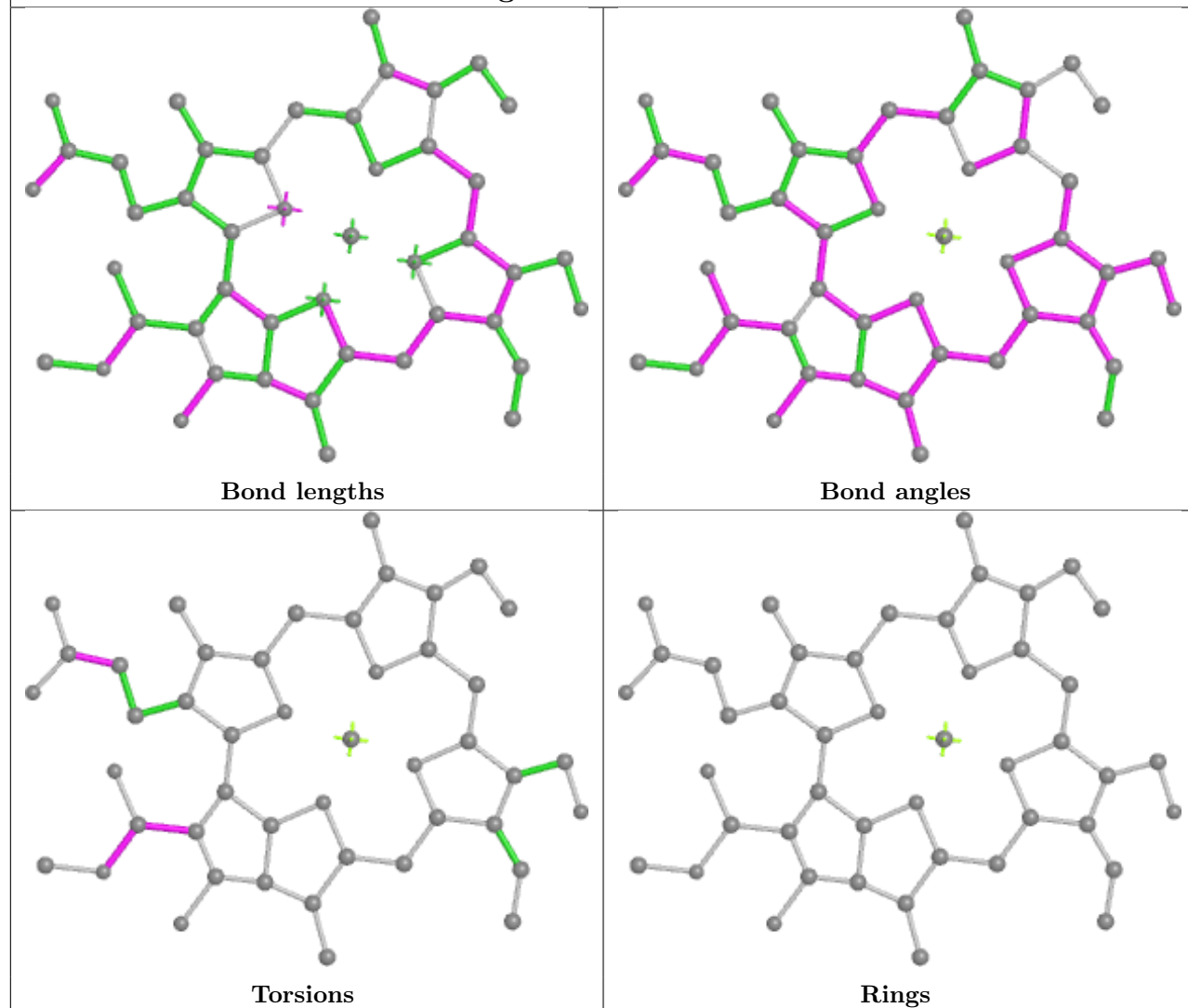
Ligand CLA B 803



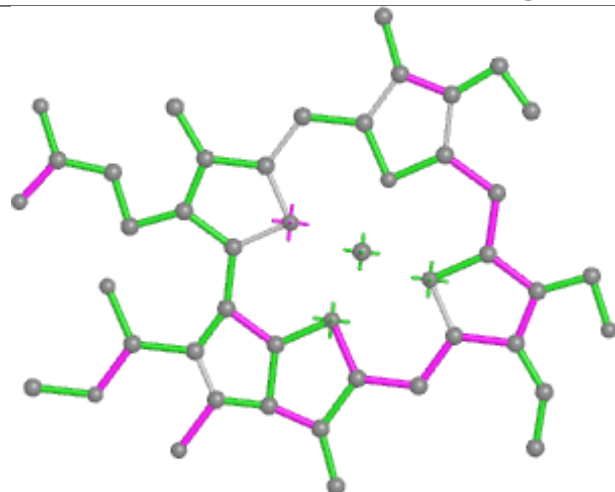
Ligand CHL 2 606



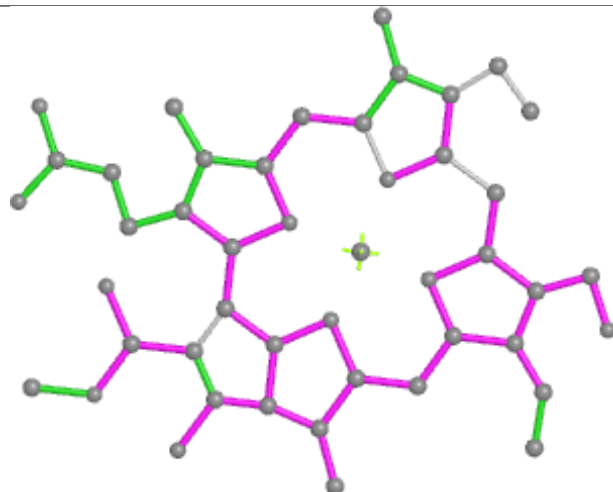
Ligand CHL a 606



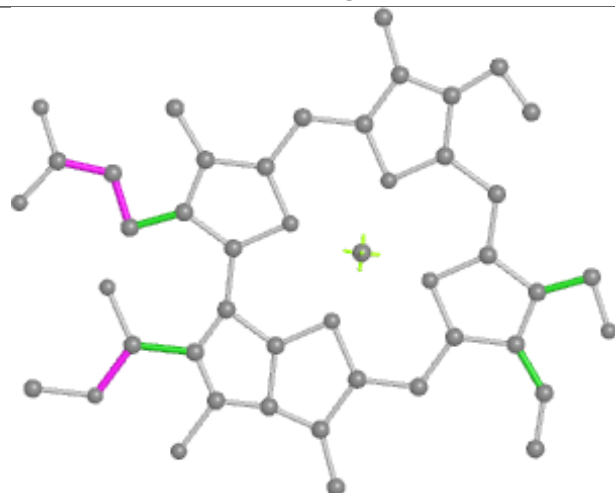
Ligand CHL 6 606



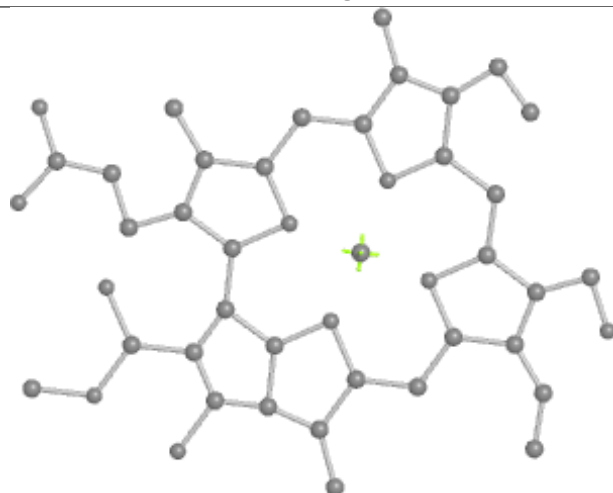
Bond lengths



Bond angles

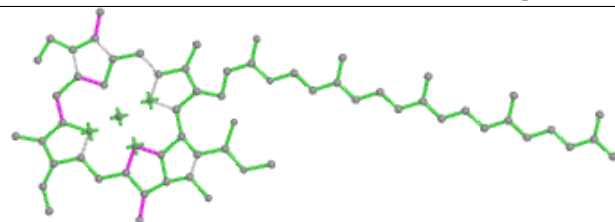


Torsions

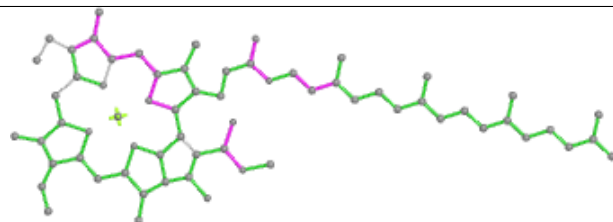


Rings

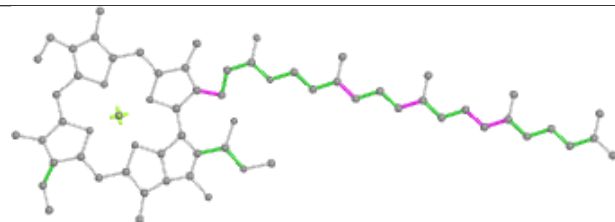
Ligand CLA B 835



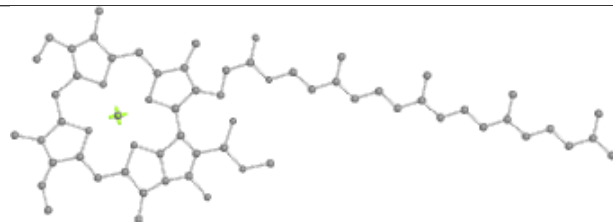
Bond lengths



Bond angles

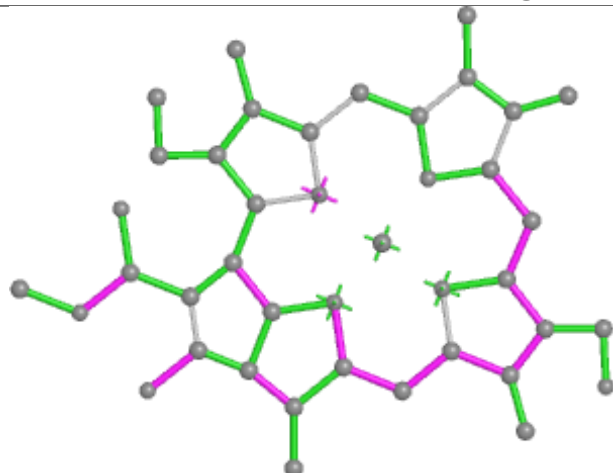


Torsions

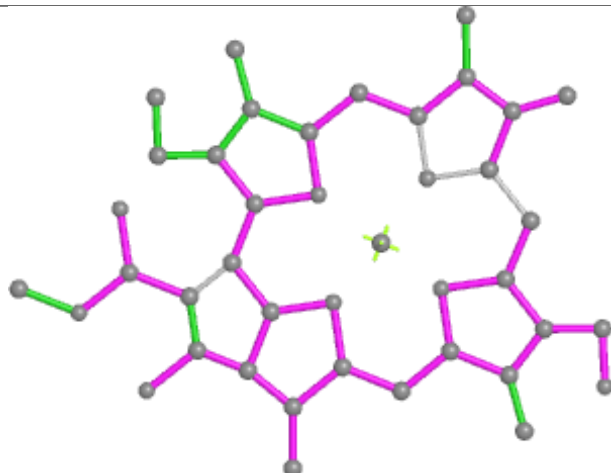


Rings

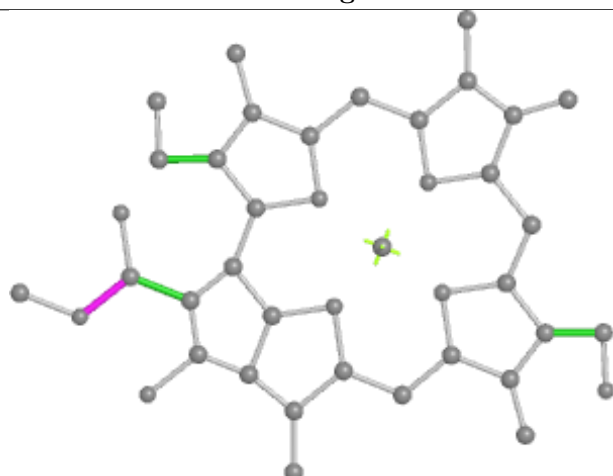
Ligand CHL 4 605



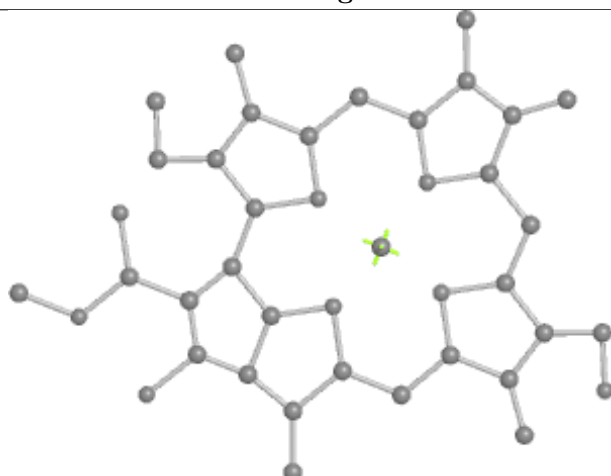
Bond lengths



Bond angles

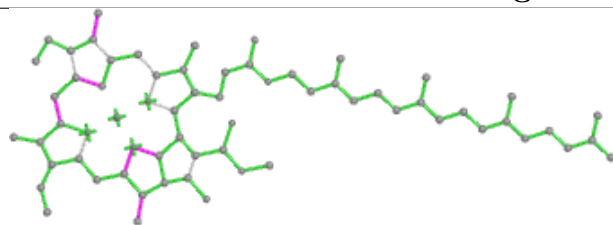


Torsions

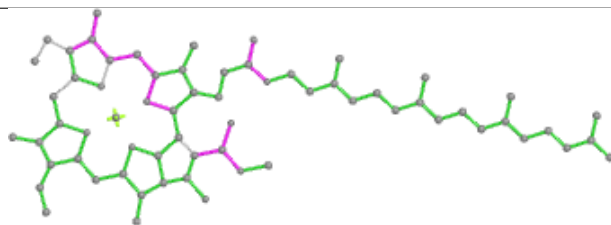


Rings

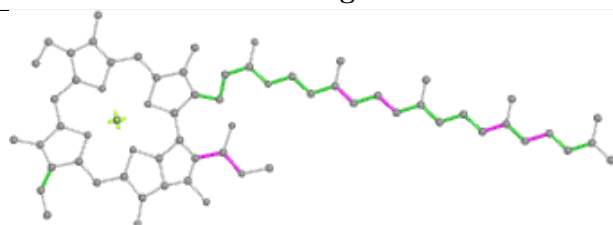
Ligand CLA A 834



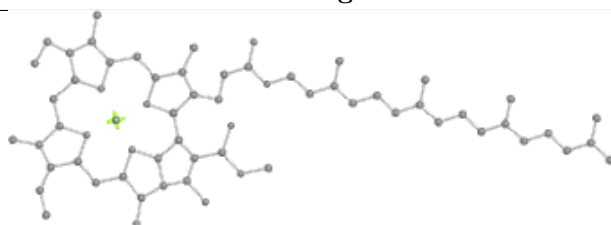
Bond lengths



Bond angles

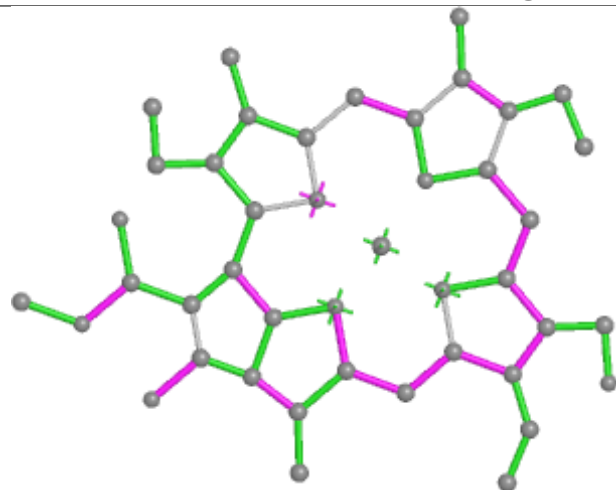


Torsions

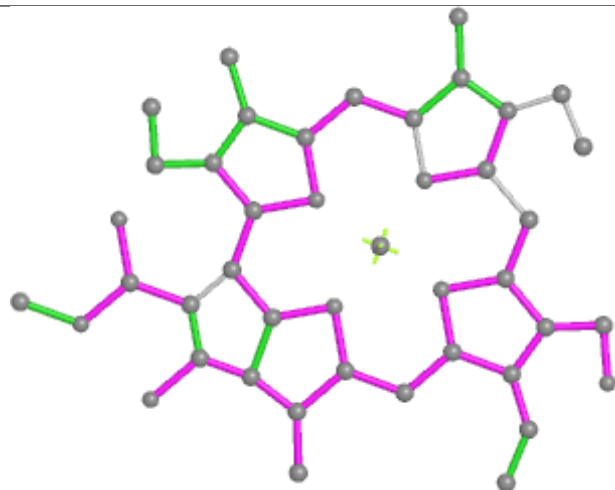


Rings

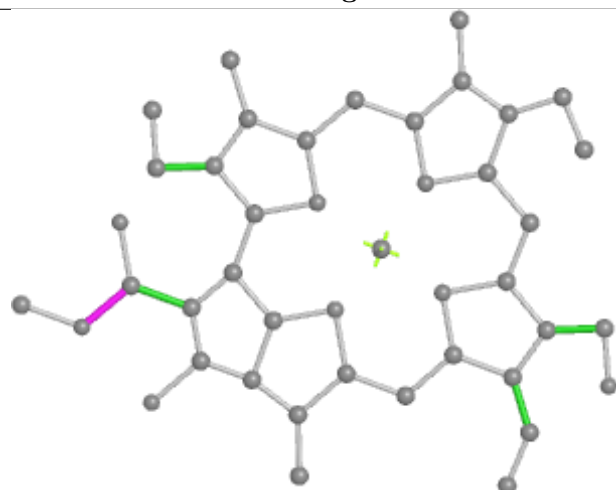
Ligand CHL 9 601



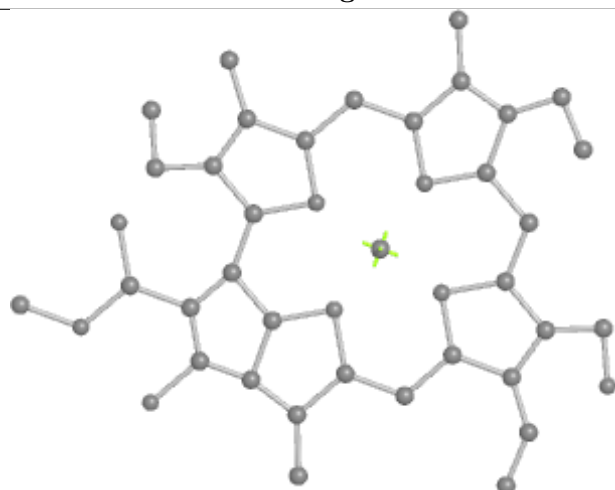
Bond lengths



Bond angles

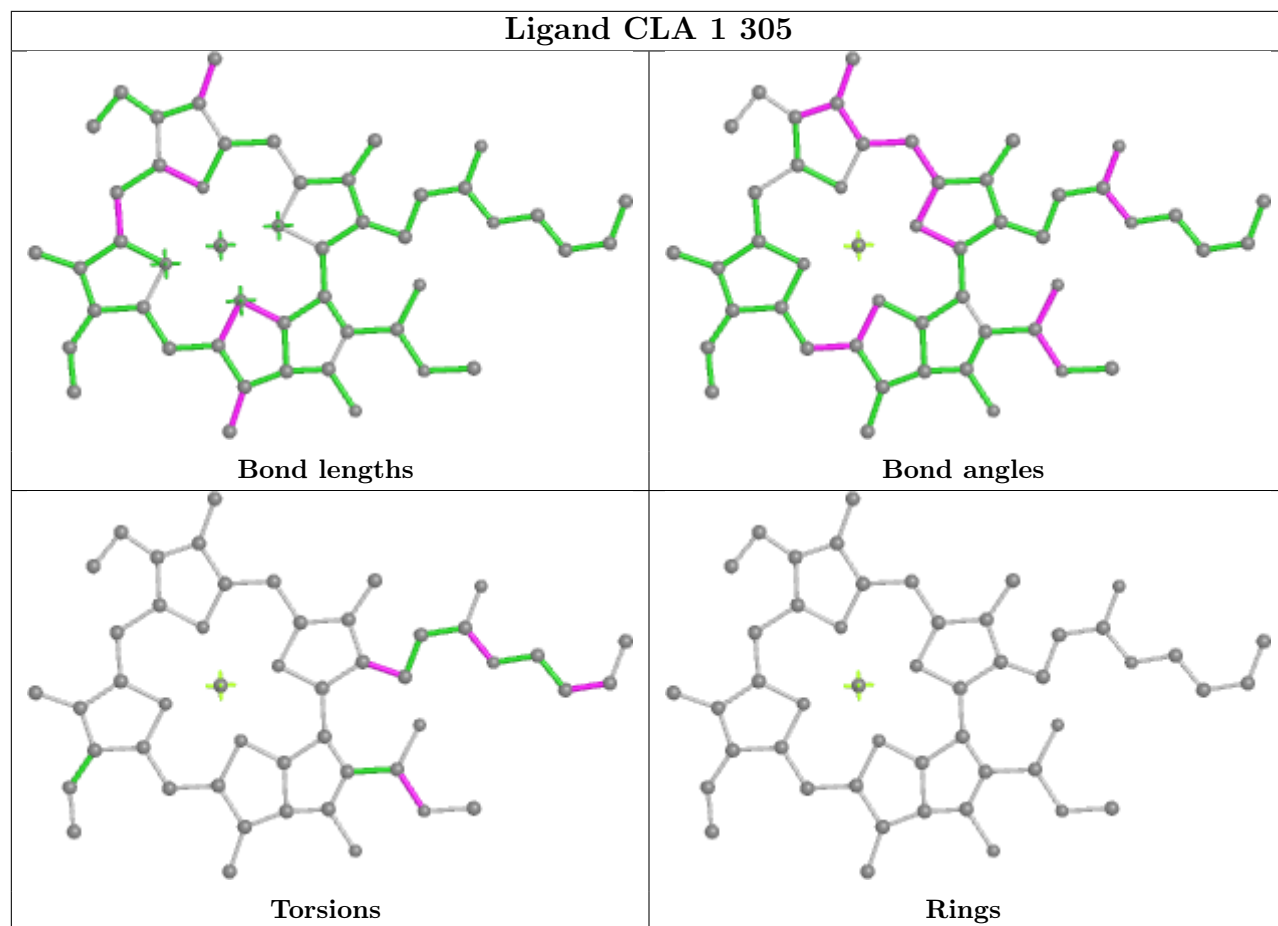


Torsions

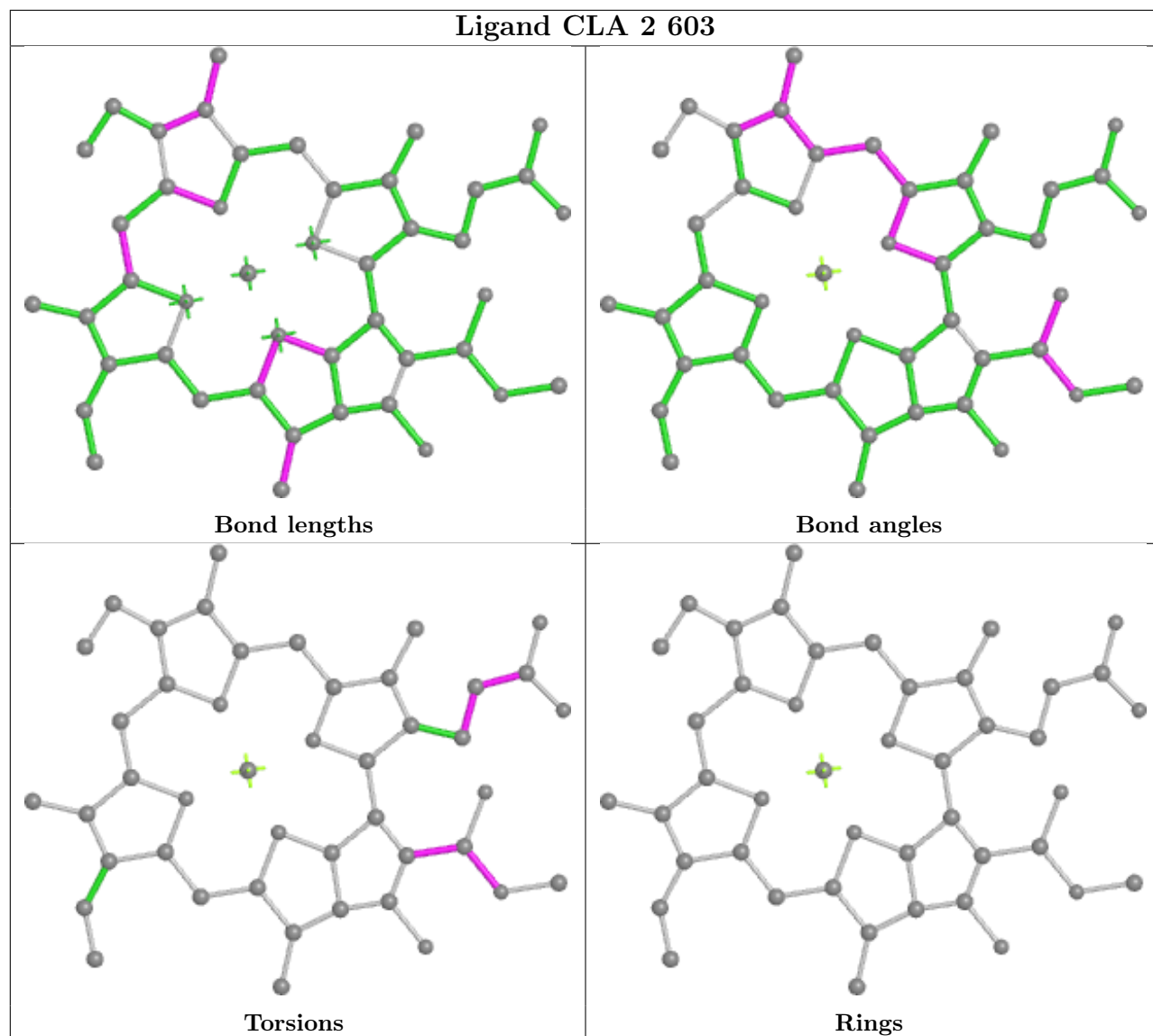


Rings

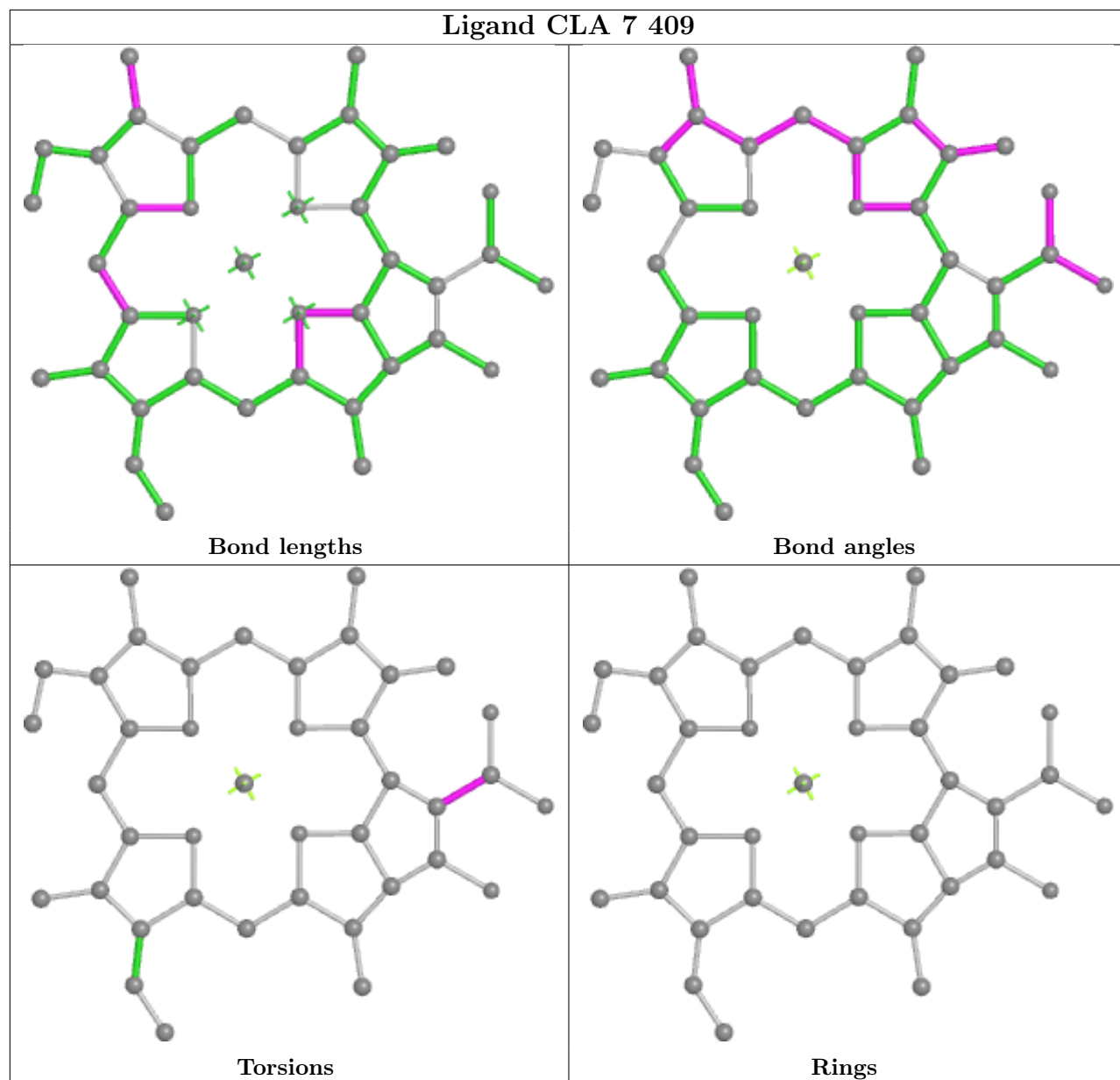
Ligand CLA 1 305



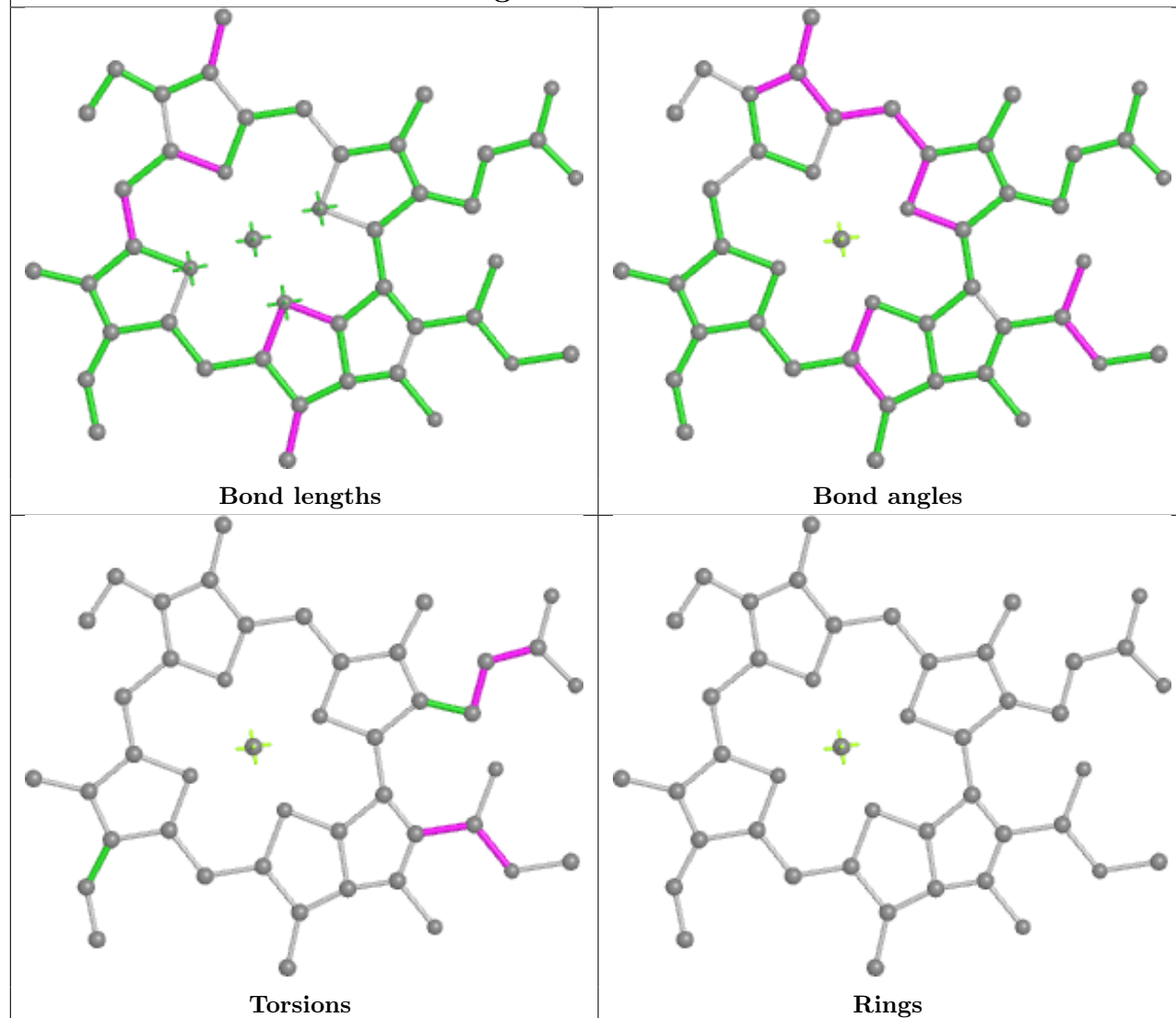
Ligand CLA 2 603



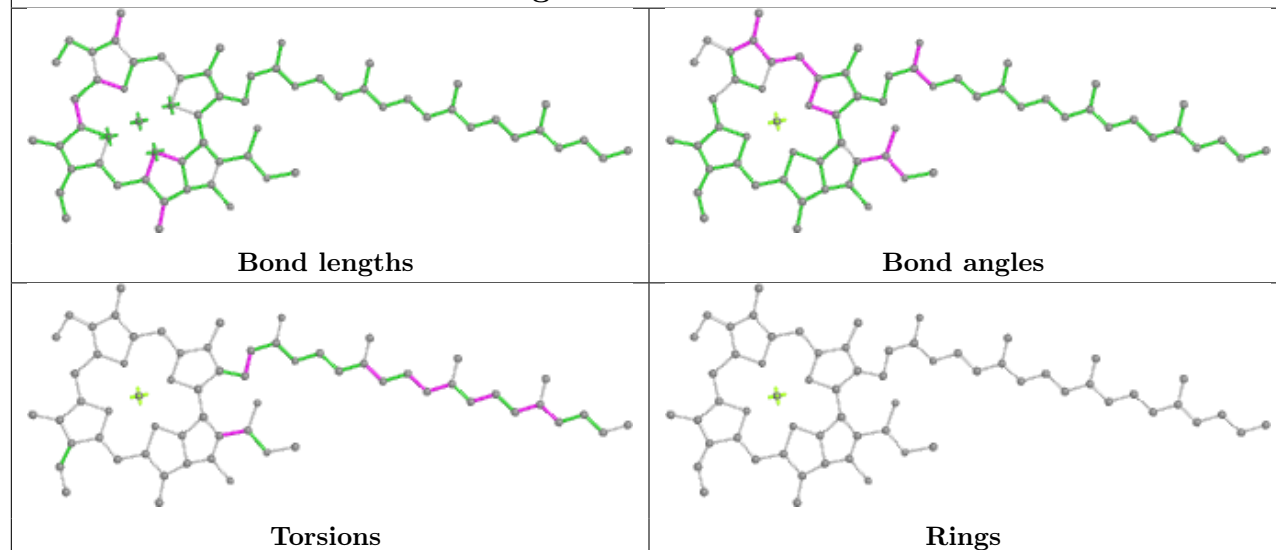
Ligand CLA 7 409



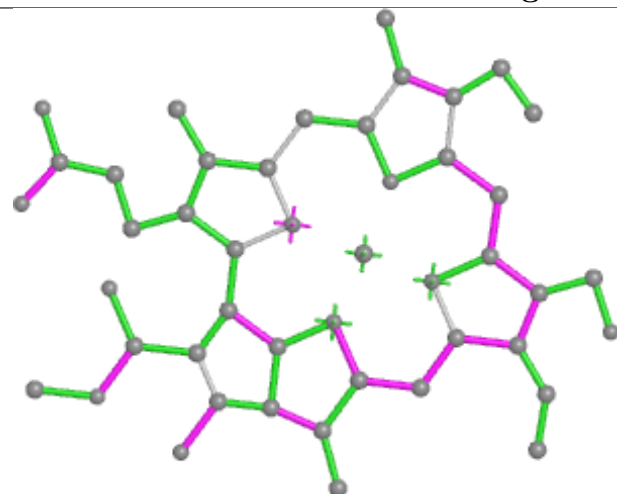
Ligand CLA 6 603



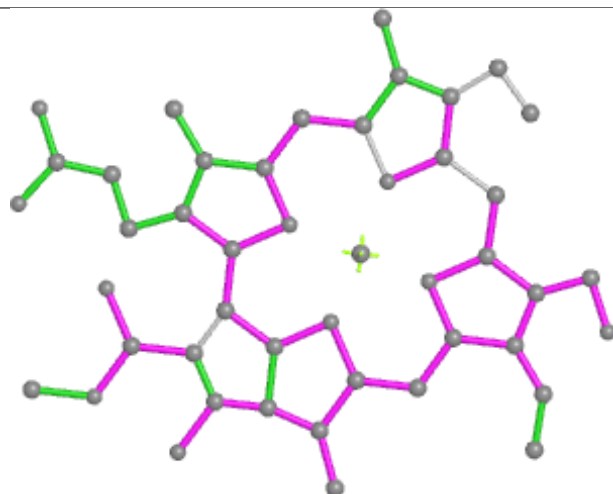
Ligand CLA B 806



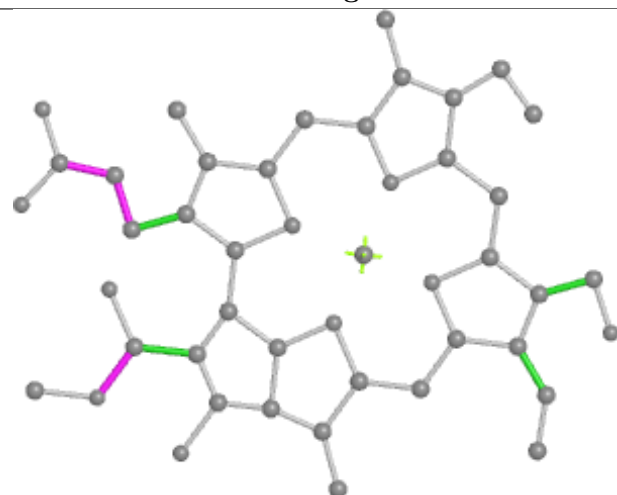
Ligand CHL 9 608



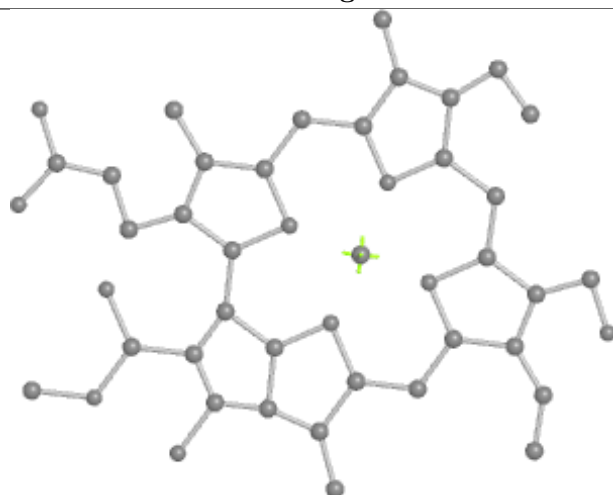
Bond lengths



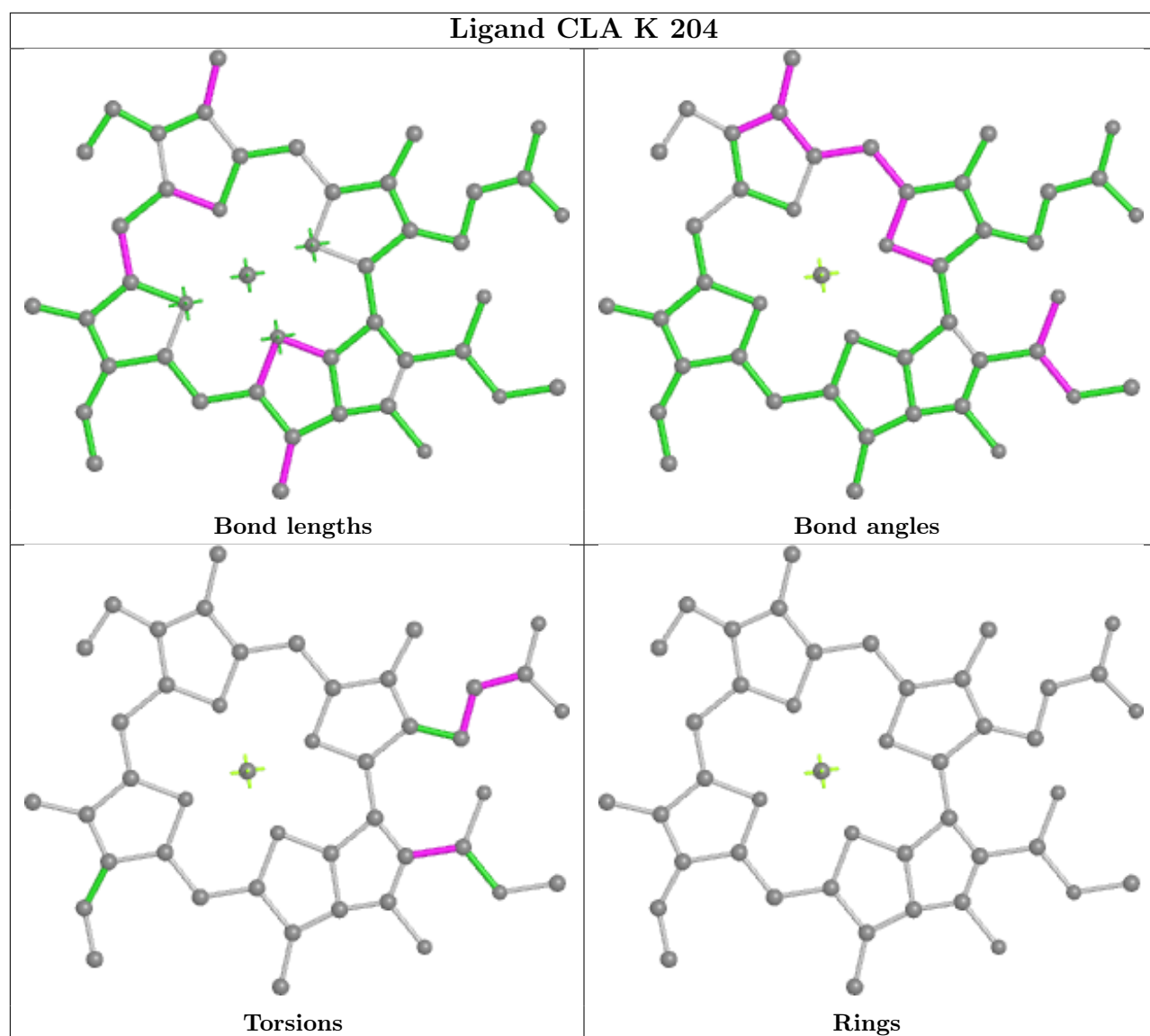
Bond angles



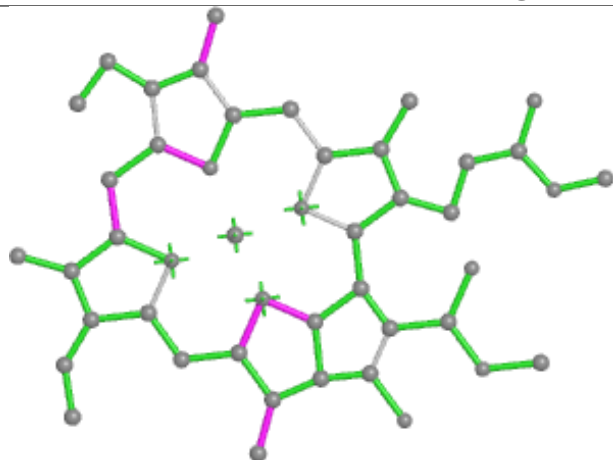
Torsions



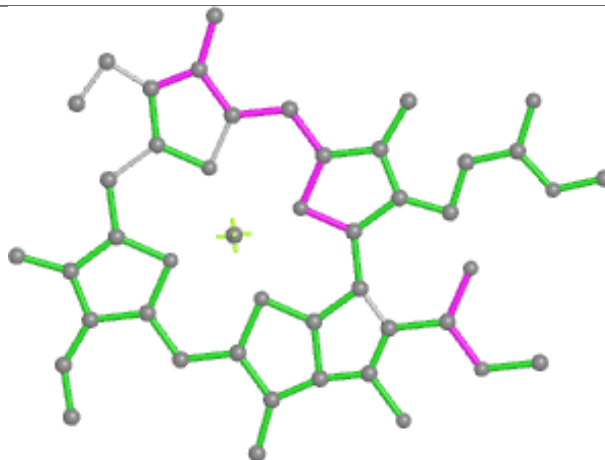
Rings



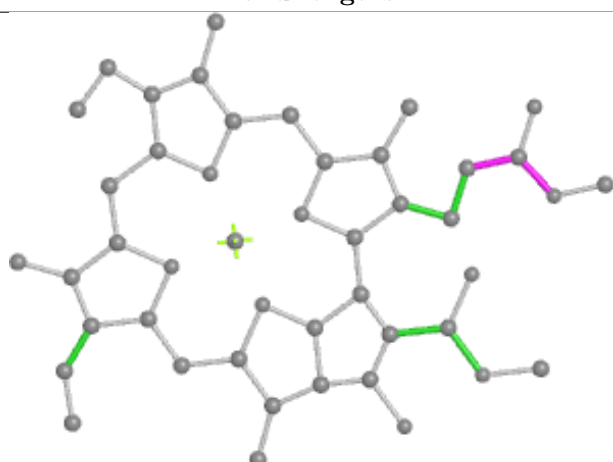
Ligand CLA K 201



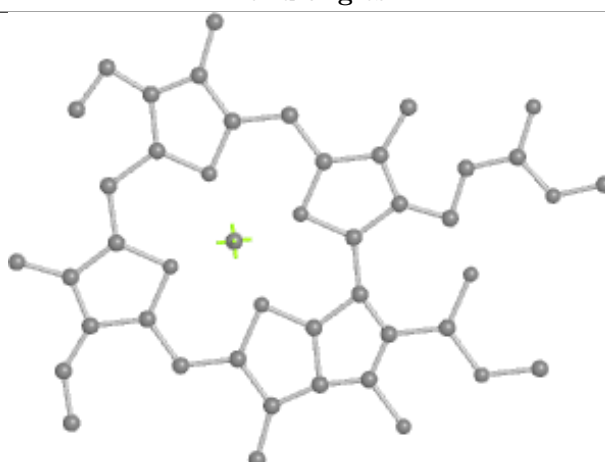
Bond lengths



Bond angles

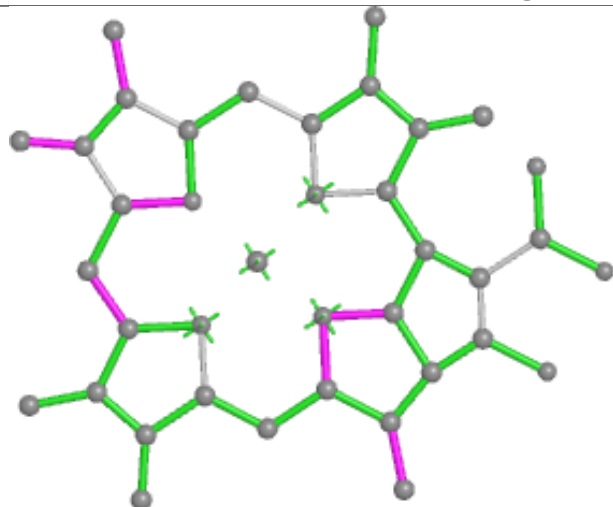


Torsions

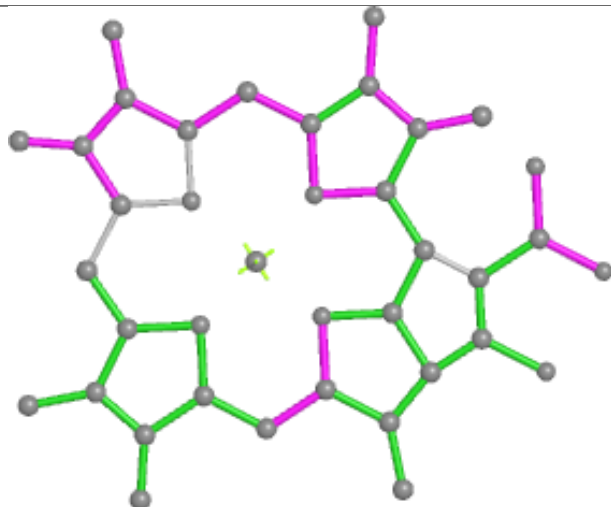


Rings

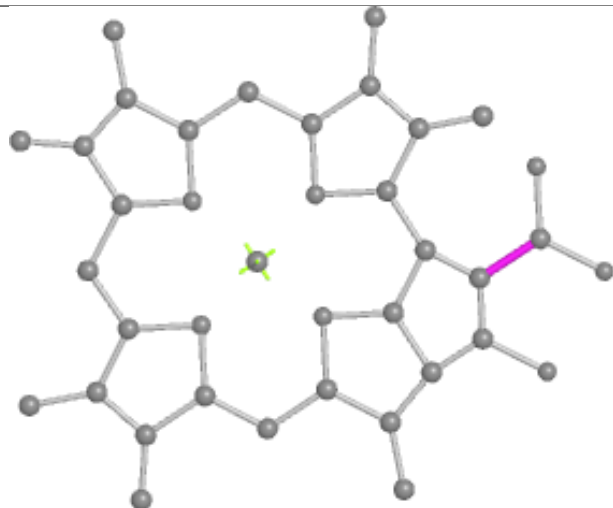
Ligand CLA 1 314



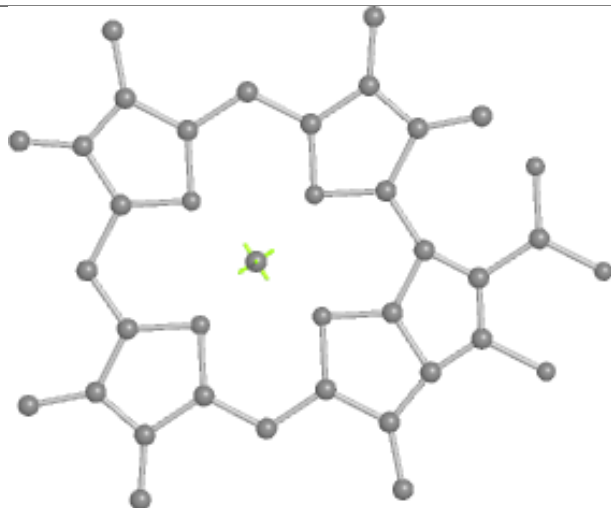
Bond lengths



Bond angles

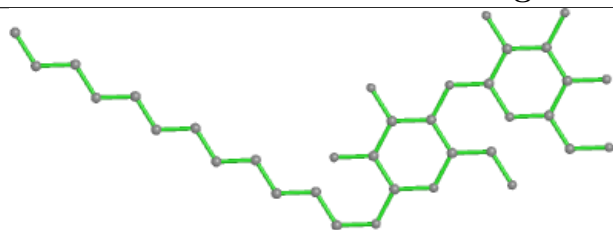


Torsions

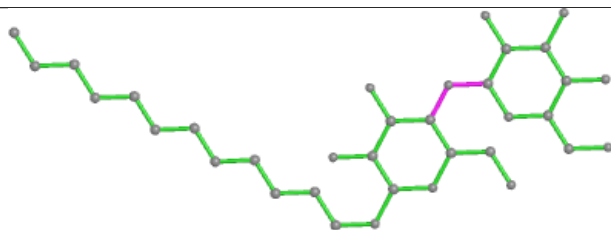


Rings

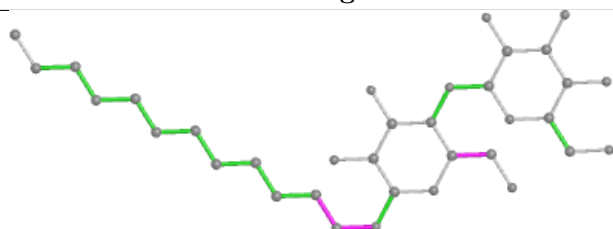
Ligand LMU 3 420



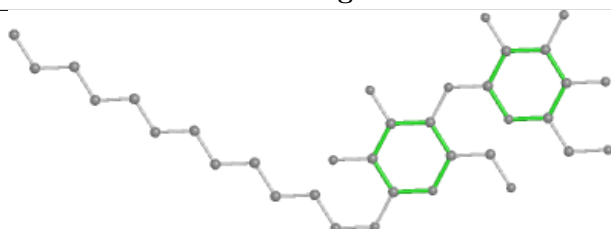
Bond lengths



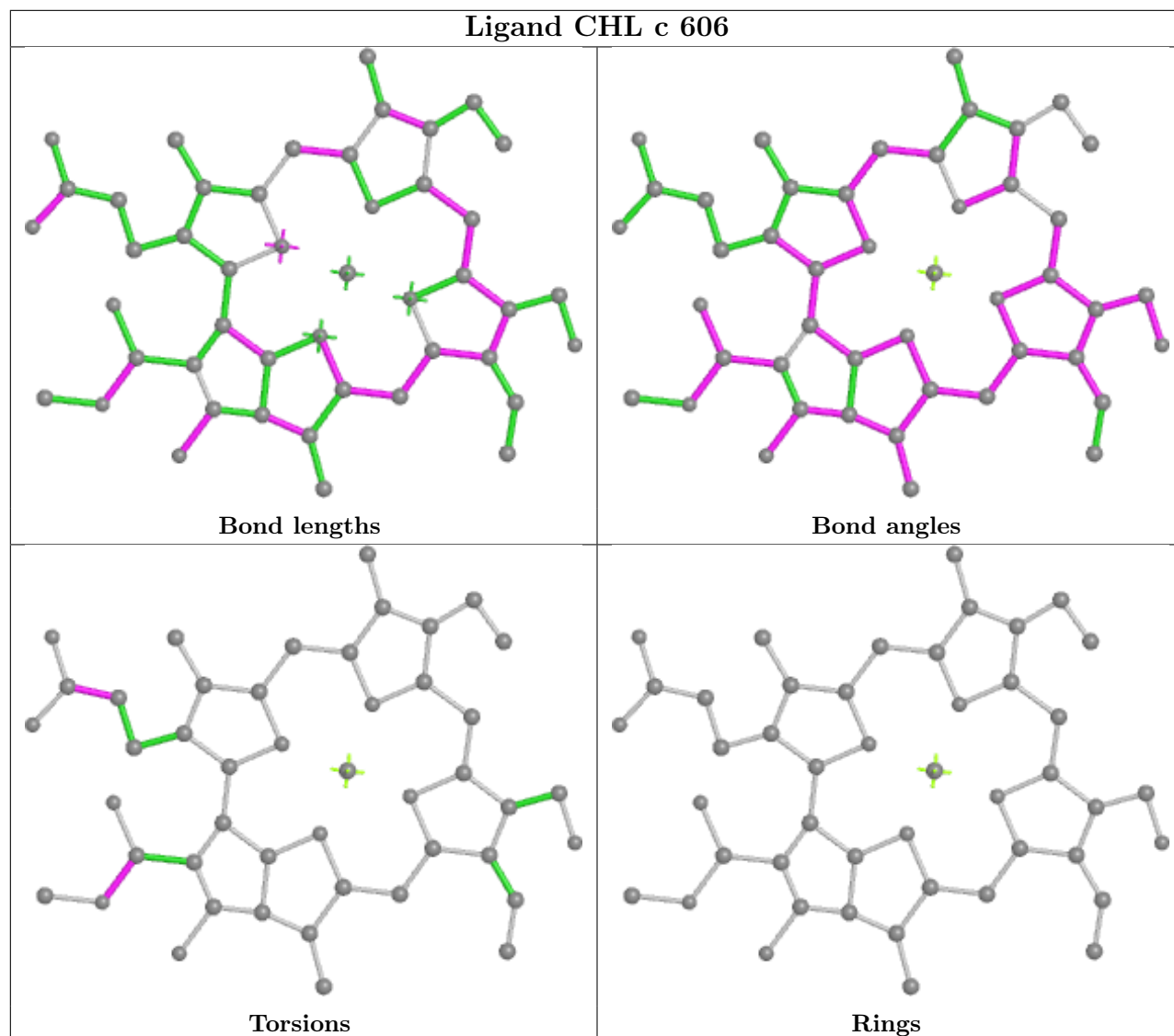
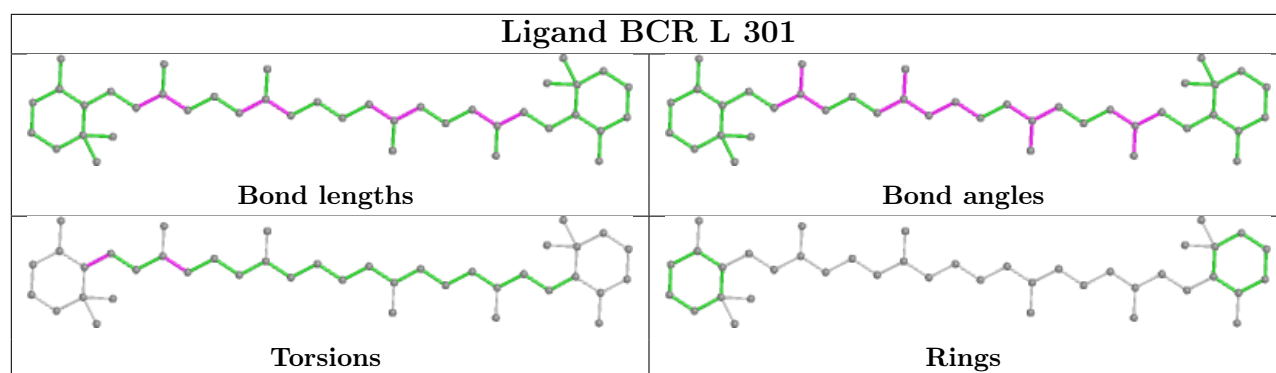
Bond angles



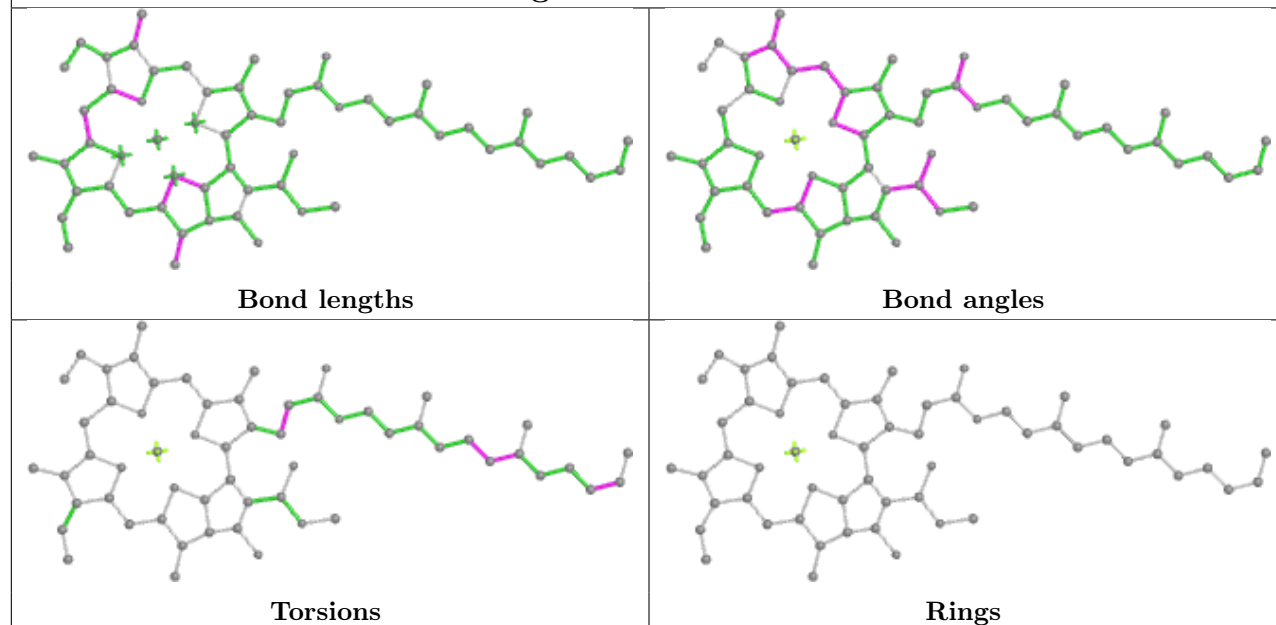
Torsions



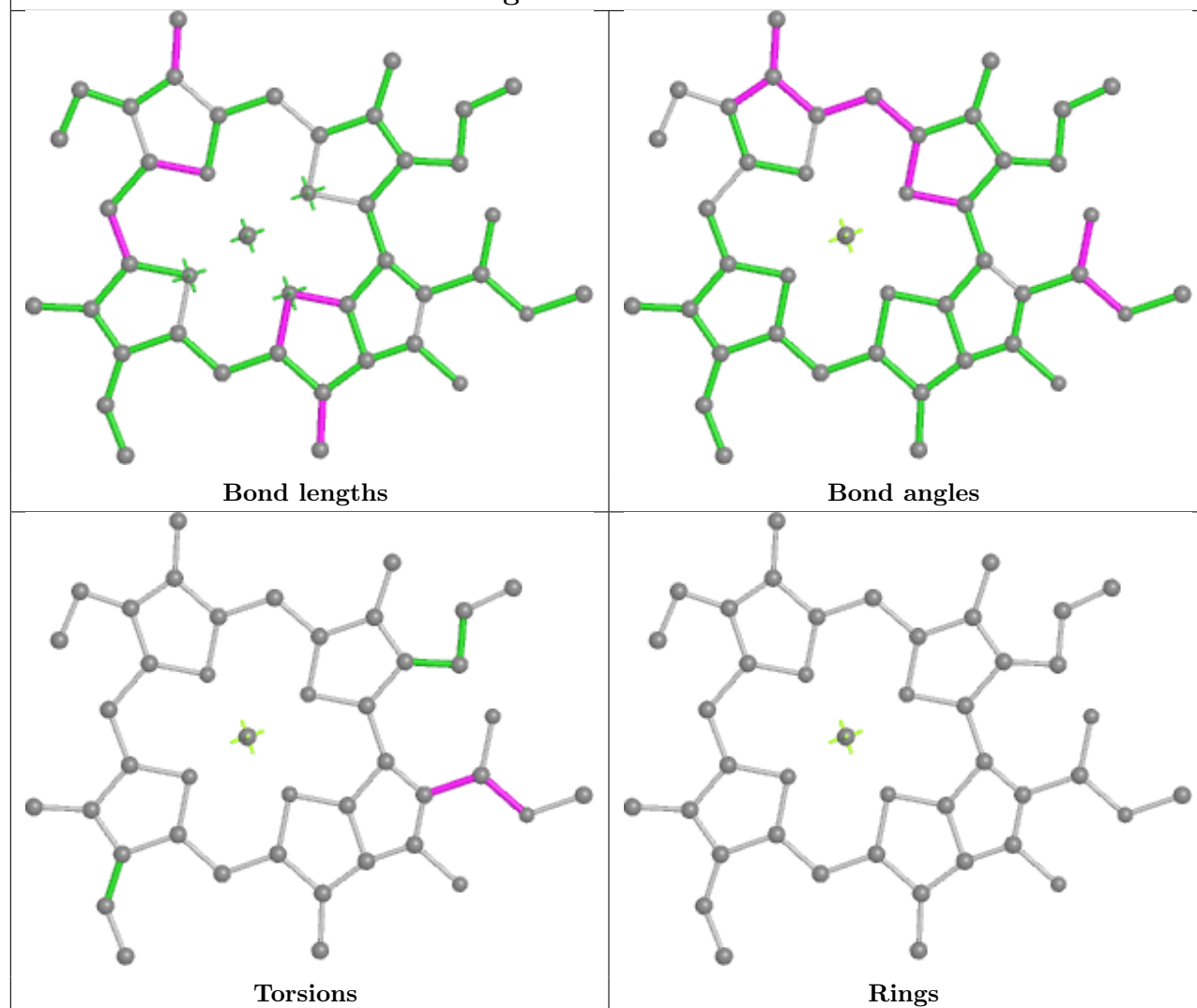
Rings



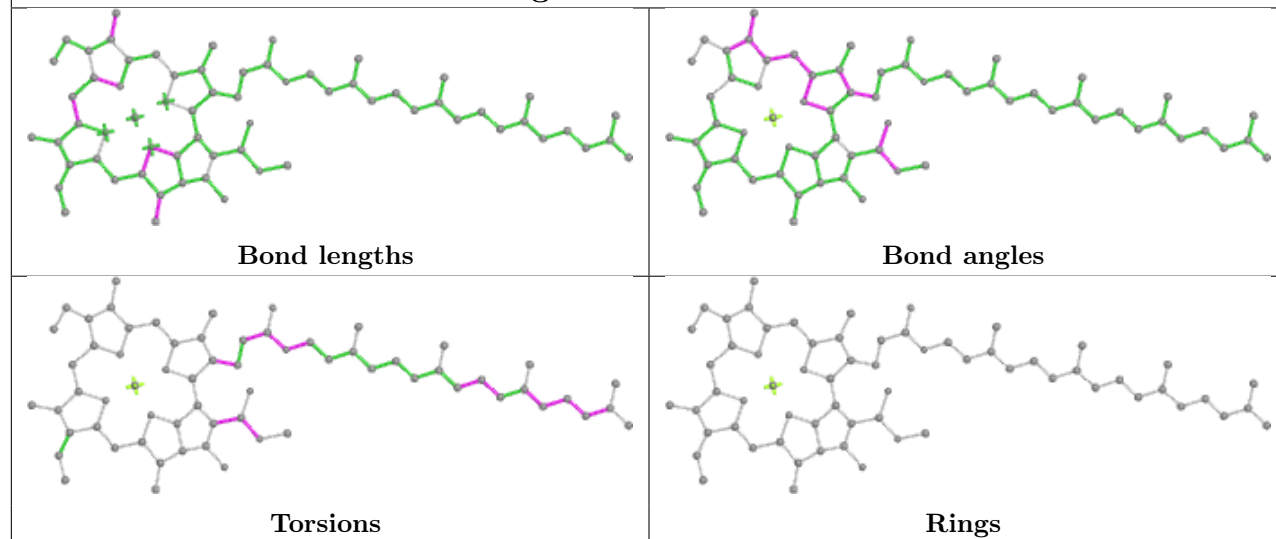
Ligand CLA A 809



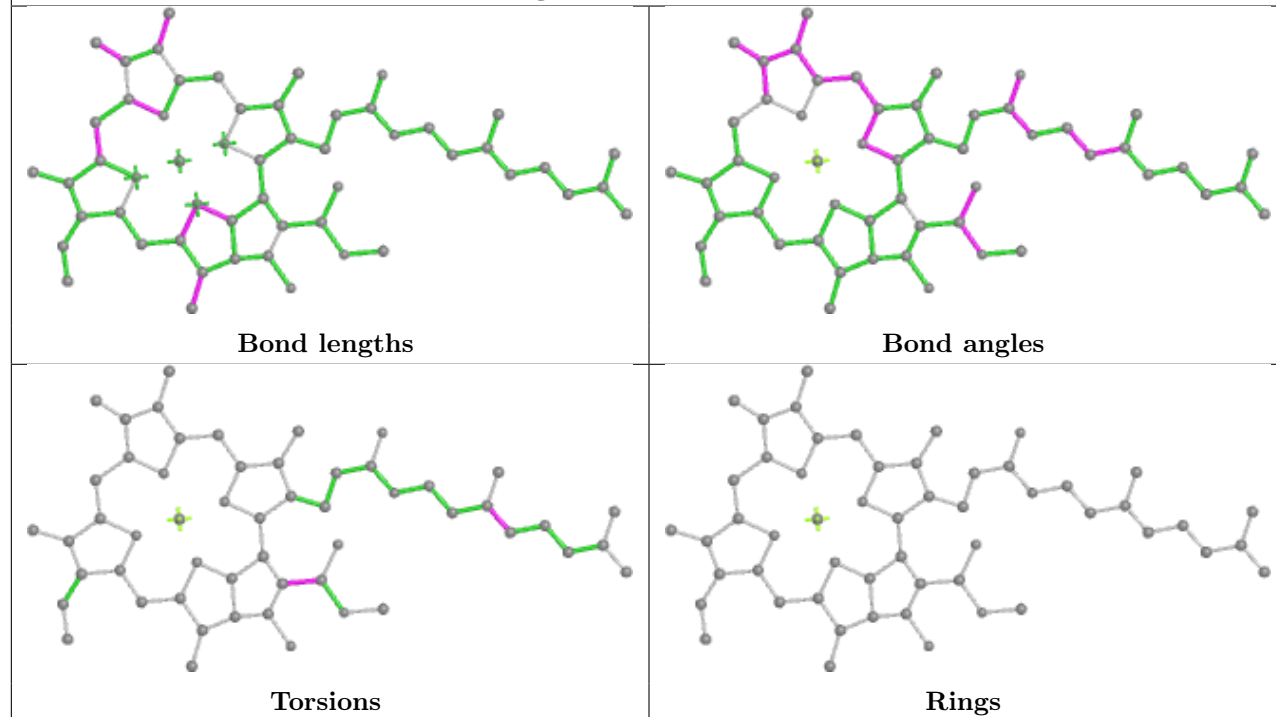
Ligand CLA 3 411

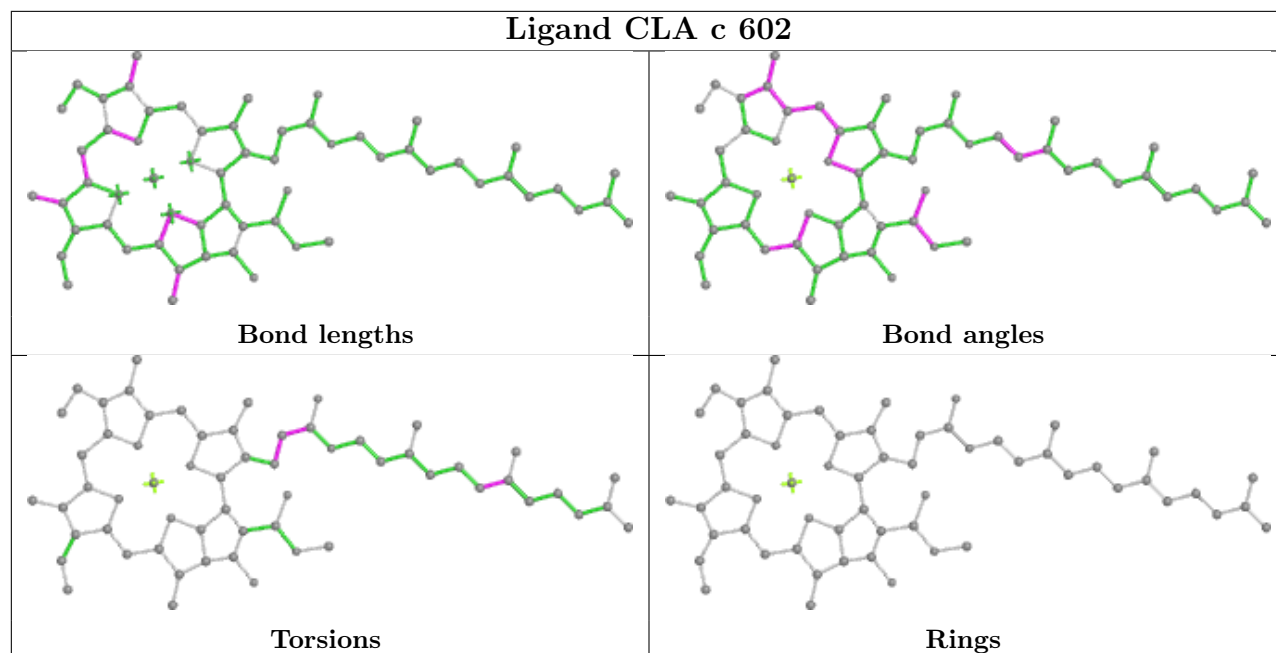
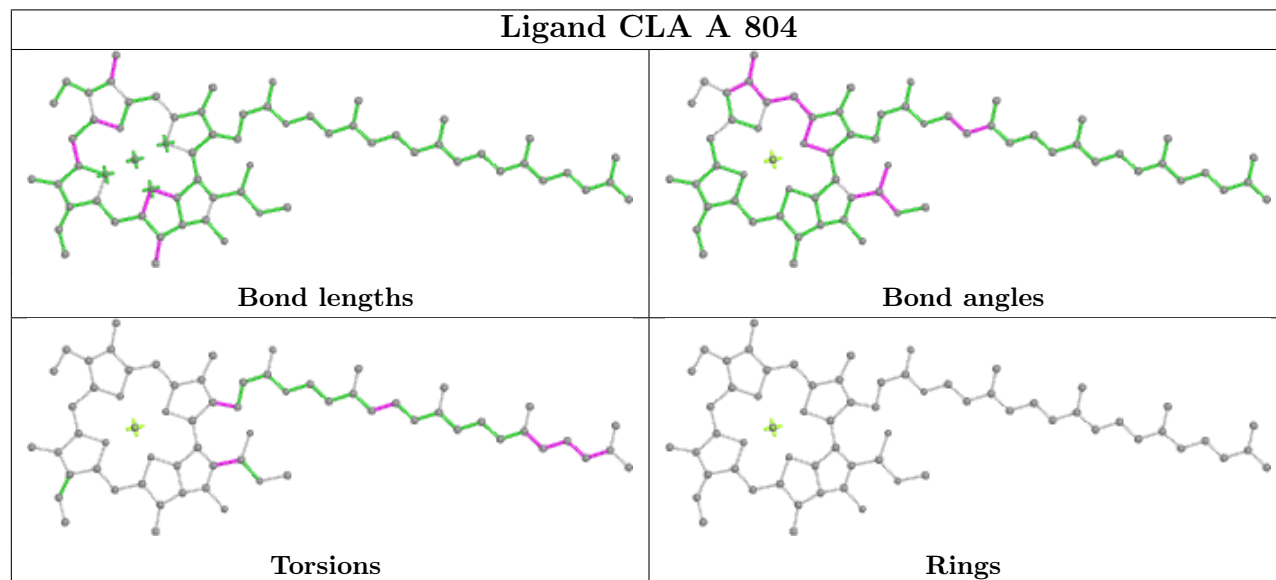
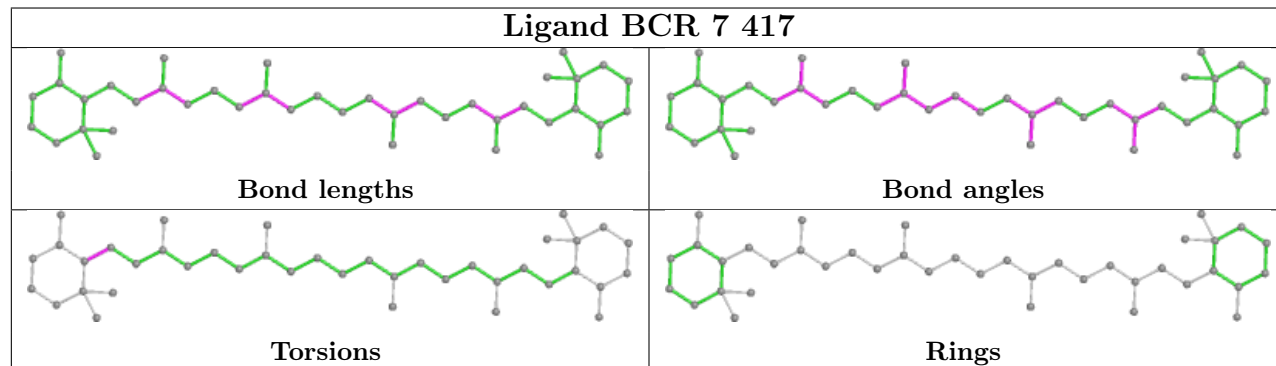


Ligand CLA A 841

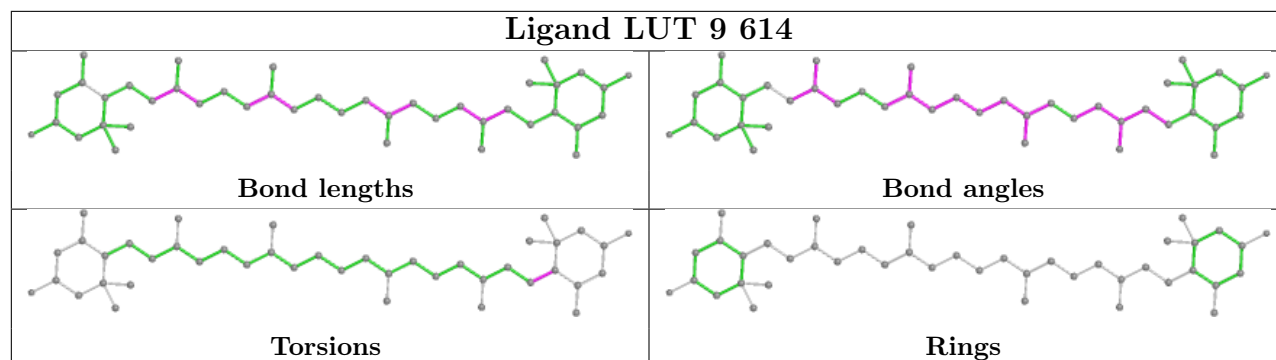


Ligand CLA B 810

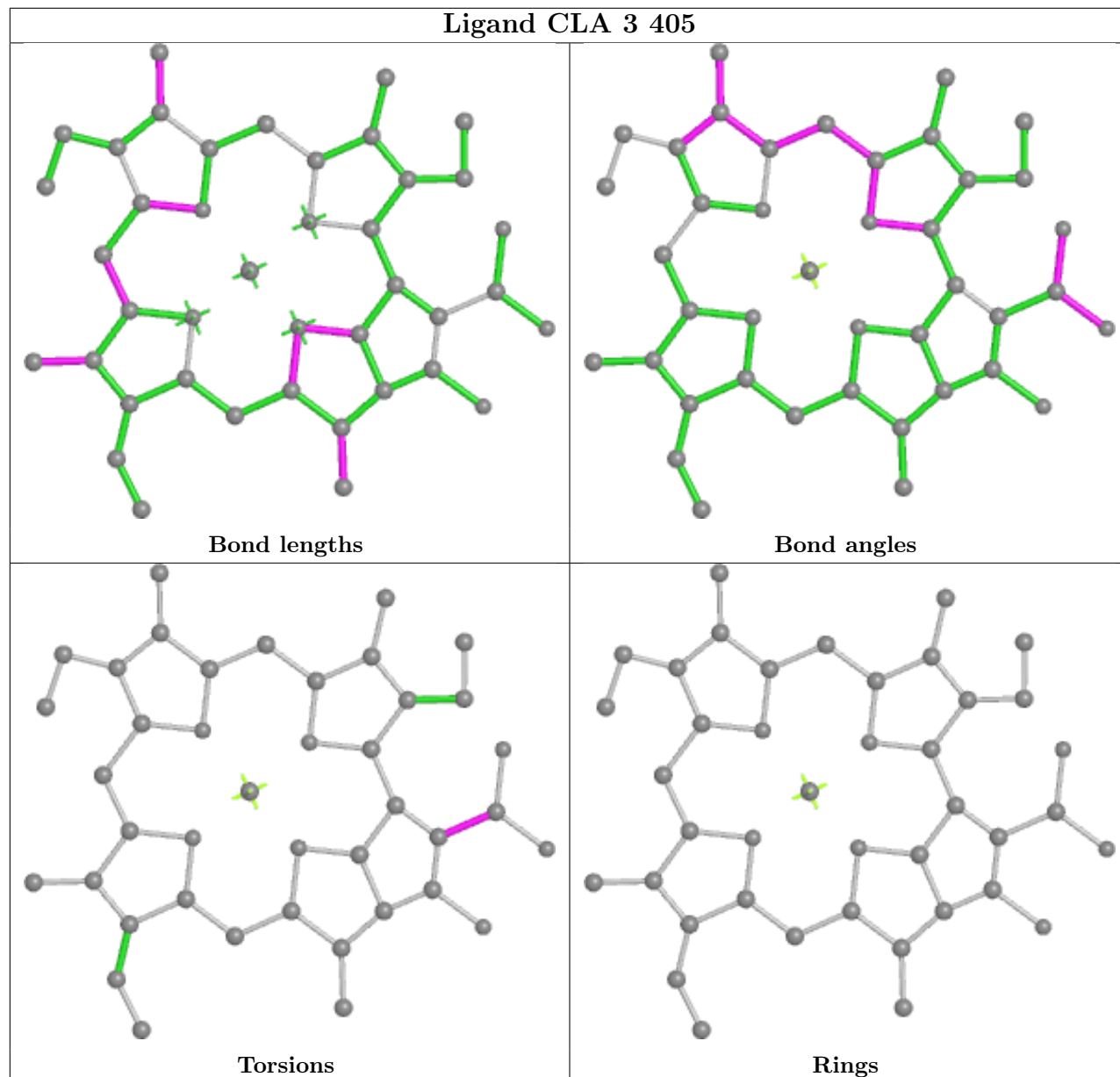


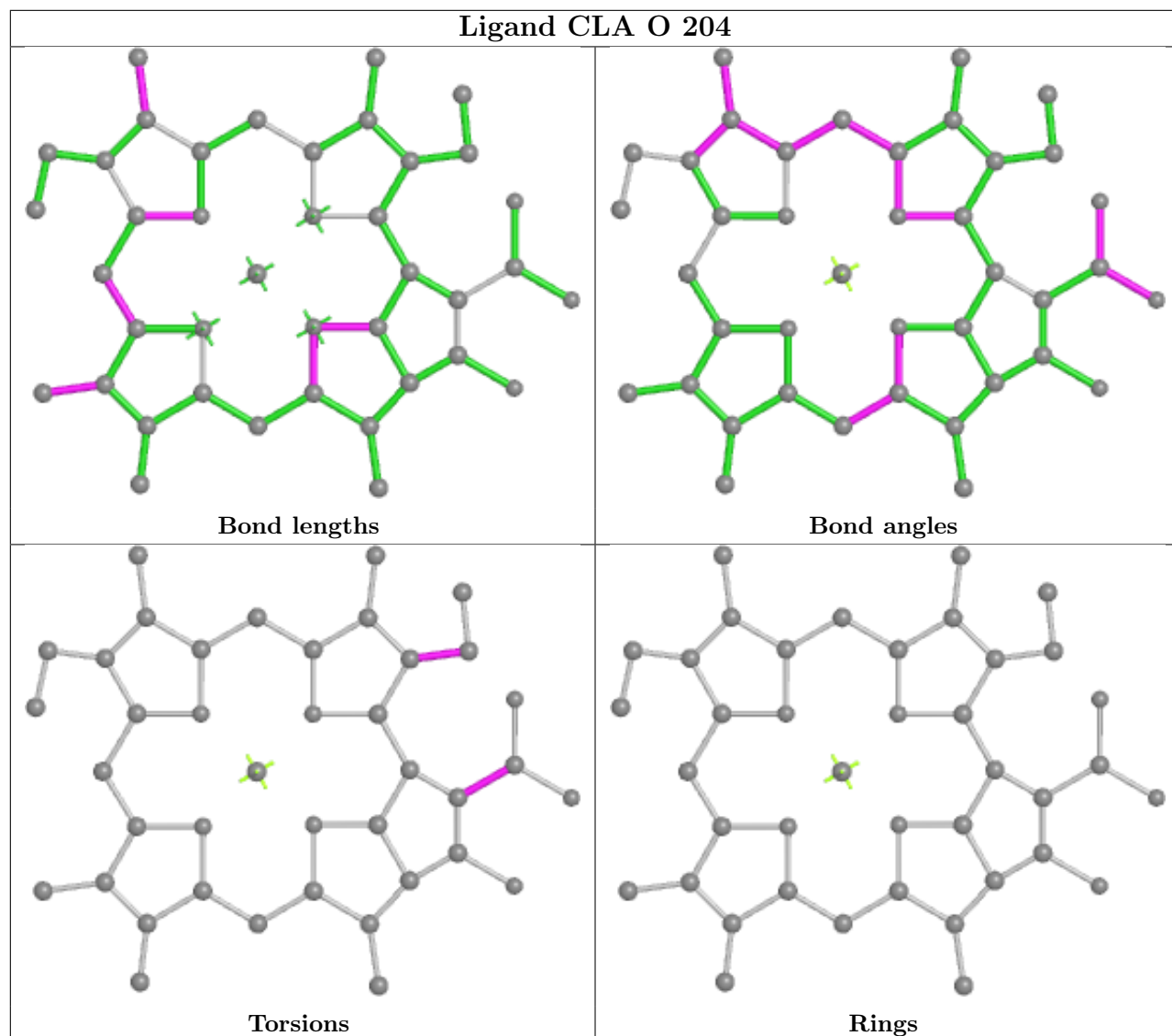
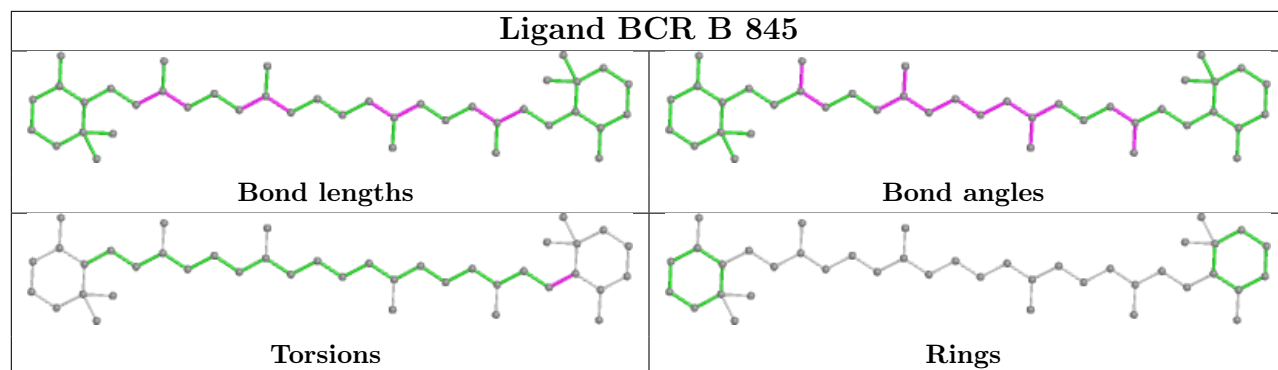
Ligand CLA c 602**Ligand CLA A 804****Ligand BCR 7 417**

Ligand LUT 9 614

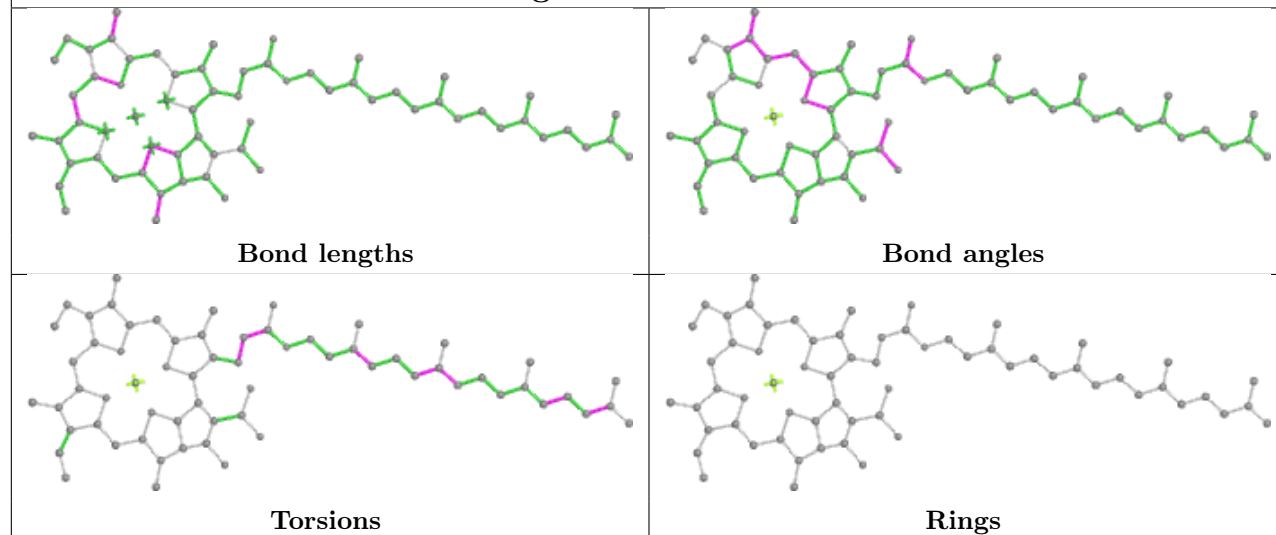


Ligand CLA 3 405

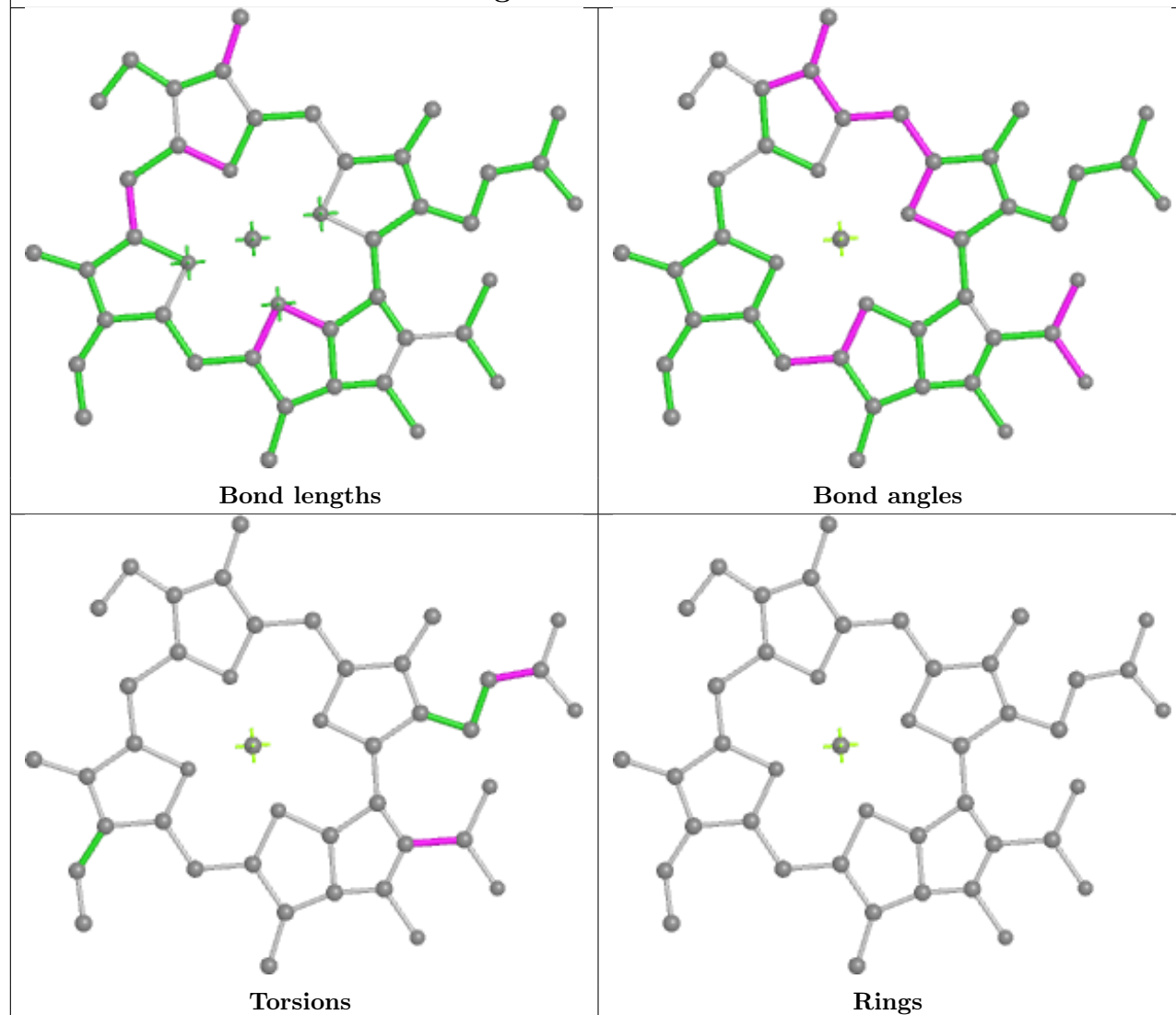


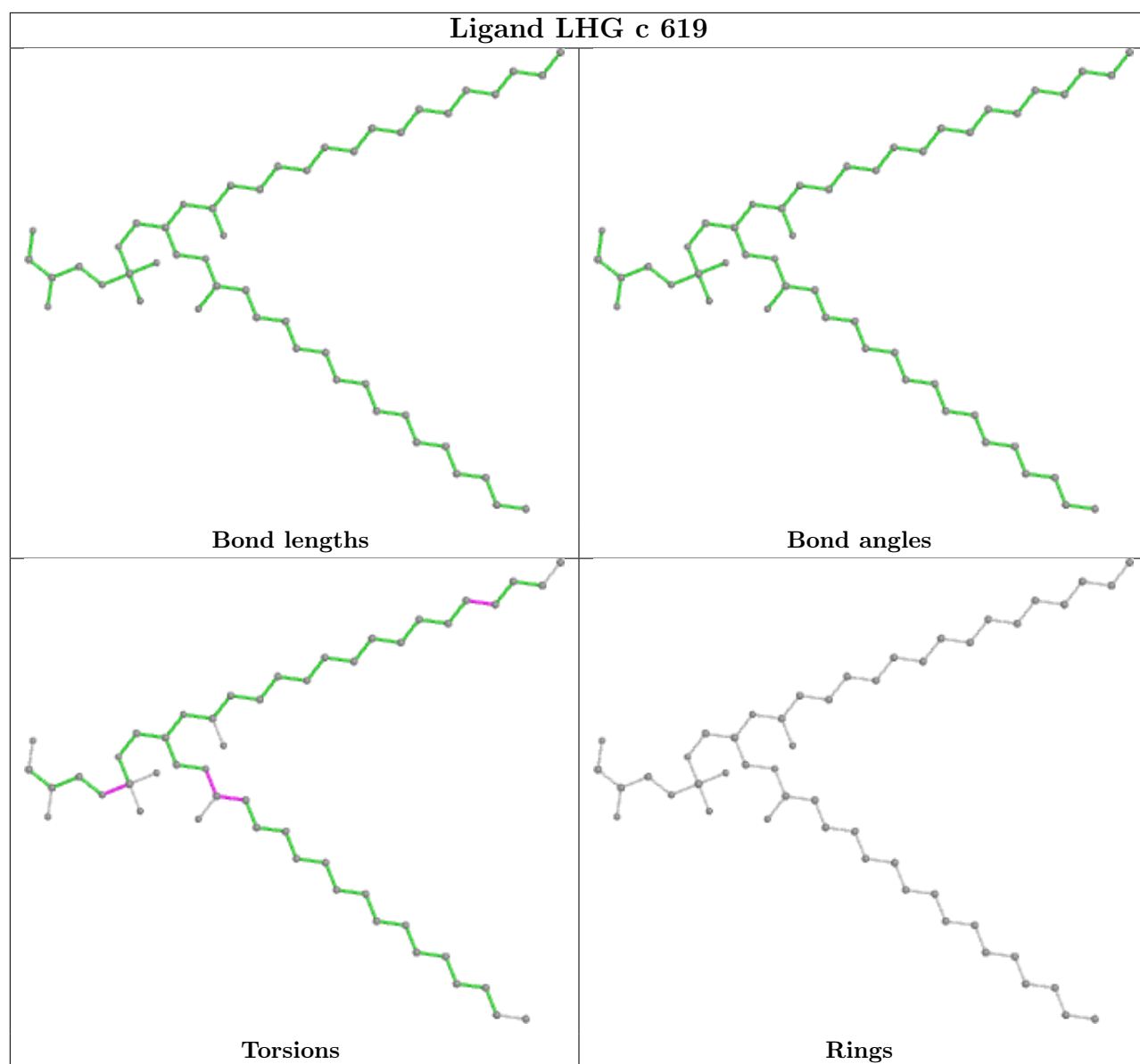


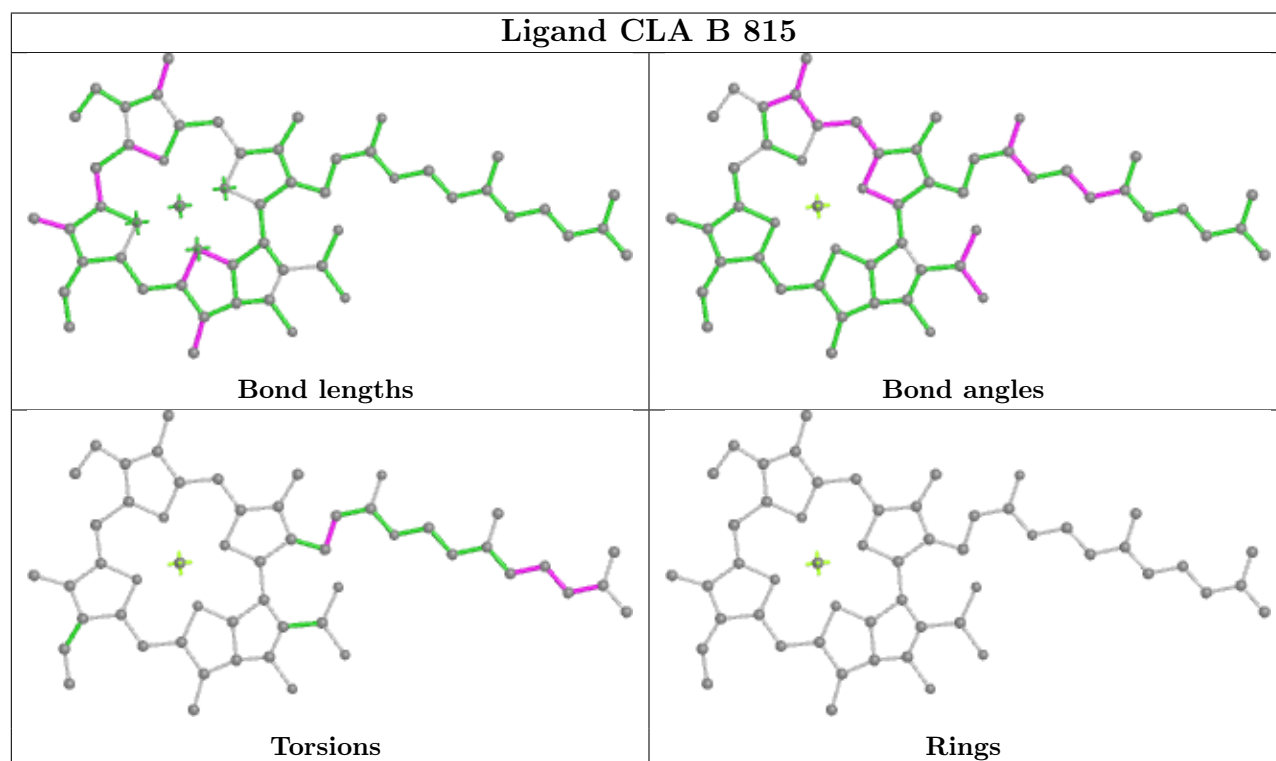
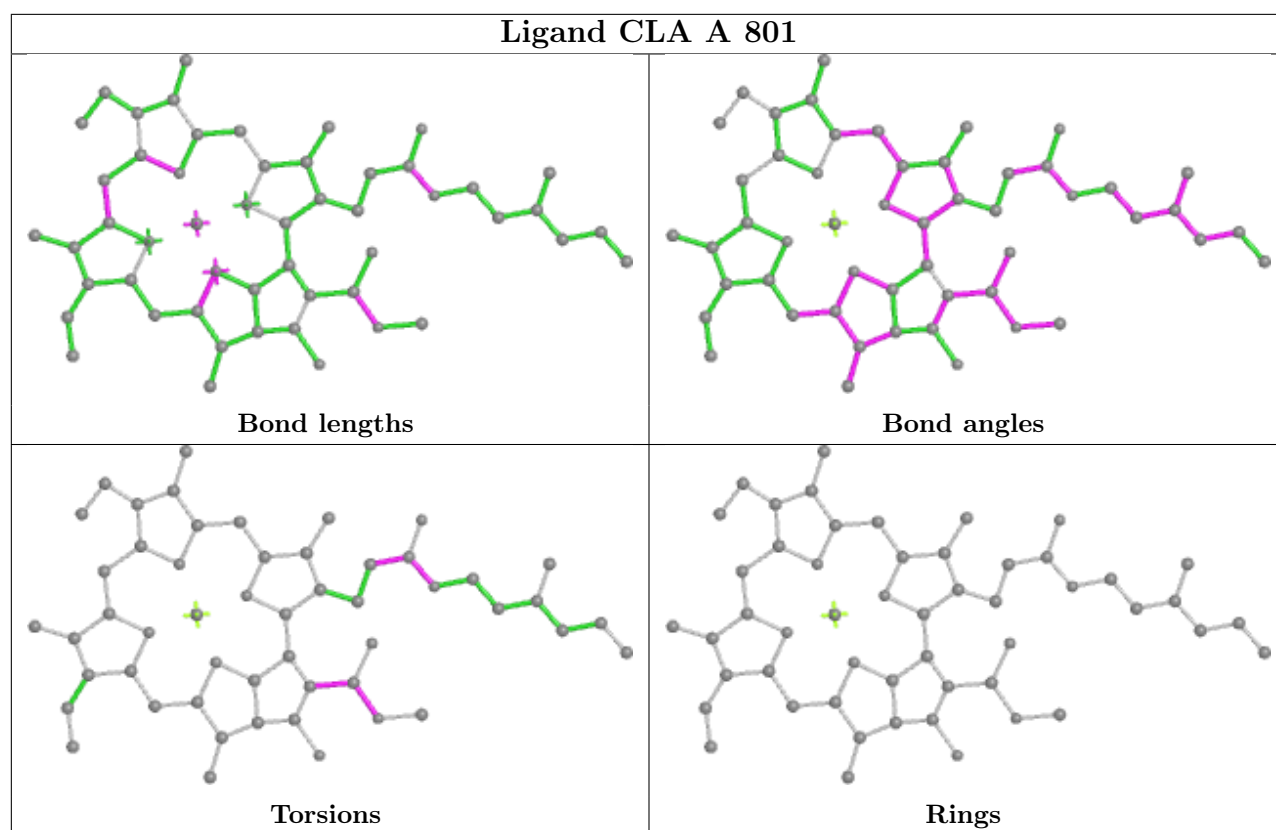
Ligand CLA B 837



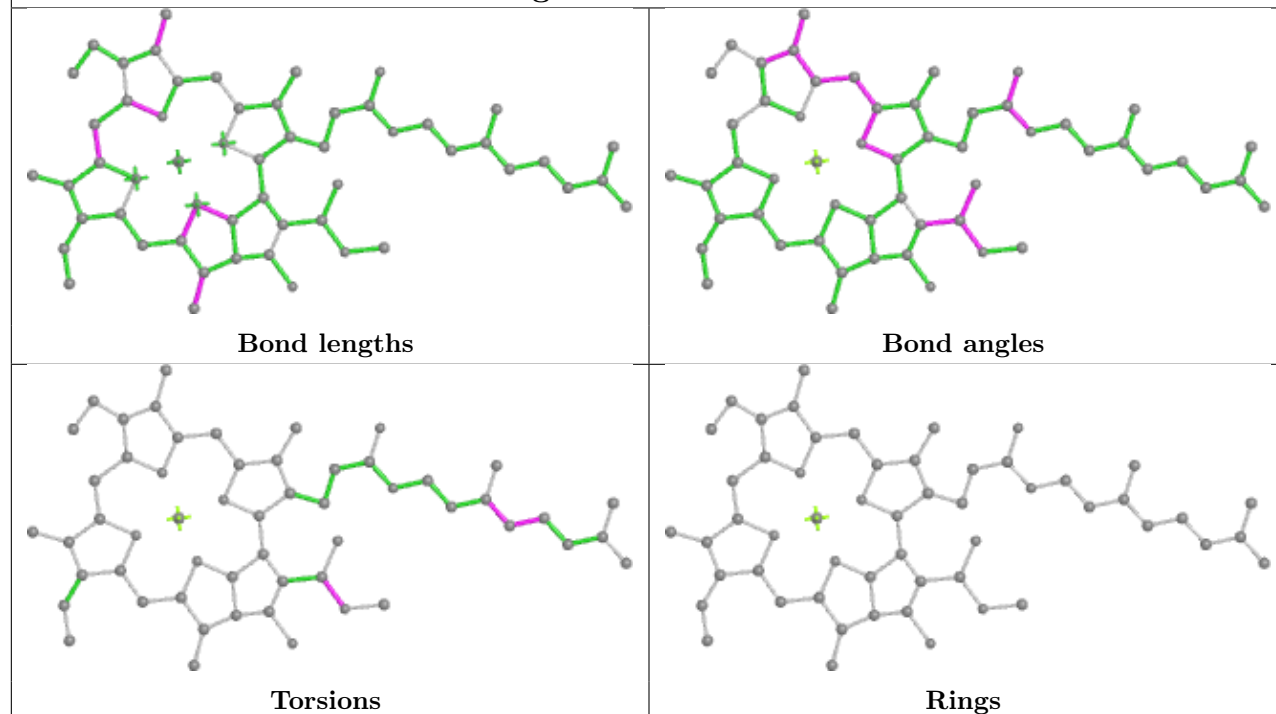
Ligand CLA 8 603



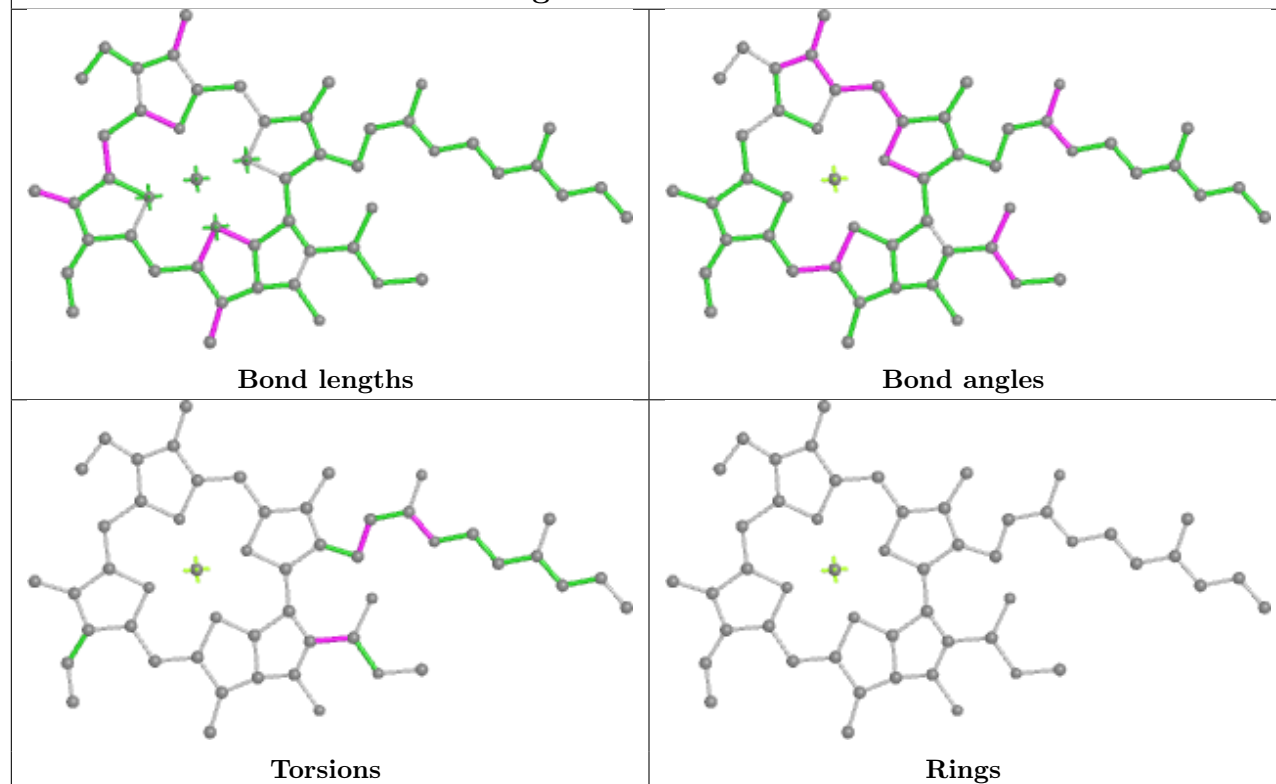




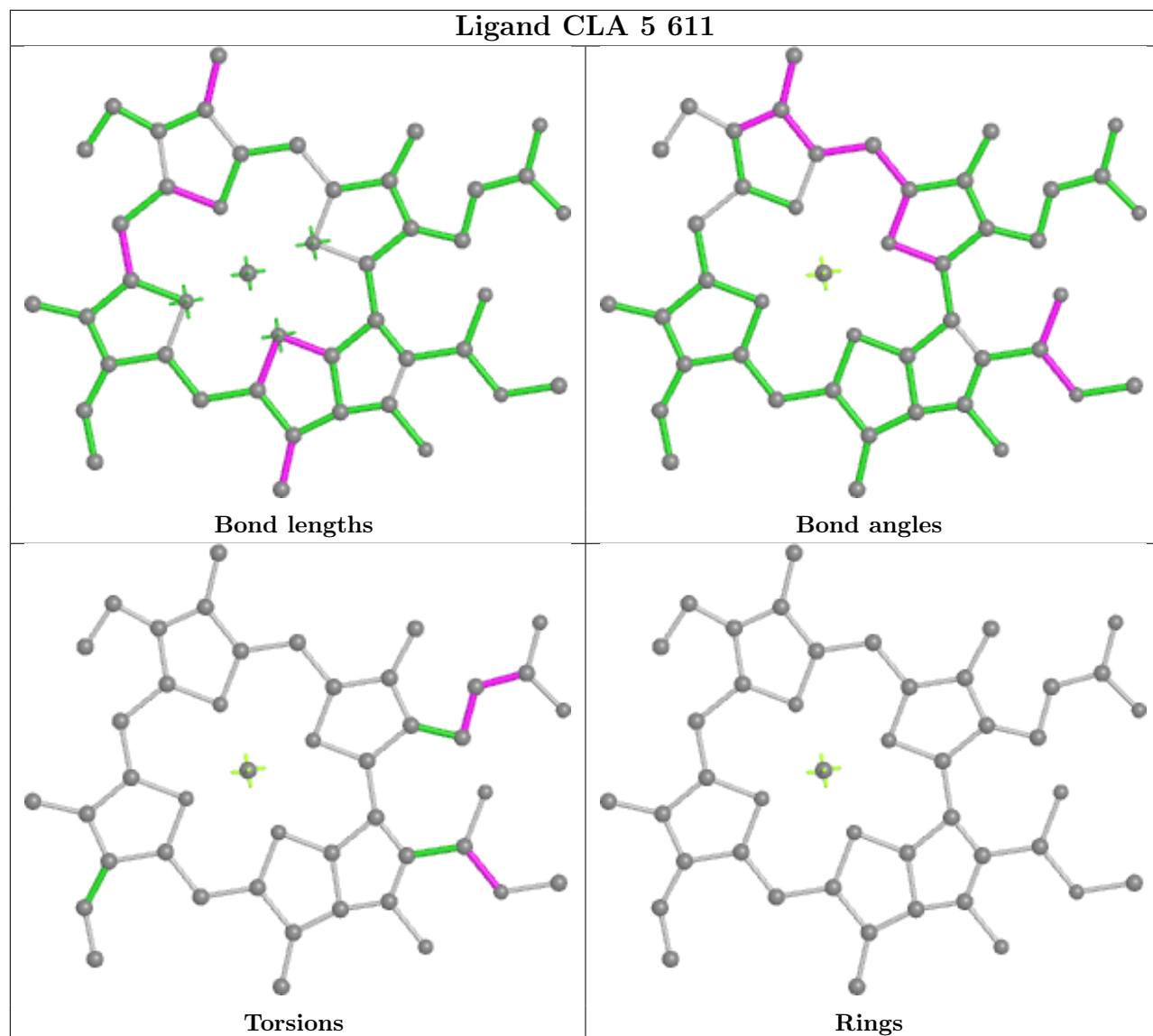
Ligand CLA B 821



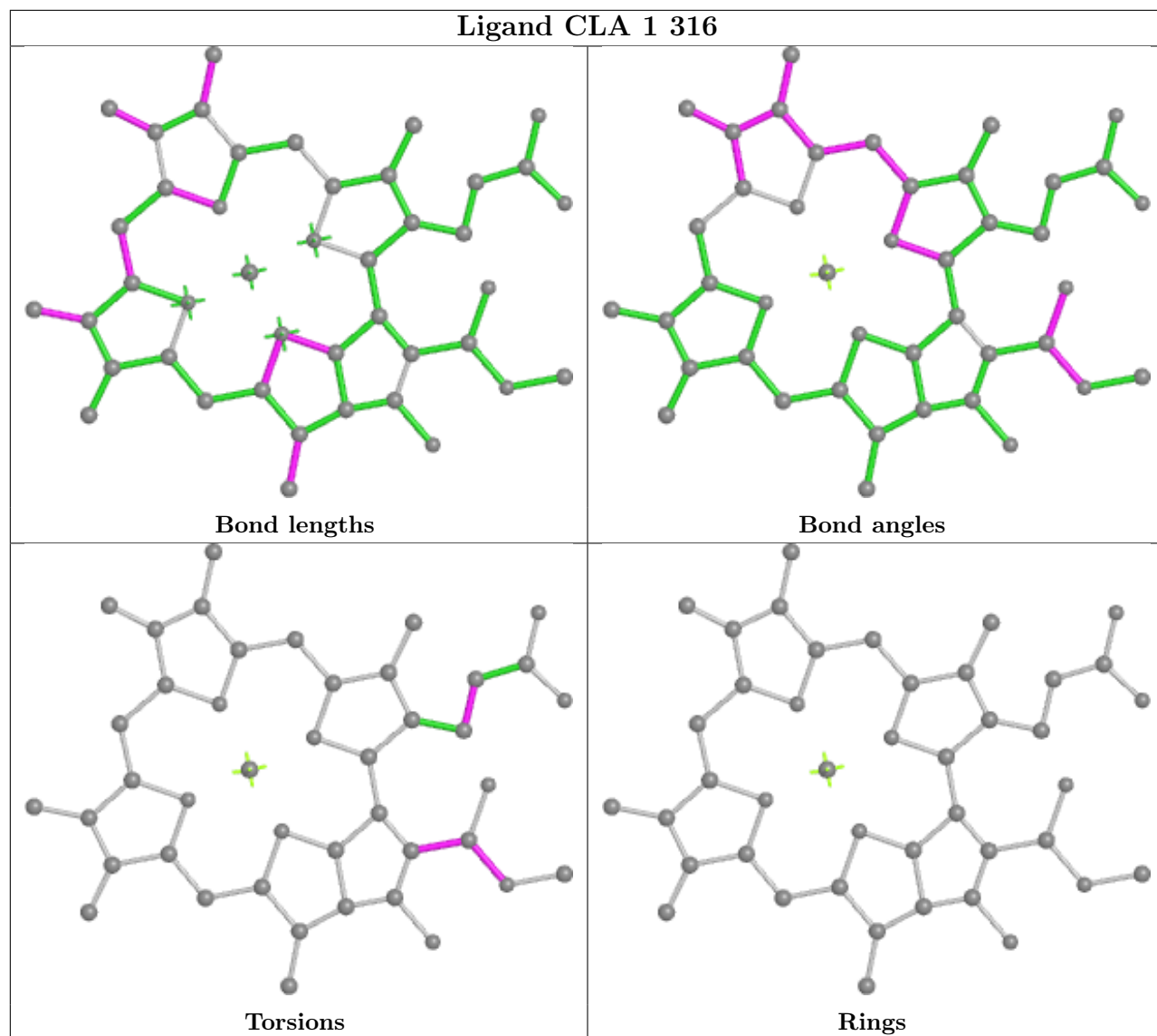
Ligand CLA B 816

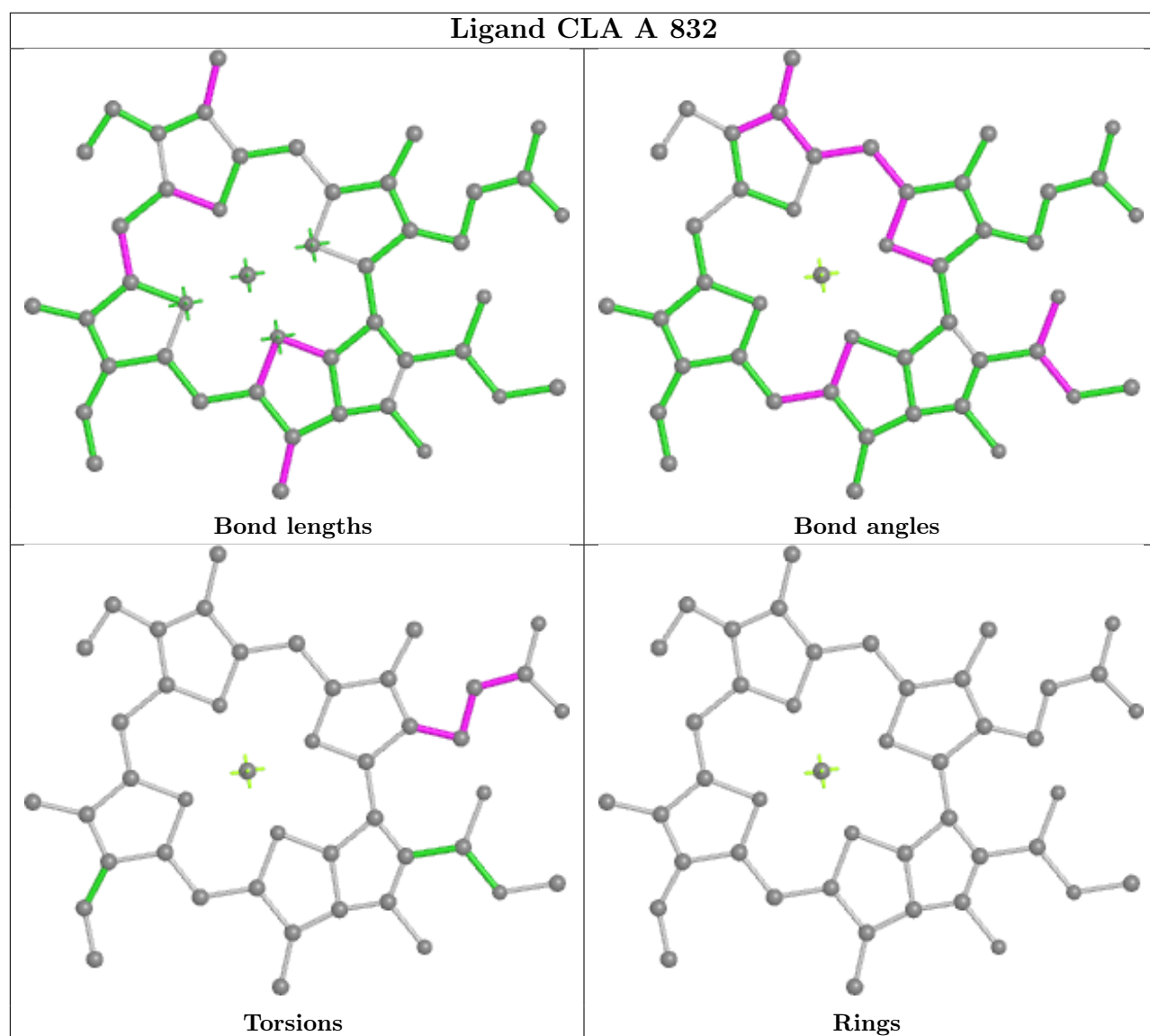


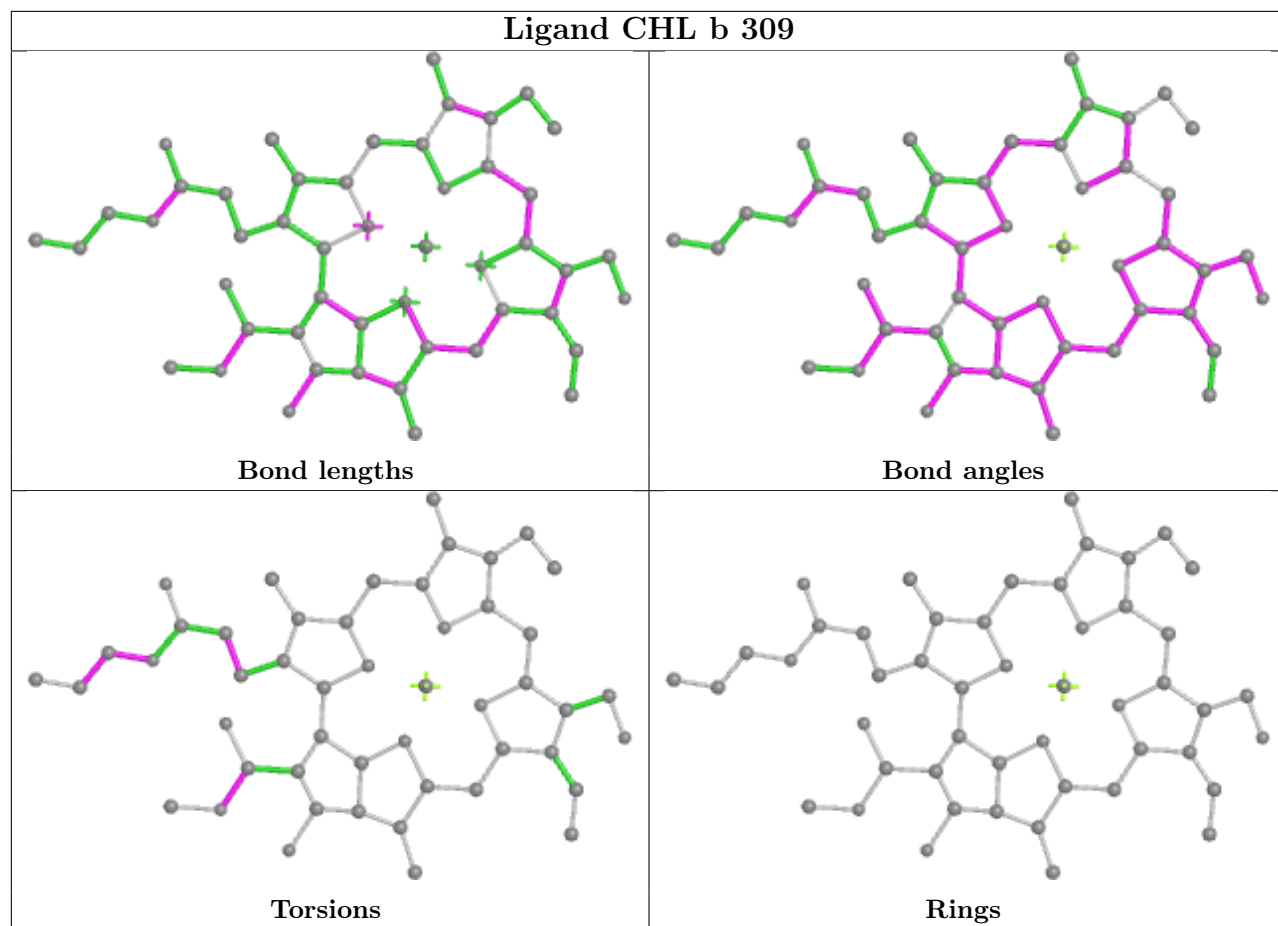
Ligand CLA 5 611



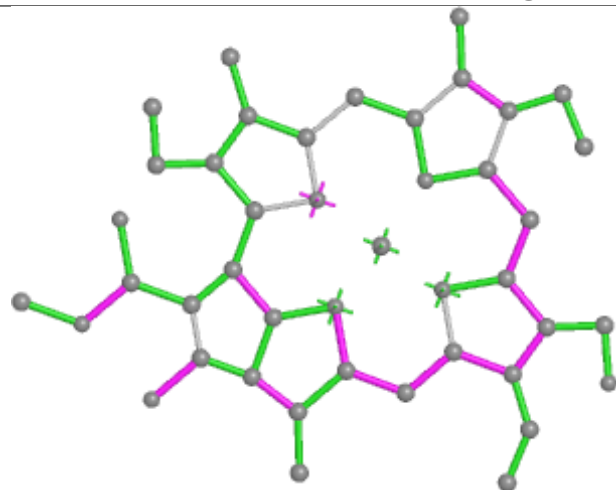
Ligand CLA 1 316



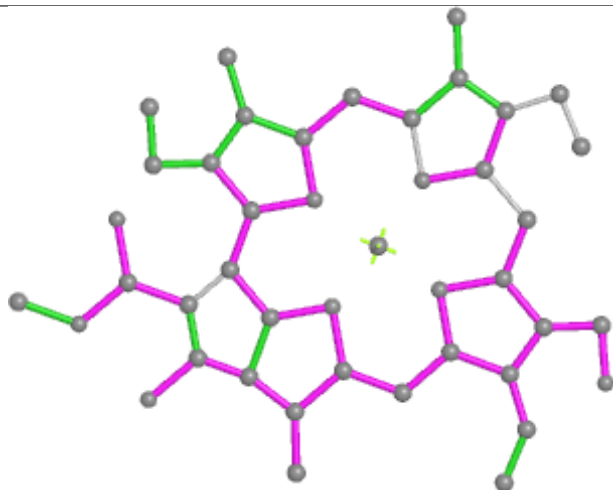




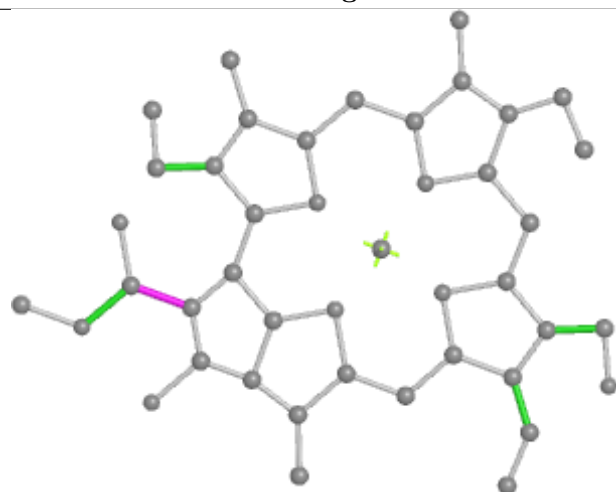
Ligand CHL a 607



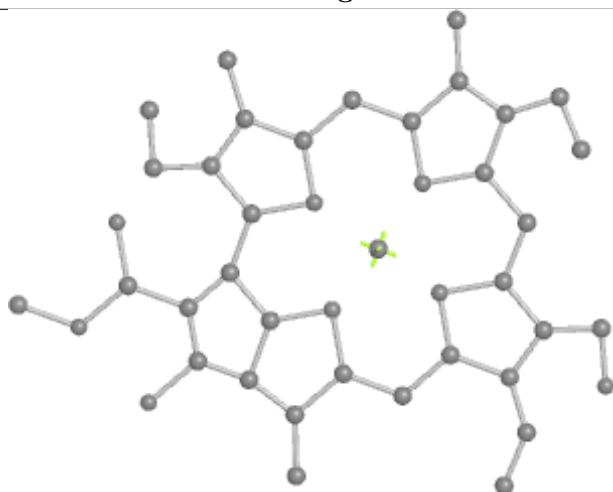
Bond lengths



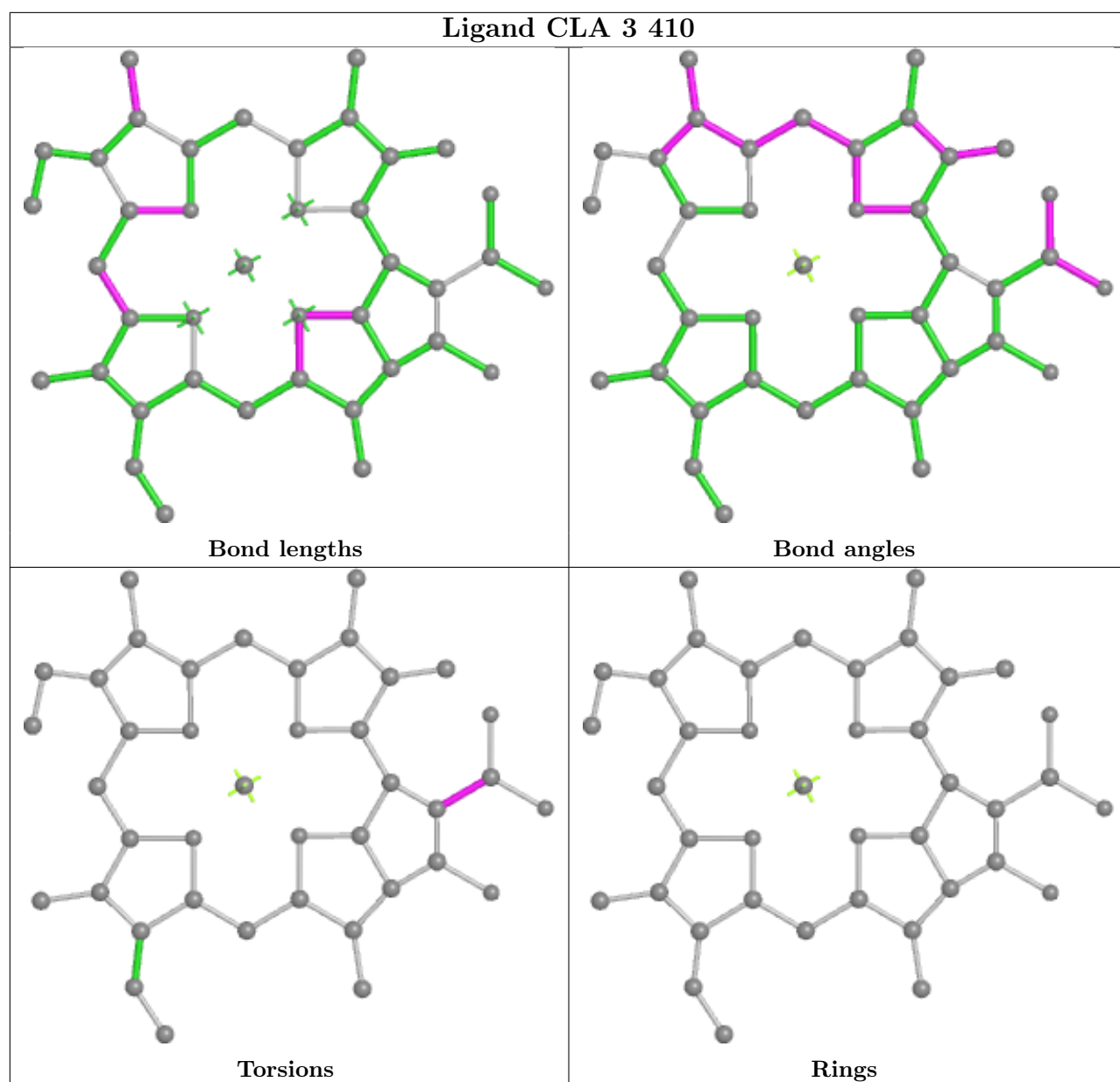
Bond angles

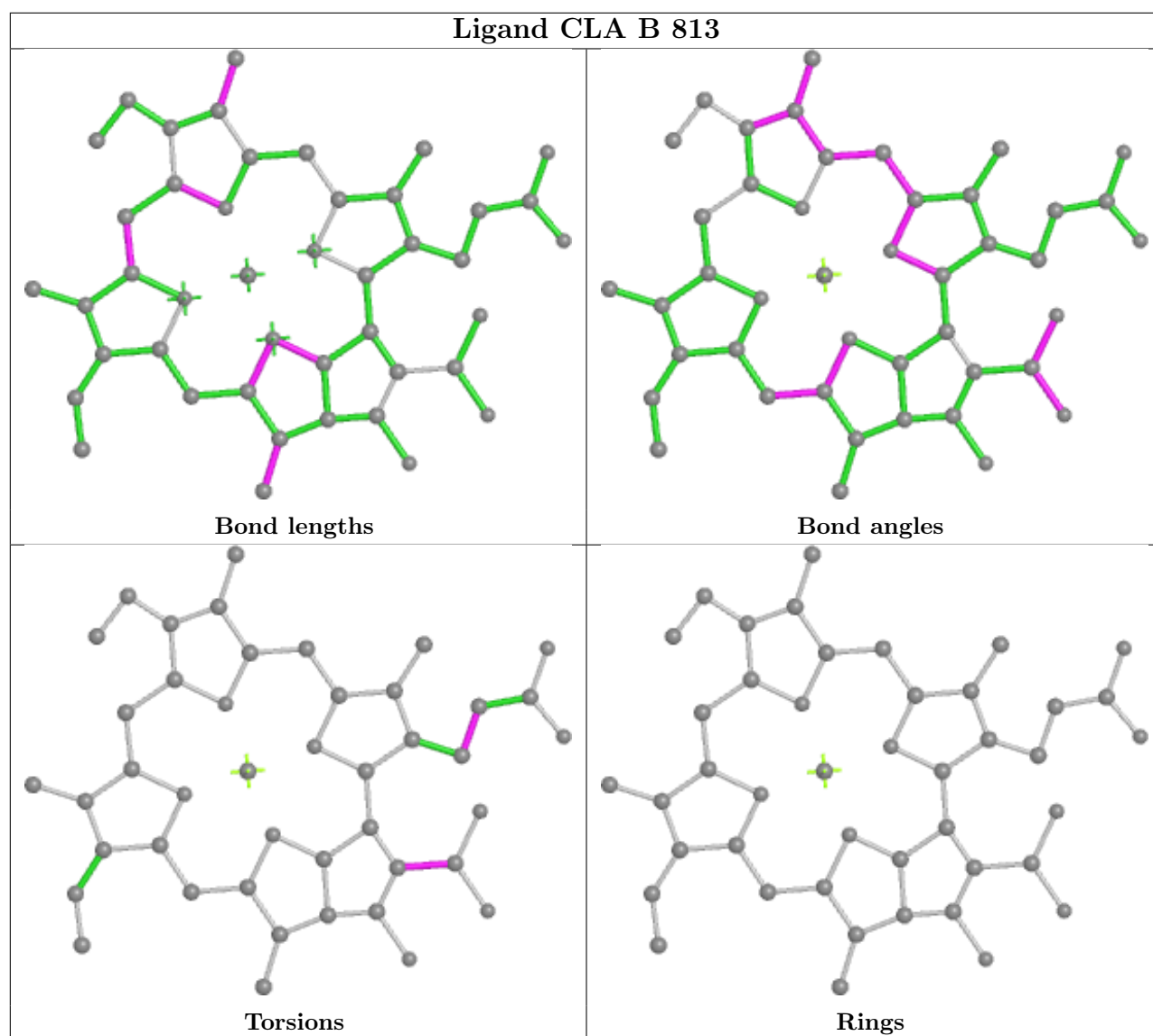


Torsions

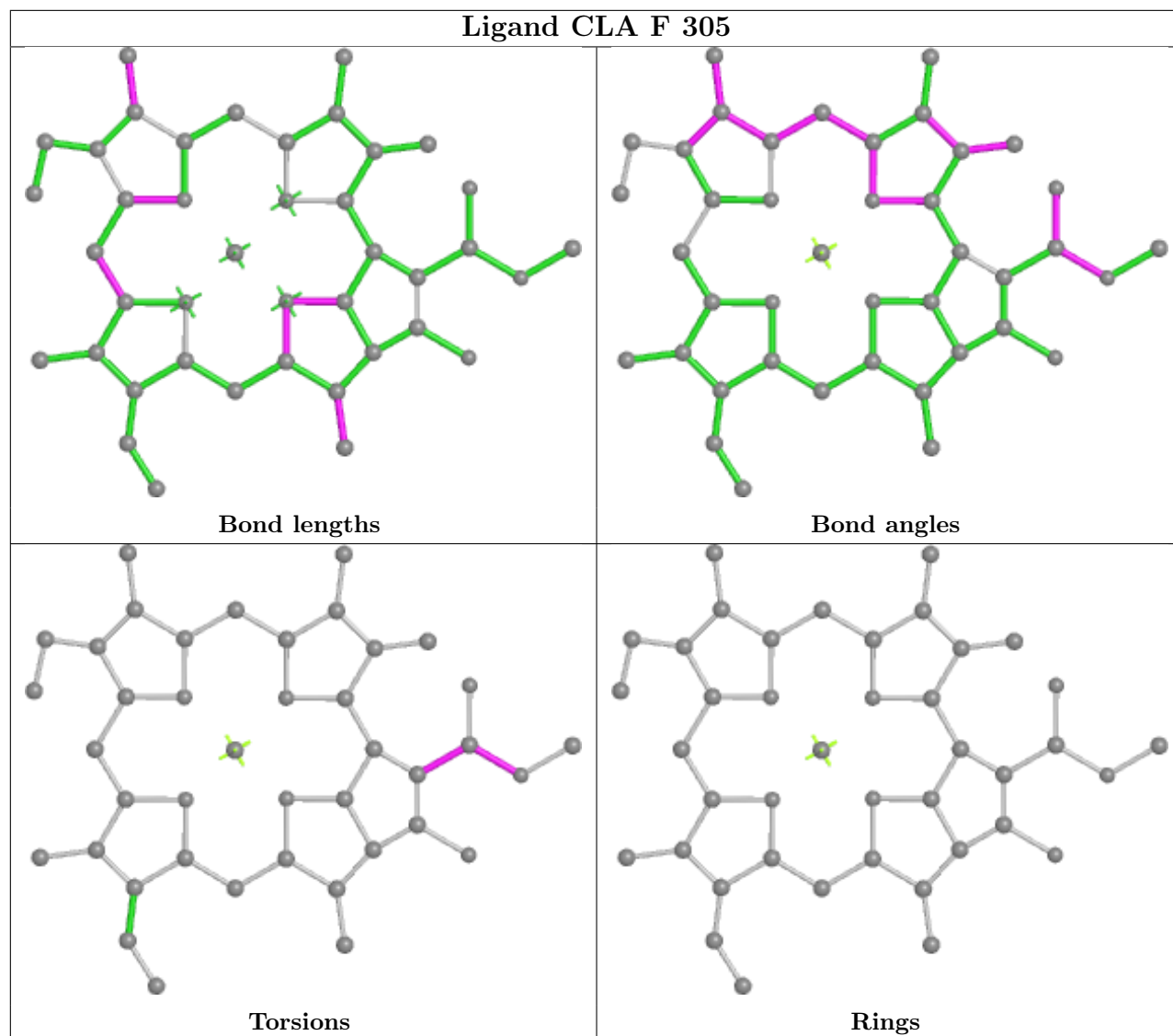


Rings

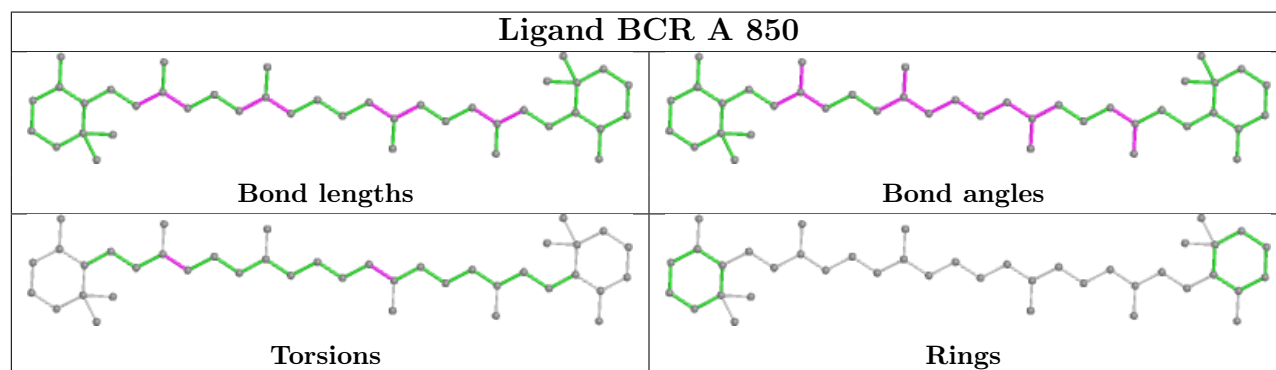




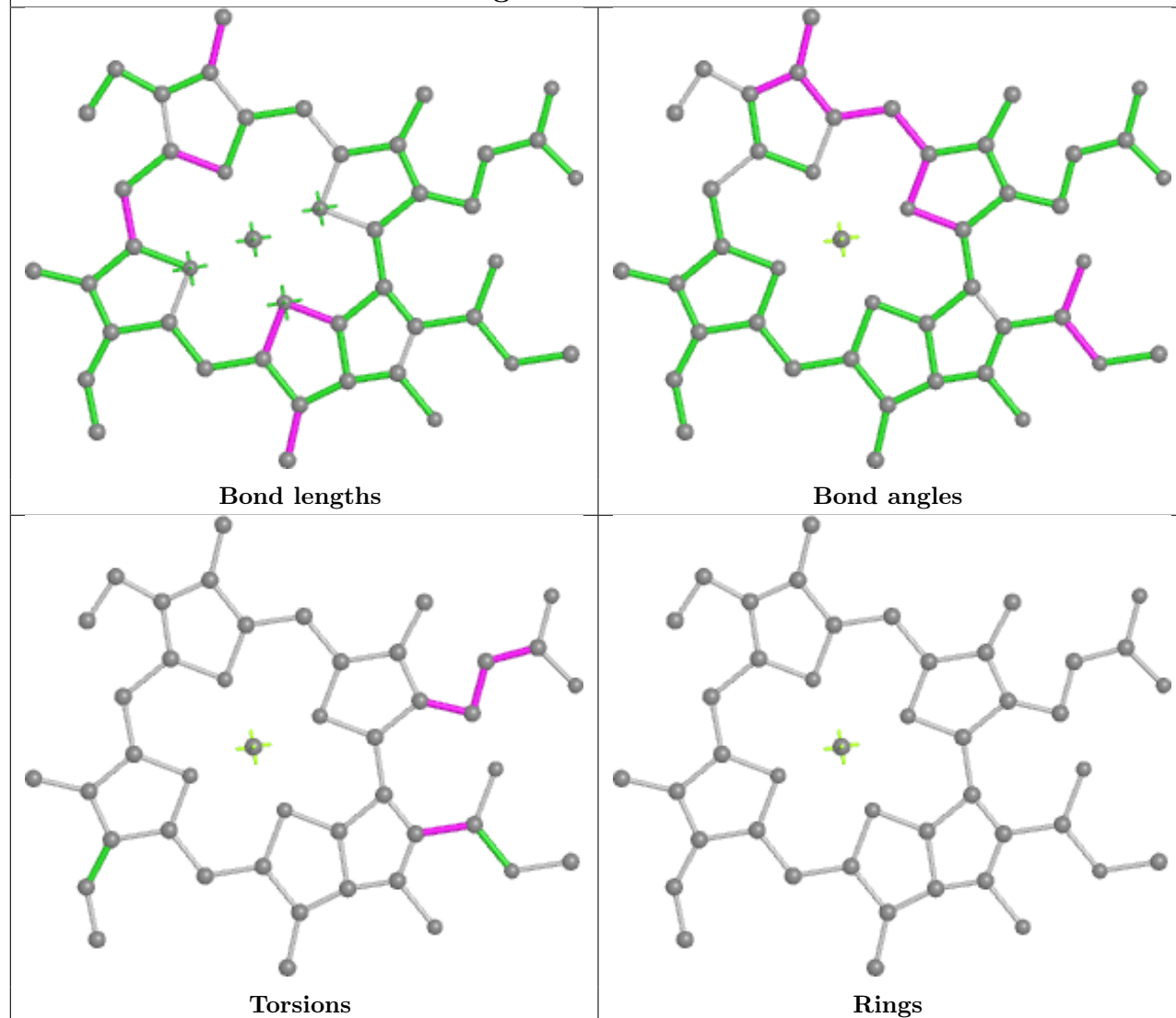
Ligand CLA F 305



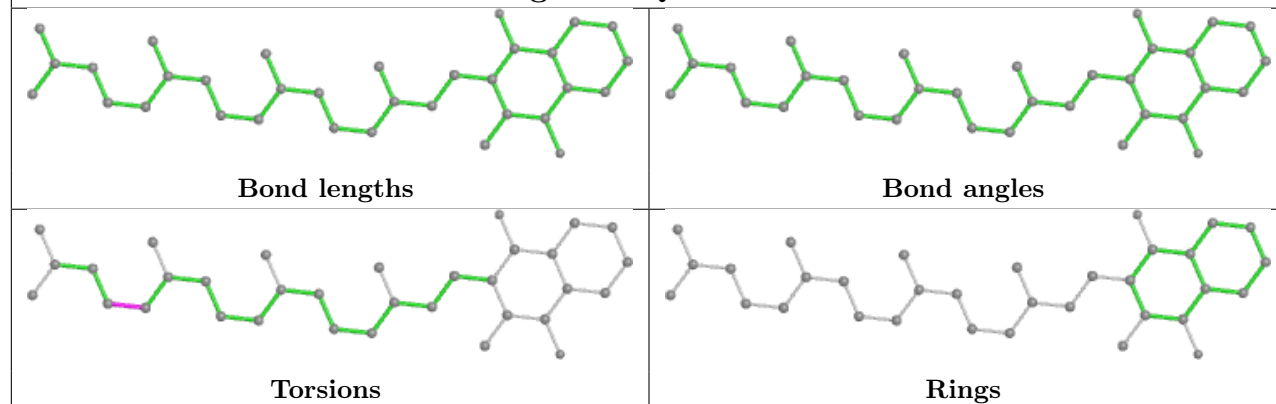
Ligand BCR A 850

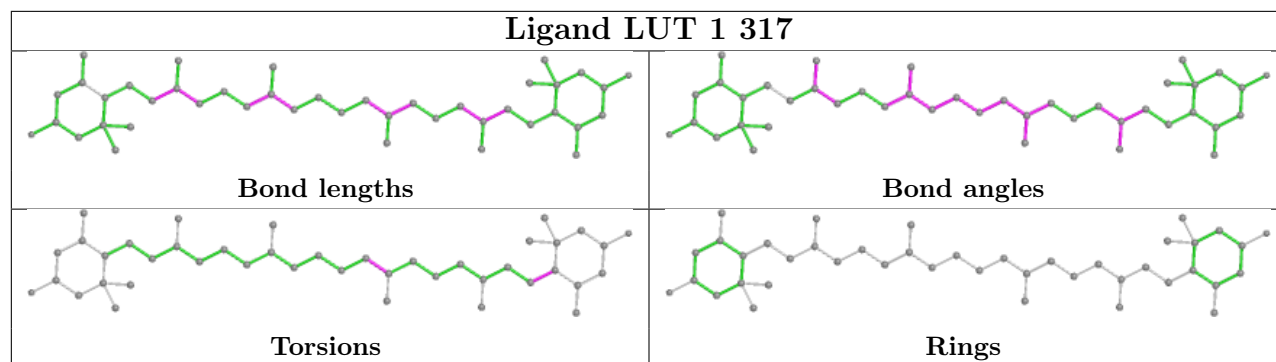
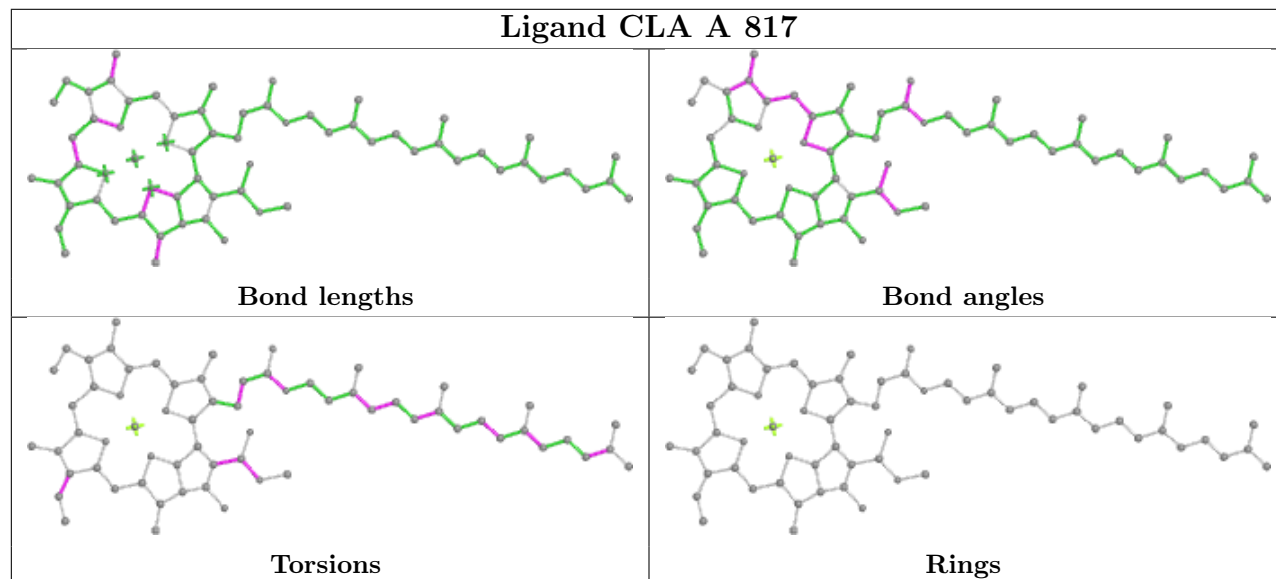
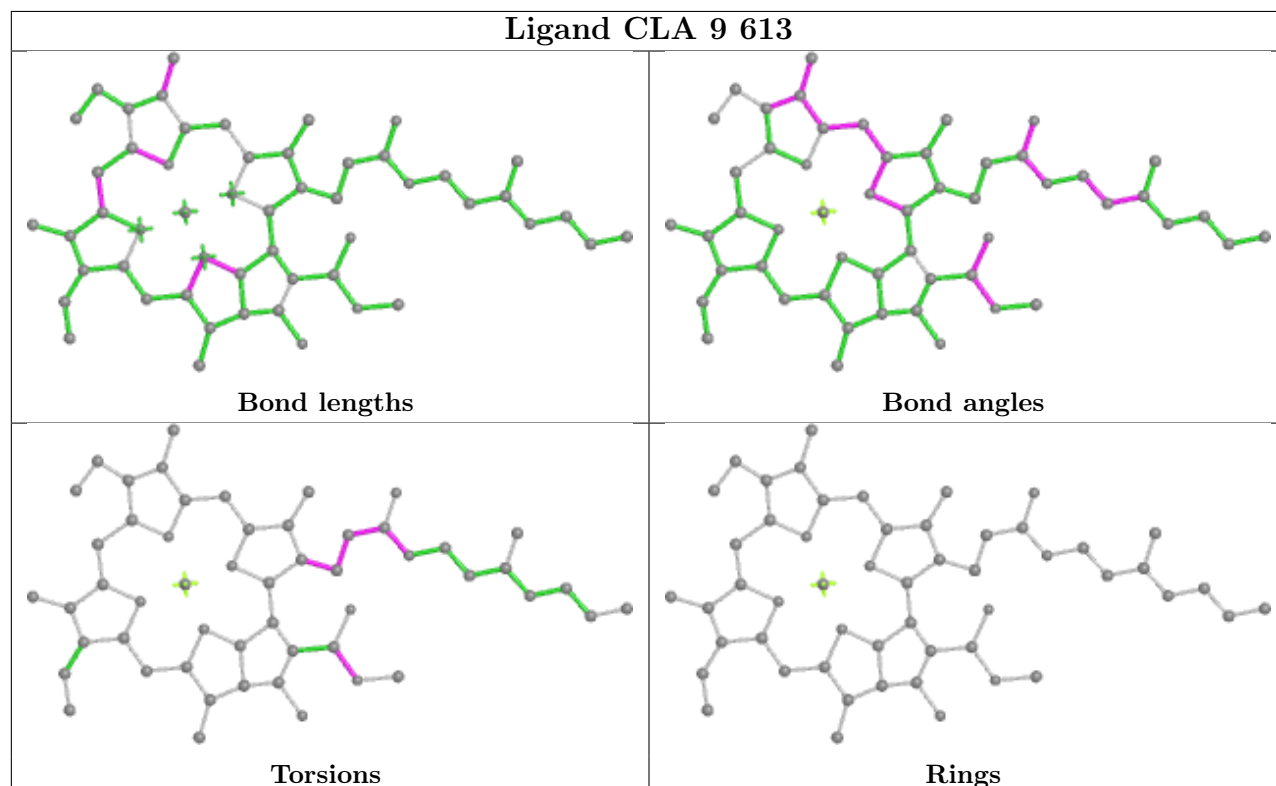


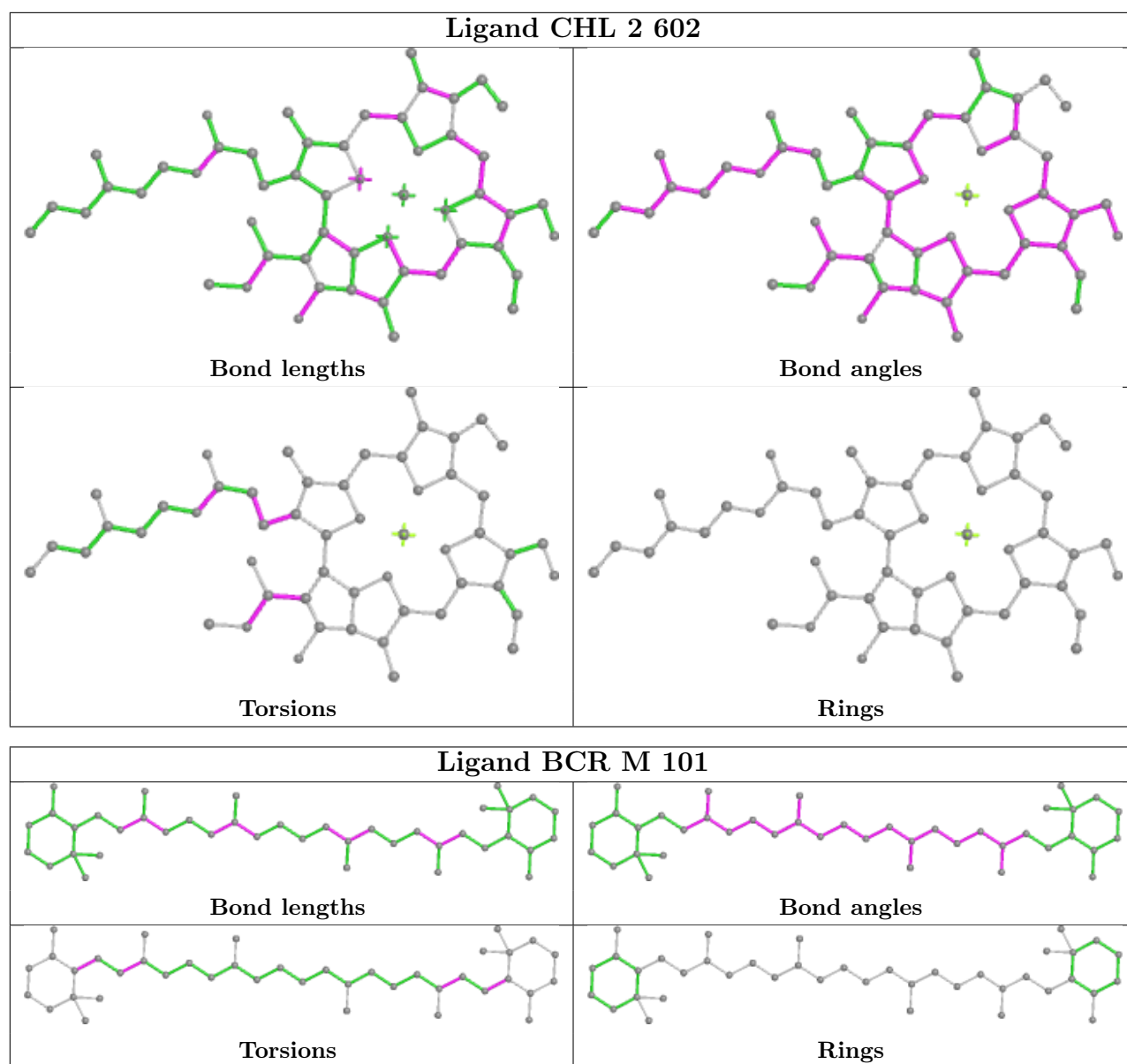
Ligand CLA b 305



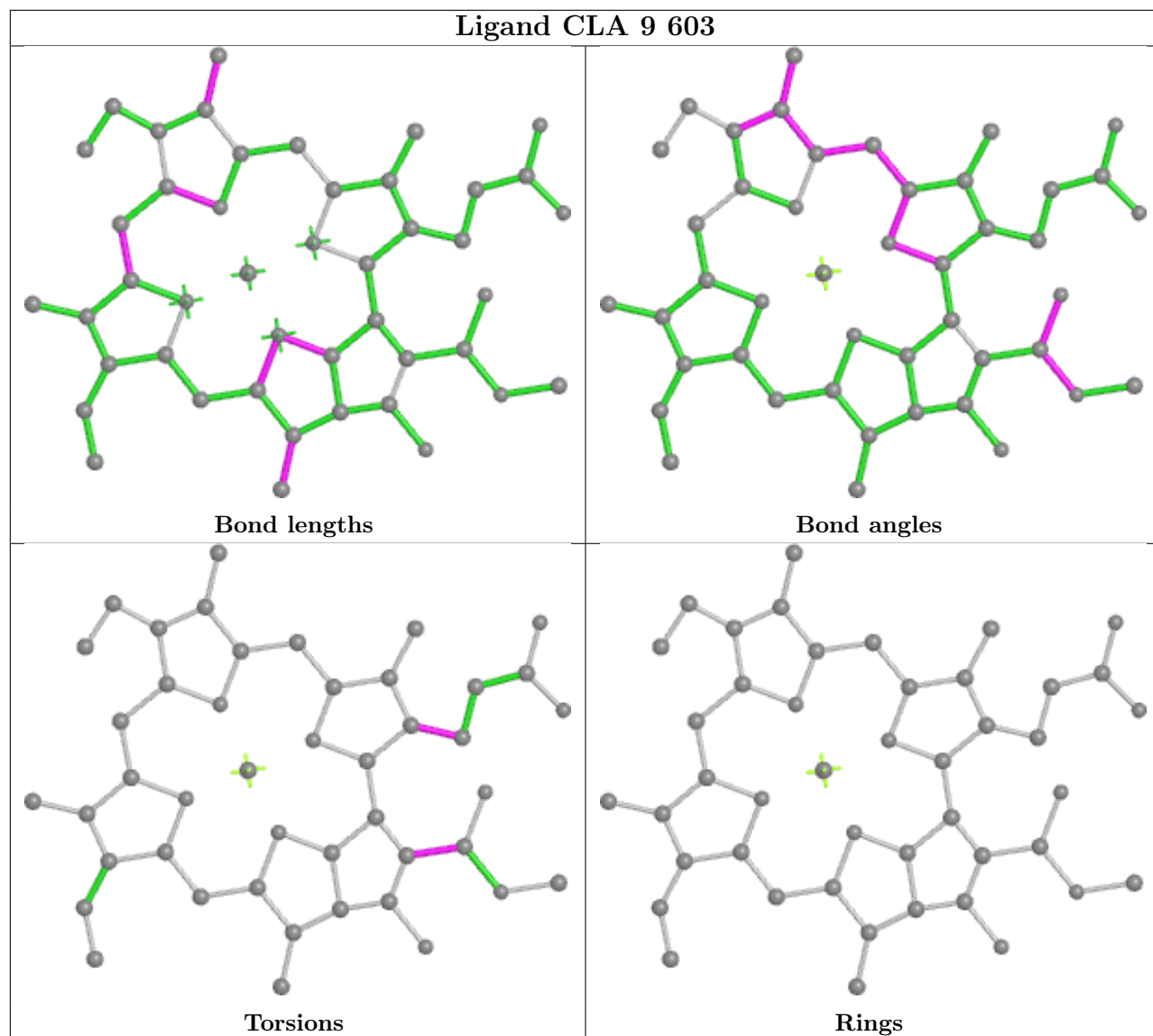
Ligand PQN B 841



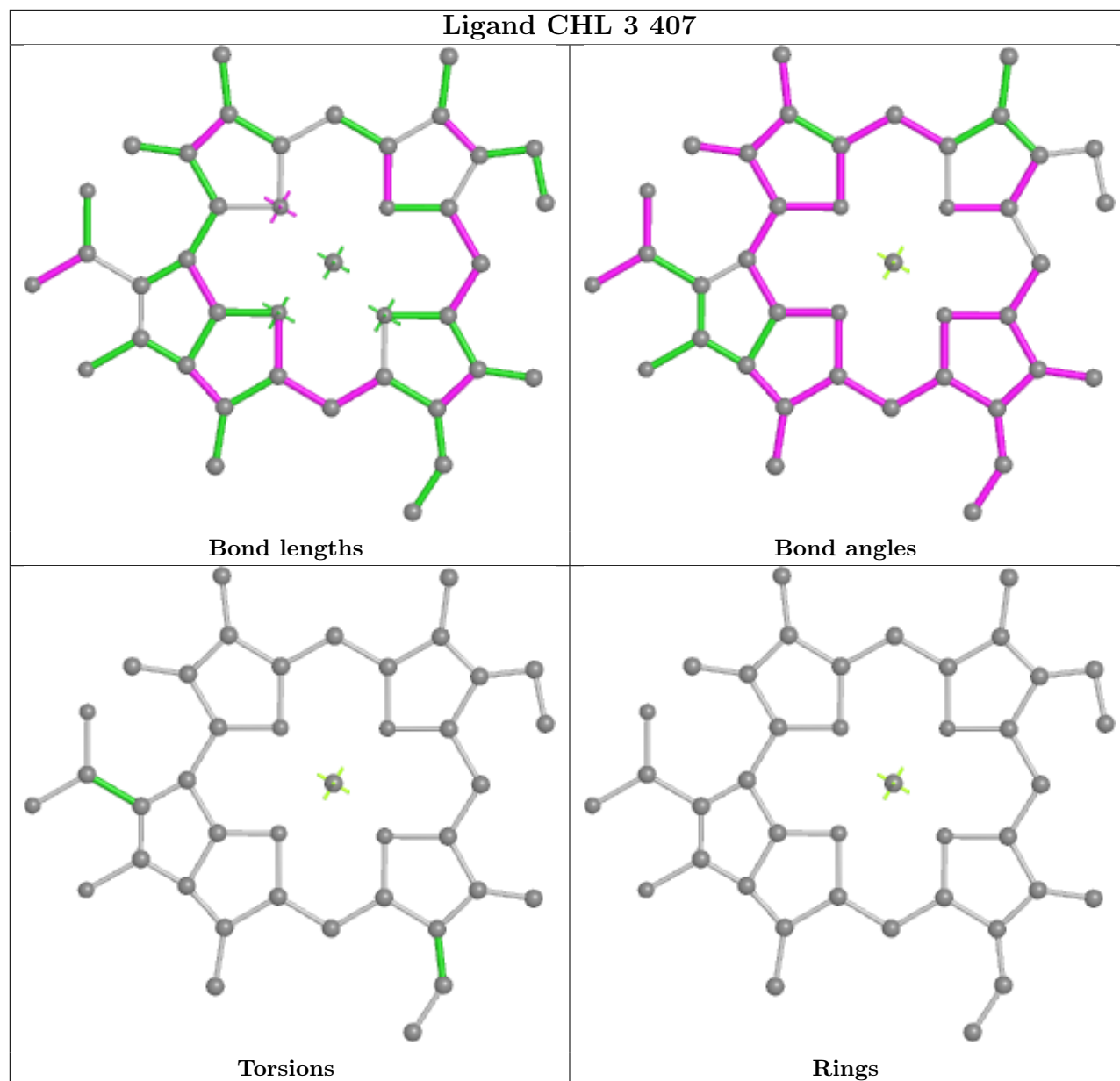
Ligand LUT 1 317**Ligand CLA A 817****Ligand CLA 9 613**



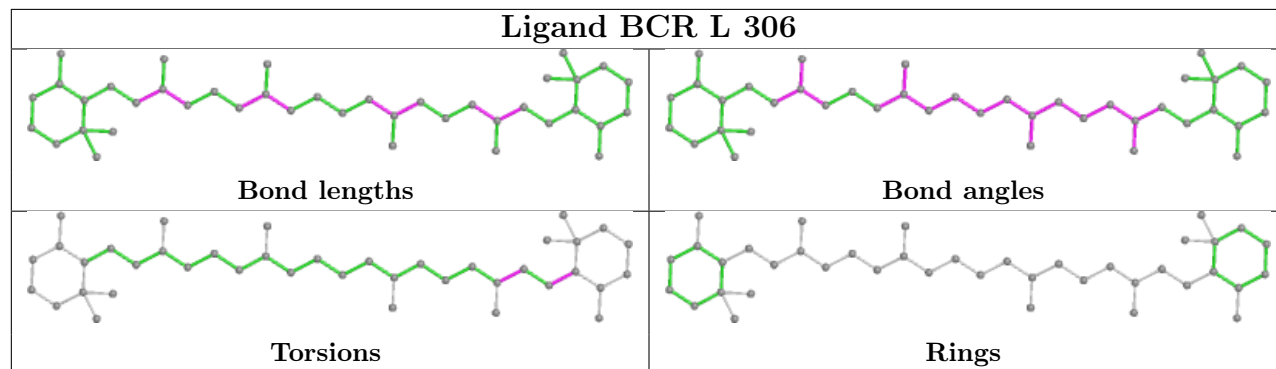
Ligand CLA 9 603



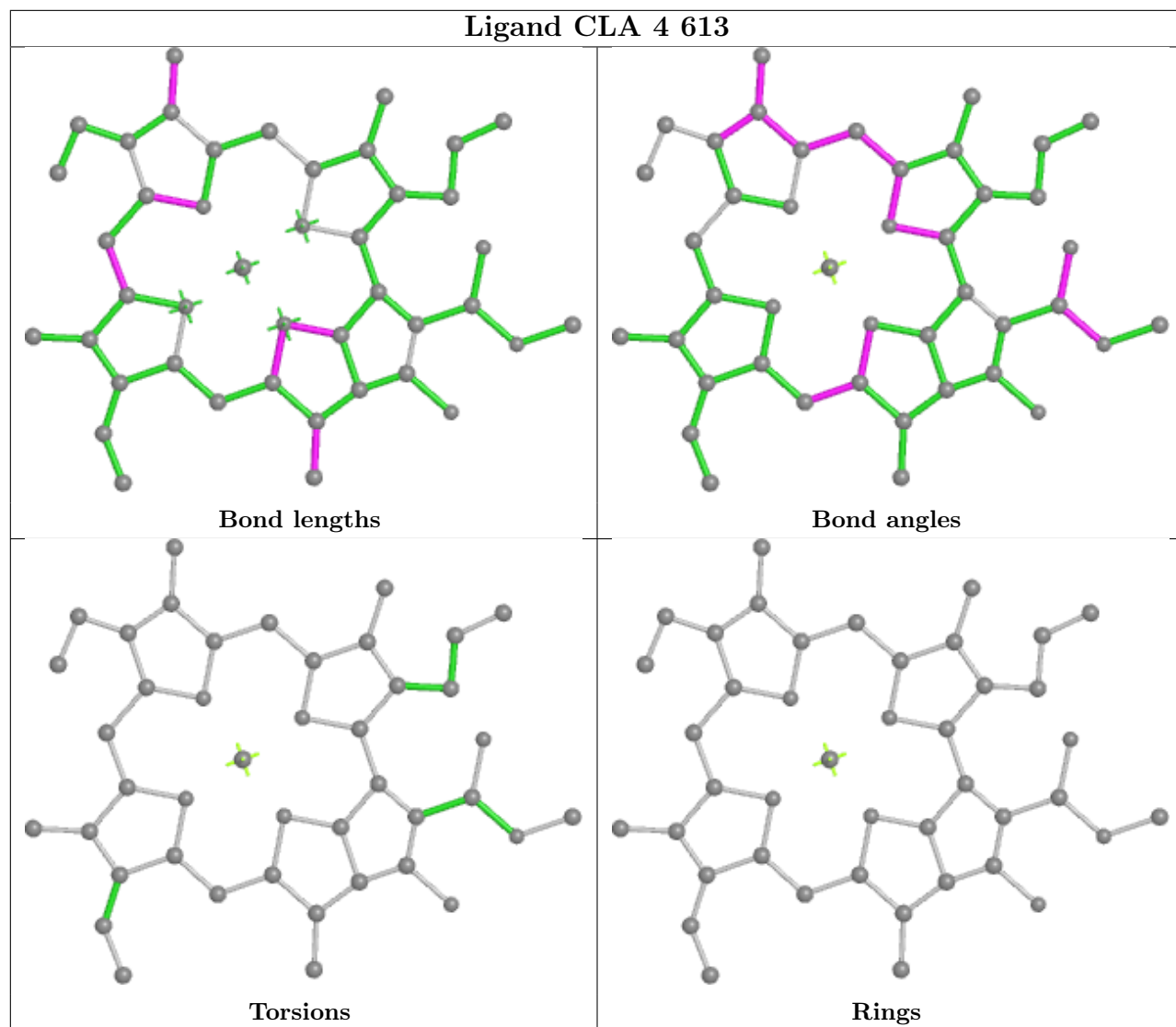
Ligand CHL 3 407



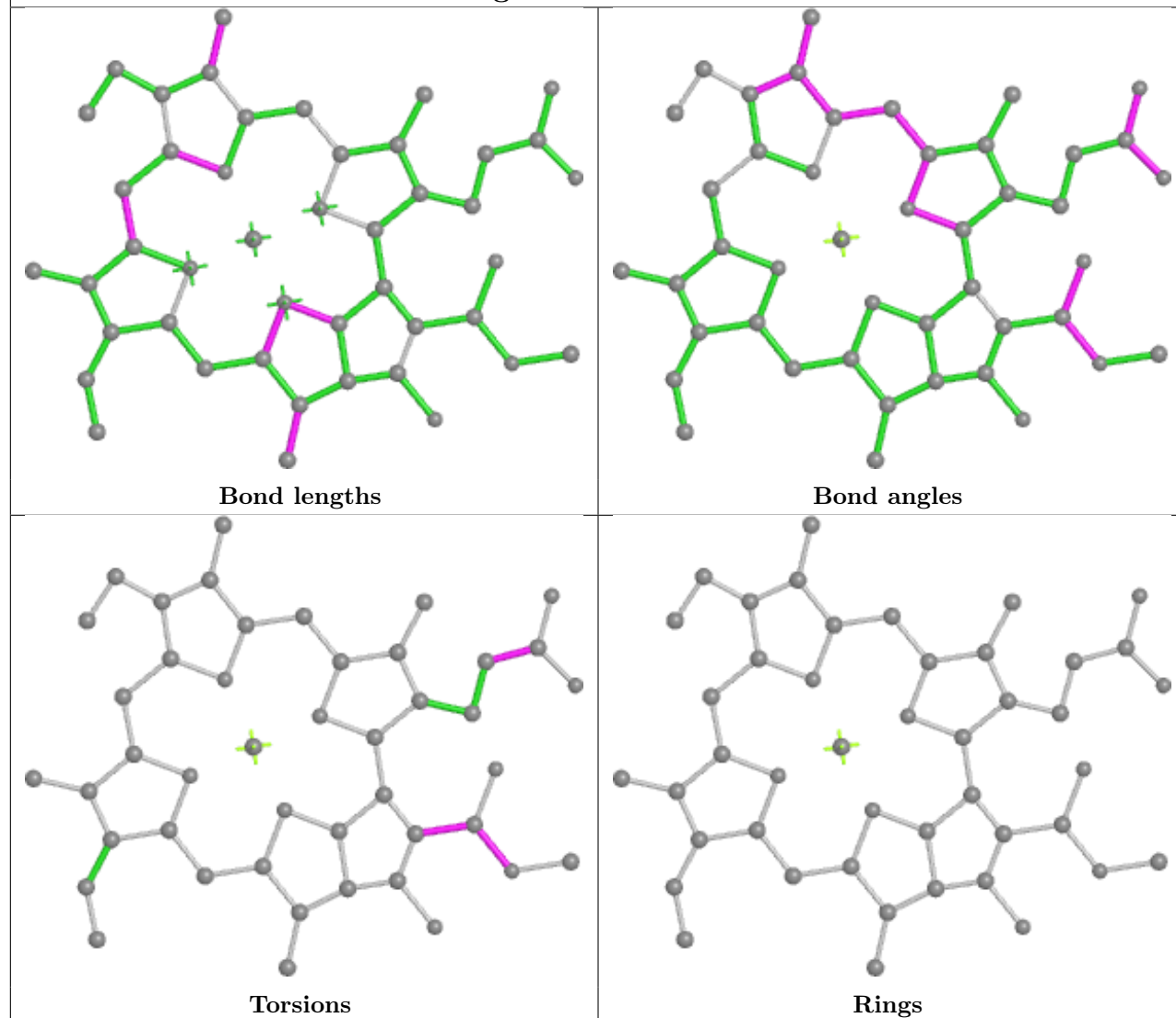
Ligand BCR L 306



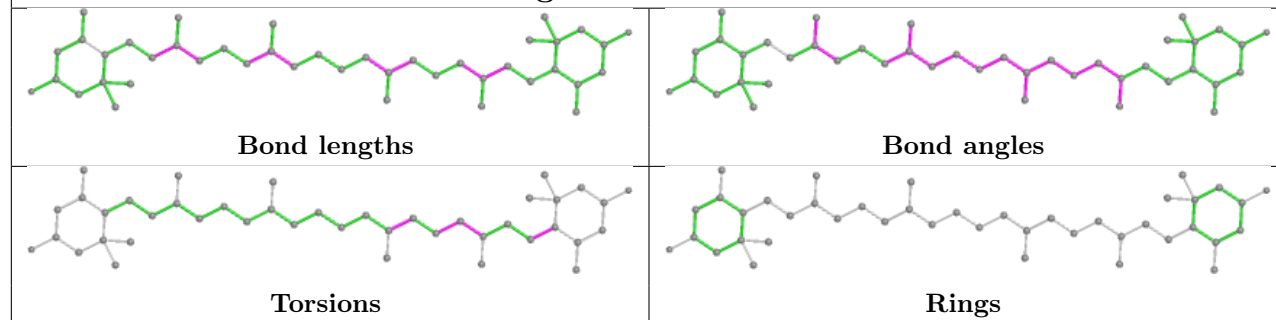
Ligand CLA 4 613

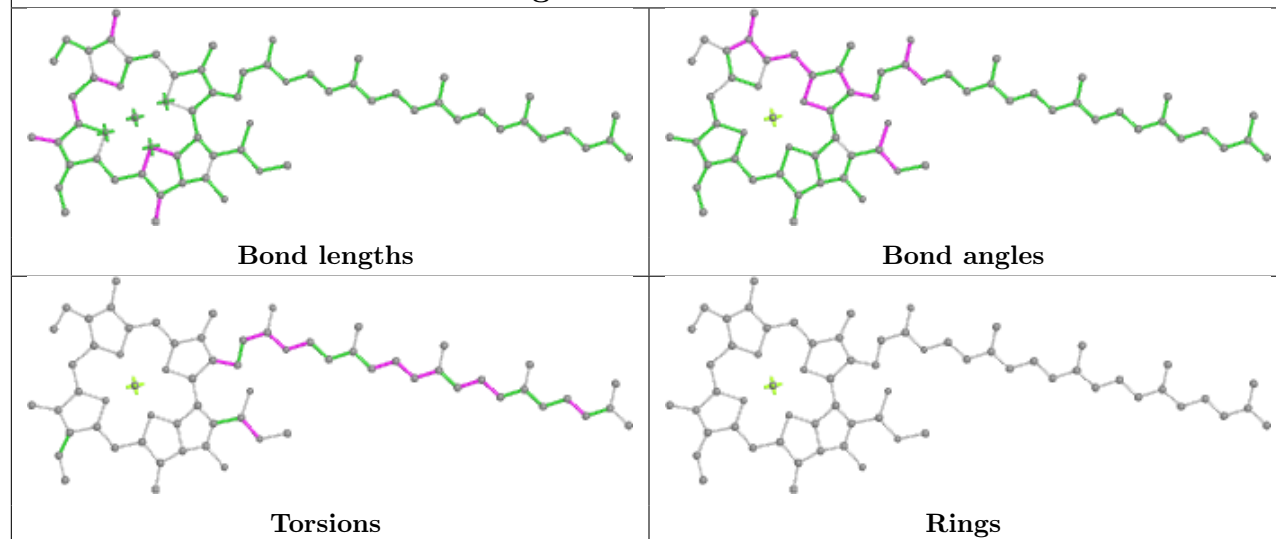
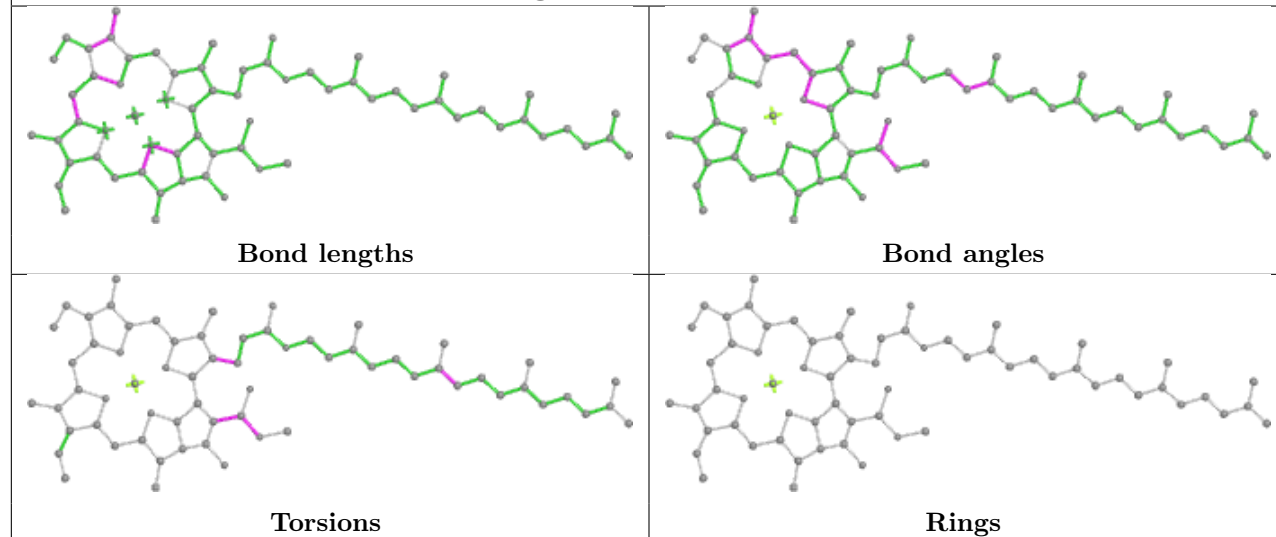


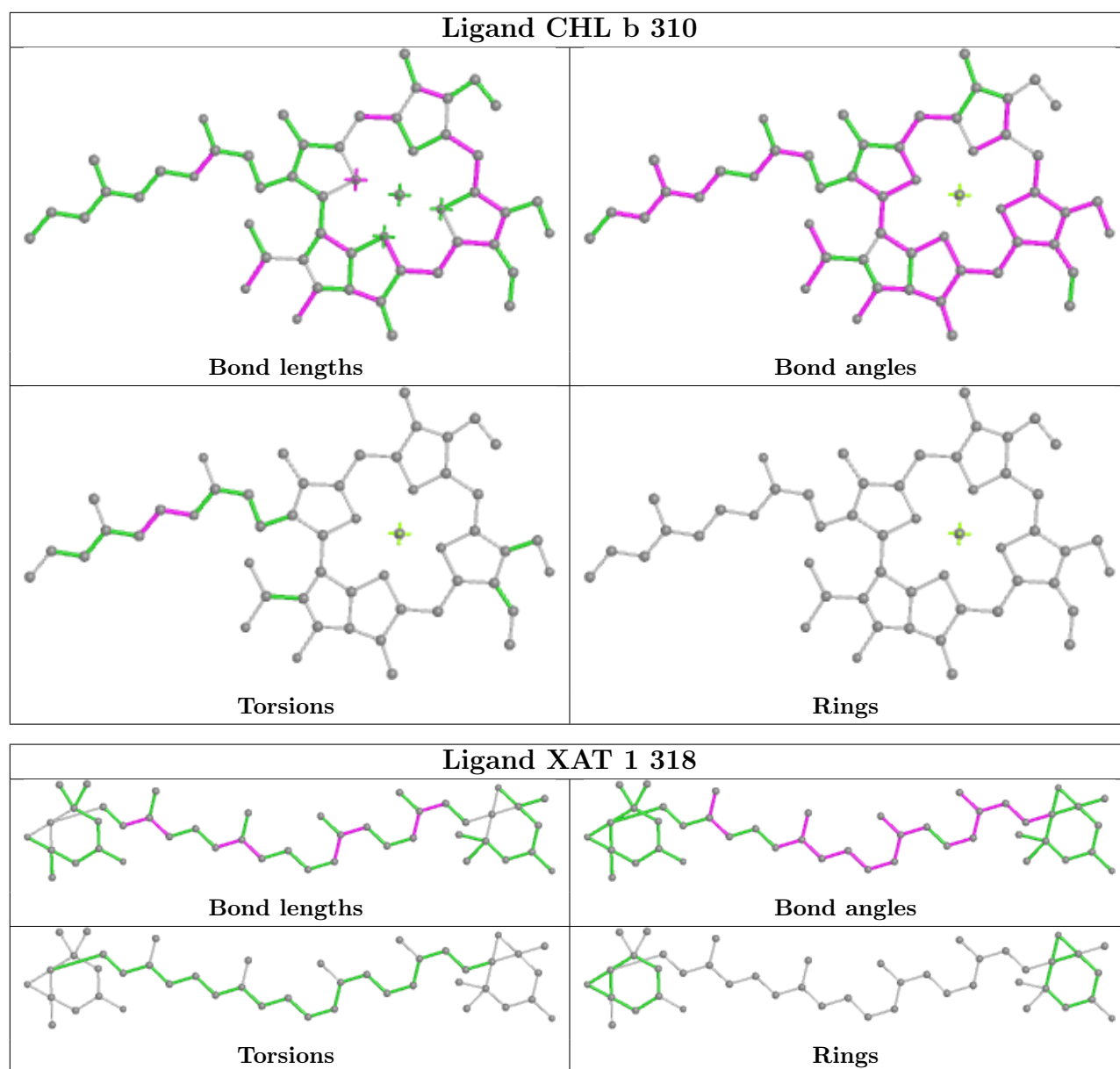
Ligand CLA b 304



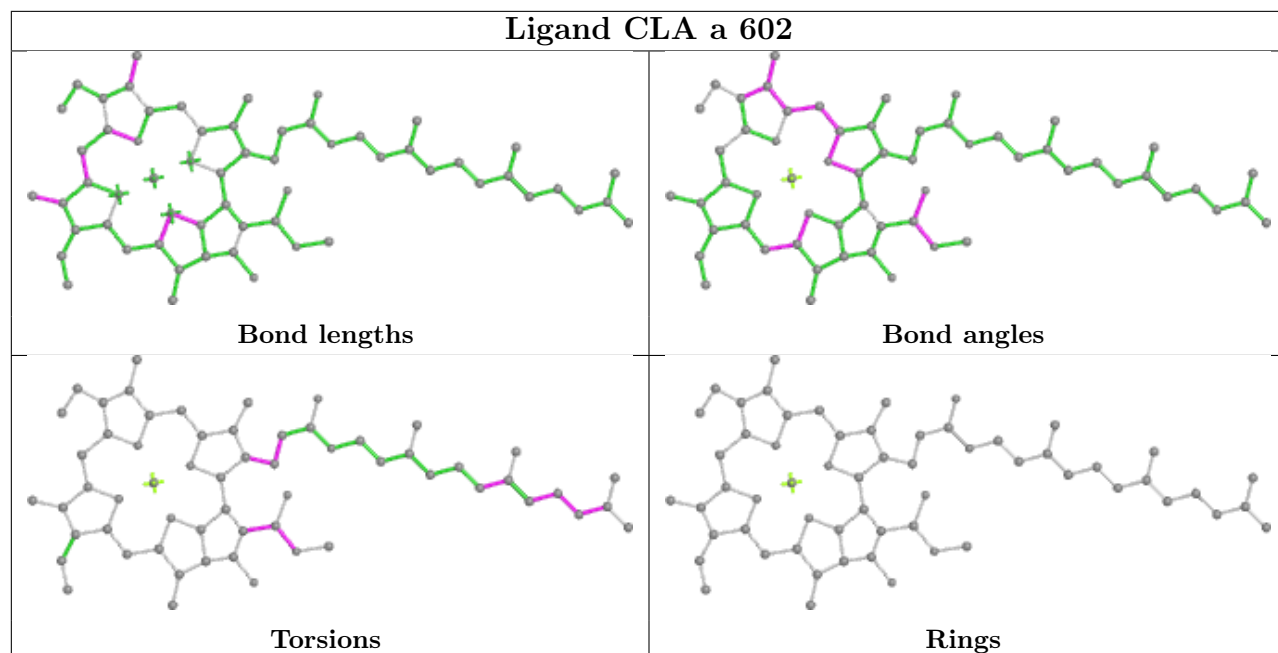
Ligand LUT 5 615



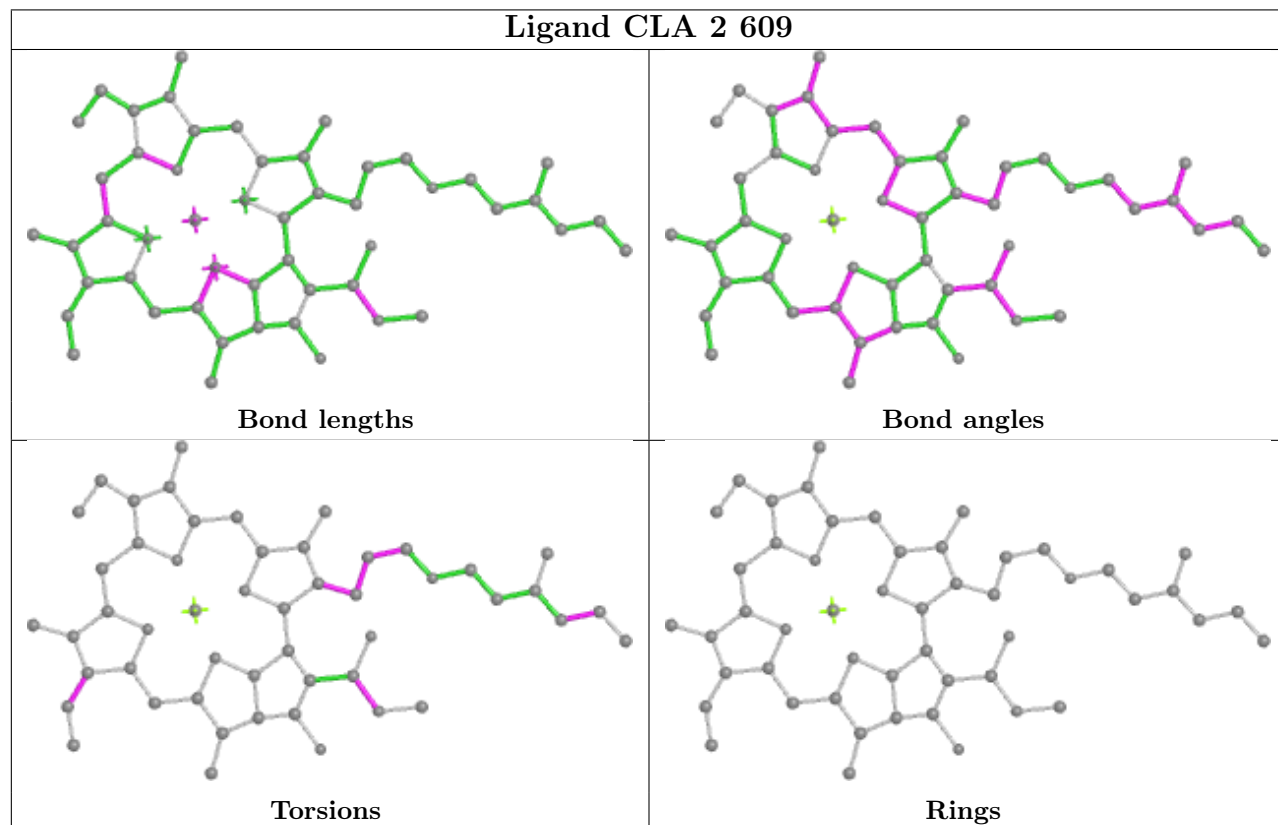
Ligand CLA B 807**Ligand CLA A 833**

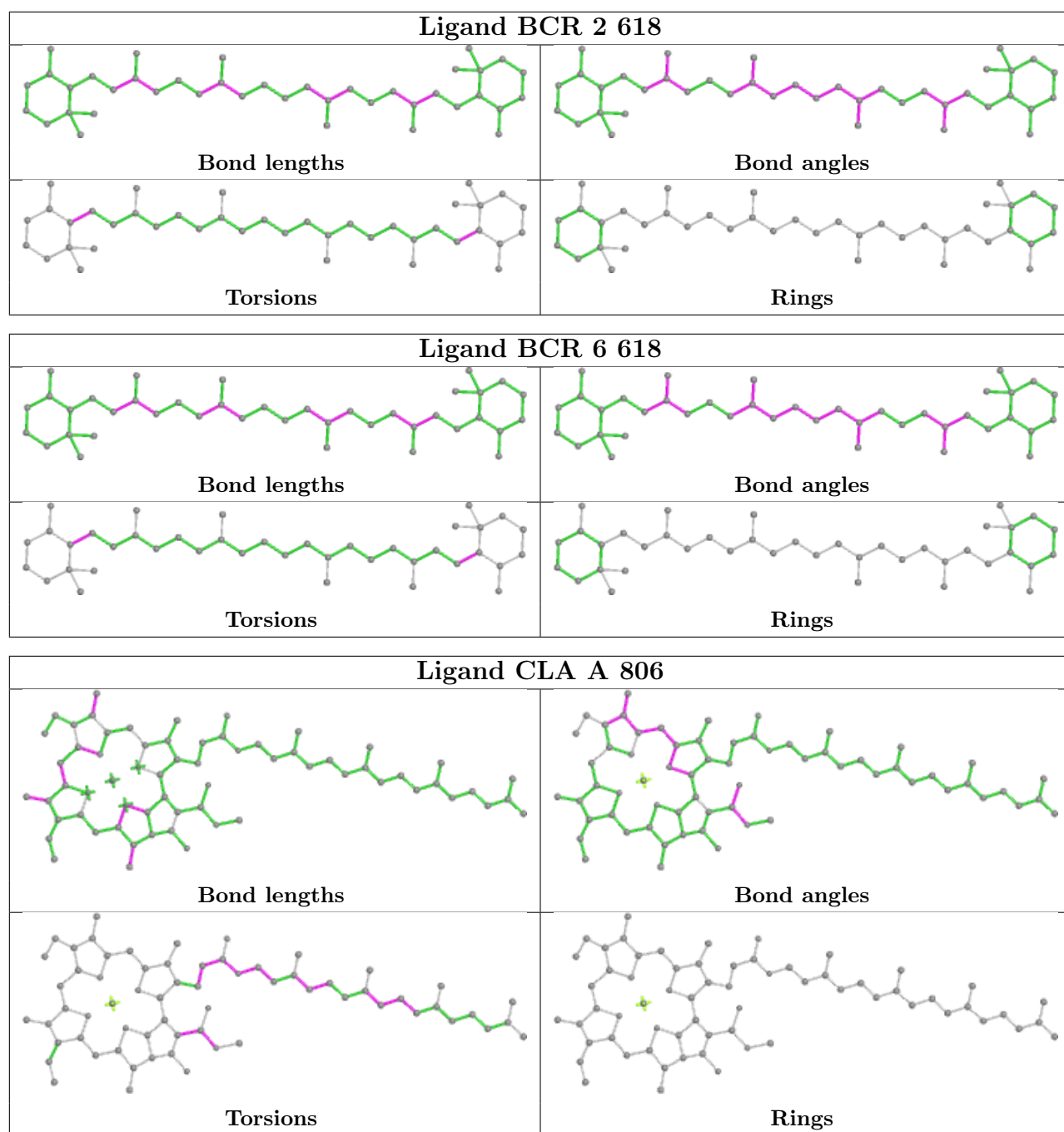


Ligand CLA a 602

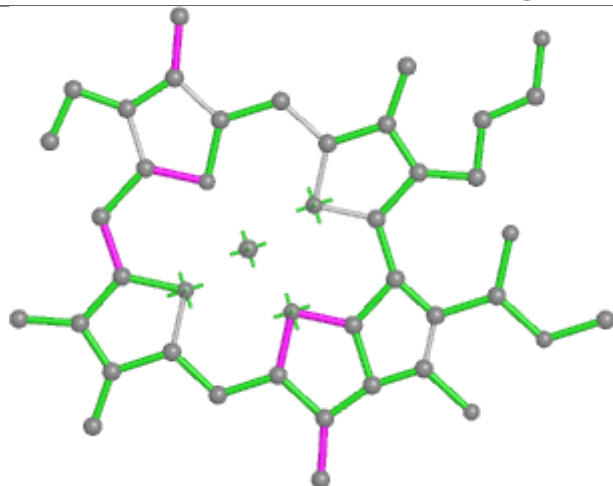


Ligand CLA 2 609

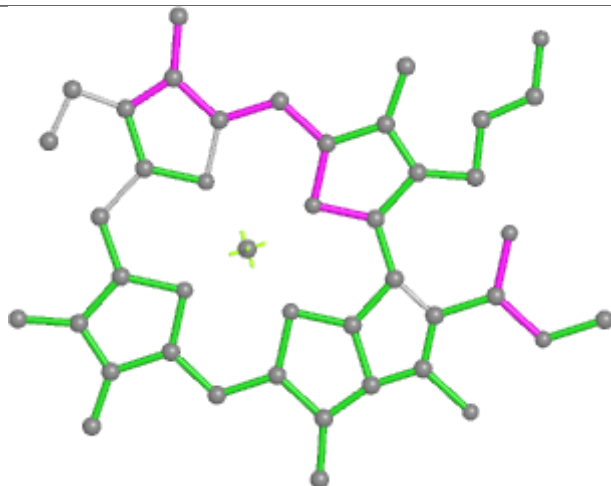




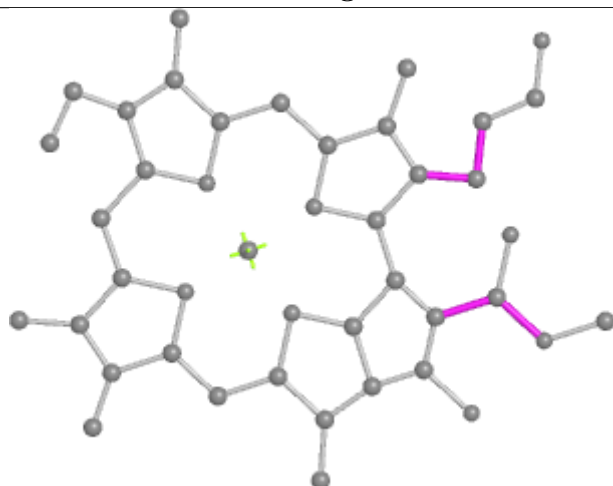
Ligand CLA 8 604



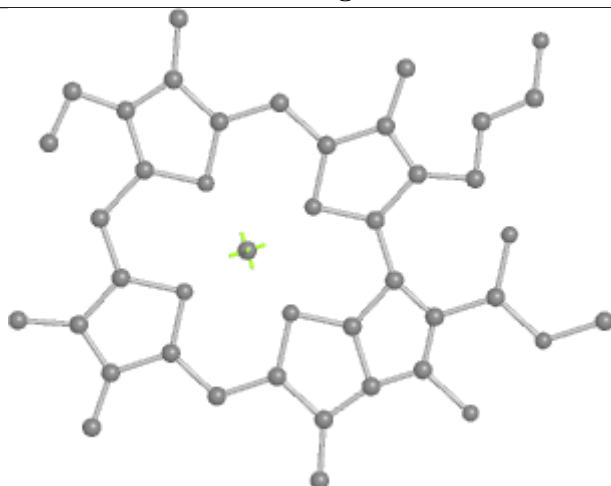
Bond lengths



Bond angles

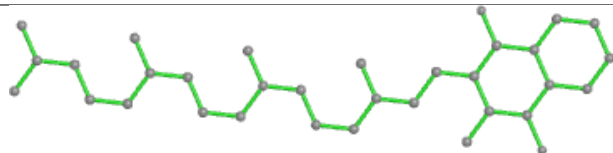


Torsions

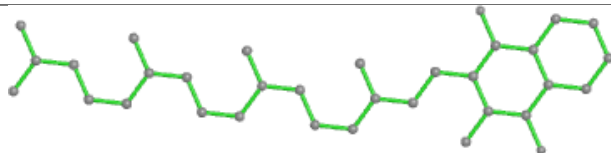


Rings

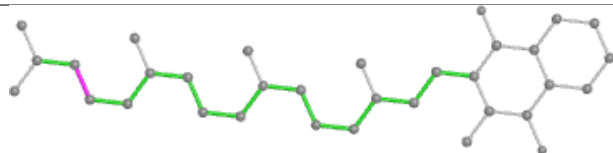
Ligand PQN A 843



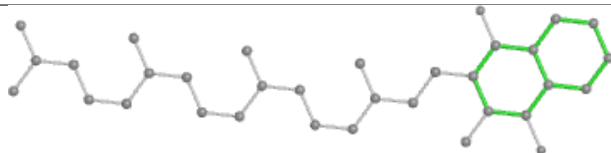
Bond lengths



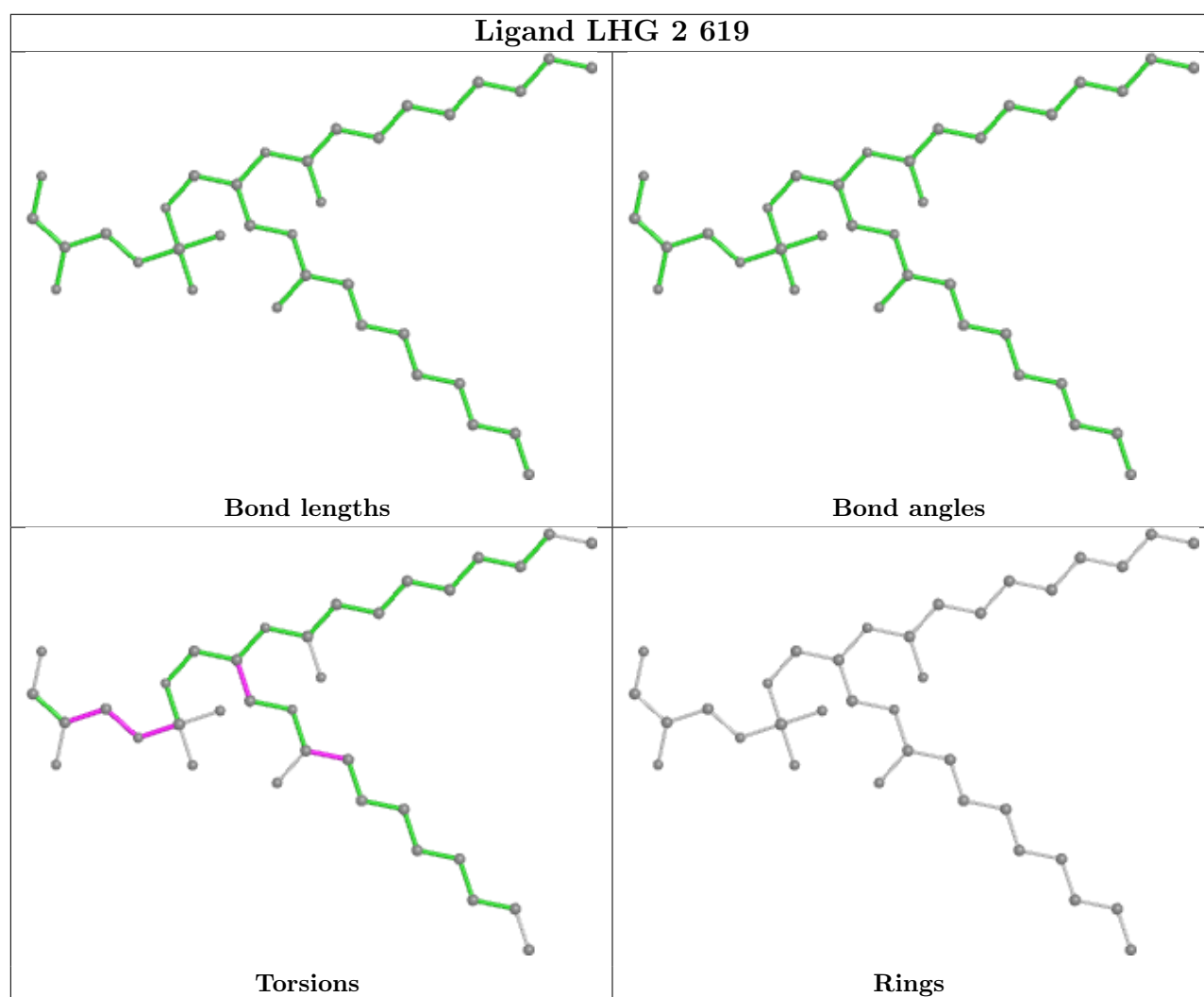
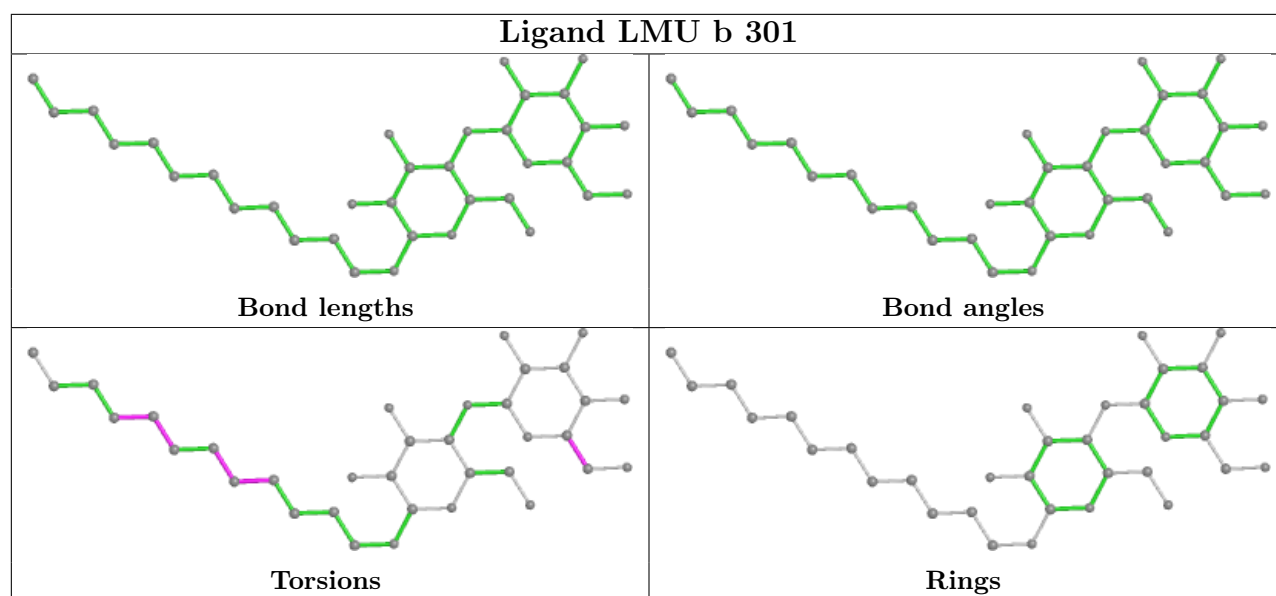
Bond angles



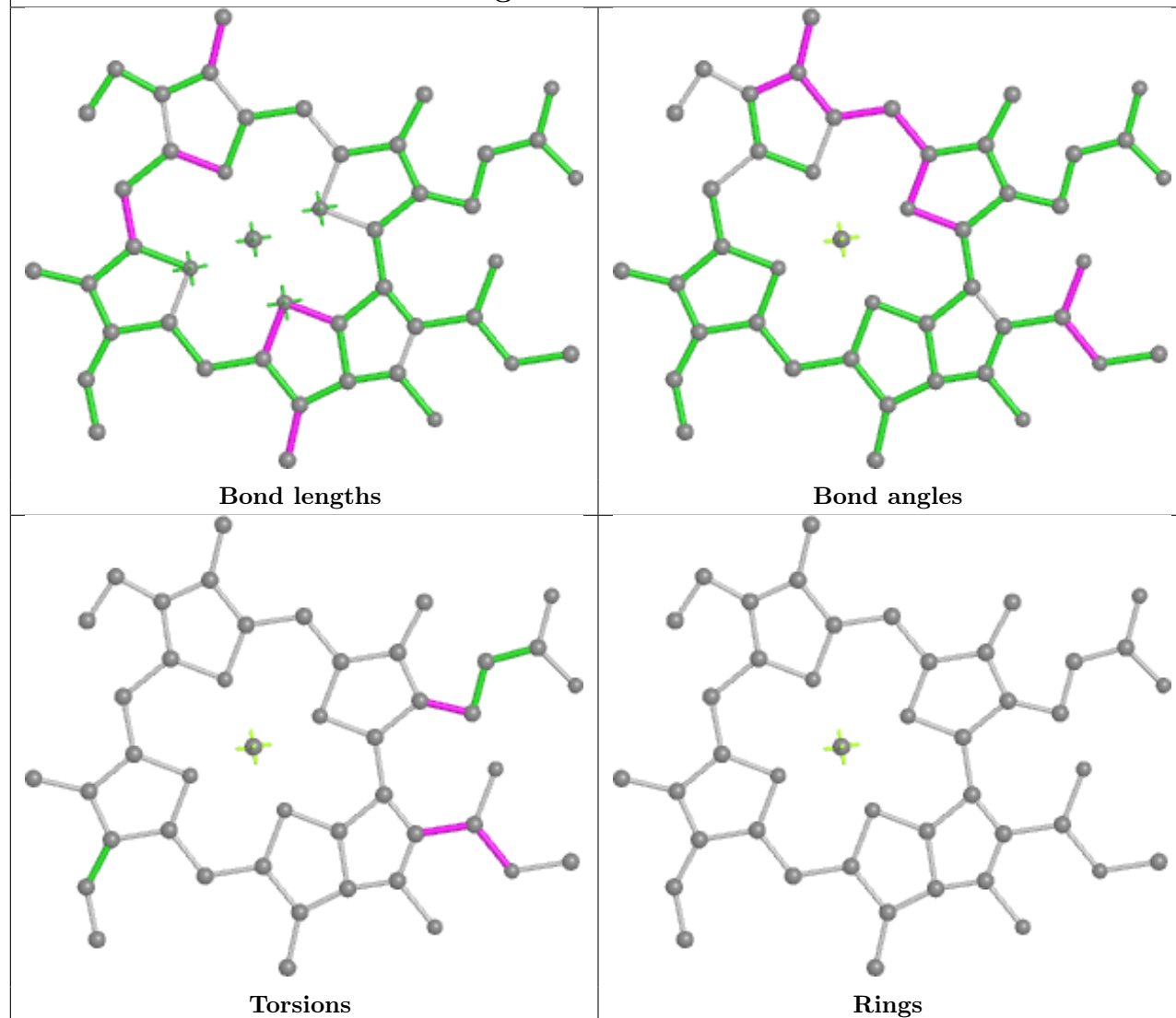
Torsions



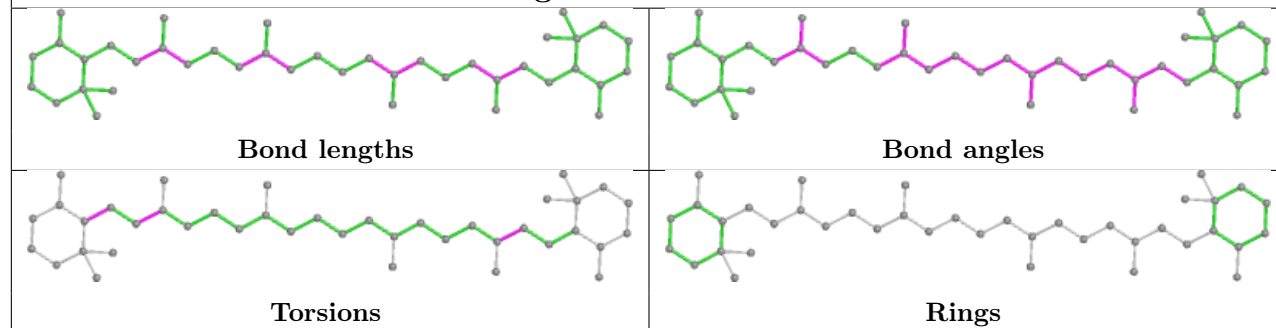
Rings

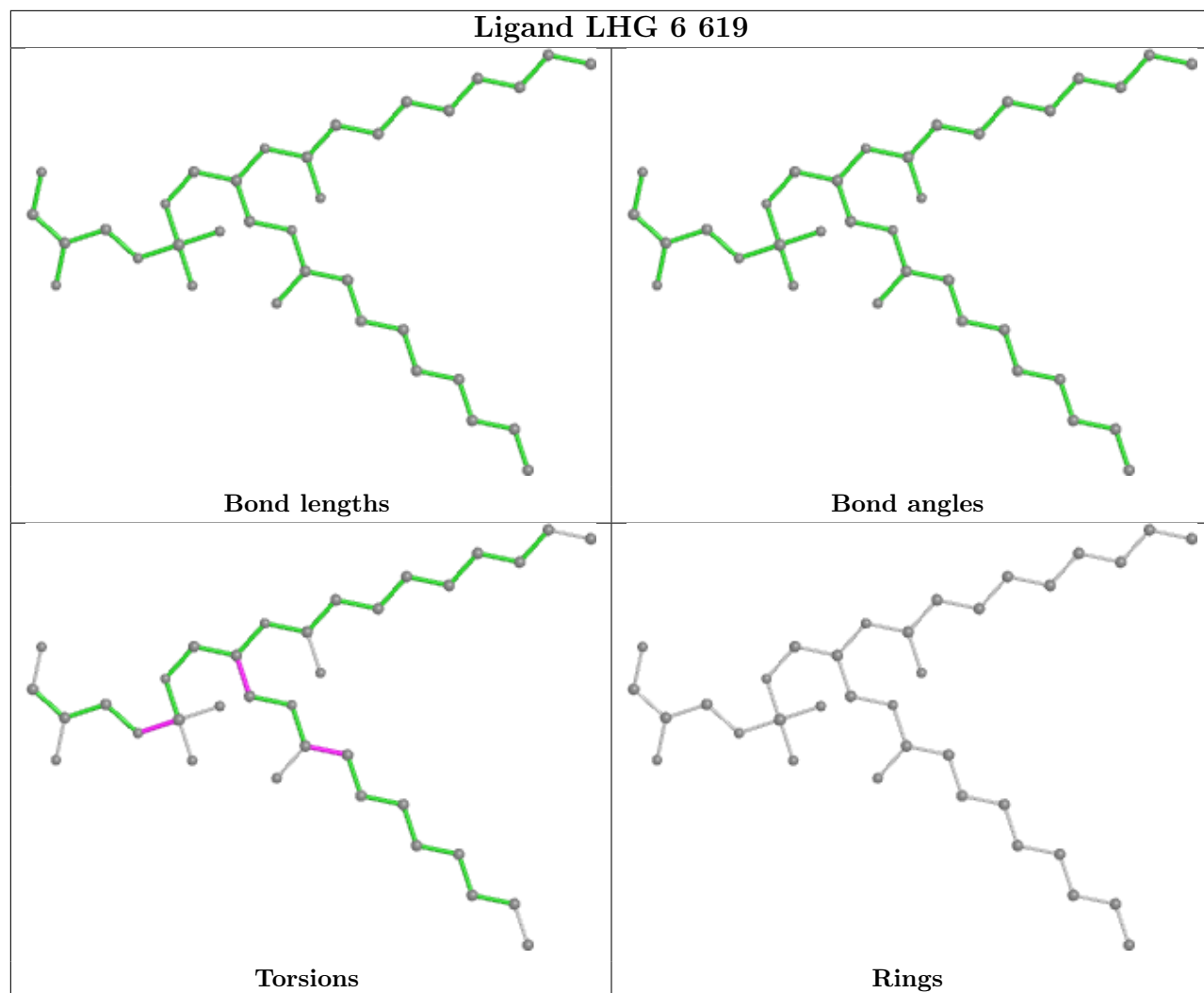


Ligand CLA c 614

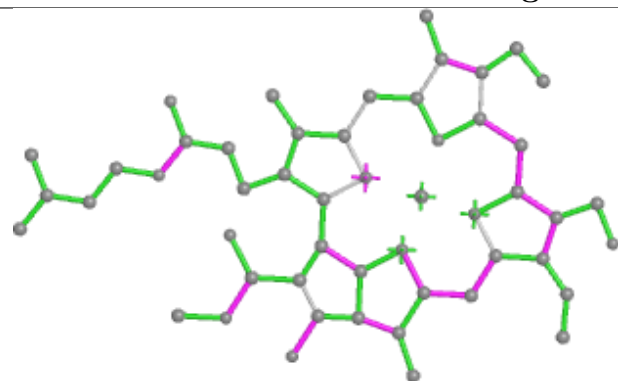


Ligand BCR 7 418

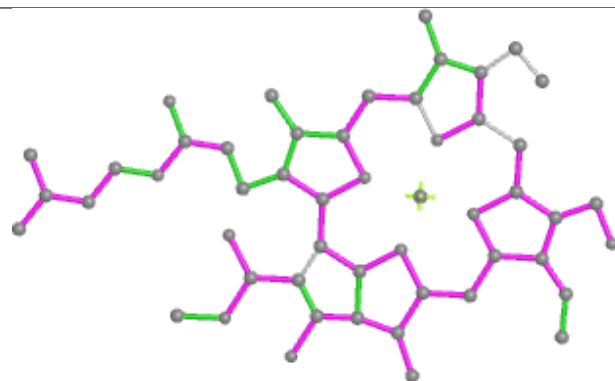




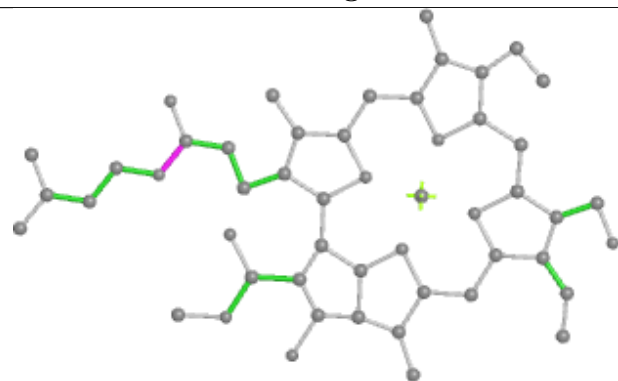
Ligand CHL 1 307



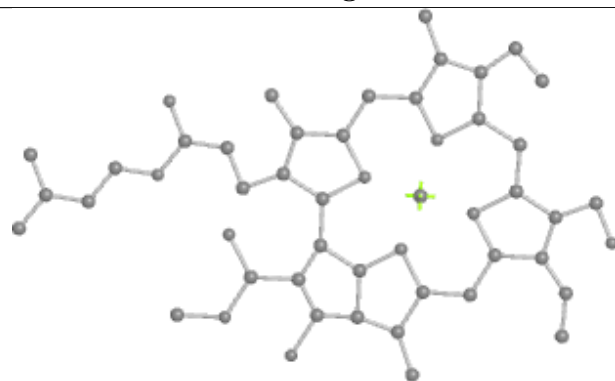
Bond lengths



Bond angles

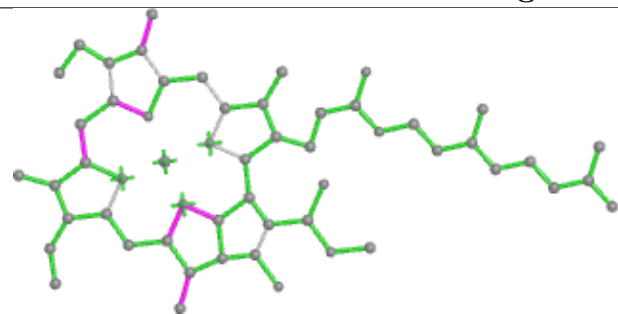


Torsions

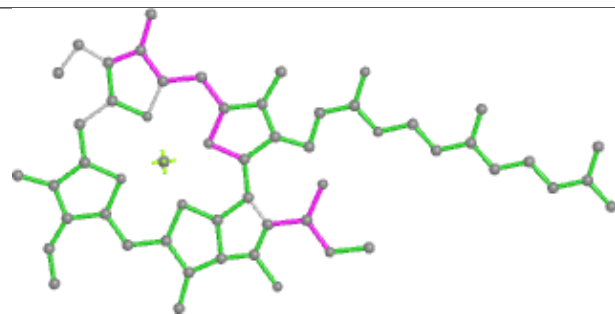


Rings

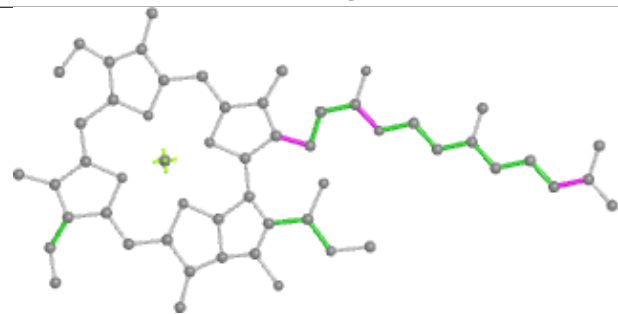
Ligand CLA A 805



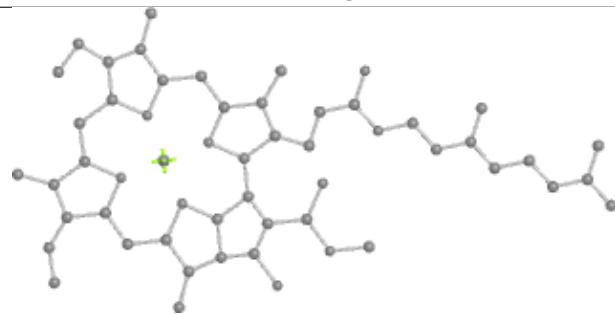
Bond lengths



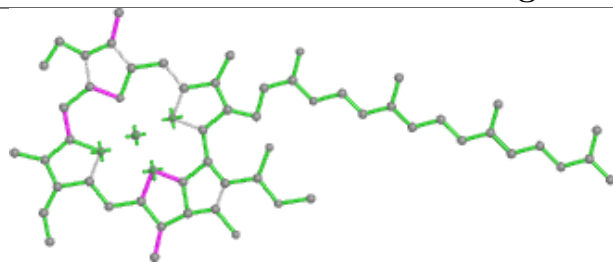
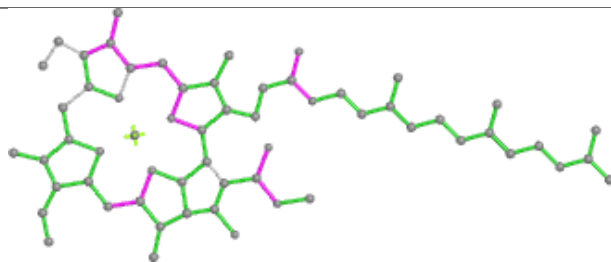
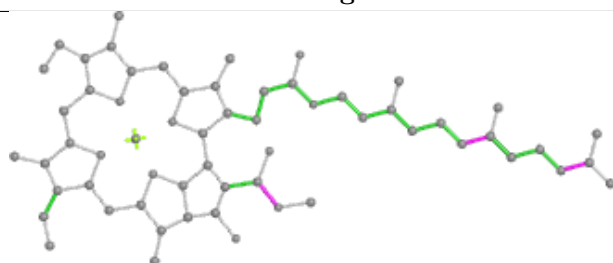
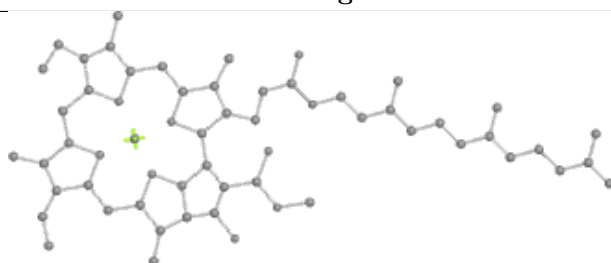
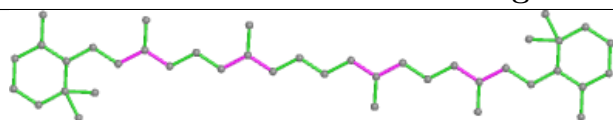
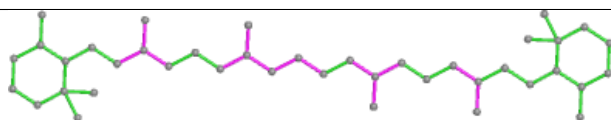
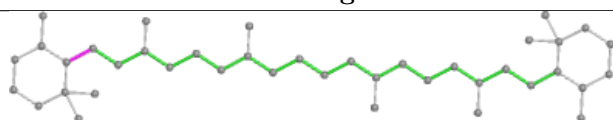
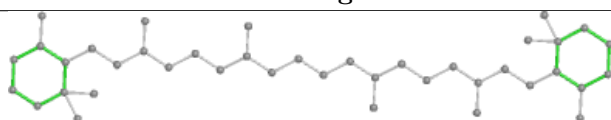
Bond angles



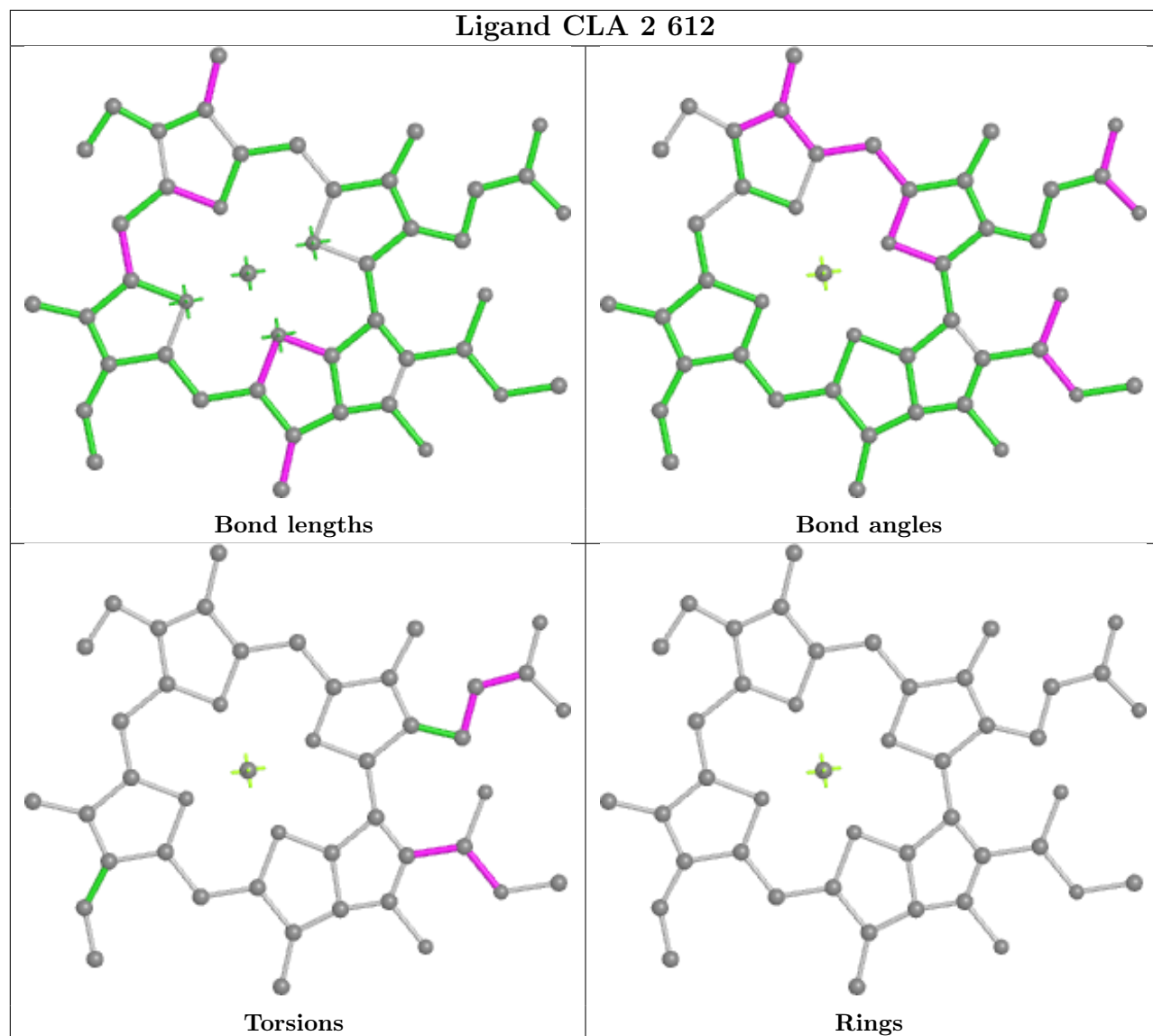
Torsions

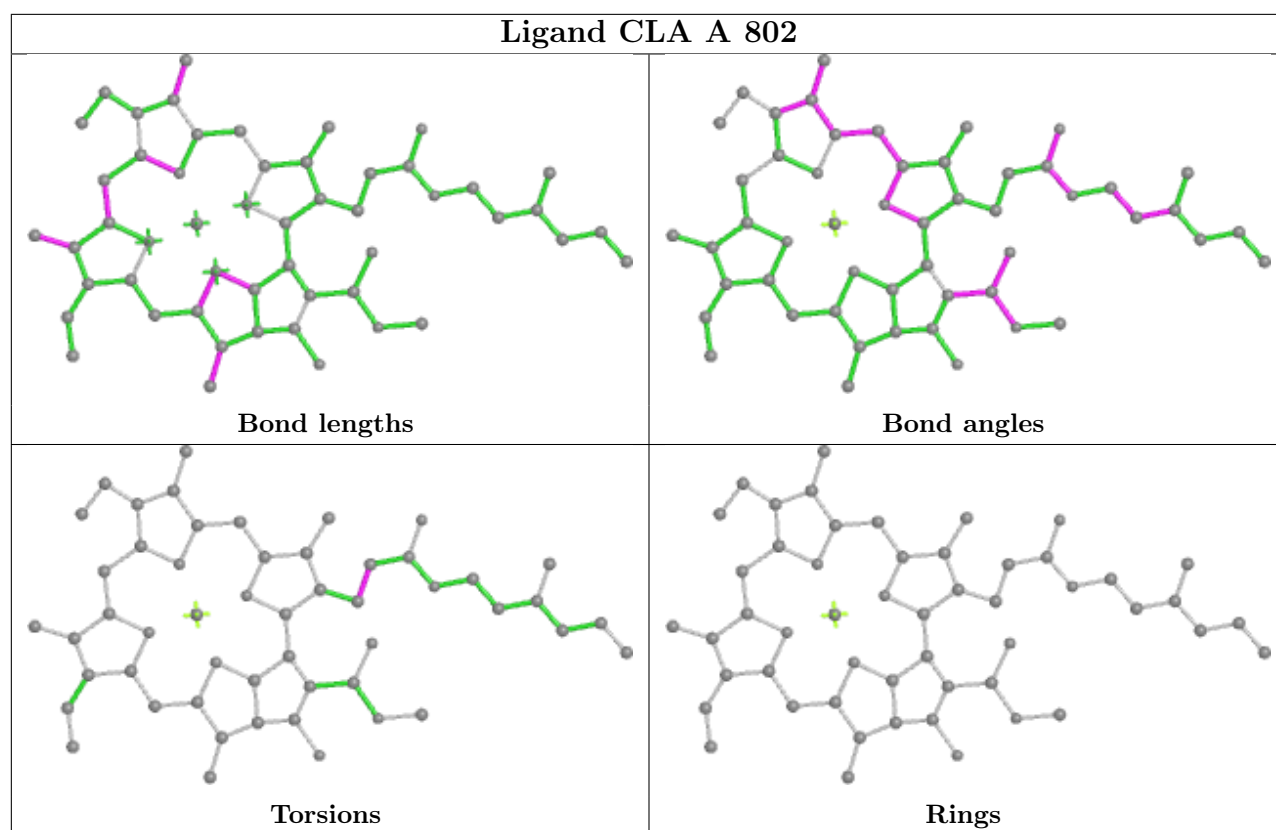


Rings

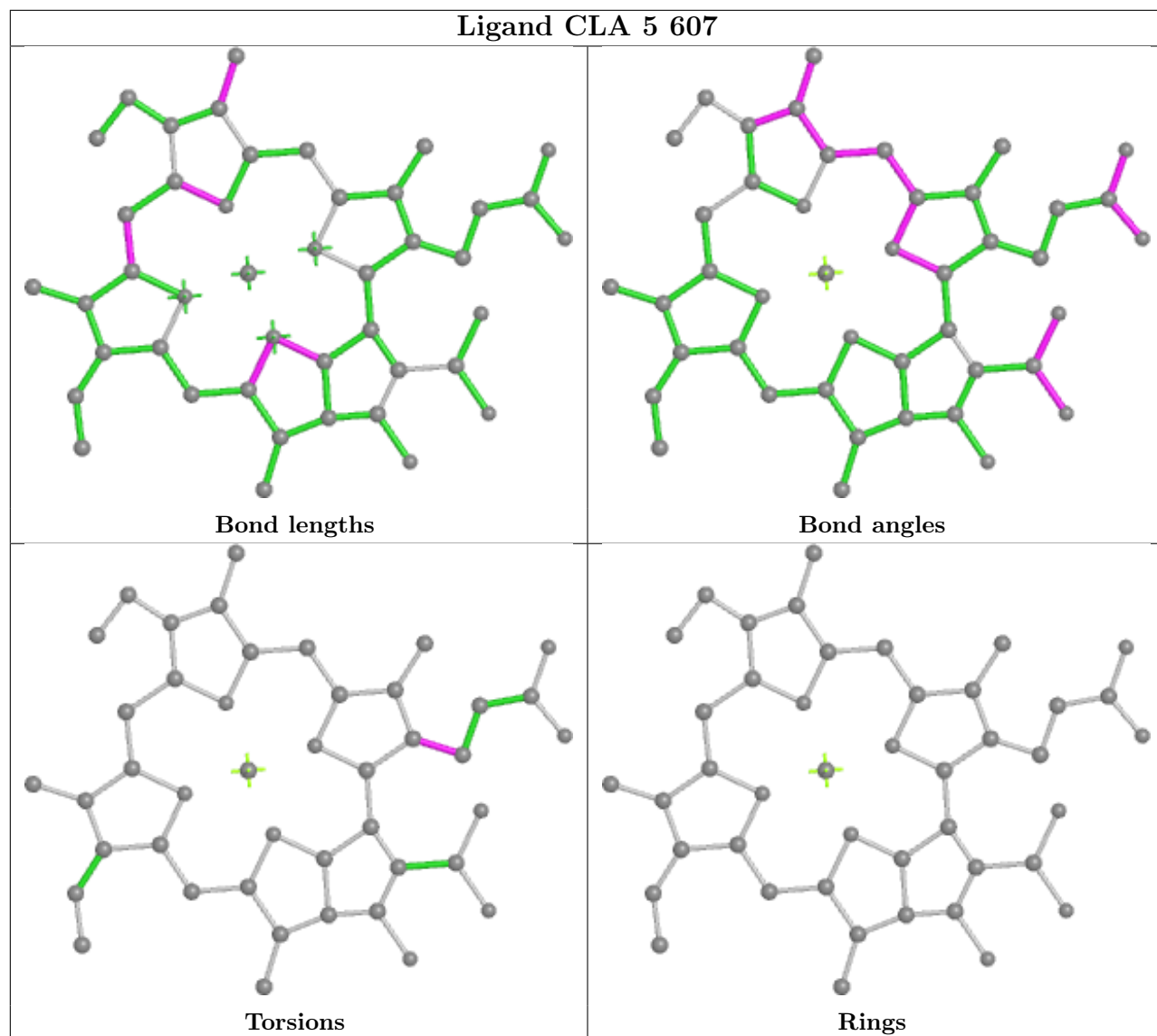
Ligand CLA 3 402**Bond lengths****Bond angles****Torsions****Rings****Ligand BCR A 848****Bond lengths****Bond angles****Torsions****Rings**

Ligand CLA 2 612

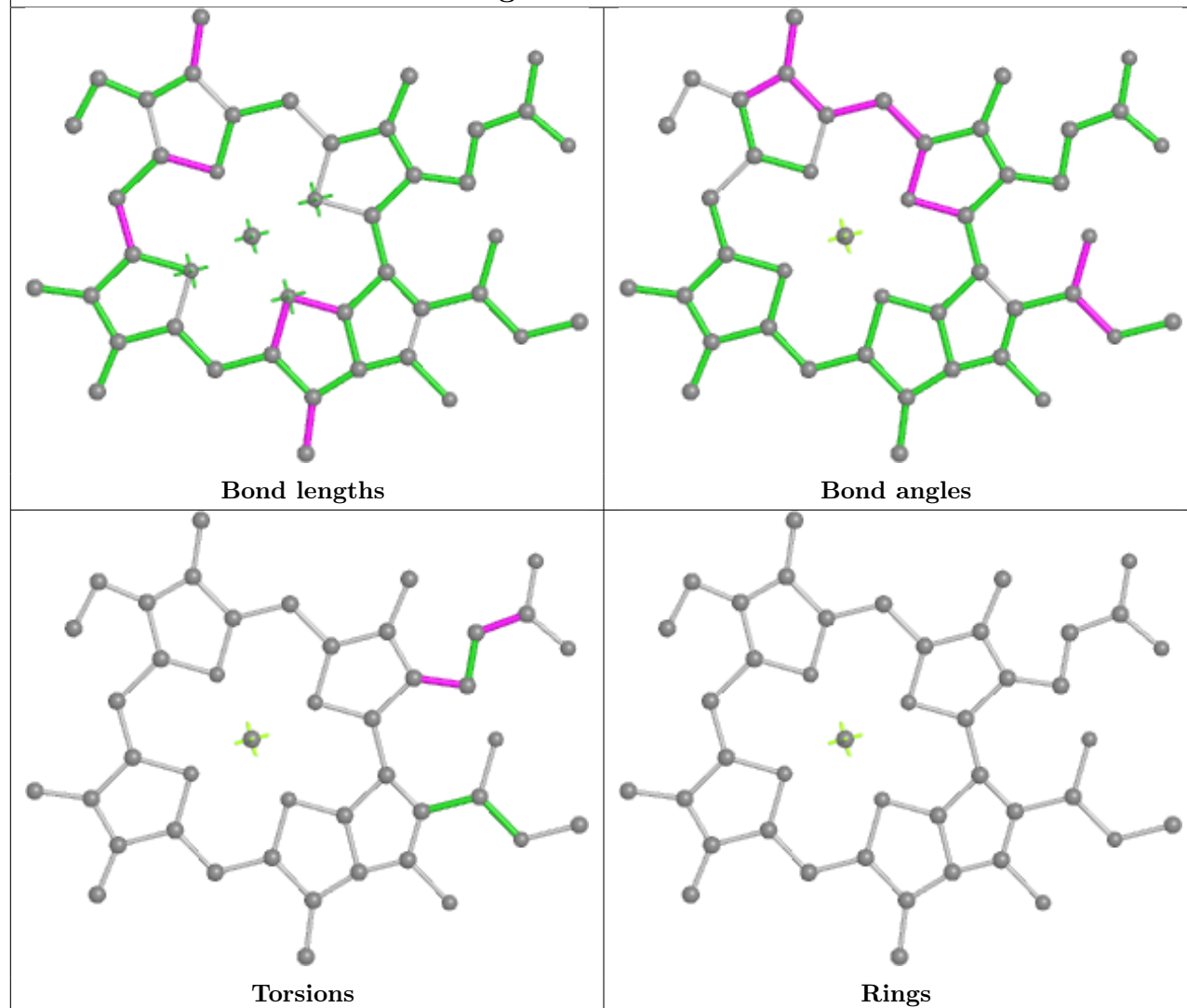




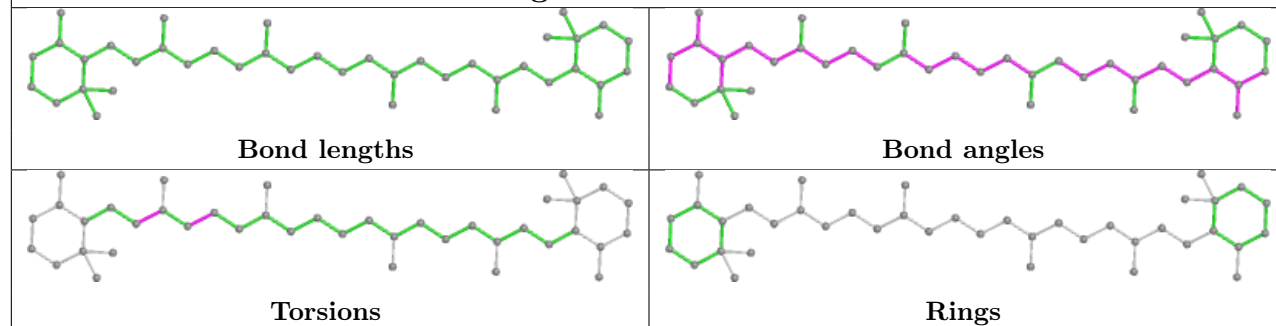
Ligand CLA 5 607



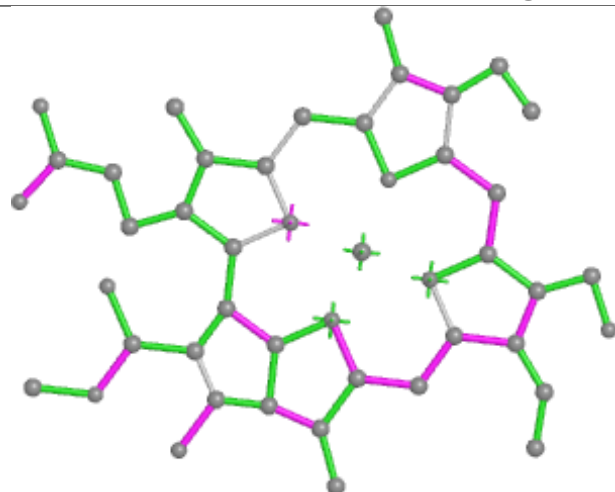
Ligand CLA 4 611



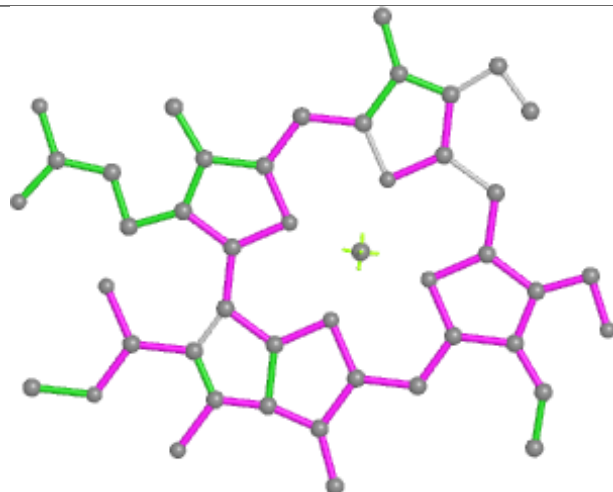
Ligand BCR B 846



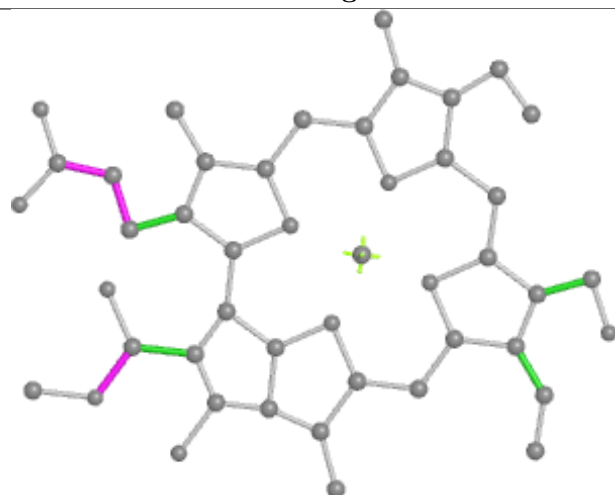
Ligand CHL 4 606



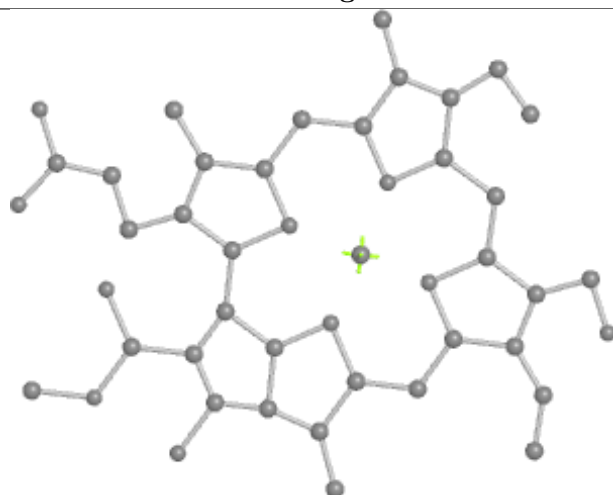
Bond lengths



Bond angles

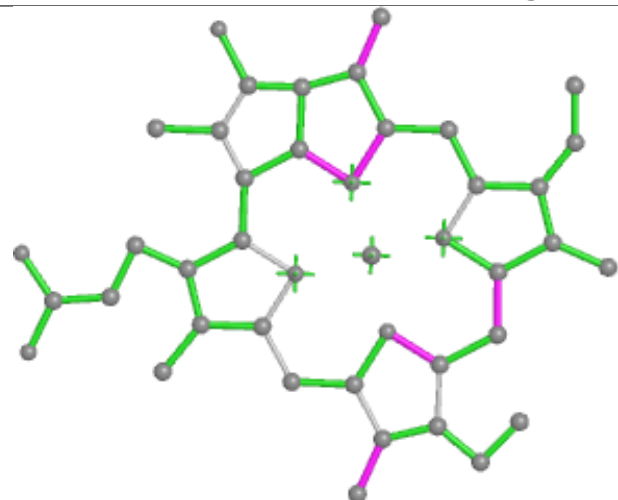


Torsions

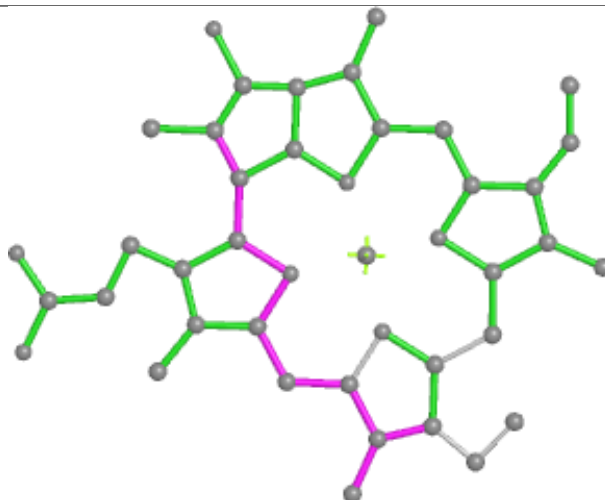


Rings

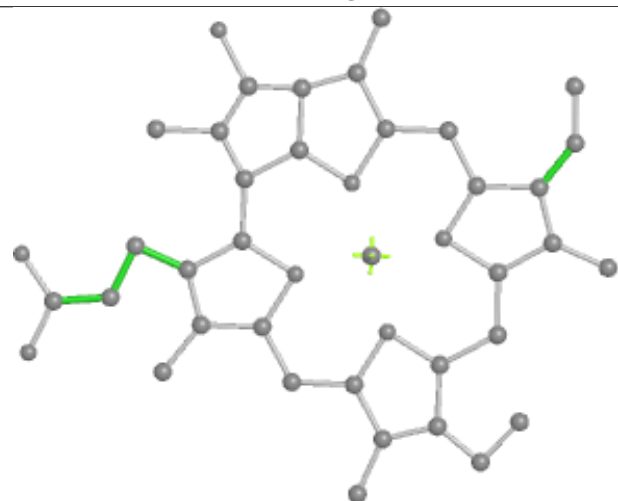
Ligand CLA 6 610



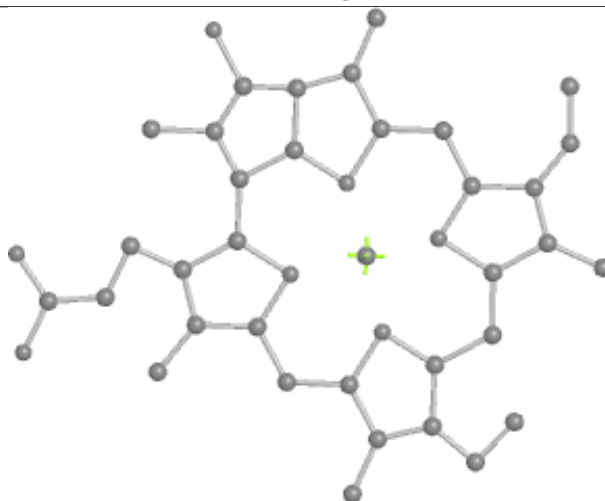
Bond lengths



Bond angles

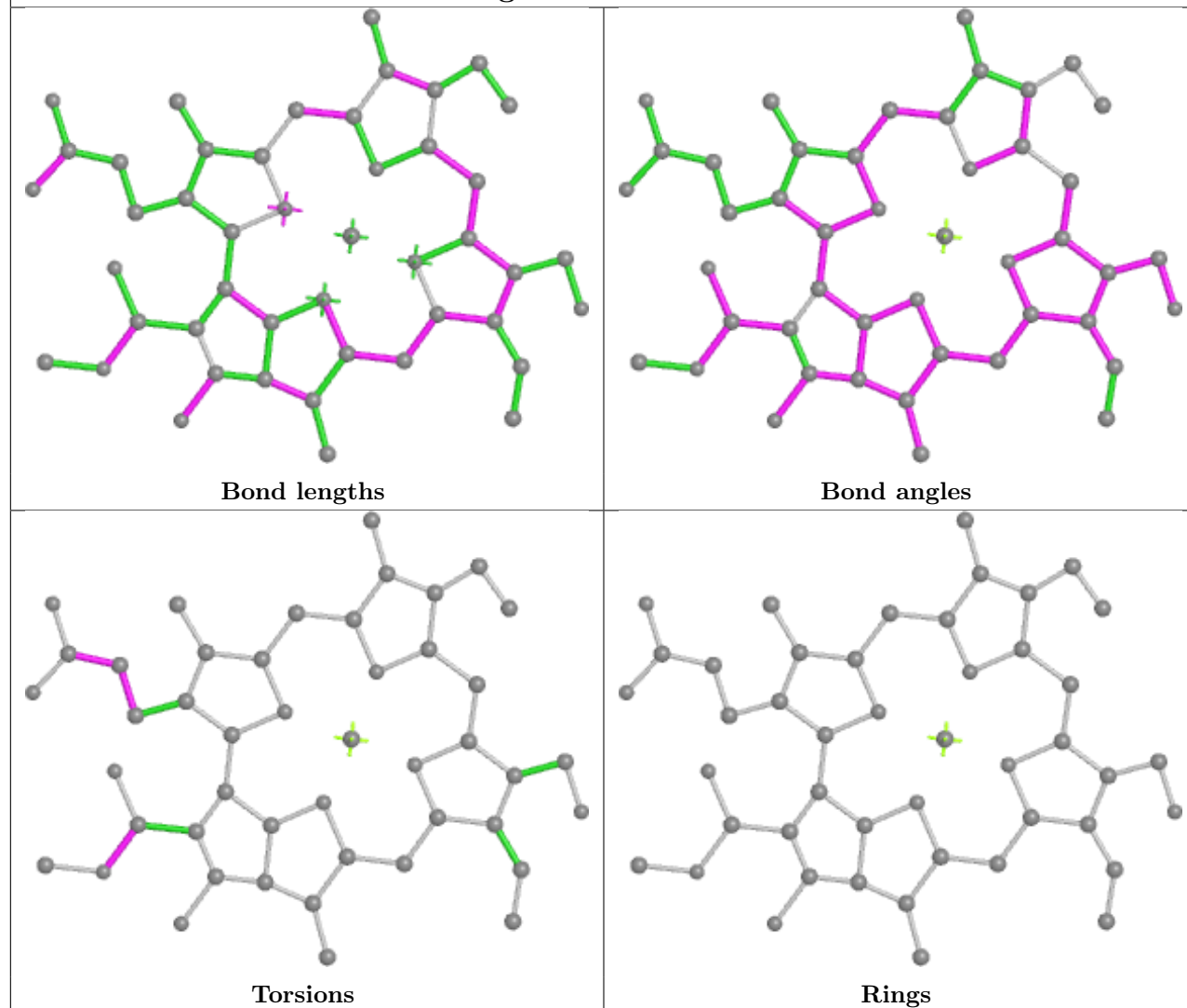


Torsions

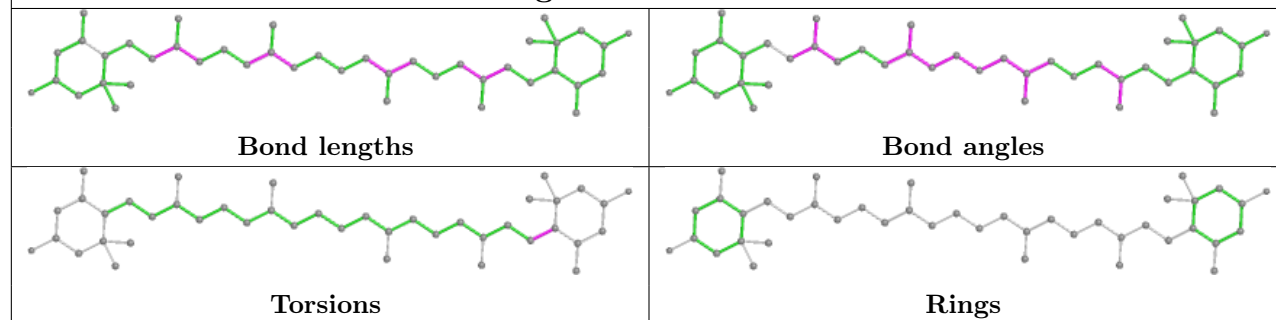


Rings

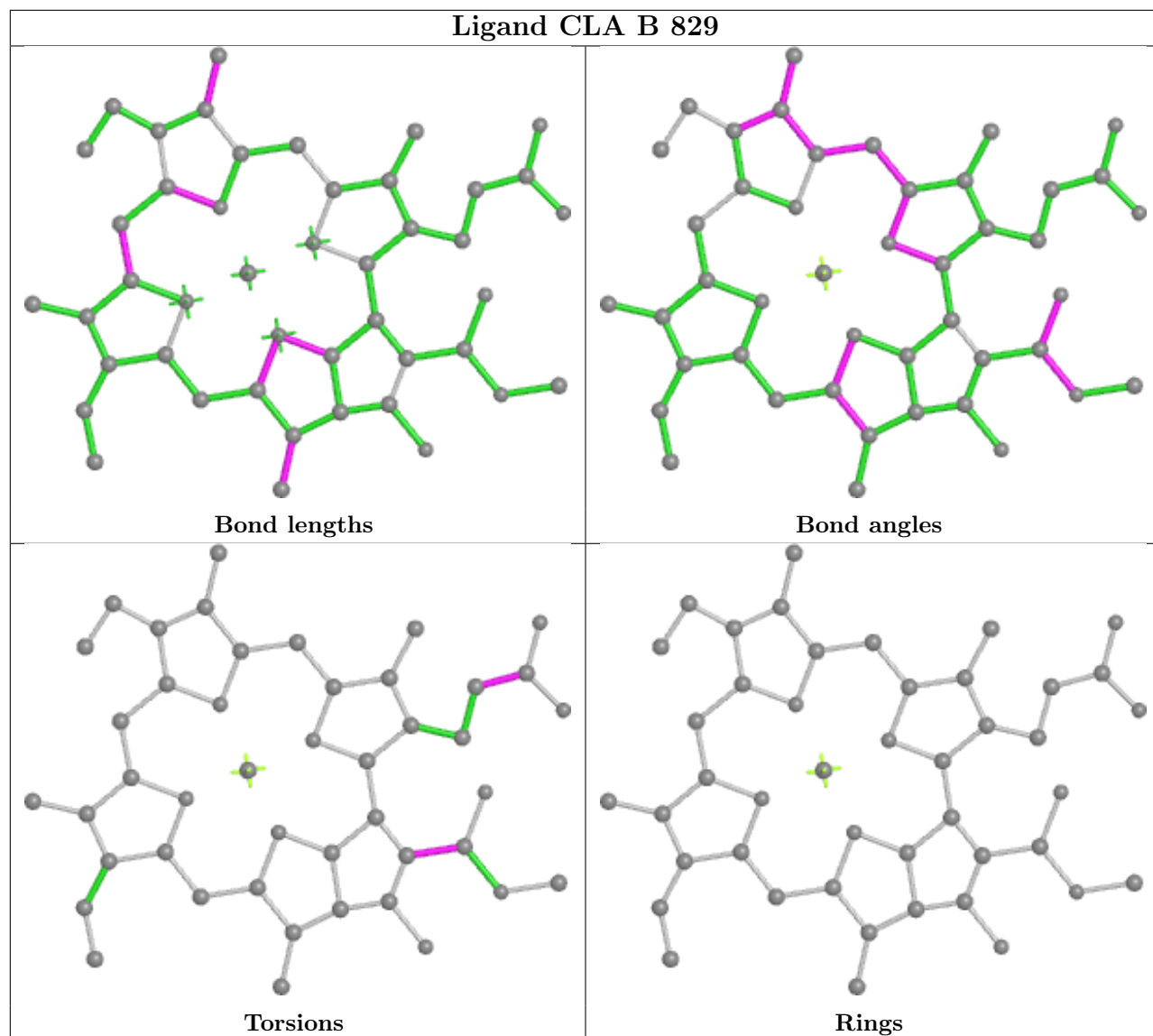
Ligand CHL a 608



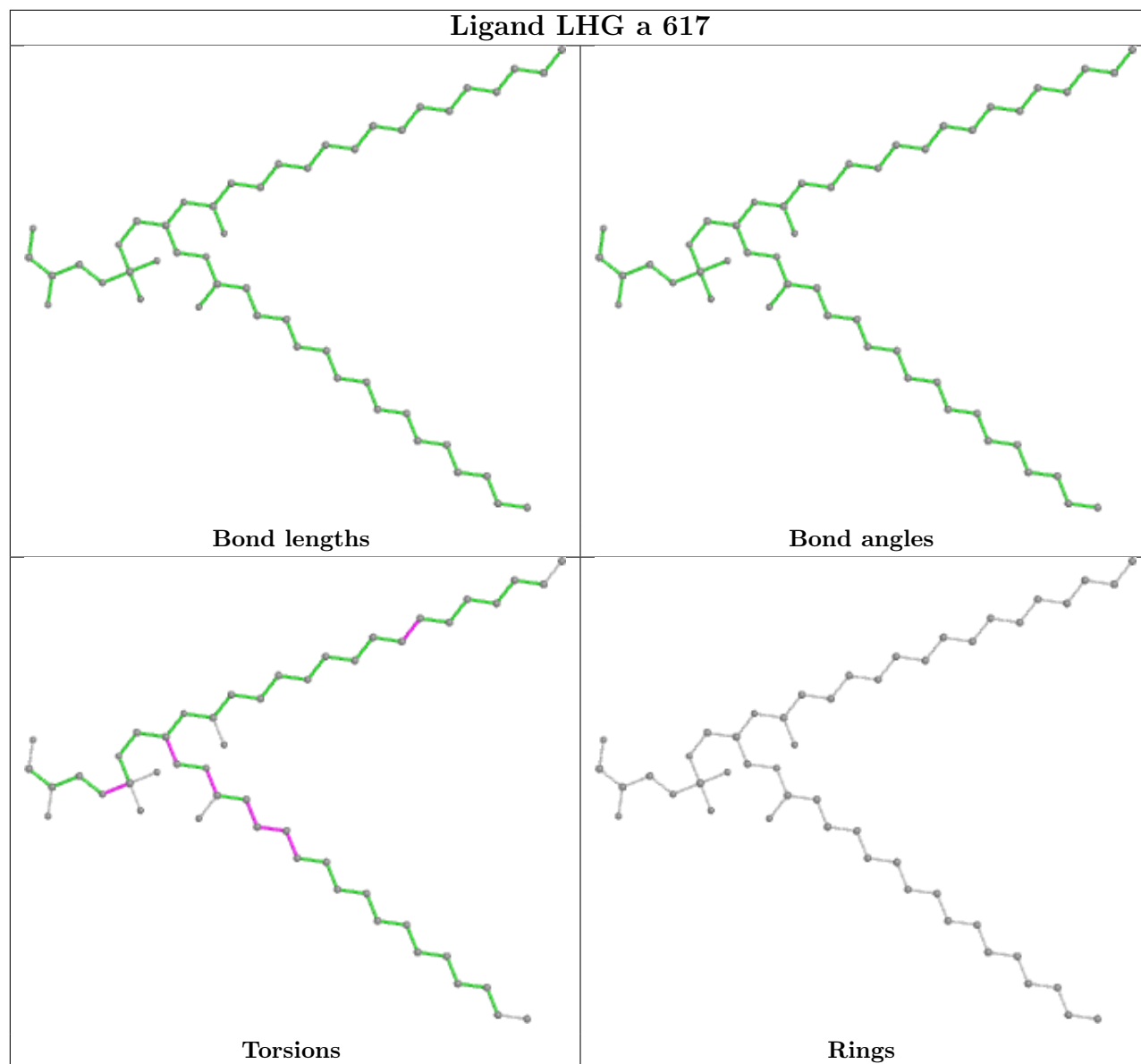
Ligand LUT b 316



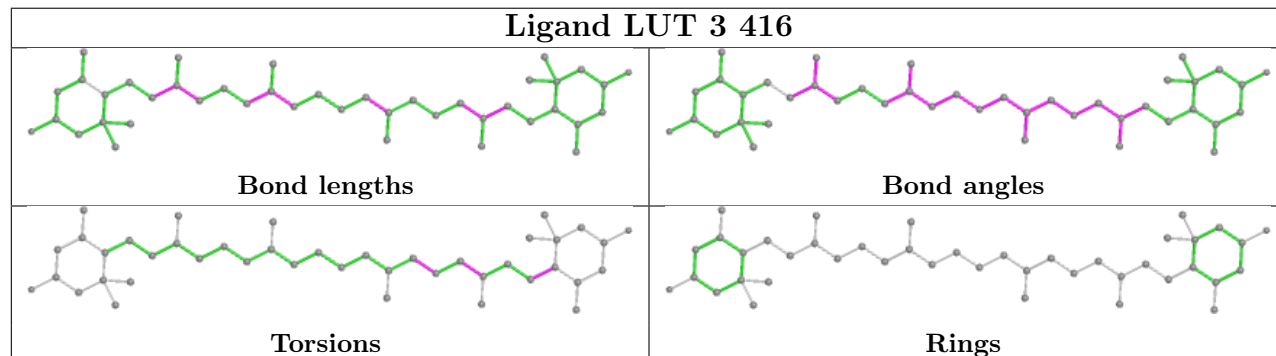
Ligand CLA B 829

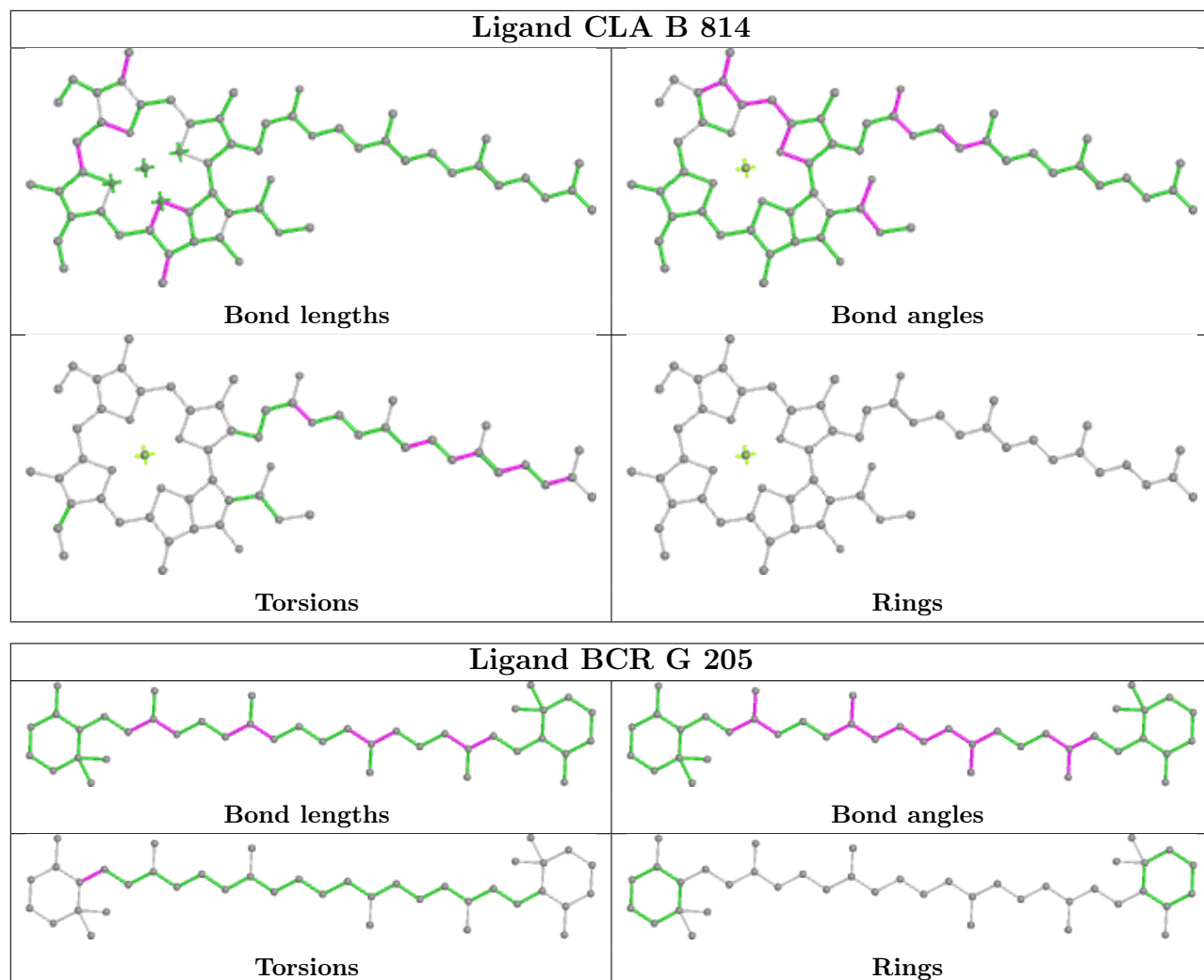


Ligand LHG a 617

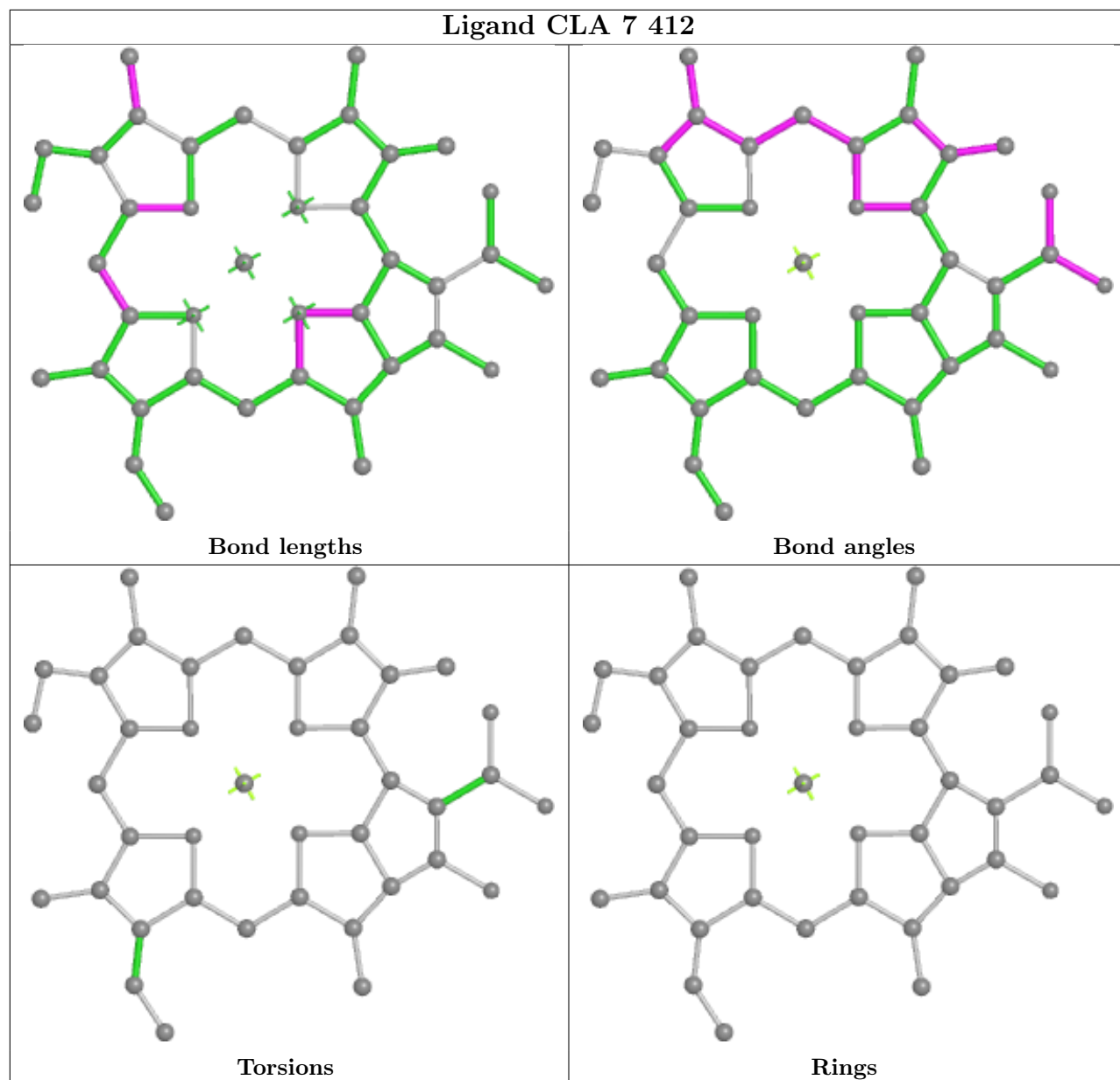


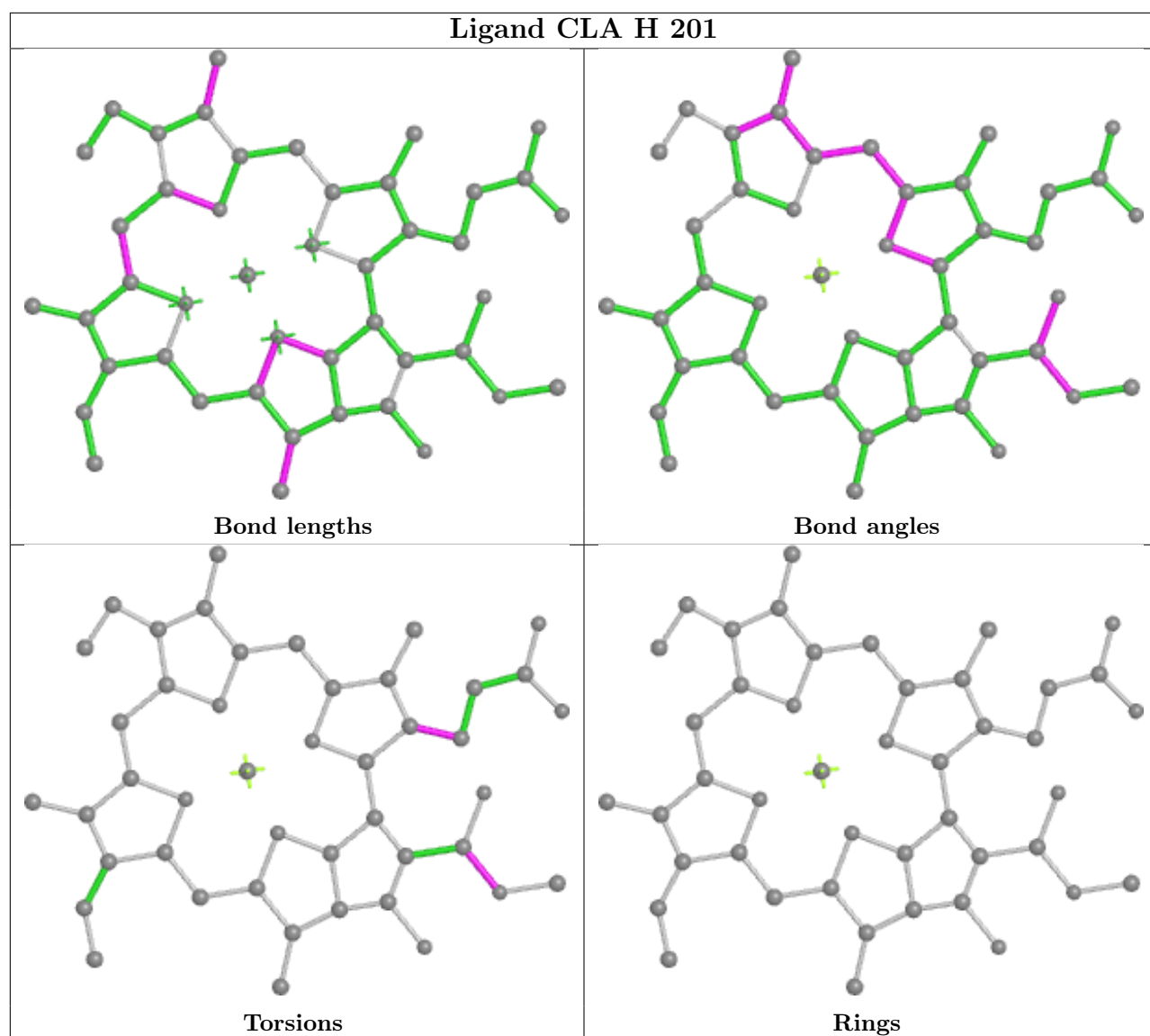
Ligand LUT 3 416

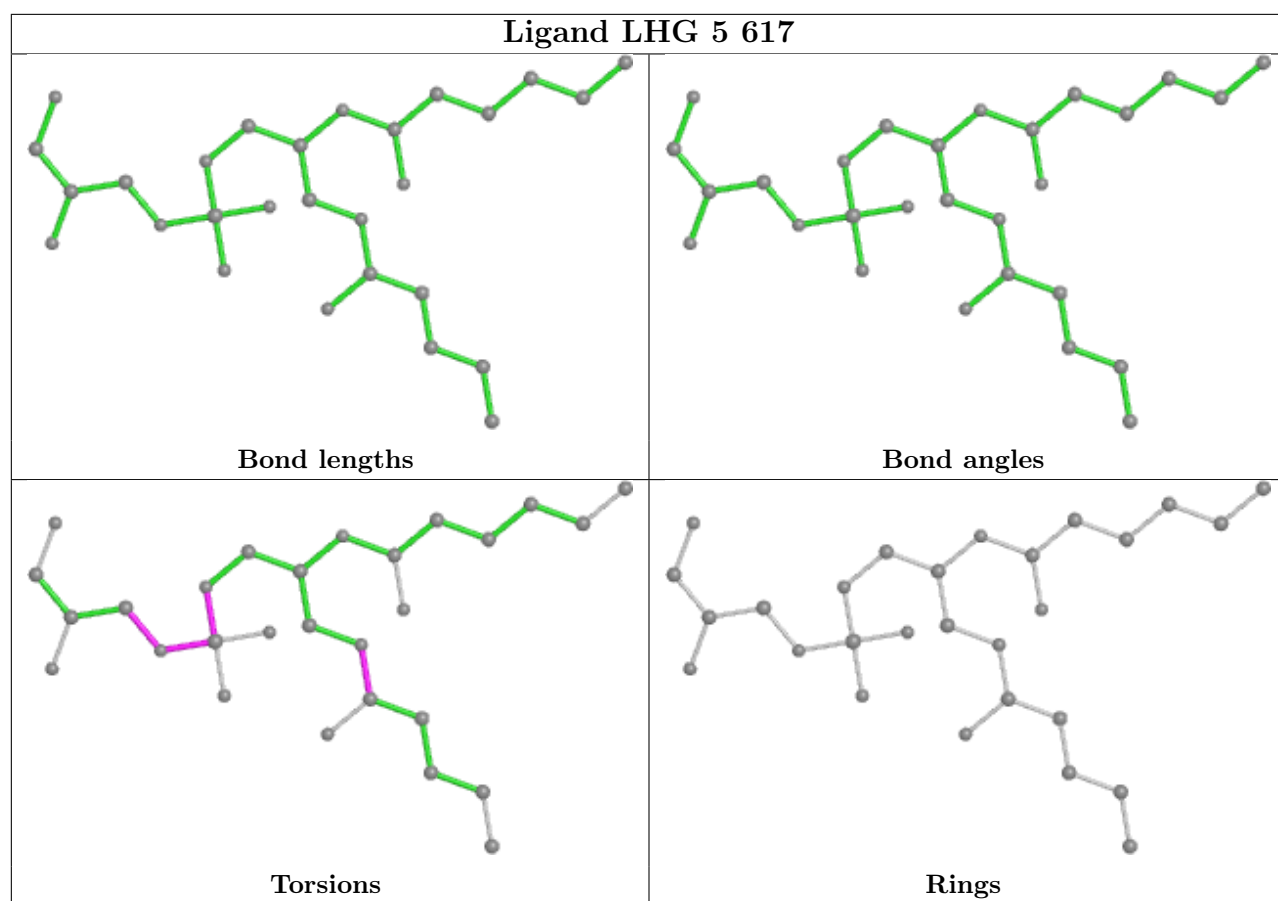


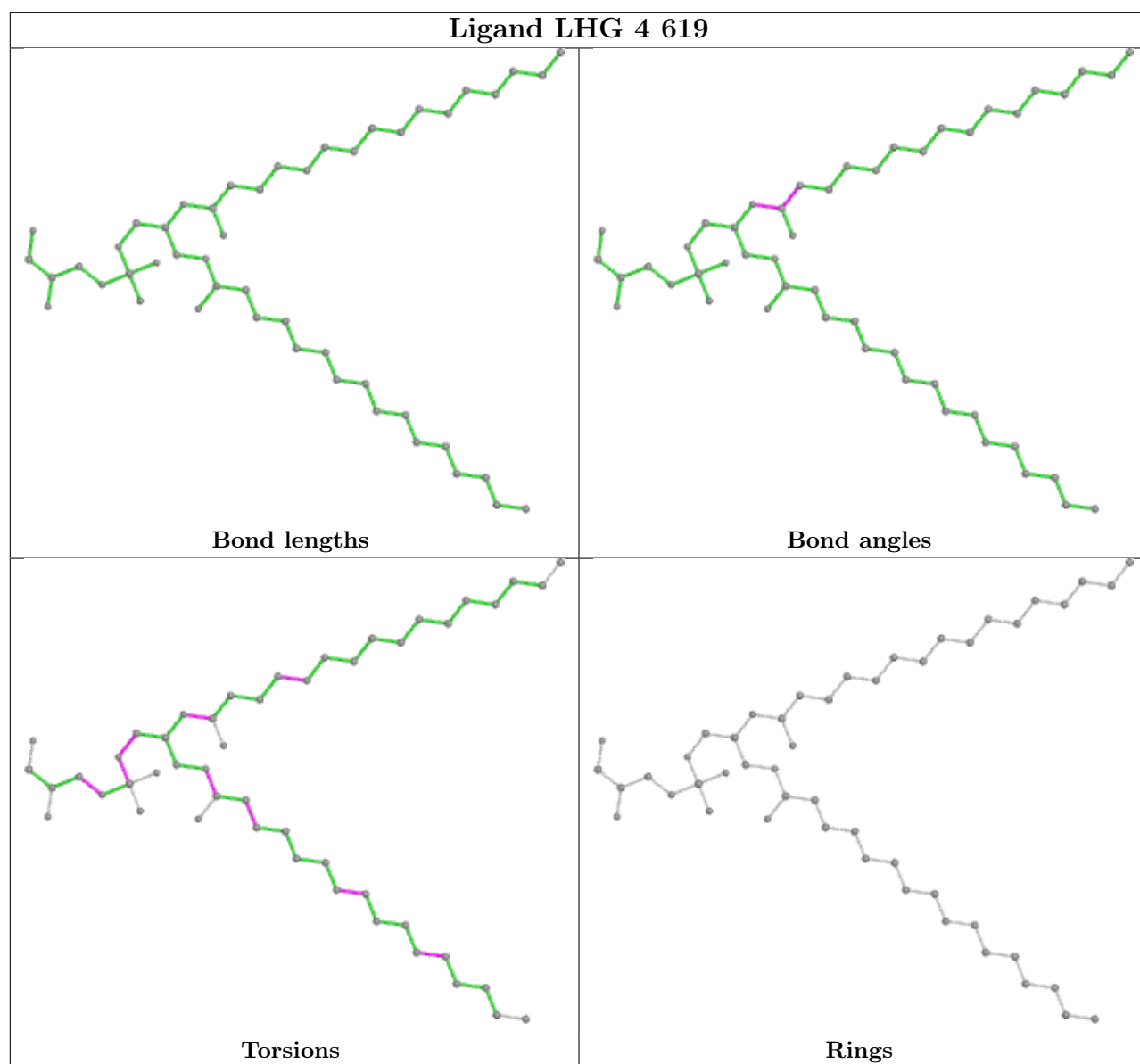


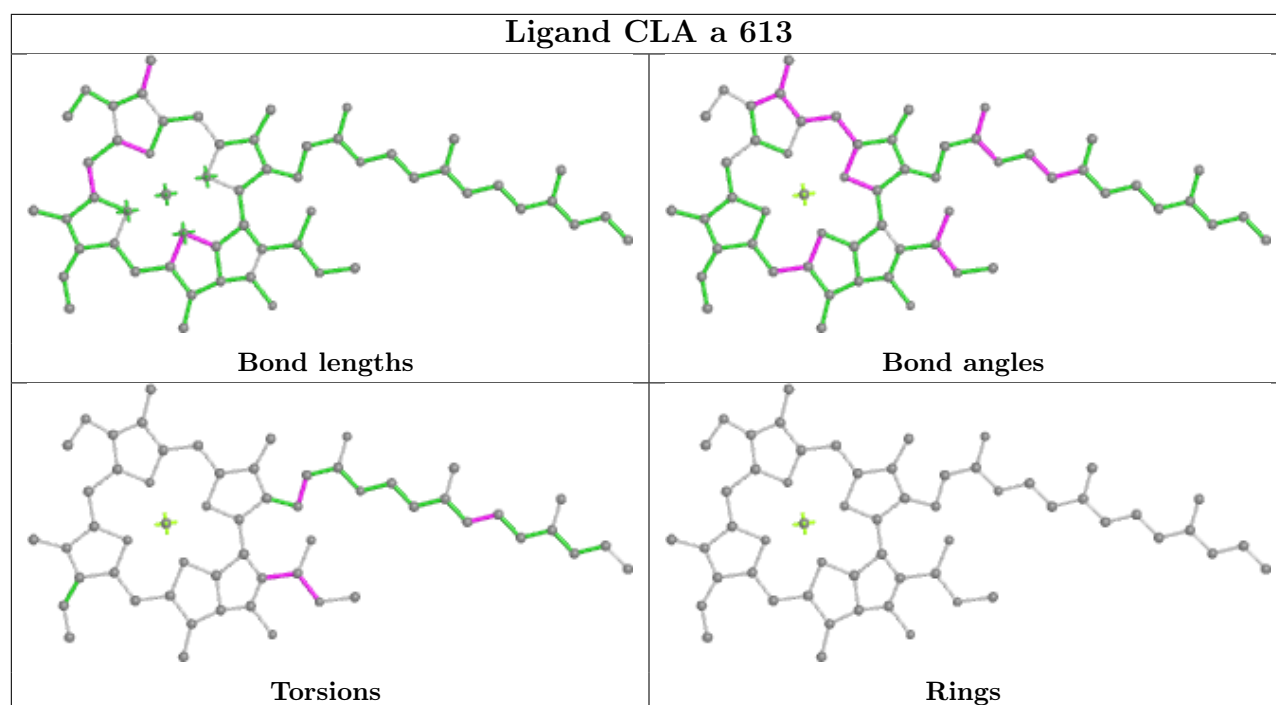
Ligand CLA 7 412



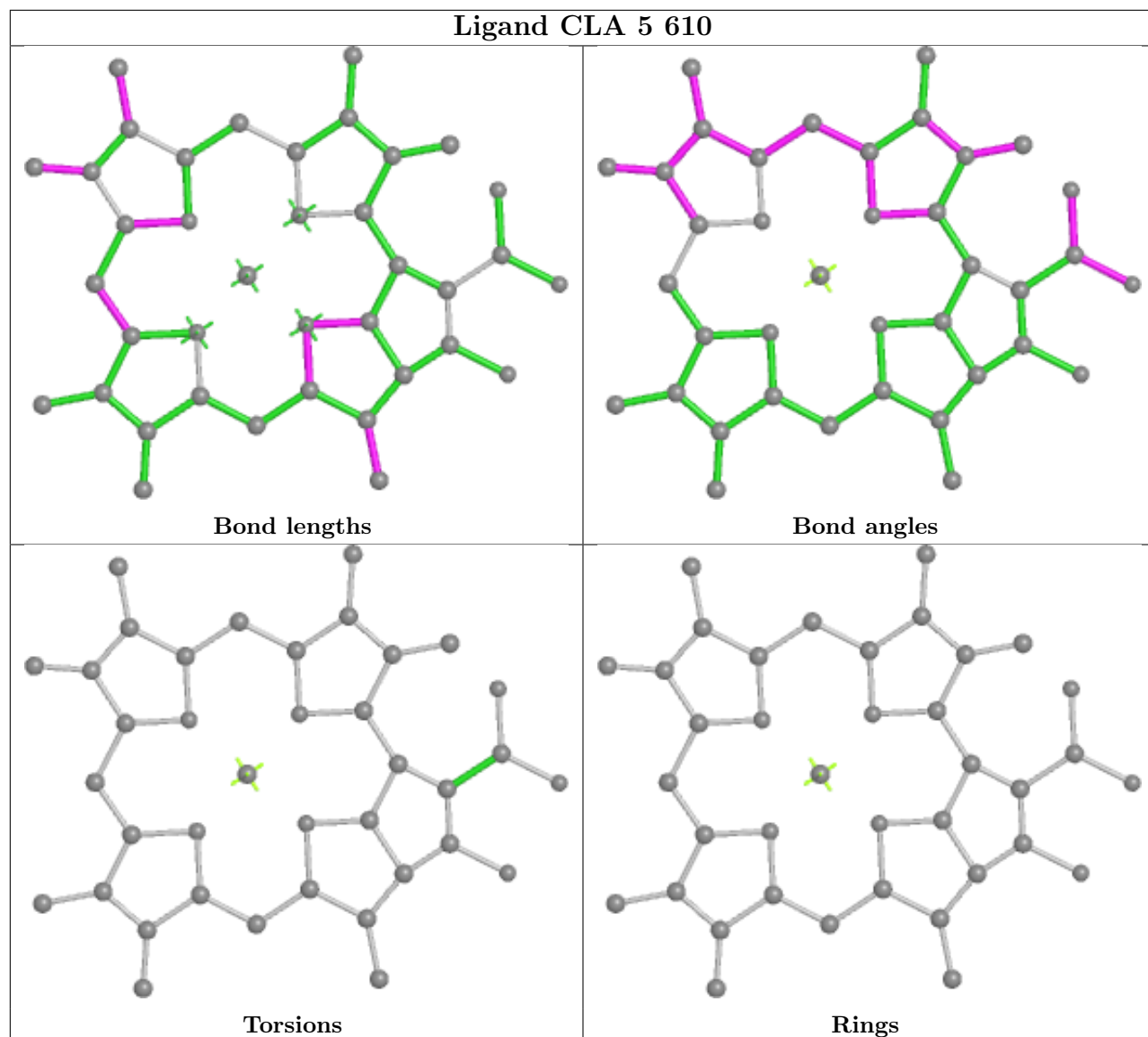




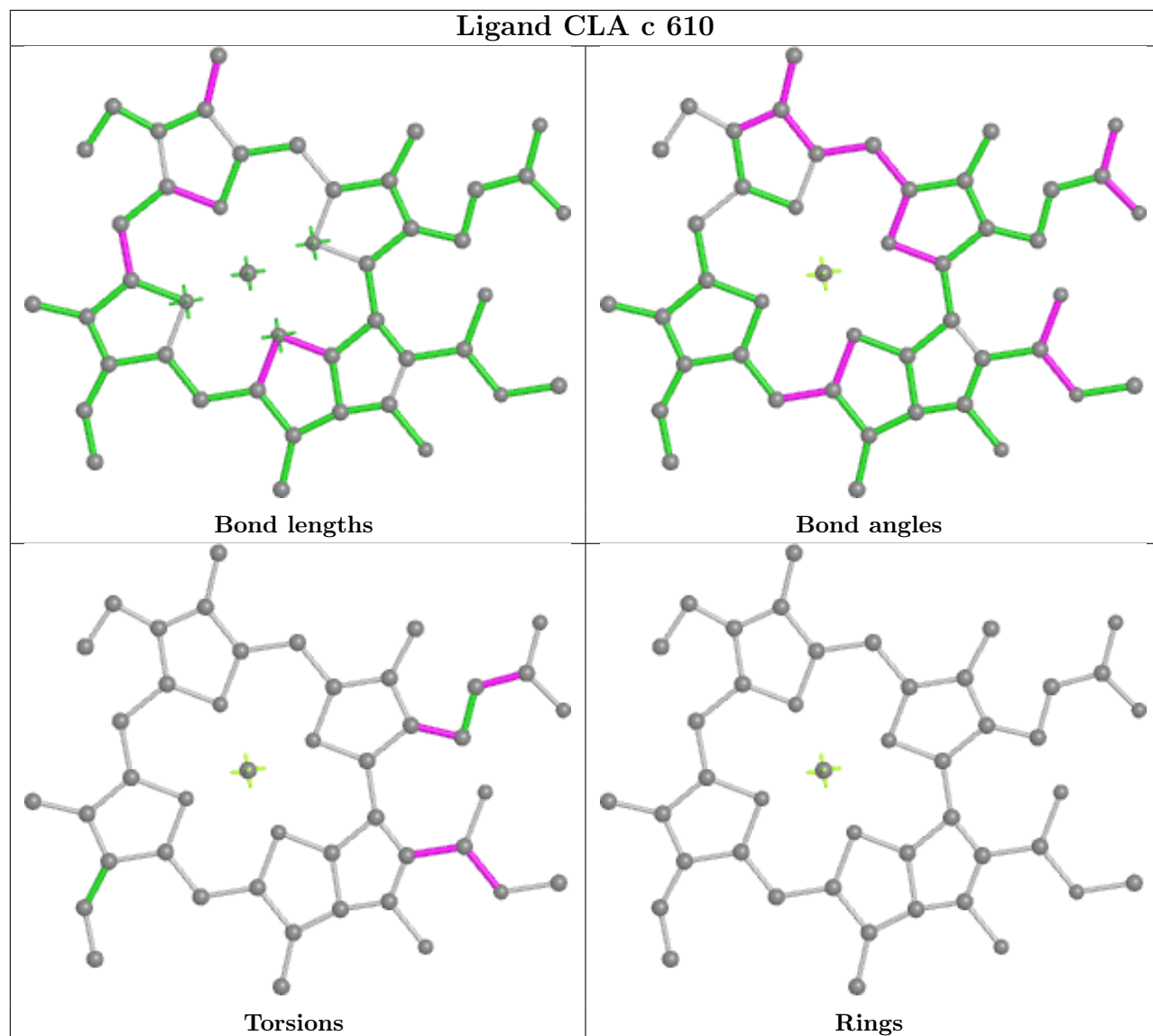




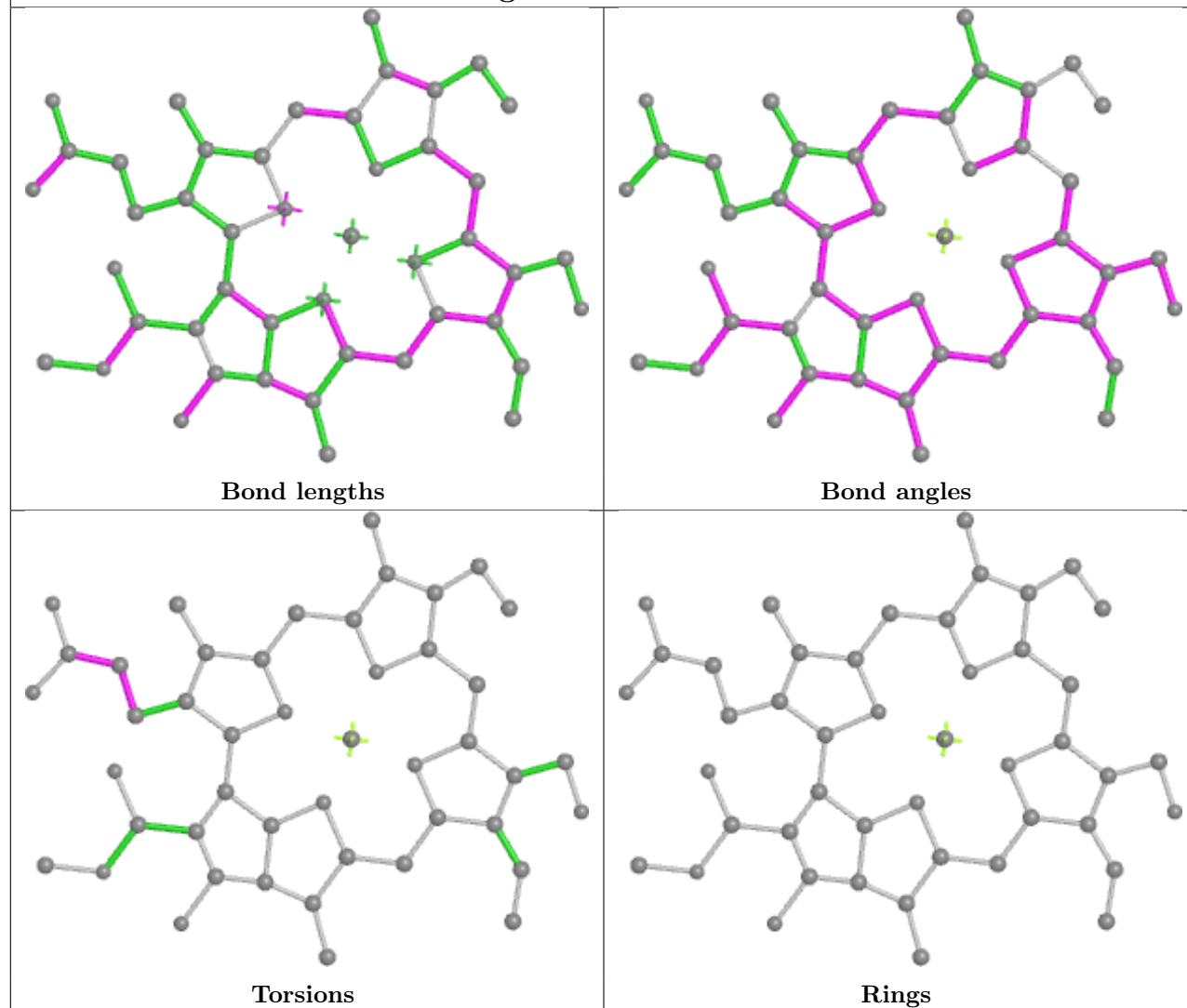
Ligand CLA 5 610

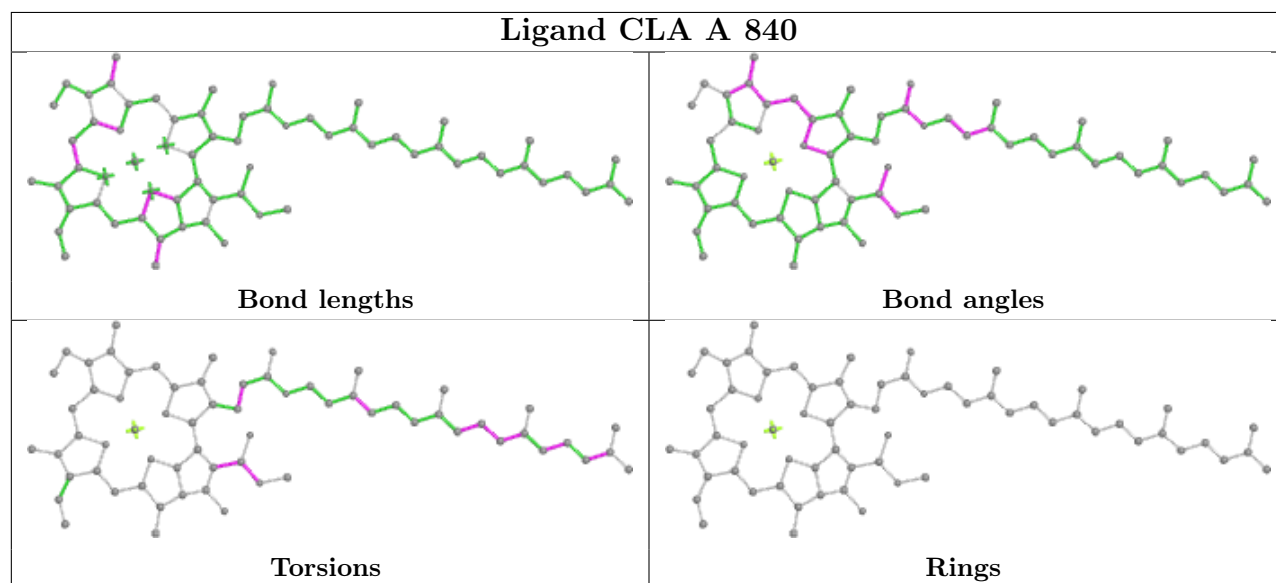
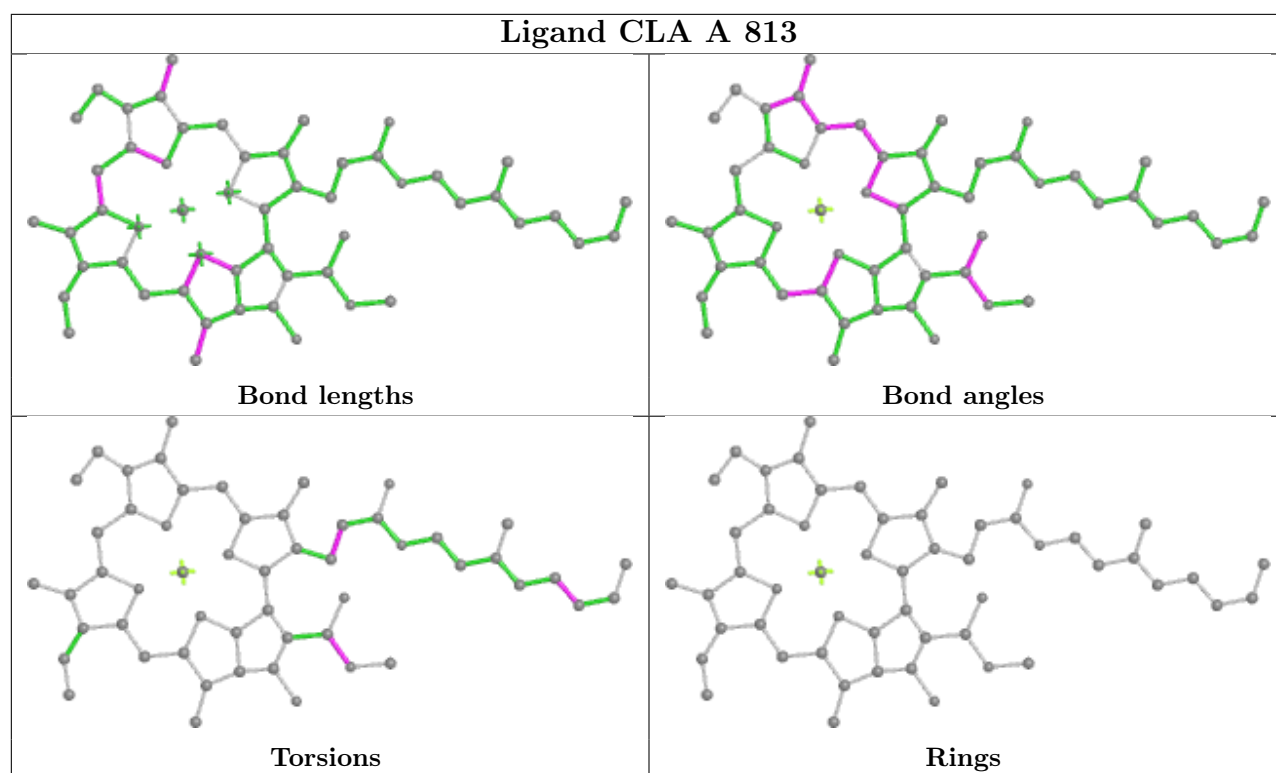


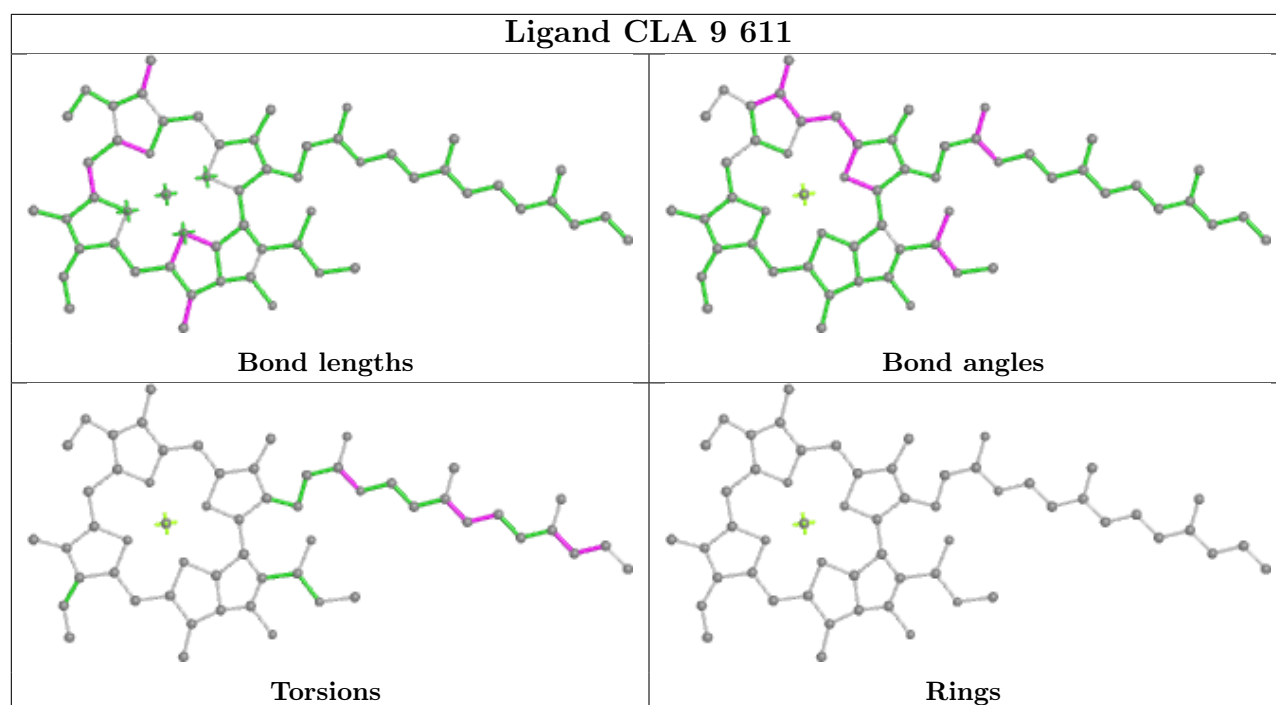
Ligand CLA c 610



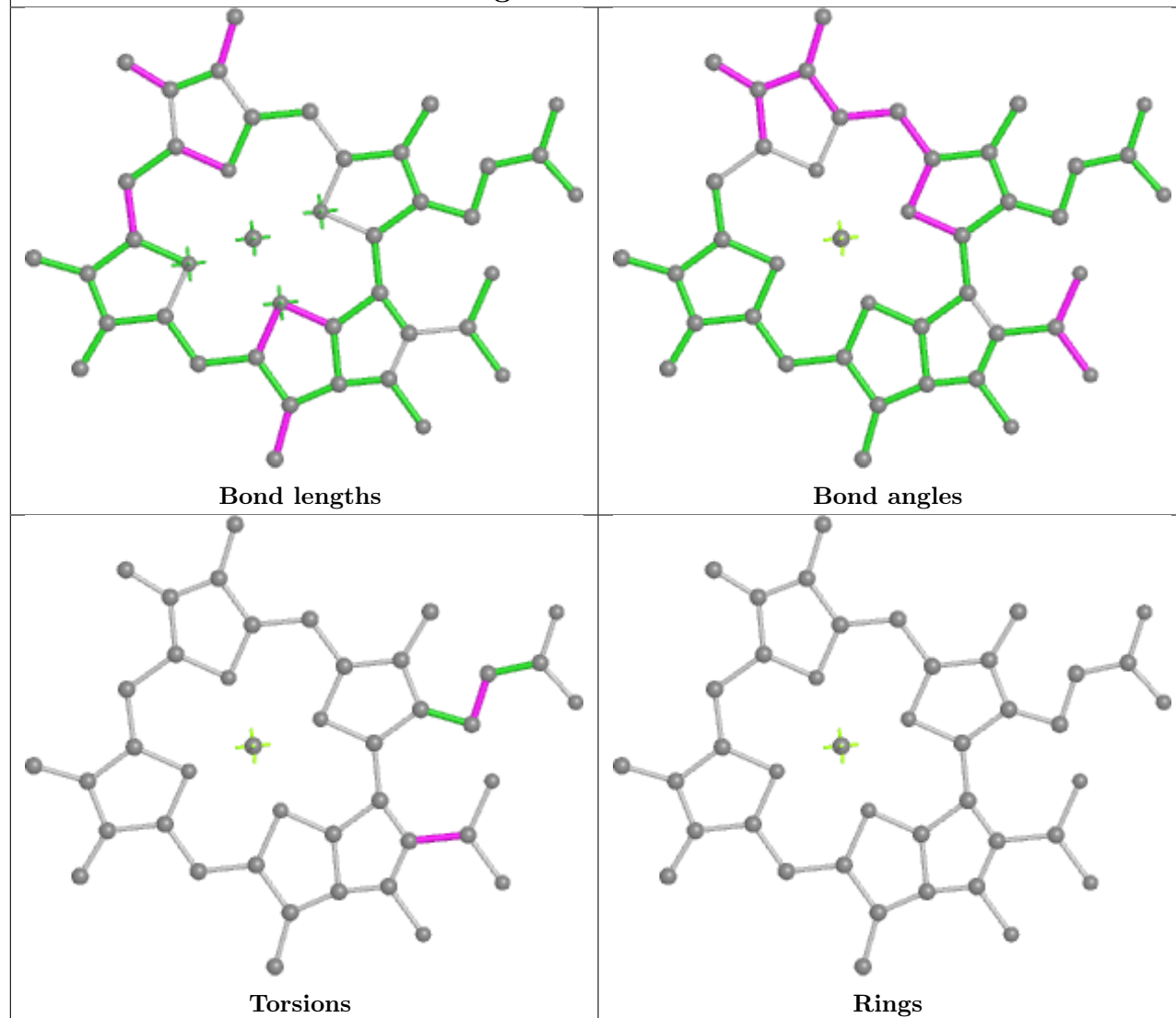
Ligand CHL c 607



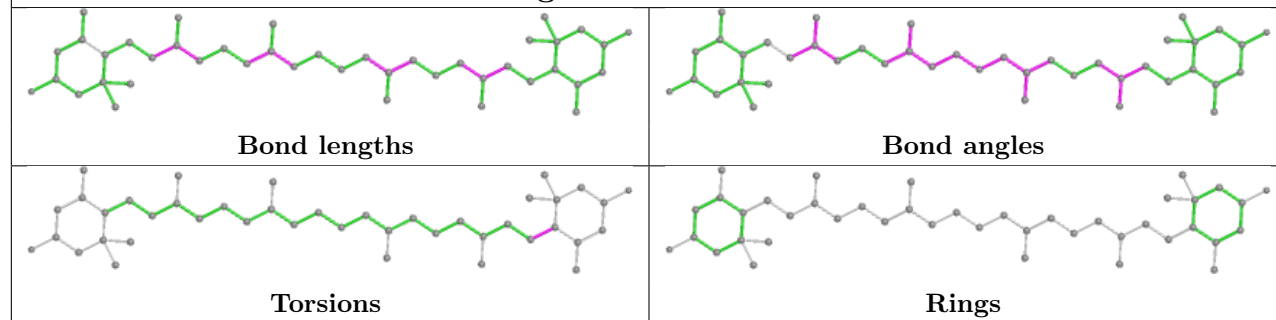




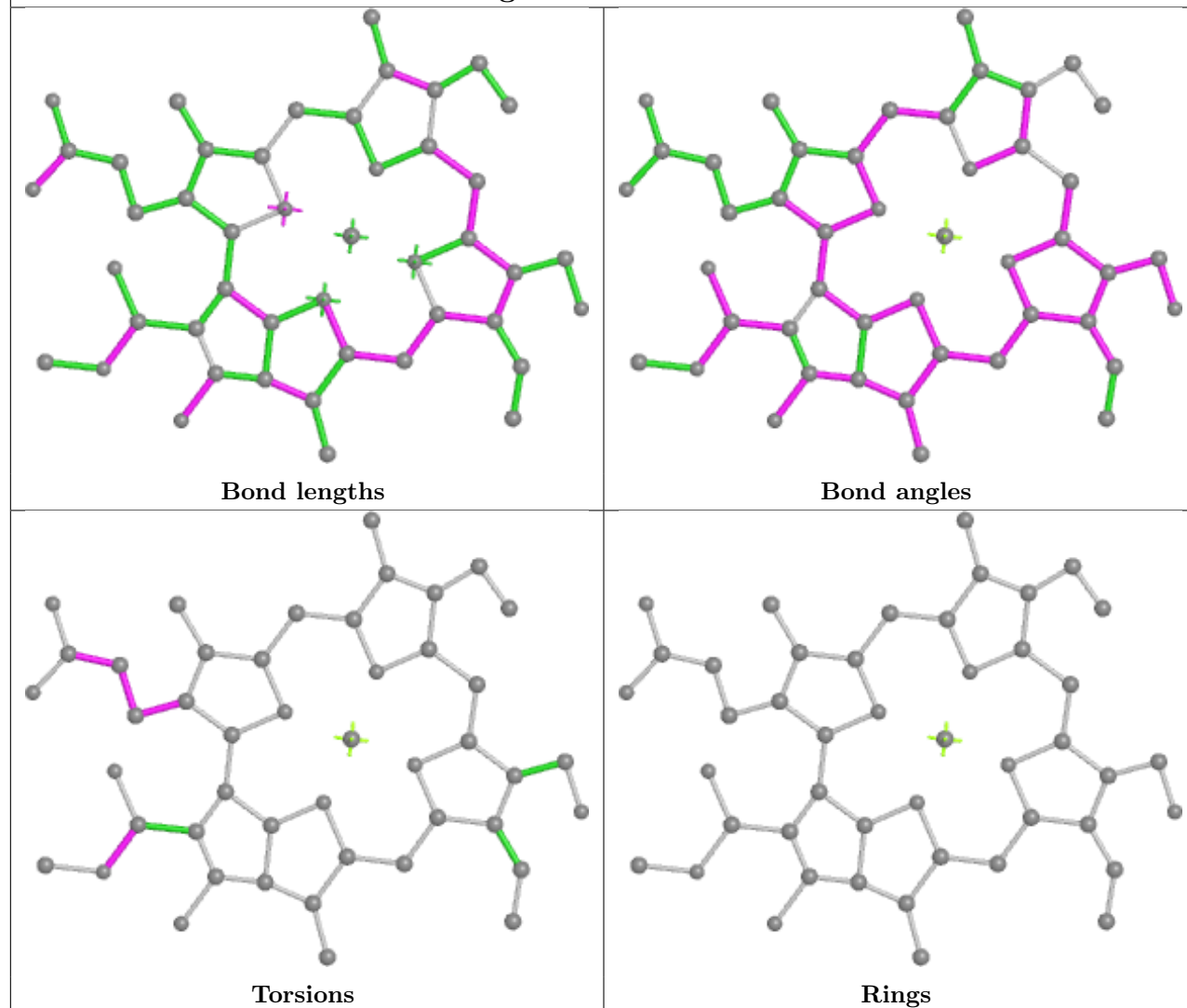
Ligand CLA 7 403



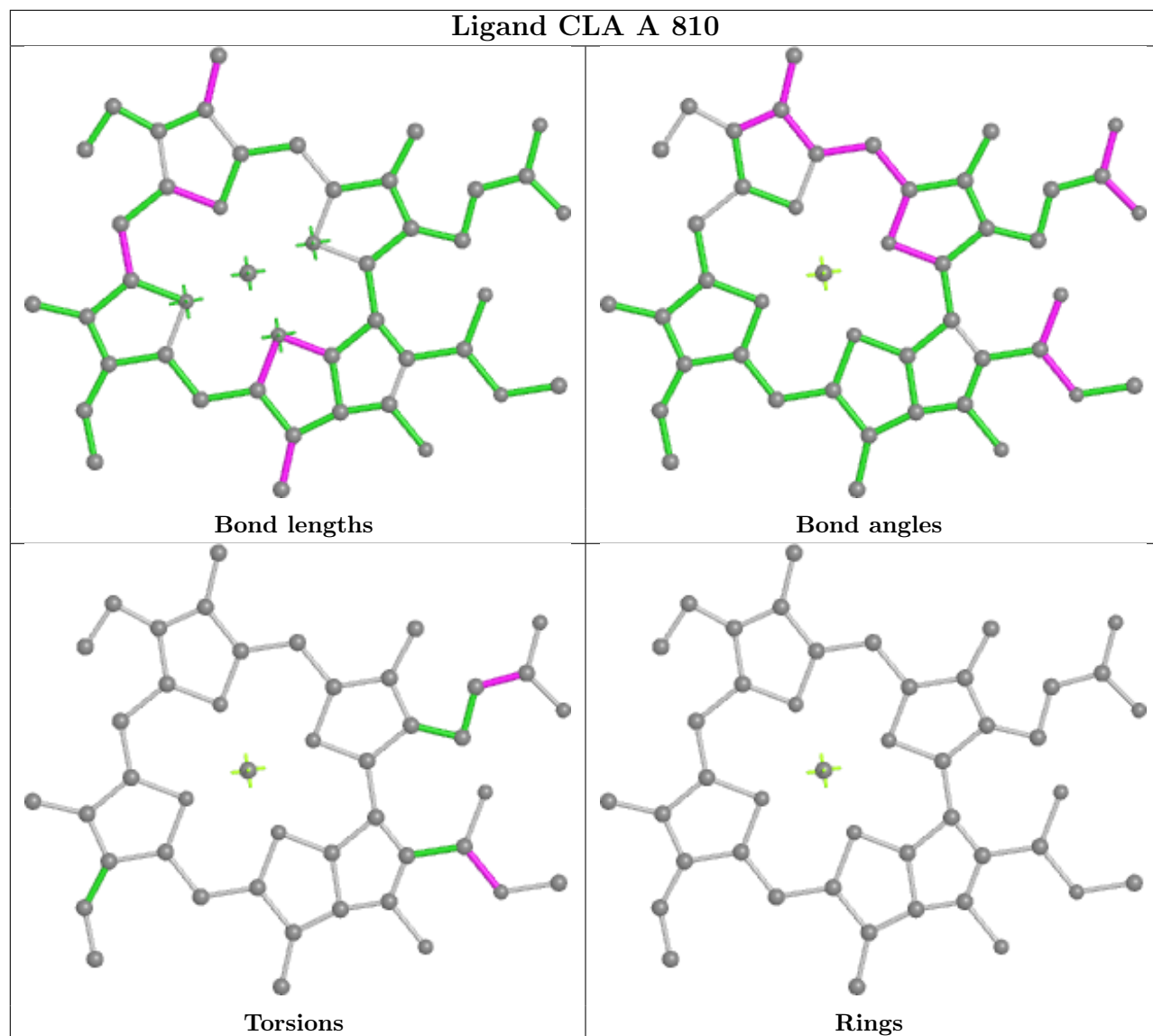
Ligand LUT c 615



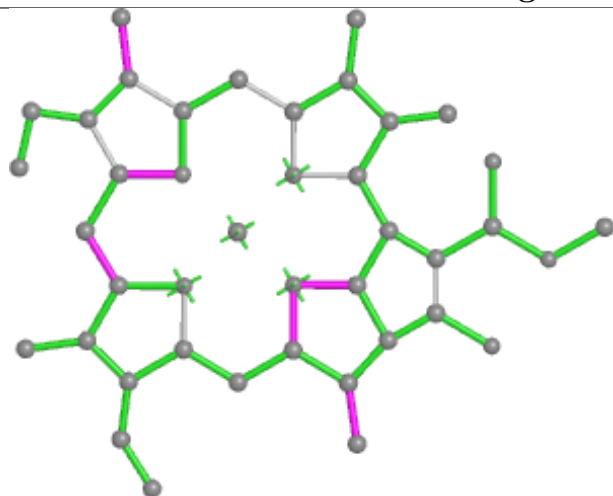
Ligand CHL c 608



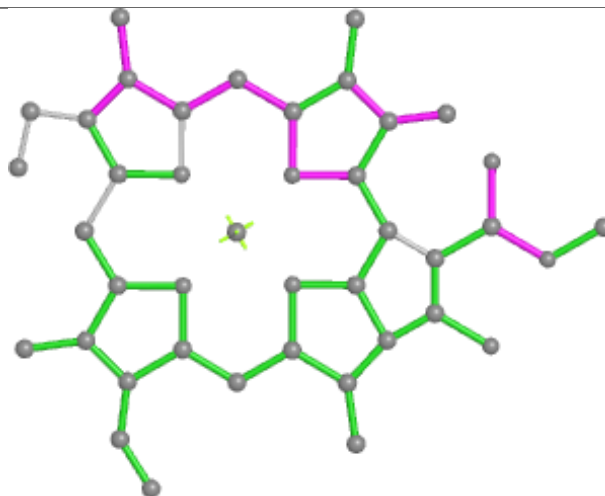
Ligand CLA A 810



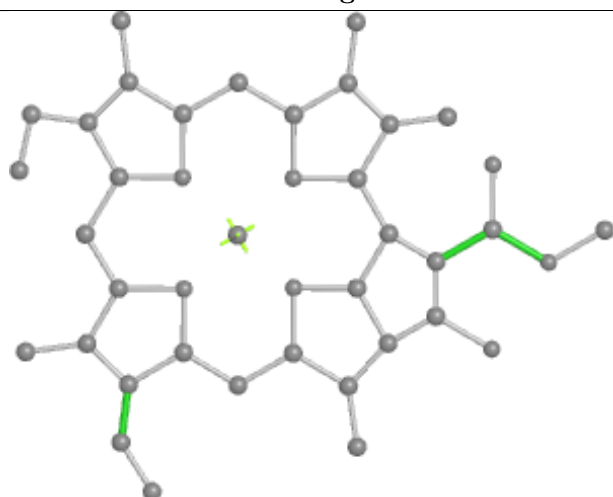
Ligand CLA a 603



Bond lengths



Bond angles

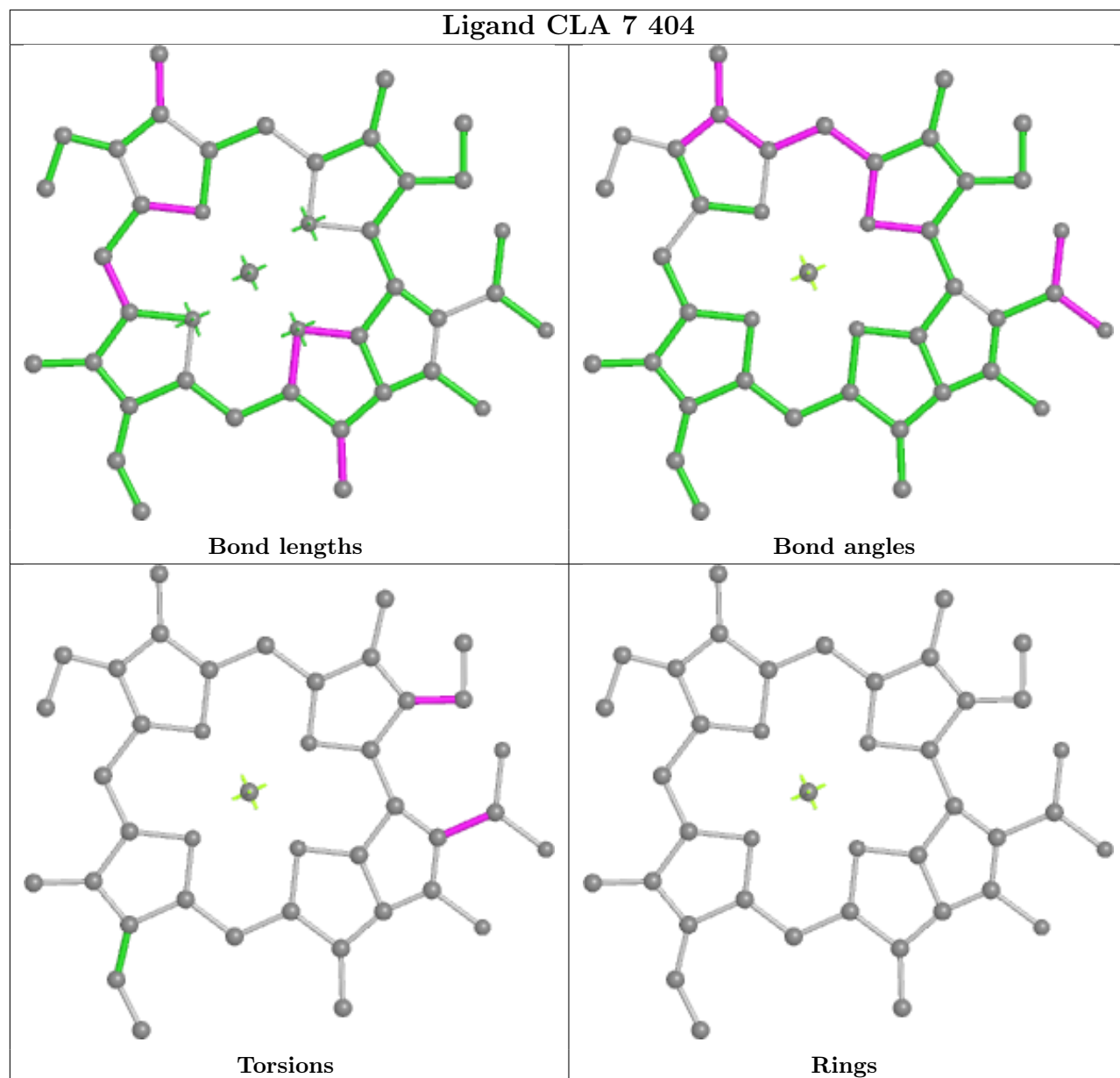


Torsions

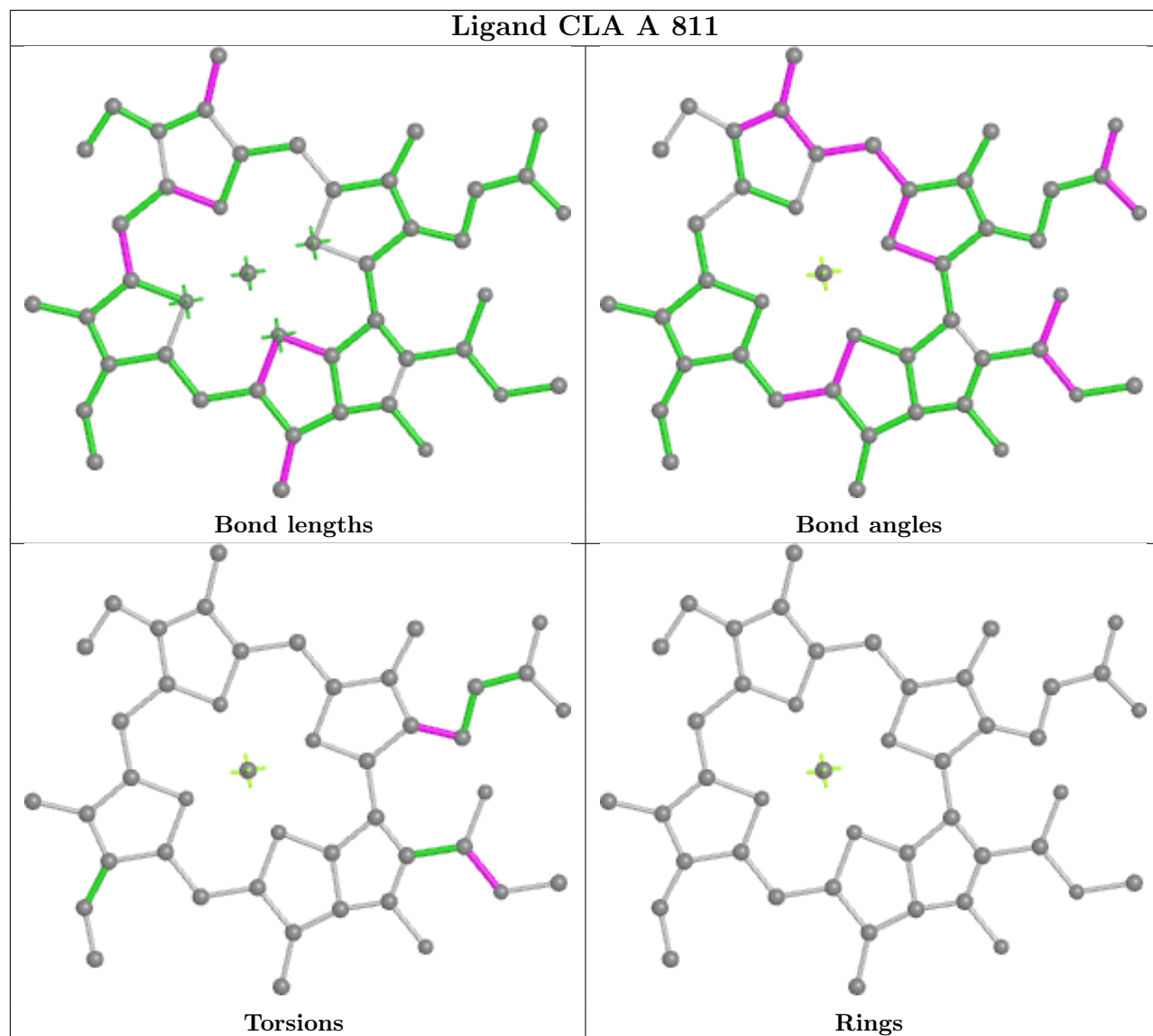


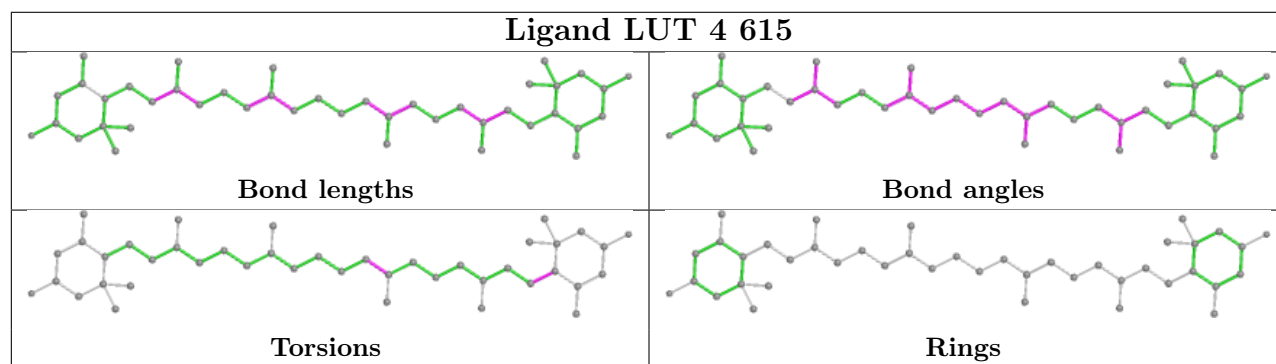
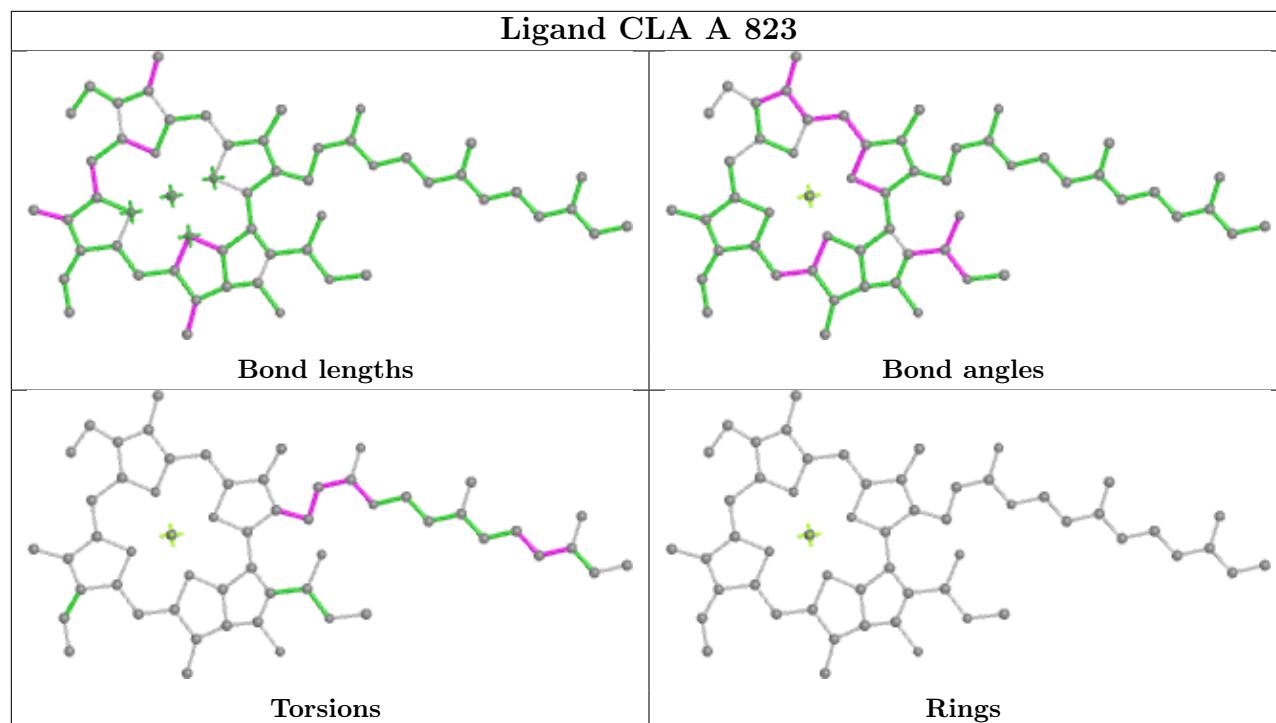
Rings

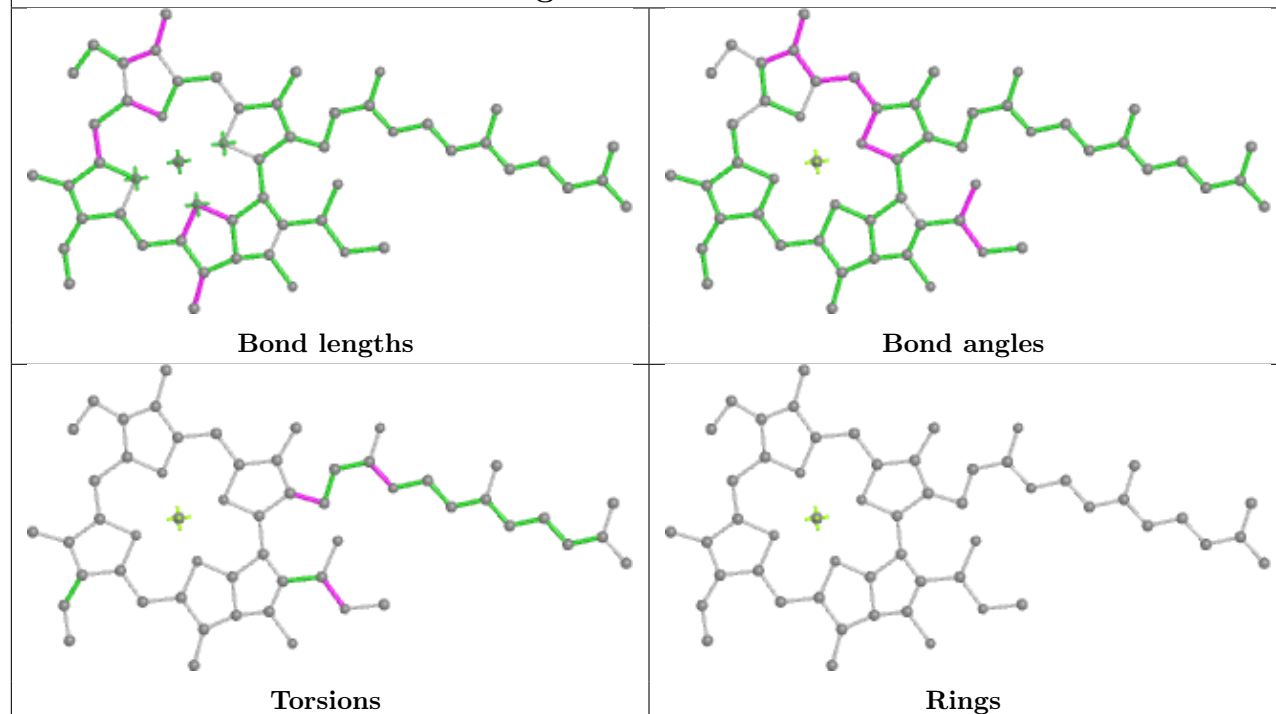
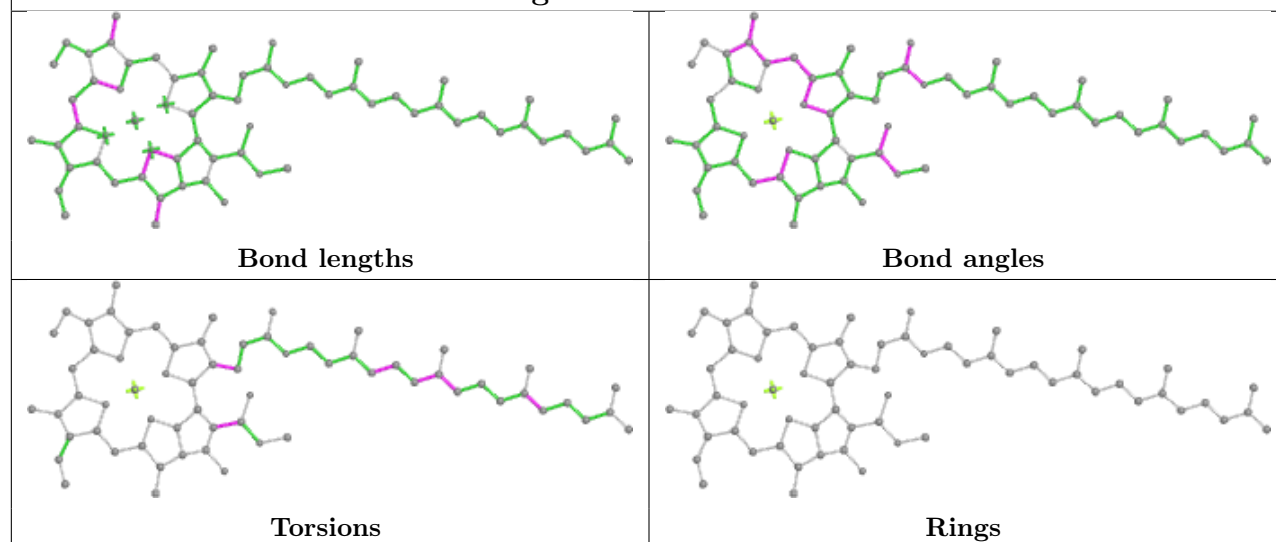
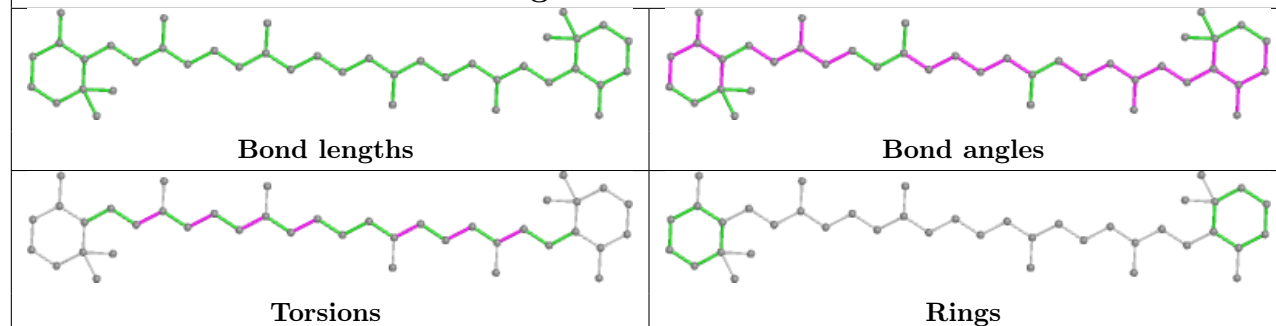
Ligand CLA 7 404



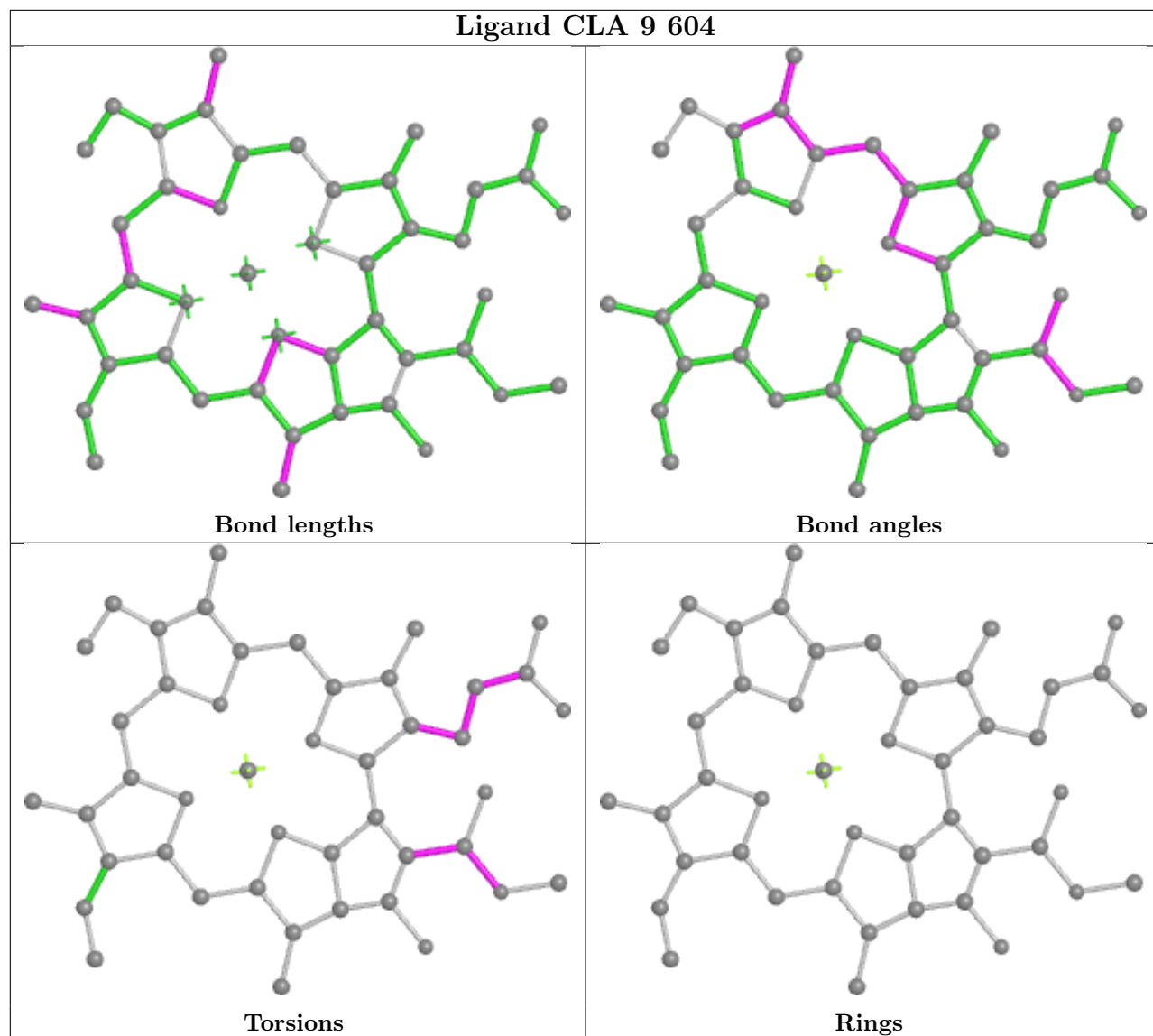
Ligand CLA A 811



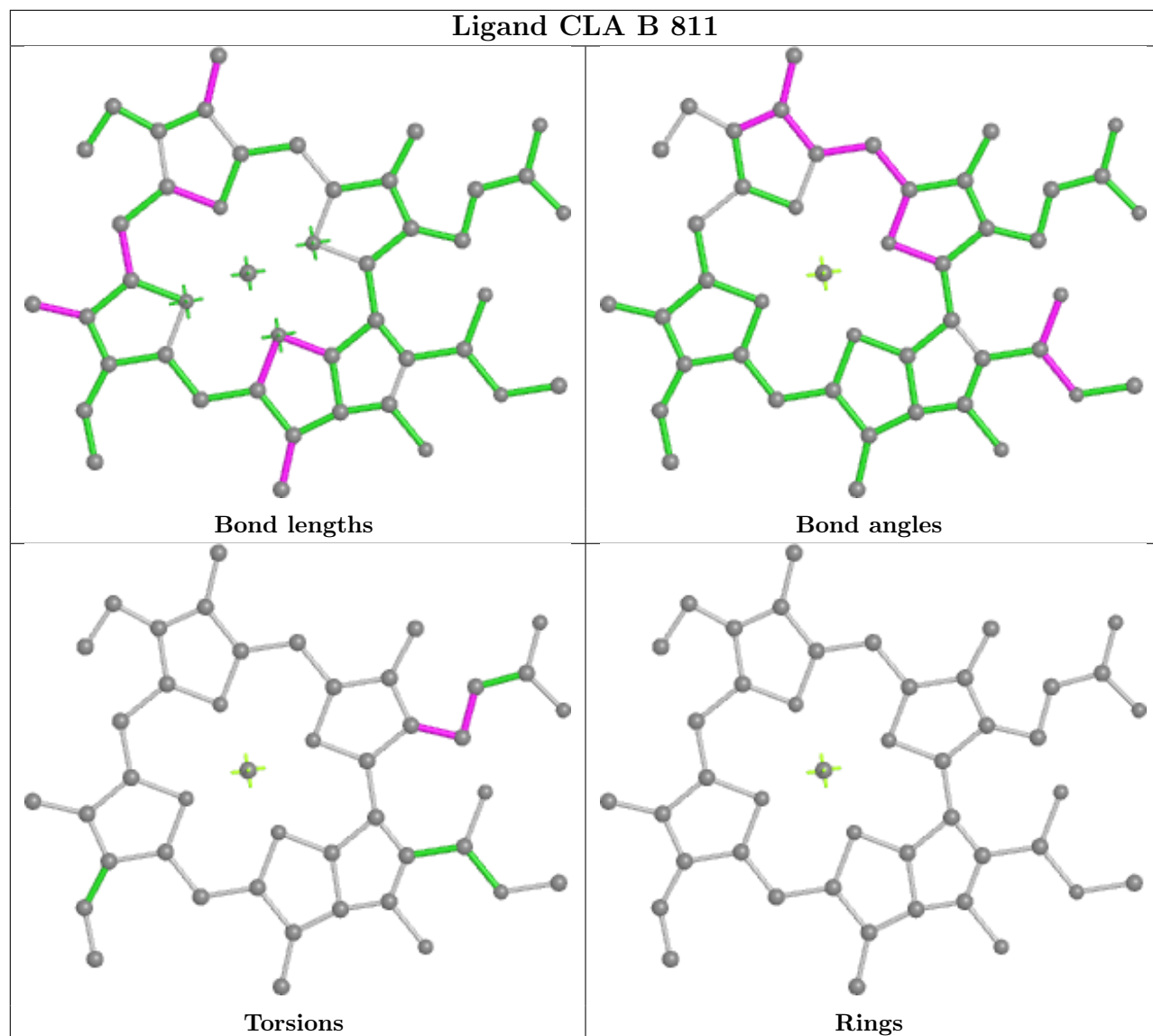


Ligand CLA 3 403**Ligand CLA A 826****Ligand BCR B 844**

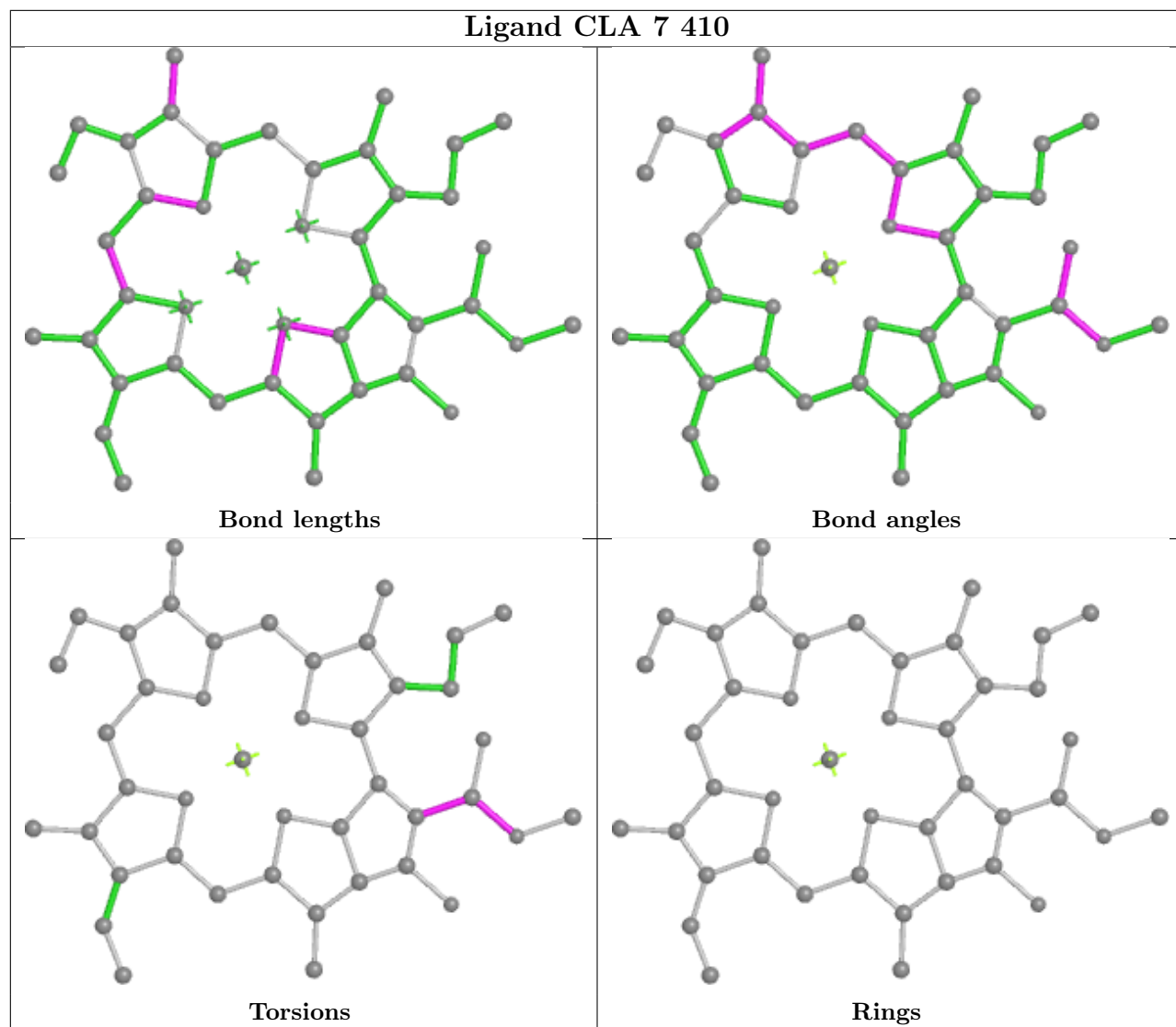
Ligand CLA 9 604



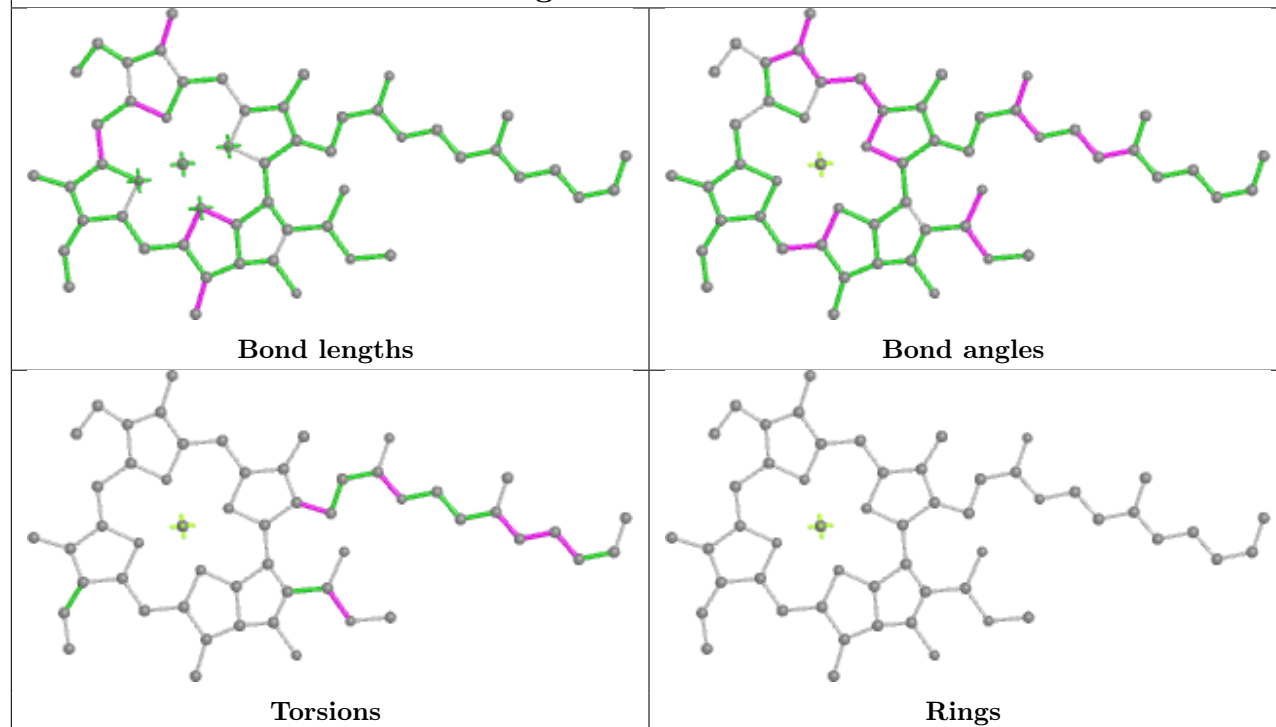
Ligand CLA B 811



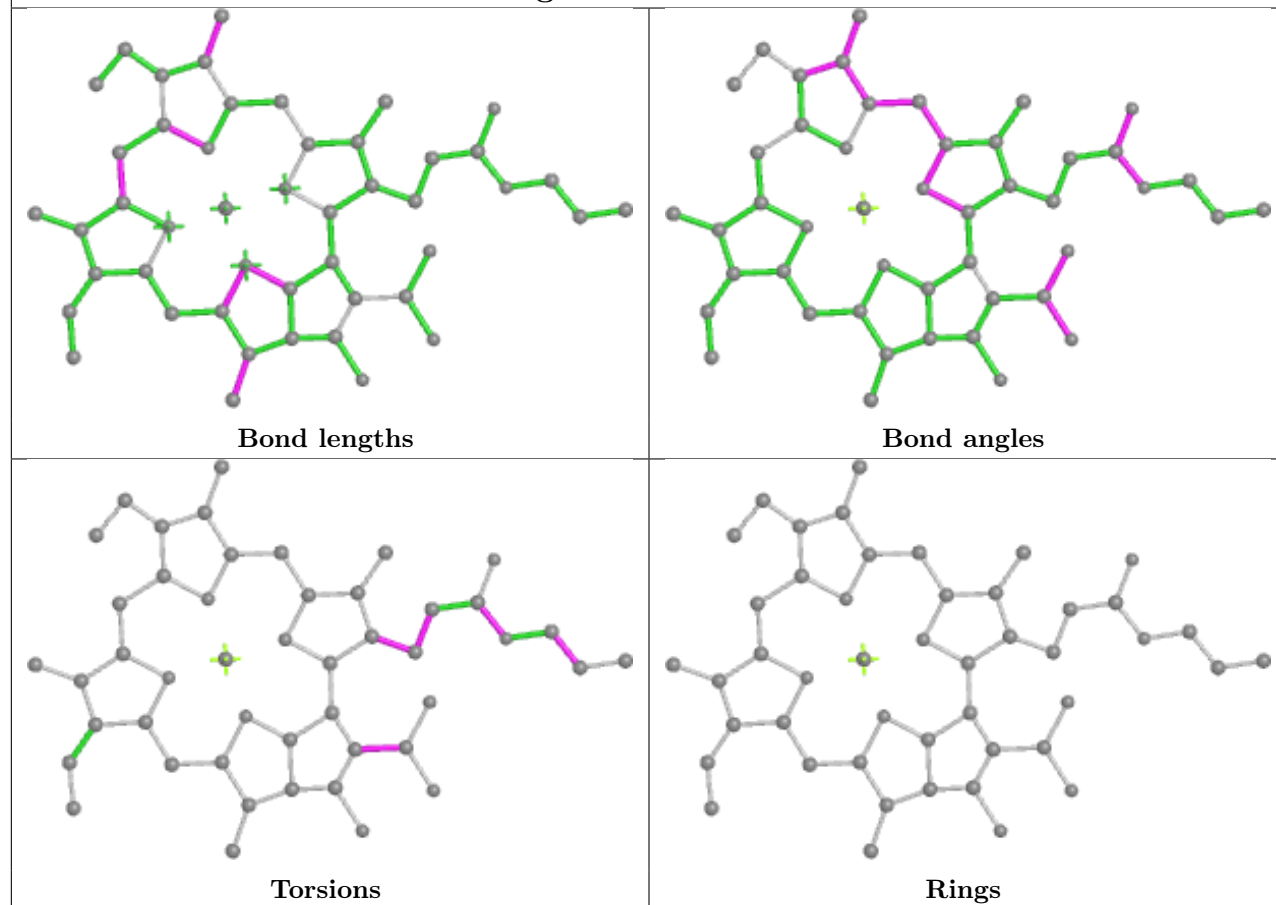
Ligand CLA 7 410

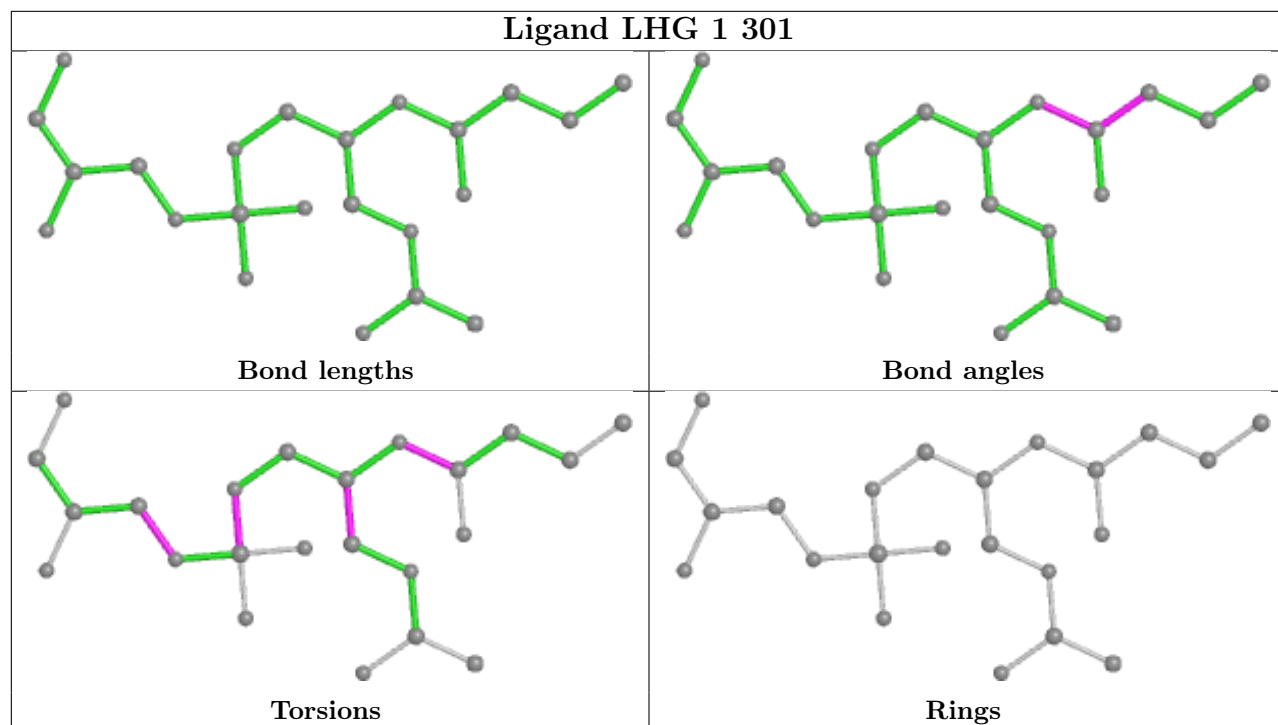


Ligand CLA b 311

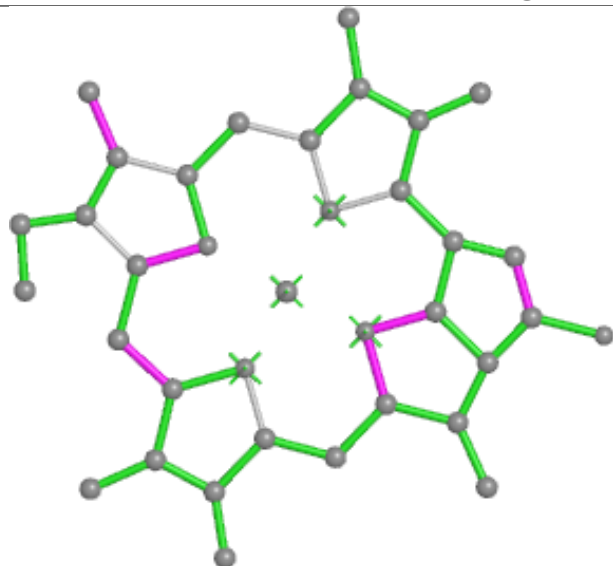


Ligand CLA a 604

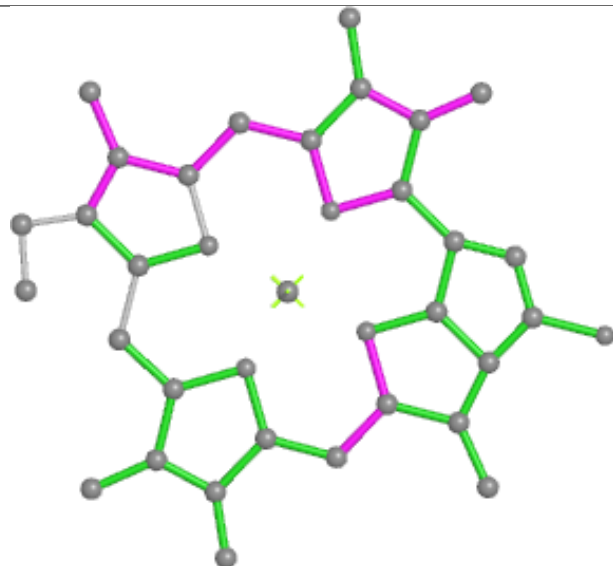




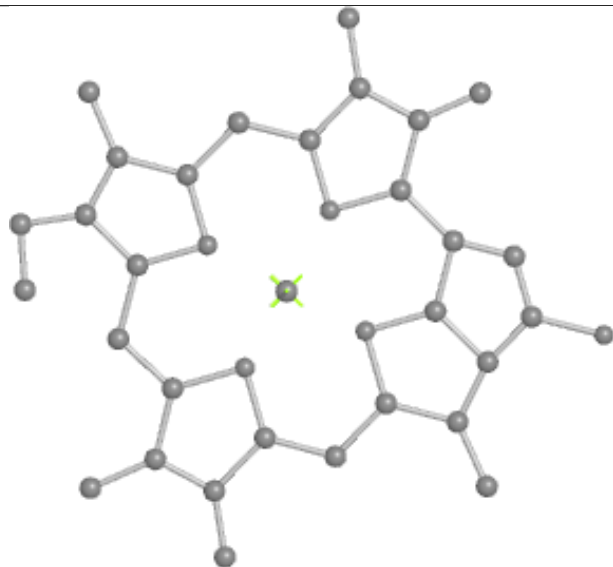
Ligand CLA 7 413



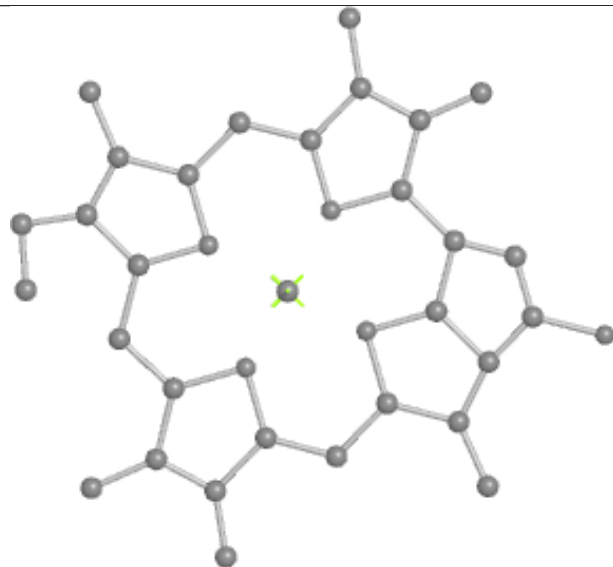
Bond lengths



Bond angles

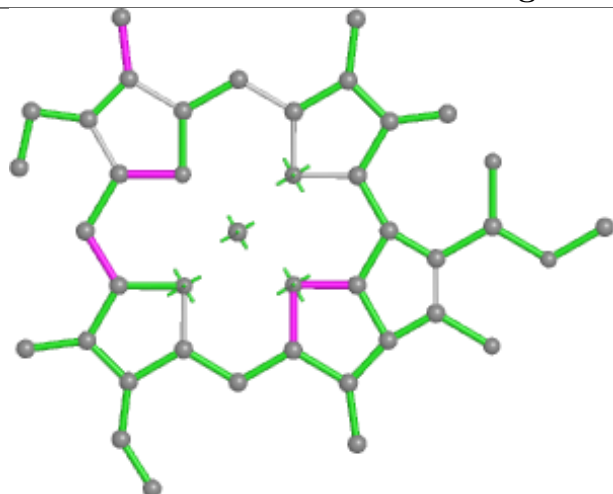


Torsions

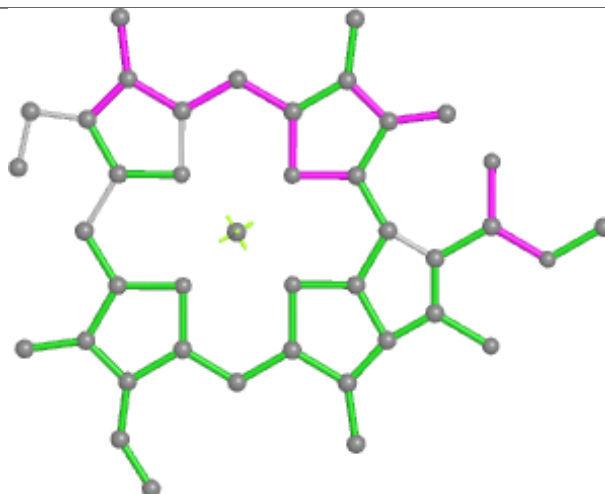


Rings

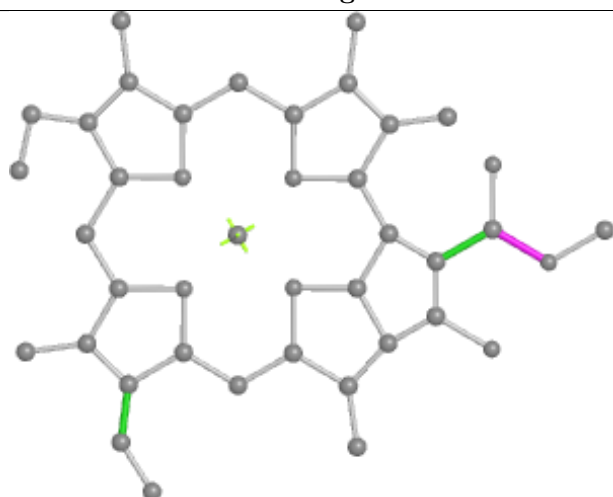
Ligand CLA 7 408



Bond lengths



Bond angles

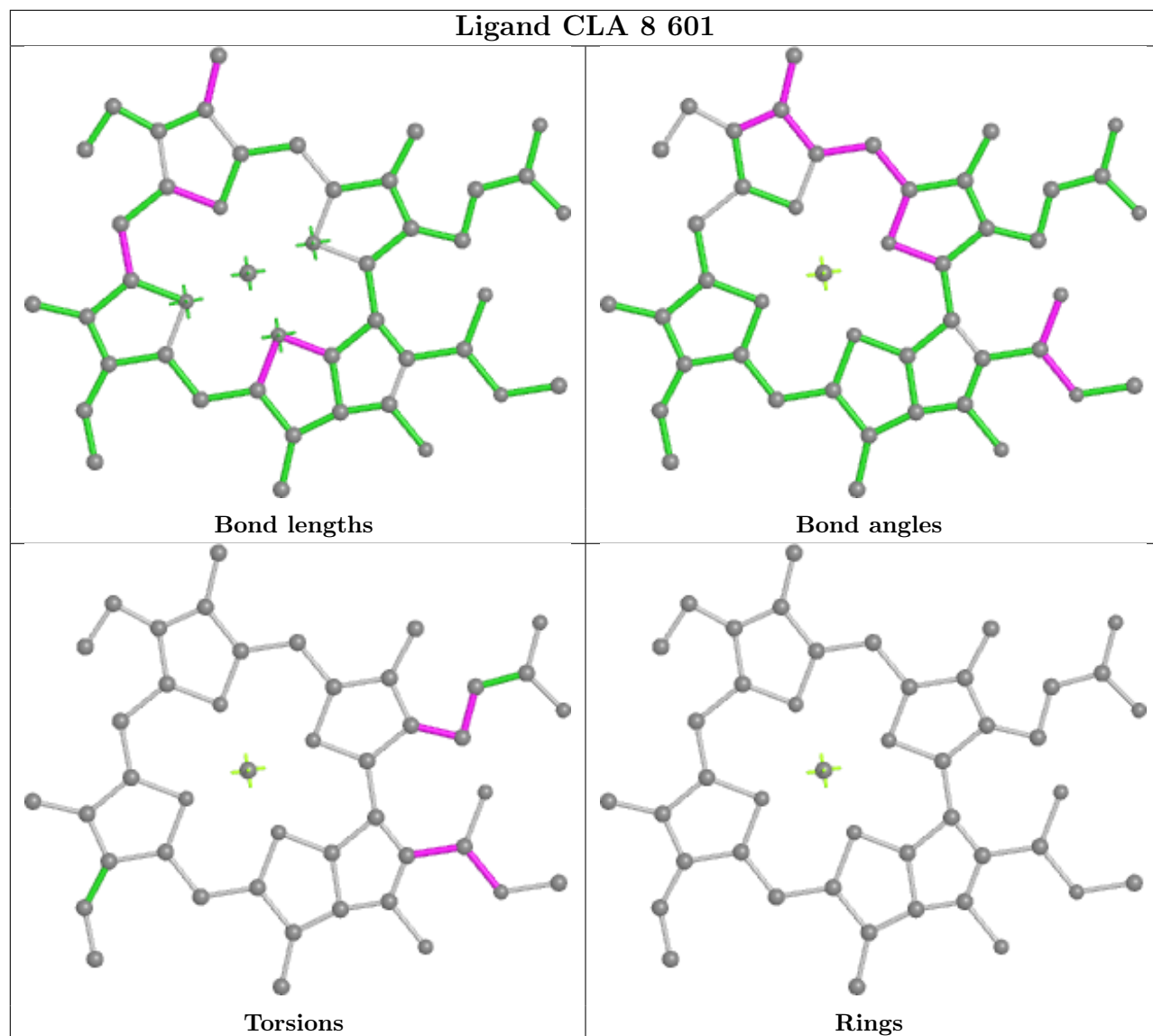


Torsions

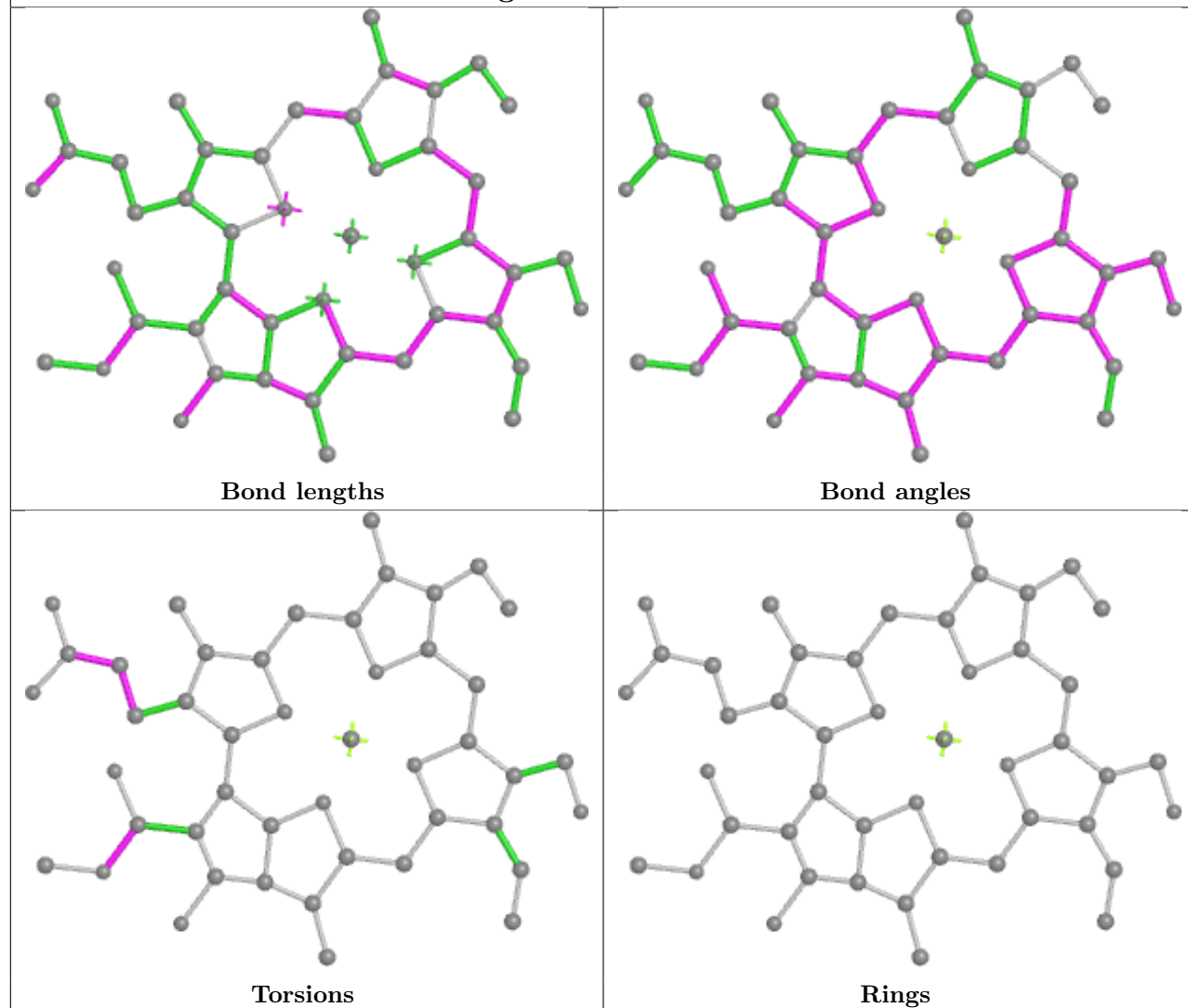


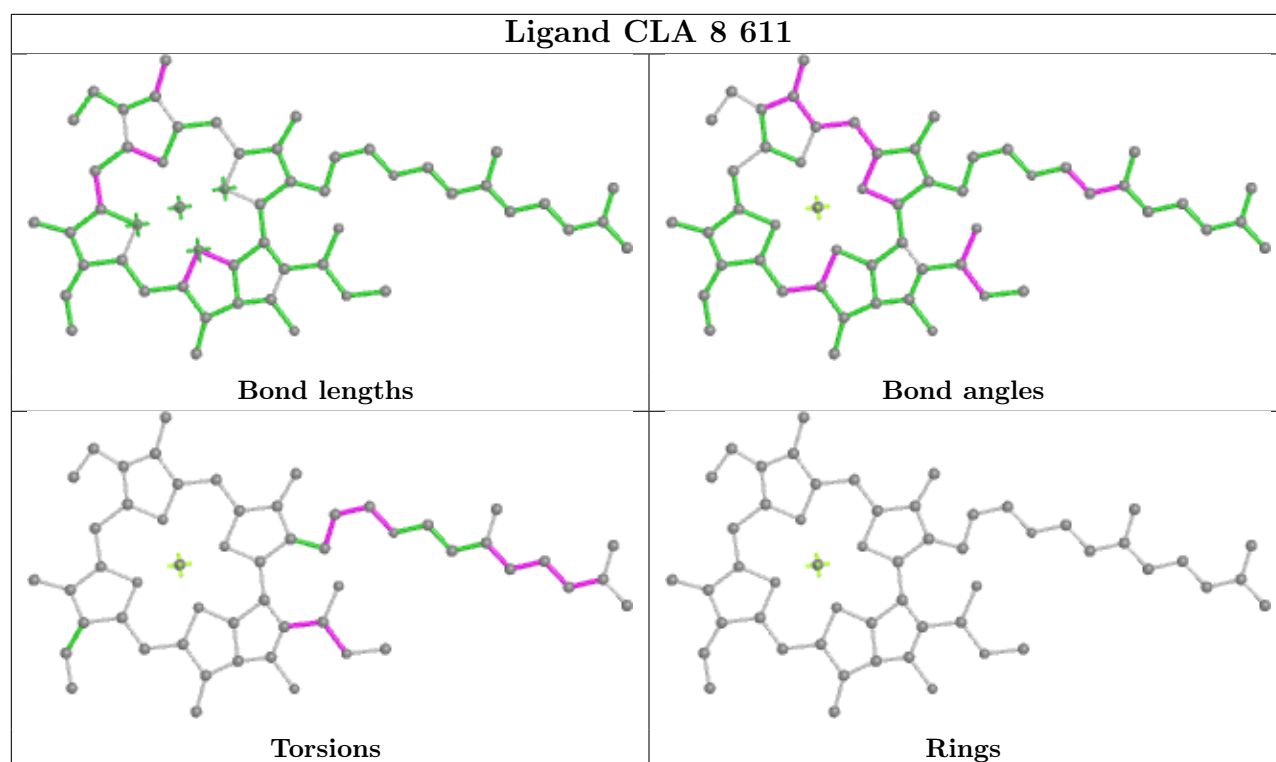
Rings

Ligand CLA 8 601

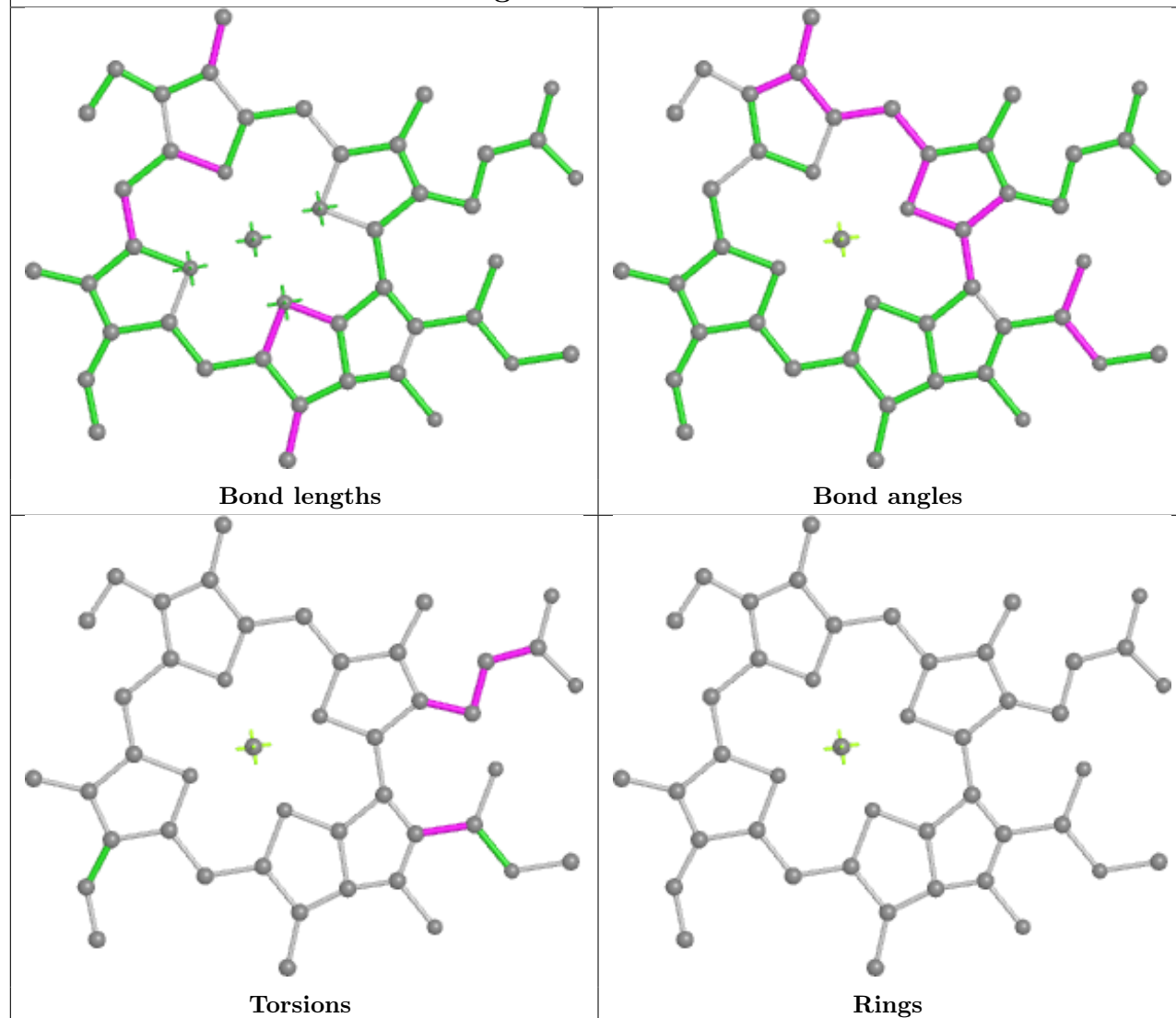


Ligand CHL a 609

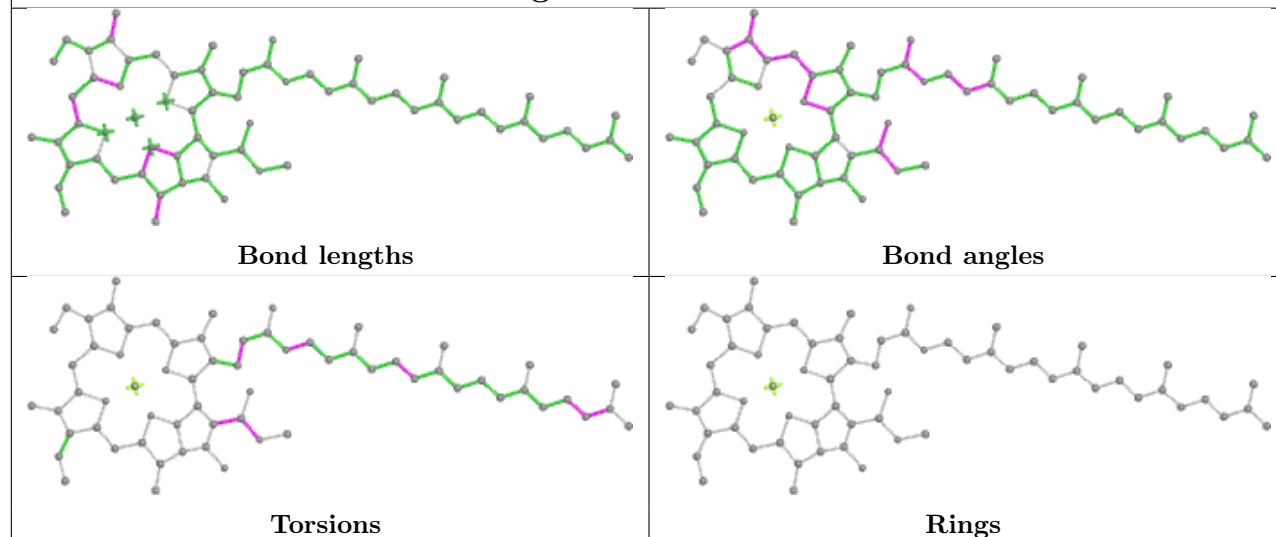




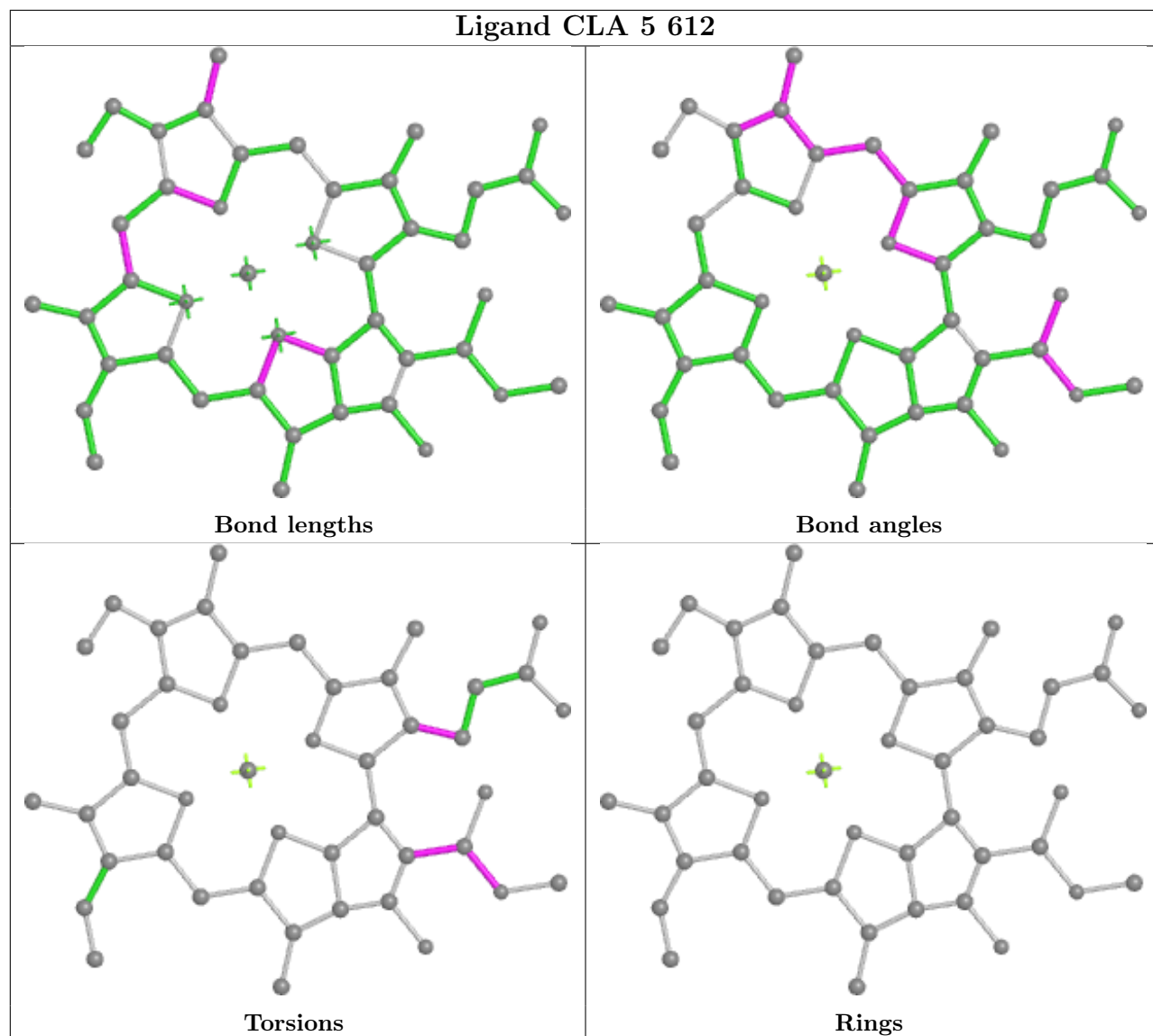
Ligand CLA 7 402



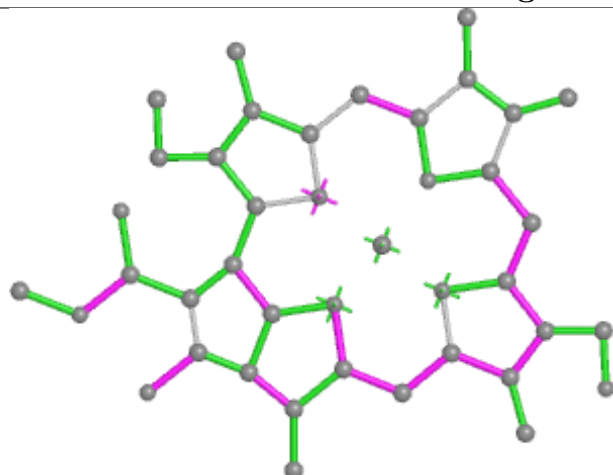
Ligand CLA A 814



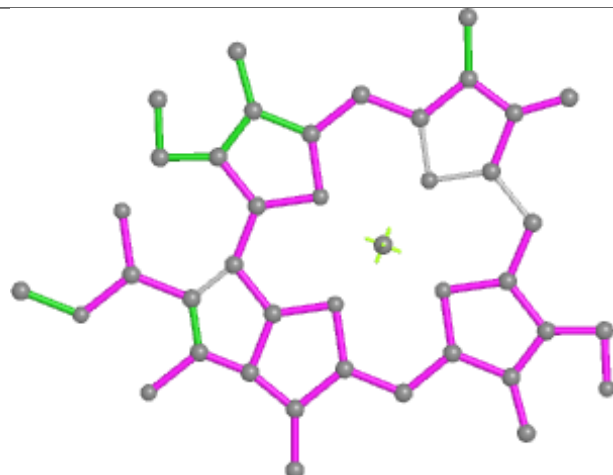
Ligand CLA 5 612



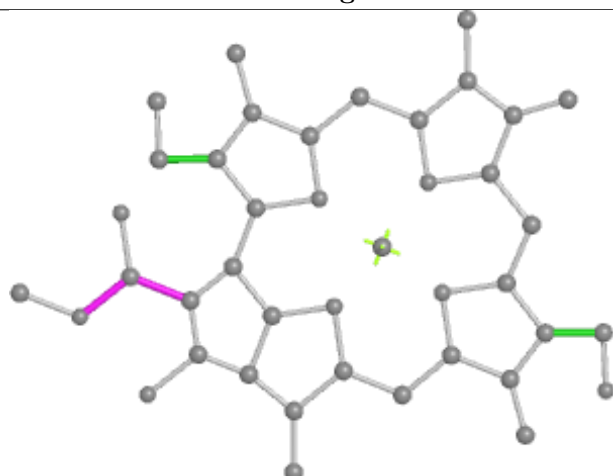
Ligand CHL 8 605



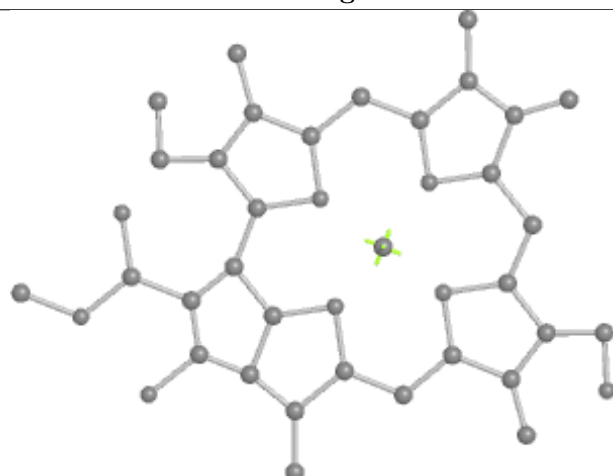
Bond lengths



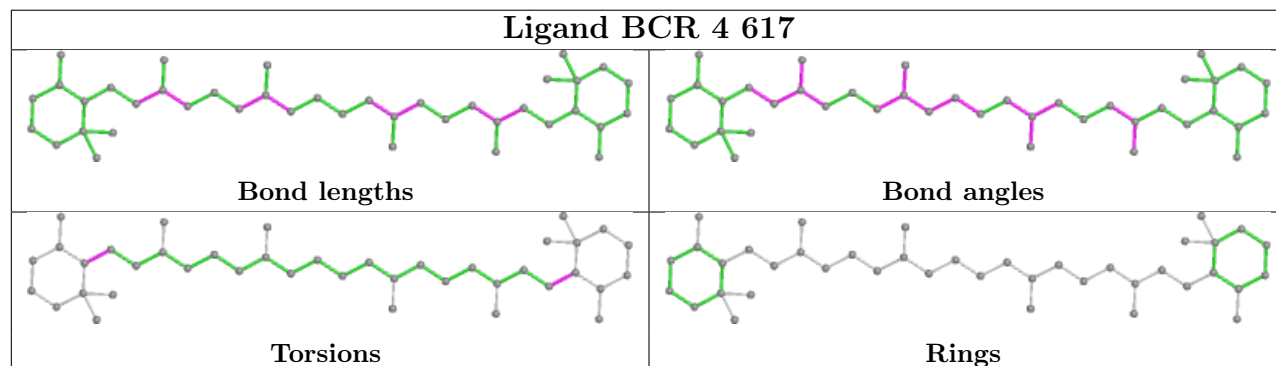
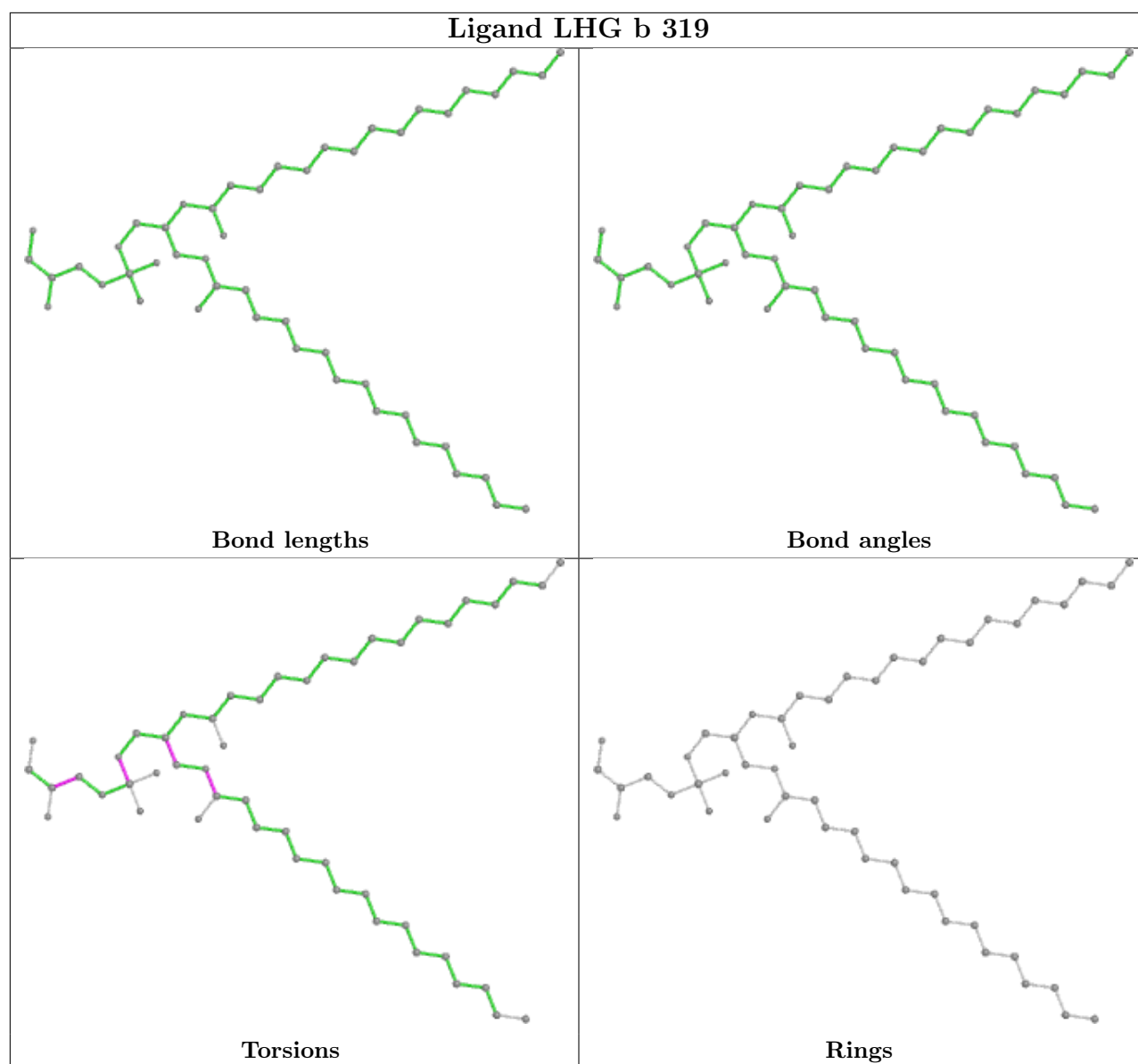
Bond angles



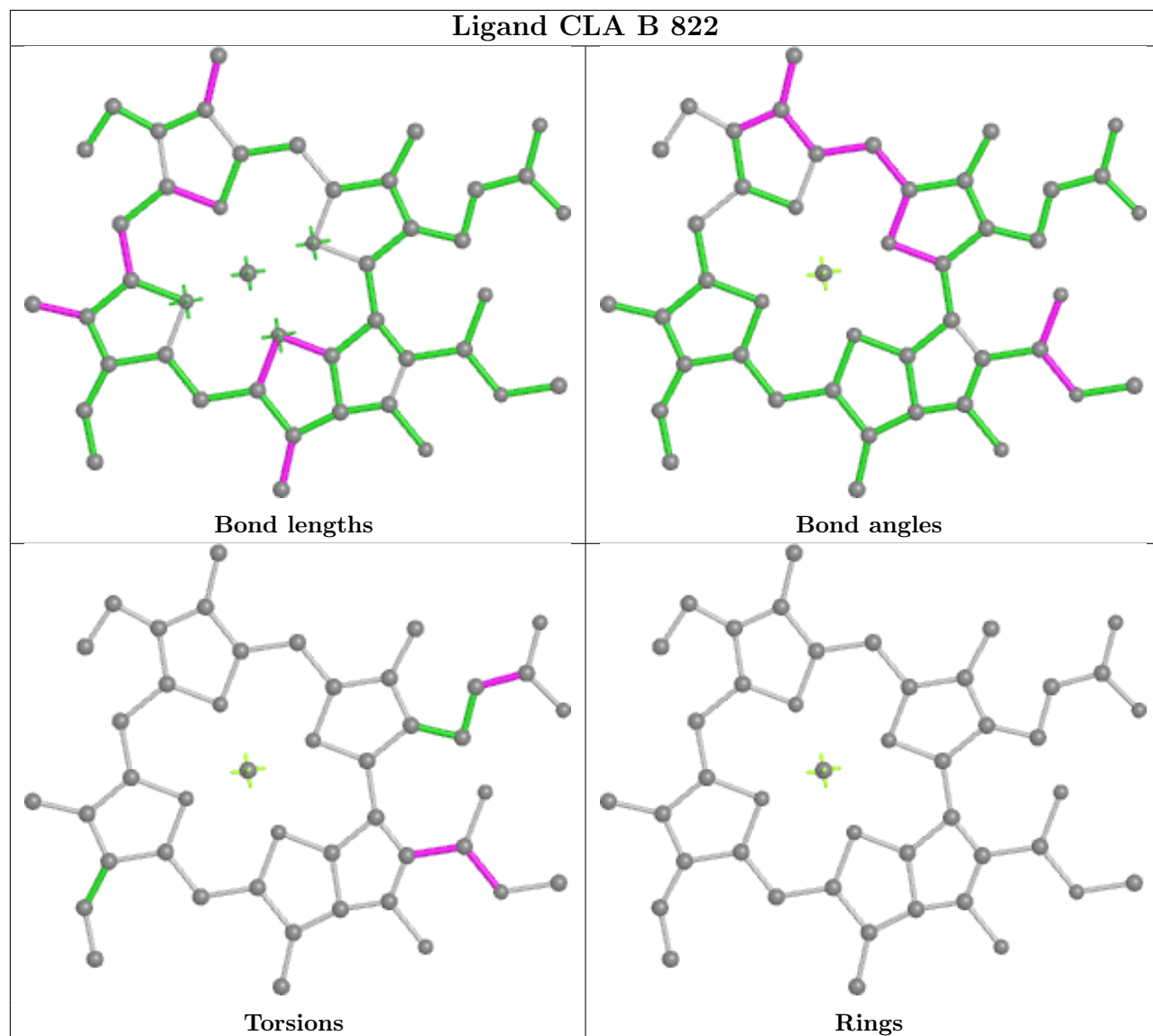
Torsions

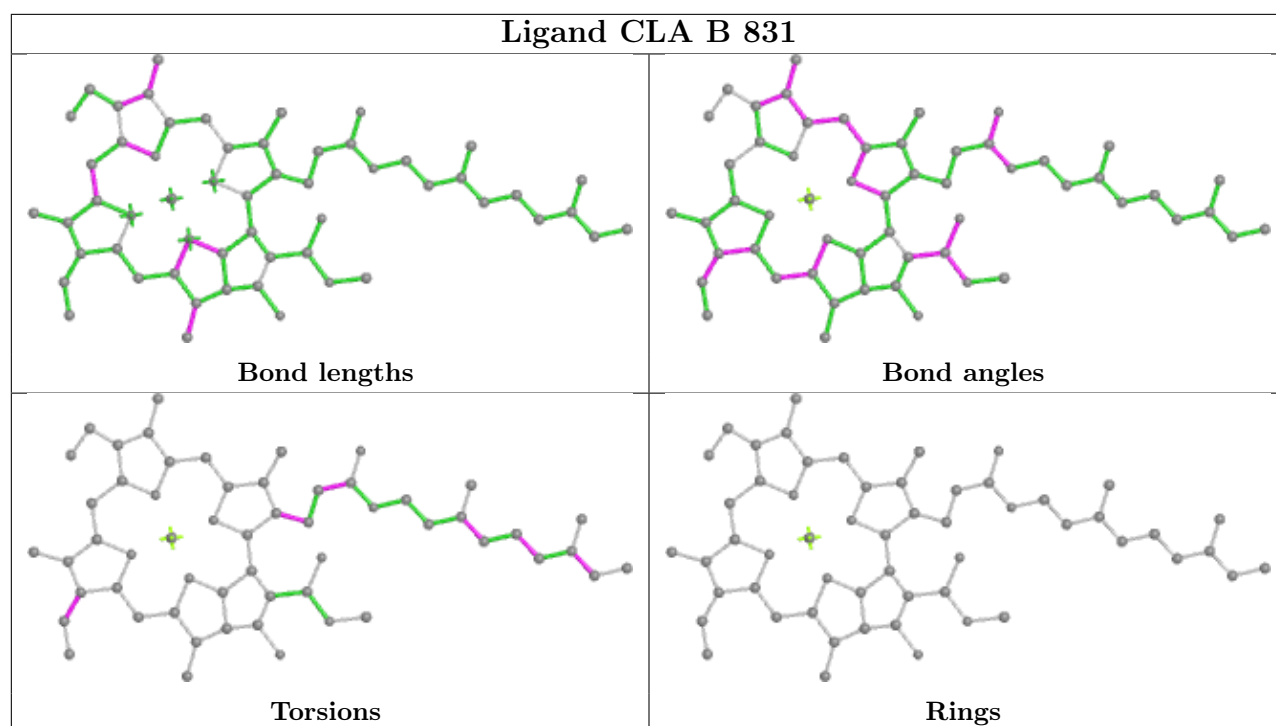


Rings

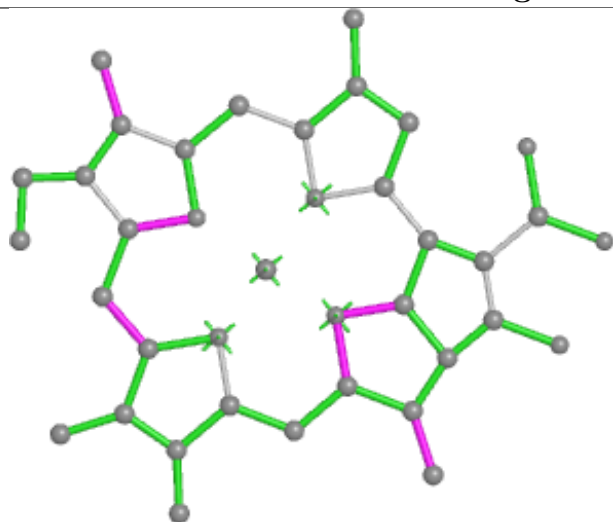


Ligand CLA B 822

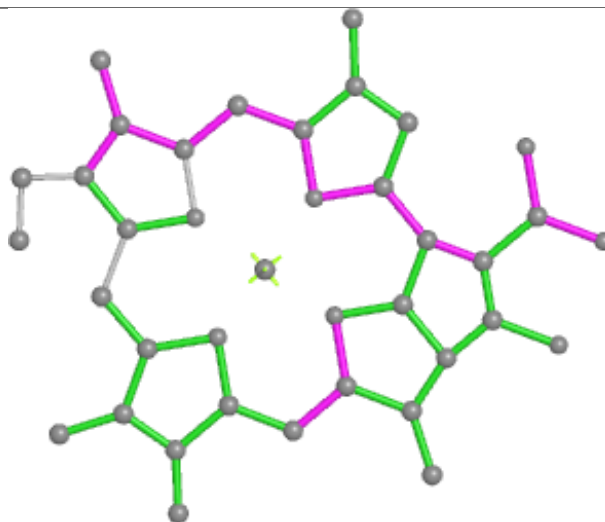




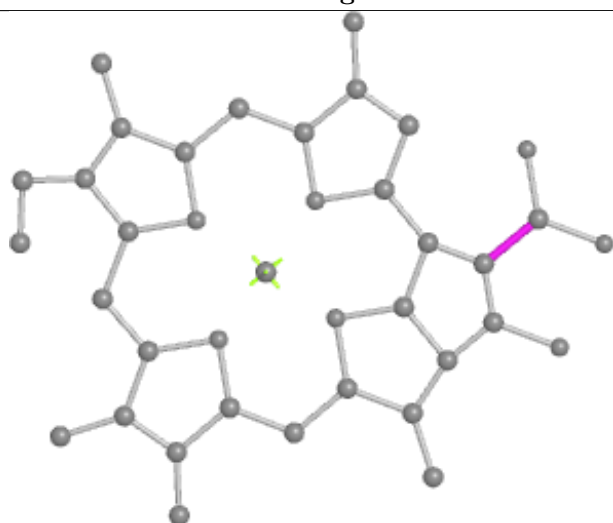
Ligand CLA O 202



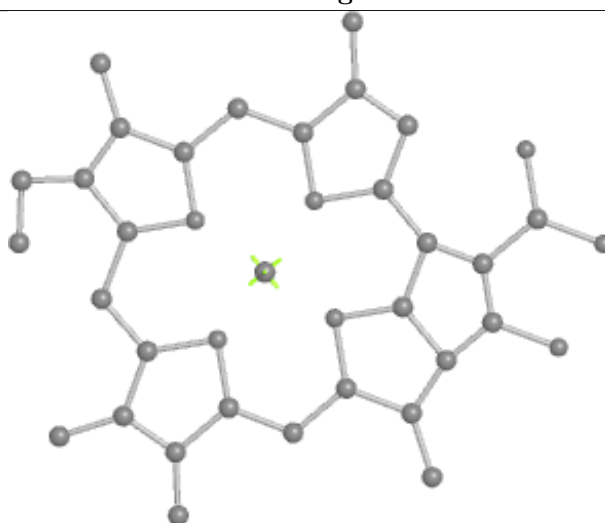
Bond lengths



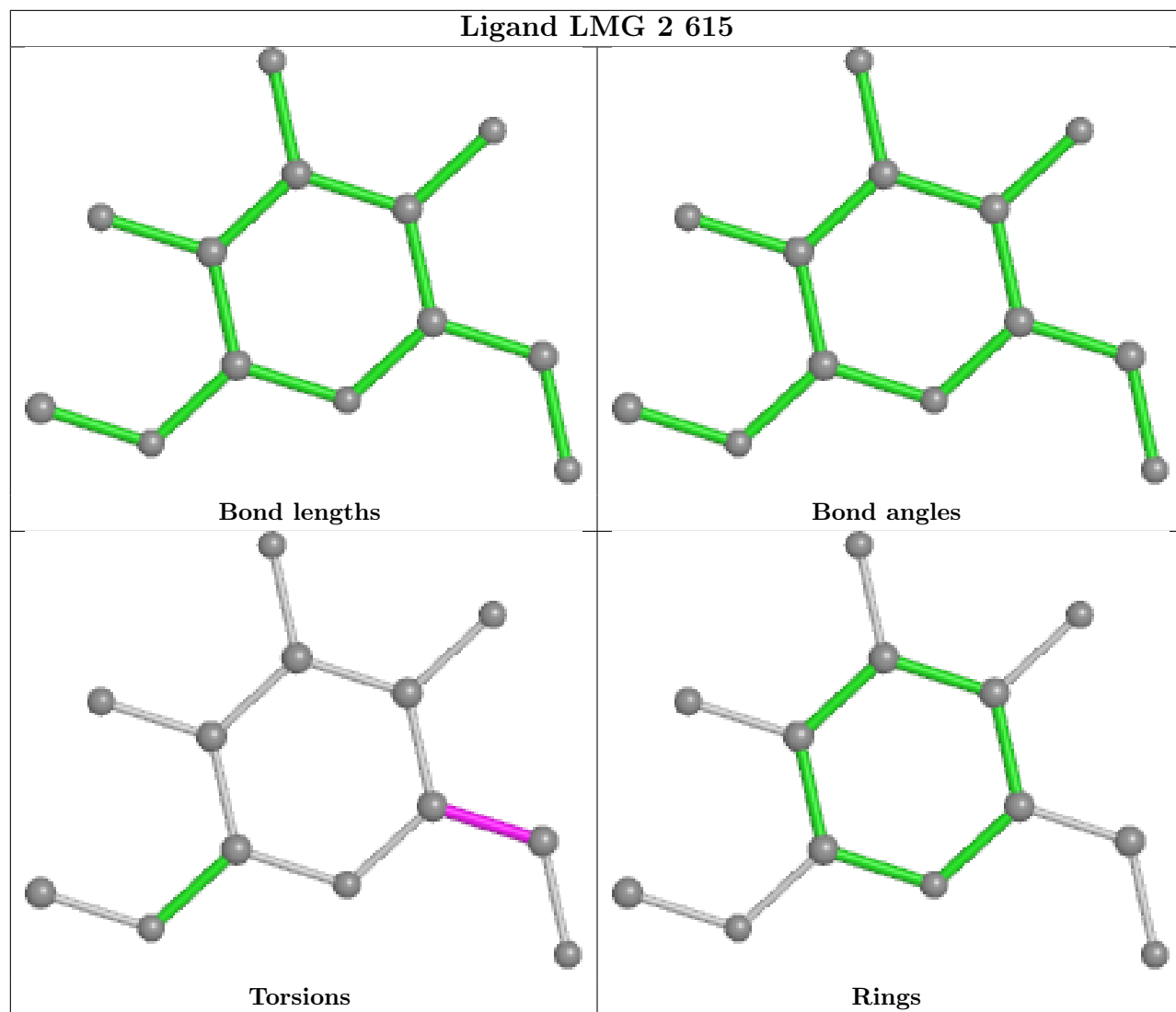
Bond angles



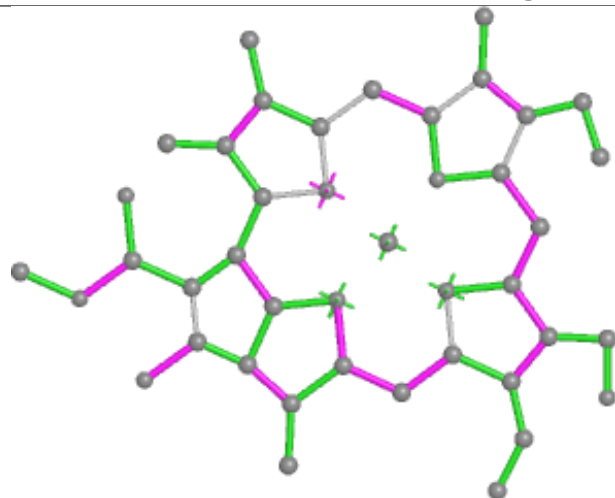
Torsions



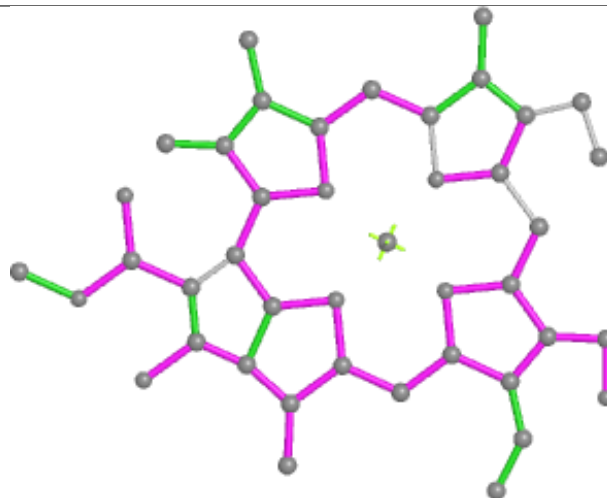
Rings



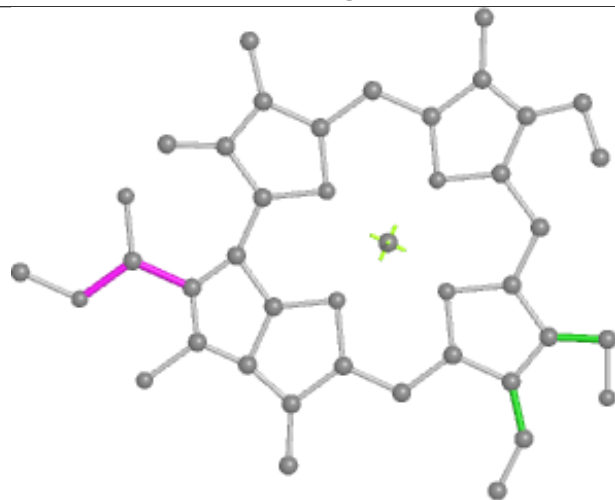
Ligand CHL 8 613



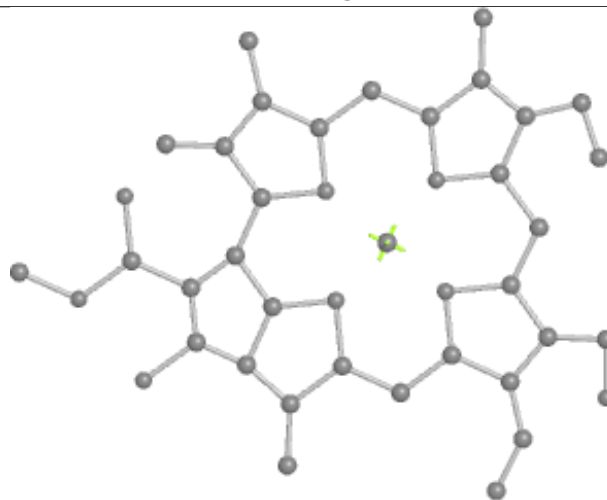
Bond lengths



Bond angles

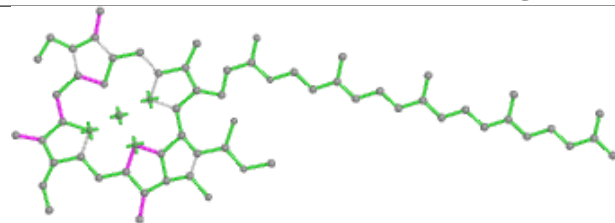


Torsions

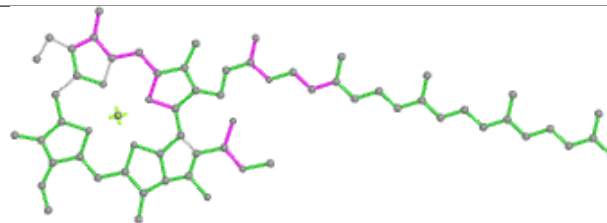


Rings

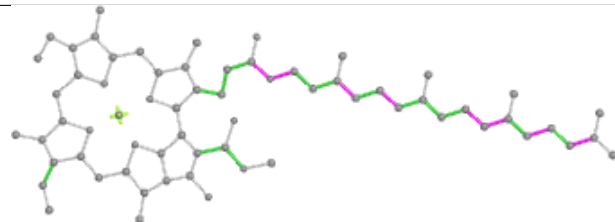
Ligand CLA B 825



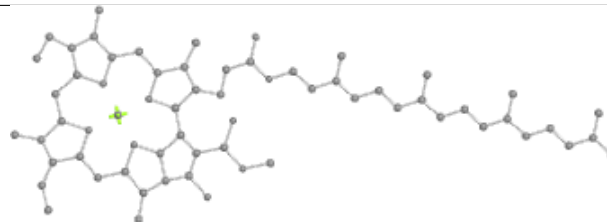
Bond lengths



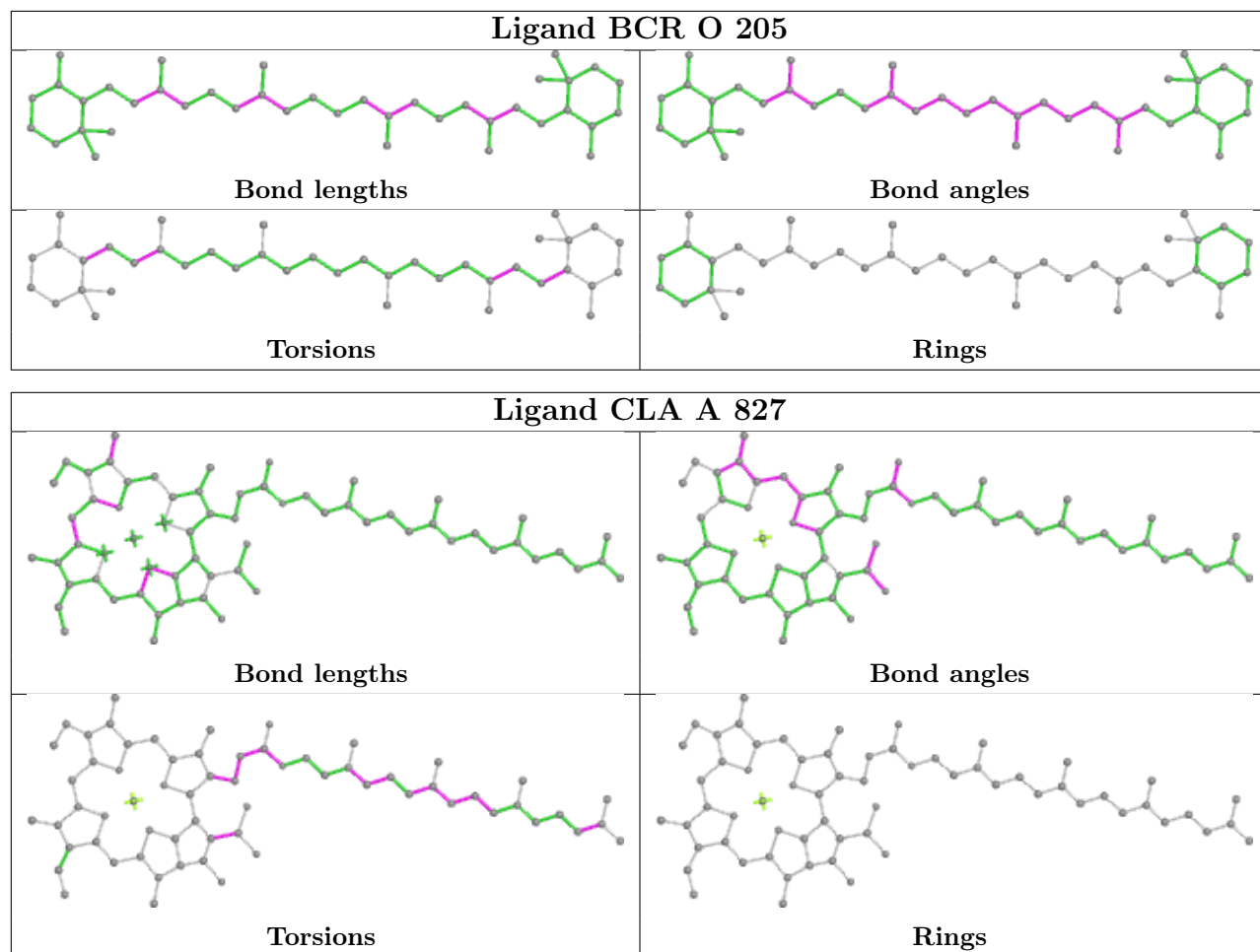
Bond angles



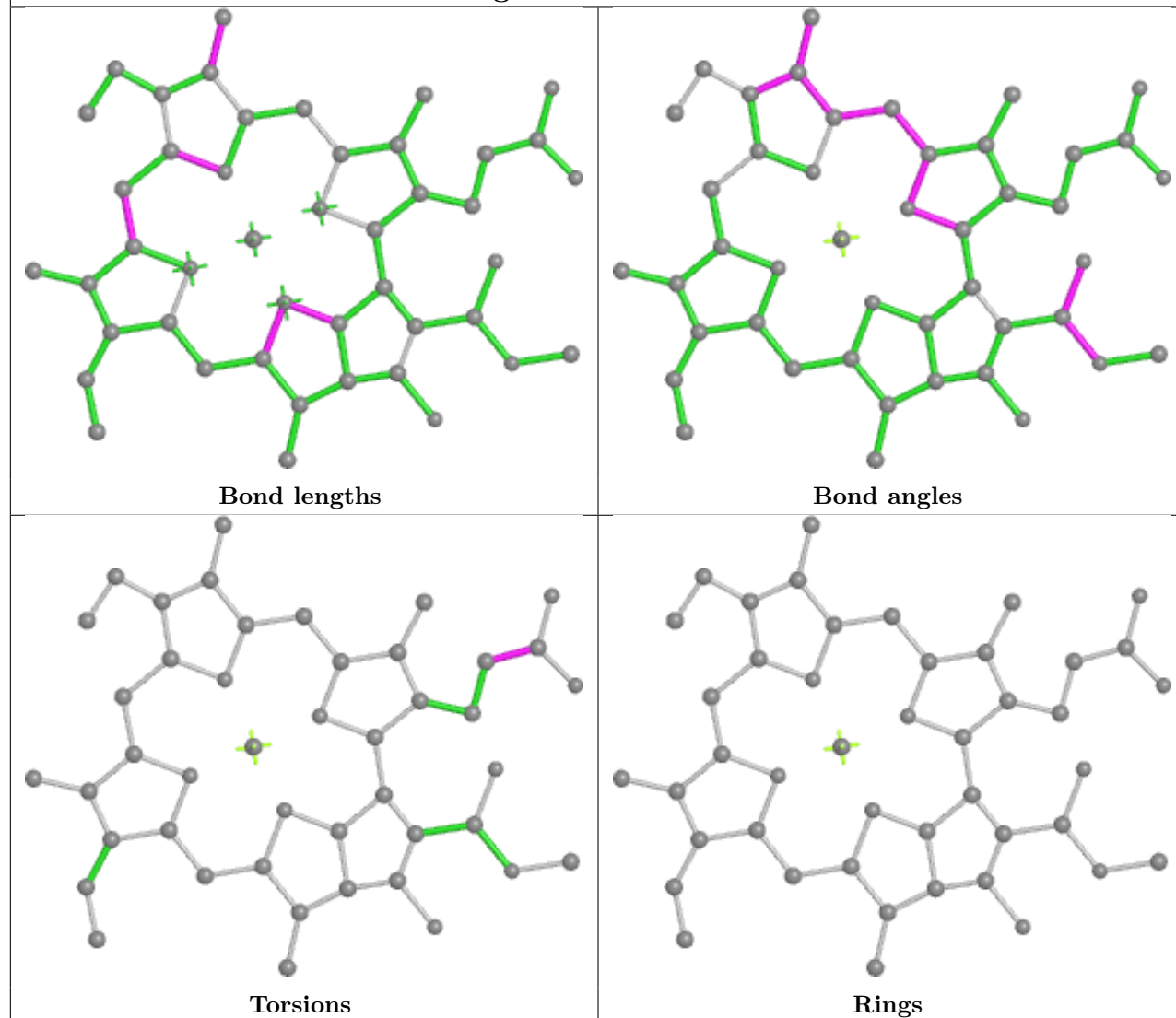
Torsions



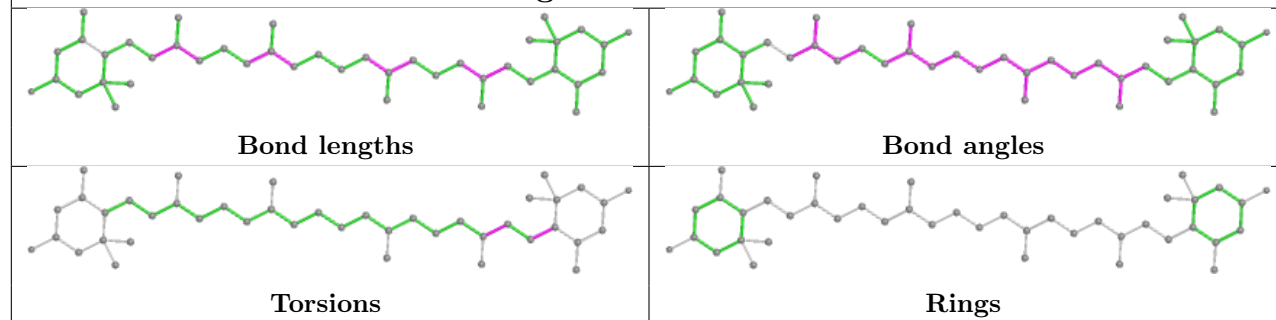
Rings



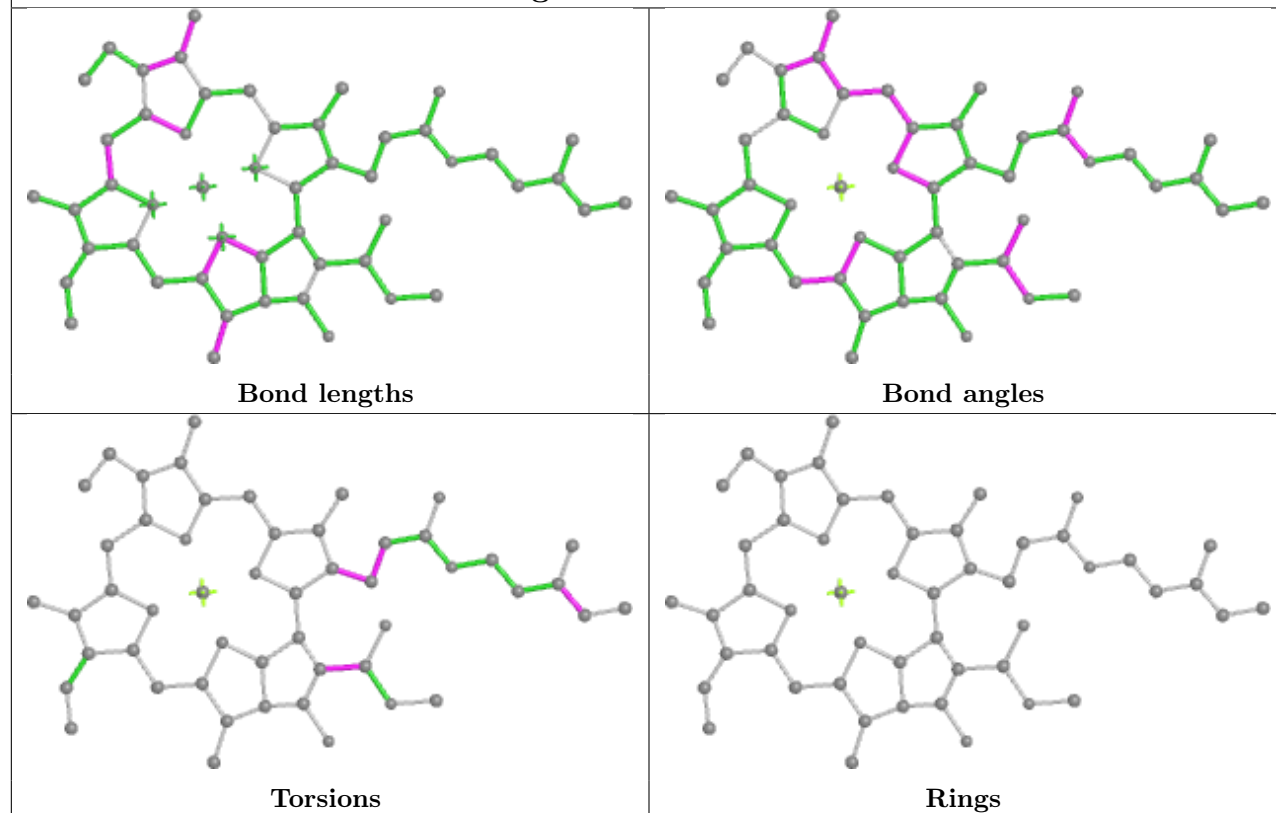
Ligand CLA b 312



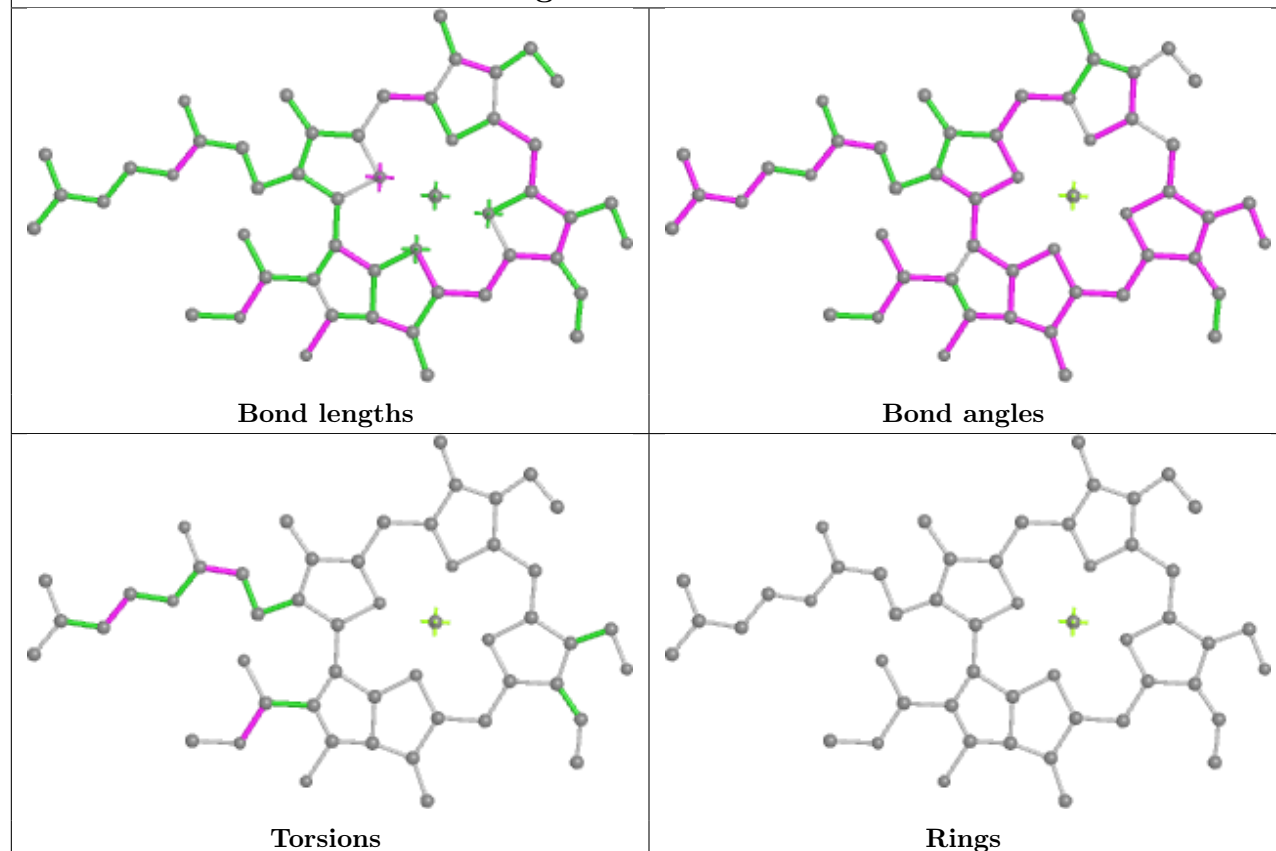
Ligand LUT 2 616



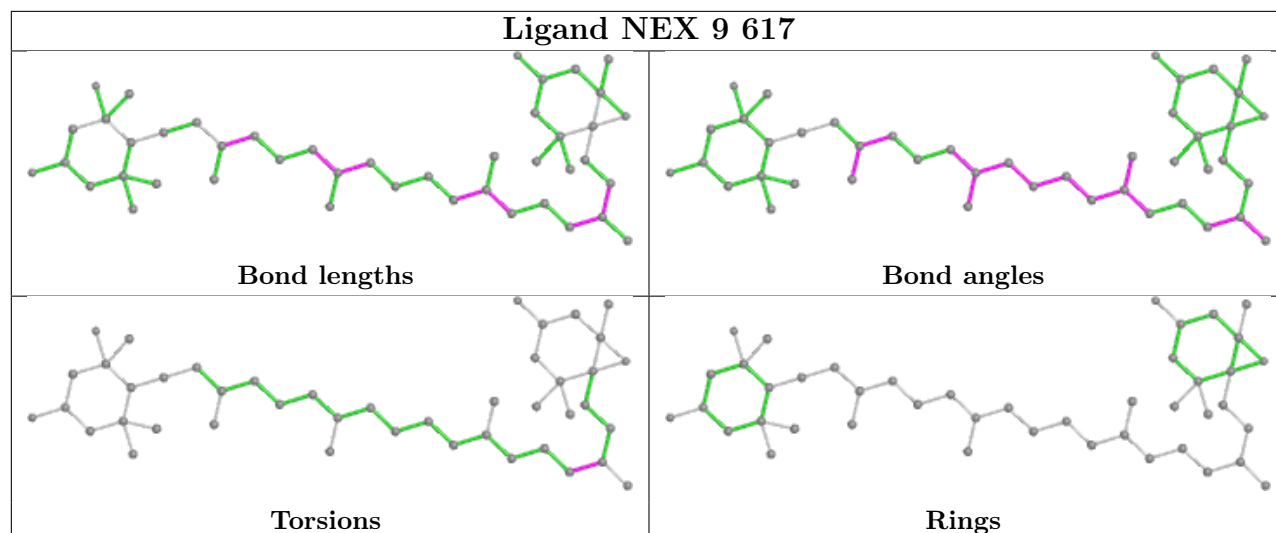
Ligand CLA A 837



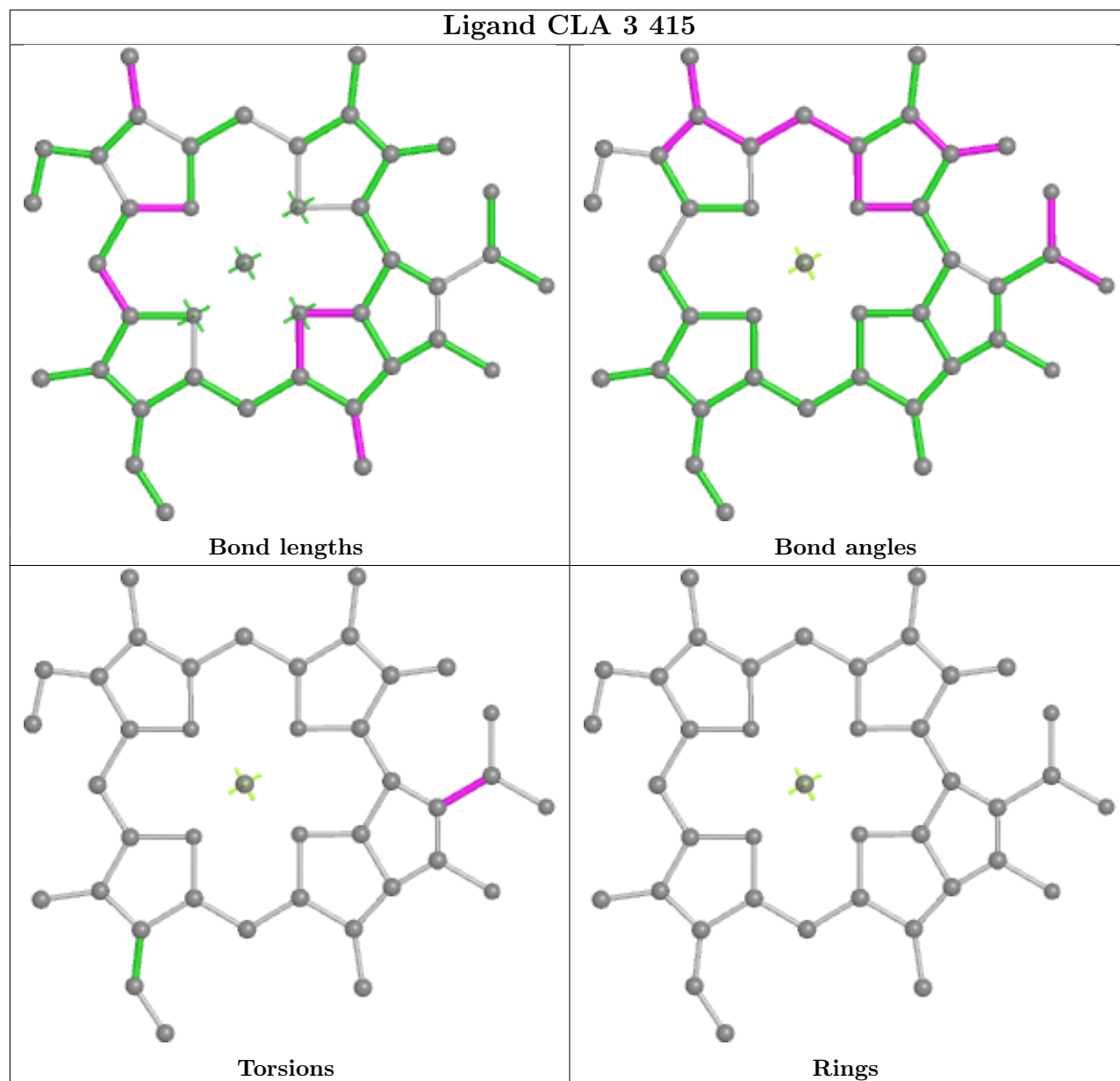
Ligand CHL 6 607



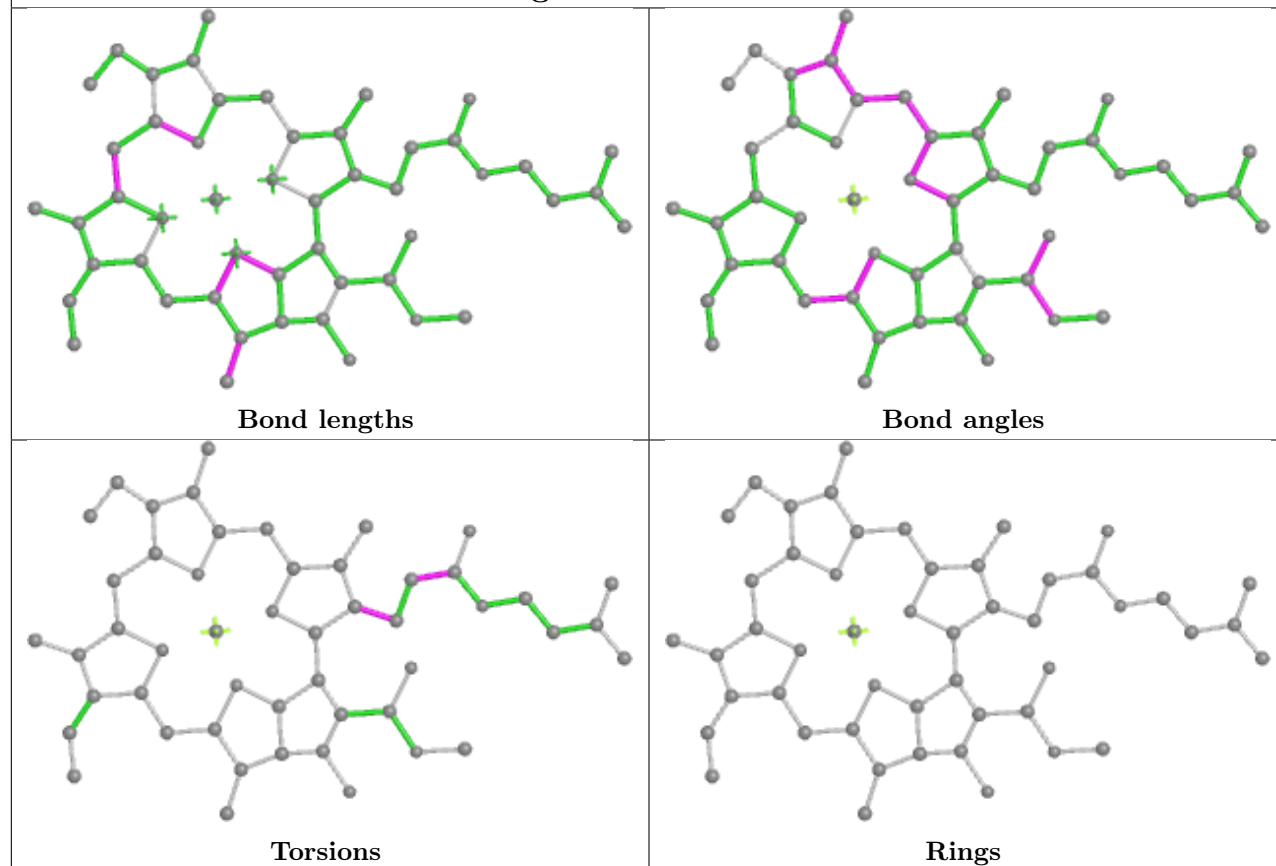
Ligand NEX 9 617



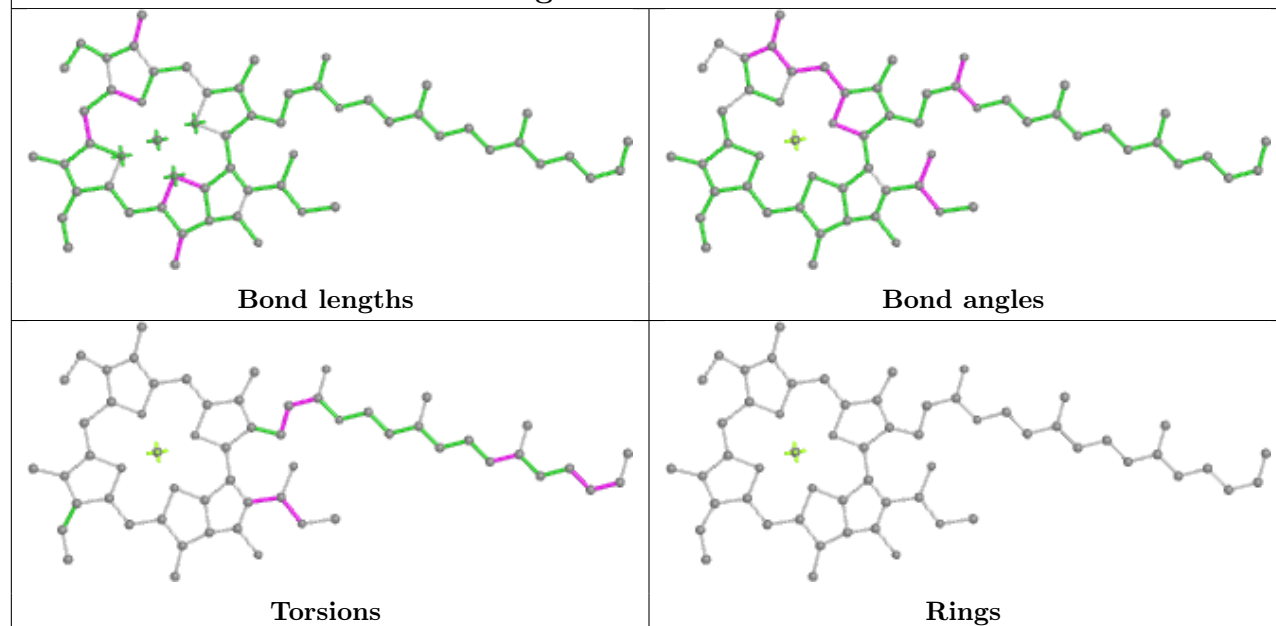
Ligand CLA 3 415



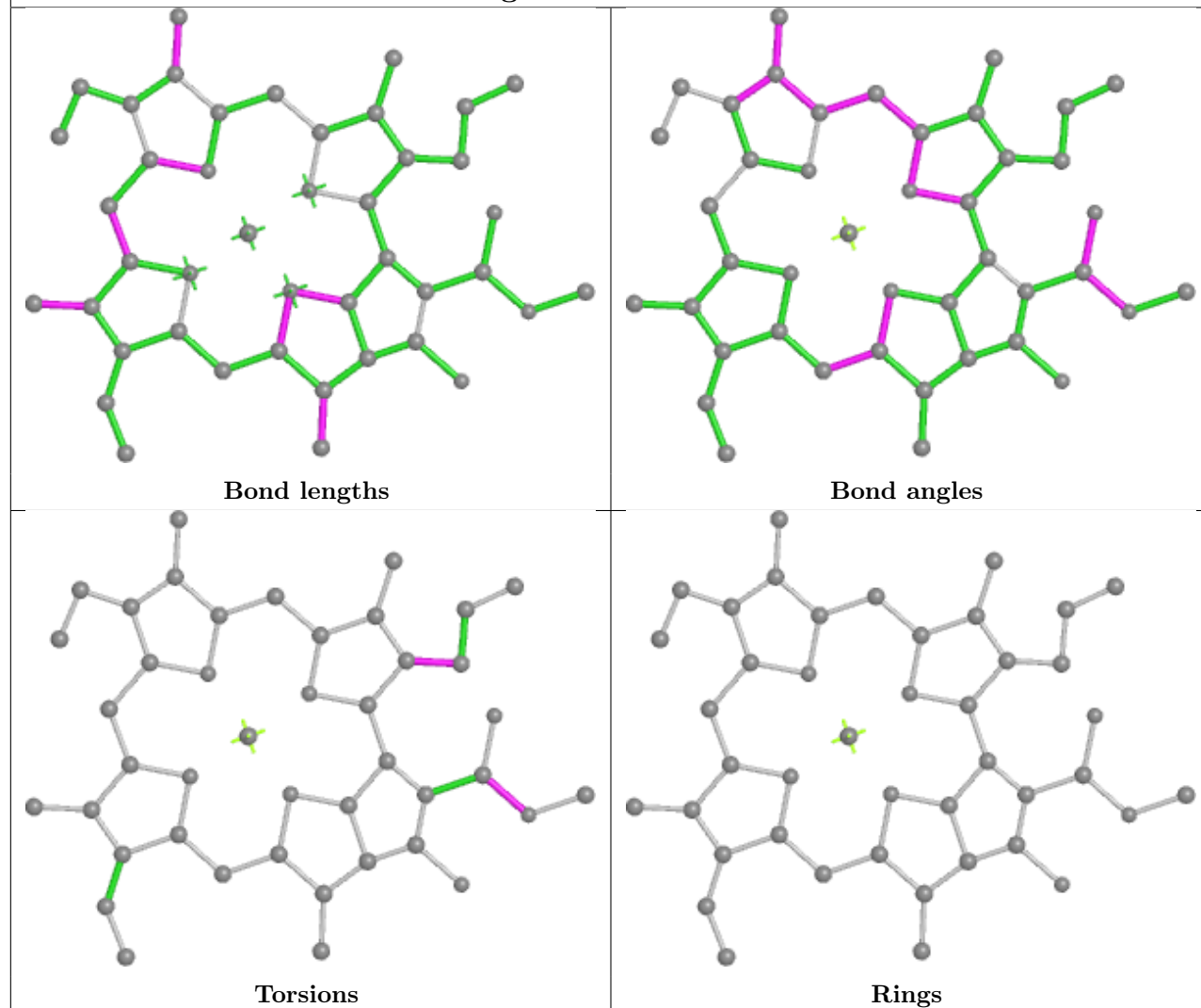
Ligand CLA A 835



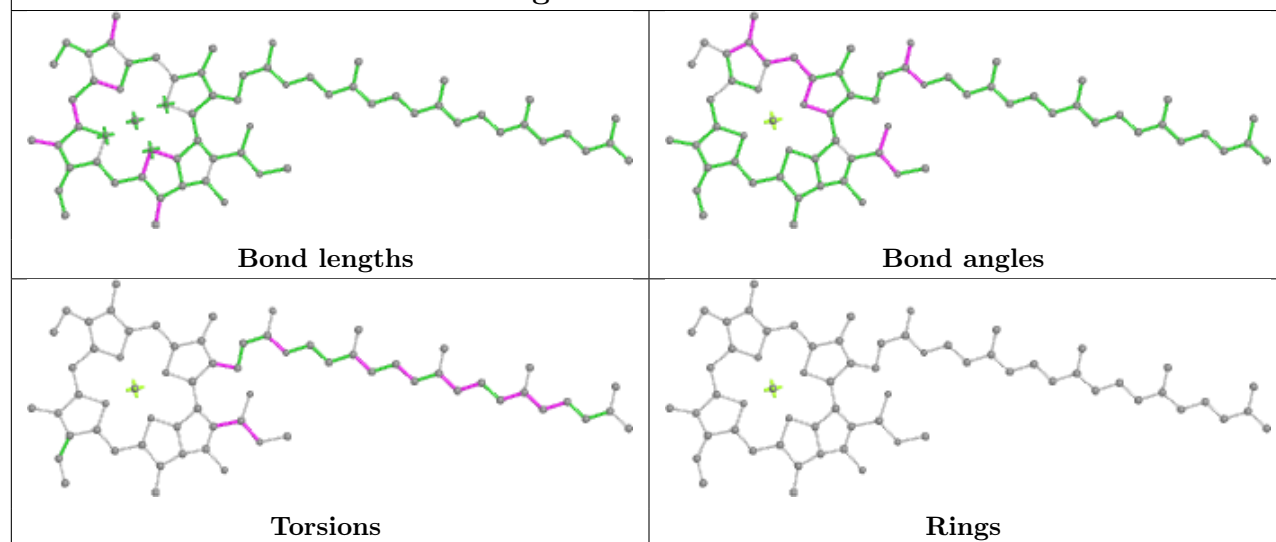
Ligand CLA b 303



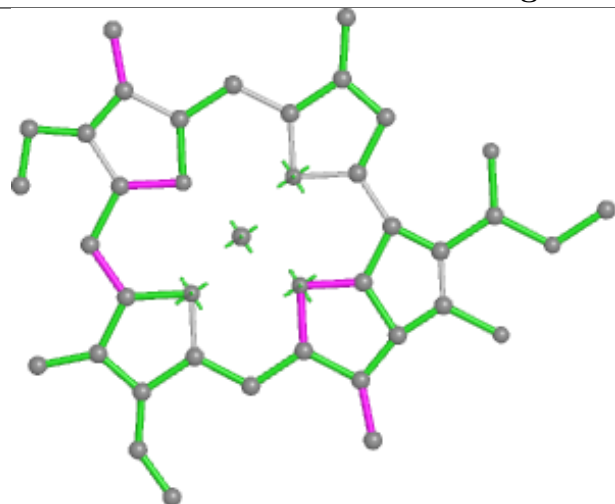
Ligand CLA B 819



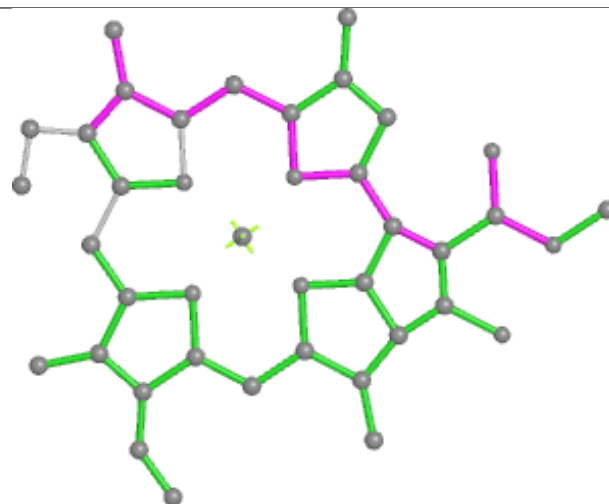
Ligand CLA B 802



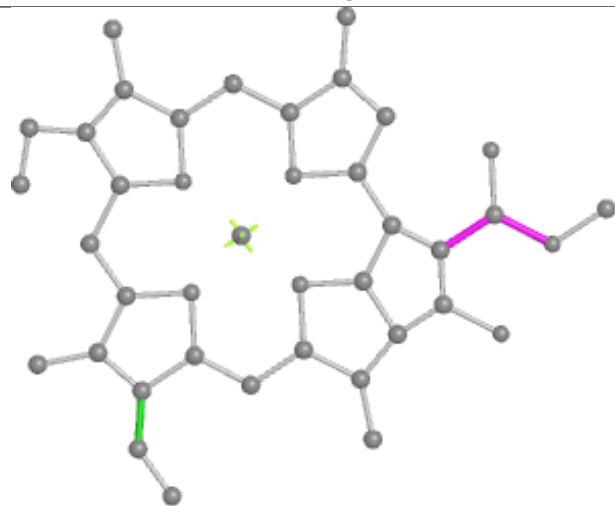
Ligand CLA 1 306



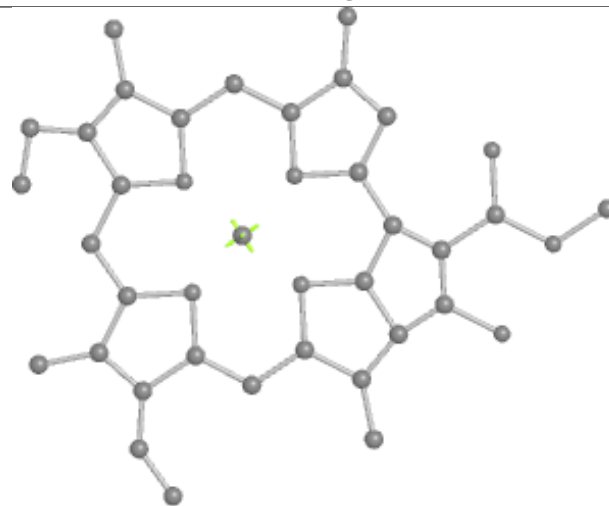
Bond lengths



Bond angles

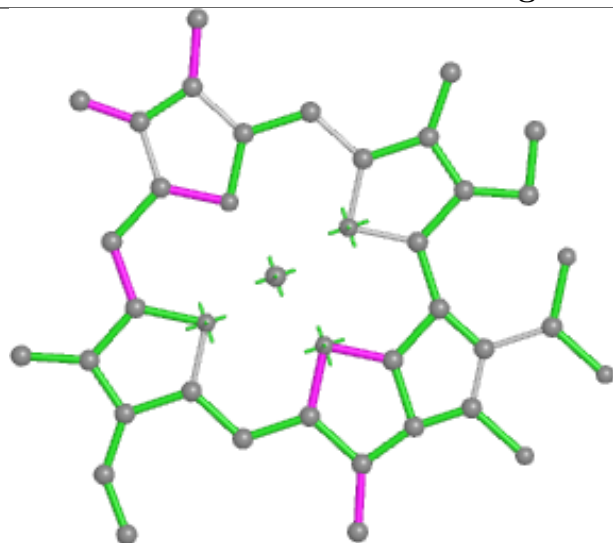


Torsions

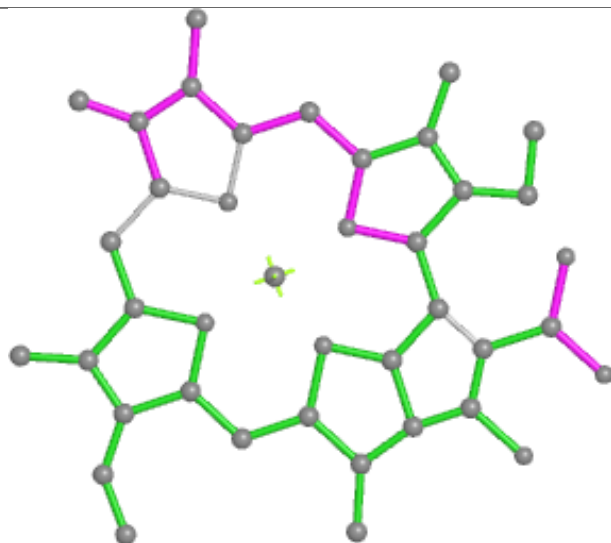


Rings

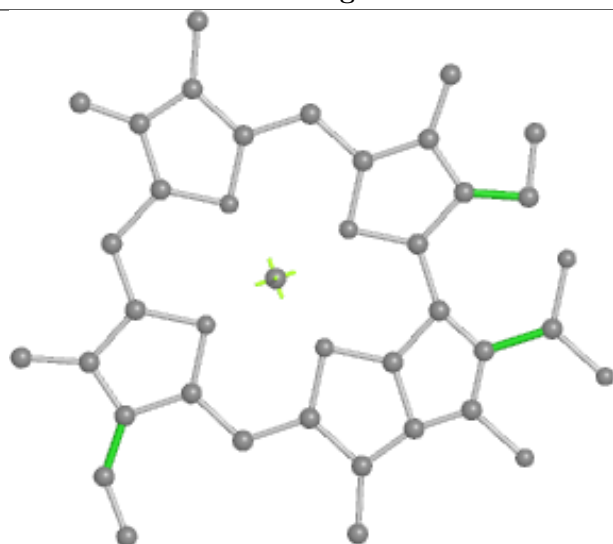
Ligand CLA 3 406



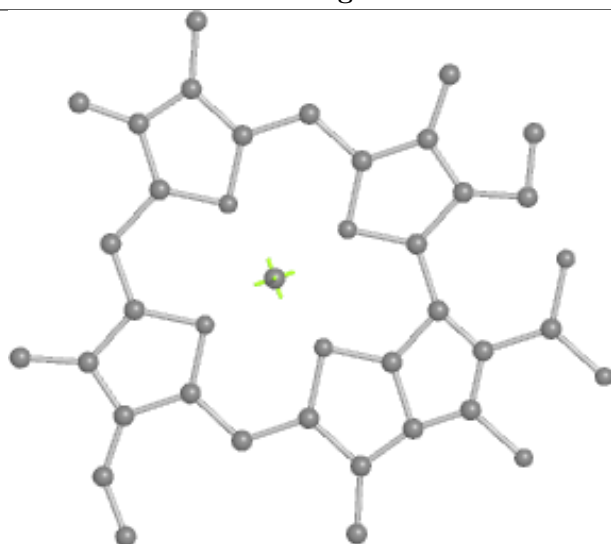
Bond lengths



Bond angles

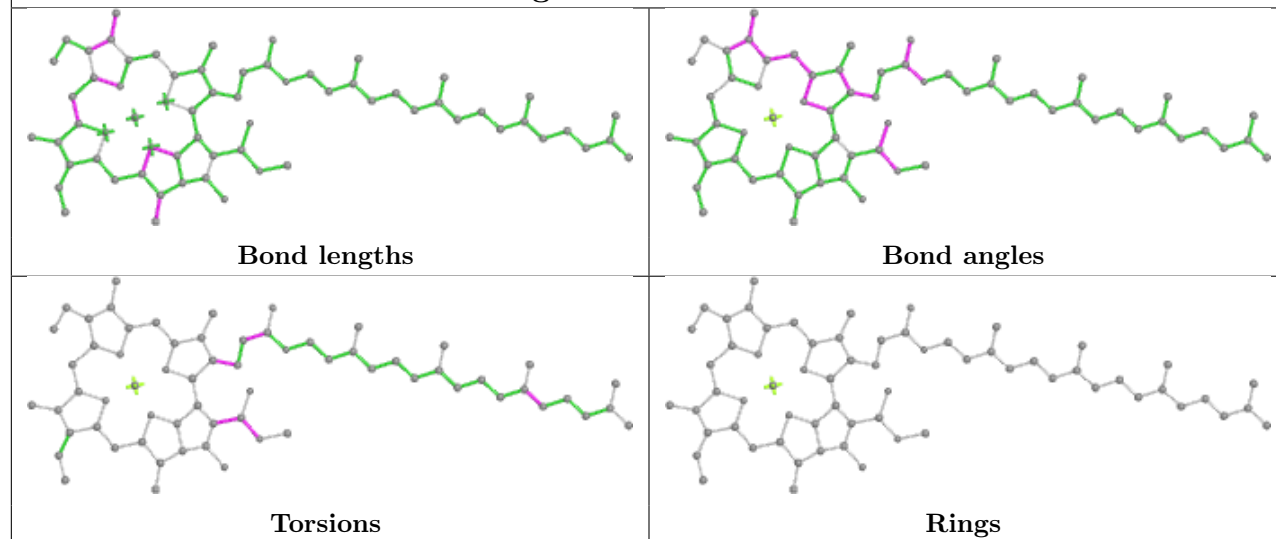


Torsions

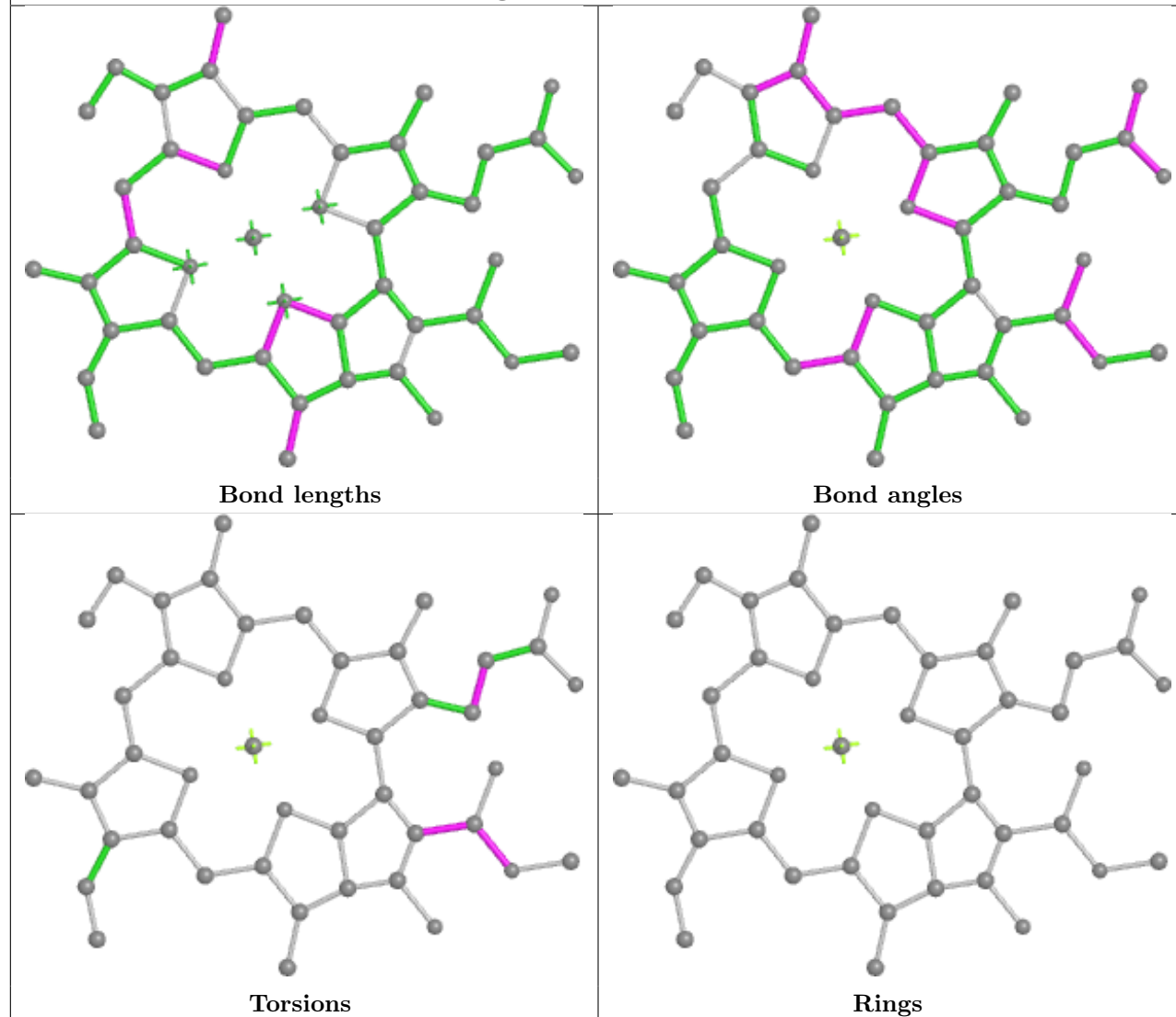


Rings

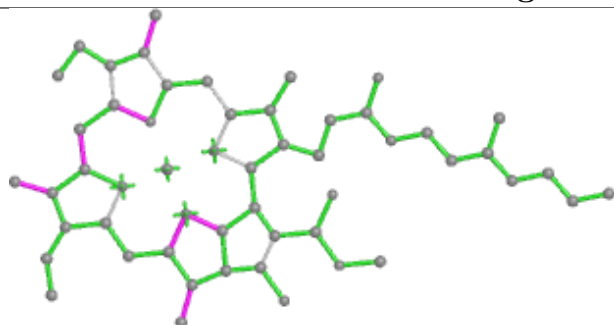
Ligand CLA B 839



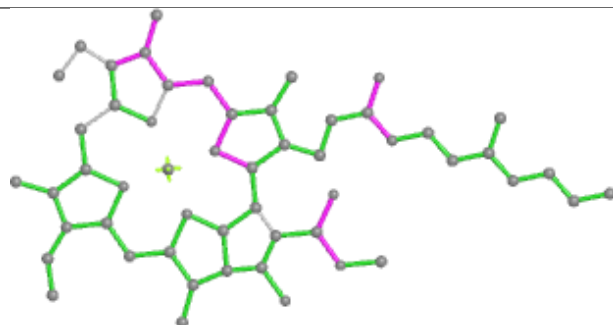
Ligand CLA 1 313



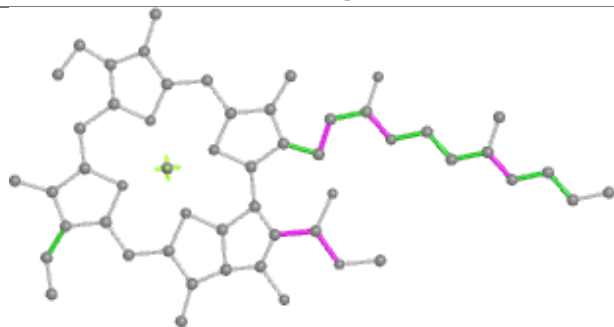
Ligand CLA b 314



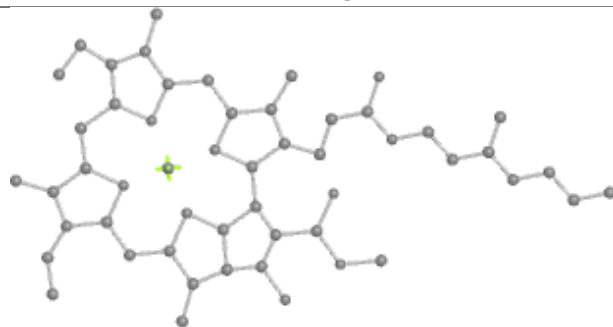
Bond lengths



Bond angles

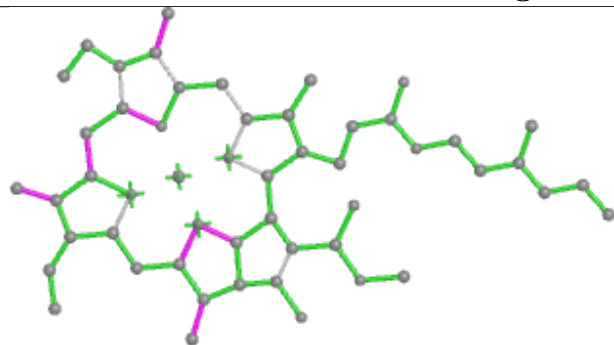


Torsions

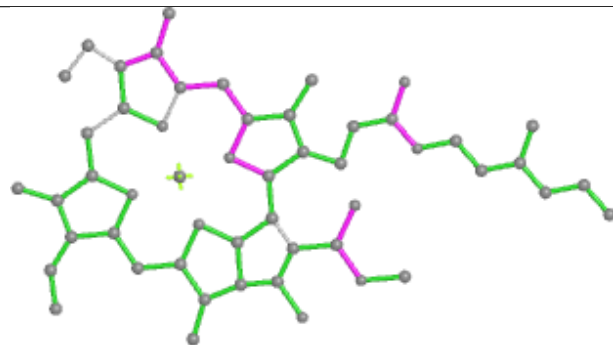


Rings

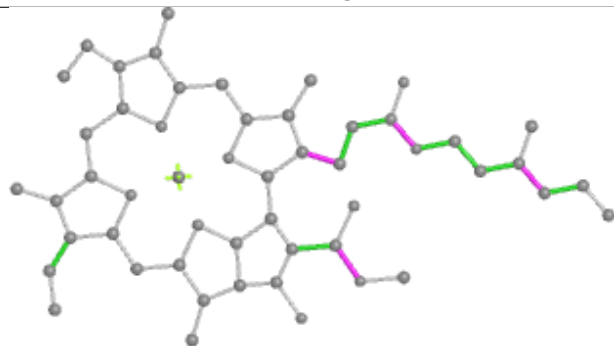
Ligand CLA B 828



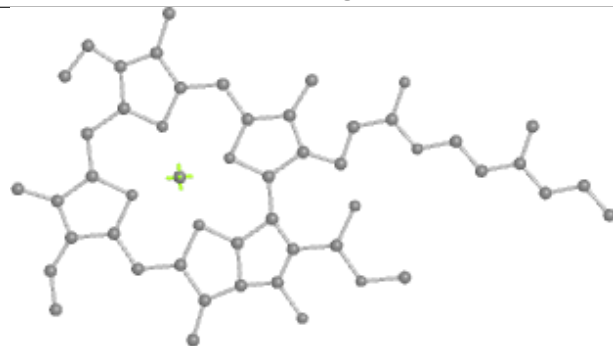
Bond lengths



Bond angles

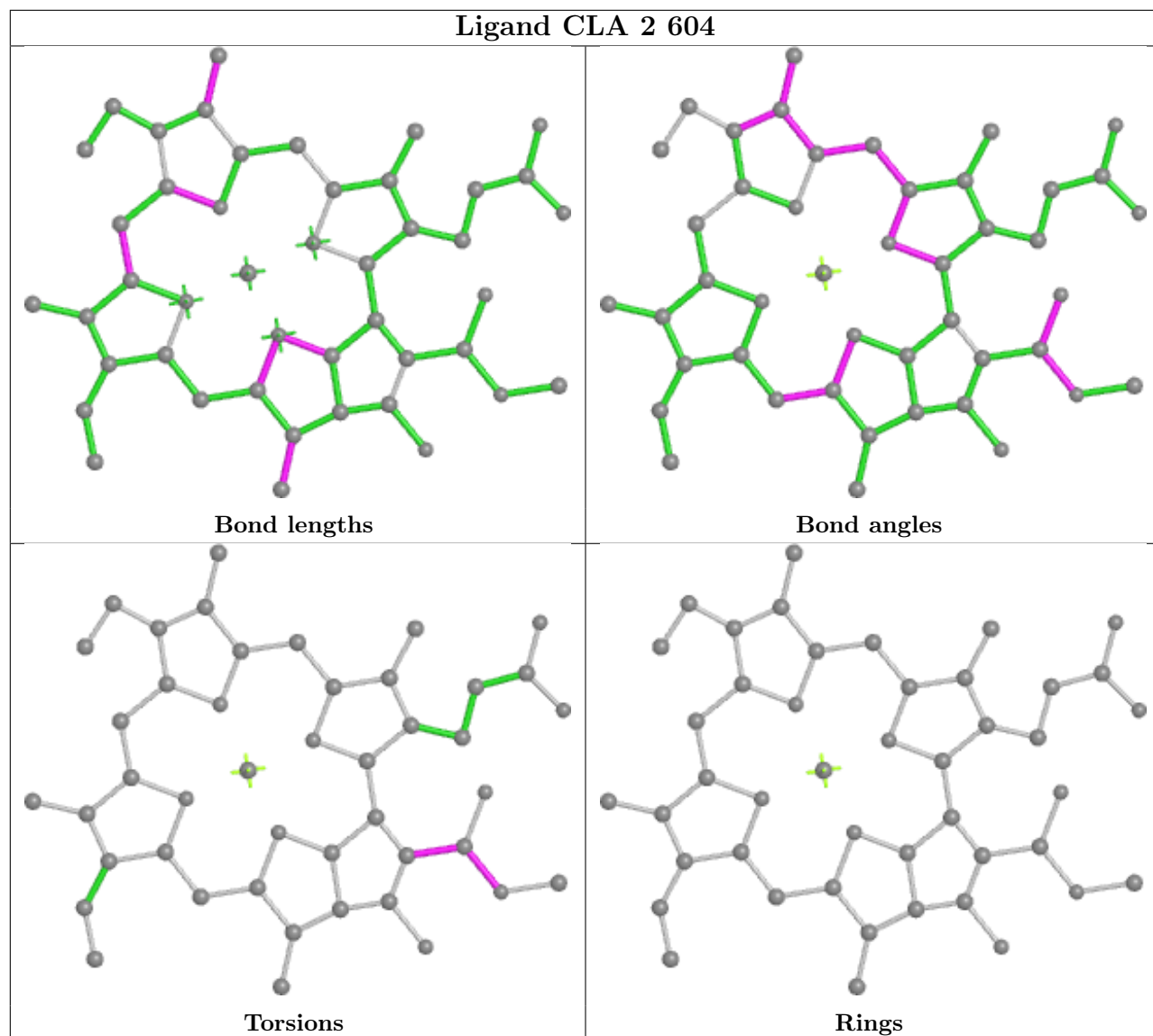


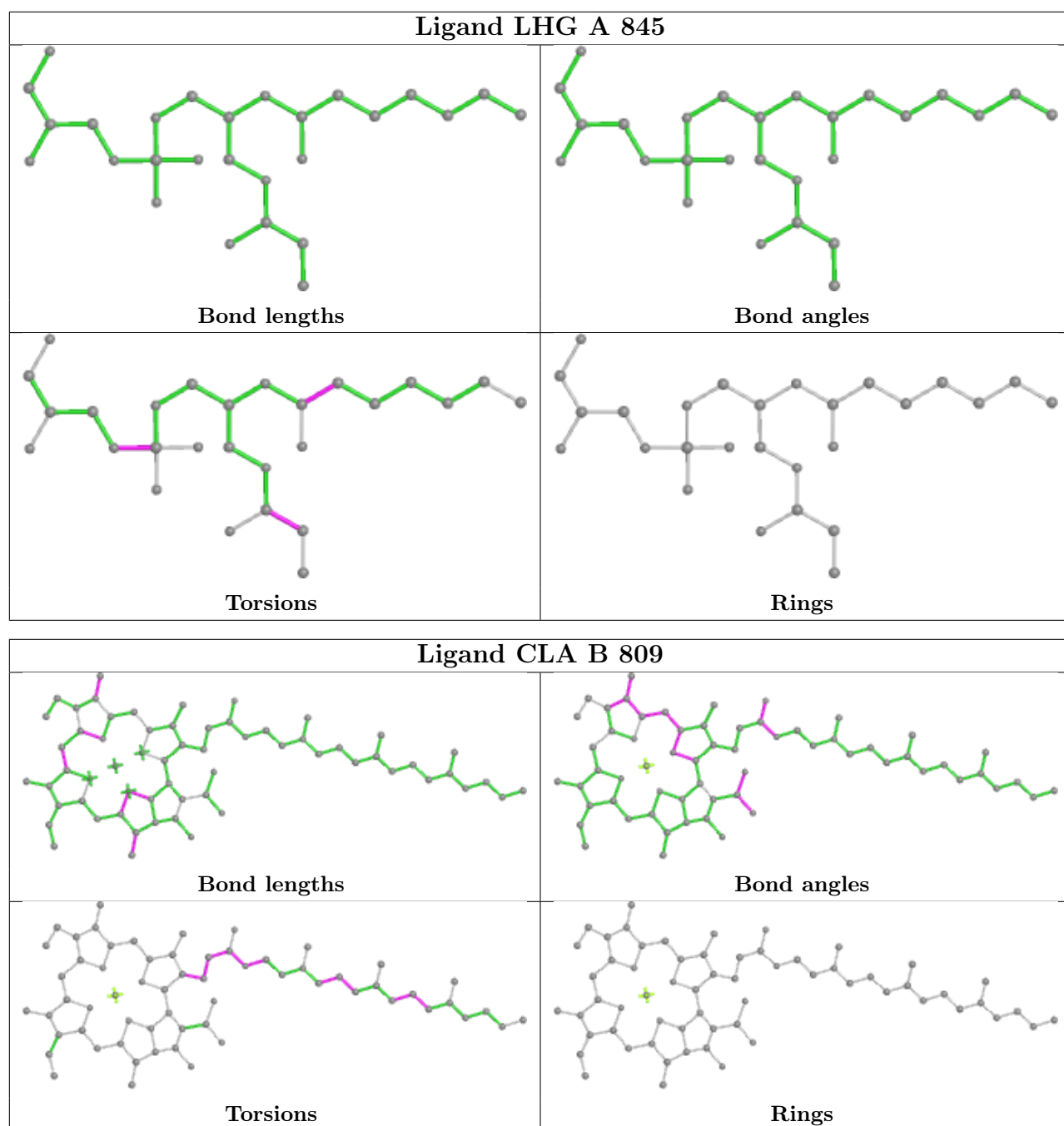
Torsions



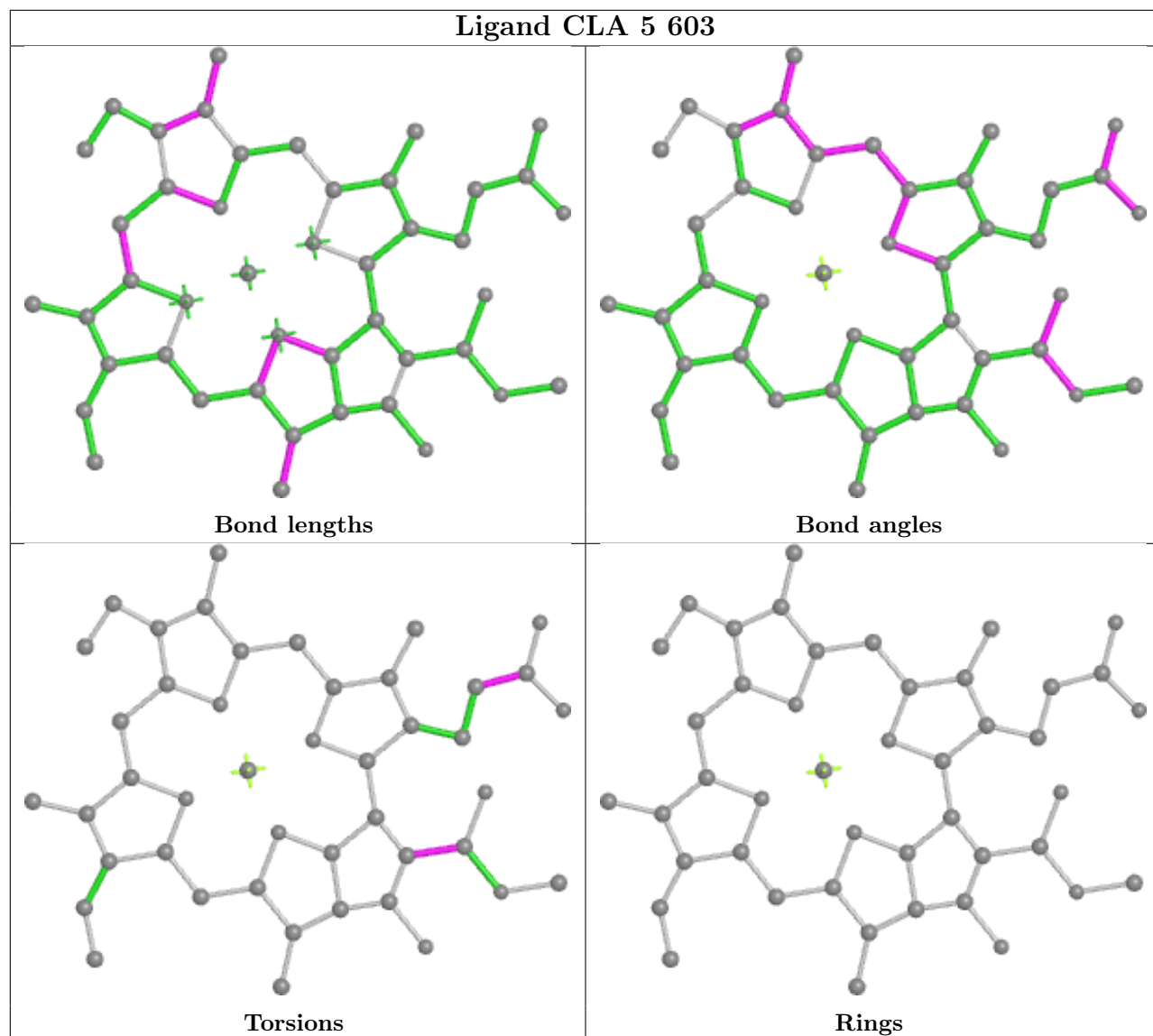
Rings

Ligand CLA 2 604

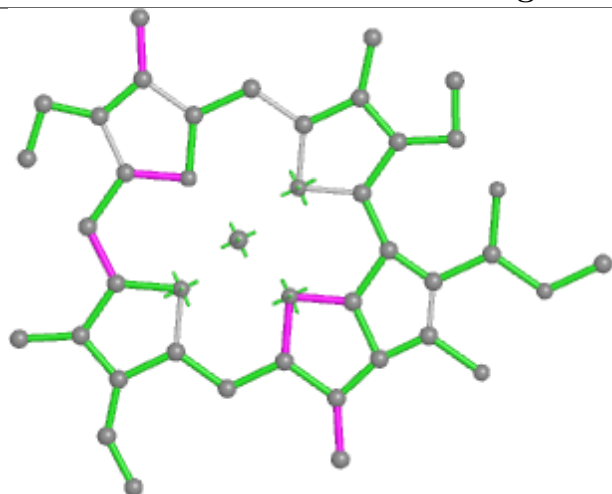




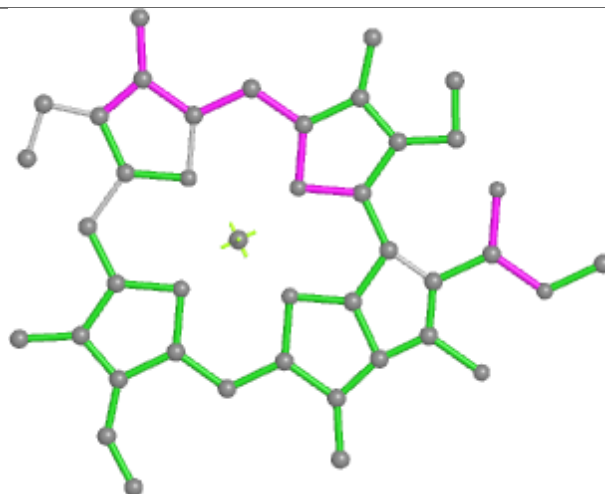
Ligand CLA 5 603



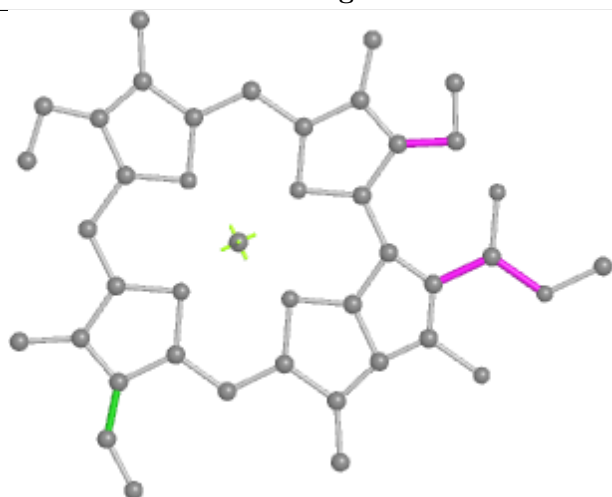
Ligand CLA J 102



Bond lengths



Bond angles

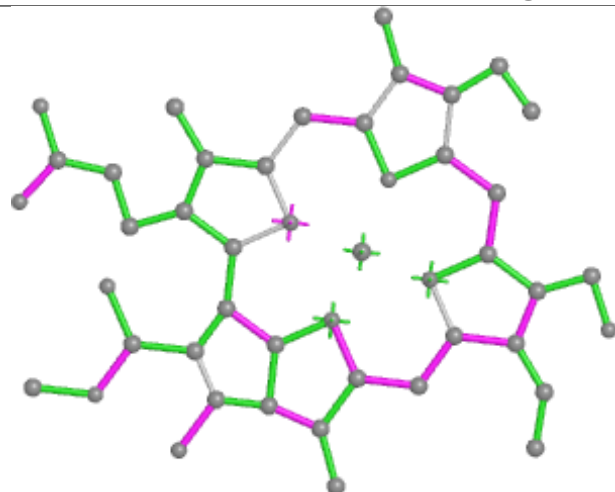


Torsions

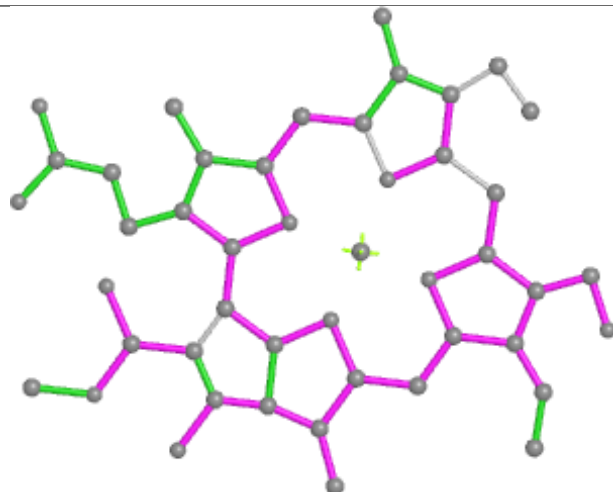


Rings

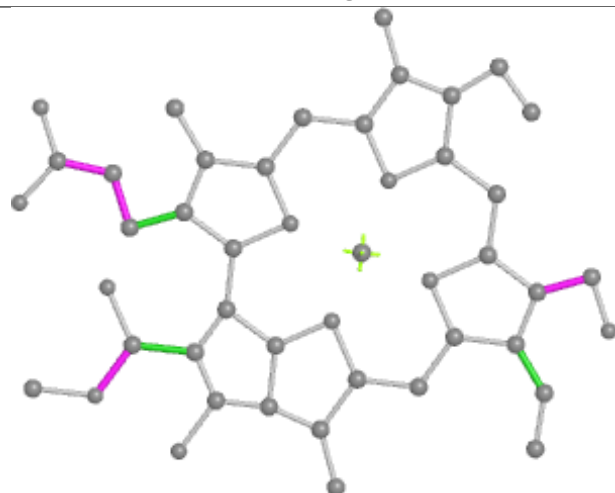
Ligand CHL 9 607



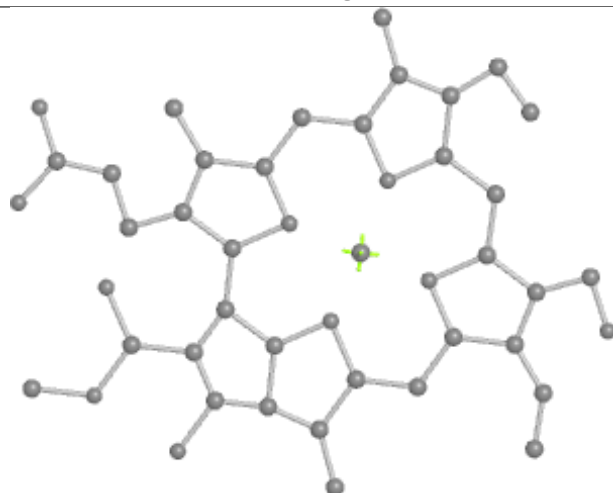
Bond lengths



Bond angles

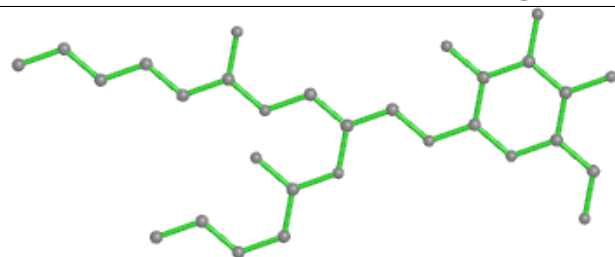


Torsions

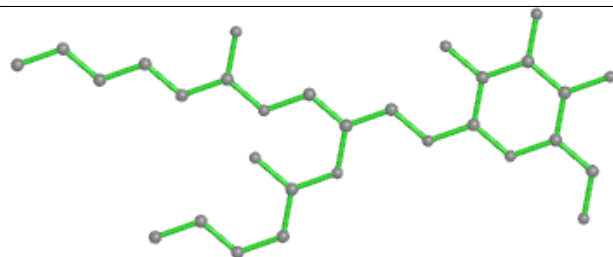


Rings

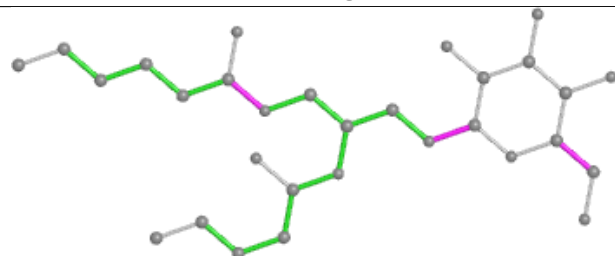
Ligand LMG J 105



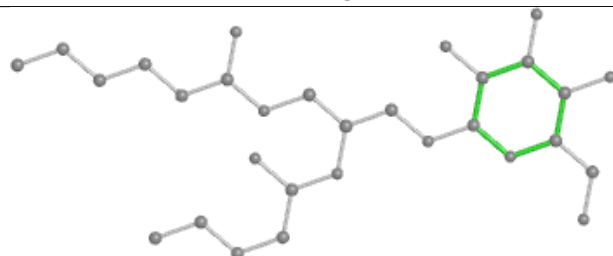
Bond lengths



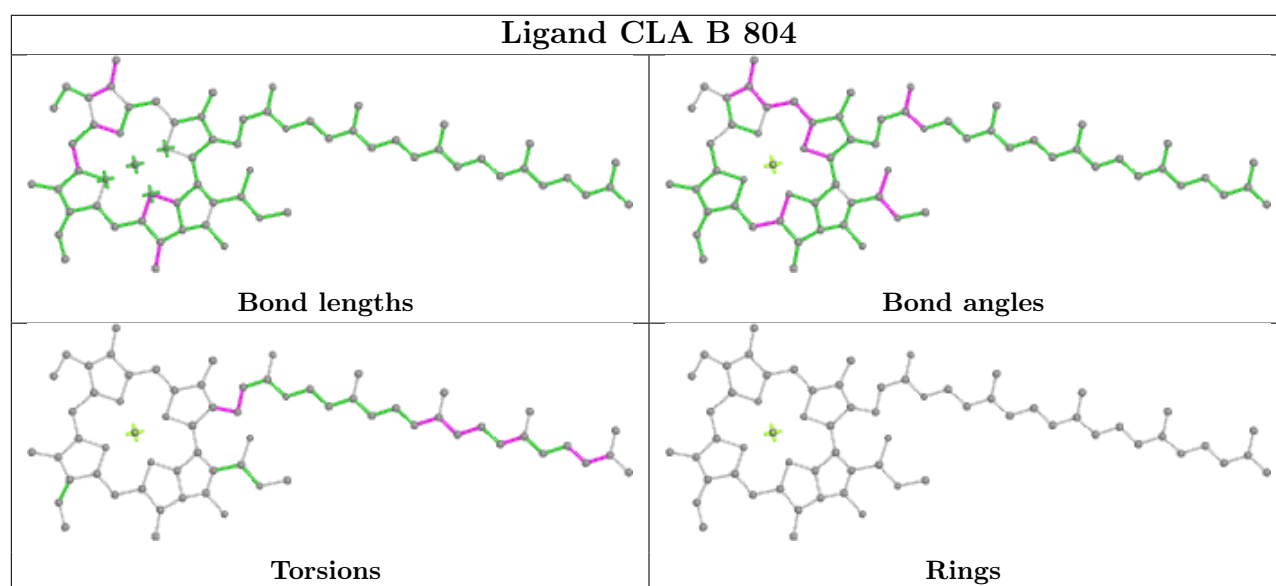
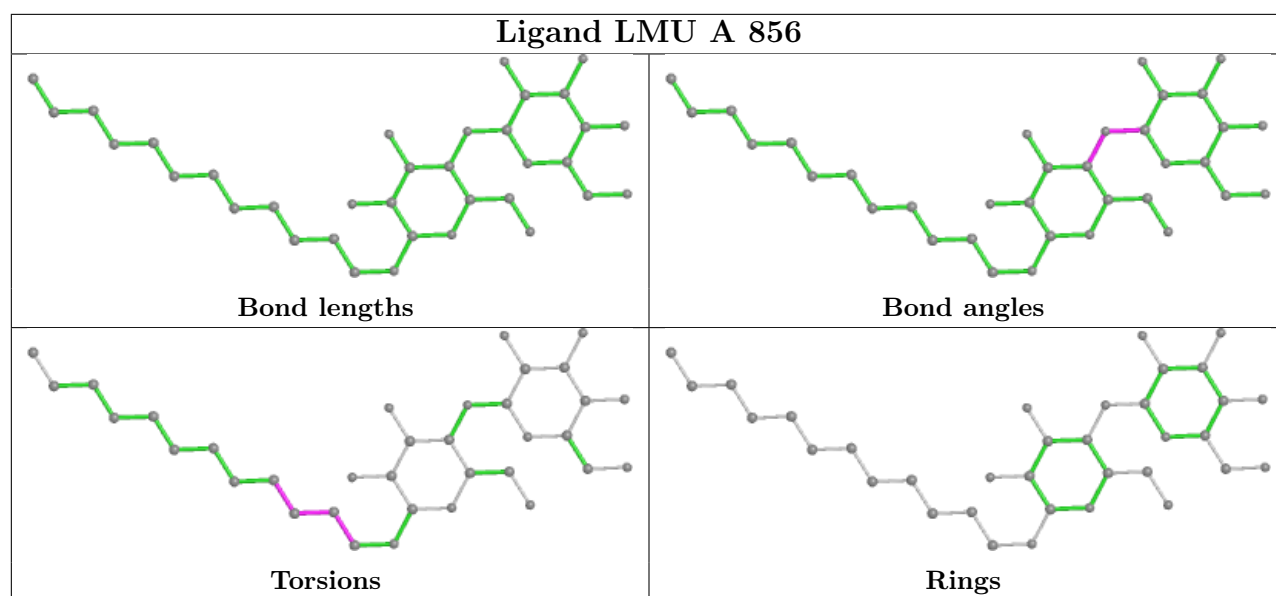
Bond angles

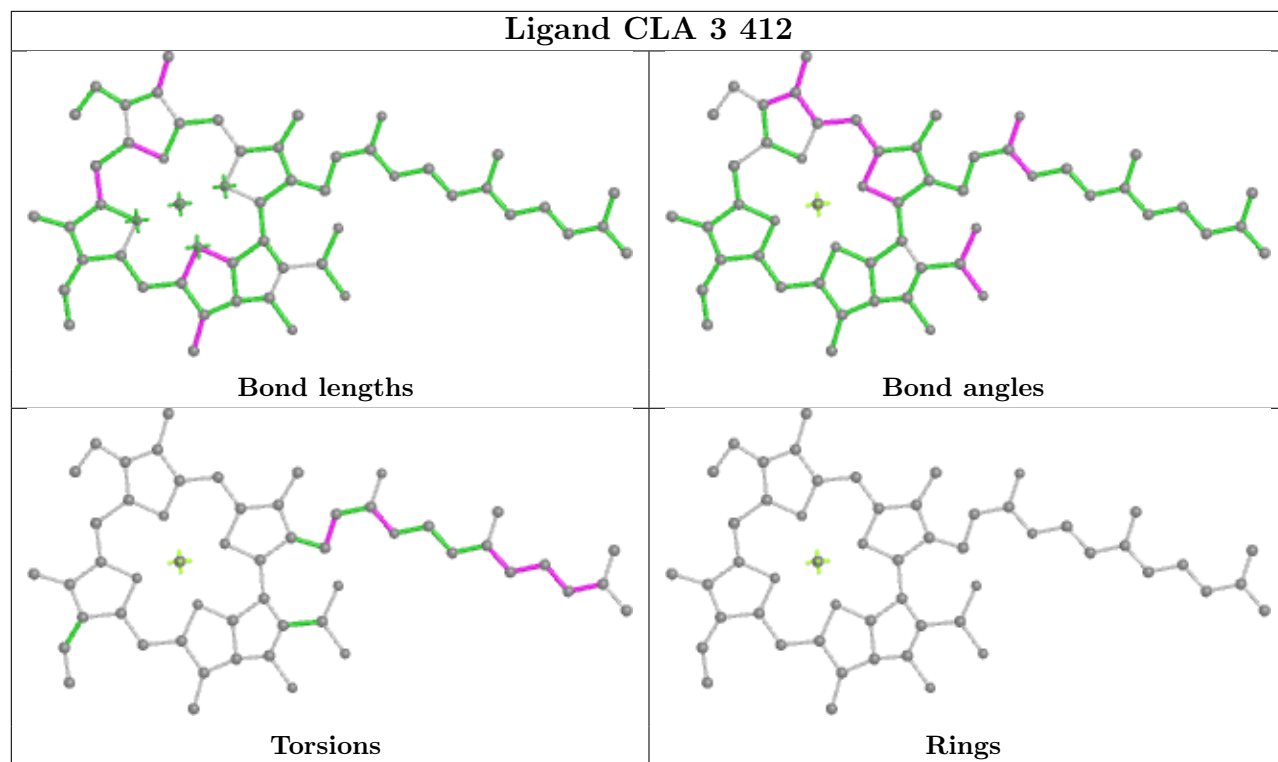


Torsions

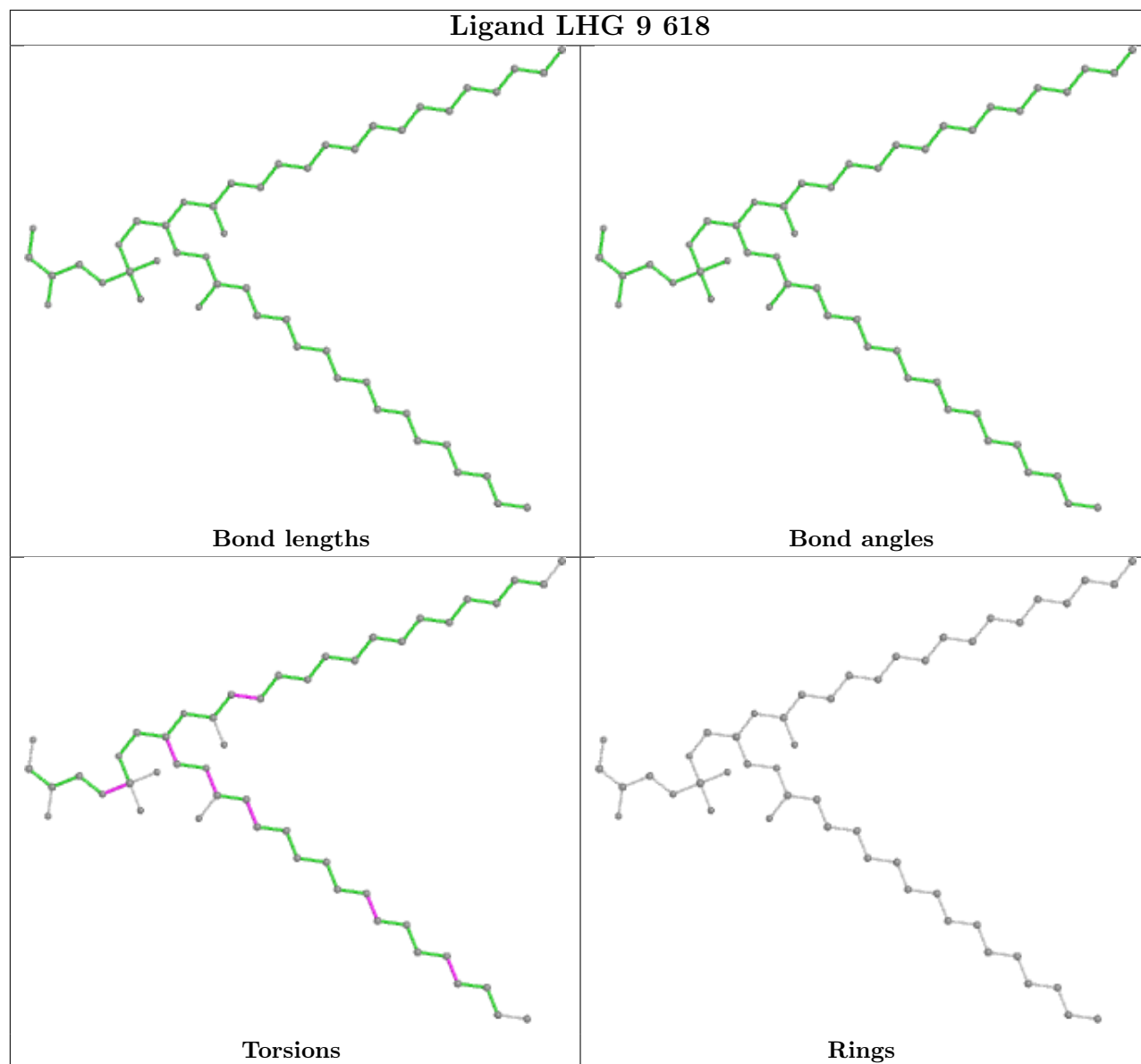


Rings

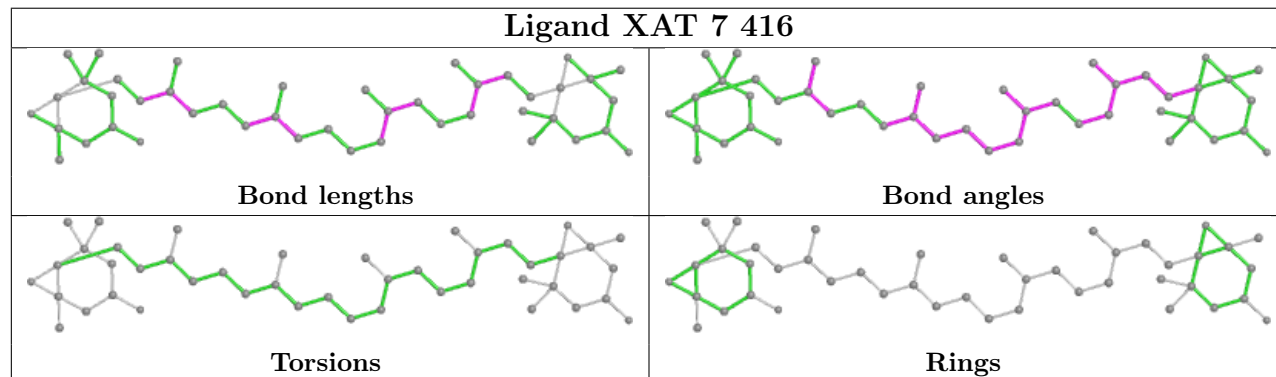


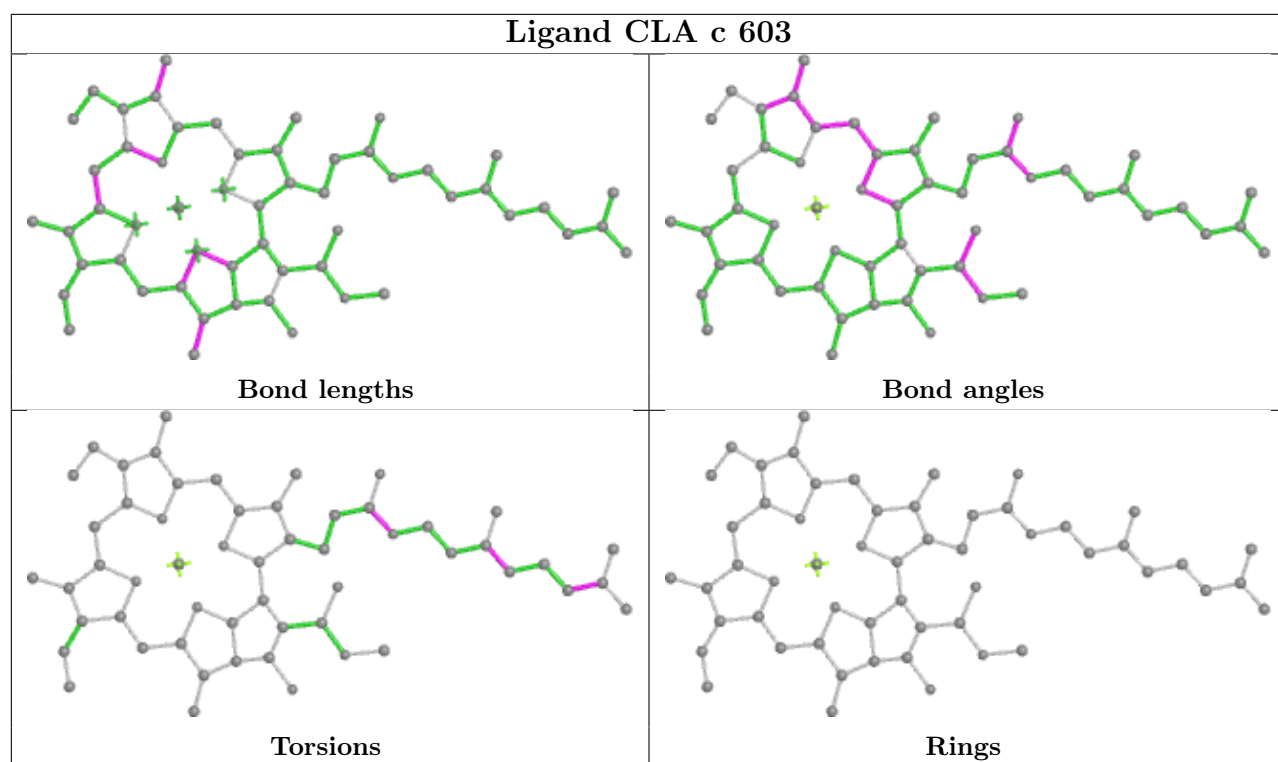


Ligand LHG 9 618

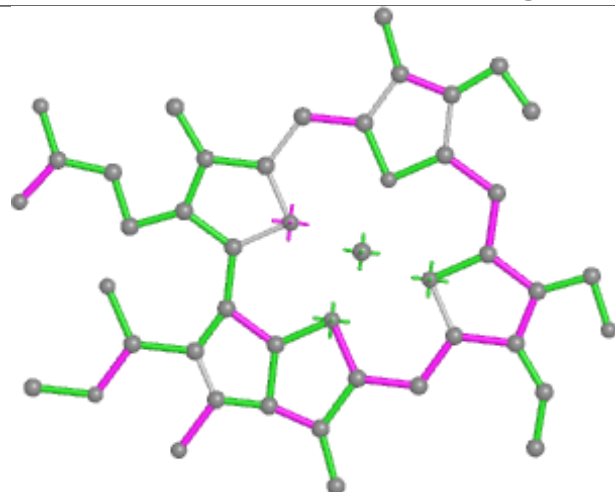


Ligand XAT 7 416

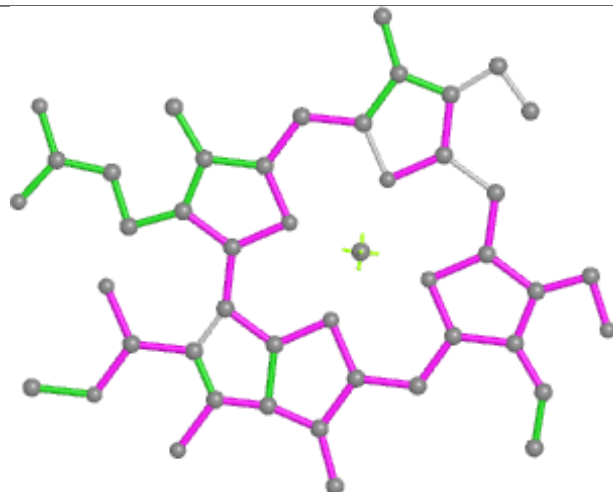




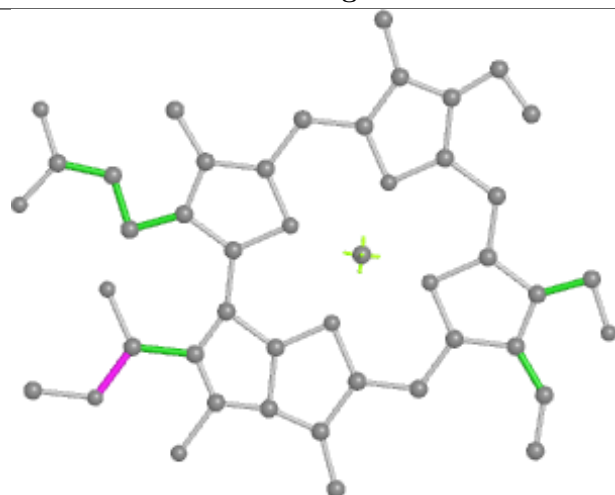
Ligand CHL 9 605



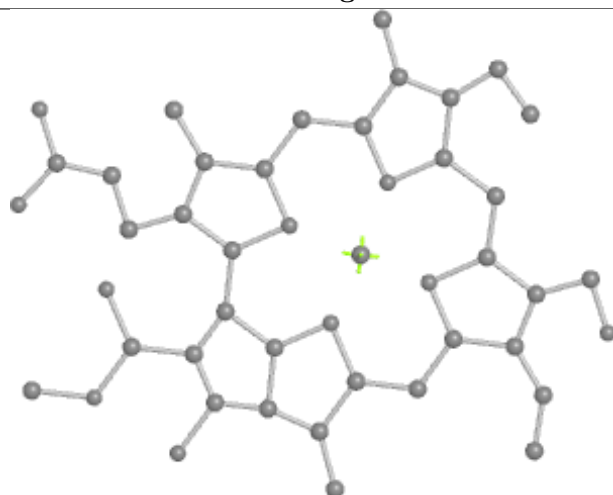
Bond lengths



Bond angles

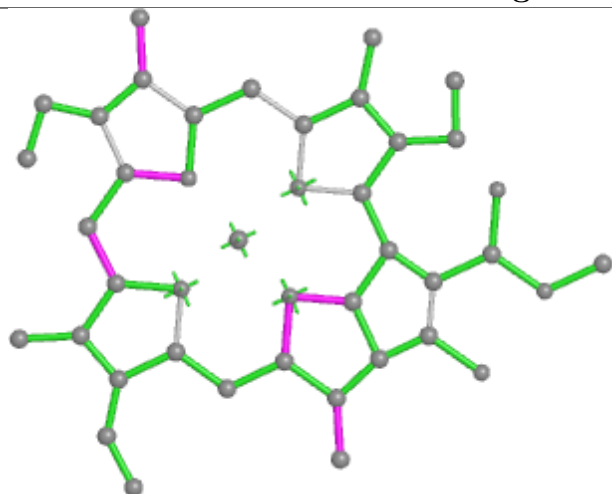


Torsions

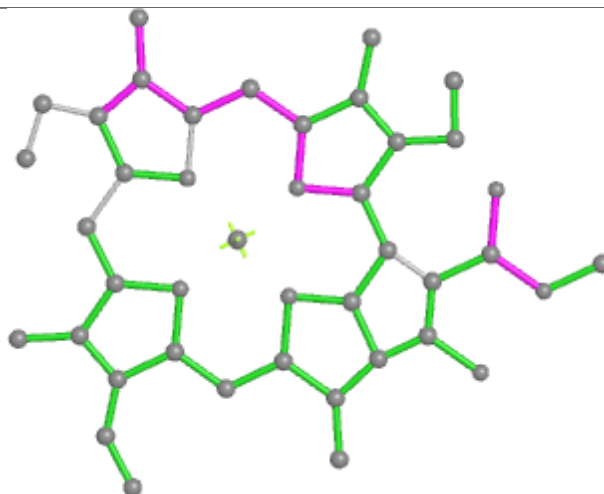


Rings

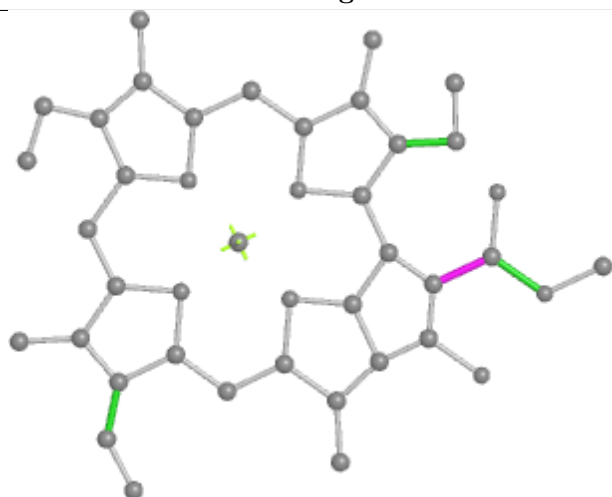
Ligand CLA O 201



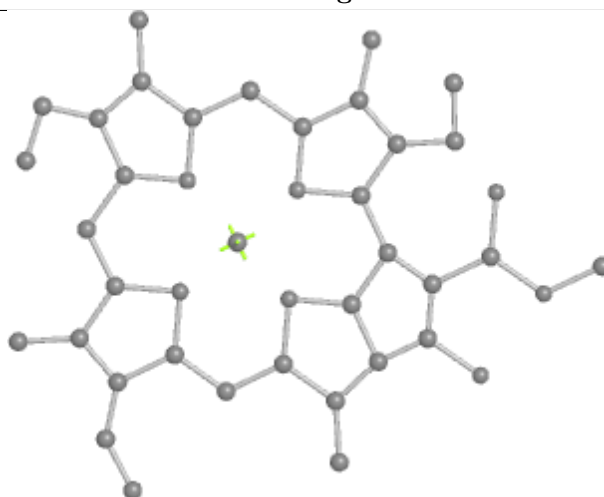
Bond lengths



Bond angles

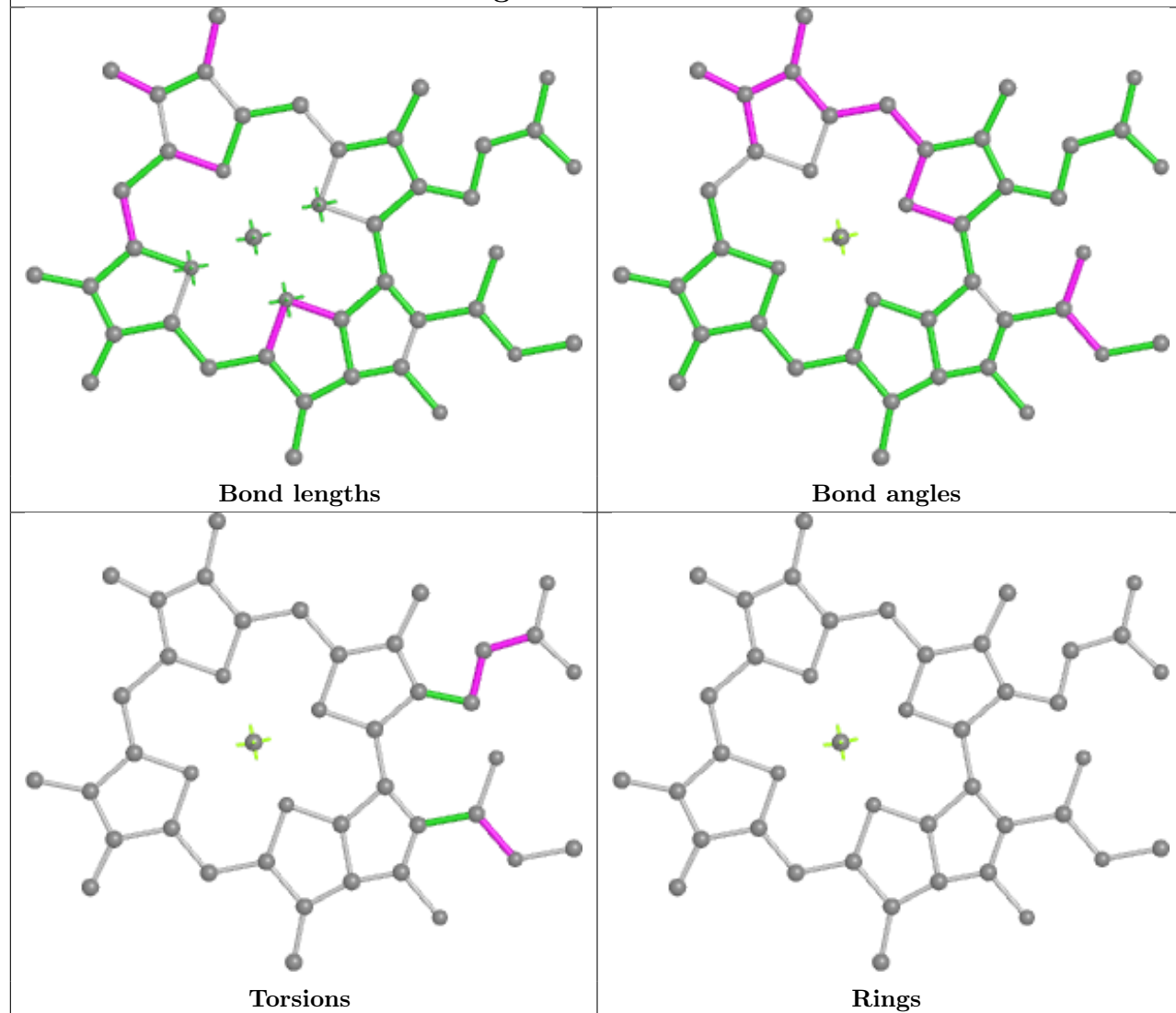


Torsions

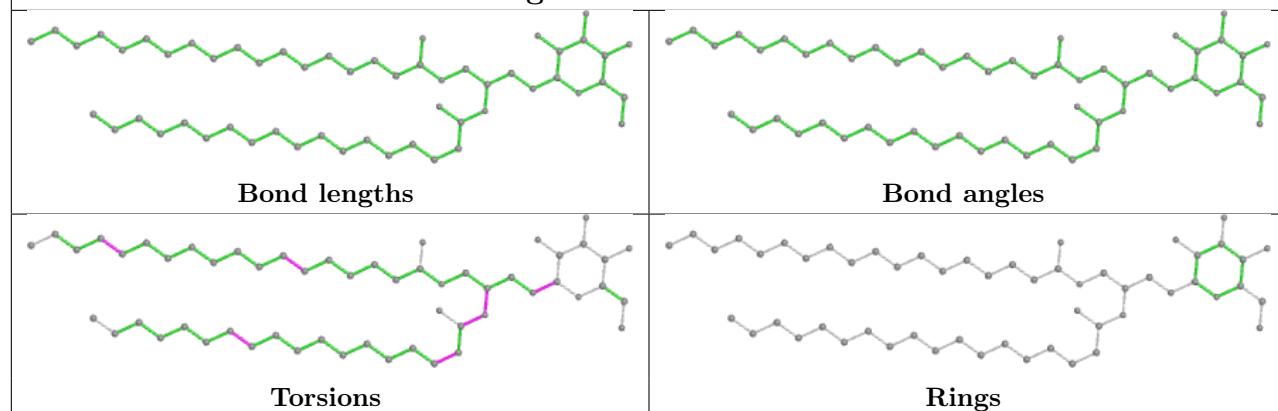


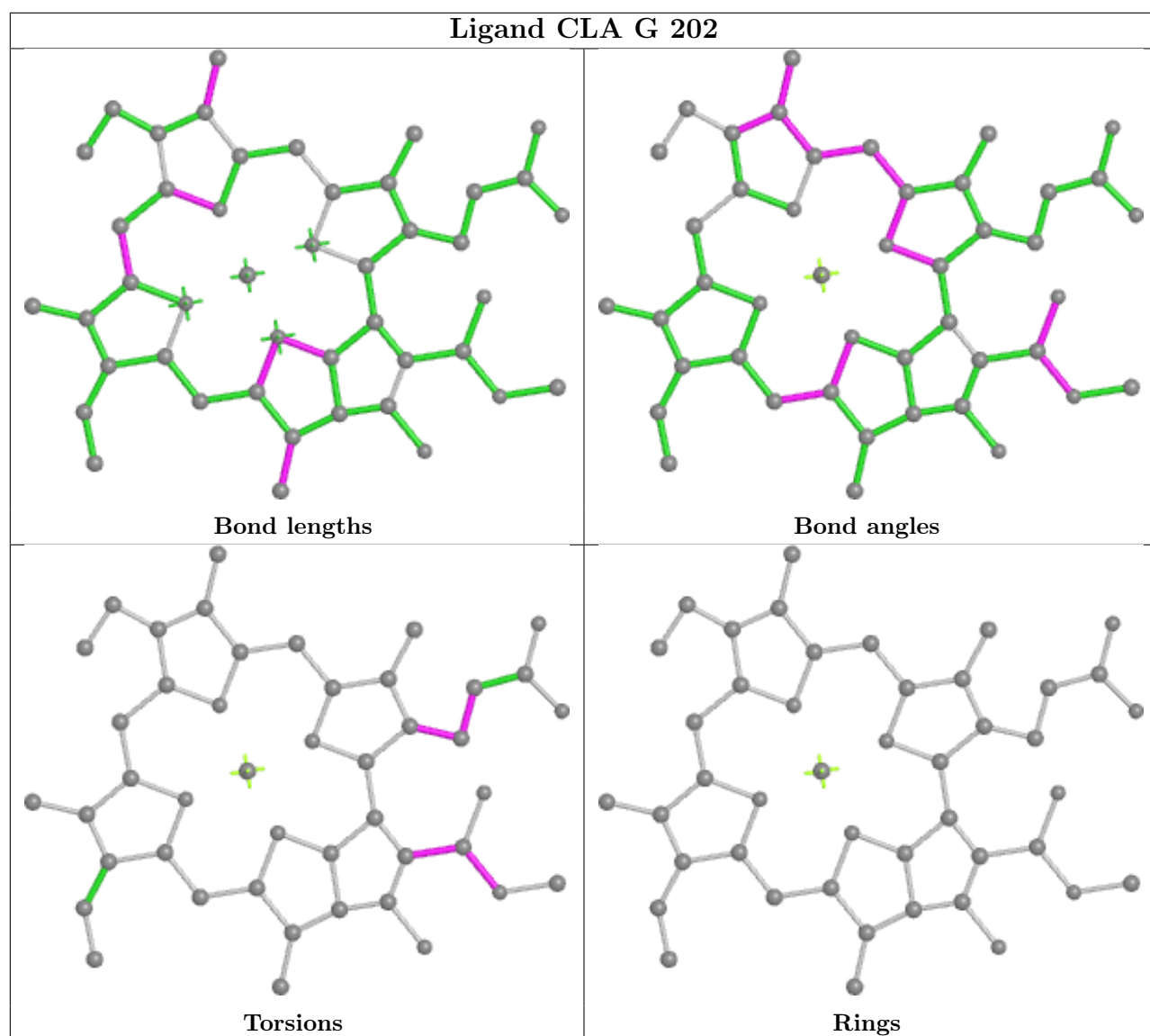
Rings

Ligand CLA 5 614

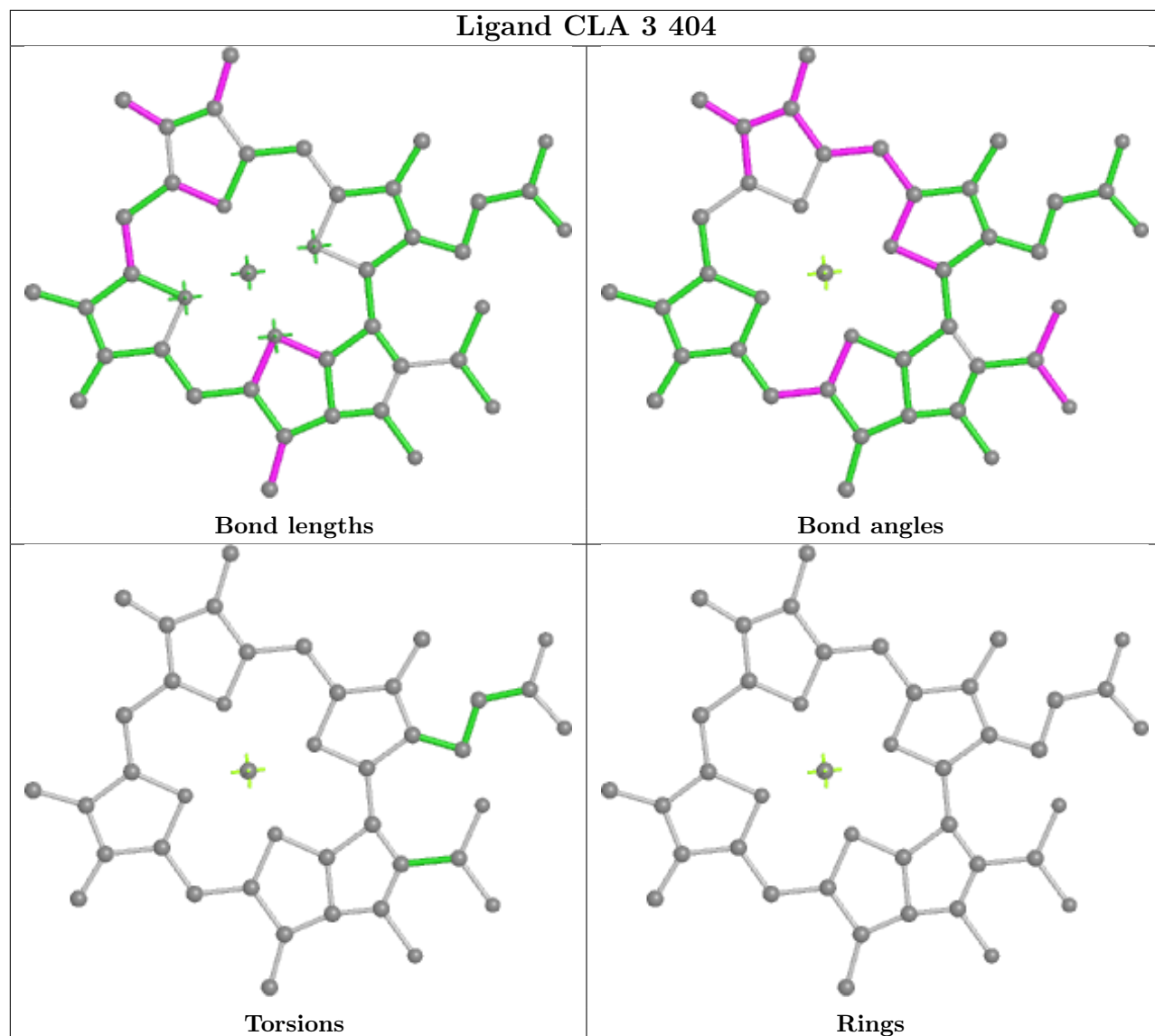


Ligand LMG G 206

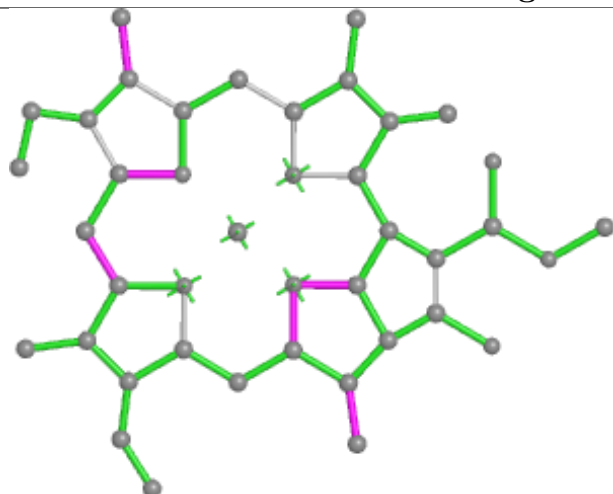




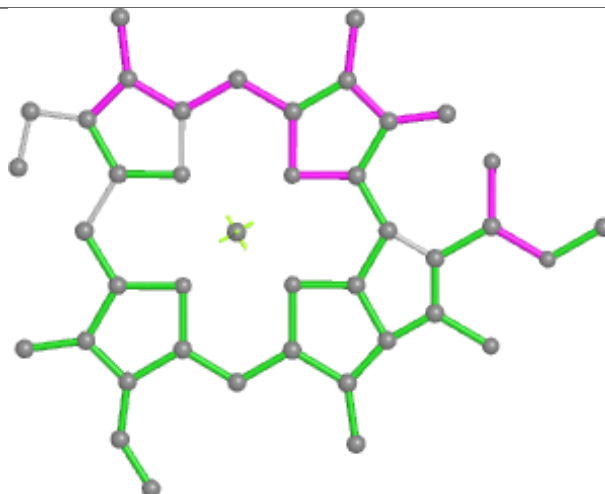
Ligand CLA 3 404



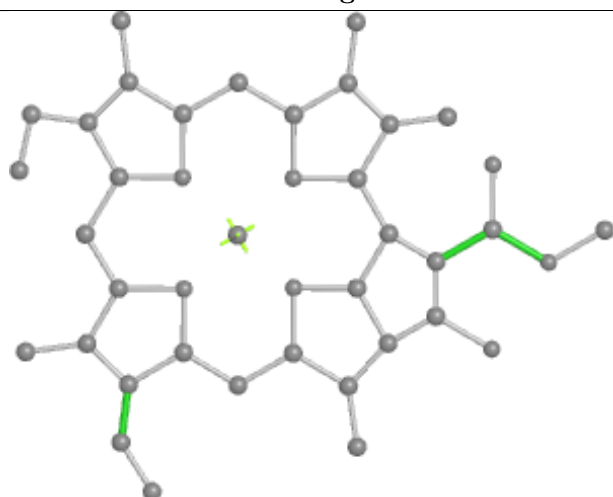
Ligand CLA 2 611



Bond lengths



Bond angles

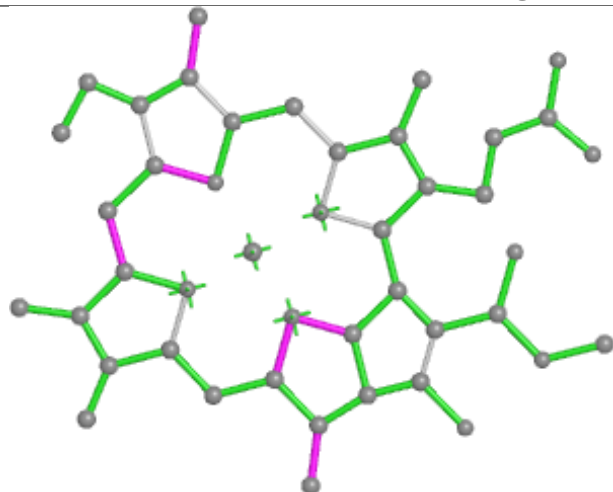


Torsions

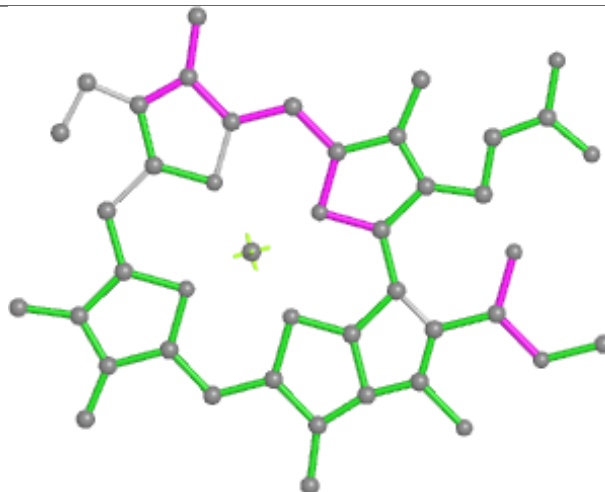


Rings

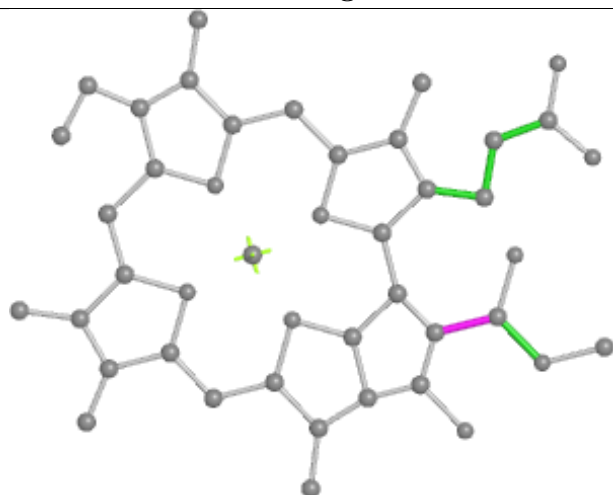
Ligand CLA A 820



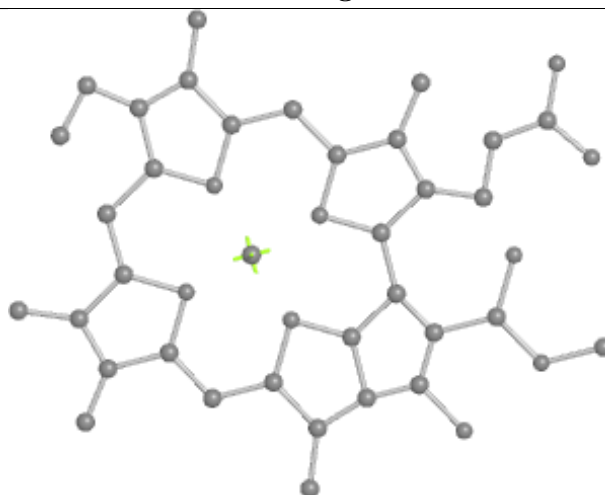
Bond lengths



Bond angles

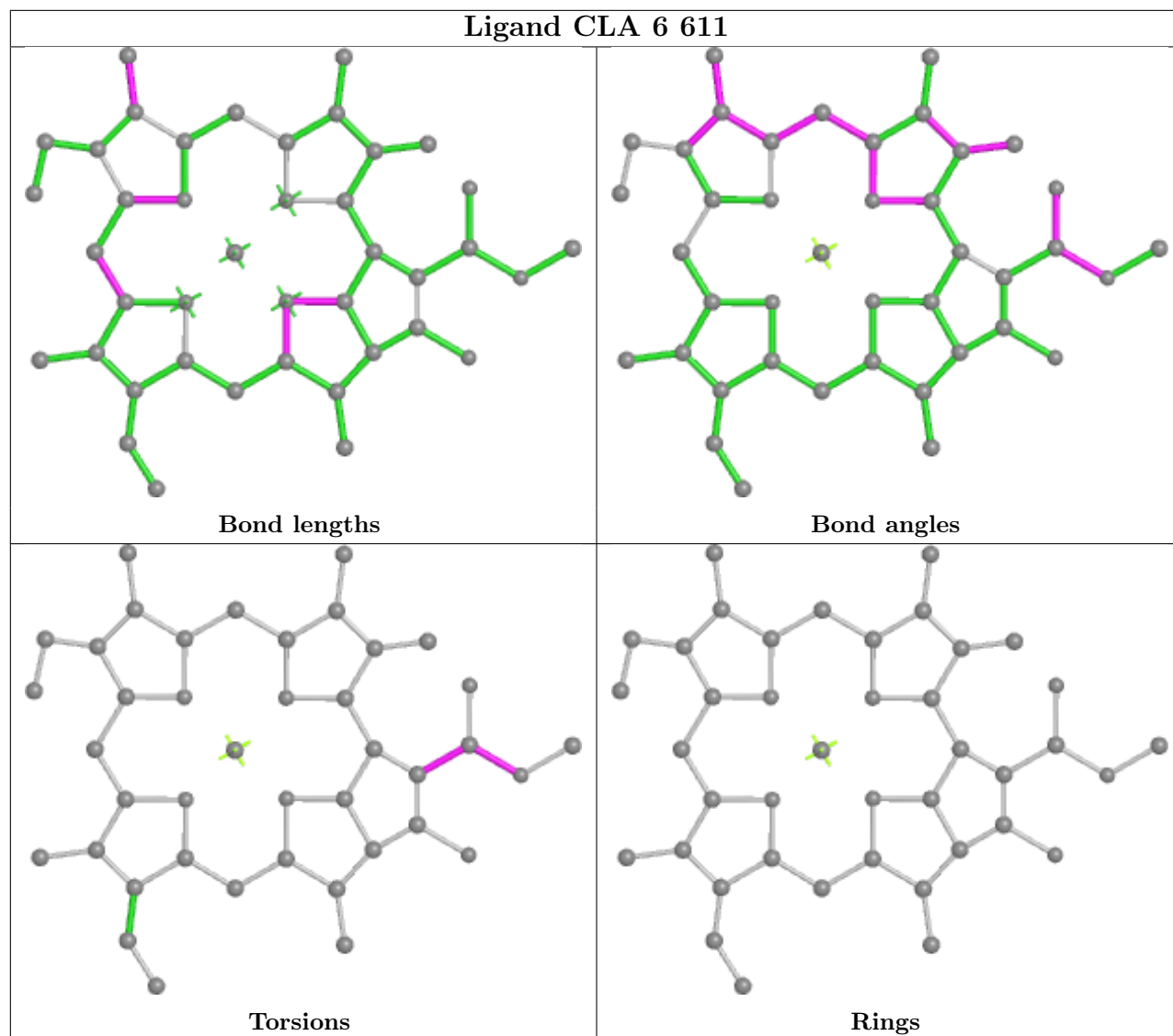


Torsions

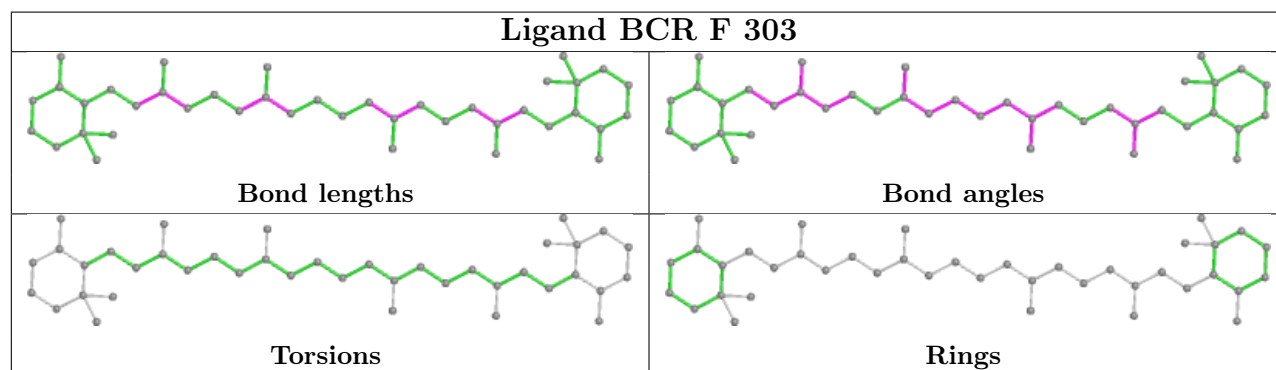


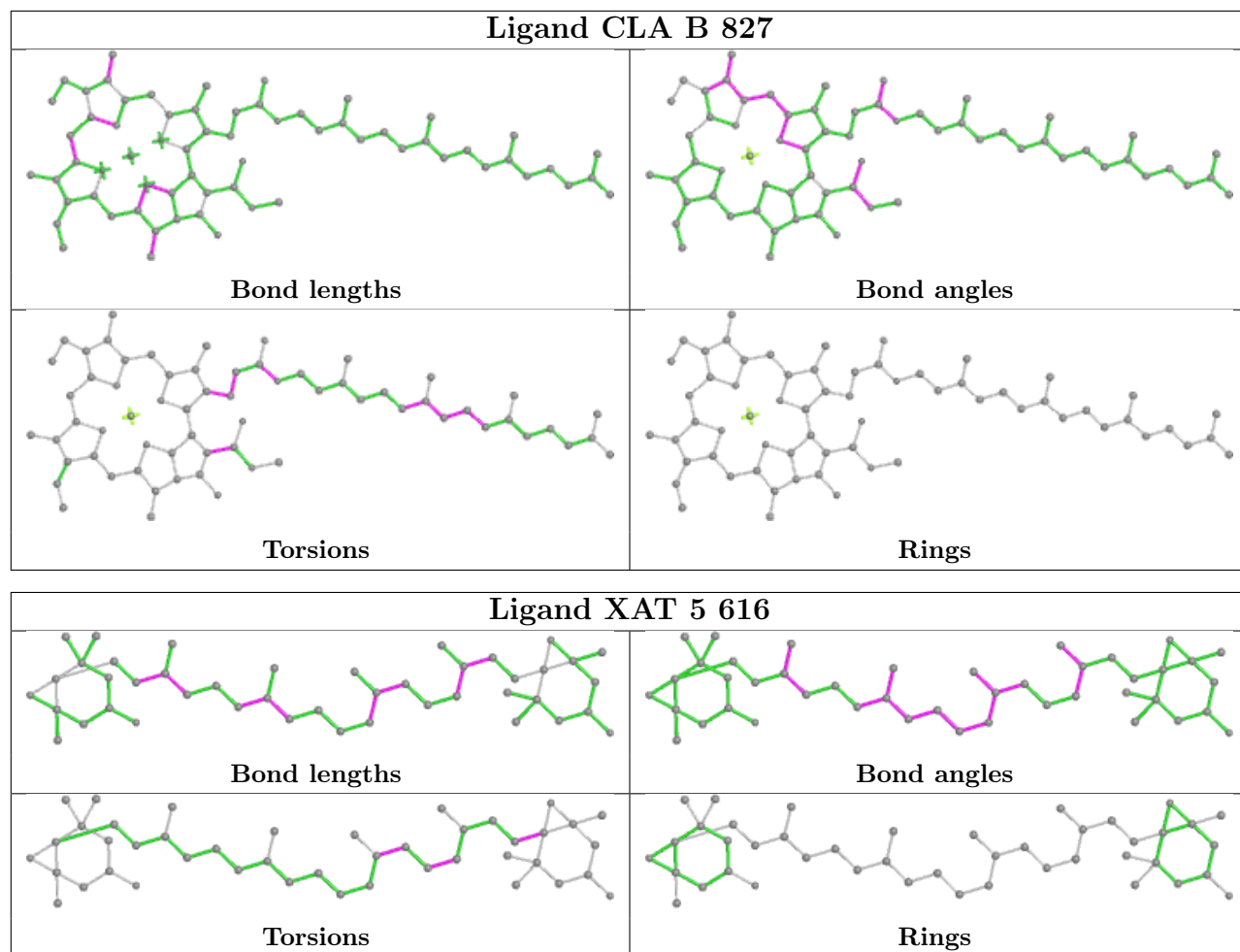
Rings

Ligand CLA 6 611

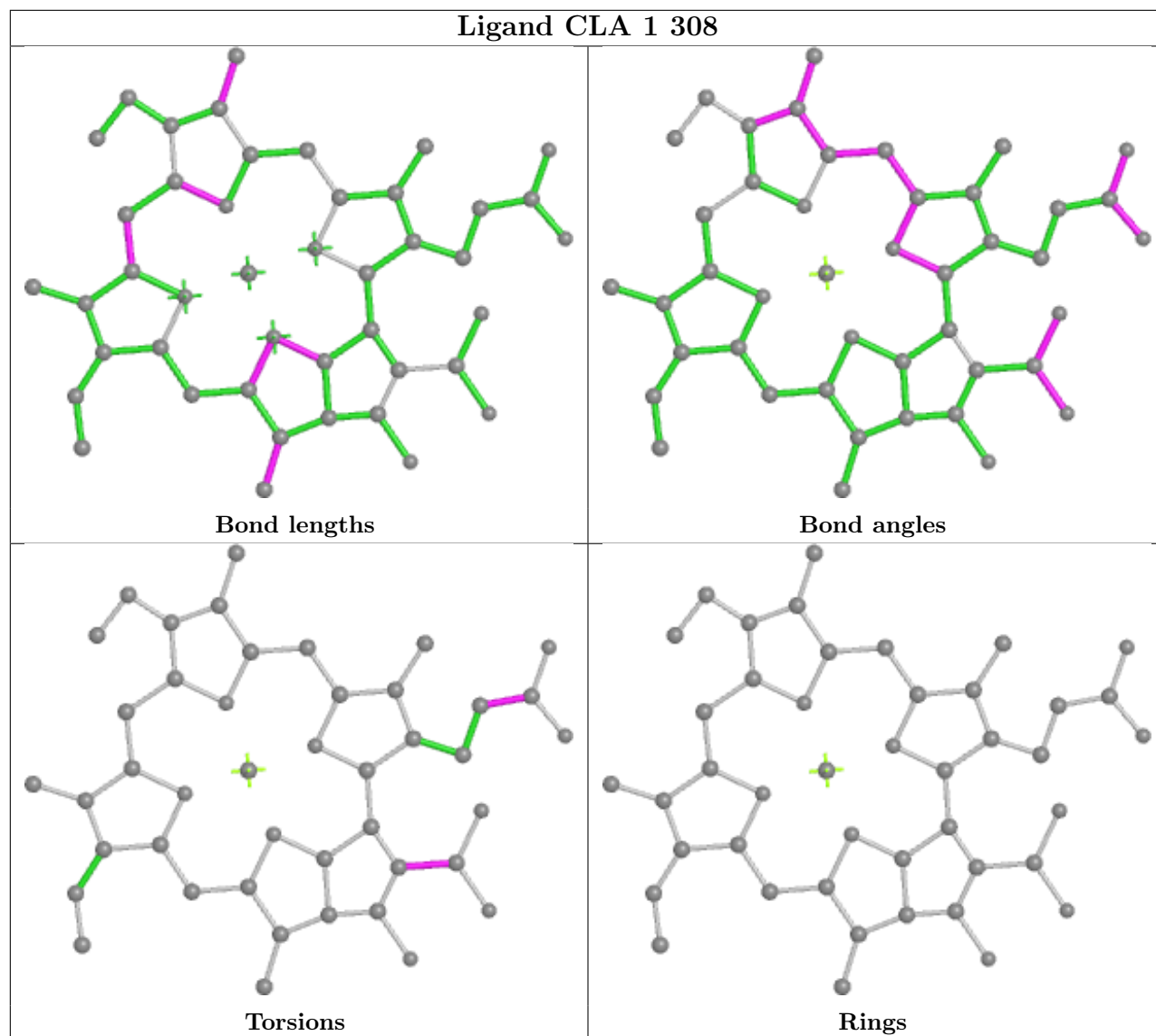


Ligand BCR F 303

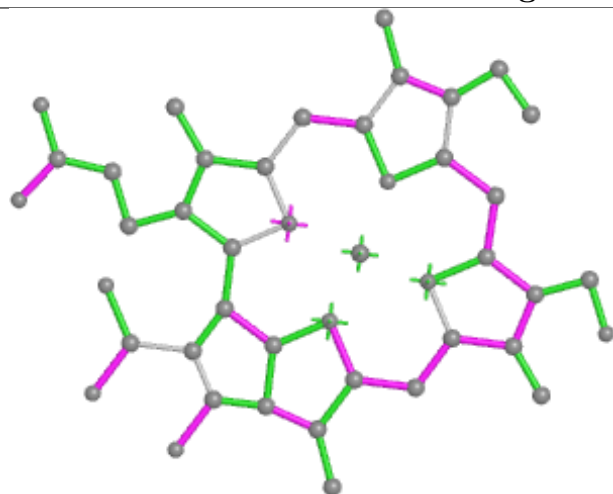




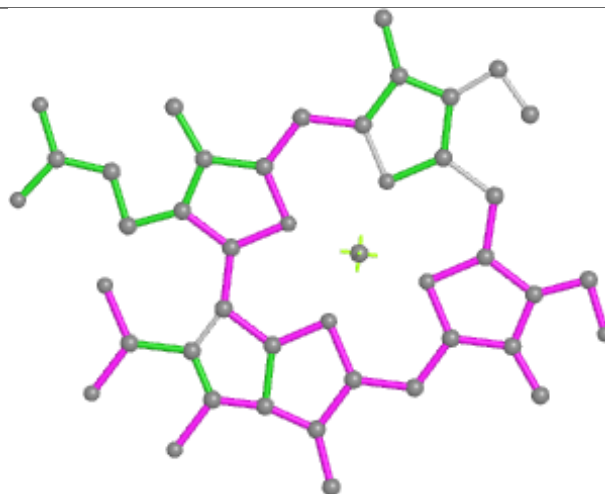
Ligand CLA 1 308



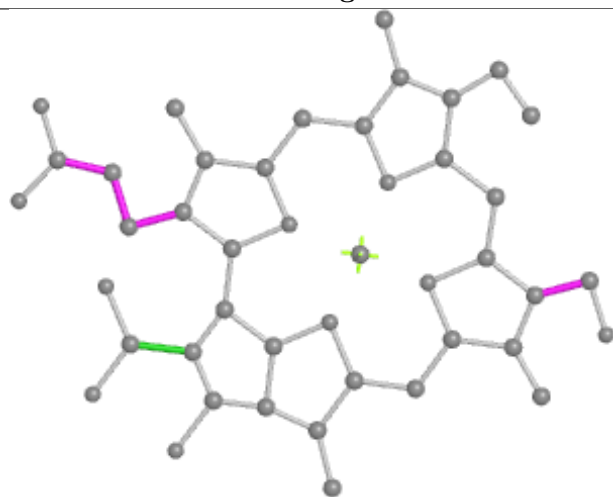
Ligand CHL c 609



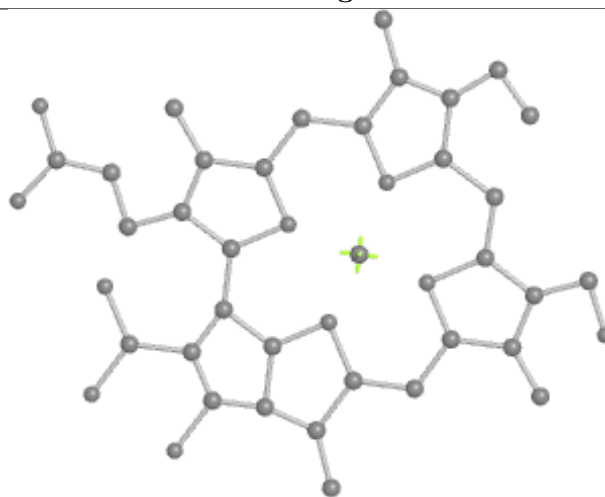
Bond lengths



Bond angles

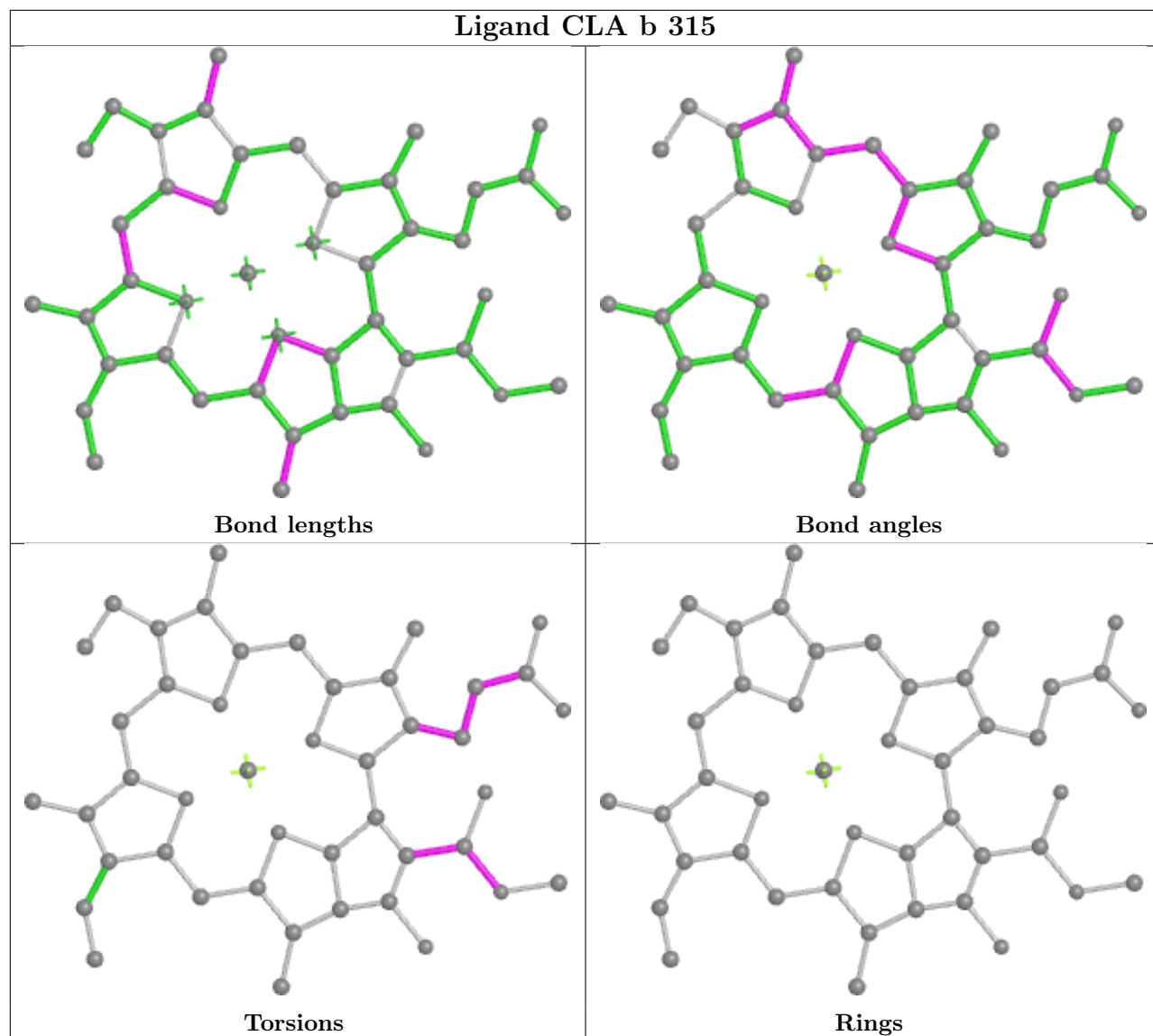


Torsions

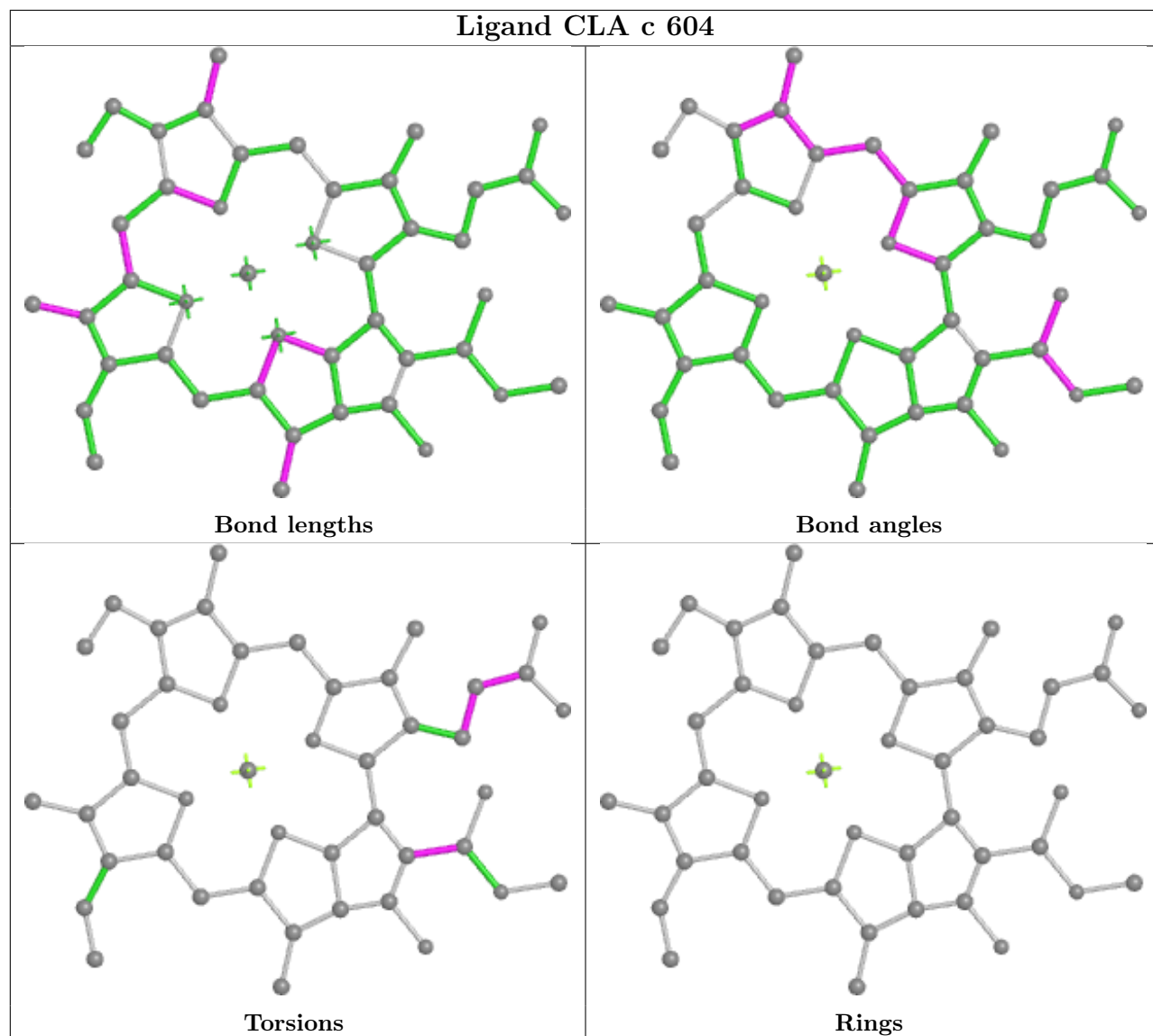


Rings

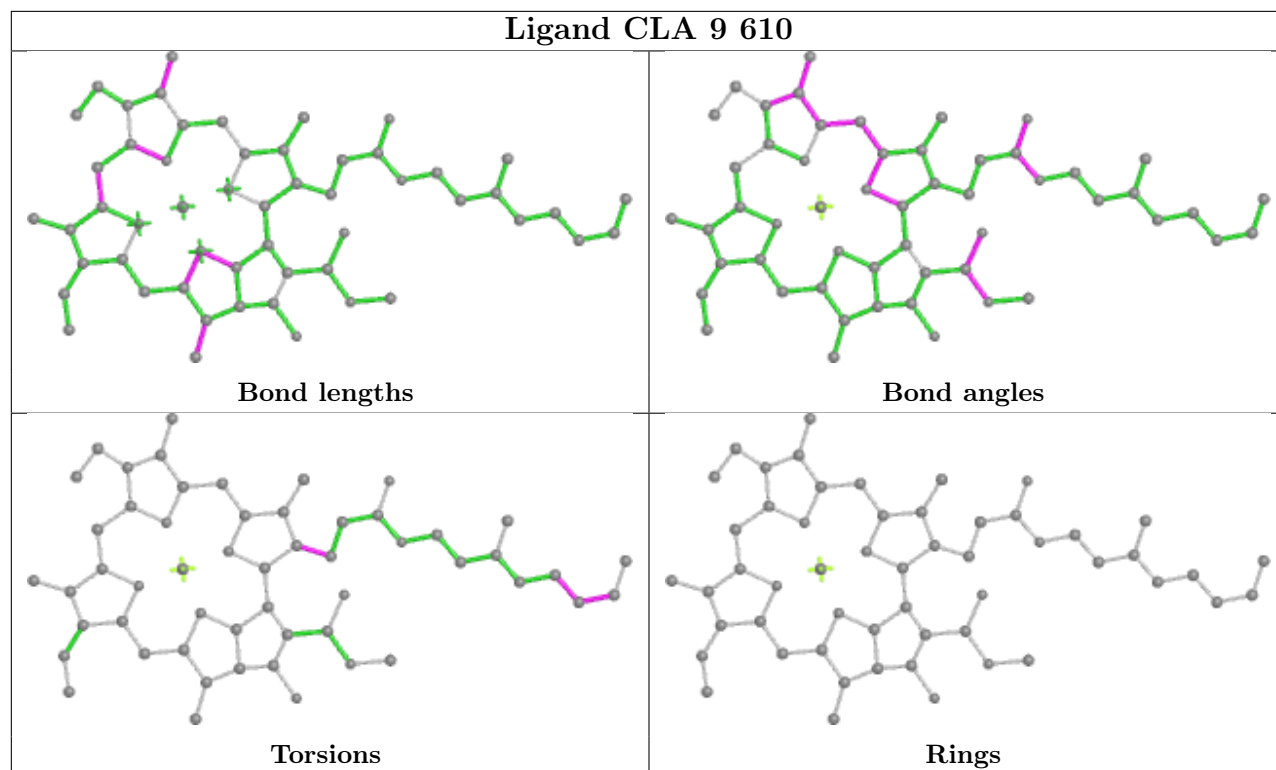
Ligand CLA b 315



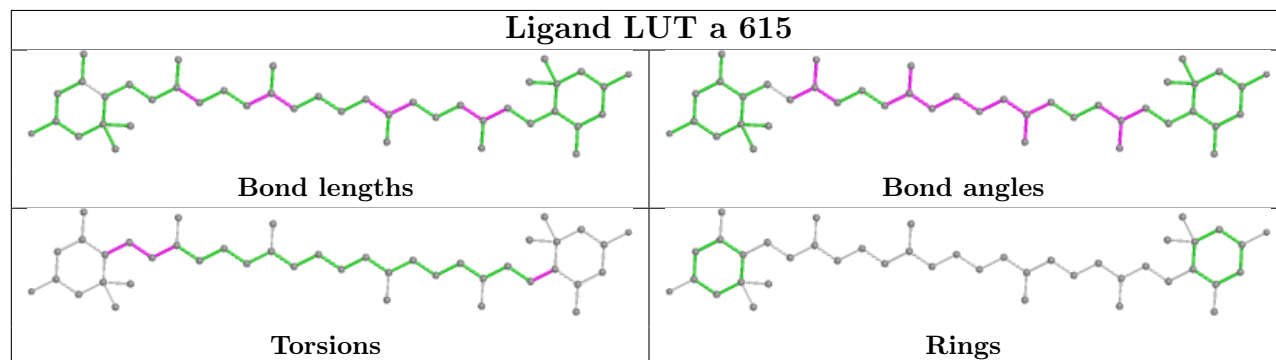
Ligand CLA c 604



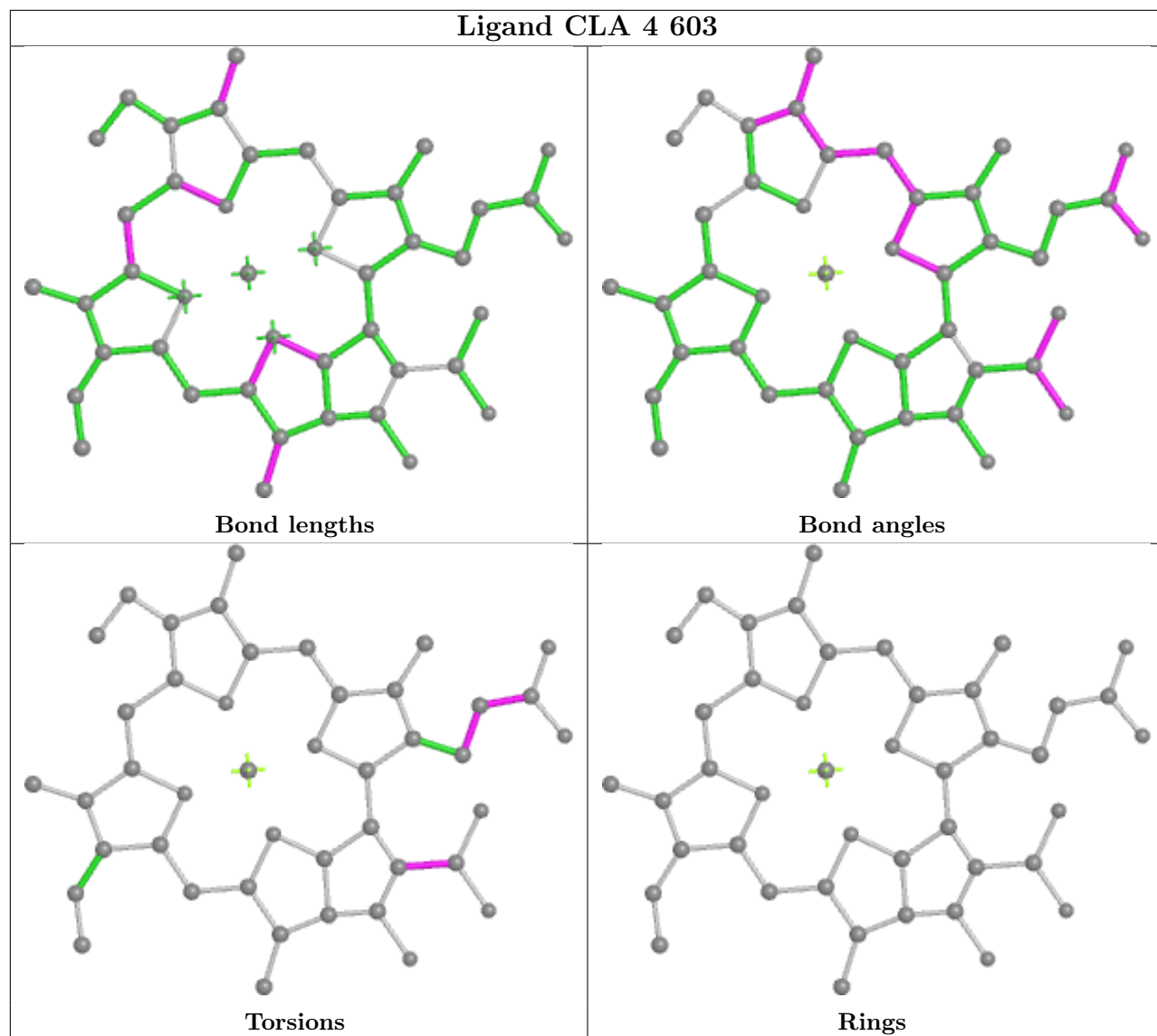
Ligand CLA 9 610



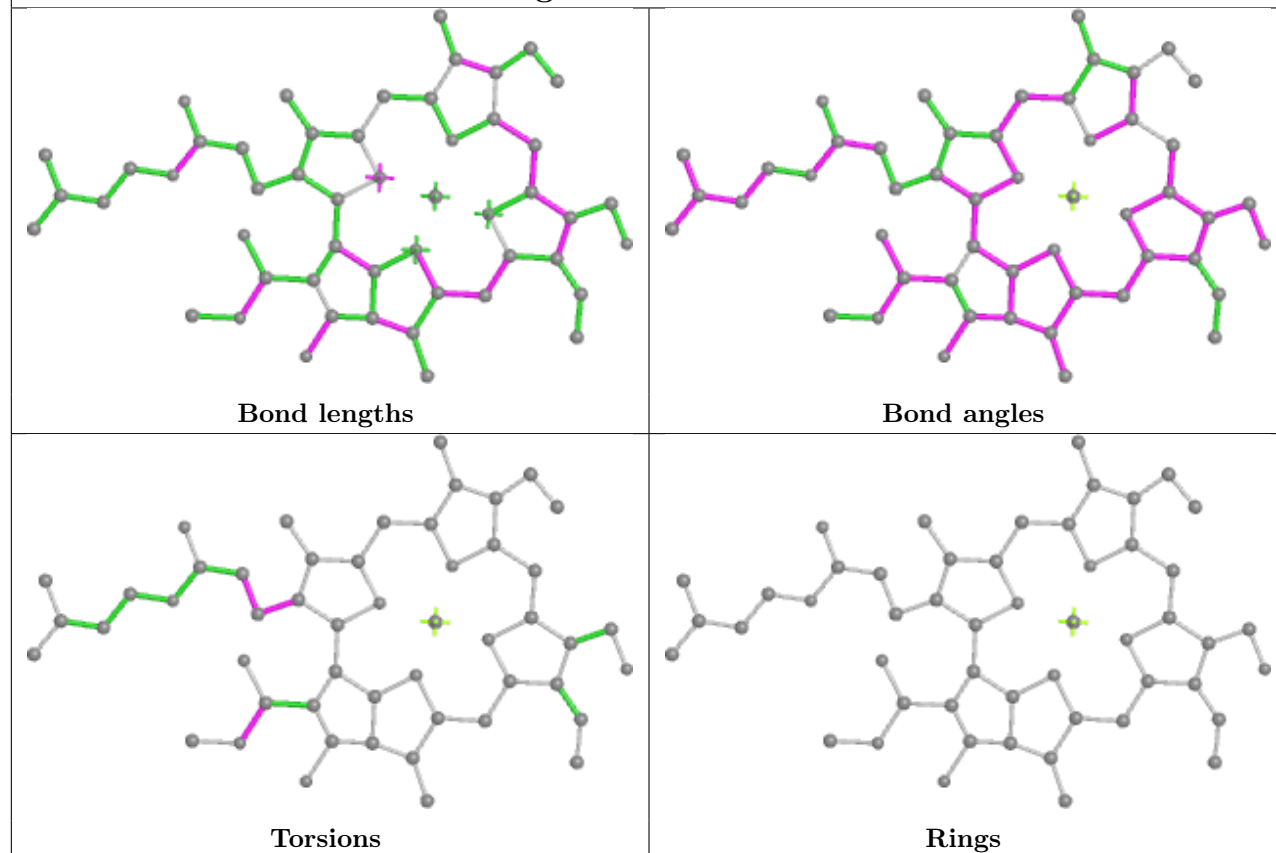
Ligand LUT a 615



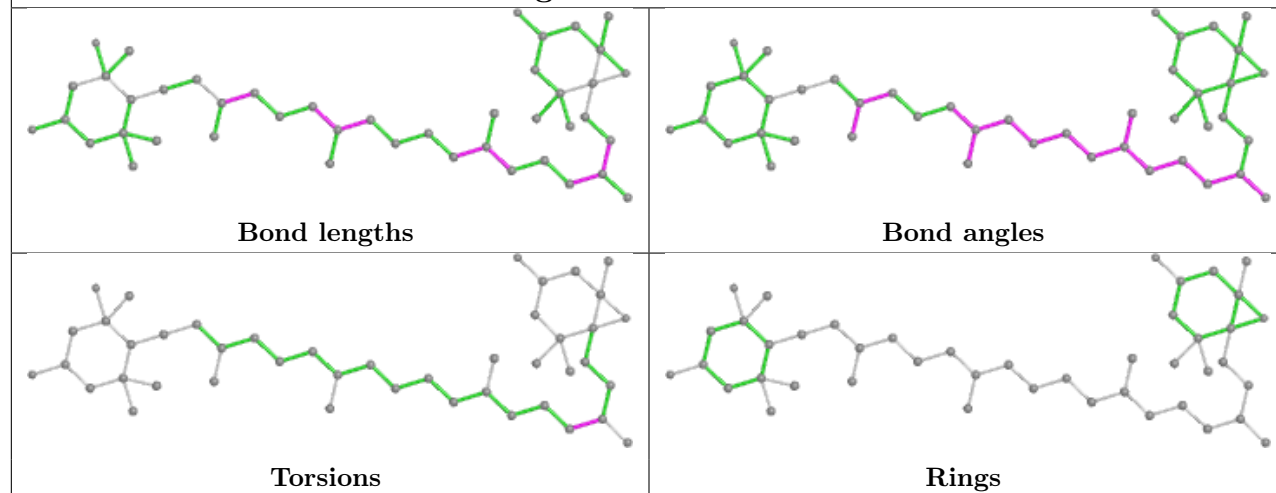
Ligand CLA 4 603



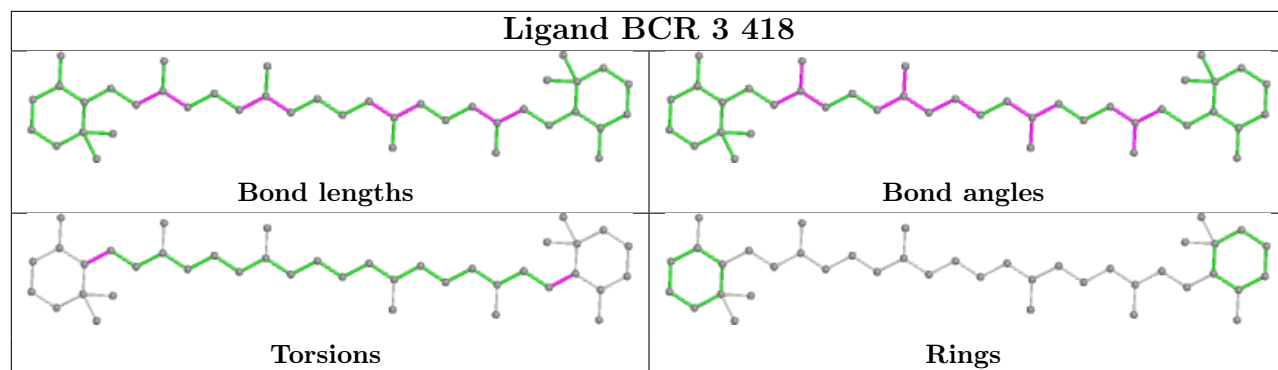
Ligand CHL 4 607



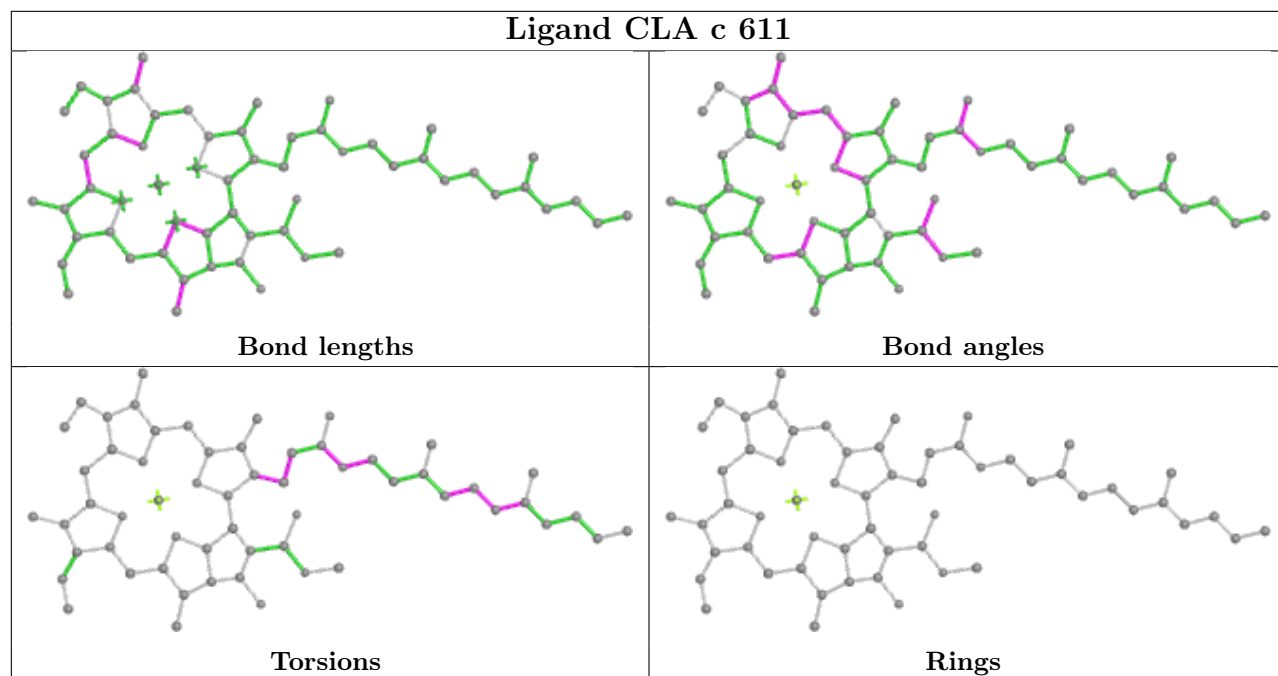
Ligand NEX c 618



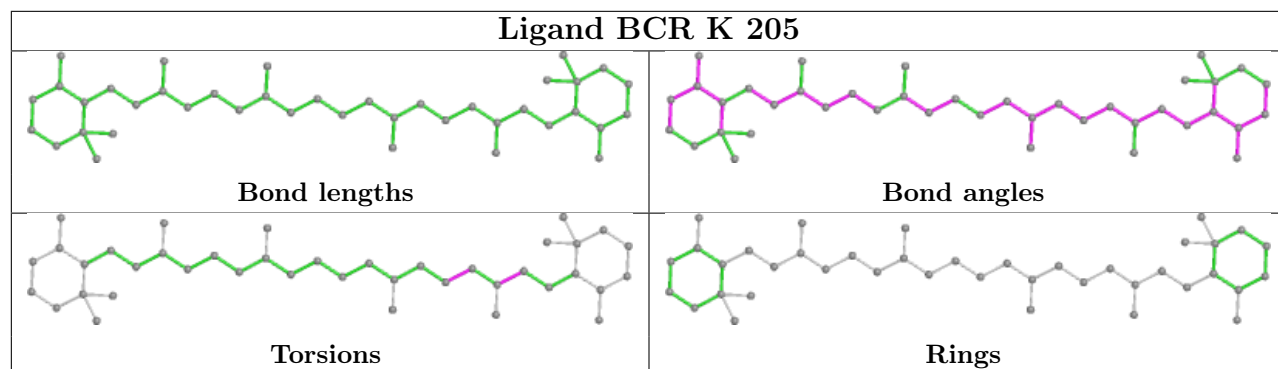
Ligand BCR 3 418



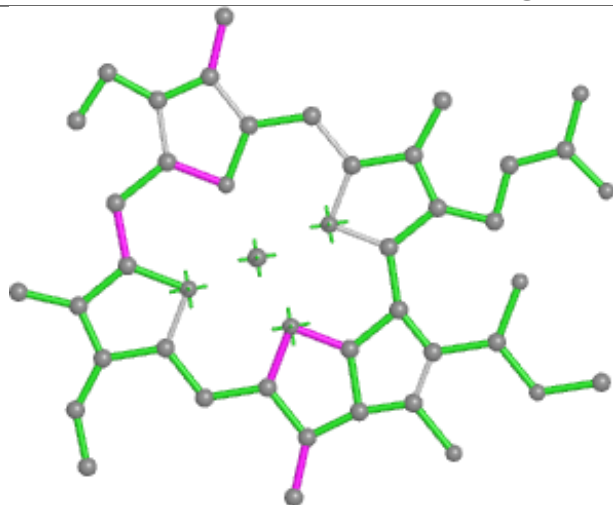
Ligand CLA c 611



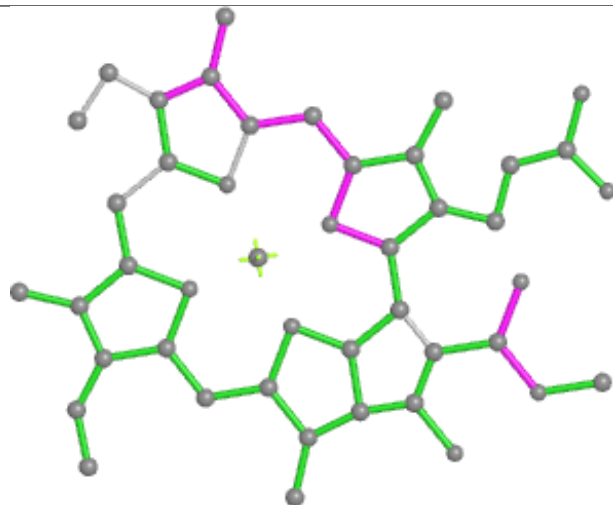
Ligand BCR K 205



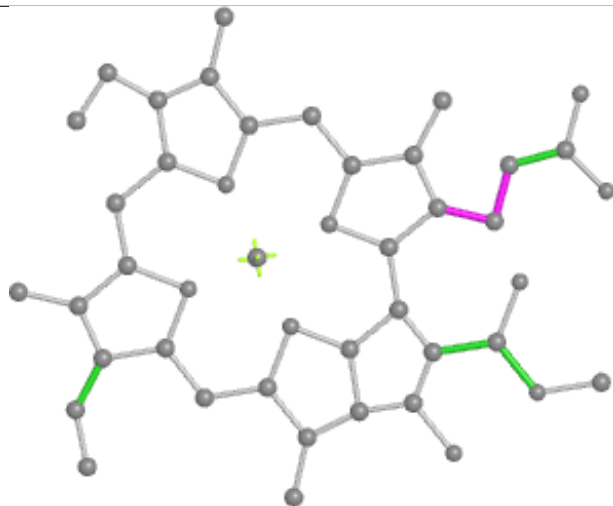
Ligand CLA 4 610



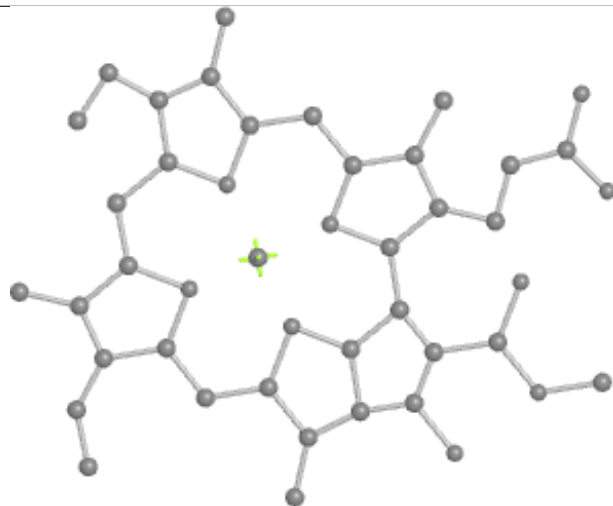
Bond lengths



Bond angles

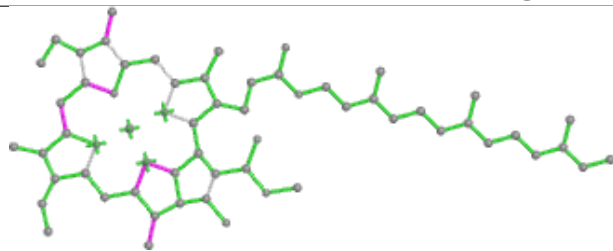


Torsions

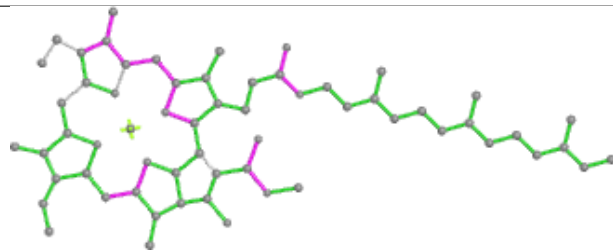


Rings

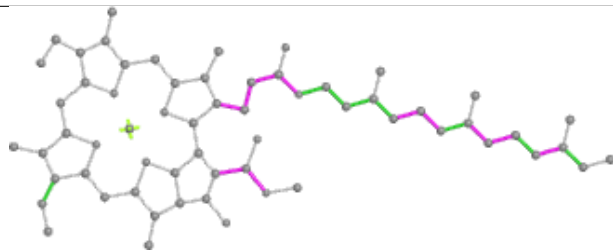
Ligand CLA 5 602



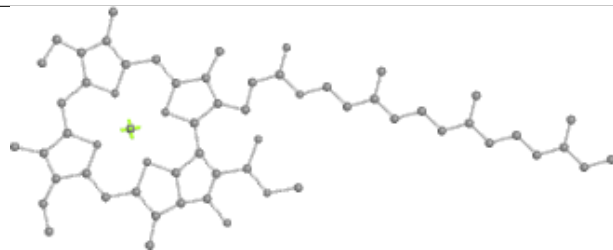
Bond lengths



Bond angles

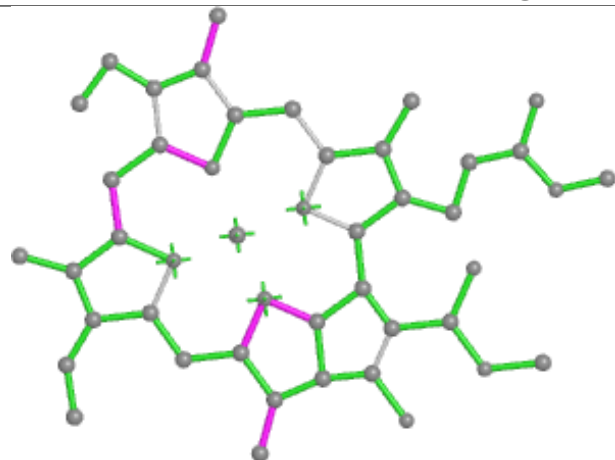


Torsions

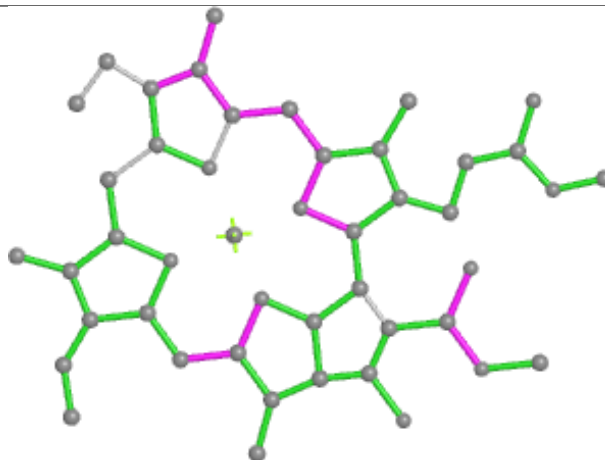


Rings

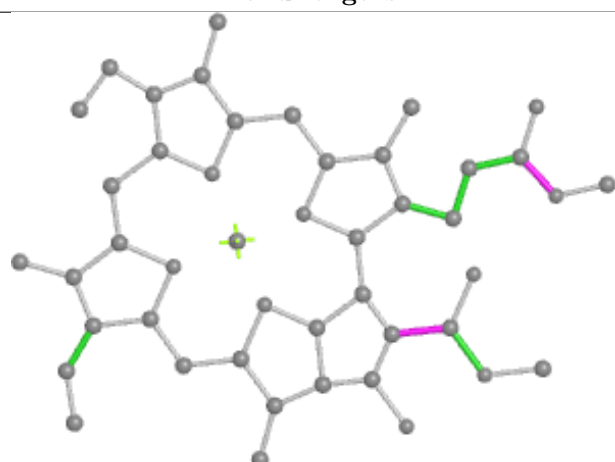
Ligand CLA B 820



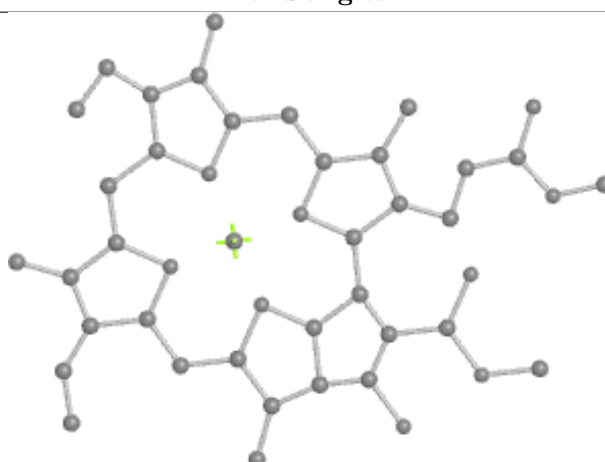
Bond lengths



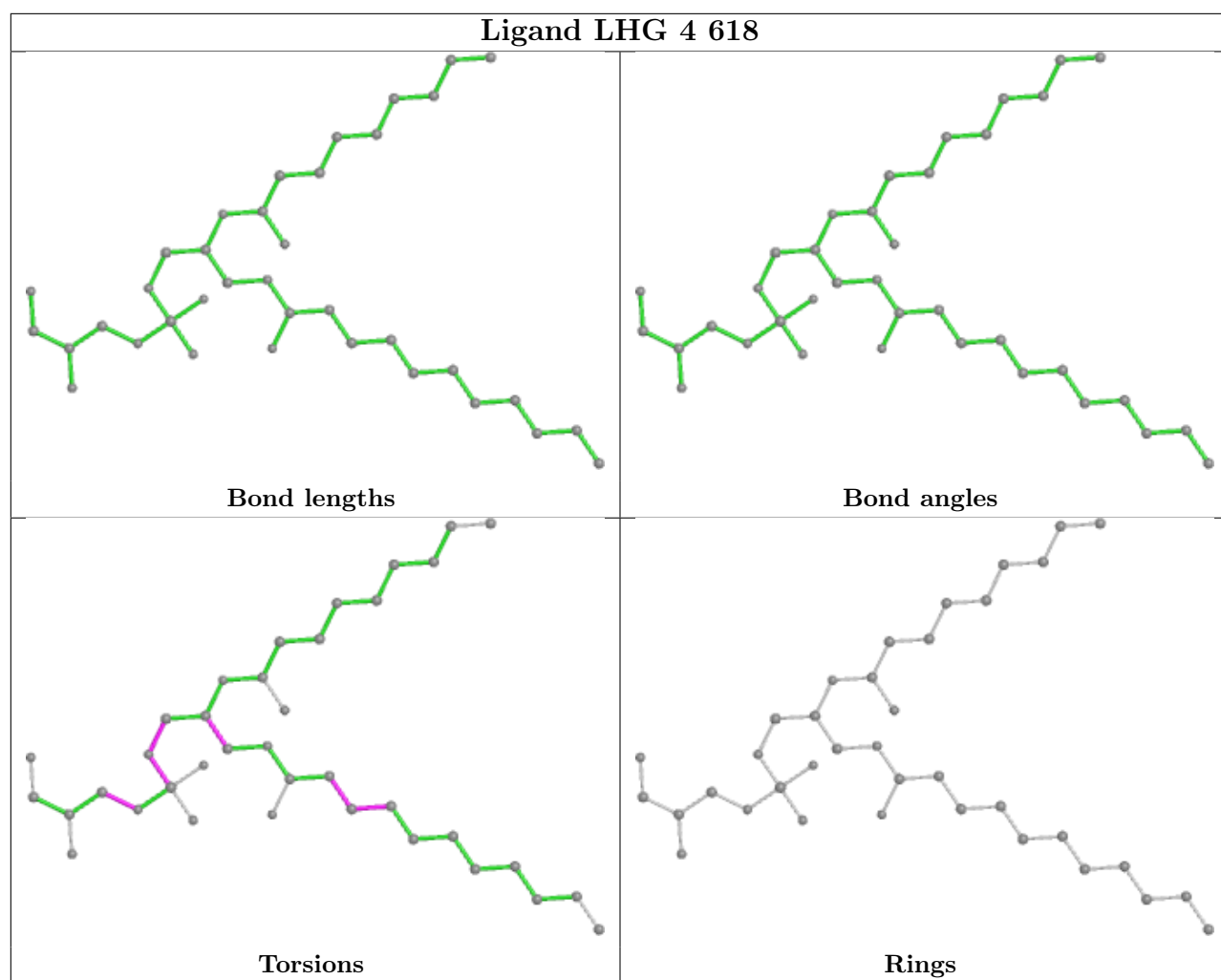
Bond angles



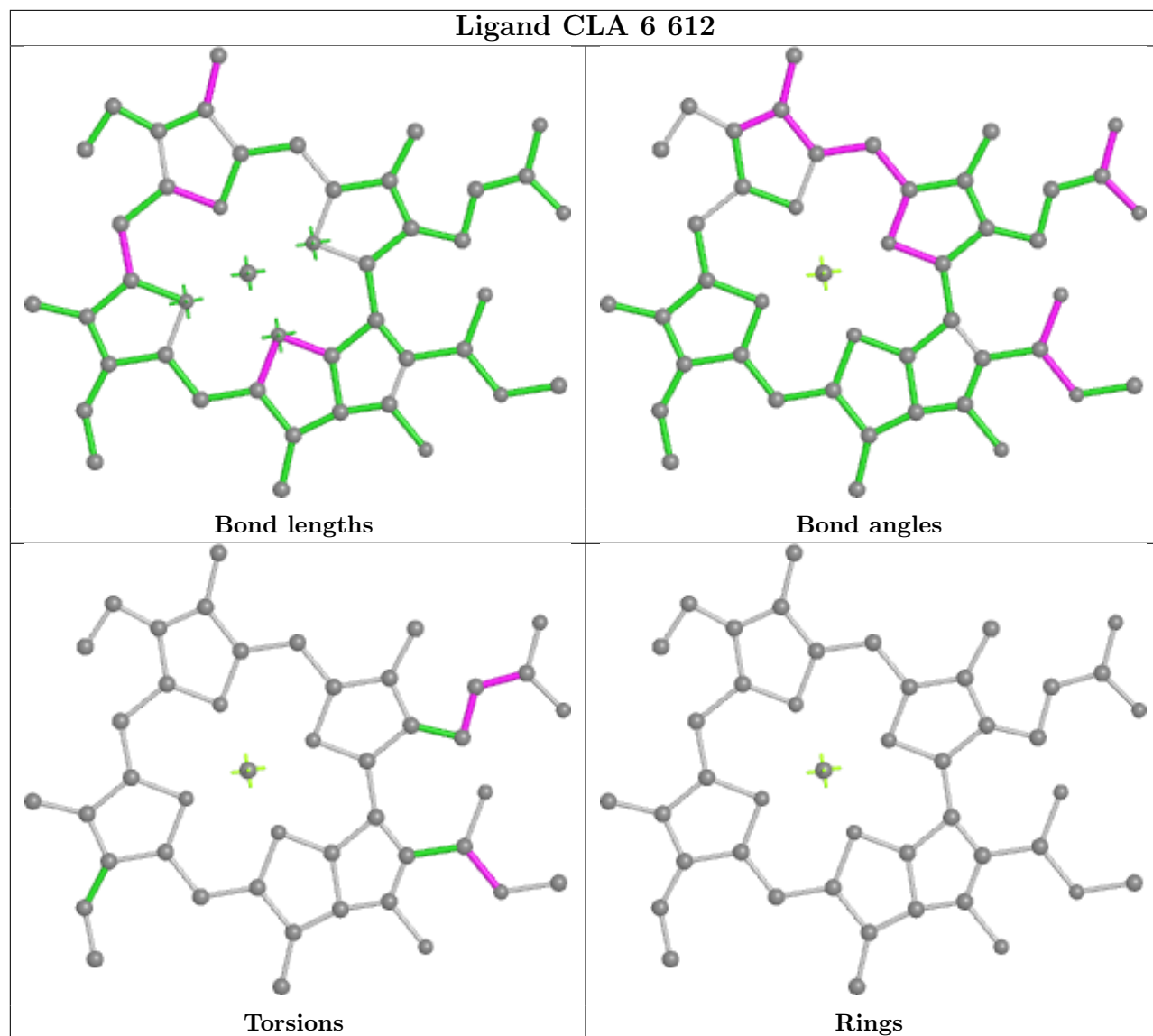
Torsions



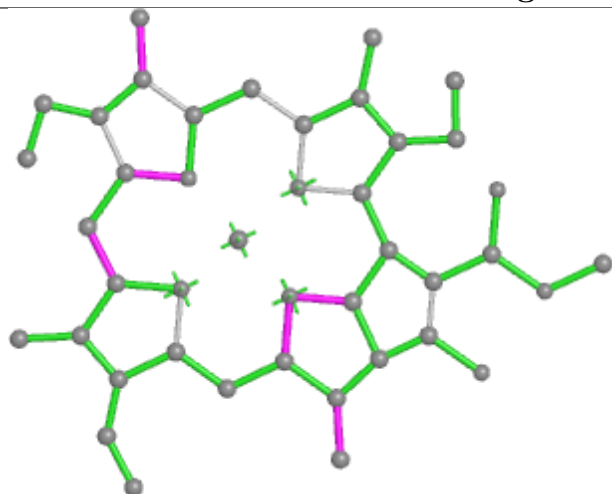
Rings



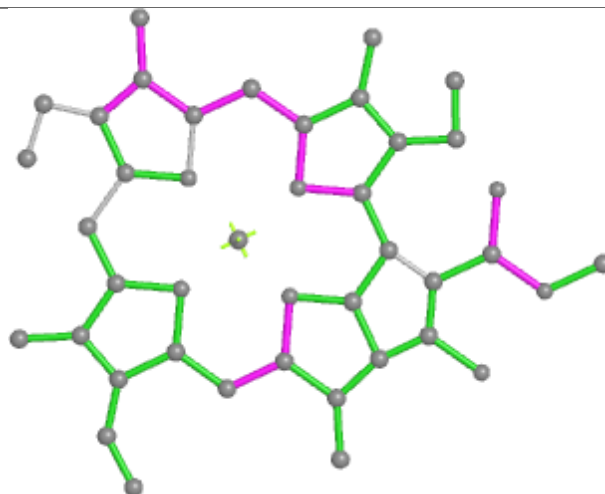
Ligand CLA 6 612



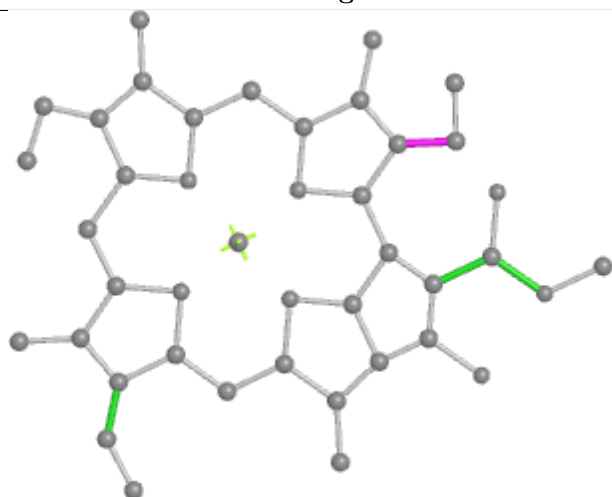
Ligand CLA 2 613



Bond lengths



Bond angles

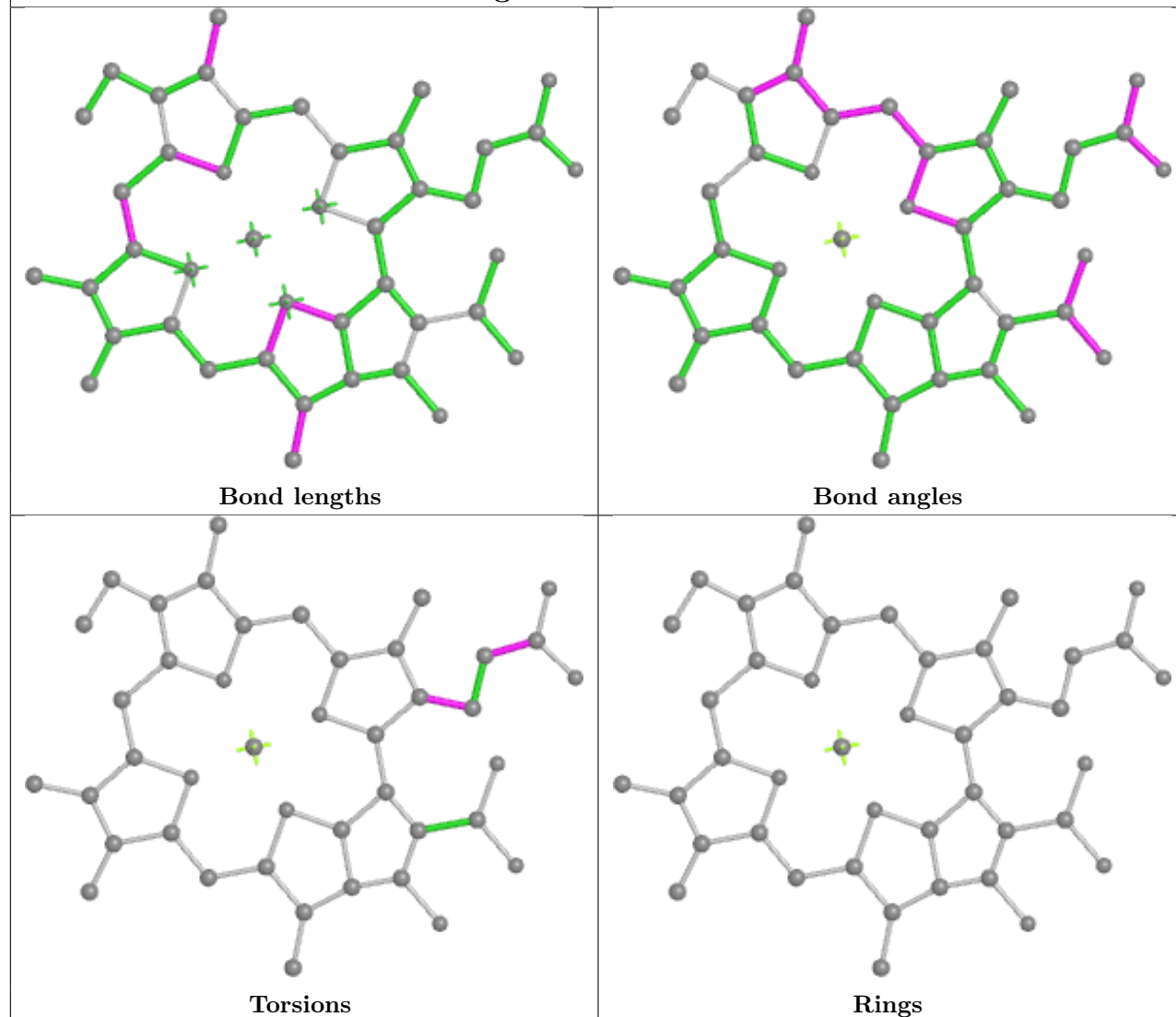


Torsions

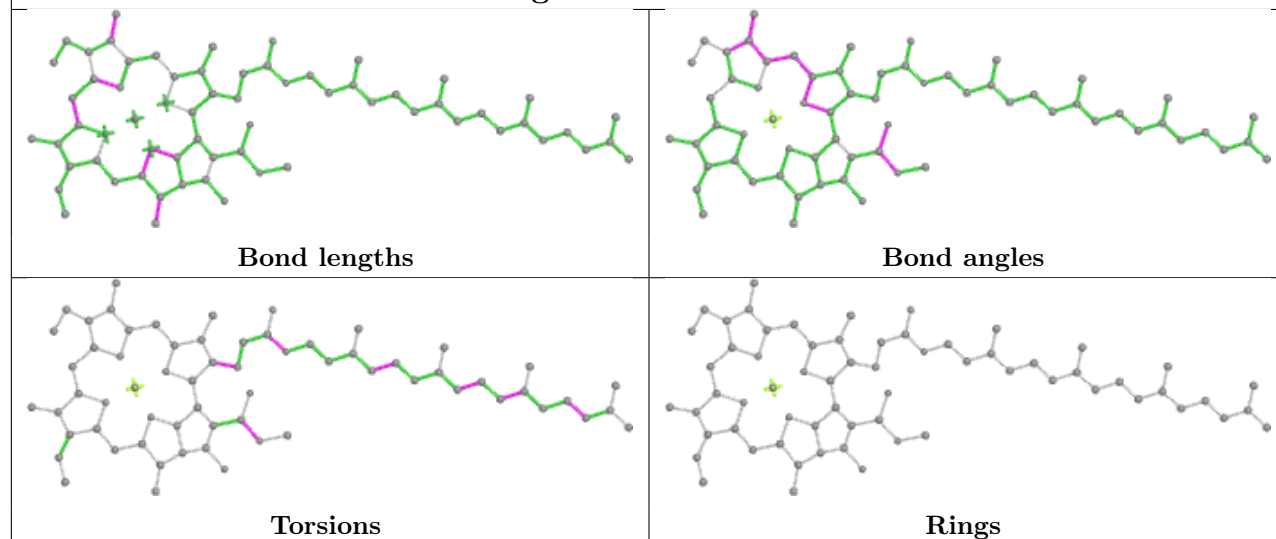


Rings

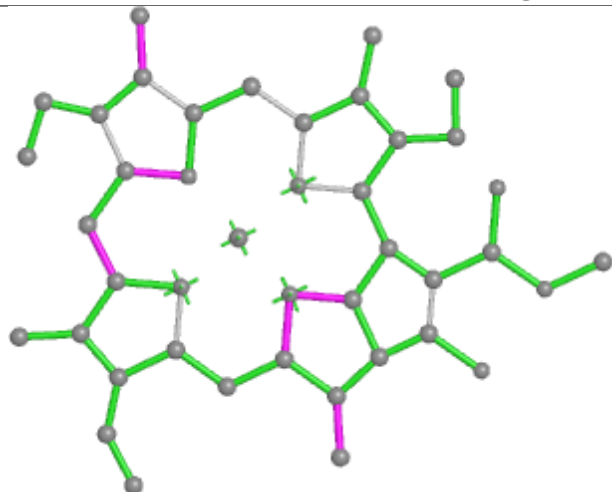
Ligand CLA 1 310



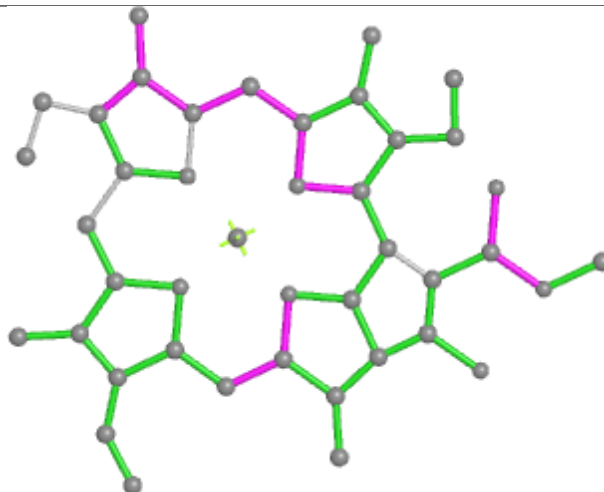
Ligand CLA A 807



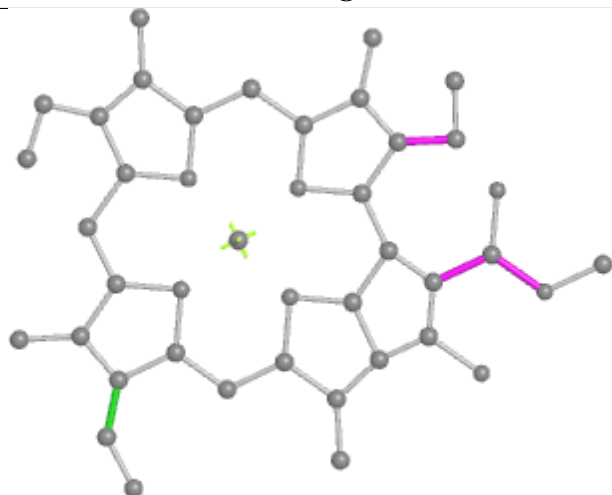
Ligand CLA 6 613



Bond lengths



Bond angles

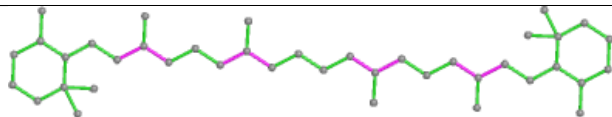


Torsions

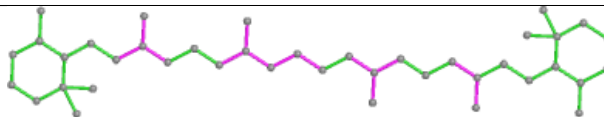


Rings

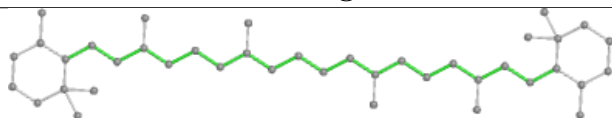
Ligand BCR B 842



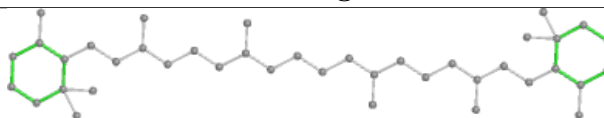
Bond lengths



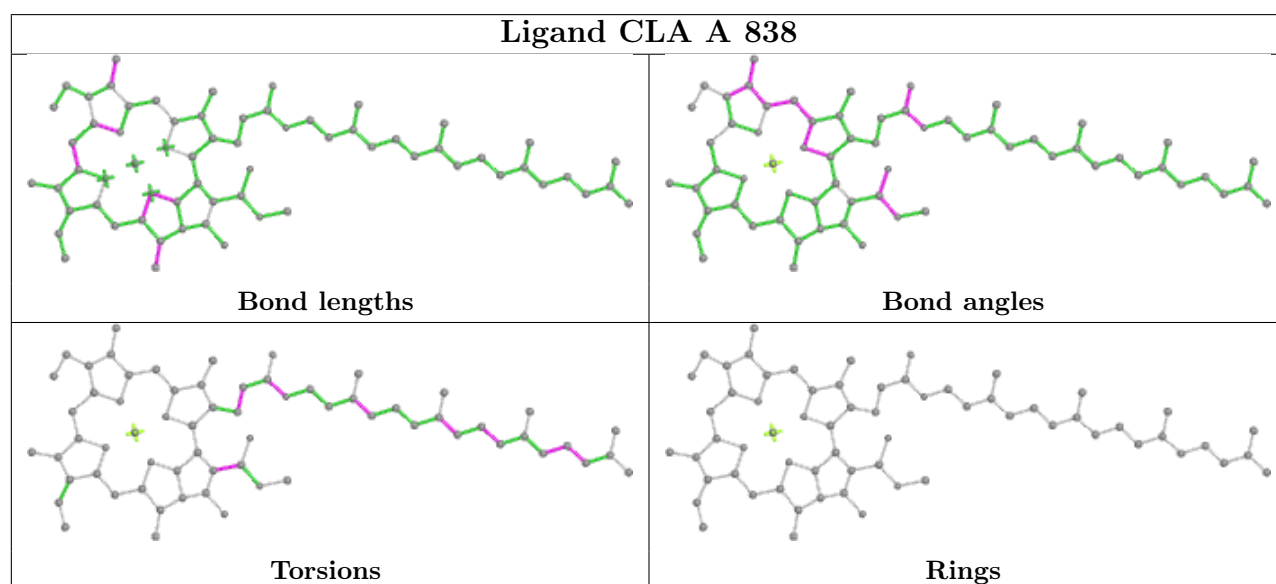
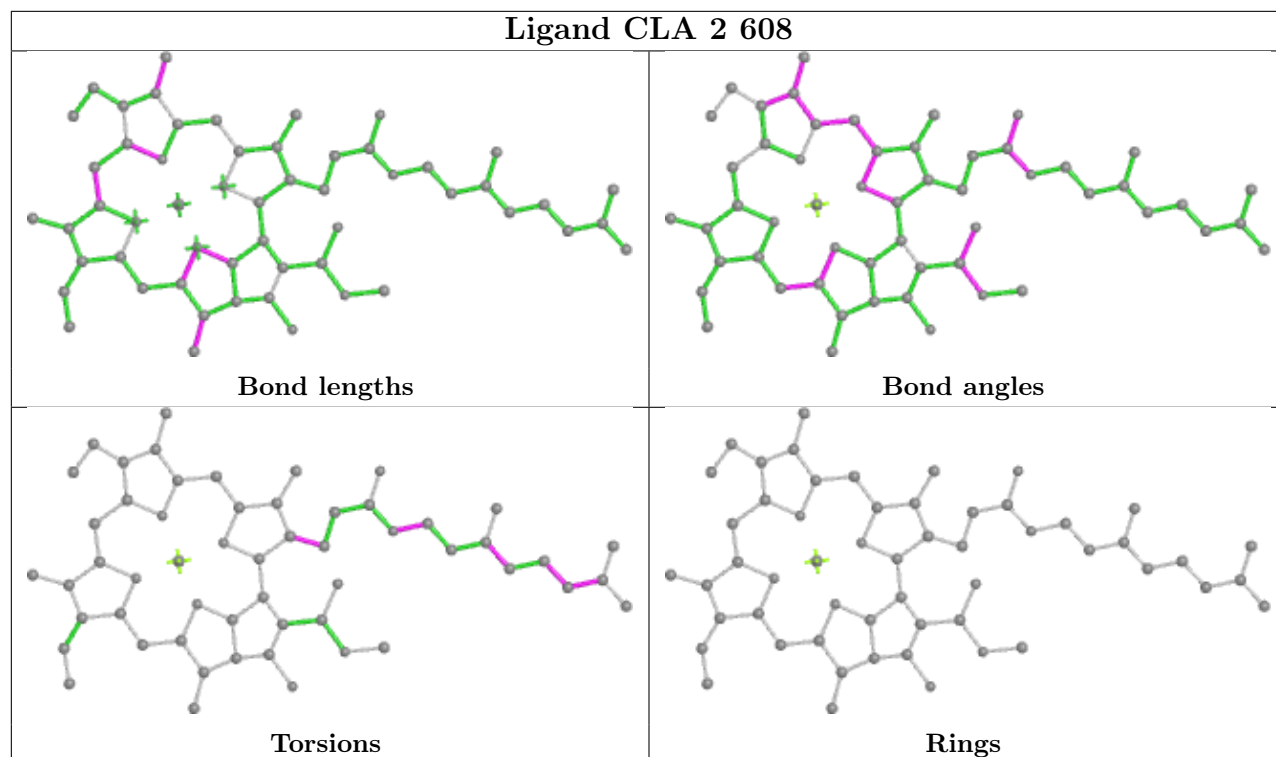
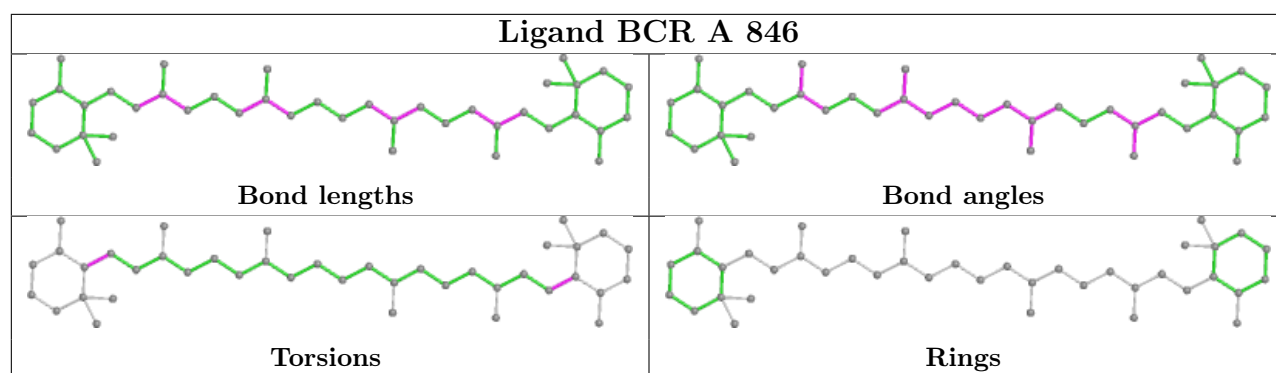
Bond angles

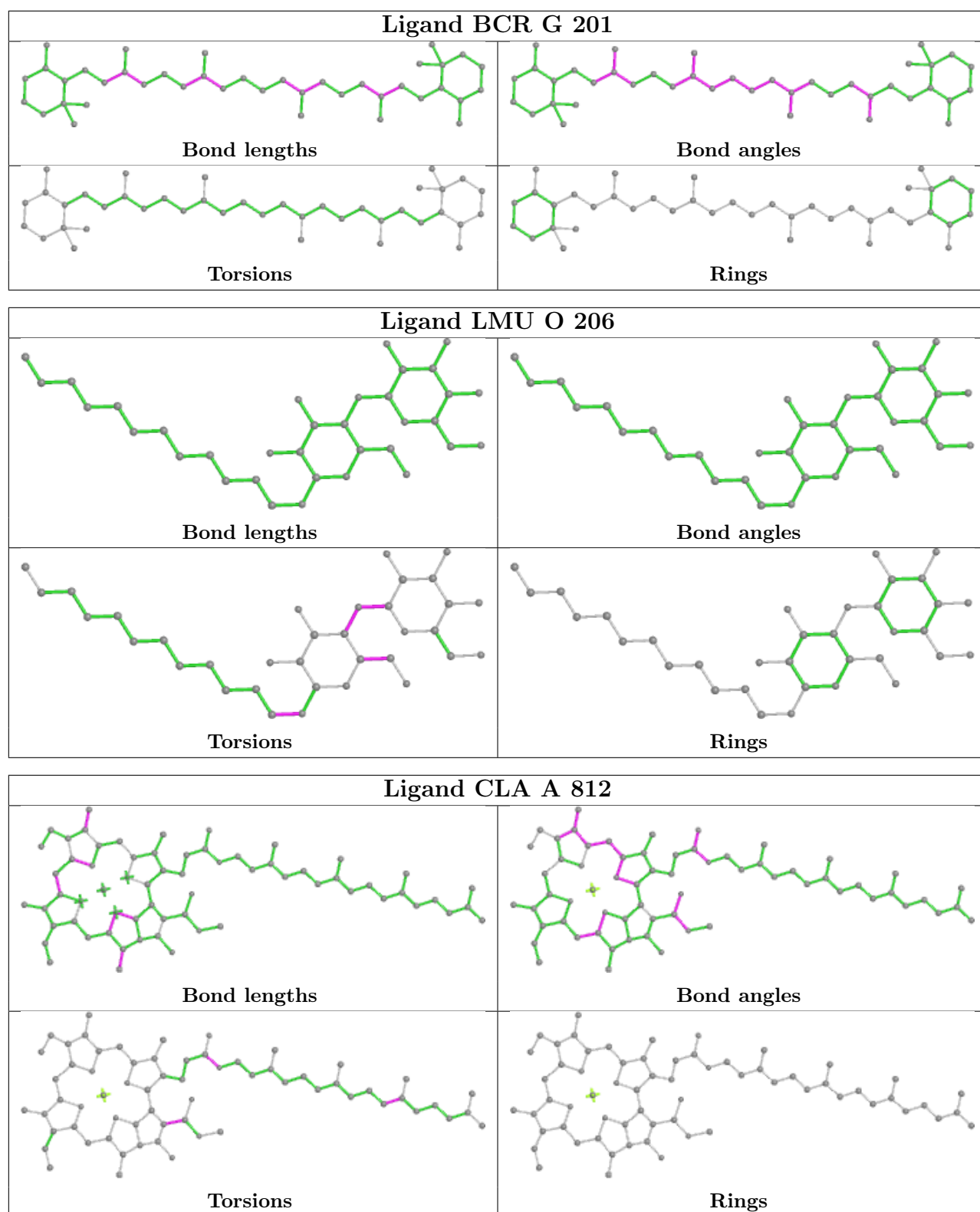


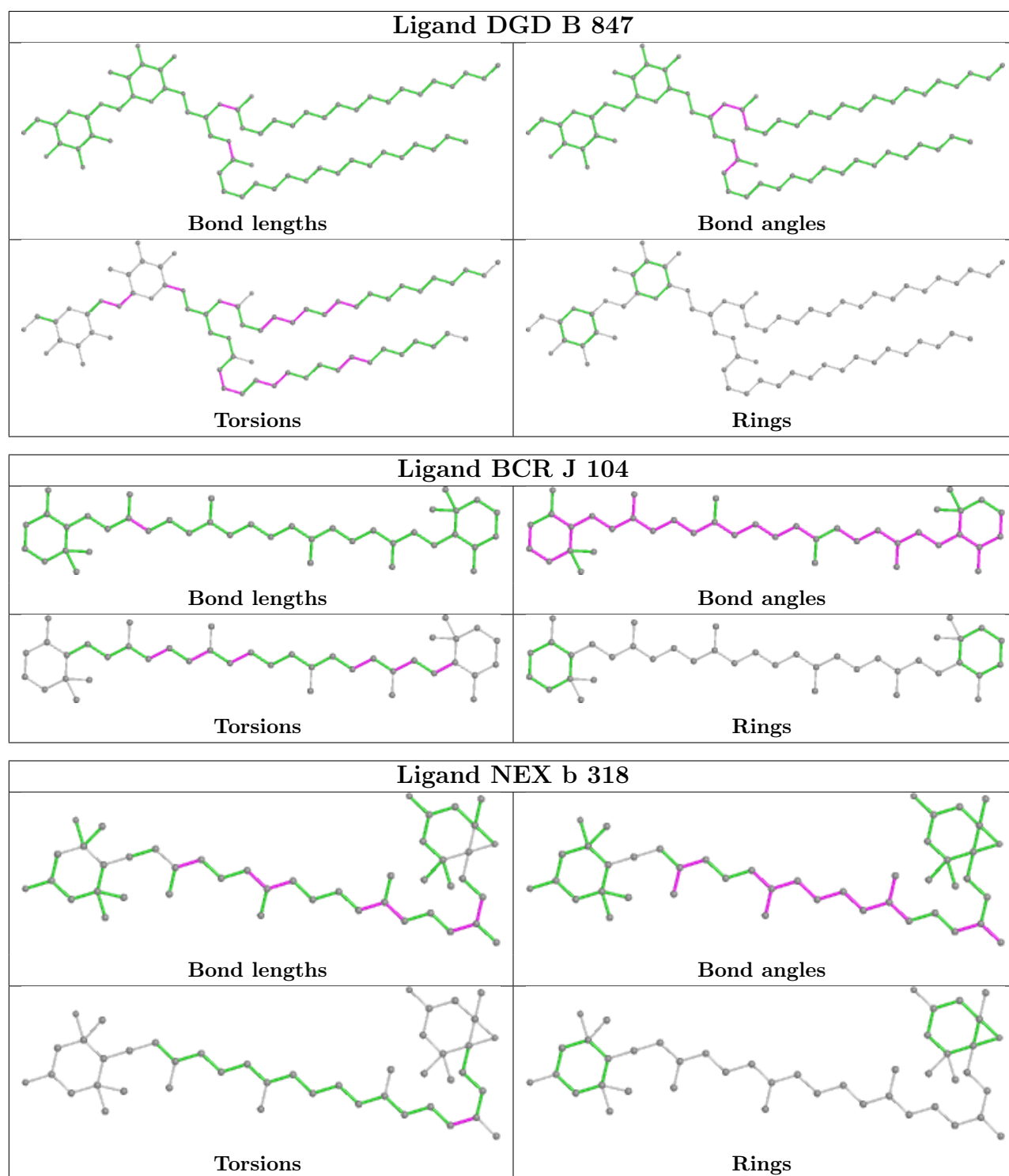
Torsions



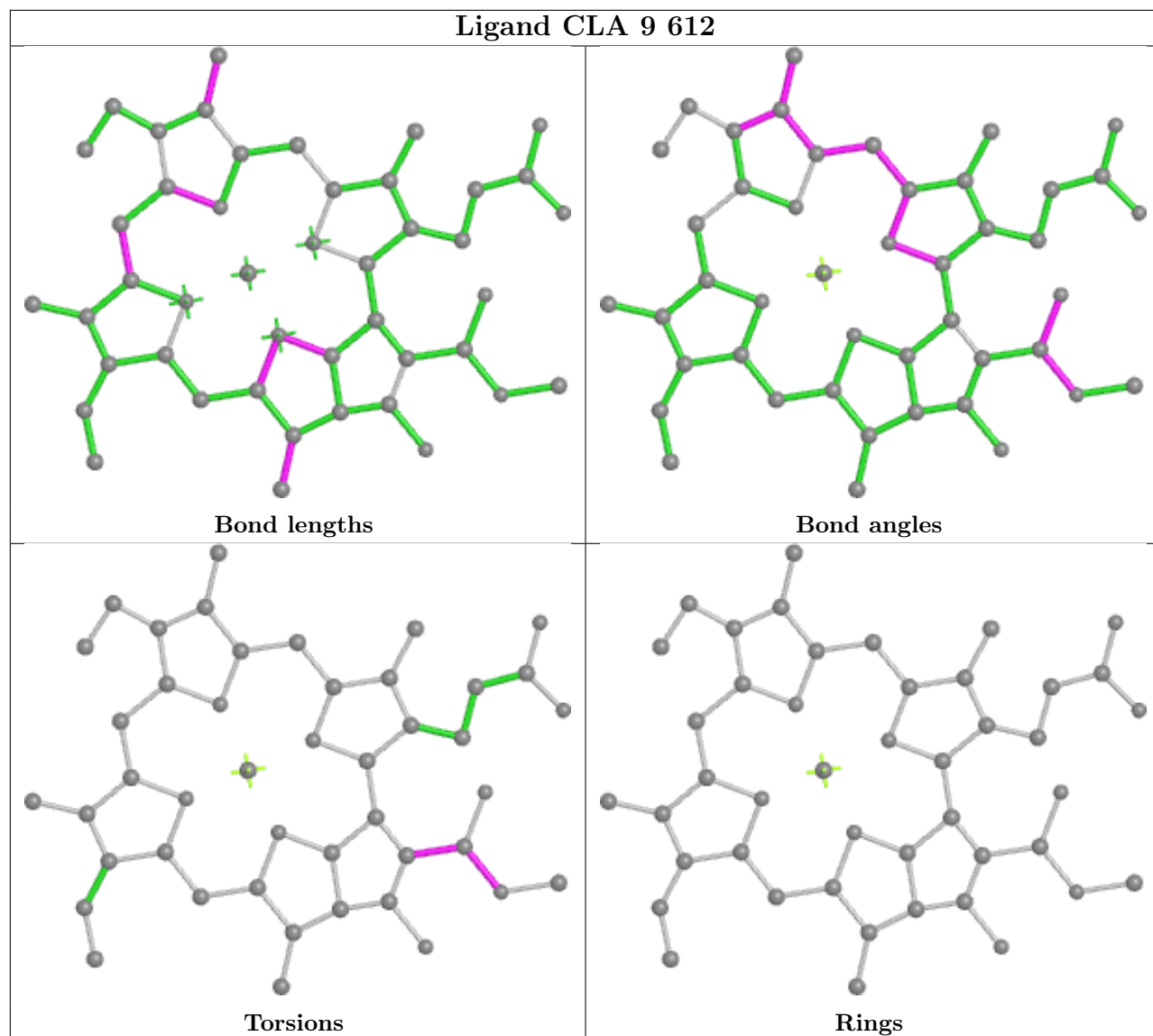
Rings

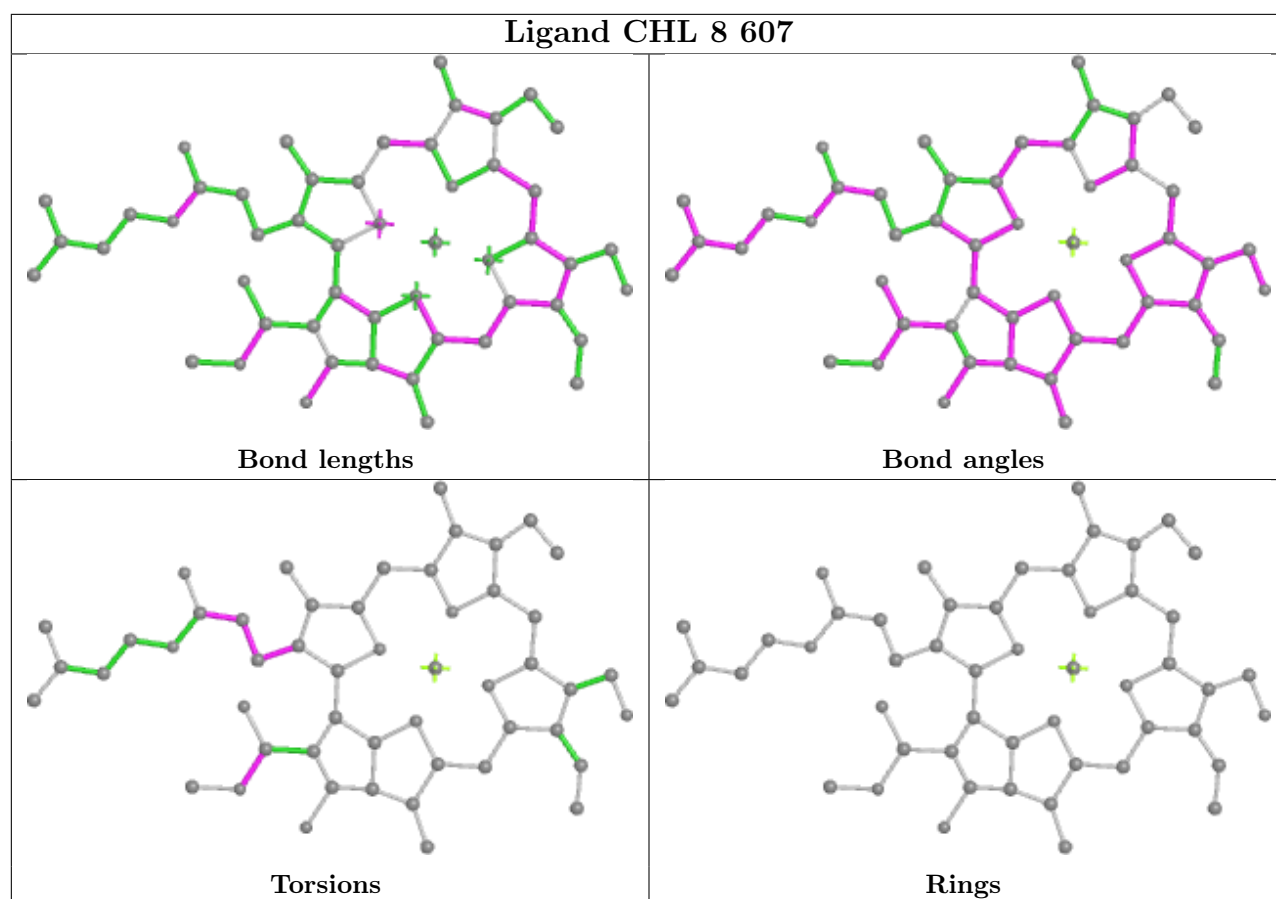




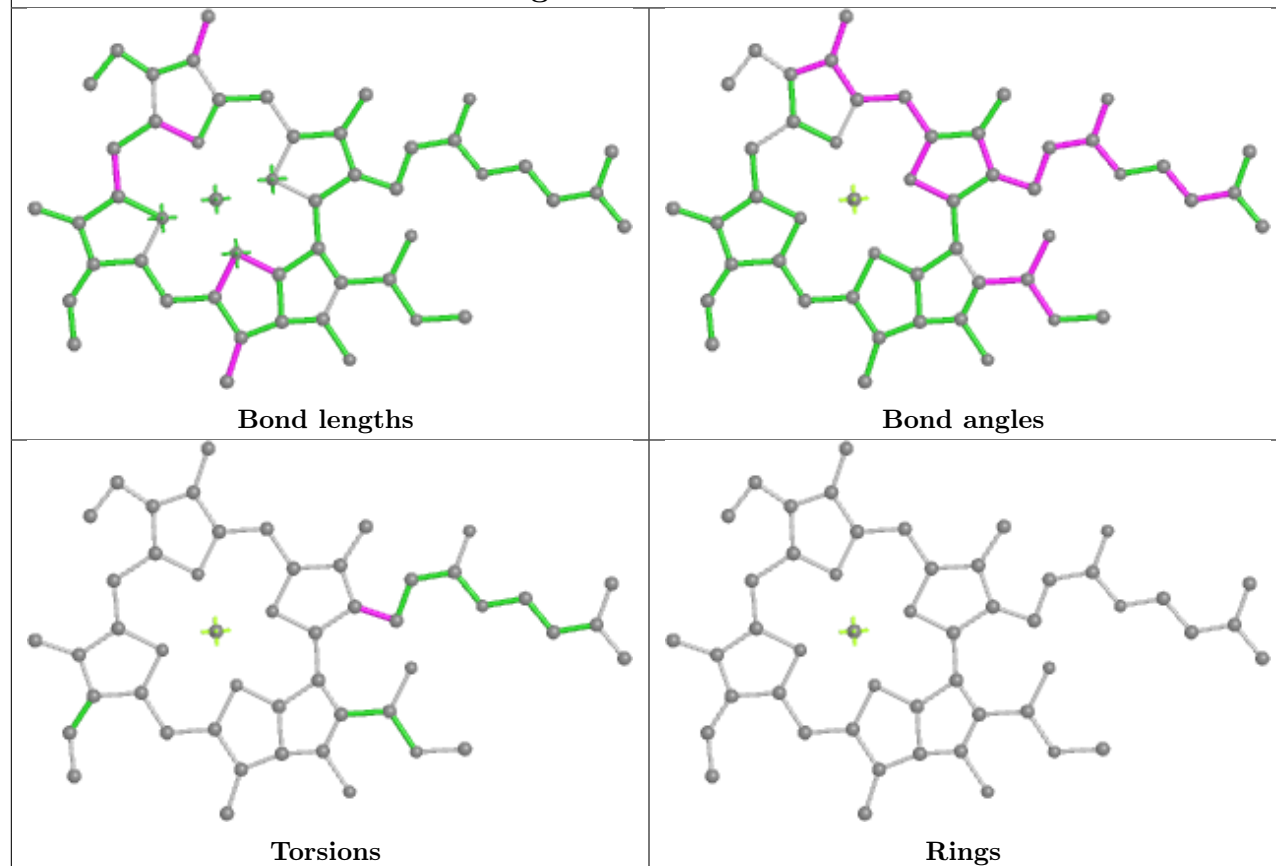


Ligand CLA 9 612

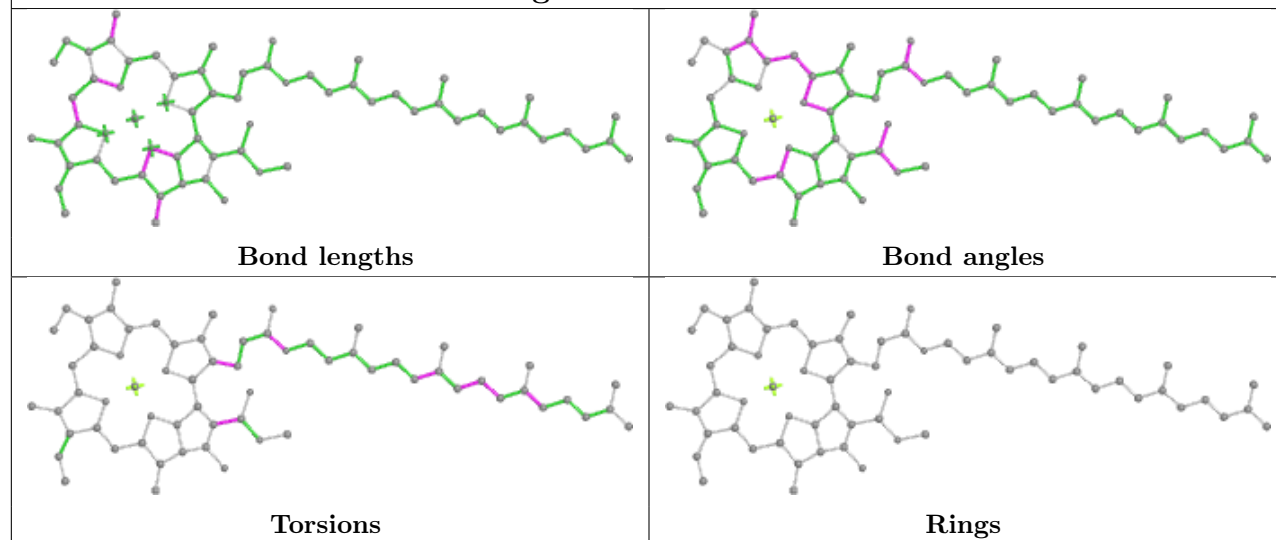




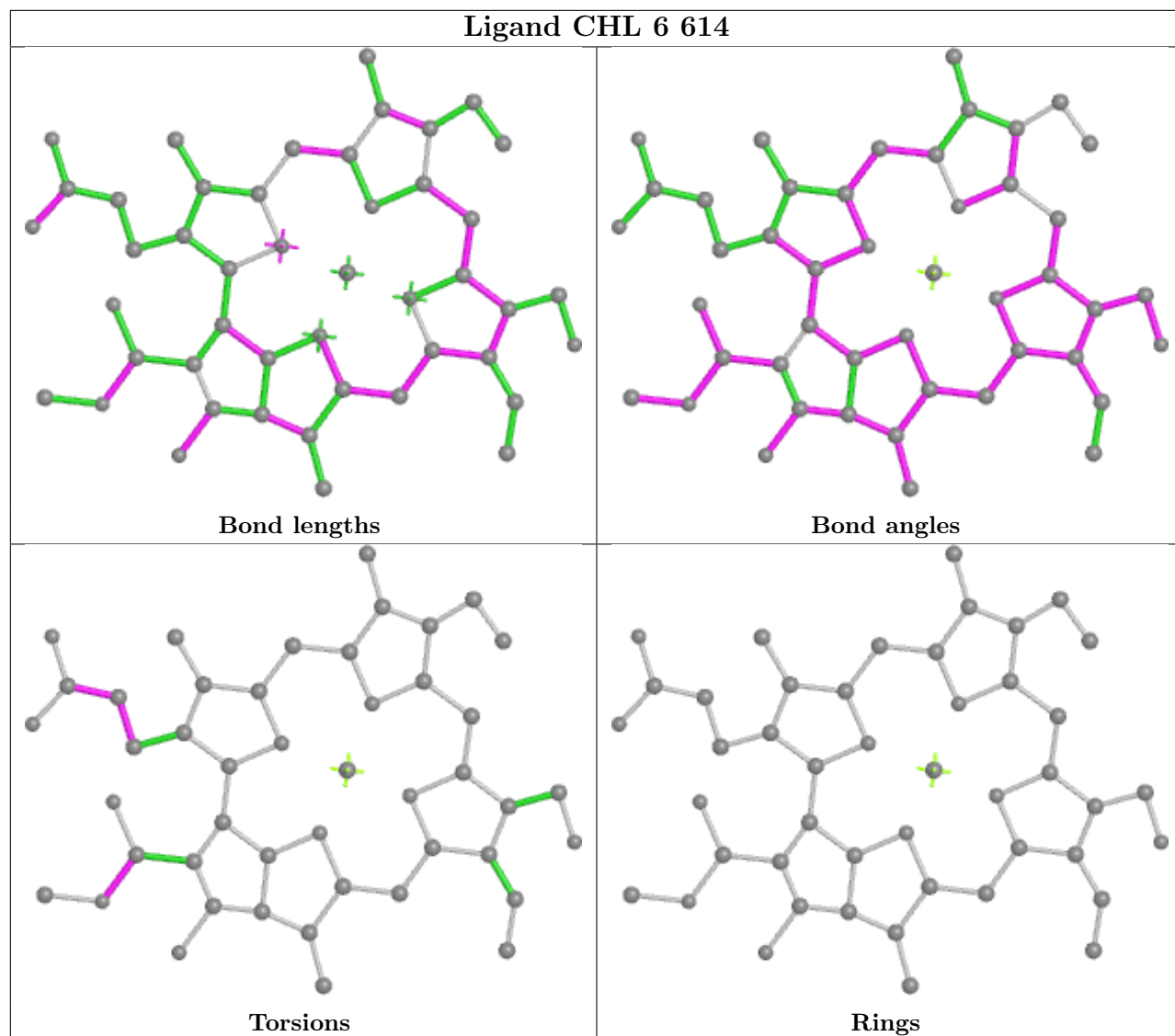
Ligand CLA K 202

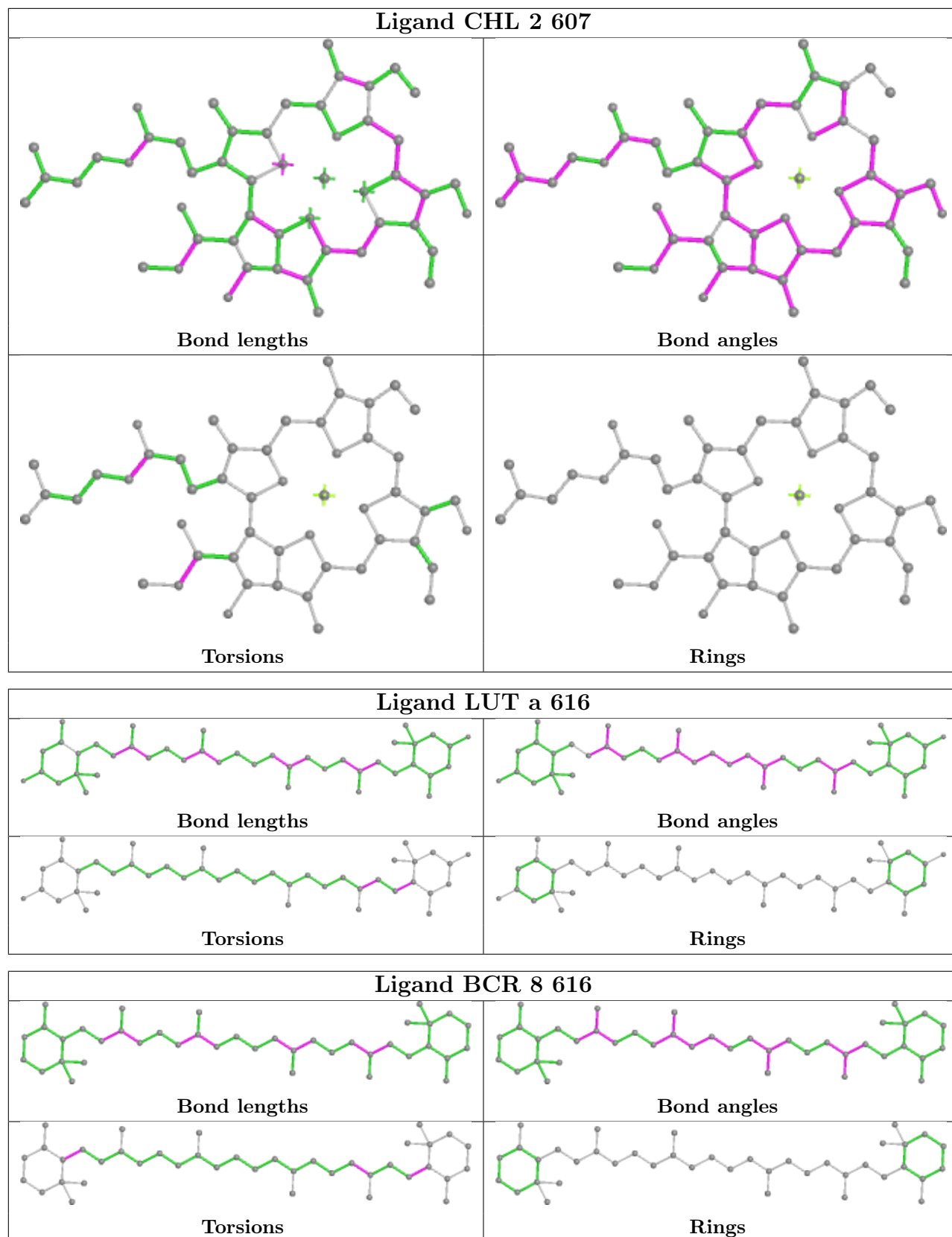


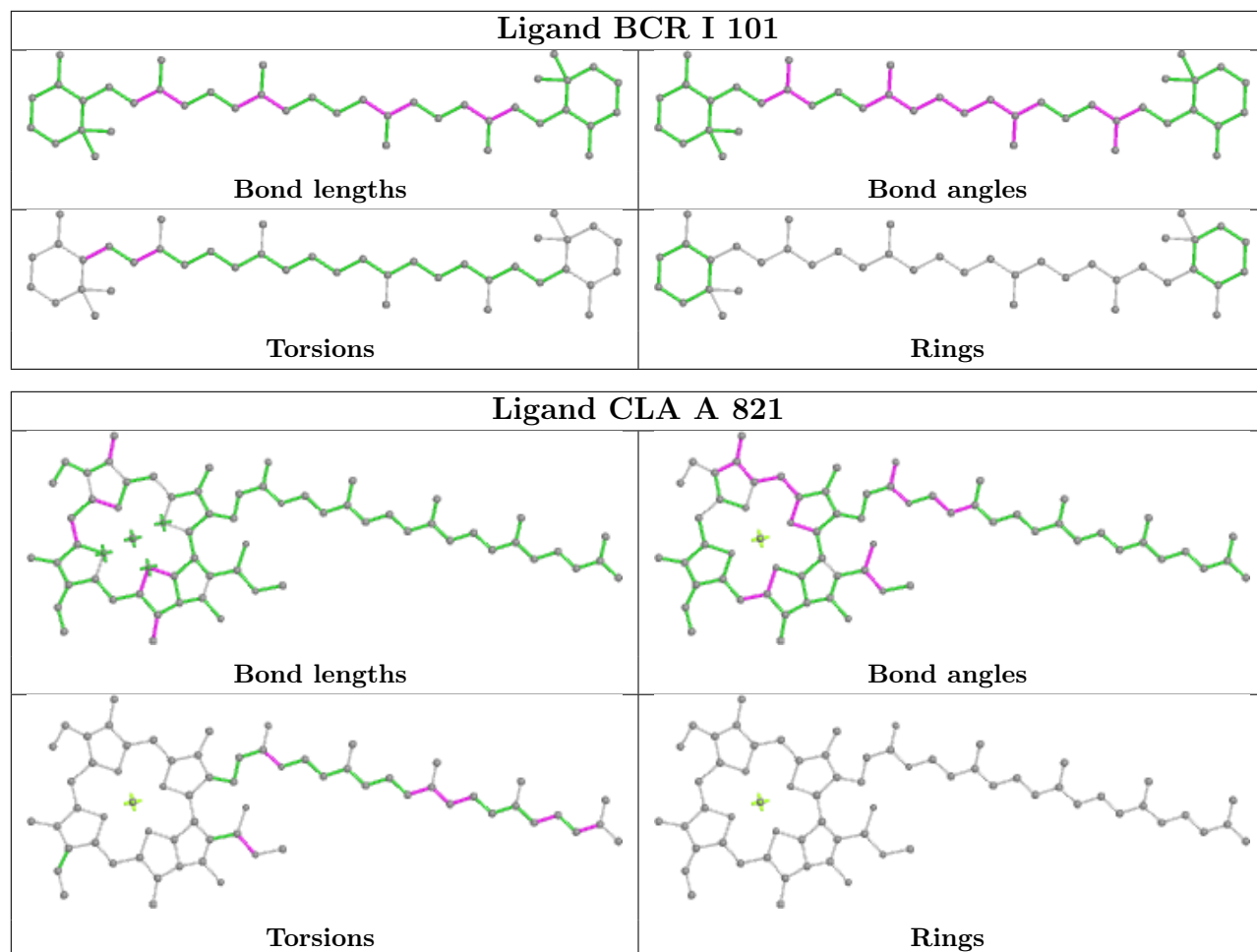
Ligand CLA B 824



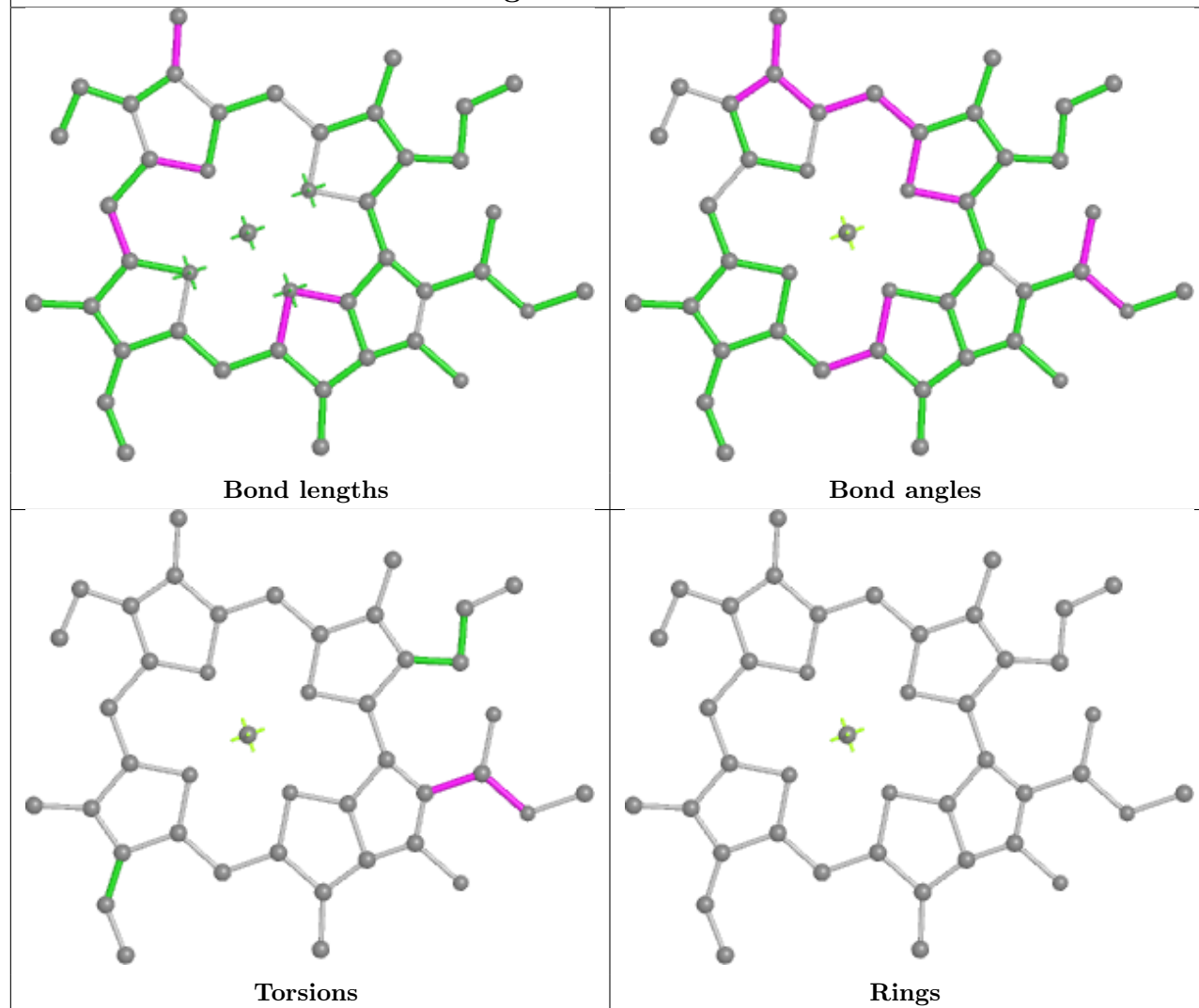
Ligand CHL 6 614



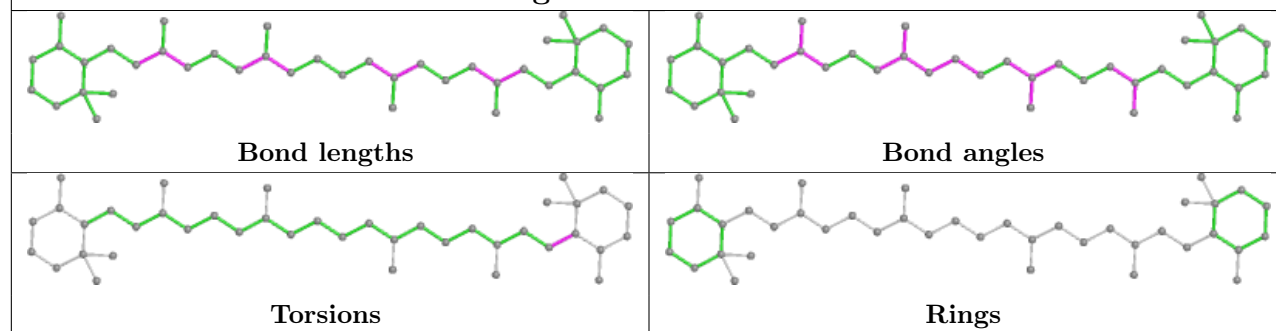




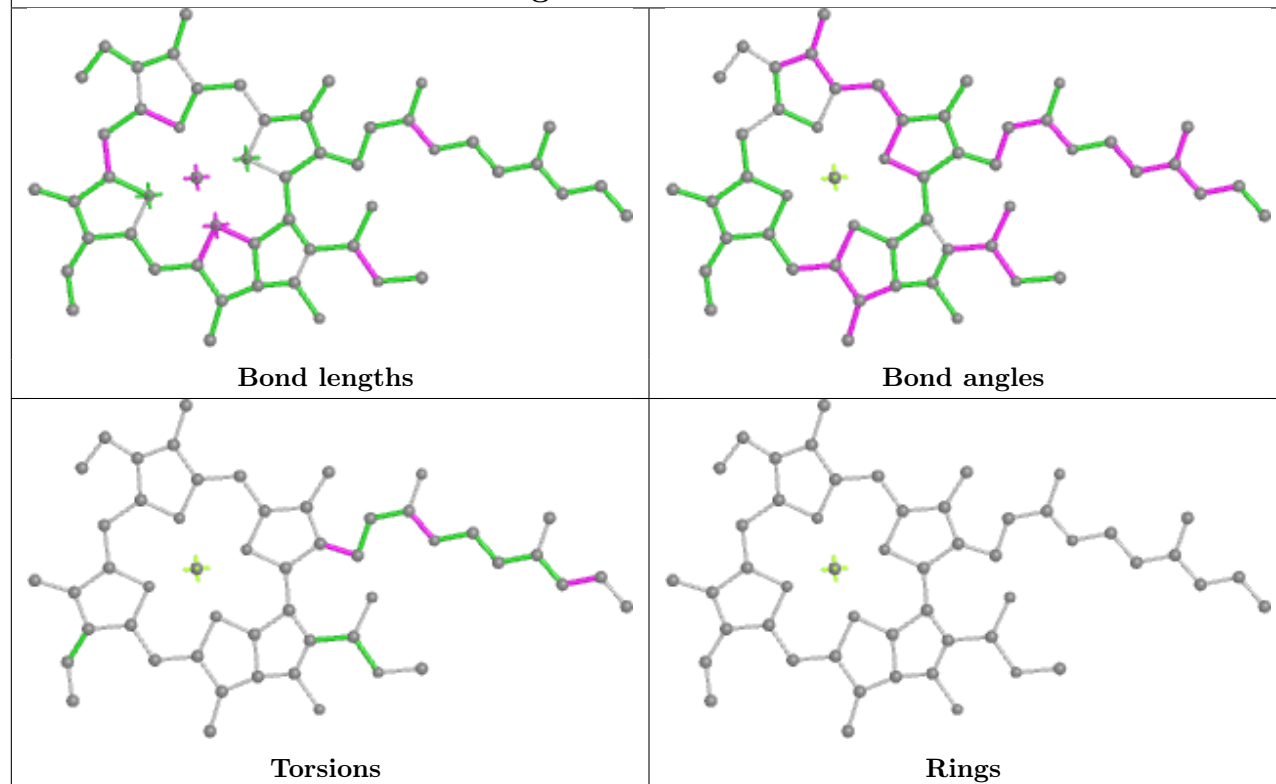
Ligand CLA 8 612



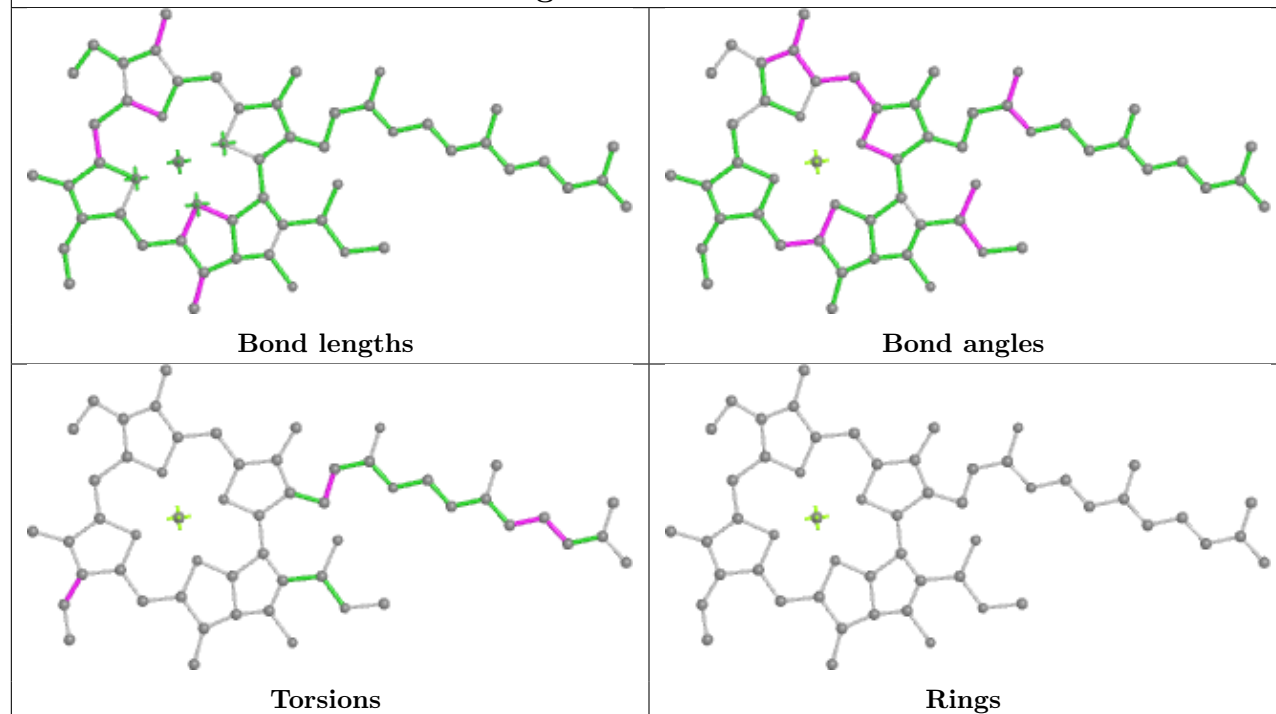
Ligand BCR L 305



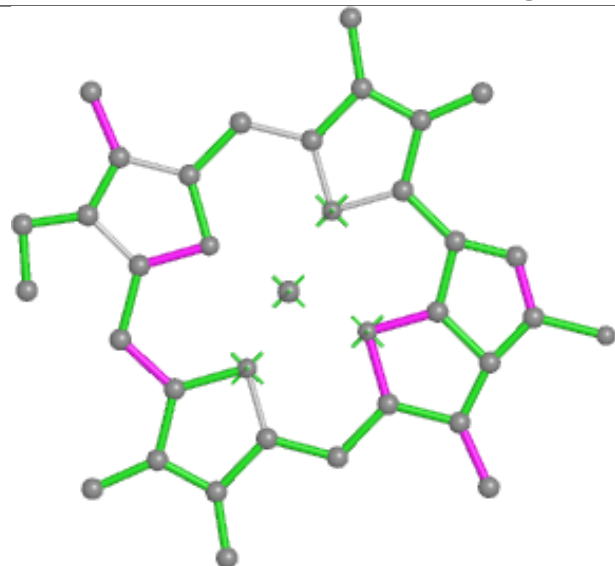
Ligand CLA A 830



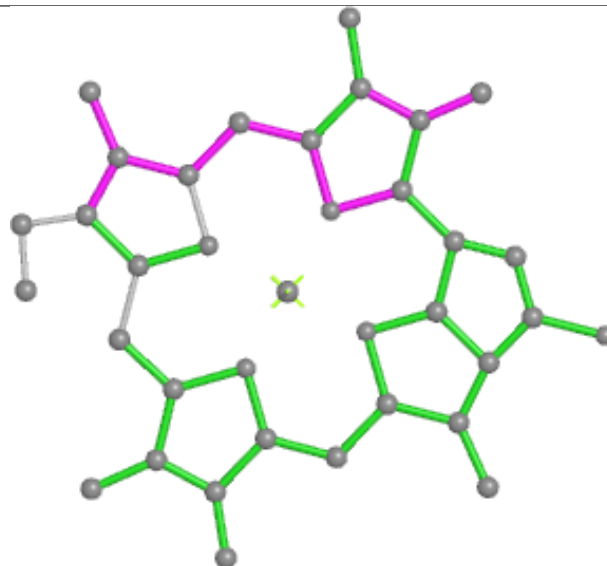
Ligand CLA 4 612



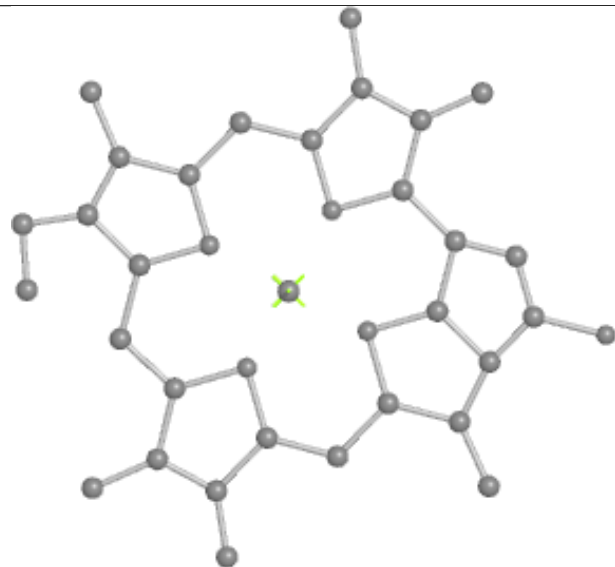
Ligand CLA 3 414



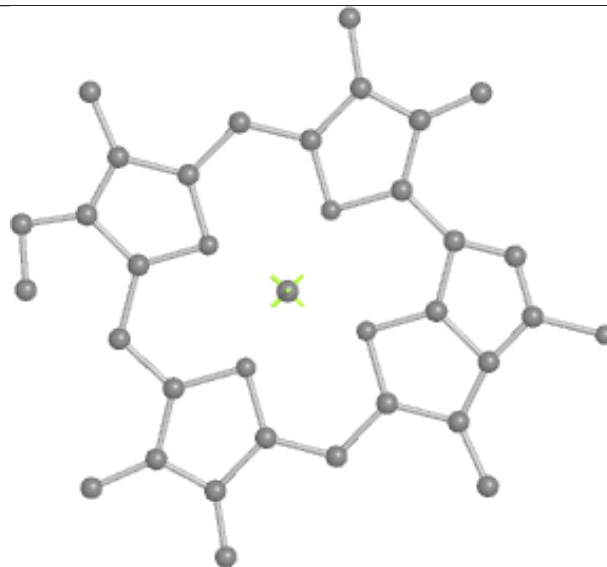
Bond lengths



Bond angles

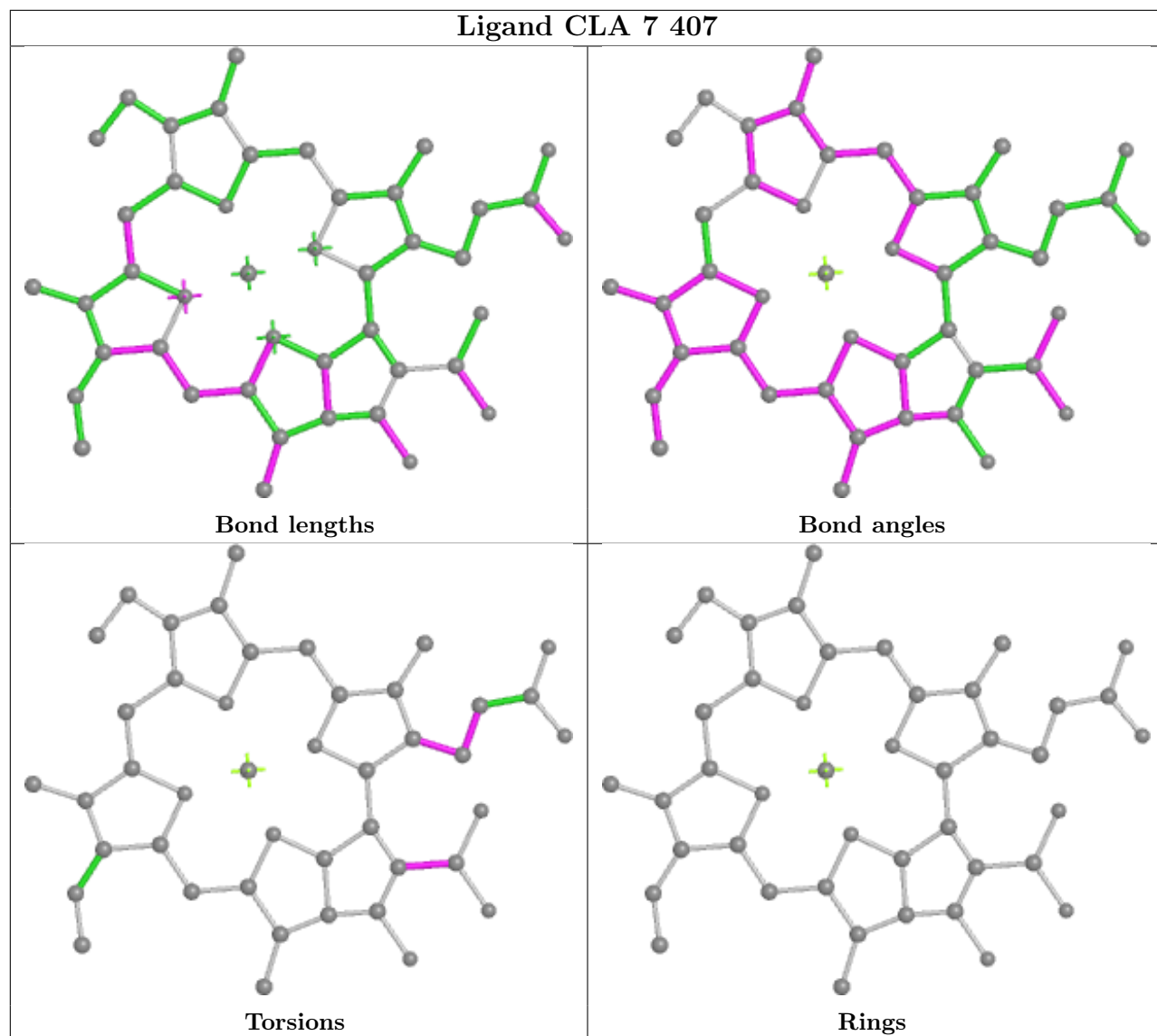


Torsions

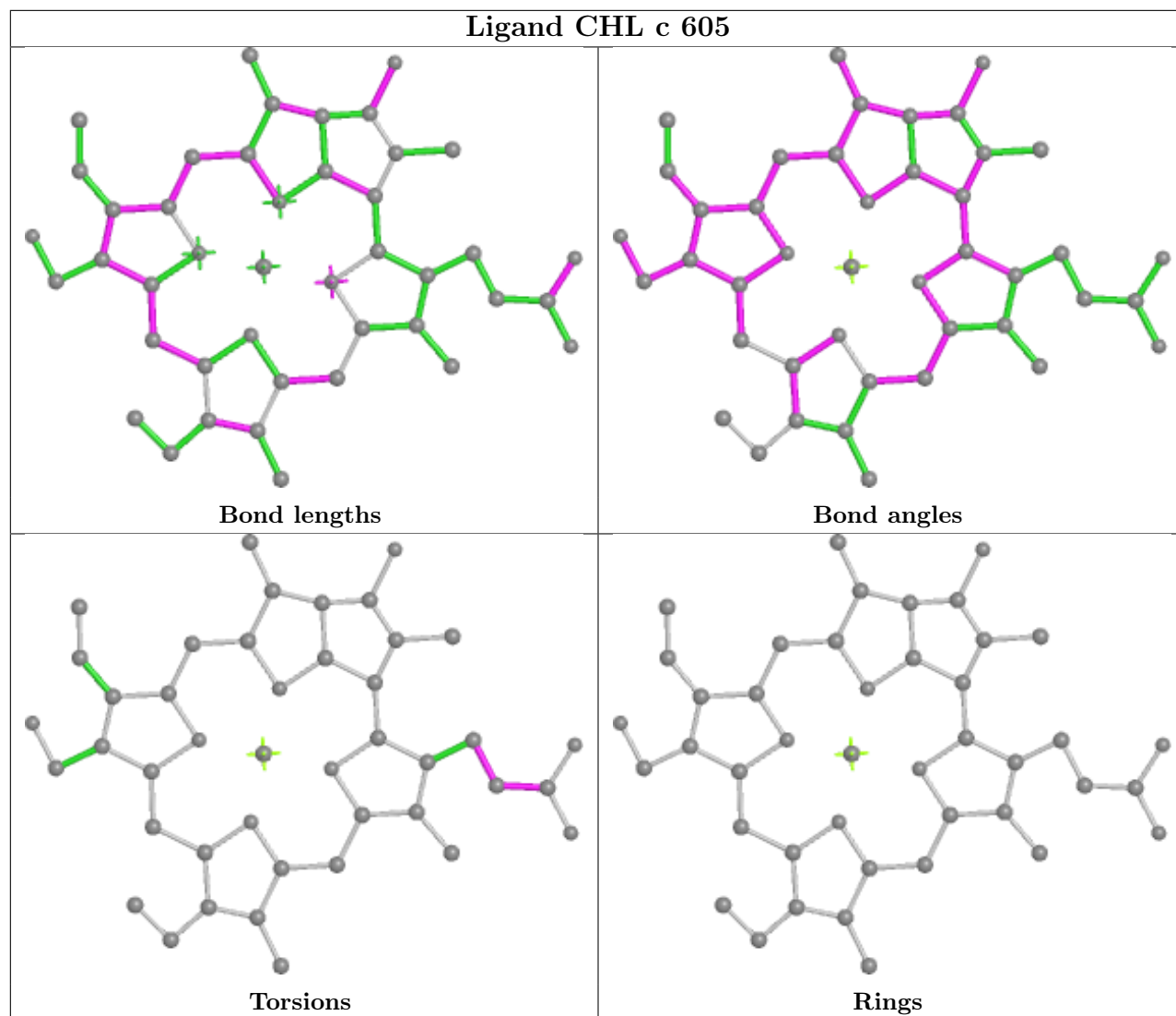


Rings

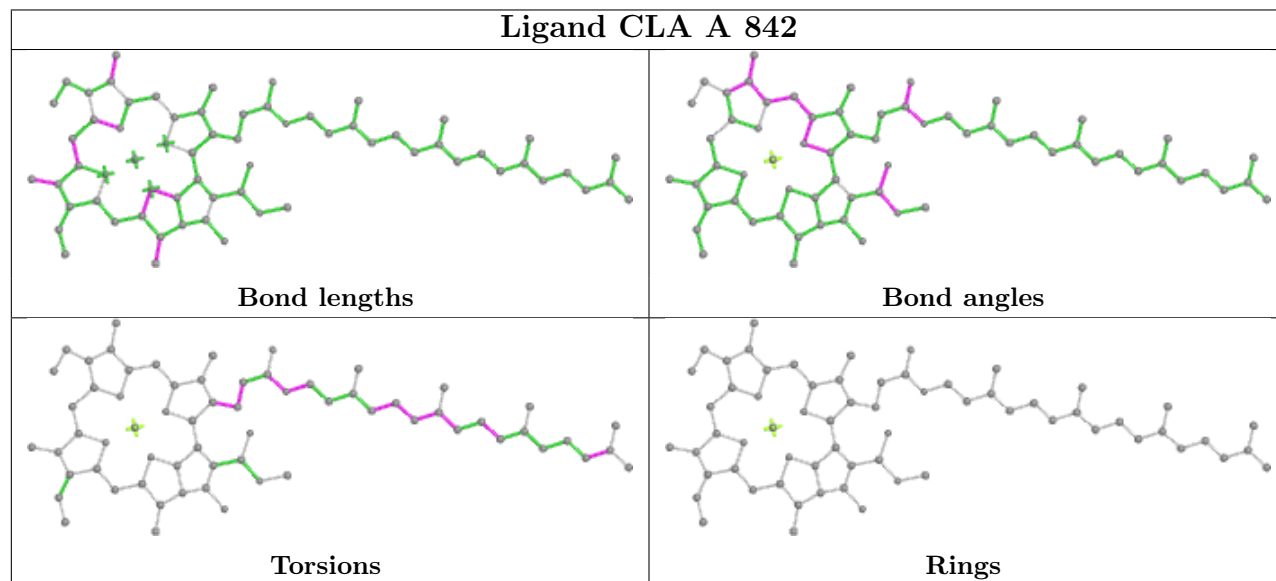
Ligand CLA 7 407



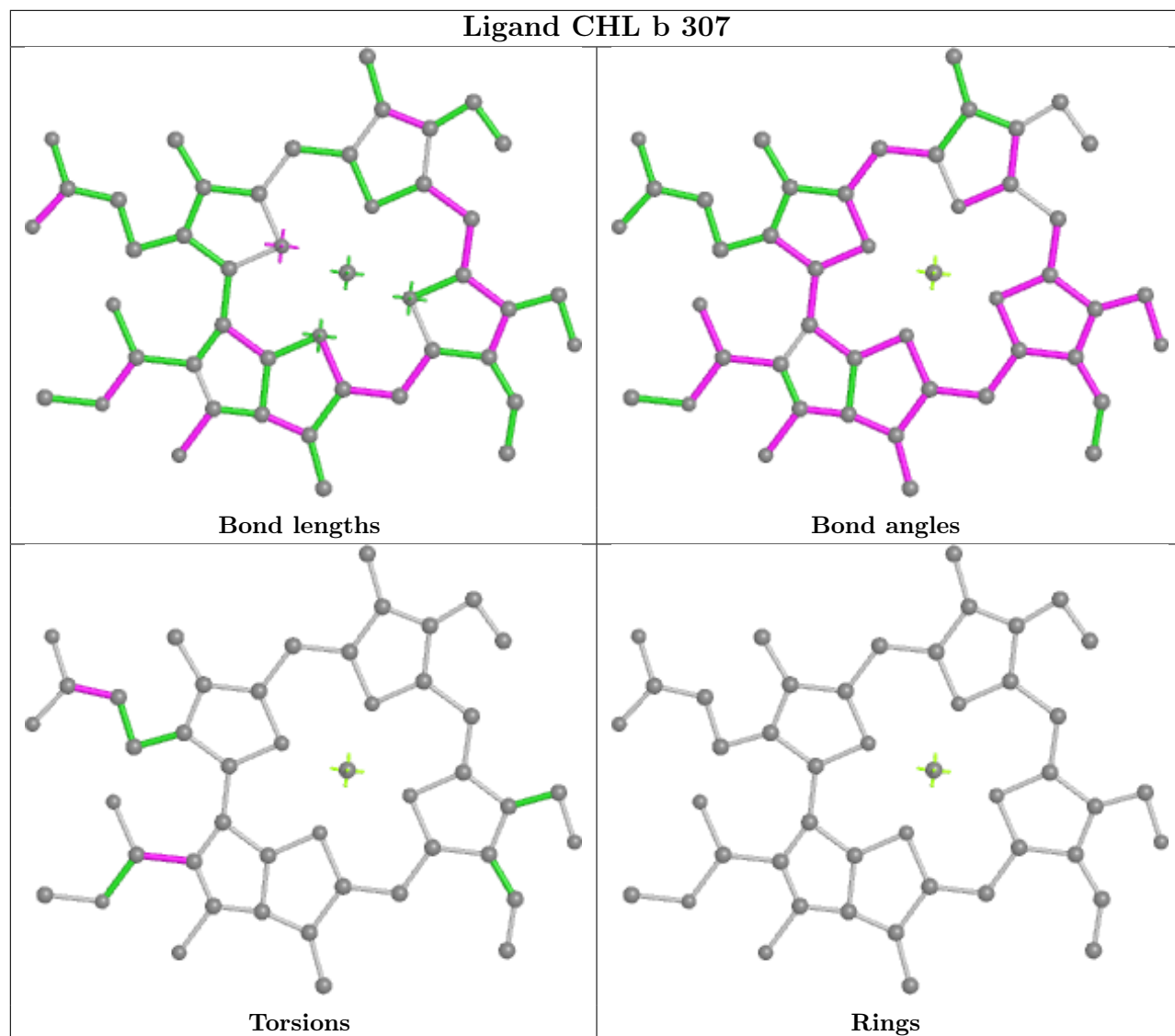
Ligand CHL c 605

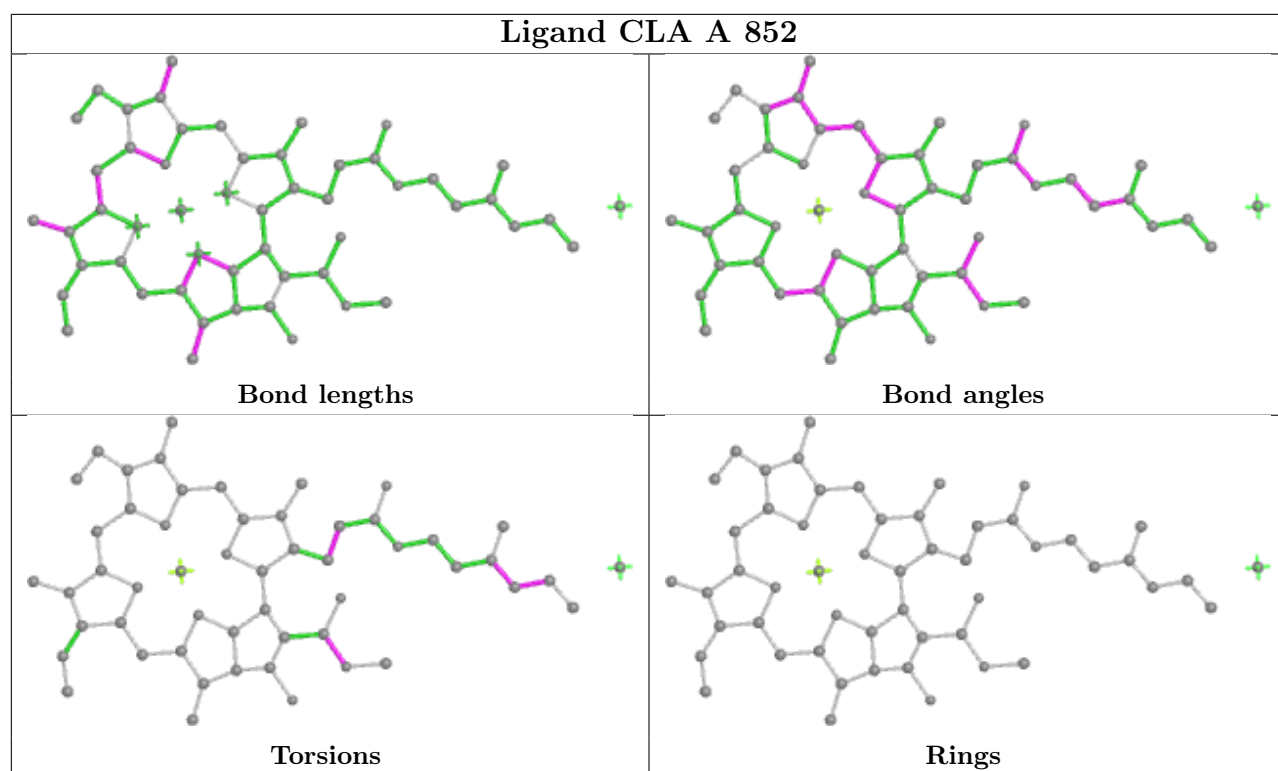


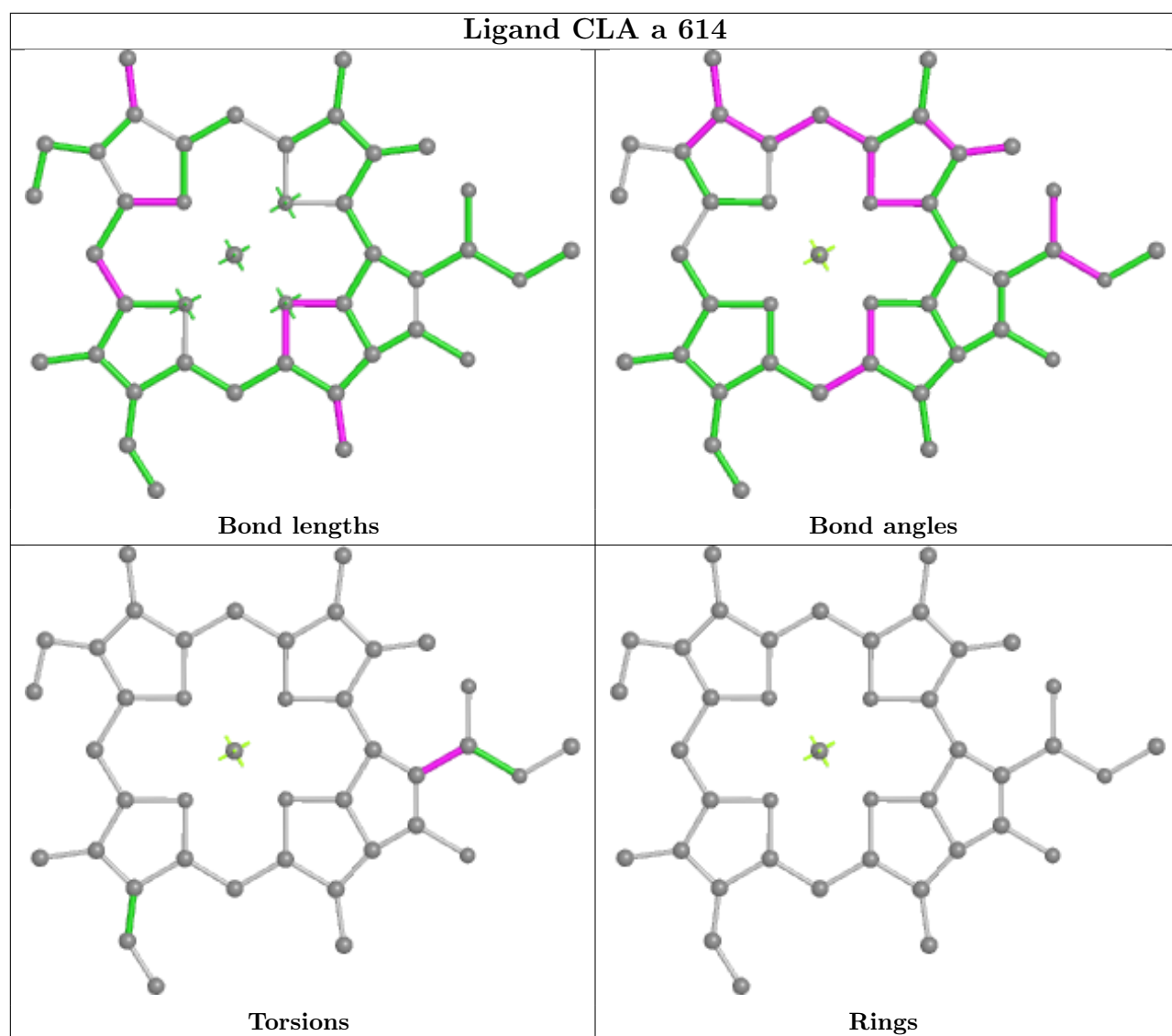
Ligand CLA A 842

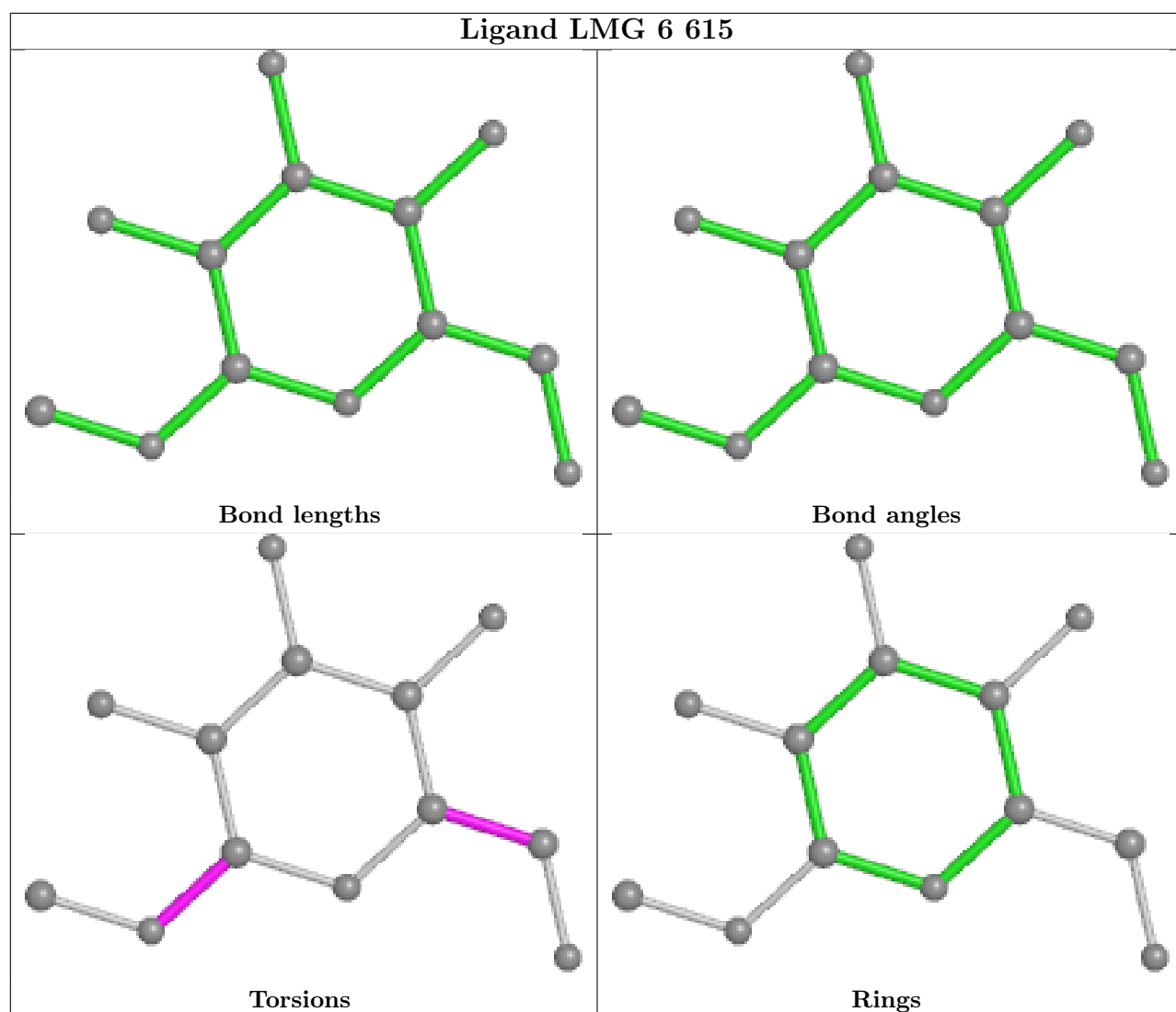


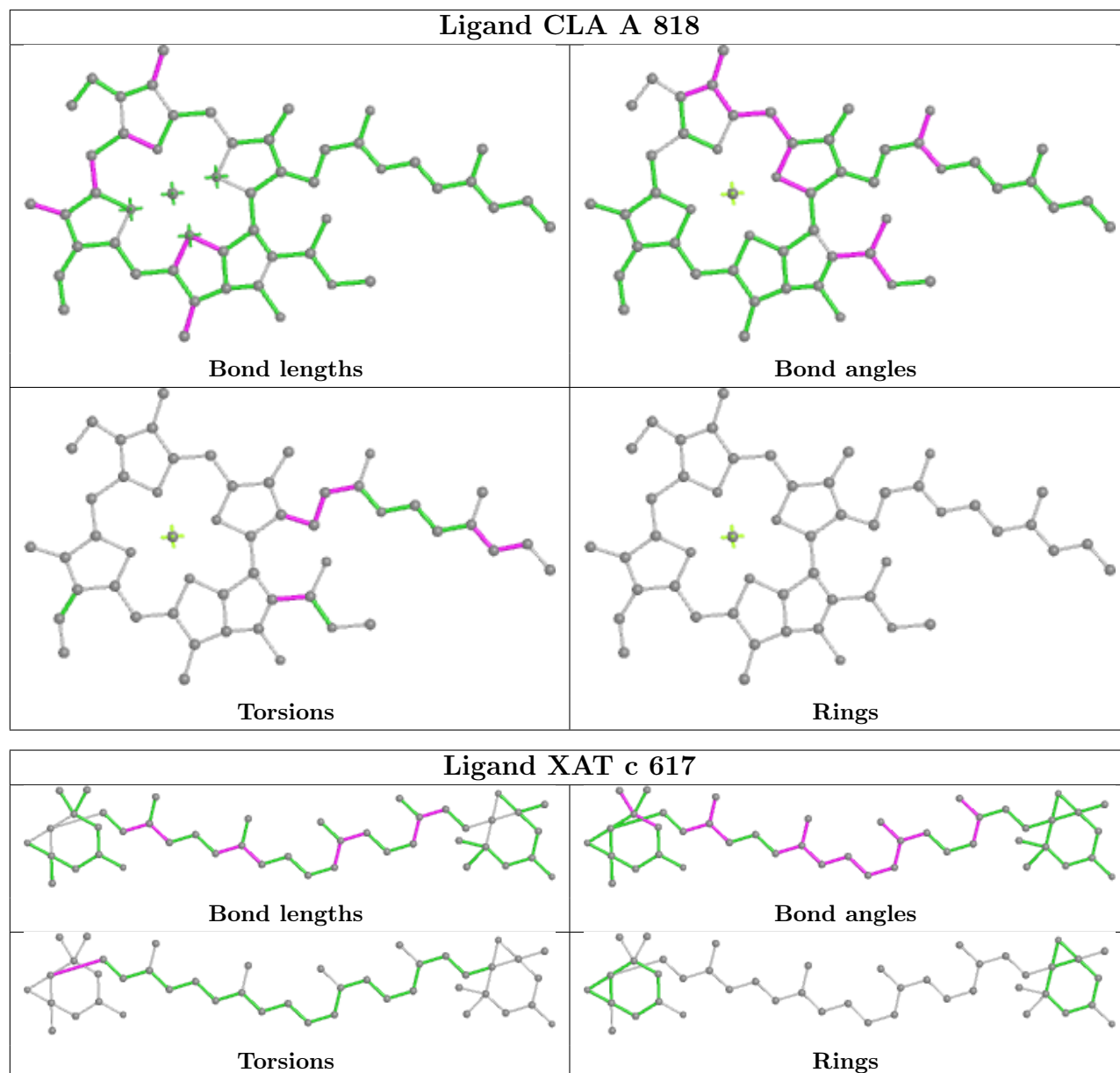
Ligand CHL b 307



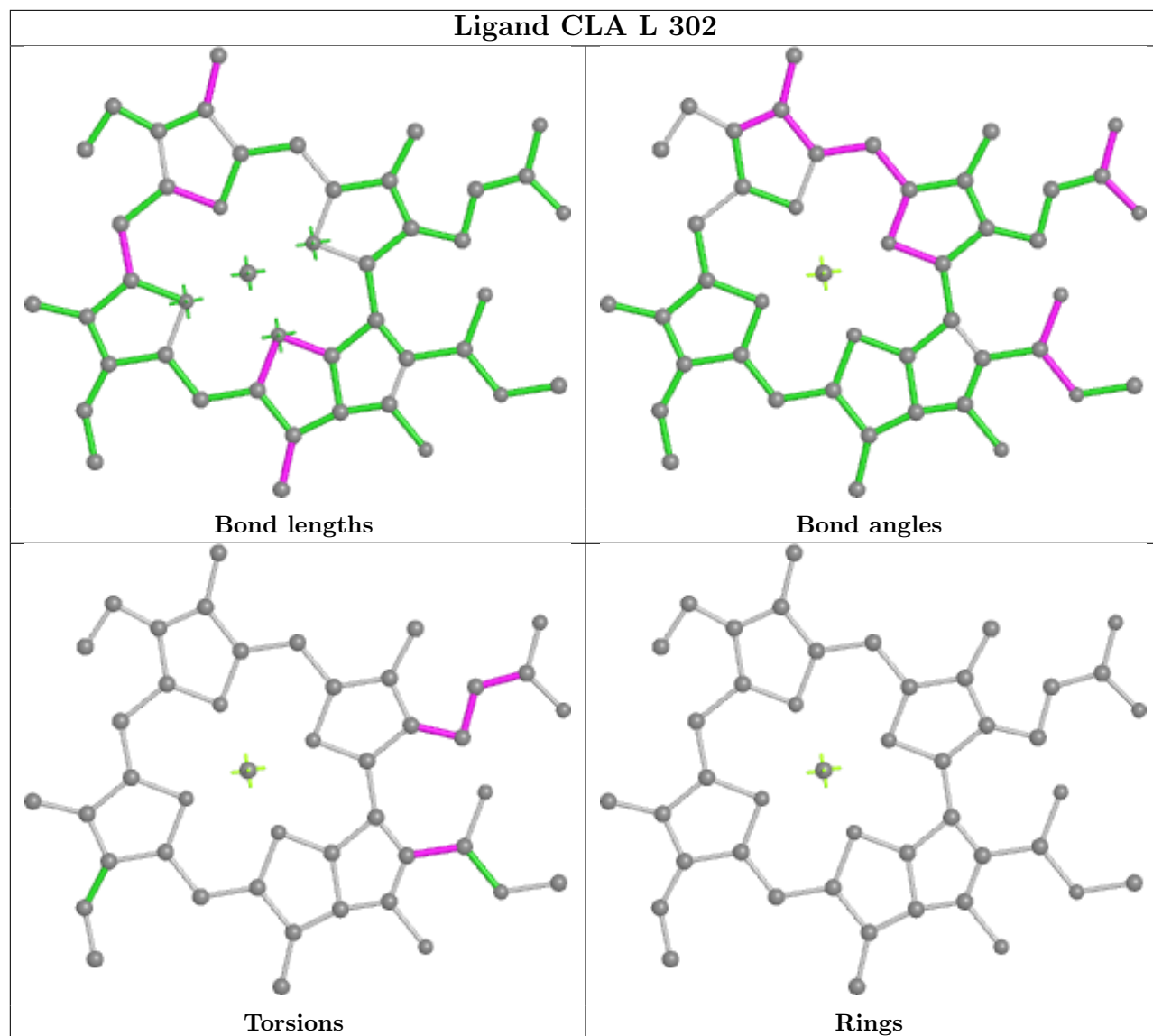




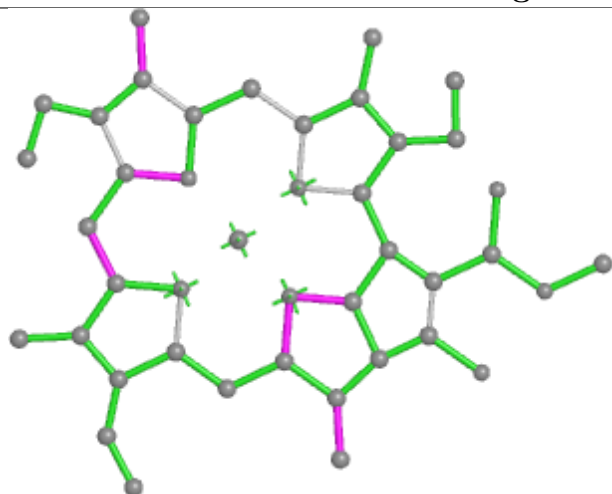




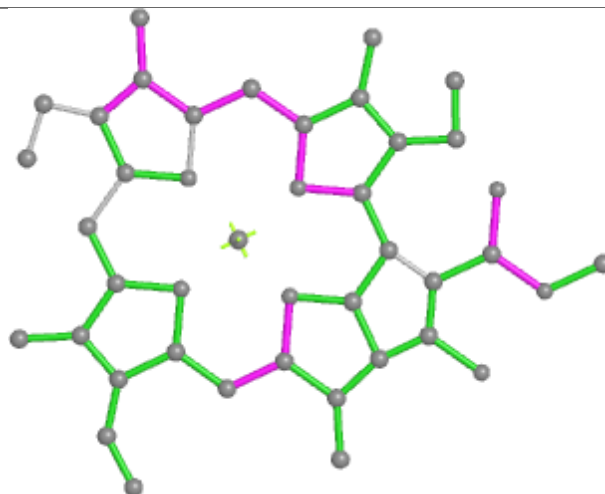
Ligand CLA L 302



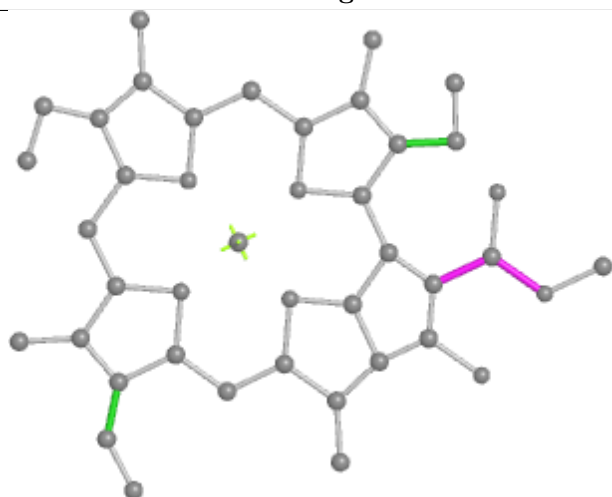
Ligand CLA A 816



Bond lengths



Bond angles

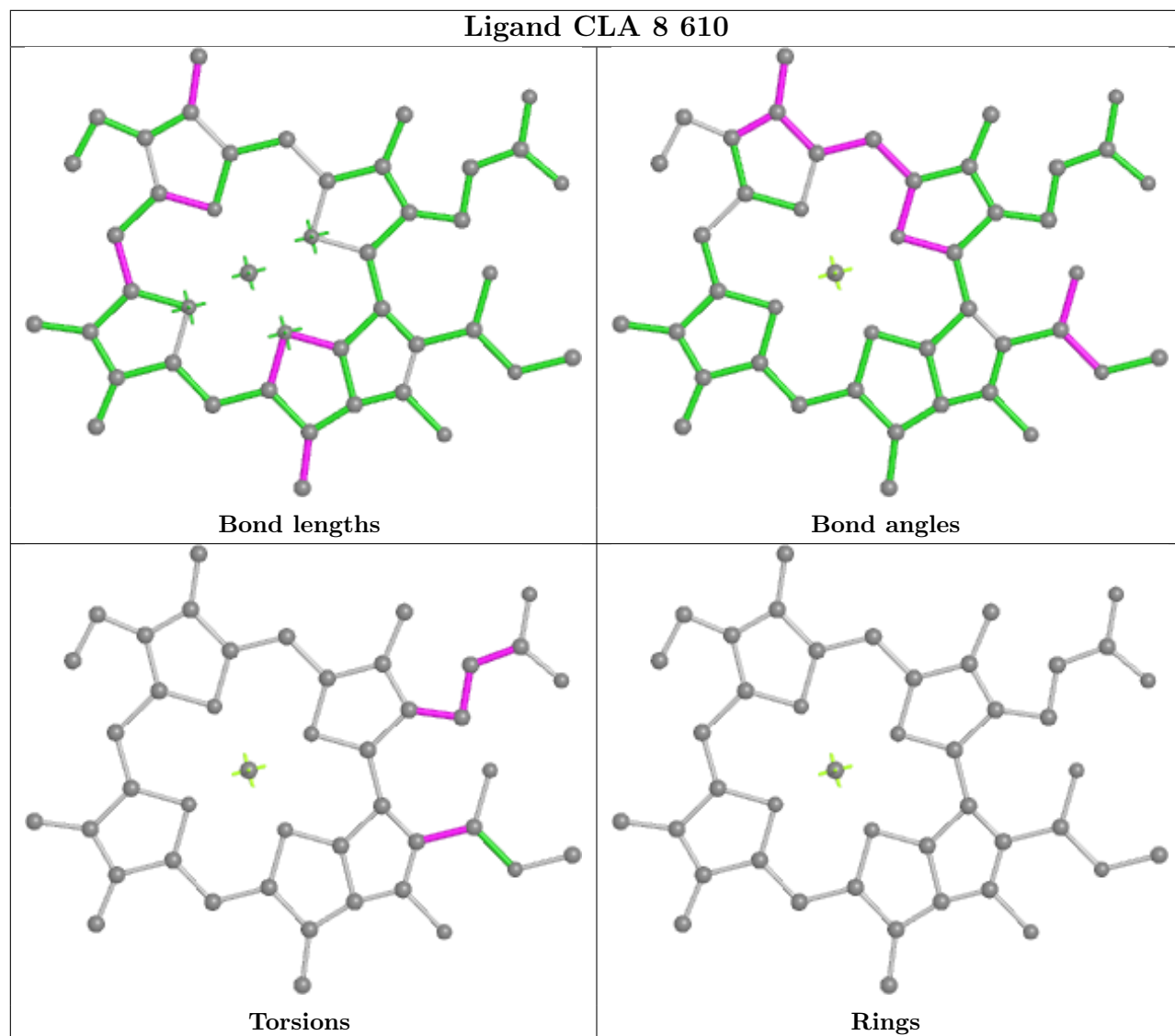


Torsions

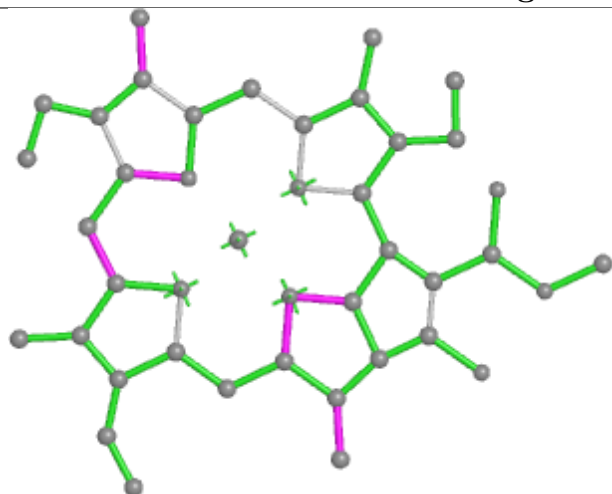


Rings

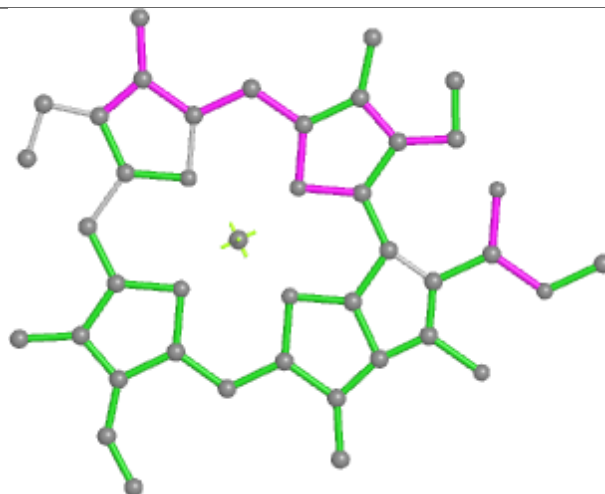
Ligand CLA 8 610



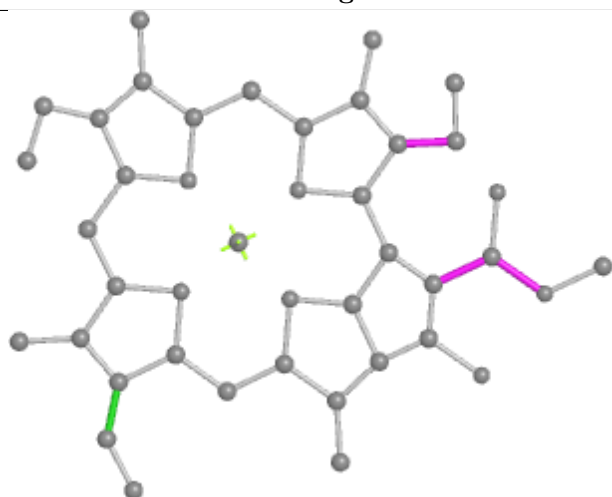
Ligand CLA 6 609



Bond lengths



Bond angles

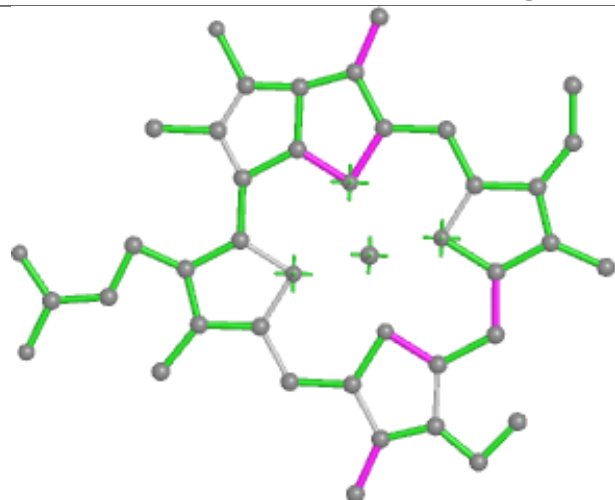


Torsions

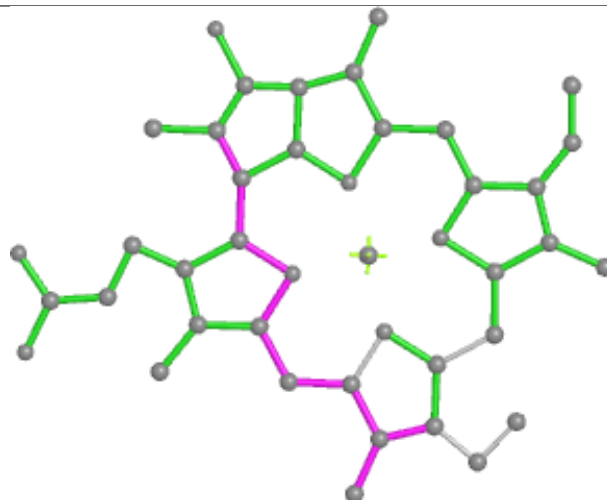


Rings

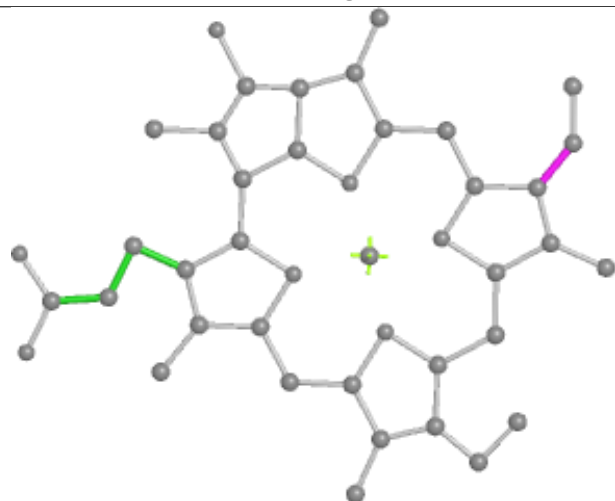
Ligand CLA 2 610



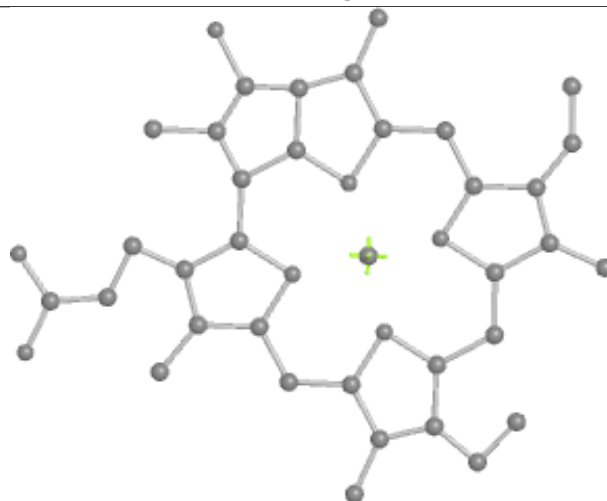
Bond lengths



Bond angles

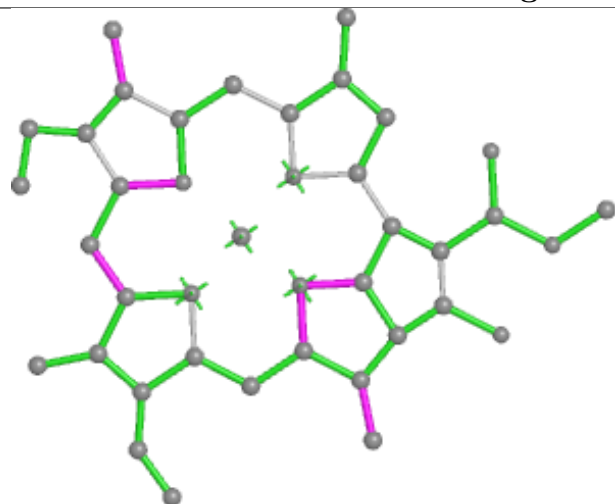


Torsions

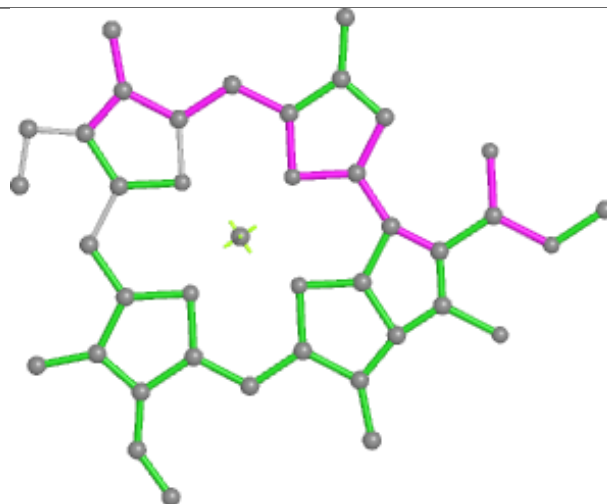


Rings

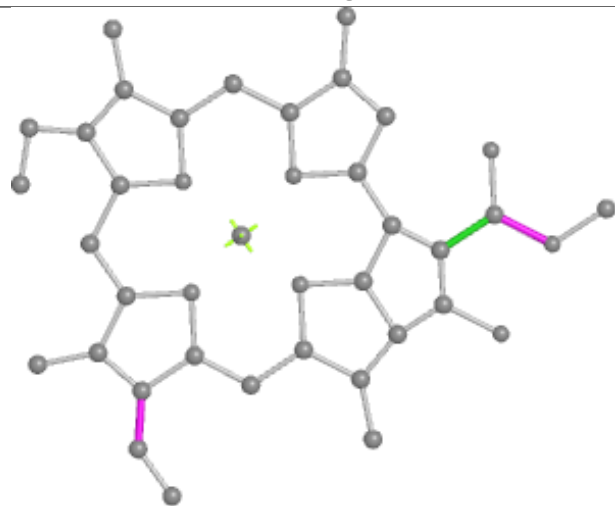
Ligand CLA 5 605



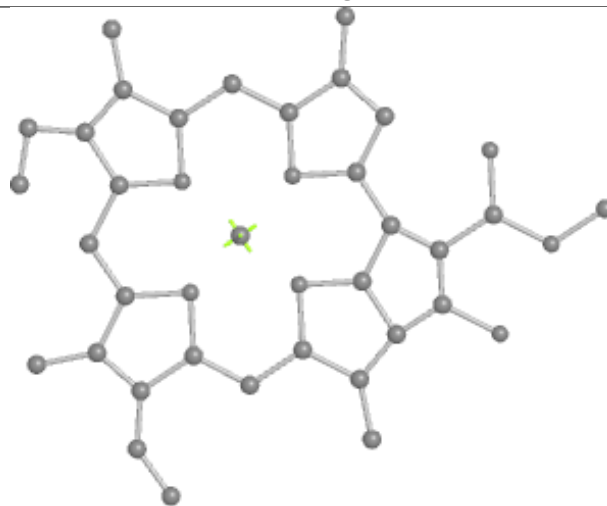
Bond lengths



Bond angles

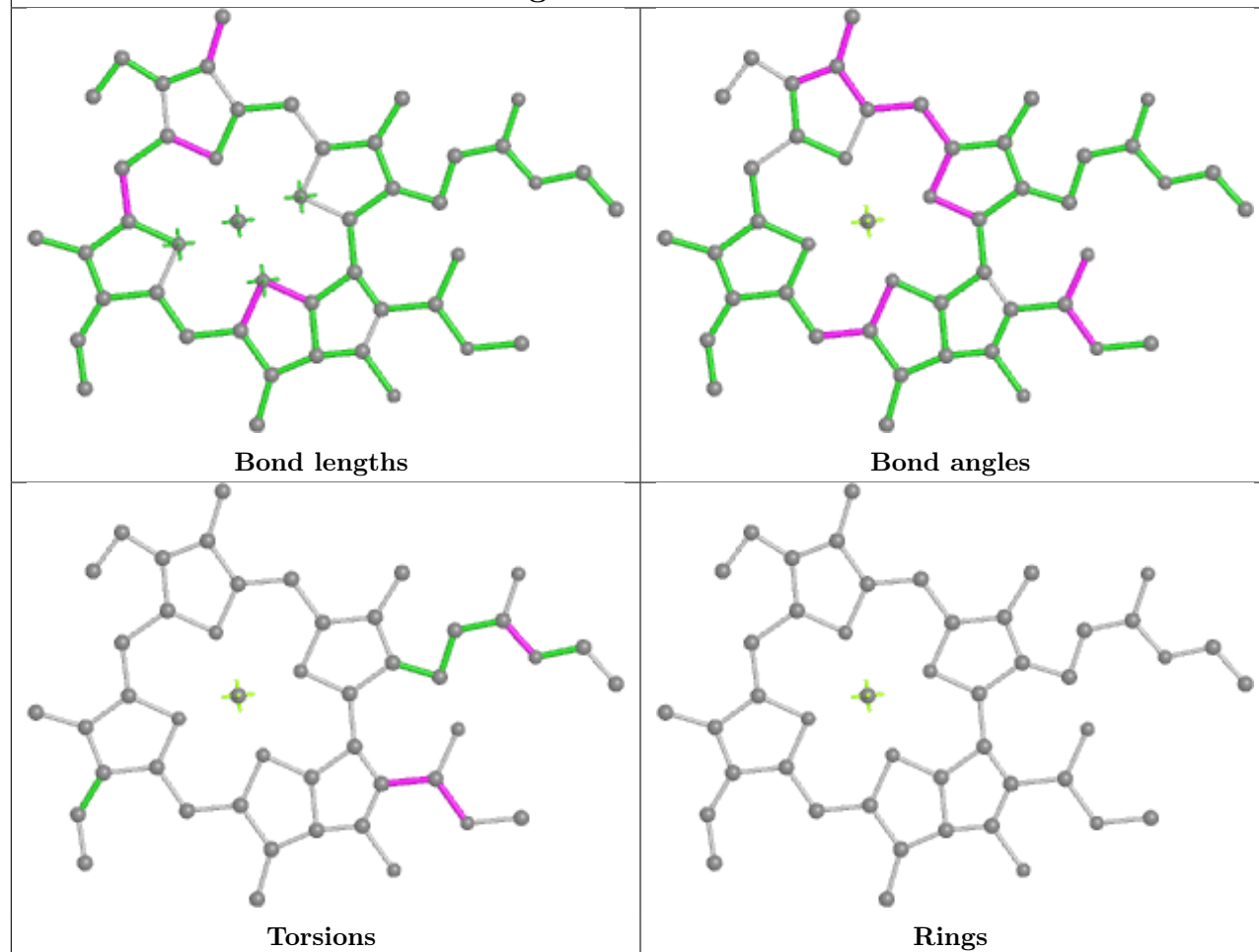


Torsions

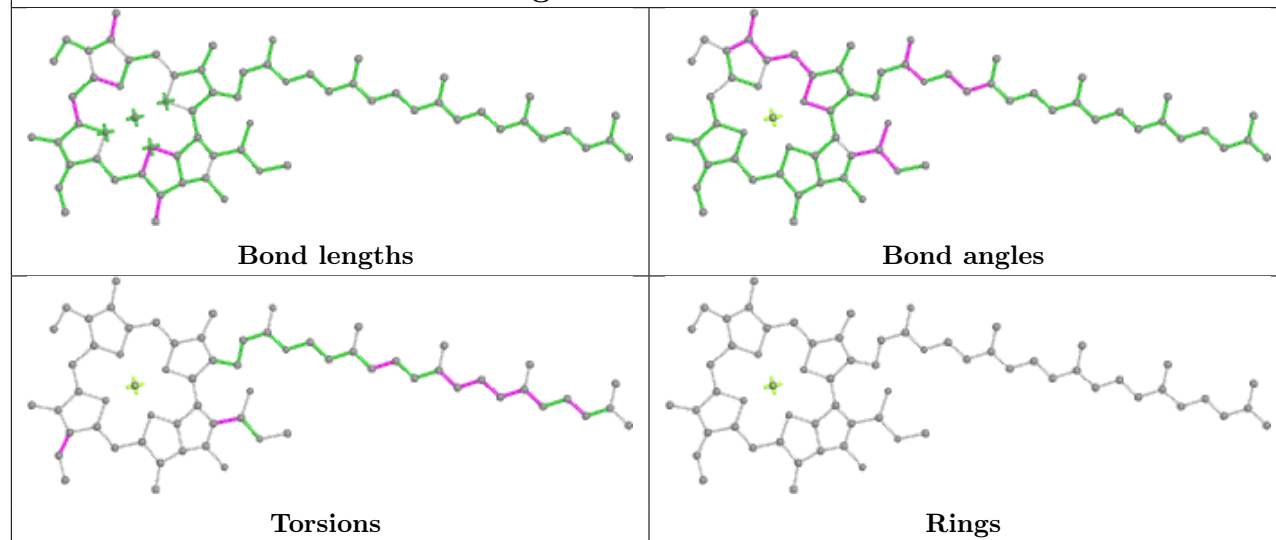


Rings

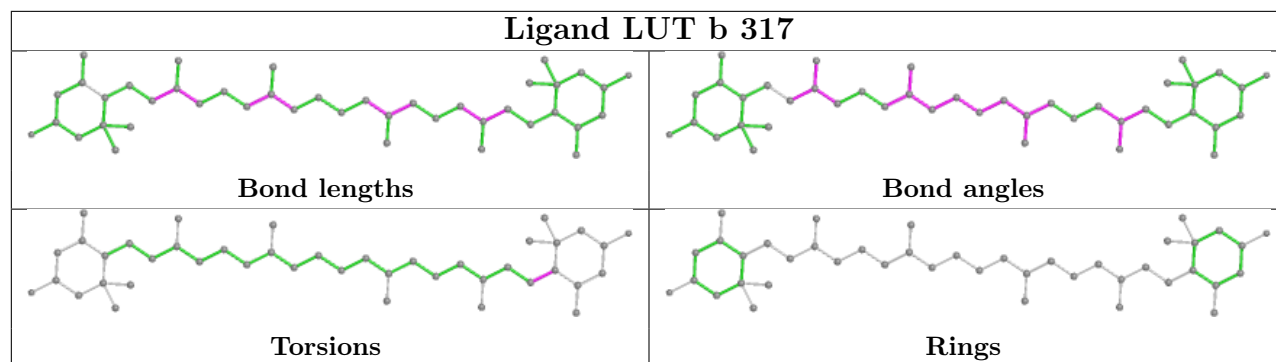
Ligand CLA a 611



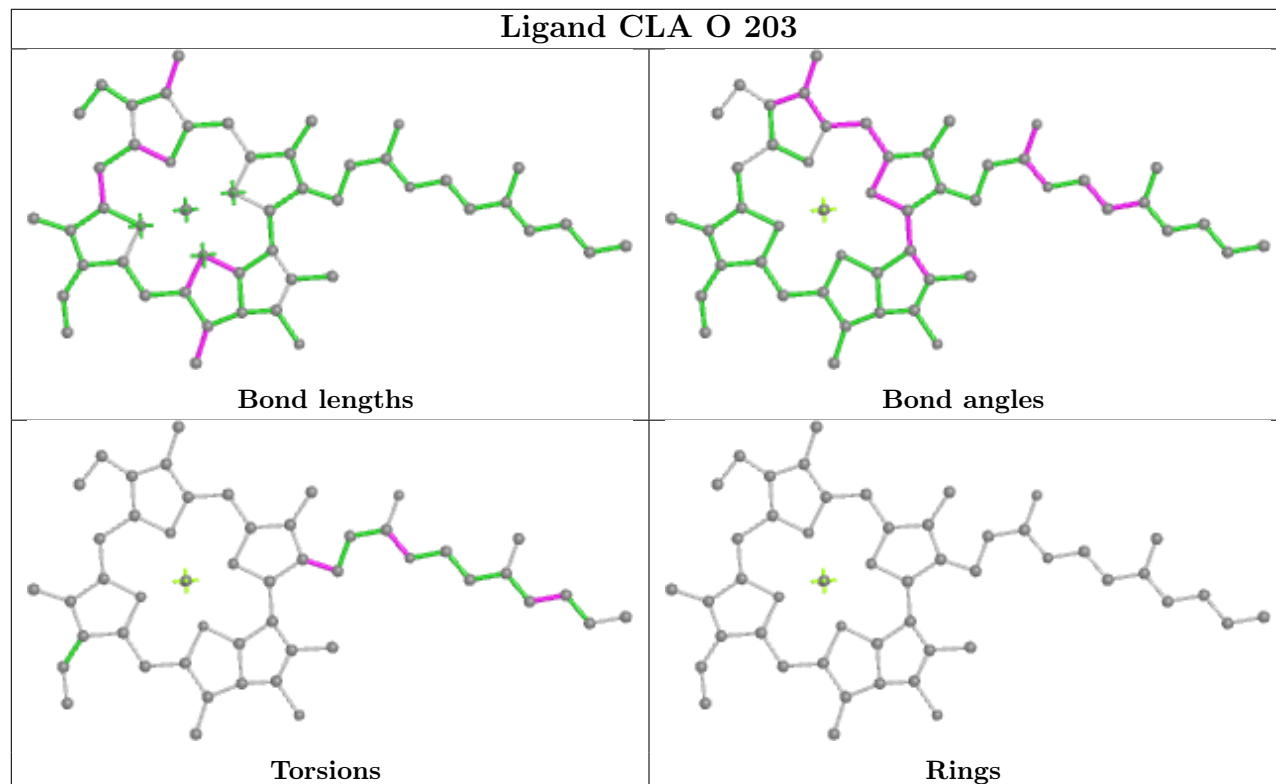
Ligand CLA B 823



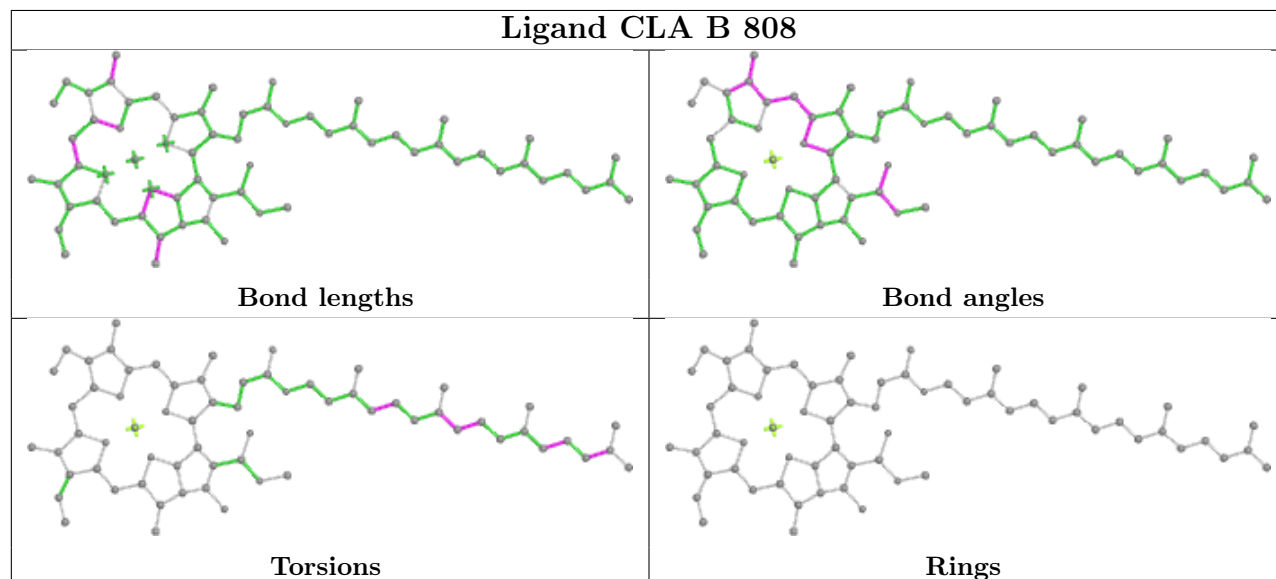
Ligand LUT b 317

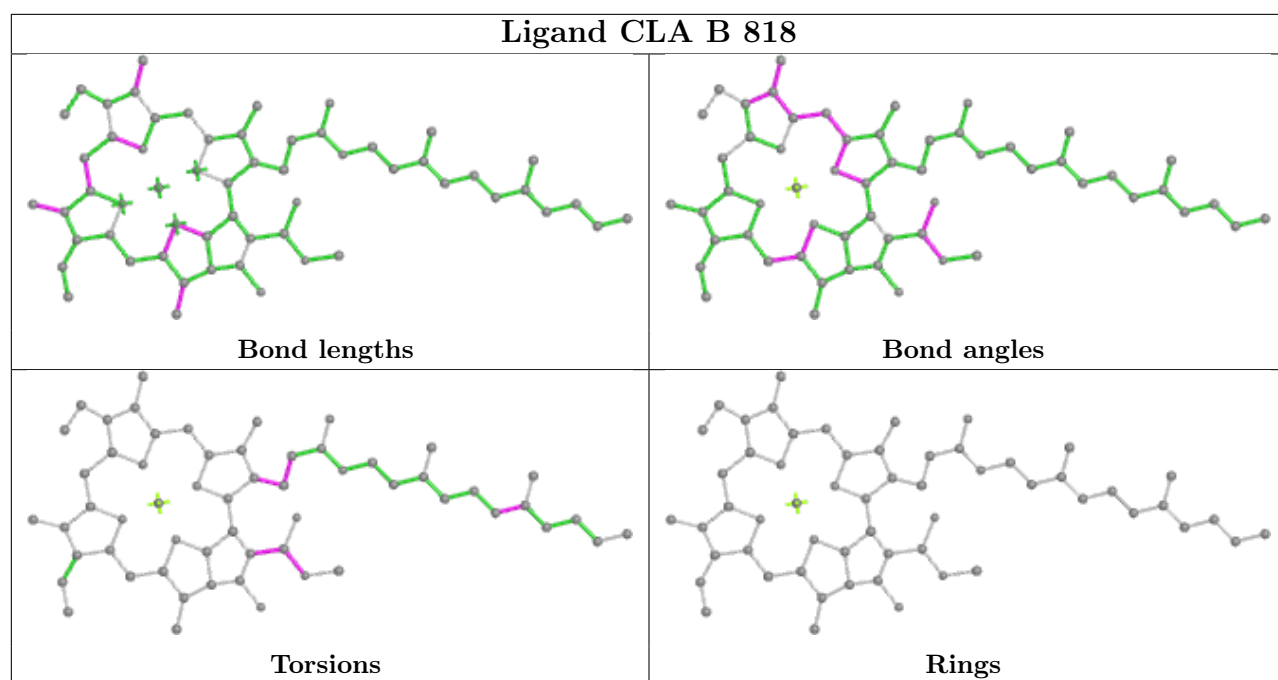


Ligand CLA O 203

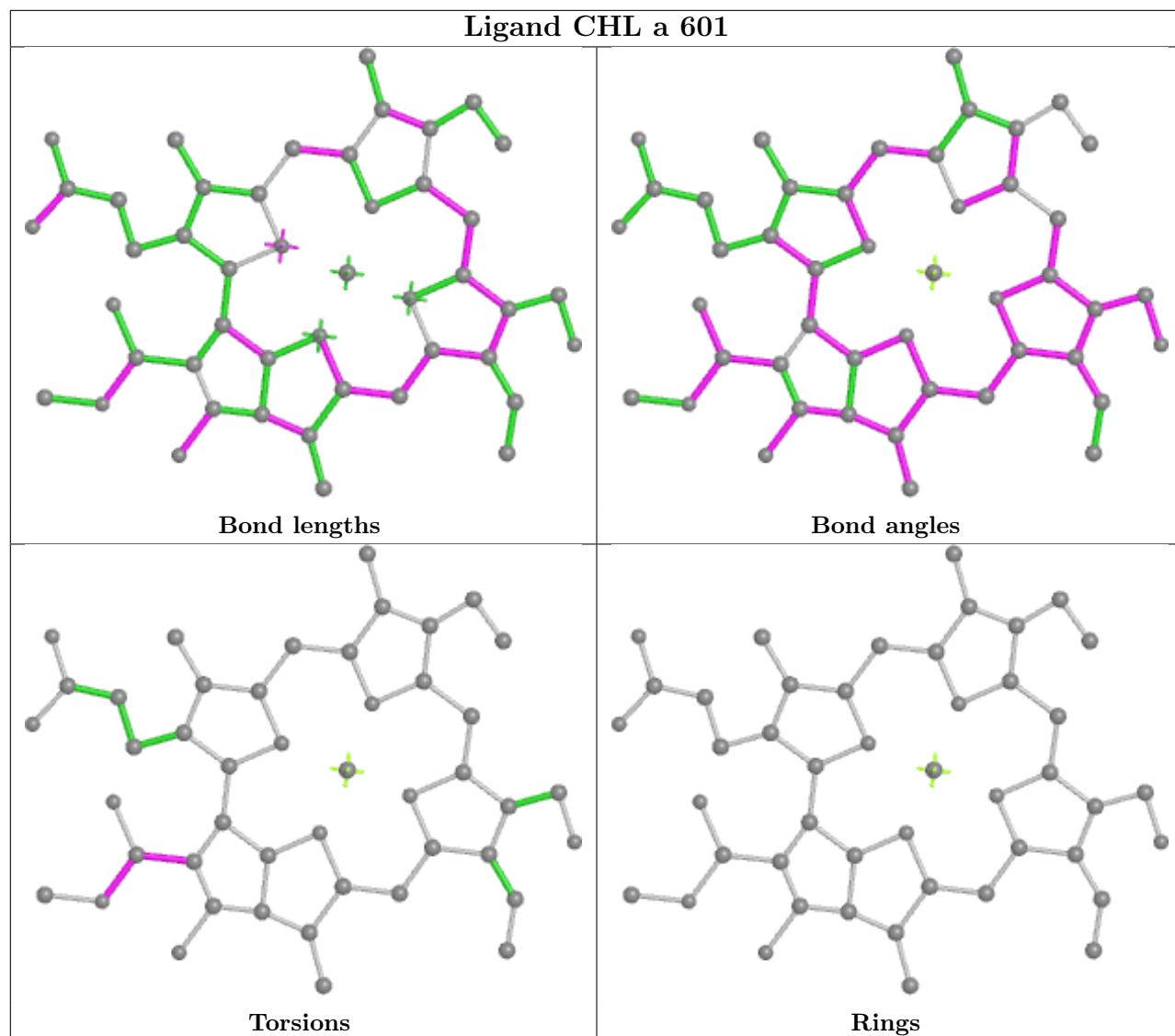


Ligand CLA B 808

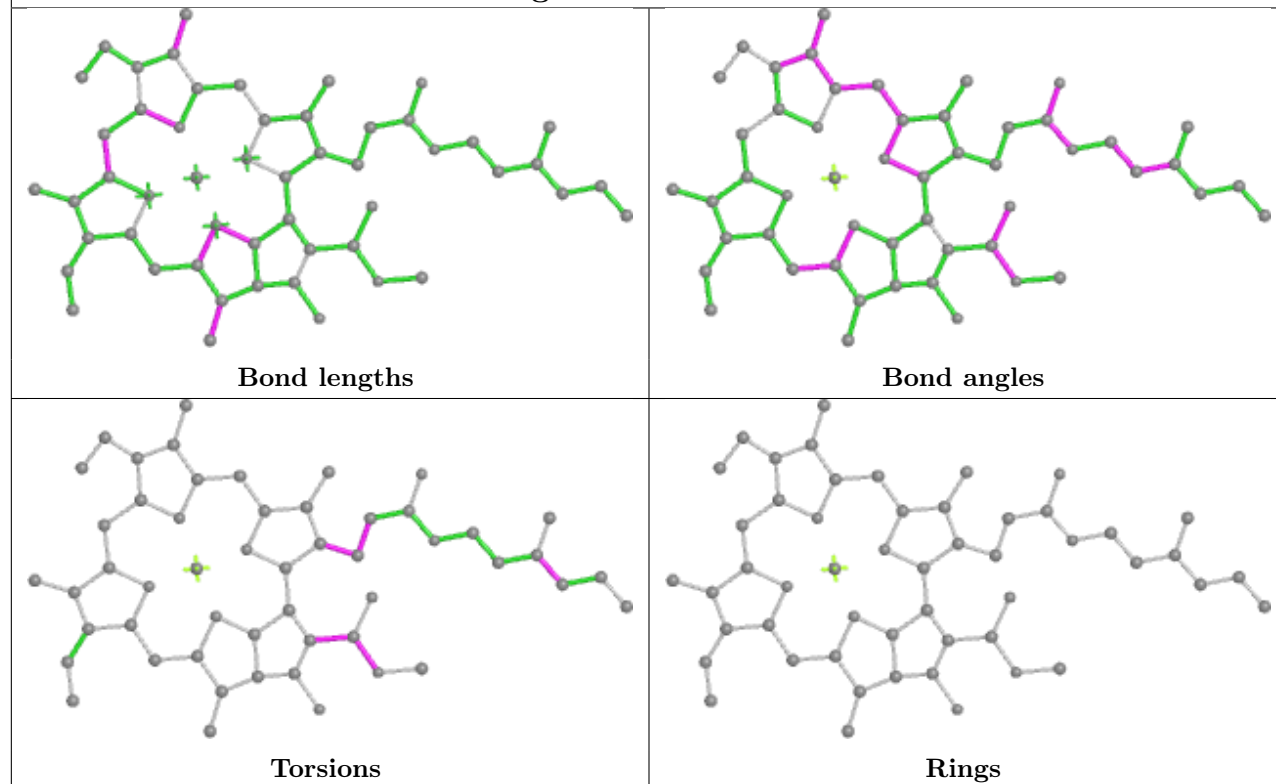




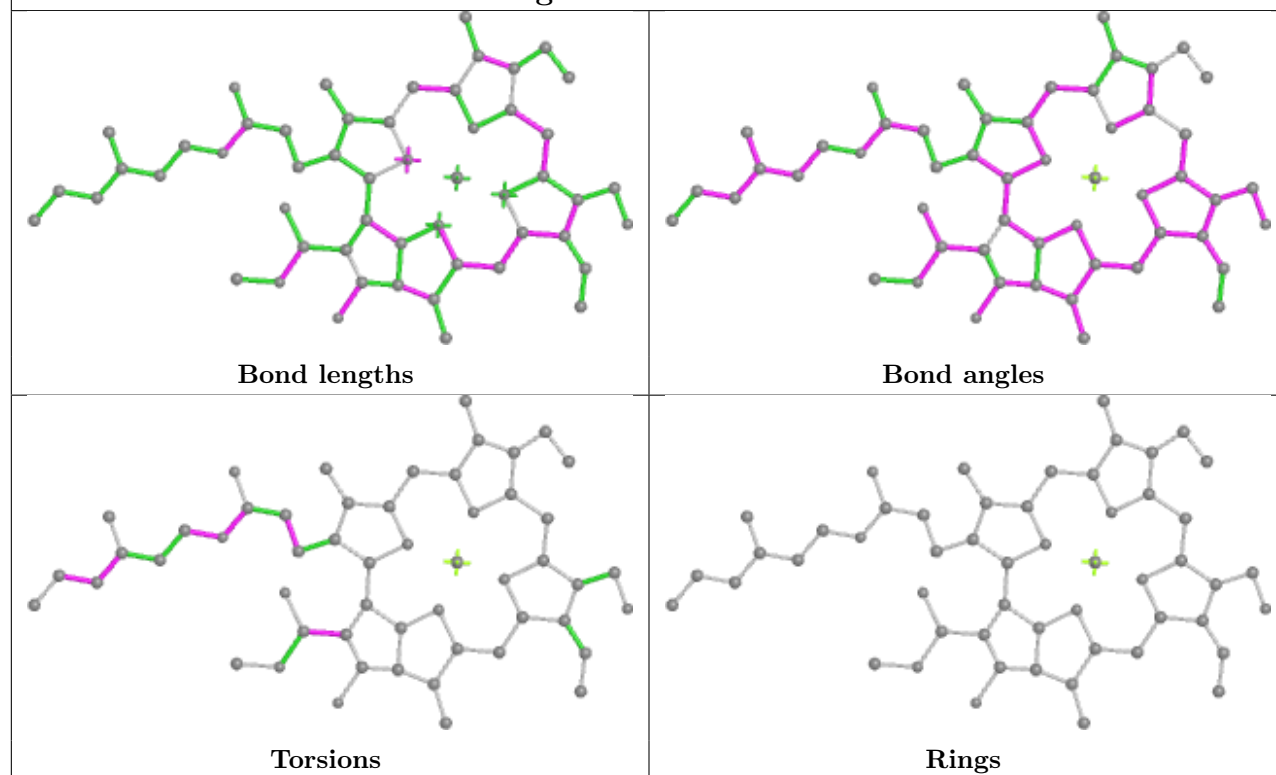
Ligand CHL a 601



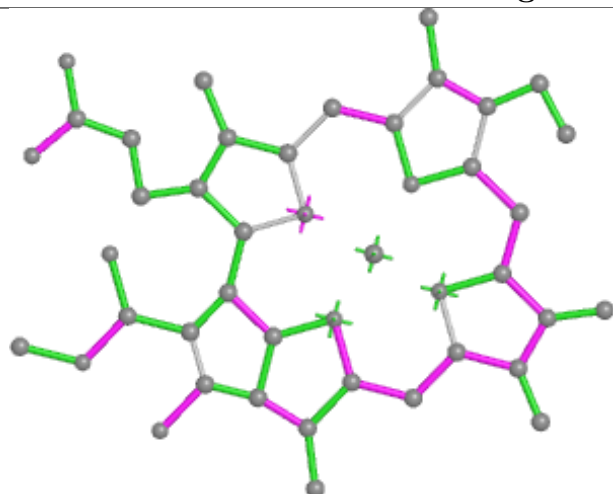
Ligand CLA A 803



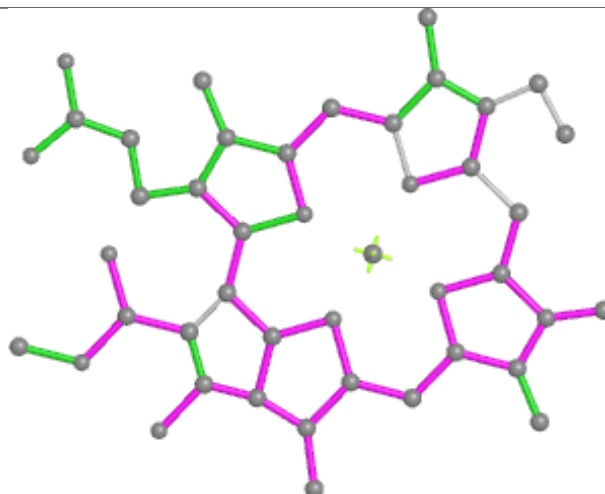
Ligand CHL 2 601



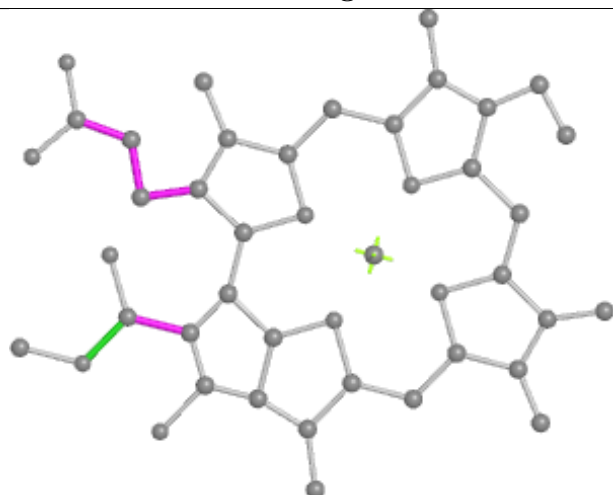
Ligand CHL 6 601



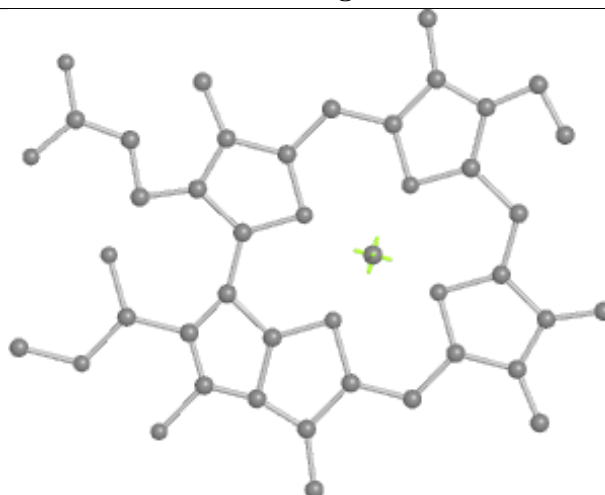
Bond lengths



Bond angles

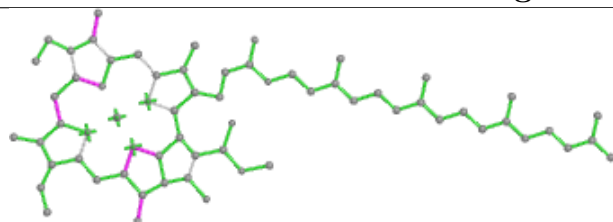


Torsions

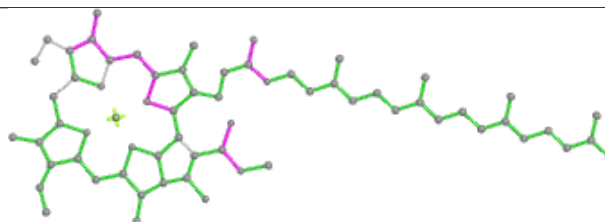


Rings

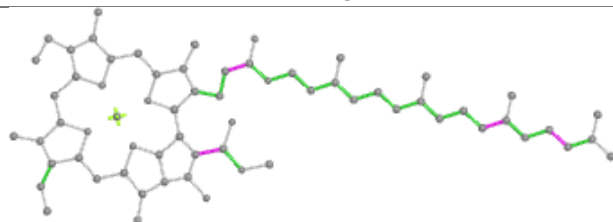
Ligand CLA B 840



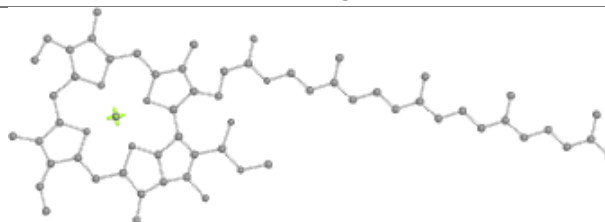
Bond lengths



Bond angles

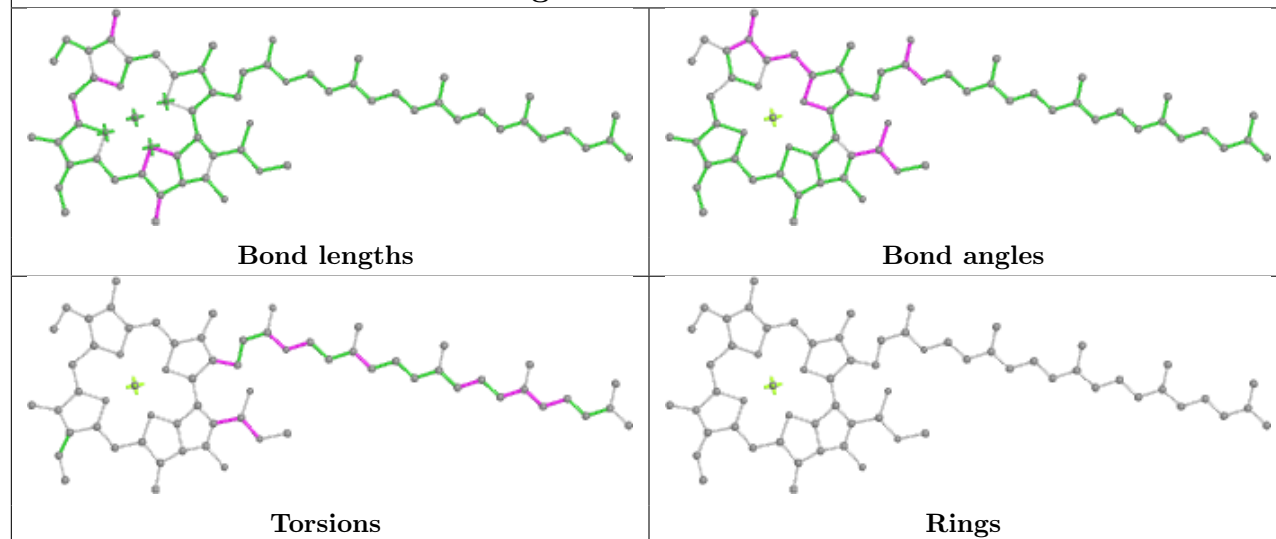


Torsions

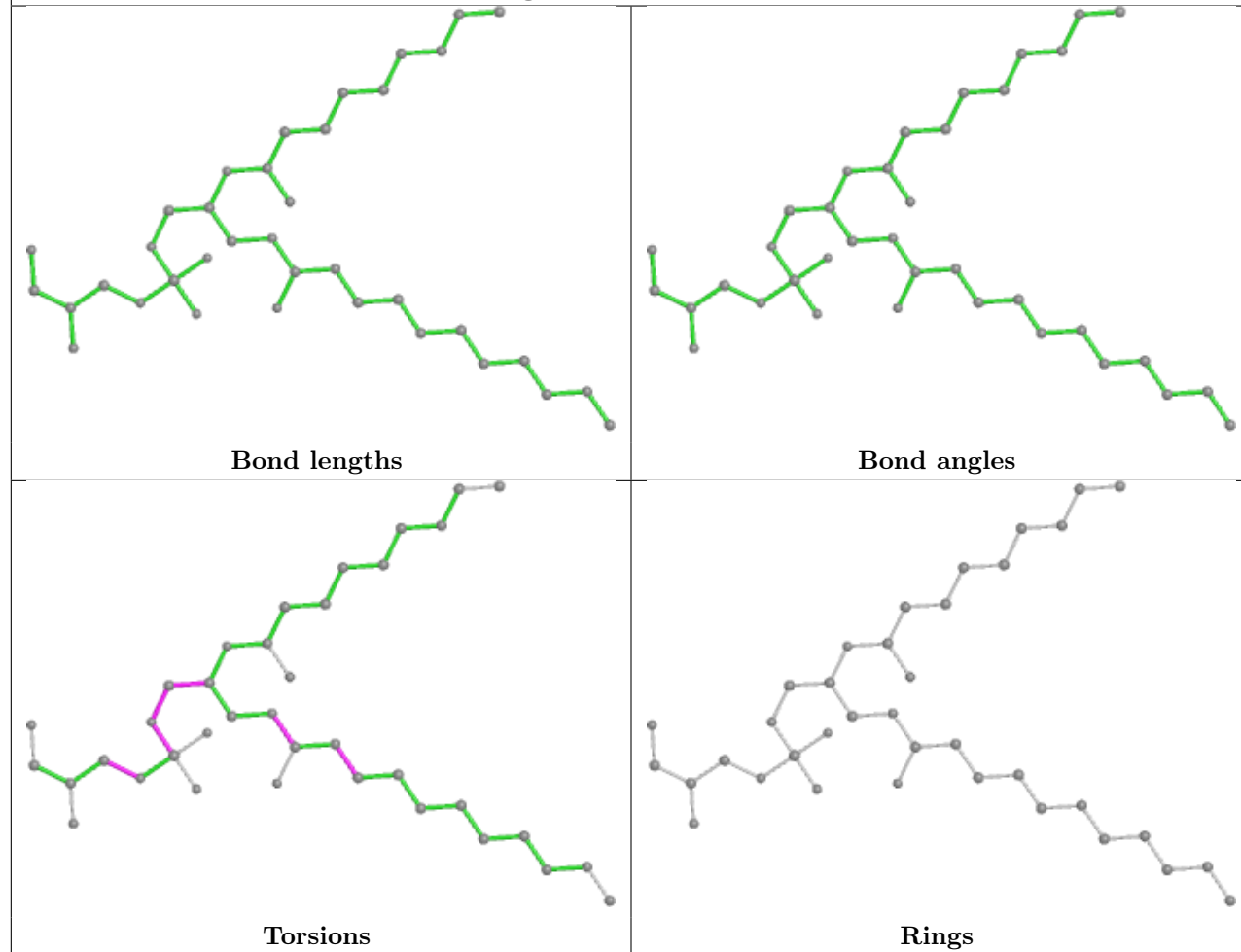


Rings

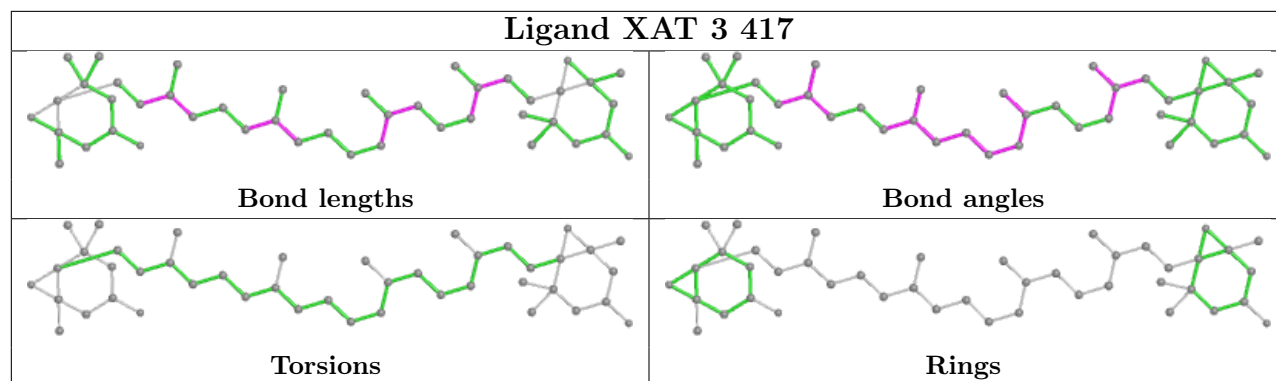
Ligand CLA A 819



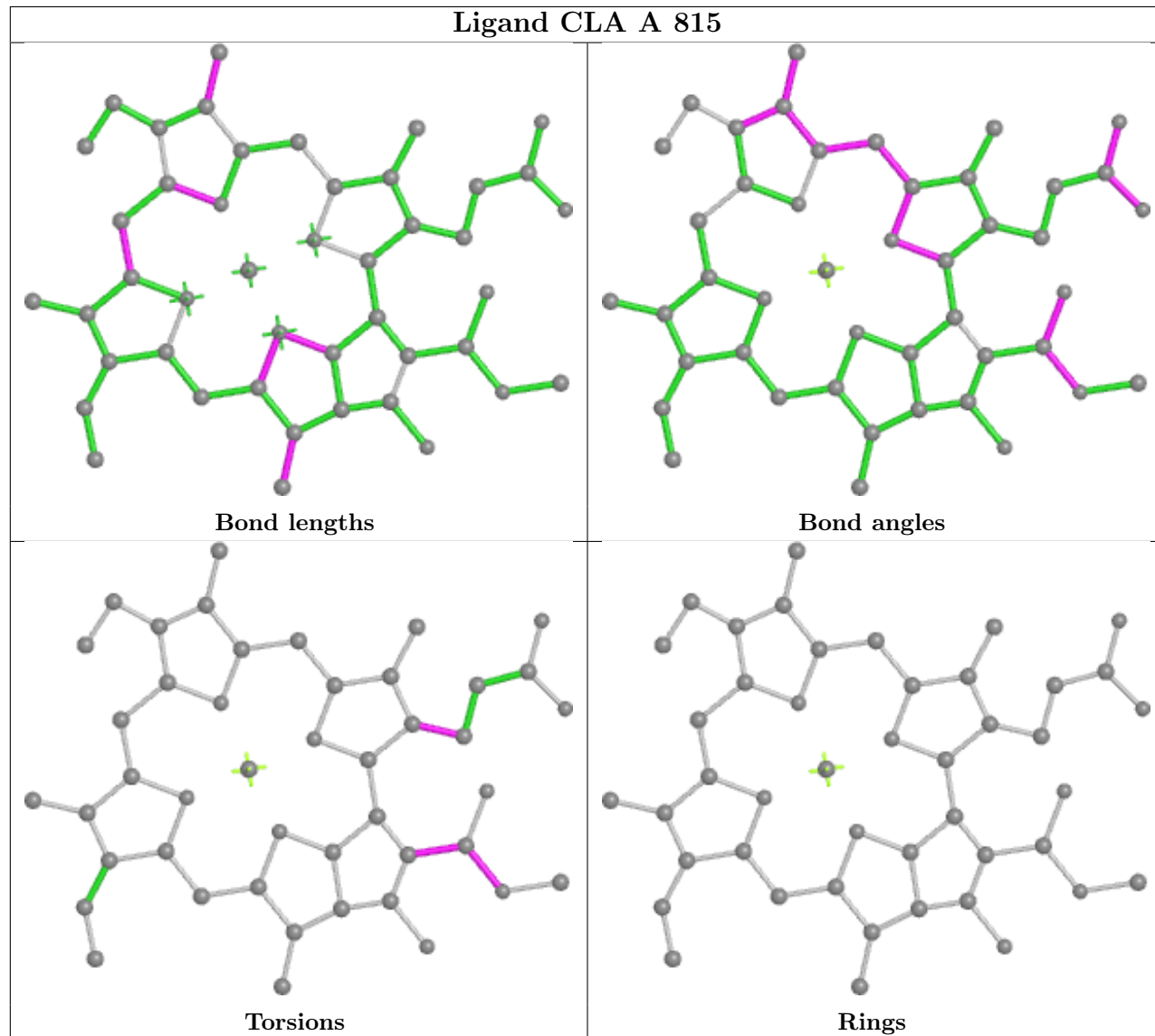
Ligand LHG 8 617



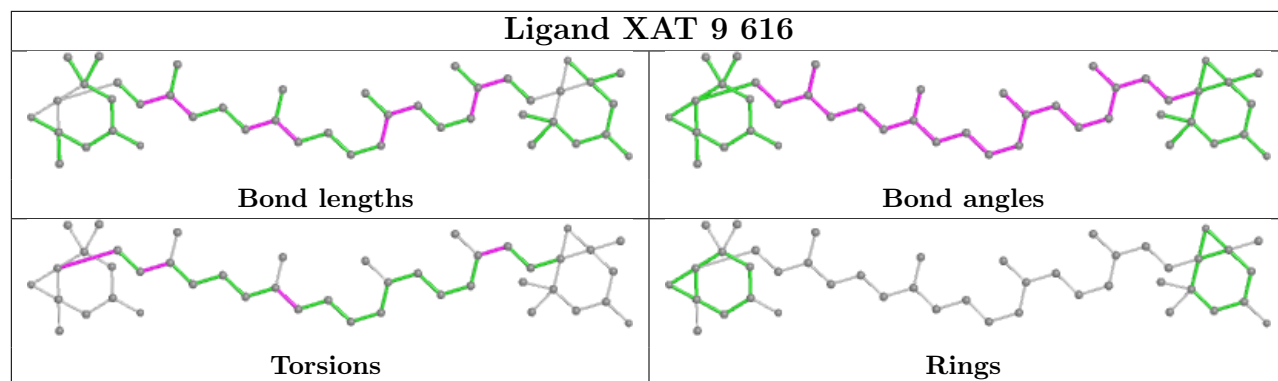
Ligand XAT 3 417



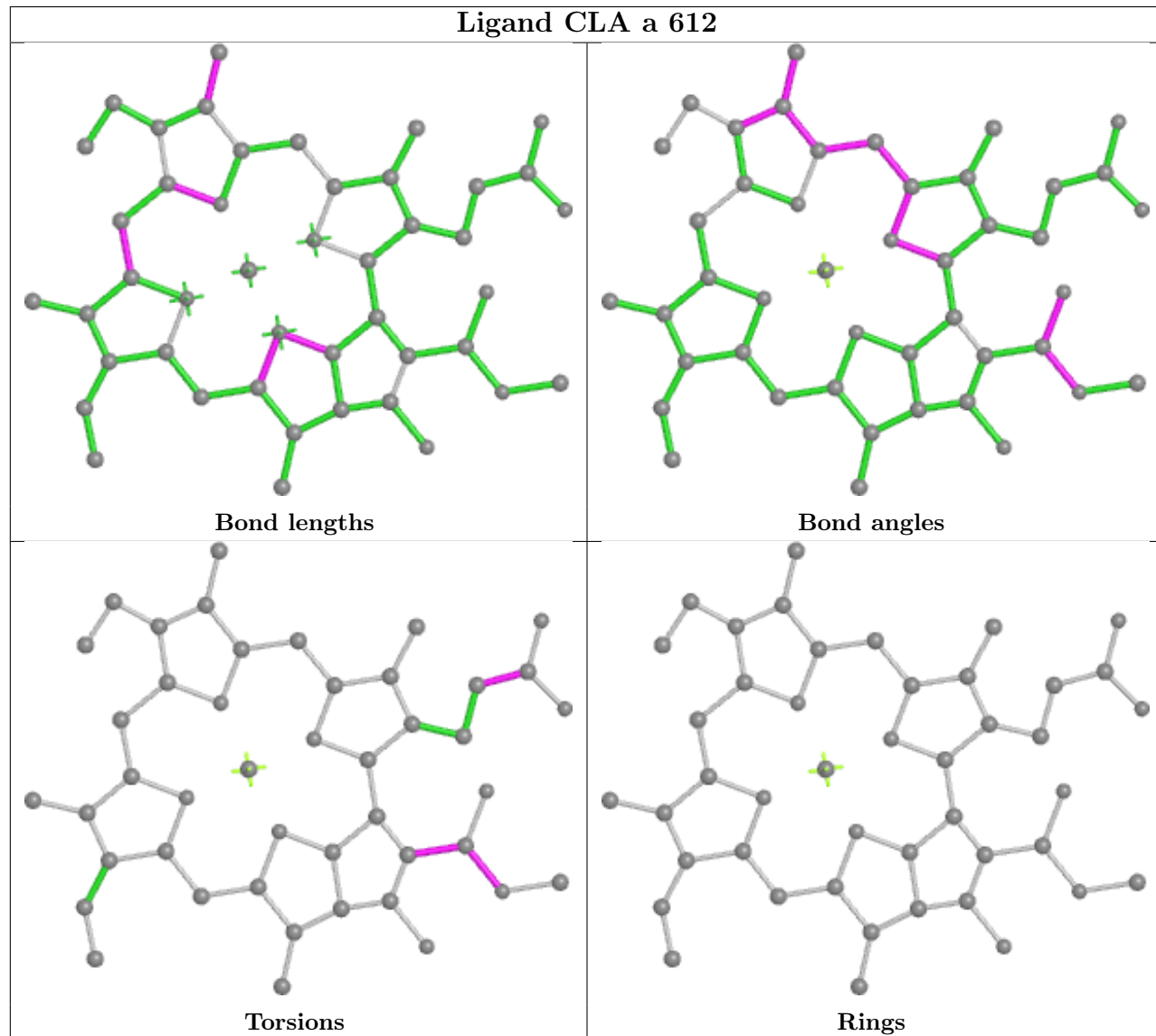
Ligand CLA A 815



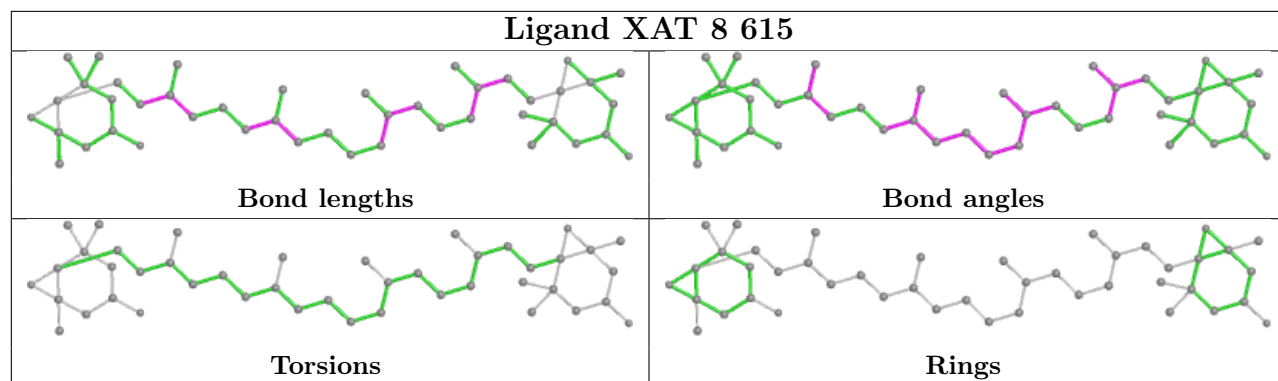
Ligand XAT 9 616



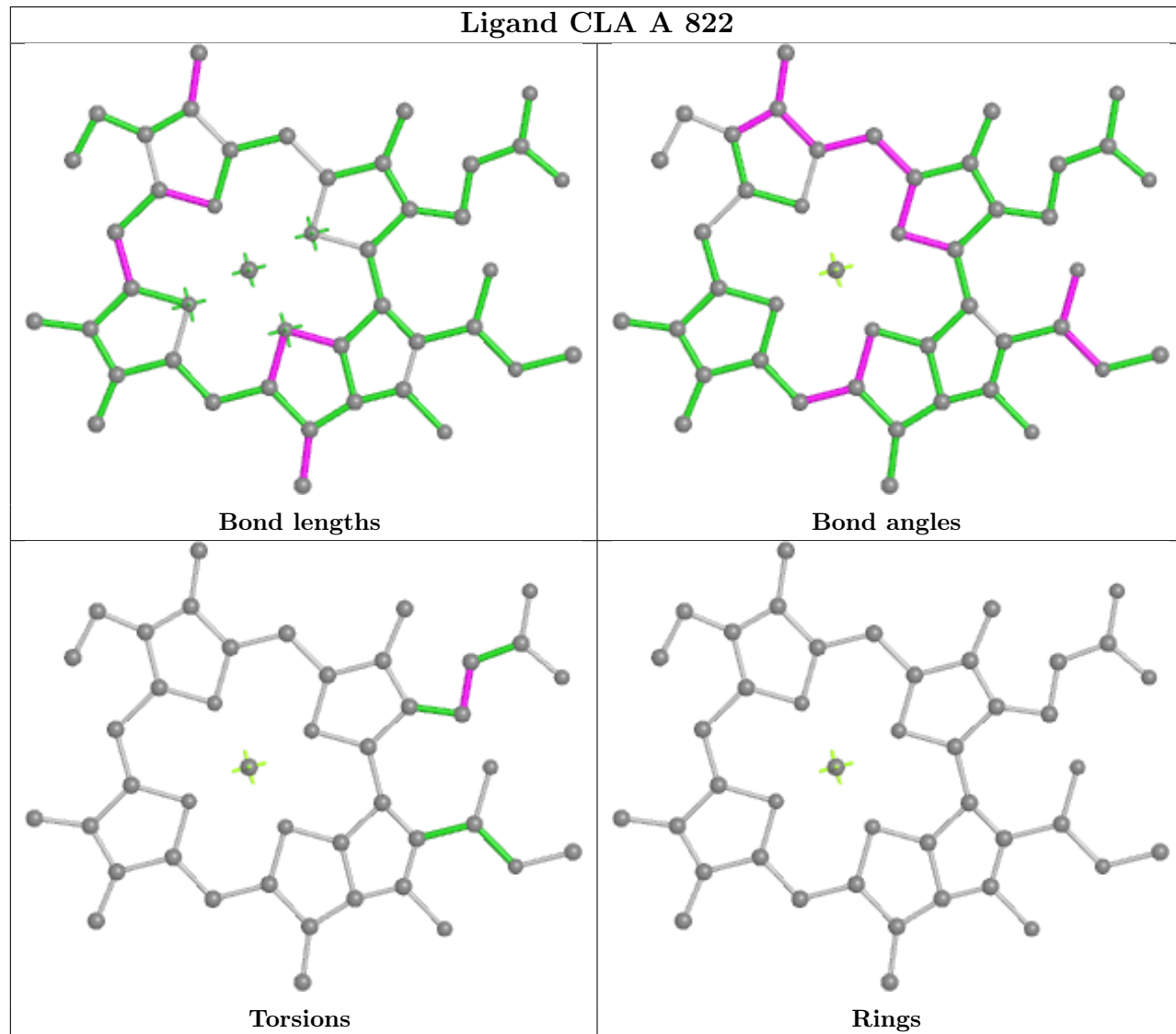
Ligand CLA a 612

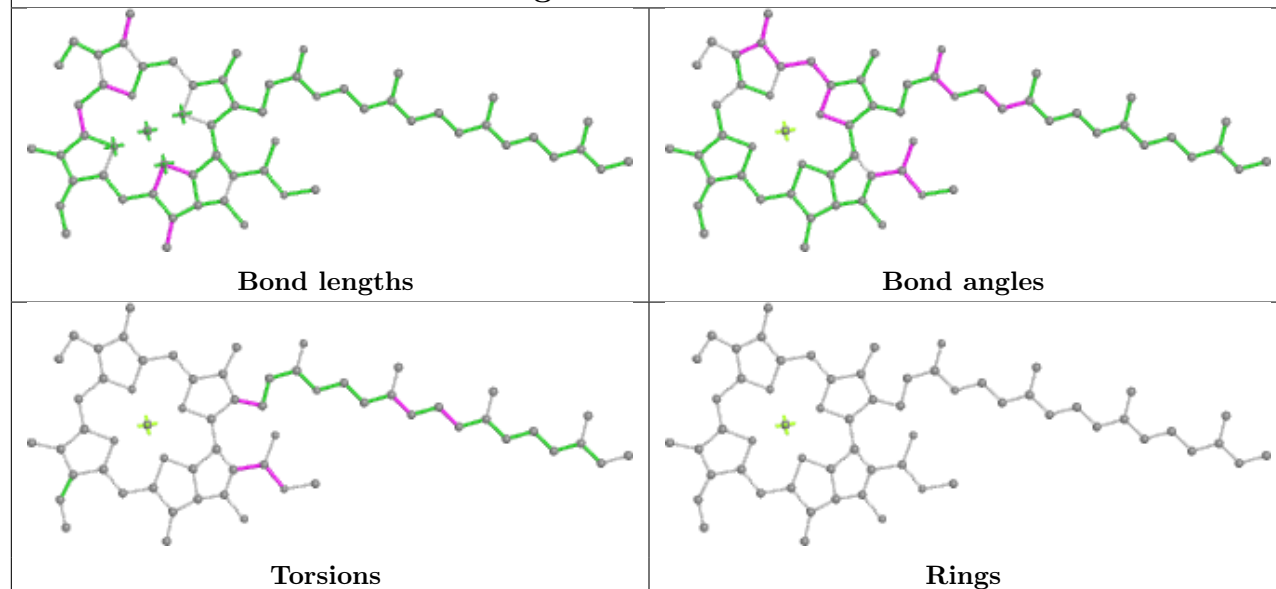
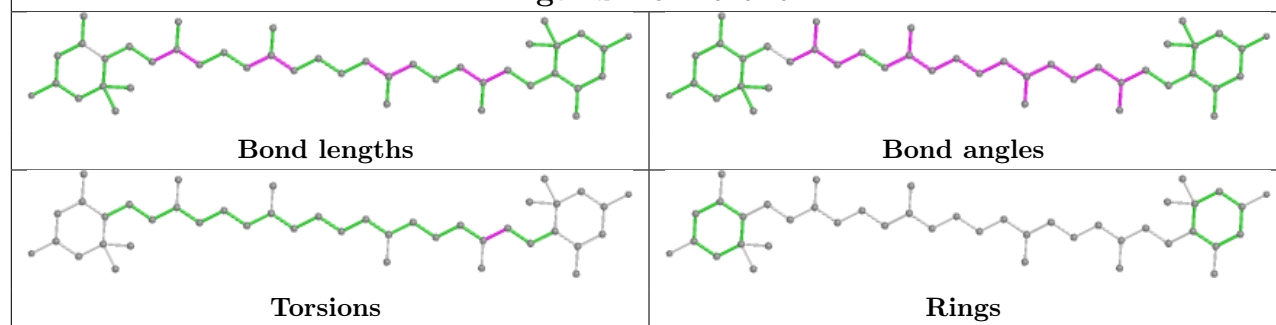


Ligand XAT 8 615

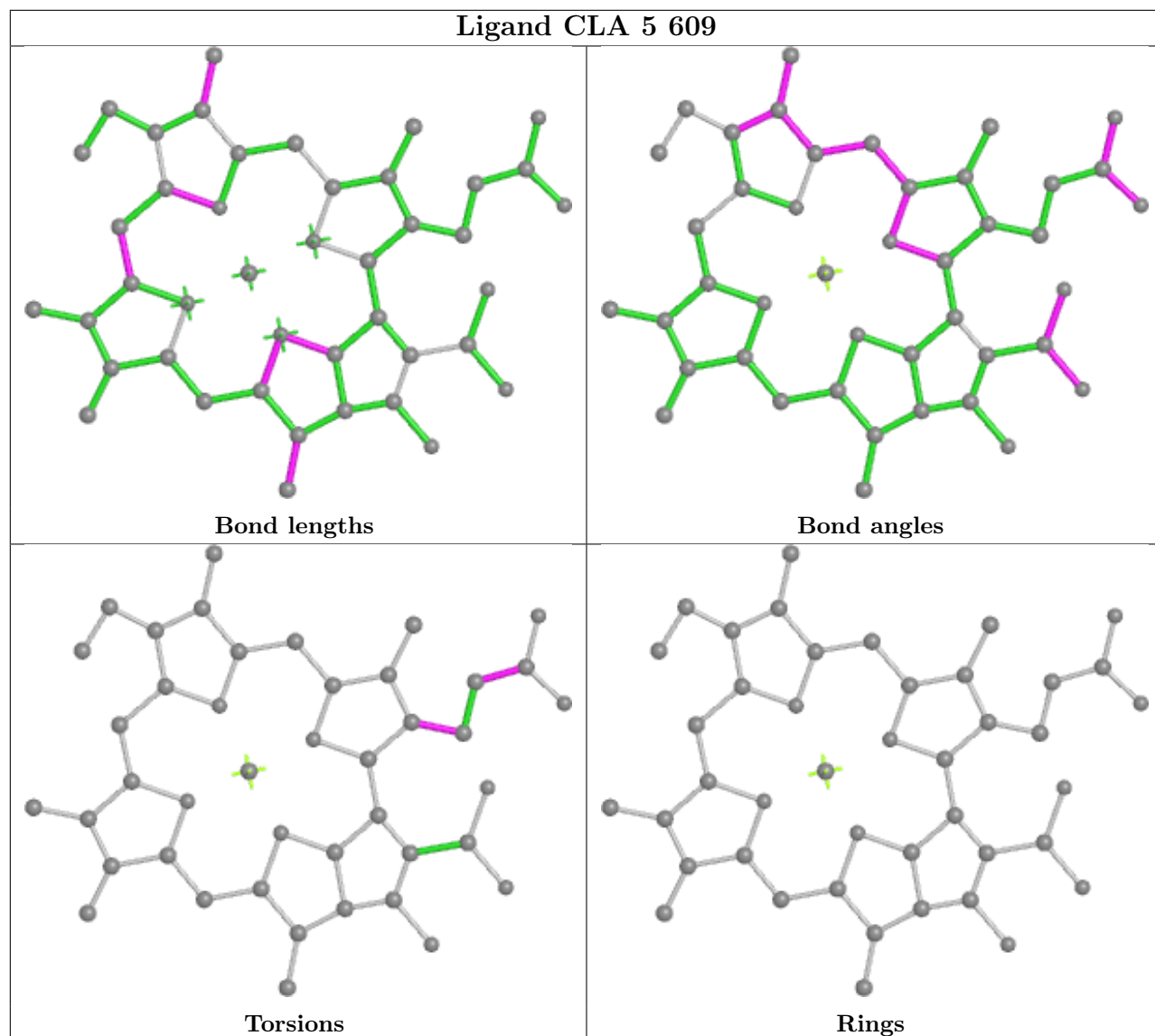


Ligand CLA A 822

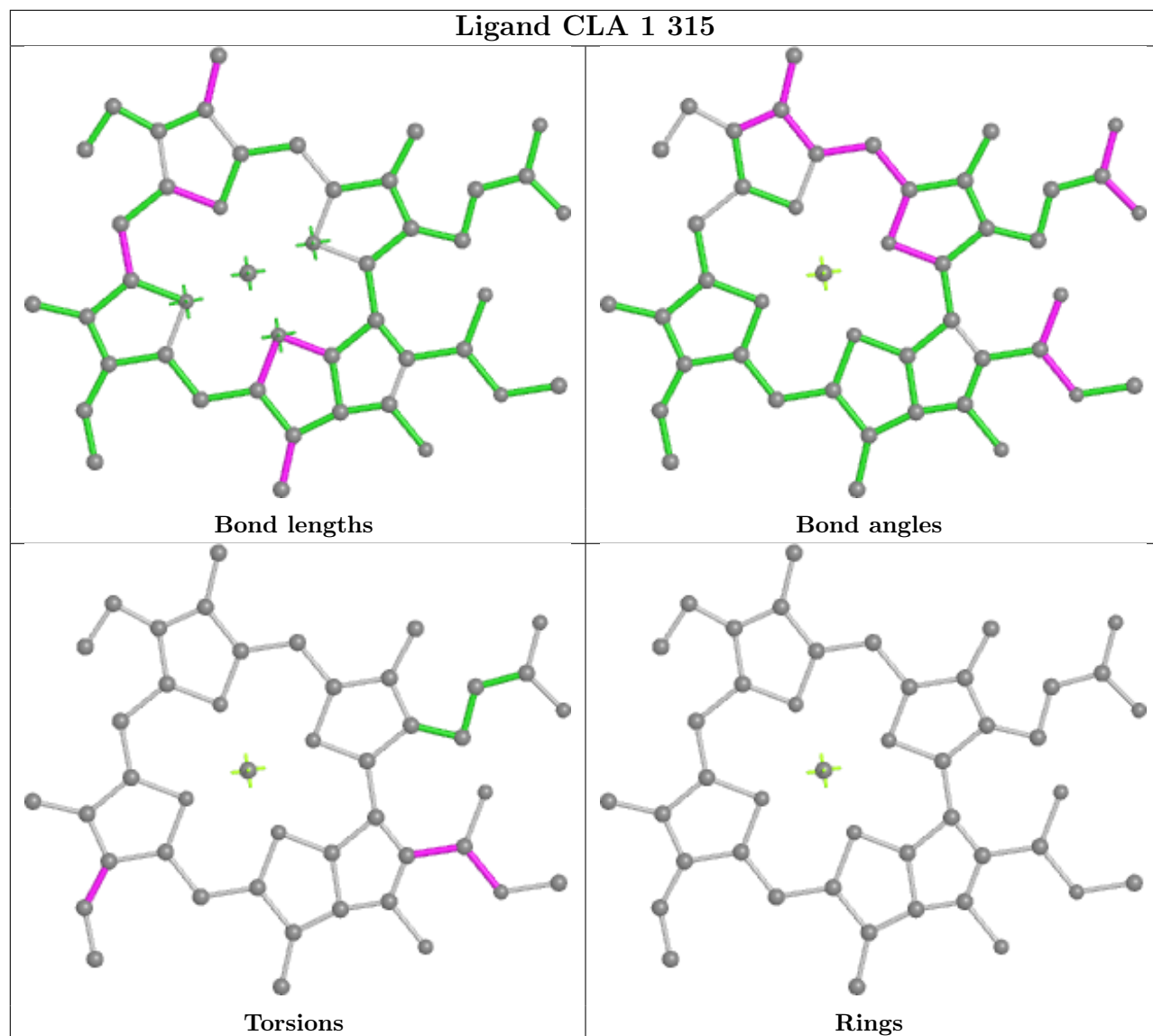


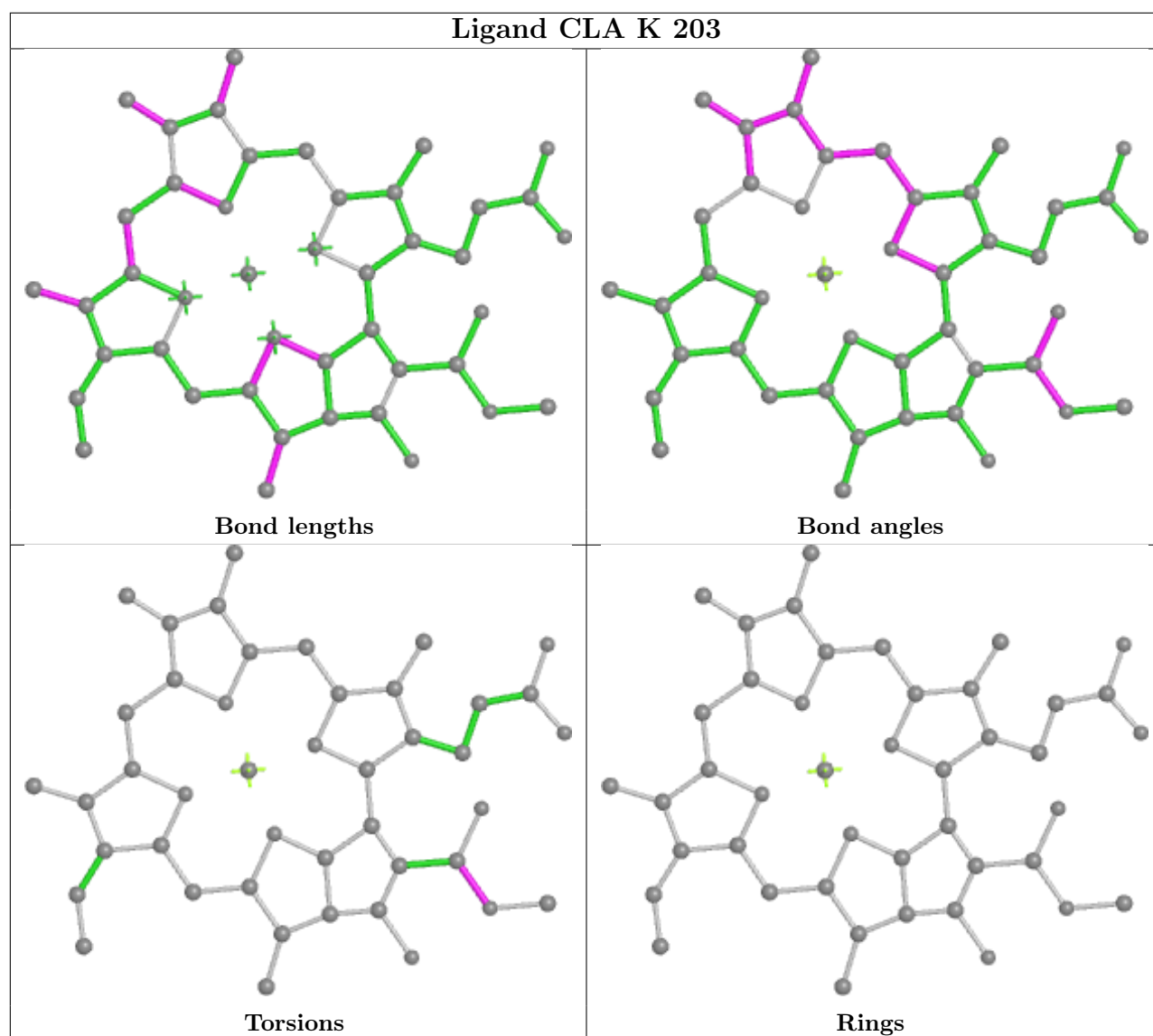
Ligand CLA F 302**Ligand LUT 6 616**

Ligand CLA 5 609



Ligand CLA 1 315





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.

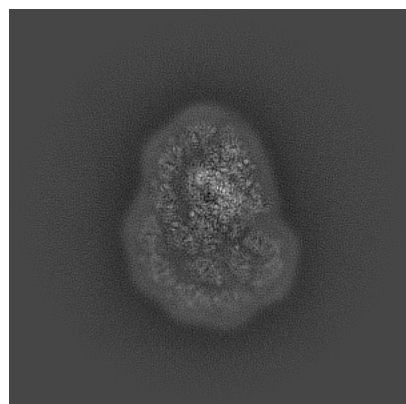
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33401. These allow visual inspection of the internal detail of the map and identification of artifacts.

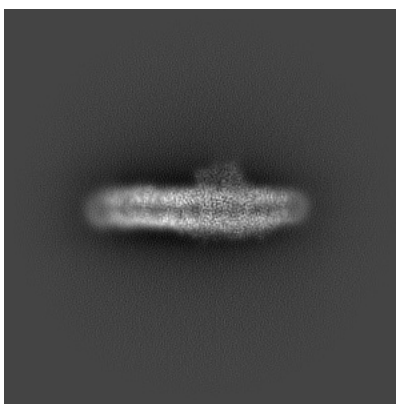
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

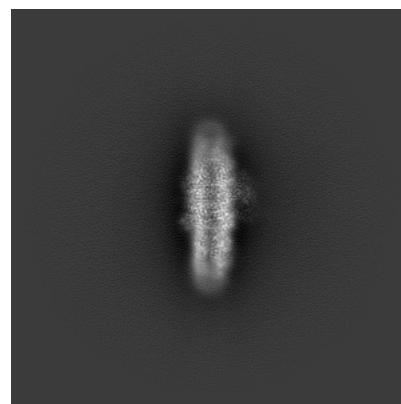
6.1.1 Primary map



X

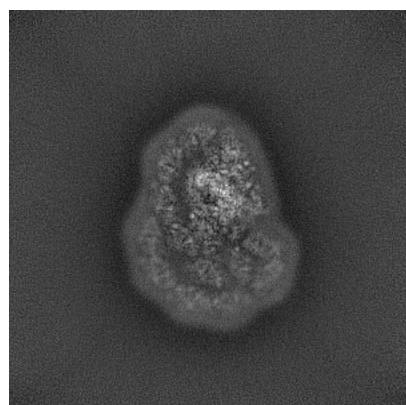


Y

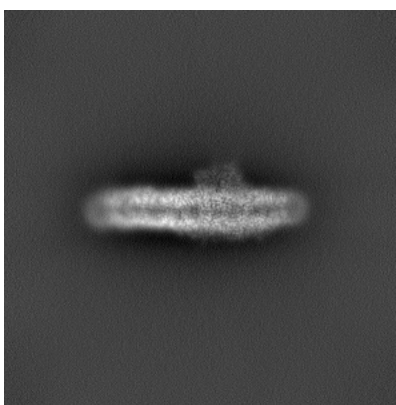


Z

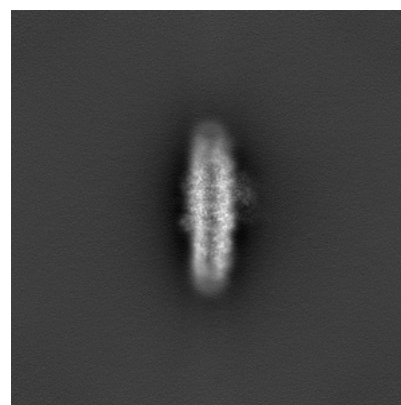
6.1.2 Raw map



X



Y

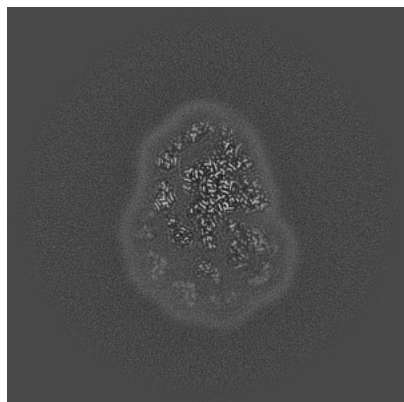


Z

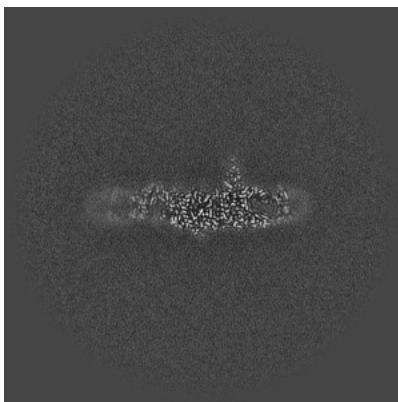
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

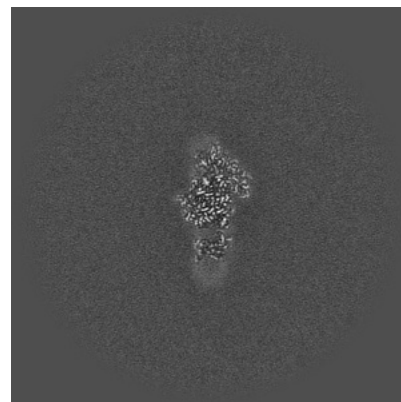
6.2.1 Primary map



X Index: 240

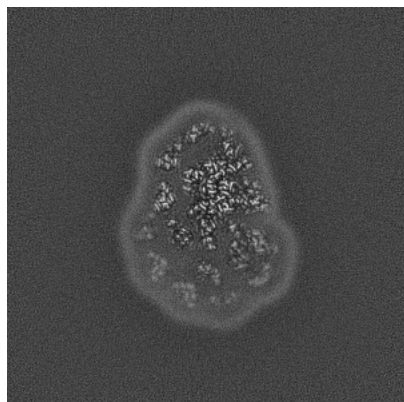


Y Index: 240

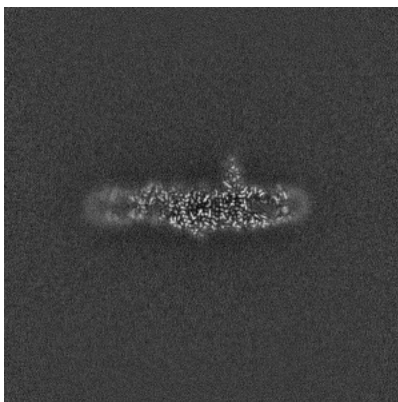


Z Index: 240

6.2.2 Raw map



X Index: 240



Y Index: 240

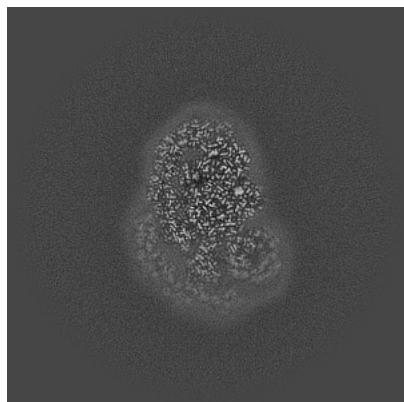


Z Index: 240

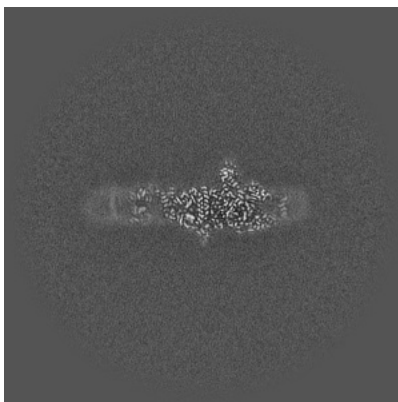
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

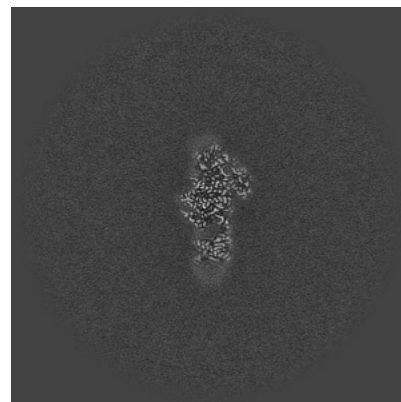
6.3.1 Primary map



X Index: 252

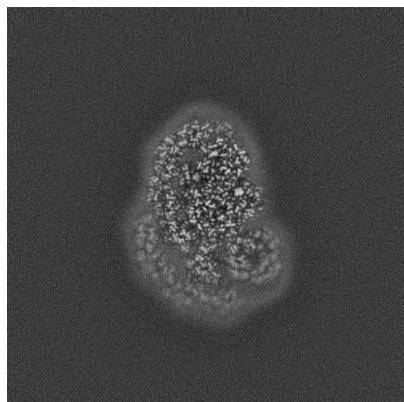


Y Index: 247

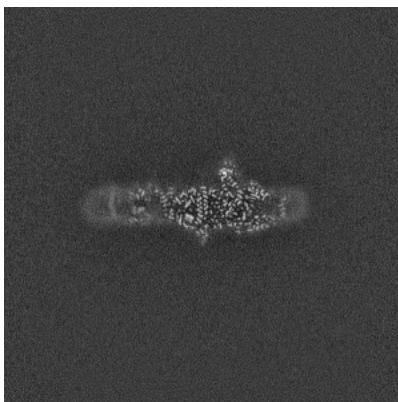


Z Index: 243

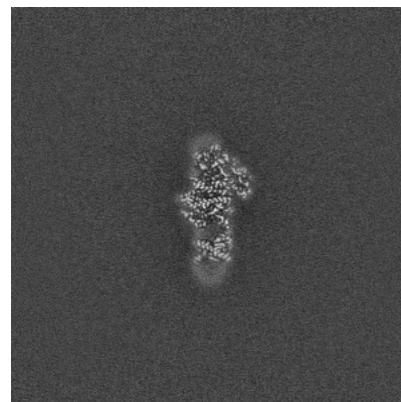
6.3.2 Raw map



X Index: 252



Y Index: 247

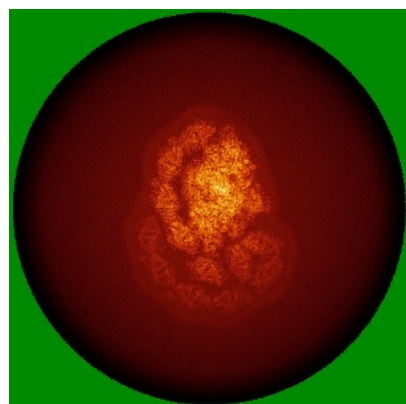


Z Index: 242

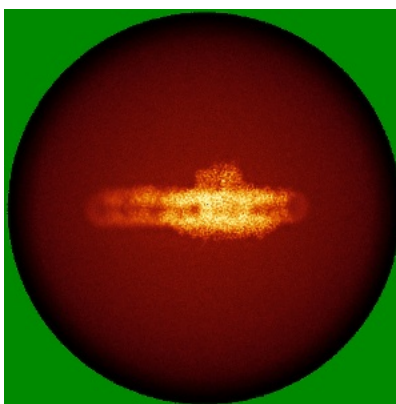
The images above show the largest variance slices of the map in three orthogonal directions.

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

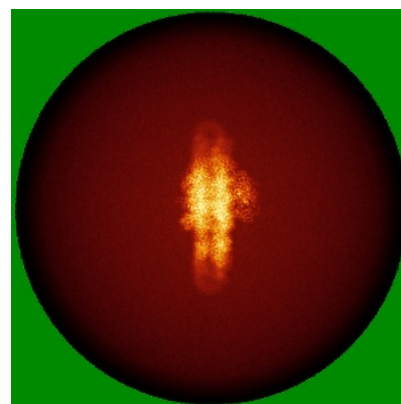
6.4.1 Primary map



X

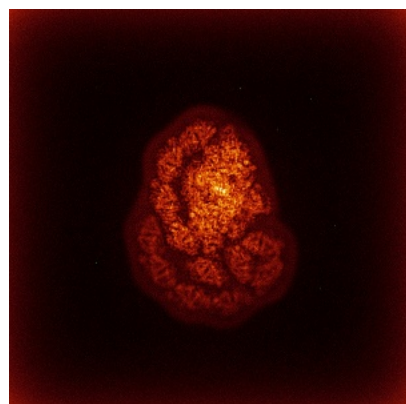


Y

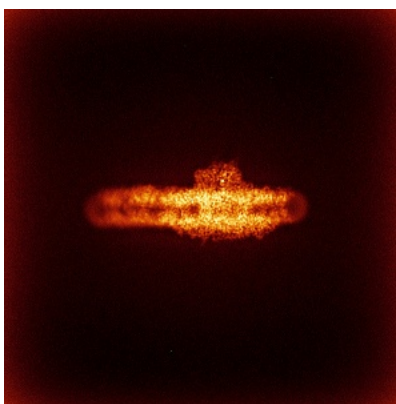


Z

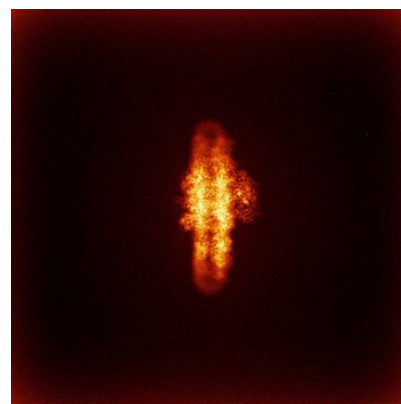
6.4.2 Raw map



X



Y

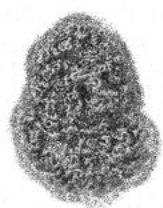


Z

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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.45. 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



X



Y



Z

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.

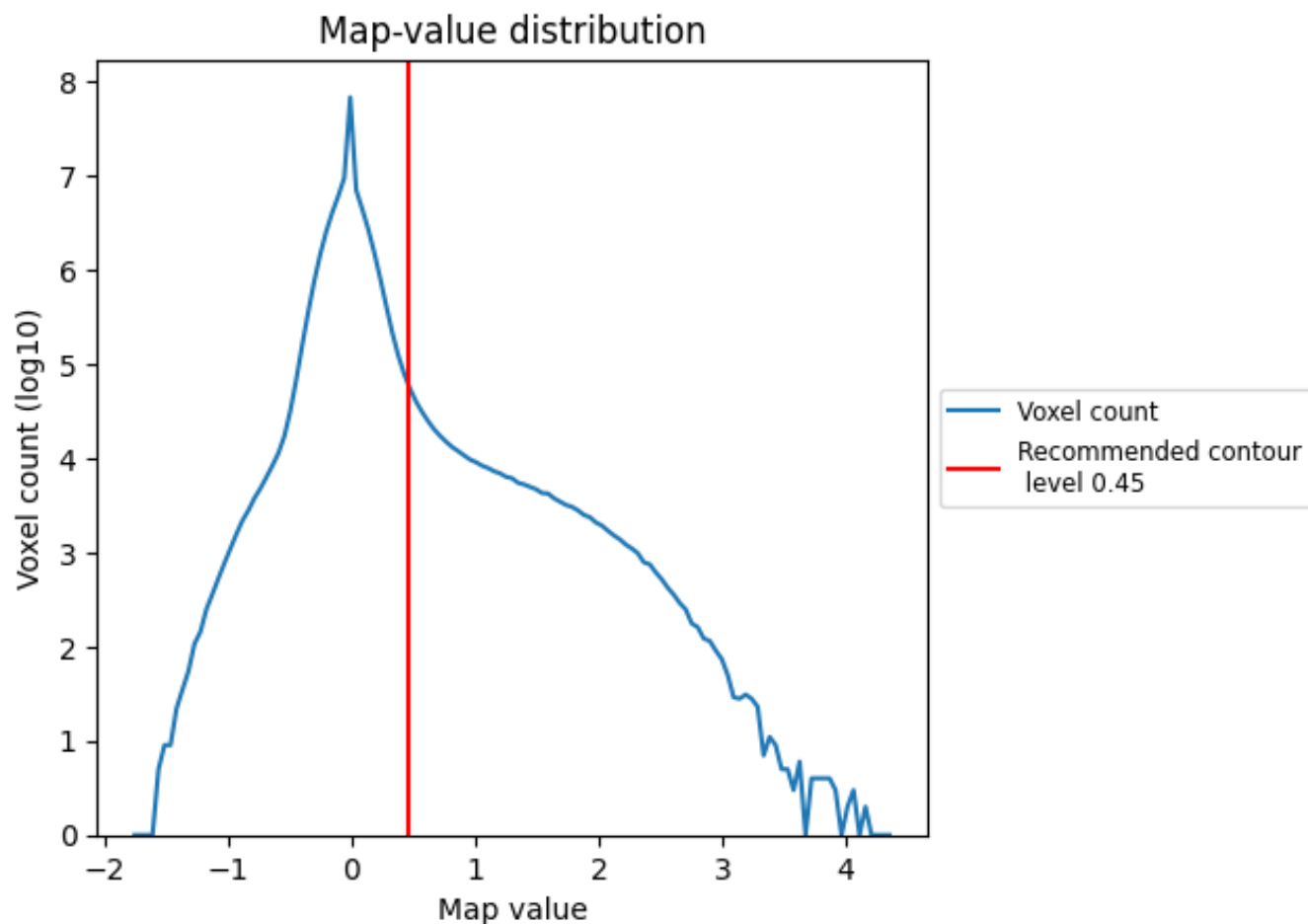
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

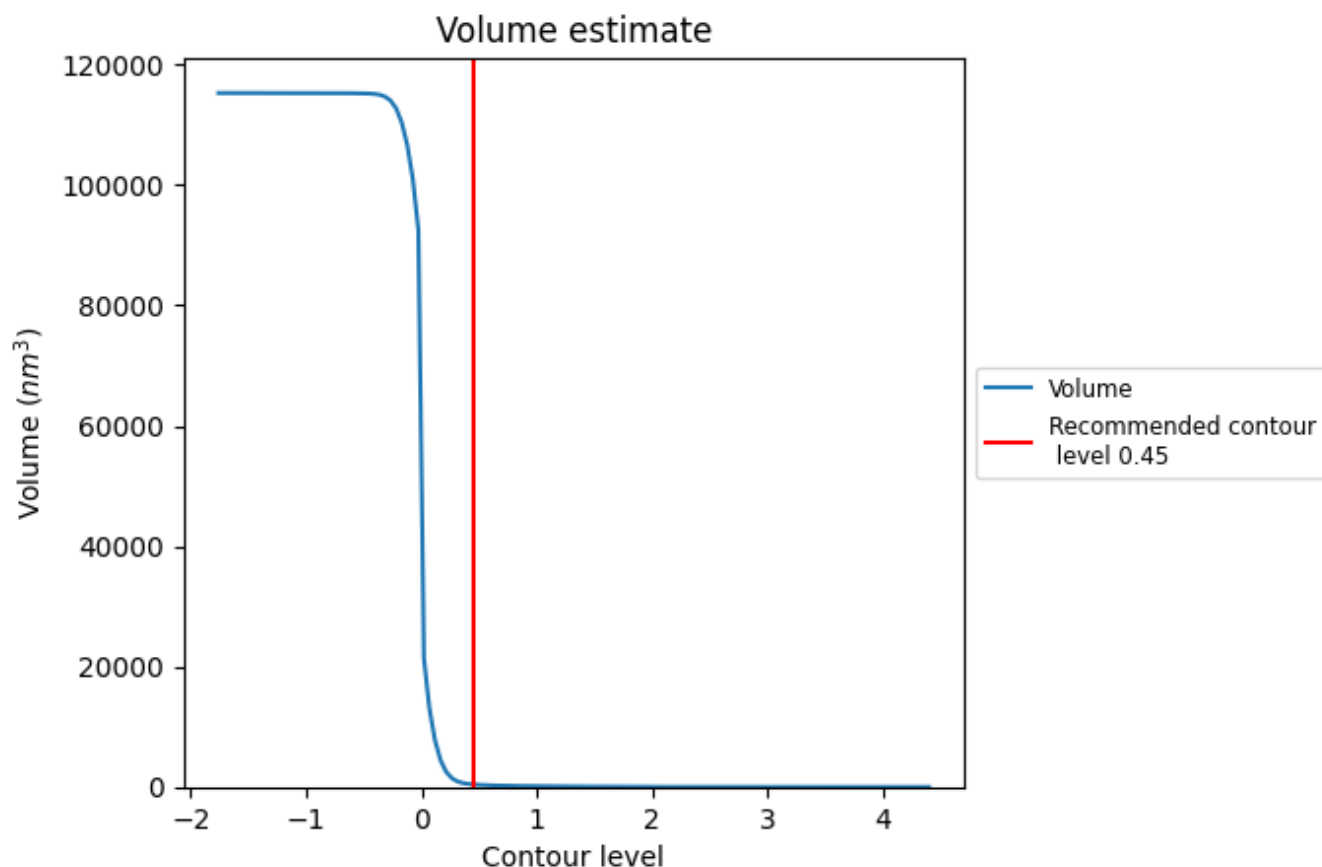
This section contains the results of statistical analysis of the map.

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.

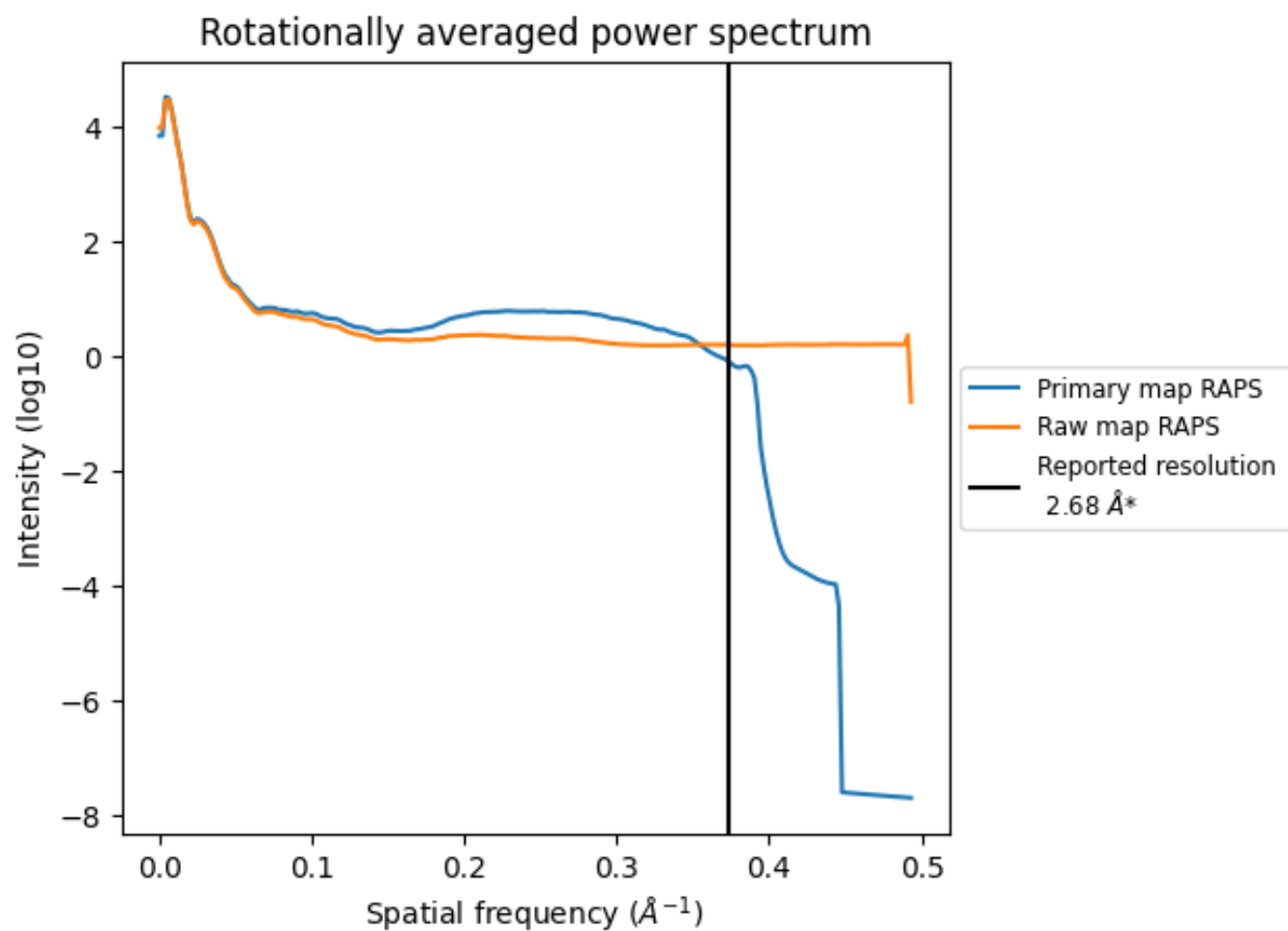
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 418 nm³; this corresponds to an approximate mass of 378 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 ⓘ

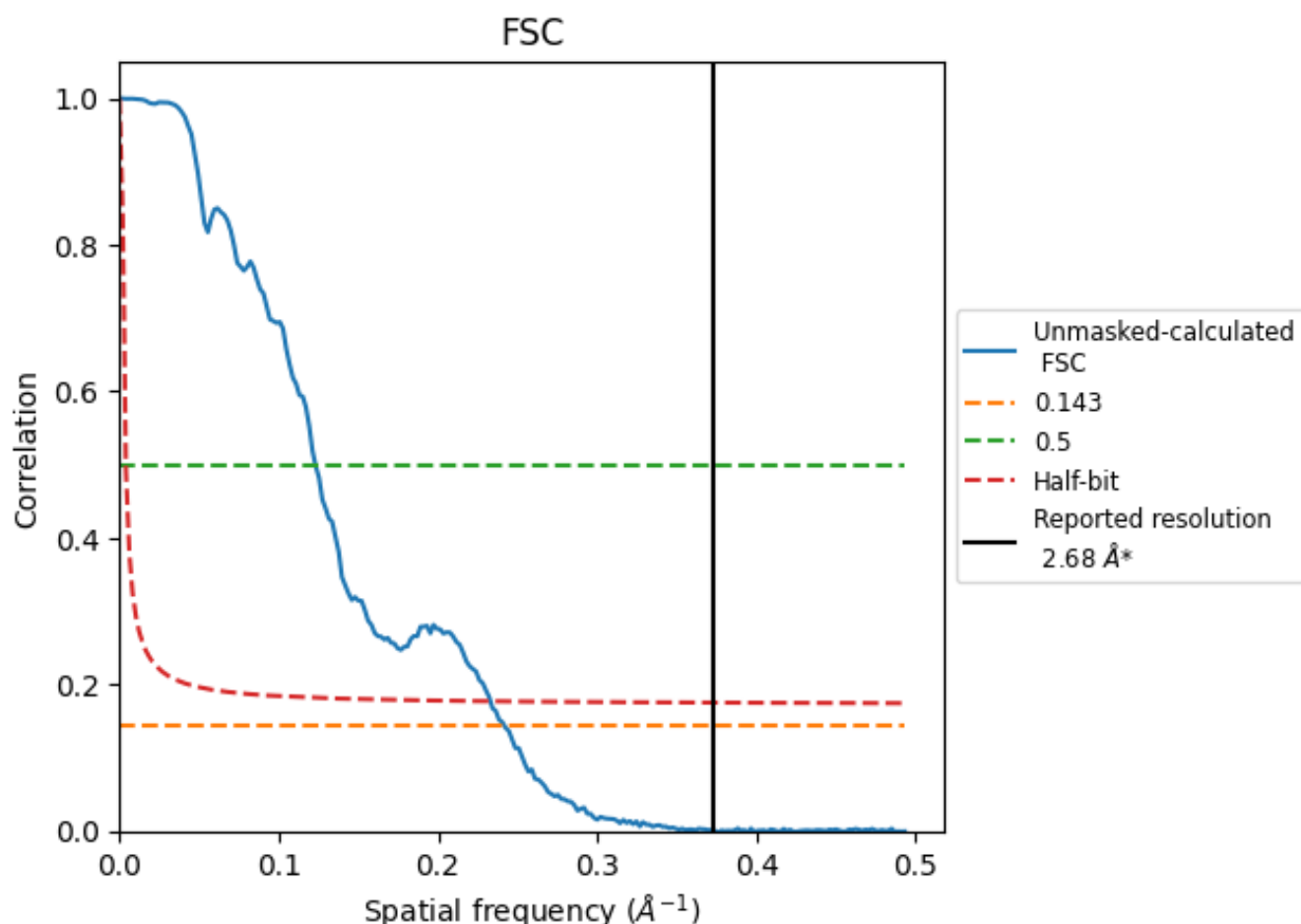


*Reported resolution corresponds to spatial frequency of 0.373 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.373 \AA^{-1}

8.2 Resolution estimates [i](#)

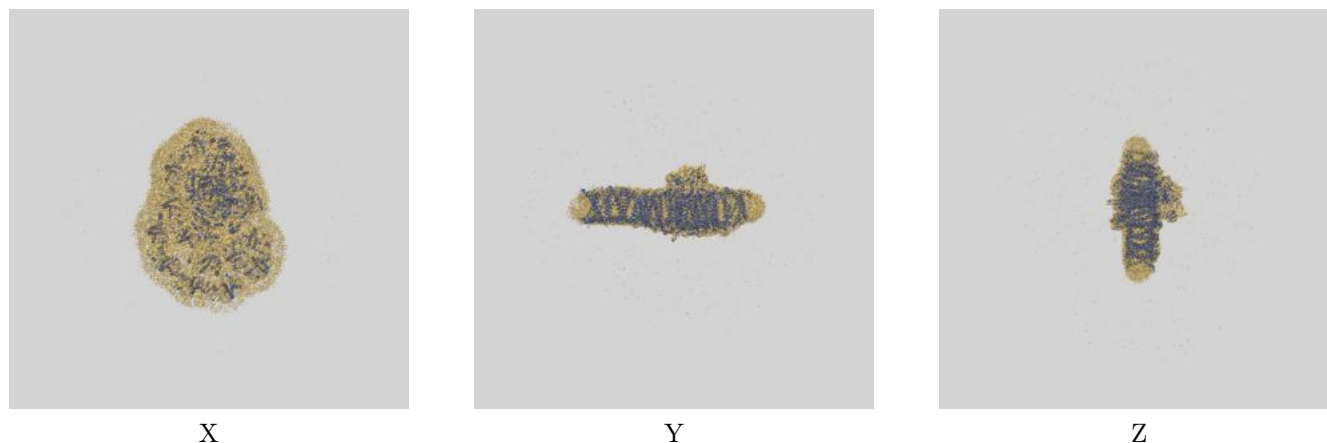
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.68	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.14	8.13	4.29

*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 4.14 differs from the reported value 2.68 by more than 10 %

9 Map-model fit [i](#)

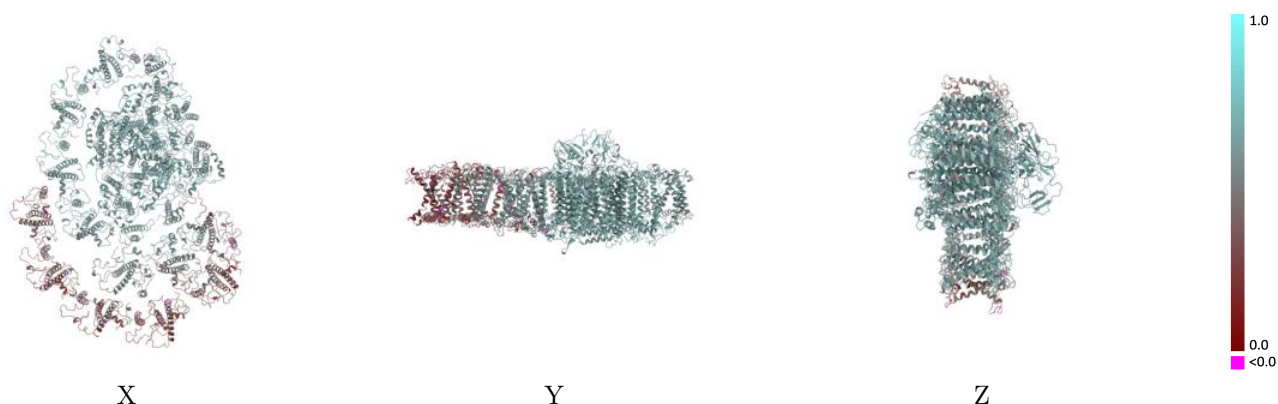
This section contains information regarding the fit between EMDB map EMD-33401 and PDB model 7XQP. Per-residue inclusion information can be found in section [3](#) on page [38](#).

9.1 Map-model overlay [i](#)



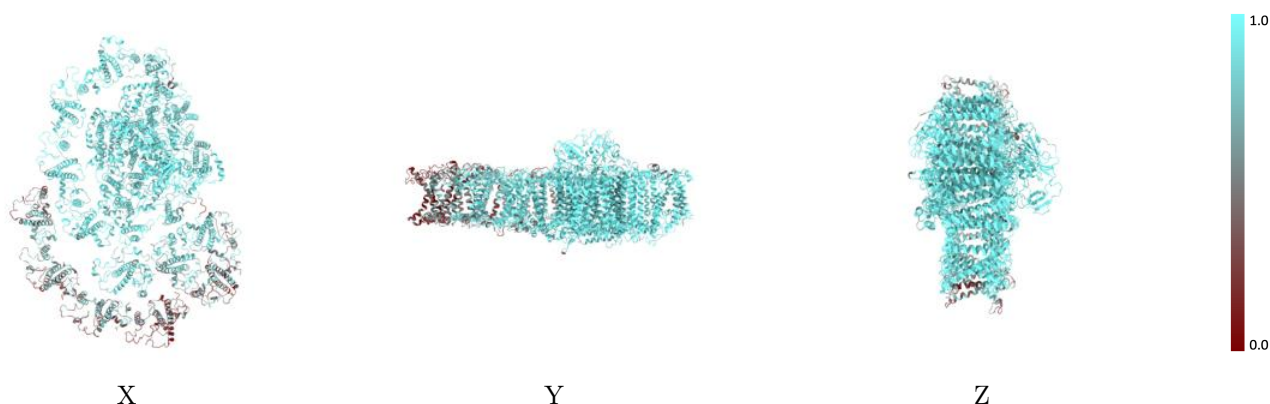
The images above show the 3D surface view of the map at the recommended contour level 0.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



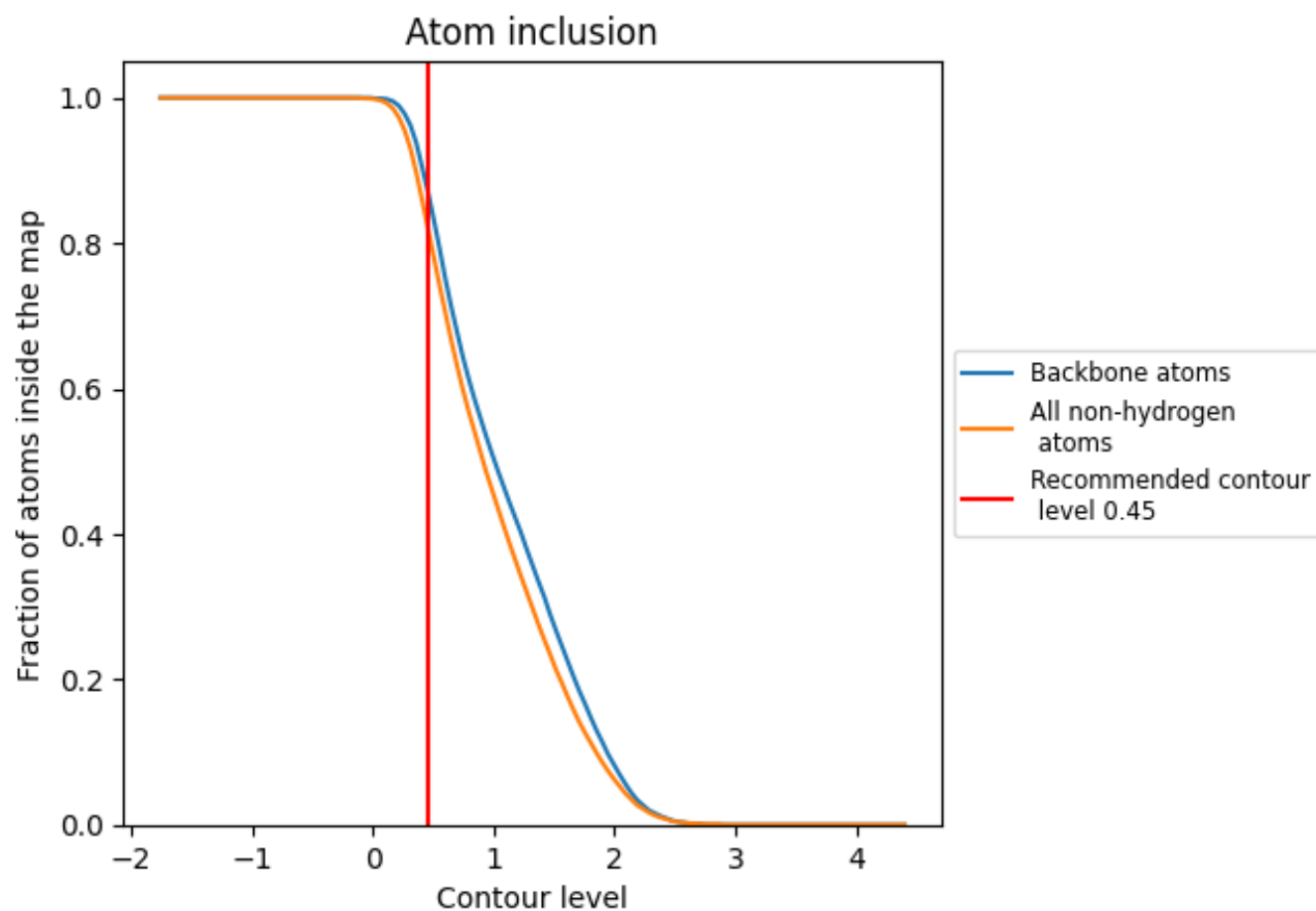
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.45).























































9.4 Atom inclusion ⓘ



At the recommended contour level, 88% of all backbone atoms, 83% 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 (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8260	 0.5360
1	 0.9160	 0.5760
2	 0.9220	 0.5910
3	 0.9350	 0.6030
4	 0.9200	 0.5810
5	 0.5830	 0.3590
6	 0.5300	 0.3330
7	 0.3390	 0.2870
8	 0.5420	 0.3320
9	 0.8250	 0.5250
A	 0.9620	 0.6340
B	 0.9610	 0.6300
C	 0.9730	 0.6210
D	 0.9470	 0.6150
E	 0.9410	 0.6070
F	 0.9220	 0.6030
G	 0.7980	 0.5530
H	 0.8880	 0.5780
I	 0.9470	 0.6180
J	 0.9350	 0.6110
K	 0.9400	 0.6090
L	 0.9430	 0.6120
M	 0.8980	 0.5880
O	 0.8320	 0.5260
a	 0.5470	 0.3560
b	 0.7680	 0.4910
c	 0.7450	 0.4660

