



Full wwPDB EM Validation Report ⓘ

Oct 1, 2024 – 05:49 PM JST

PDB ID : 8HTU
EMDB ID : EMD-35018
Title : Cryo-EM structure of PpPSI-L
Authors : Li, M.; Pan, X.W.; Sun, H.Y.
Deposited on : 2022-12-21
Resolution : 2.87 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

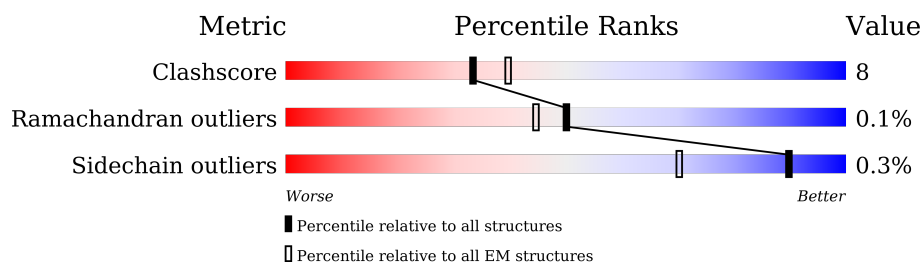
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.87 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	U	265	
1	V	265	
1	W	265	
2	1	245	
2	5	245	
3	2	273	
3	6	273	
4	3	323	

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Mol	Chain	Length	Quality of chain
4	7	323	
5	4	270	
5	8	270	
6	A	750	
7	B	734	
8	C	81	
9	D	210	
10	E	132	
11	F	246	
12	G	155	
13	H	139	
14	I	36	
15	J	41	
16	K	132	
17	L	223	
18	M	32	
19	O	143	
20	9	311	

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	CHL	1	601	X	-	-	-
21	CHL	1	607	X	-	-	-
21	CHL	2	601	X	-	-	-
21	CHL	2	602	X	-	-	-
21	CHL	2	606	X	-	-	-
21	CHL	2	607	X	-	-	-
21	CHL	2	608	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CHL	2	618	X	-	-	-
21	CHL	3	608	X	-	-	-
21	CHL	4	606	X	-	-	-
21	CHL	4	607	X	-	-	-
21	CHL	4	608	X	-	-	-
21	CHL	4	618	X	-	-	-
21	CHL	5	601	X	-	-	-
21	CHL	5	607	X	-	-	-
21	CHL	6	601	X	-	-	-
21	CHL	6	602	X	-	-	-
21	CHL	6	606	X	-	-	-
21	CHL	6	607	X	-	-	-
21	CHL	6	608	X	-	-	-
21	CHL	6	618	X	-	-	-
21	CHL	7	608	X	-	-	-
21	CHL	8	606	X	-	-	-
21	CHL	8	607	X	-	-	-
21	CHL	8	608	X	-	-	-
21	CHL	8	618	X	-	-	-
21	CHL	9	601	X	-	-	-
21	CHL	9	605	X	-	-	-
21	CHL	9	606	X	-	-	-
21	CHL	9	607	X	-	-	-
21	CHL	9	608	X	-	-	-
21	CHL	U	601	X	-	-	-
21	CHL	U	605	X	-	-	-
21	CHL	U	606	X	-	-	-
21	CHL	U	607	X	-	-	-
21	CHL	U	608	X	-	-	-
21	CHL	U	609	X	-	-	-
21	CHL	V	601	X	-	-	-
21	CHL	V	605	X	-	-	-
21	CHL	V	606	X	-	-	-
21	CHL	V	607	X	-	-	-
21	CHL	V	608	X	-	-	-
21	CHL	V	609	X	-	-	-
21	CHL	W	601	X	-	-	-
21	CHL	W	605	X	-	-	-
21	CHL	W	606	X	-	-	-
21	CHL	W	607	X	-	-	-
21	CHL	W	608	X	-	-	-
21	CHL	W	609	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	1	602	X	-	-	-
22	CLA	1	603	X	-	-	-
22	CLA	1	606	X	-	-	-
22	CLA	1	608	X	-	-	-
22	CLA	1	609	X	-	-	-
22	CLA	1	610	X	-	-	-
22	CLA	1	611	X	-	-	-
22	CLA	1	612	X	-	-	-
22	CLA	1	613	X	-	-	-
22	CLA	1	614	X	-	-	-
22	CLA	1	616	X	-	-	-
22	CLA	2	603	X	-	-	-
22	CLA	2	604	X	-	-	-
22	CLA	2	609	X	-	-	-
22	CLA	2	610	X	-	-	-
22	CLA	2	611	X	-	-	-
22	CLA	2	612	X	-	-	-
22	CLA	2	613	X	-	-	-
22	CLA	2	614	X	-	-	-
22	CLA	3	602	X	-	-	-
22	CLA	3	603	X	-	-	-
22	CLA	3	604	X	-	-	-
22	CLA	3	606	X	-	-	-
22	CLA	3	607	X	-	-	-
22	CLA	3	609	X	-	-	-
22	CLA	3	610	X	-	-	-
22	CLA	3	611	X	-	-	-
22	CLA	3	612	X	-	-	-
22	CLA	3	613	X	-	-	-
22	CLA	3	614	X	-	-	-
22	CLA	3	615	X	-	-	-
22	CLA	3	617	X	-	-	-
22	CLA	4	601	X	-	-	-
22	CLA	4	602	X	-	-	-
22	CLA	4	603	X	-	-	-
22	CLA	4	604	X	-	-	-
22	CLA	4	609	X	-	-	-
22	CLA	4	610	X	-	-	-
22	CLA	4	611	X	-	-	-
22	CLA	4	612	X	-	-	-
22	CLA	4	613	X	-	-	-
22	CLA	4	614	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	5	602	X	-	-	-
22	CLA	5	603	X	-	-	-
22	CLA	5	604	X	-	-	-
22	CLA	5	606	X	-	-	-
22	CLA	5	608	X	-	-	-
22	CLA	5	609	X	-	-	-
22	CLA	5	610	X	-	-	-
22	CLA	5	611	X	-	-	-
22	CLA	5	612	X	-	-	-
22	CLA	5	614	X	-	-	-
22	CLA	5	616	X	-	-	-
22	CLA	6	603	X	-	-	-
22	CLA	6	604	X	-	-	-
22	CLA	6	609	X	-	-	-
22	CLA	6	610	X	-	-	-
22	CLA	6	611	X	-	-	-
22	CLA	6	612	X	-	-	-
22	CLA	6	613	X	-	-	-
22	CLA	6	614	X	-	-	-
22	CLA	7	603	X	-	-	-
22	CLA	7	604	X	-	-	-
22	CLA	7	606	X	-	-	-
22	CLA	7	607	X	-	-	-
22	CLA	7	609	X	-	-	-
22	CLA	7	610	X	-	-	-
22	CLA	7	611	X	-	-	-
22	CLA	7	612	X	-	-	-
22	CLA	7	613	X	-	-	-
22	CLA	7	614	X	-	-	-
22	CLA	7	615	X	-	-	-
22	CLA	7	617	X	-	-	-
22	CLA	8	601	X	-	-	-
22	CLA	8	602	X	-	-	-
22	CLA	8	603	X	-	-	-
22	CLA	8	604	X	-	-	-
22	CLA	8	609	X	-	-	-
22	CLA	8	610	X	-	-	-
22	CLA	8	611	X	-	-	-
22	CLA	8	612	X	-	-	-
22	CLA	8	613	X	-	-	-
22	CLA	8	614	X	-	-	-
22	CLA	9	602	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	9	603	X	-	-	-
22	CLA	9	604	X	-	-	-
22	CLA	9	609	X	-	-	-
22	CLA	9	610	X	-	-	-
22	CLA	9	611	X	-	-	-
22	CLA	9	612	X	-	-	-
22	CLA	9	613	X	-	-	-
22	CLA	A	801	X	-	-	-
22	CLA	A	802	X	-	-	-
22	CLA	A	803	X	-	-	-
22	CLA	A	804	X	-	-	-
22	CLA	A	806	X	-	-	-
22	CLA	A	807	X	-	-	-
22	CLA	A	808	X	-	-	-
22	CLA	A	809	X	-	-	-
22	CLA	A	810	X	-	-	-
22	CLA	A	811	X	-	-	-
22	CLA	A	812	X	-	-	-
22	CLA	A	813	X	-	-	-
22	CLA	A	814	X	-	-	-
22	CLA	A	815	X	-	-	-
22	CLA	A	816	X	-	-	-
22	CLA	A	817	X	-	-	-
22	CLA	A	818	X	-	-	-
22	CLA	A	819	X	-	-	-
22	CLA	A	820	X	-	-	-
22	CLA	A	821	X	-	-	-
22	CLA	A	822	X	-	-	-
22	CLA	A	823	X	-	-	-
22	CLA	A	824	X	-	-	-
22	CLA	A	826	X	-	-	-
22	CLA	A	828	X	-	-	-
22	CLA	A	829	X	-	-	-
22	CLA	A	830	X	-	-	-
22	CLA	A	831	X	-	-	-
22	CLA	A	832	X	-	-	-
22	CLA	A	833	X	-	-	-
22	CLA	A	834	X	-	-	-
22	CLA	A	835	X	-	-	-
22	CLA	A	836	X	-	-	-
22	CLA	A	838	X	-	-	-
22	CLA	A	839	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	A	840	X	-	-	-
22	CLA	A	841	X	-	-	-
22	CLA	A	842	X	-	-	-
22	CLA	A	843	X	-	-	-
22	CLA	A	845	X	-	-	-
22	CLA	A	854	X	-	-	-
22	CLA	B	802	X	-	-	-
22	CLA	B	803	X	-	-	-
22	CLA	B	804	X	-	-	-
22	CLA	B	805	X	-	-	-
22	CLA	B	806	X	-	-	-
22	CLA	B	808	X	-	-	-
22	CLA	B	809	X	-	-	-
22	CLA	B	810	X	-	-	-
22	CLA	B	811	X	-	-	-
22	CLA	B	812	X	-	-	-
22	CLA	B	813	X	-	-	-
22	CLA	B	814	X	-	-	-
22	CLA	B	815	X	-	-	-
22	CLA	B	816	X	-	-	-
22	CLA	B	817	X	-	-	-
22	CLA	B	818	X	-	-	-
22	CLA	B	819	X	-	-	-
22	CLA	B	820	X	-	-	-
22	CLA	B	821	X	-	-	-
22	CLA	B	822	X	-	-	-
22	CLA	B	823	X	-	-	-
22	CLA	B	824	X	-	-	-
22	CLA	B	825	X	-	-	-
22	CLA	B	826	X	-	-	-
22	CLA	B	827	X	-	-	-
22	CLA	B	828	X	-	-	-
22	CLA	B	829	X	-	-	-
22	CLA	B	830	X	-	-	-
22	CLA	B	831	X	-	-	-
22	CLA	B	833	X	-	-	-
22	CLA	B	834	X	-	-	-
22	CLA	B	835	X	-	-	-
22	CLA	B	836	X	-	-	-
22	CLA	B	837	X	-	-	-
22	CLA	B	839	X	-	-	-
22	CLA	B	840	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	B	841	X	-	-	-
22	CLA	F	301	X	-	-	-
22	CLA	F	303	X	-	-	-
22	CLA	F	304	X	-	-	-
22	CLA	G	201	X	-	-	-
22	CLA	G	203	X	-	-	-
22	CLA	G	204	X	-	-	-
22	CLA	H	201	X	-	-	-
22	CLA	J	101	X	-	-	-
22	CLA	K	201	X	-	-	-
22	CLA	K	203	X	-	-	-
22	CLA	K	204	X	-	-	-
22	CLA	K	206	X	-	-	-
22	CLA	L	302	X	-	-	-
22	CLA	L	303	X	-	-	-
22	CLA	L	304	X	-	-	-
22	CLA	O	2001	X	-	-	-
22	CLA	O	2002	X	-	-	-
22	CLA	O	2003	X	-	-	-
22	CLA	U	602	X	-	-	-
22	CLA	U	603	X	-	-	-
22	CLA	U	604	X	-	-	-
22	CLA	U	610	X	-	-	-
22	CLA	U	611	X	-	-	-
22	CLA	U	612	X	-	-	-
22	CLA	U	613	X	-	-	-
22	CLA	U	614	X	-	-	-
22	CLA	V	603	X	-	-	-
22	CLA	V	604	X	-	-	-
22	CLA	V	610	X	-	-	-
22	CLA	V	611	X	-	-	-
22	CLA	V	612	X	-	-	-
22	CLA	V	613	X	-	-	-
22	CLA	V	614	X	-	-	-
22	CLA	W	602	X	-	-	-
22	CLA	W	603	X	-	-	-
22	CLA	W	604	X	-	-	-
22	CLA	W	610	X	-	-	-
22	CLA	W	611	X	-	-	-
22	CLA	W	612	X	-	-	-
22	CLA	W	613	X	-	-	-
22	CLA	W	614	X	-	-	-

2 Entry composition [i](#)

There are 33 unique types of molecules in this entry. The entry contains 57715 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
1	U	219	Total	C	N	O	S	0	0	
			1659	1073	270	311	5			
1	V	215	Total	C	N	O	S	0	0	
			1630	1052	265	308	5			
1	W	228	Total	C	N	O	P	S	0	0
			1734	1113	286	329	1	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	193	Total	C	N	O	S	0	0
			1478	964	248	265	1		
2	5	192	Total	C	N	O	S	0	0
			1473	961	247	264	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	211	Total	C	N	O	S	0	0
			1625	1055	273	293	4		
3	6	205	Total	C	N	O	S	0	0
			1583	1029	265	285	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	222	Total	C	N	O	S	0	0
			1719	1125	281	306	7		
4	7	219	Total	C	N	O	S	0	0
			1687	1105	274	301	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	206	Total	C	N	O	S	0	0
			1600	1040	267	288	5		
5	8	204	Total	C	N	O	S	0	0
			1582	1028	265	284	5		

- Molecule 6 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	742	Total	C	N	O	S	0	0
			5837	3827	993	998	19		

- Molecule 7 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	733	Total	C	N	O	S	0	0
			5850	3839	996	999	16		

- Molecule 8 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	80	Total	C	N	O	S	0	0
			595	365	103	116	11		

- Molecule 9 is a protein called Photosystem I reaction center subunit II, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	142	Total	C	N	O	S	0	0
			1114	714	197	200	3		

- Molecule 10 is a protein called Photosystem I reaction center subunit IV, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	E	64	Total	C	N	O	0	0
			507	322	90	95		

- Molecule 11 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	161	Total	C	N	O	S	0	0
			1251	808	217	223	3		

- Molecule 12 is a protein called Photosystem I reaction center subunit V, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	G	97	Total	C	N	O	0	0
			740	478	127	135		

- Molecule 13 is a protein called Photosystem I reaction center subunit VI, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	H	95	Total	C	N	O	S	0	0
			736	472	125	138	1		

- Molecule 14 is a protein called Photosystem I reaction center subunit VIII.

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

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

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

- Molecule 16 is a protein called Photosystem I subunit X.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	K	81	Total	C	N	O	S	0	0
			565	356	98	108	3		

- Molecule 17 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	163	Total	C	N	O	S	0	0
			1228	809	197	220	2		

- Molecule 18 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	M	31	Total	C	N	O	0	0
			230	150	37	43		

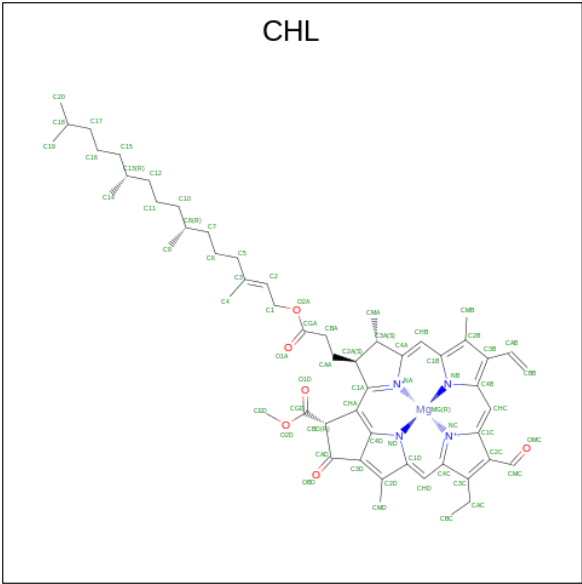
- Molecule 19 is a protein called Photosystem I subunit O.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	O	90	Total	C	N	O	S	0	0
			711	477	117	116	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	9	221	Total	C	N	O	S	0	0
			1713	1113	283	308	9		

- Molecule 21 is CHLOROPHYLL B (three-letter code: CHL) (formula: C₅₅H₇₀MgN₄O₆).



Mol	Chain	Residues	Atoms					AltConf
21	U	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
21	U	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
21	U	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
21	U	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
21	U	1	Total	C	Mg	N	O	0
			40	31	1	4	4	
21	U	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
21	V	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
21	V	1	Total	C	Mg	N	O	0
			42	33	1	4	4	

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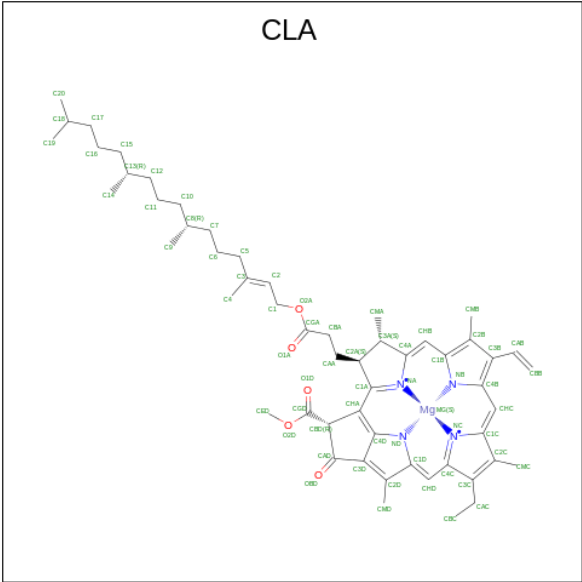
Mol	Chain	Residues	Atoms					AltConf
21	V	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
21	V	1	Total	C	Mg	N	O	0
			40	31	1	4	4	
21	V	1	Total	C	Mg	N	O	0
			40	31	1	4	4	
21	V	1	Total	C	Mg	N	O	0
			40	33	1	4	2	
21	W	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
21	W	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
21	W	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
21	W	1	Total	C	Mg	N	O	0
			40	31	1	4	4	
21	W	1	Total	C	Mg	N	O	0
			40	31	1	4	4	
21	W	1	Total	C	Mg	N	O	0
			40	33	1	4	2	
21	1	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
21	1	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
21	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
21	2	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
21	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
21	2	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
21	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
21	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
21	3	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
21	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
21	4	1	Total	C	Mg	N	O	0
			47	36	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
21	4	1	Total 46	C 35	Mg 1	N 4	O 6	0
21	4	1	Total 43	C 34	Mg 1	N 4	O 4	0
21	5	1	Total 51	C 40	Mg 1	N 4	O 6	0
21	5	1	Total 39	C 32	Mg 1	N 4	O 2	0
21	6	1	Total 66	C 55	Mg 1	N 4	O 6	0
21	6	1	Total 56	C 45	Mg 1	N 4	O 6	0
21	6	1	Total 46	C 35	Mg 1	N 4	O 6	0
21	6	1	Total 47	C 36	Mg 1	N 4	O 6	0
21	6	1	Total 48	C 37	Mg 1	N 4	O 6	0
21	6	1	Total 47	C 36	Mg 1	N 4	O 6	0
21	7	1	Total 46	C 35	Mg 1	N 4	O 6	0
21	8	1	Total 46	C 35	Mg 1	N 4	O 6	0
21	8	1	Total 46	C 35	Mg 1	N 4	O 6	0
21	8	1	Total 51	C 40	Mg 1	N 4	O 6	0
21	8	1	Total 43	C 34	Mg 1	N 4	O 4	0
21	9	1	Total 39	C 32	Mg 1	N 4	O 2	0
21	9	1	Total 38	C 31	Mg 1	N 4	O 2	0
21	9	1	Total 44	C 35	Mg 1	N 4	O 4	0
21	9	1	Total 43	C 34	Mg 1	N 4	O 4	0
21	9	1	Total 43	C 34	Mg 1	N 4	O 4	0

- Molecule 22 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
22	U	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	U	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	U	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	U	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	U	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	U	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	U	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	U	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	V	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
22	V	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	V	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	V	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
22	V	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
22	V	1	Total	C	Mg	N	O	0
			38	30	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
22	V	1	Total	C	Mg	N	O	0
			56	47	1	4	4	
22	V	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	W	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	W	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
22	W	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	W	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	W	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
22	W	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
22	W	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	W	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
22	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	2	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	2	1	Total 57	C 47	Mg 1	N 4	O 5	0
22	2	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	3	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	3	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	3	1	Total 53	C 43	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	3	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 62	C 52	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 54	C 44	Mg 1	N 4	O 5	0
22	A	1	Total 62	C 52	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 61	C 51	Mg 1	N 4	O 5	0
22	B	1	Total 44	C 34	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 64	C 54	Mg 1	N 4	O 5	0
22	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	G	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	H	1	Total	C	Mg	N	O	0
			38	32	1	4	1	
22	J	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	K	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
22	K	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	K	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	K	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	L	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	O	1	Total	C	Mg	N		0
			27	22	1	4		
22	O	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	O	1	Total	C	Mg	N		0
			27	22	1	4		
22	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
22	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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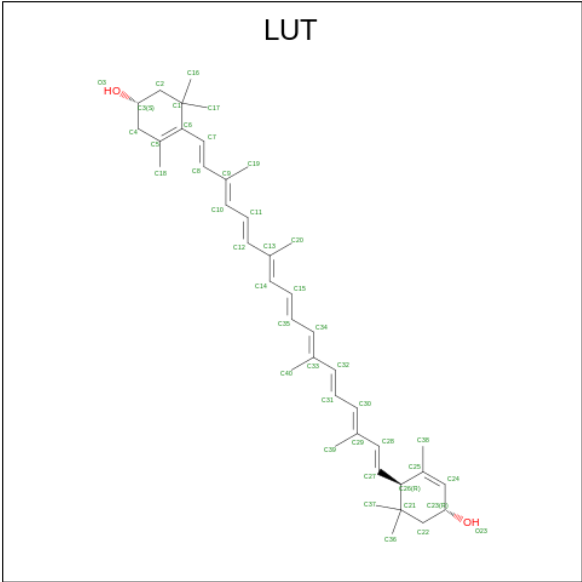
Mol	Chain	Residues	Atoms					AltConf
22	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	6	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	6	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	6	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	7	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	7	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	7	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	7	1	Total 57	C 47	Mg 1	N 4	O 5	0
22	7	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	7	1	Total 41	C 33	Mg 1	N 4	O 3	0
22	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	7	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	7	1	Total 41	C 33	Mg 1	N 4	O 3	0
22	7	1	Total 40	C 32	Mg 1	N 4	O 3	0
22	7	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	9	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
22	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			39	33	1	4	1	
22	9	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

- Molecule 23 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C₄₀H₅₆O₂).



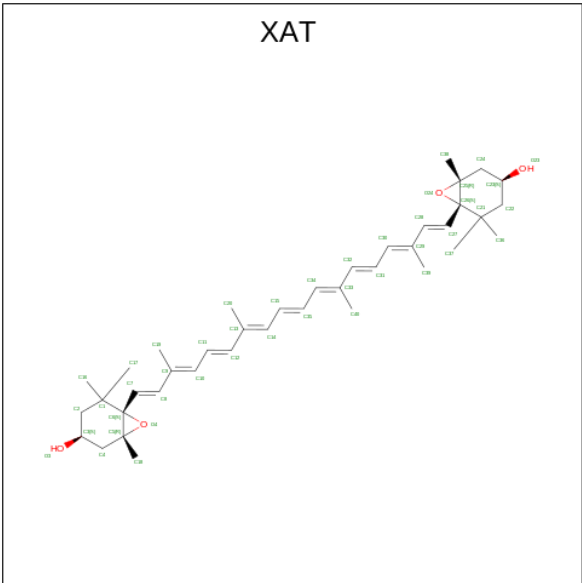
Mol	Chain	Residues	Atoms			AltConf
23	U	1	Total	C	O	0
			42	40	2	
23	U	1	Total	C	O	0
			42	40	2	
23	V	1	Total	C	O	0
			42	40	2	
23	V	1	Total	C	O	0
			42	40	2	
23	W	1	Total	C	O	0
			42	40	2	
23	W	1	Total	C	O	0
			42	40	2	
23	1	1	Total	C	O	0
			42	40	2	
23	2	1	Total	C	O	0
			42	40	2	
23	3	1	Total	C	O	0
			42	40	2	
23	4	1	Total	C	O	0
			42	40	2	
23	5	1	Total	C	O	0
			42	40	2	
23	6	1	Total	C	O	0
			42	40	2	
23	7	1	Total	C	O	0
			42	40	2	
23	8	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms			AltConf
23	9	1	Total	C	O	0
			42	40	2	
23	9	1	Total	C	O	0
			42	40	2	
23	9	1	Total	C	O	0
			42	40	2	

- Molecule 24 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).



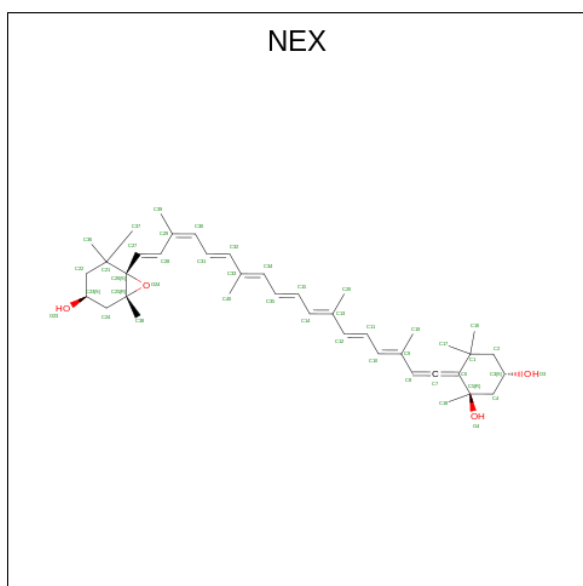
Mol	Chain	Residues	Atoms			AltConf
24	U	1	Total	C	O	0
			44	40	4	
24	V	1	Total	C	O	0
			44	40	4	
24	W	1	Total	C	O	0
			44	40	4	
24	1	1	Total	C	O	0
			44	40	4	
24	2	1	Total	C	O	0
			44	40	4	
24	3	1	Total	C	O	0
			44	40	4	
24	4	1	Total	C	O	0
			44	40	4	
24	5	1	Total	C	O	0
			44	40	4	

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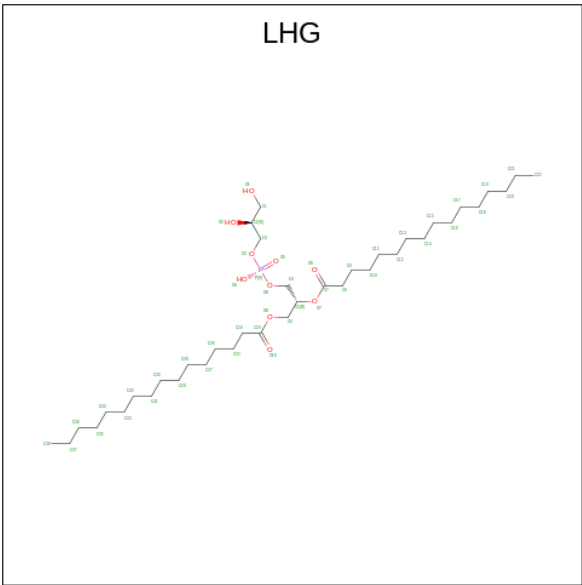
Mol	Chain	Residues	Atoms			AltConf
24	6	1	Total	C	O	0
			44	40	4	
24	7	1	Total	C	O	0
			44	40	4	
24	8	1	Total	C	O	0
			44	40	4	

- Molecule 25 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
25	U	1	Total	C	O	0
			44	40	4	
25	V	1	Total	C	O	0
			44	40	4	
25	W	1	Total	C	O	0
			44	40	4	
25	9	1	Total	C	O	0
			44	40	4	

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



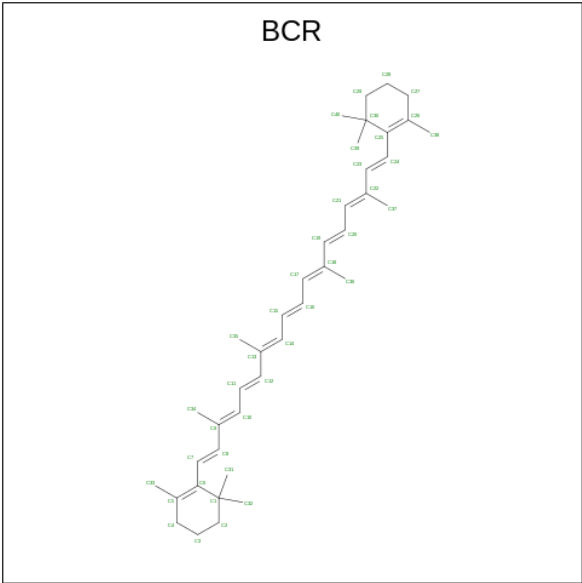
Mol	Chain	Residues	Atoms				AltConf
26	U	1	Total	C	O	P	0
			45	34	10	1	
26	V	1	Total	C	O	P	0
			42	31	10	1	
26	W	1	Total	C	O	P	0
			45	34	10	1	
26	1	1	Total	C	O	P	0
			49	38	10	1	
26	2	1	Total	C	O	P	0
			32	21	10	1	
26	3	1	Total	C	O	P	0
			32	21	10	1	
26	4	1	Total	C	O	P	0
			38	27	10	1	
26	A	1	Total	C	O	P	0
			47	36	10	1	
26	A	1	Total	C	O	P	0
			31	20	10	1	
26	B	1	Total	C	O	P	0
			35	24	10	1	
26	5	1	Total	C	O	P	0
			37	26	10	1	
26	6	1	Total	C	O	P	0
			32	21	10	1	
26	7	1	Total	C	O	P	0
			34	23	10	1	
26	8	1	Total	C	O	P	0
			38	27	10	1	

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Mol	Chain	Residues	Atoms				AltConf
26	9	1	Total	C	O	P	0
			28	17	10	1	

- Molecule 27 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



Mol	Chain	Residues	Atoms		AltConf
27	1	1	Total	C	0
			40	40	
27	2	1	Total	C	0
			40	40	
27	3	1	Total	C	0
			40	40	
27	3	1	Total	C	0
			40	40	
27	4	1	Total	C	0
			40	40	
27	A	1	Total	C	0
			40	40	
27	A	1	Total	C	0
			40	40	
27	A	1	Total	C	0
			40	40	
27	A	1	Total	C	0
			40	40	
27	A	1	Total	C	0
			40	40	

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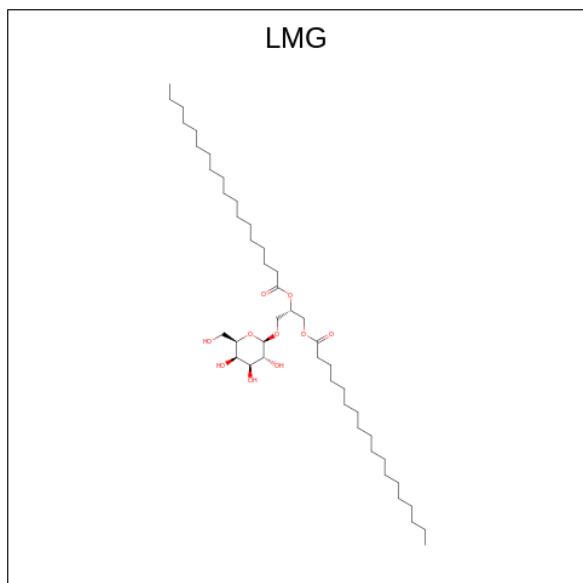
Mol	Chain	Residues	Atoms	AltConf
27	A	1	Total C 39 39	0
27	B	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	F	1	Total C 40 40	0
27	G	1	Total C 40 40	0
27	I	1	Total C 40 40	0
27	J	1	Total C 40 40	0
27	K	1	Total C 40 40	0
27	K	1	Total C 40 40	0
27	L	1	Total C 40 40	0
27	L	1	Total C 40 40	0
27	L	1	Total C 40 40	0
27	M	1	Total C 40 40	0
27	O	1	Total C 40 40	0
27	6	1	Total C 40 40	0
27	7	1	Total C 40 40	0

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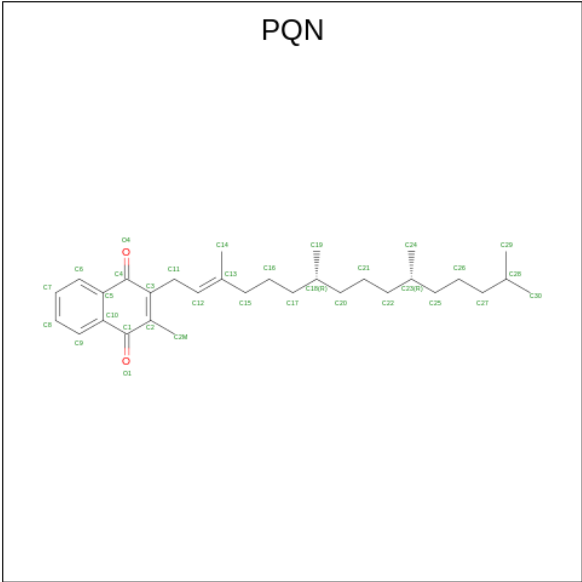
Mol	Chain	Residues	Atoms	AltConf
27	7	1	Total C 40 40	0
27	8	1	Total C 40 40	0

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



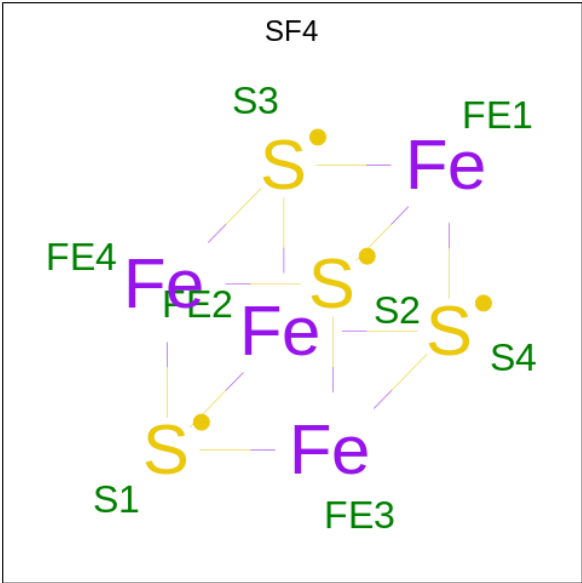
Mol	Chain	Residues	Atoms	AltConf
28	2	1	Total C O 47 37 10	0
28	A	1	Total C O 34 24 10	0
28	G	1	Total C O 32 22 10	0
28	J	1	Total C O 55 45 10	0
28	J	1	Total C O 35 25 10	0
28	L	1	Total C O 44 34 10	0

- Molecule 29 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 30 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



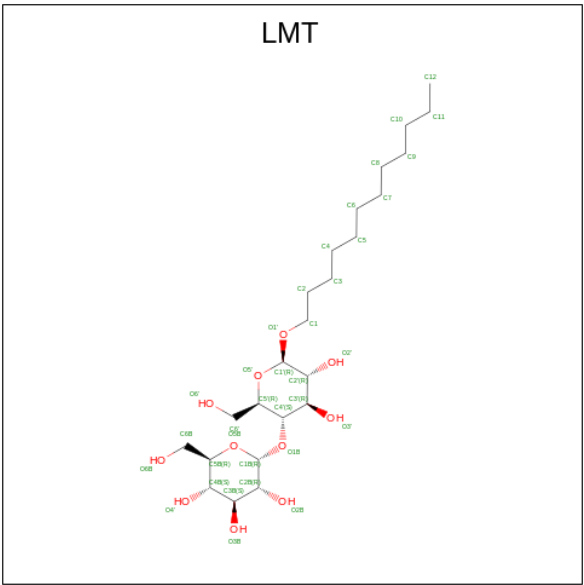
Mol	Chain	Residues	Atoms			AltConf
30	A	1	Total	Fe	S	0
			8	4	4	
30	C	1	Total	Fe	S	0
			8	4	4	

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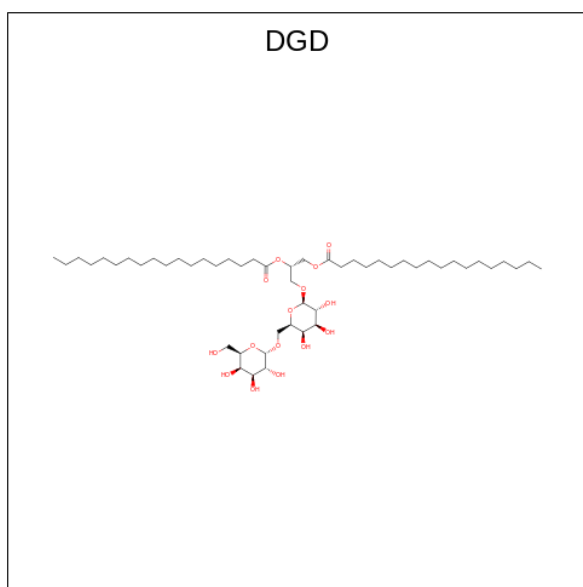
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
30	C	1	8	4	4	0

- Molecule 31 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
31	A	1	35	24	11	0
31	B	1	31	20	11	0
31	G	1	35	24	11	0
31	K	1	35	24	11	0

- Molecule 32 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



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

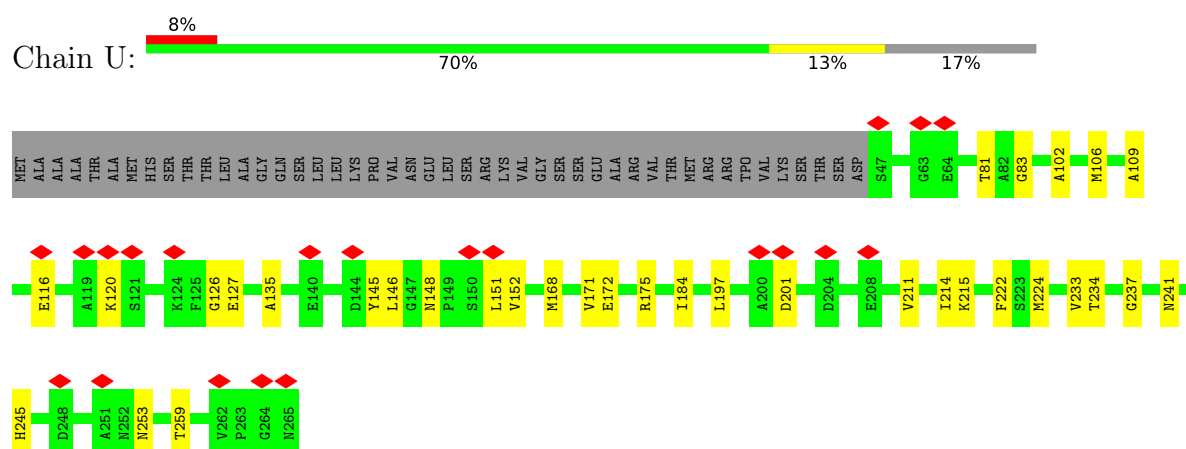
- Molecule 33 is water.

Mol	Chain	Residues	Atoms		AltConf
33	A	2	Total	O	0
			2	2	

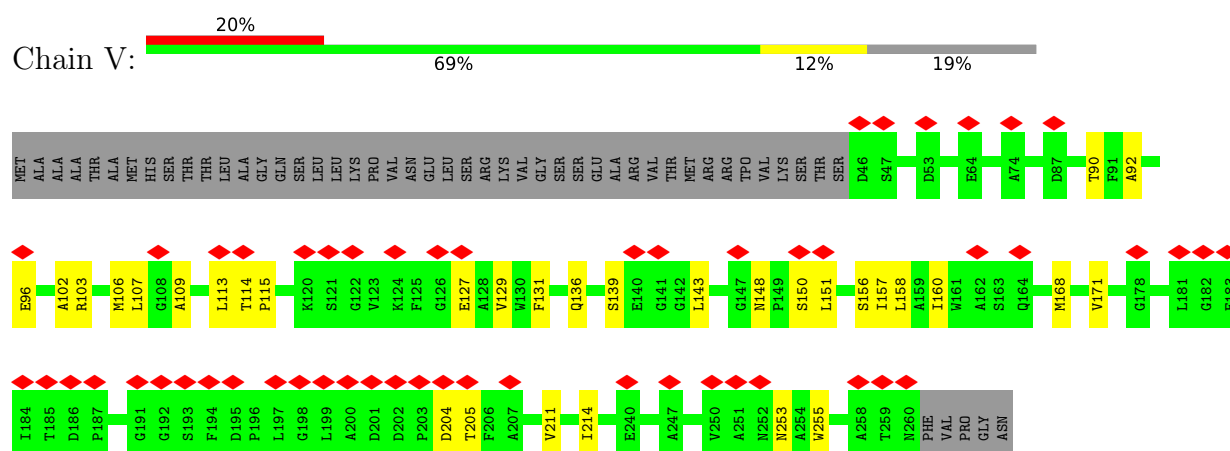
3 Residue-property plots

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.

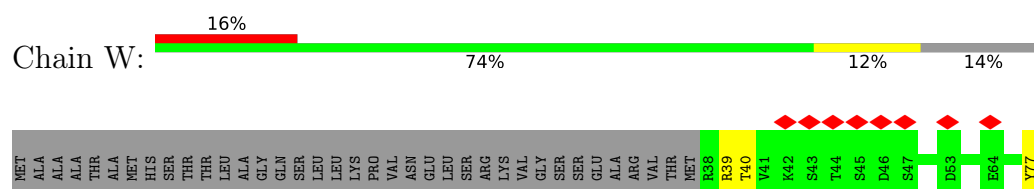
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic

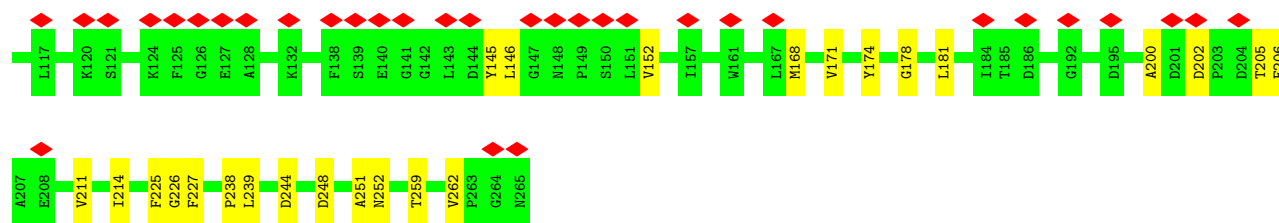


- Molecule 1: Chlorophyll a-b binding protein, chloroplastic

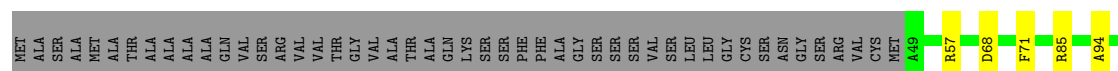


- Molecule 1: Chlorophyll a-b binding protein, chloroplastic

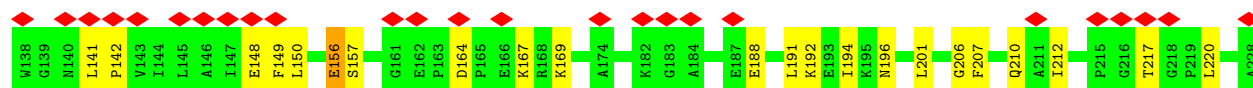
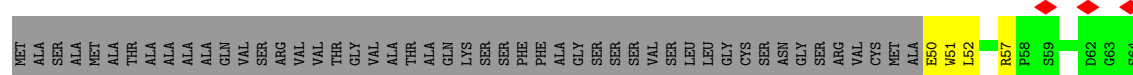




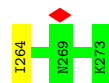
- Molecule 2: Chlorophyll a-b binding protein, chloroplastic



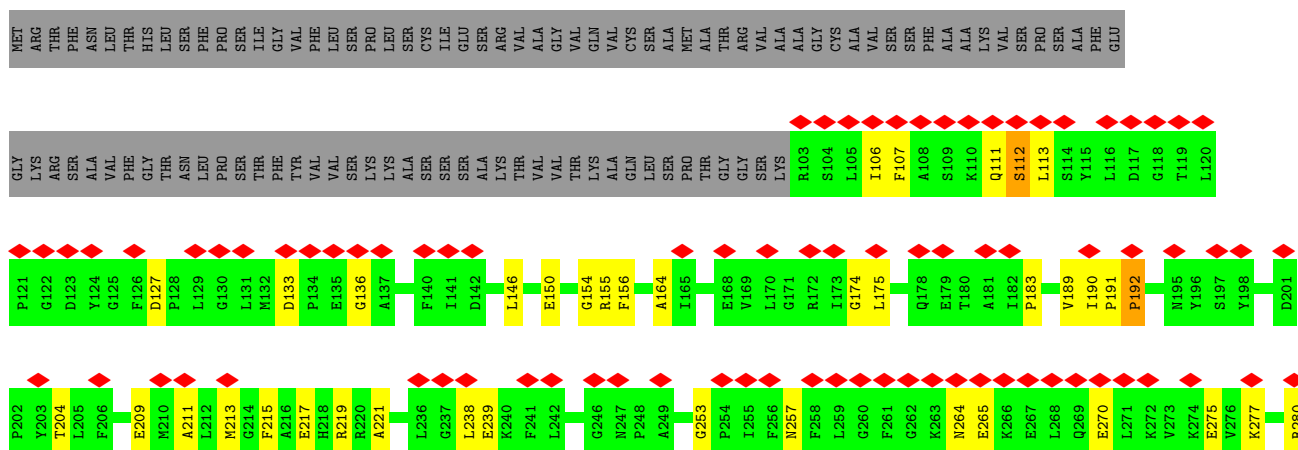
- Molecule 2: Chlorophyll a-b binding protein, chloroplastic

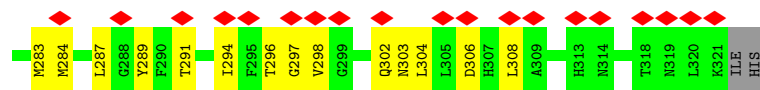


- Molecule 3: Chlorophyll a-b binding protein, chloroplastic

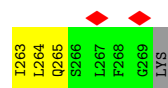
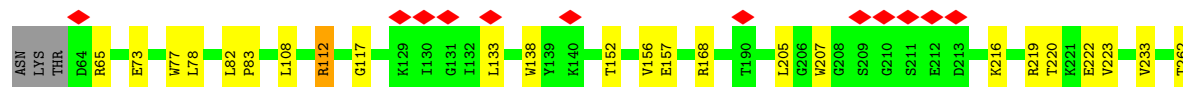


- Chain 6:

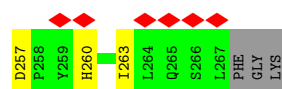
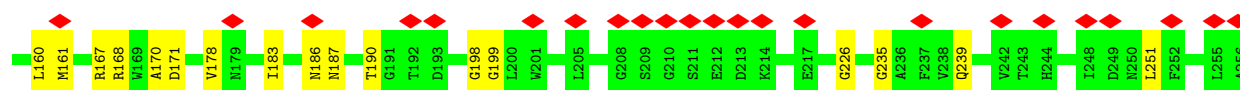
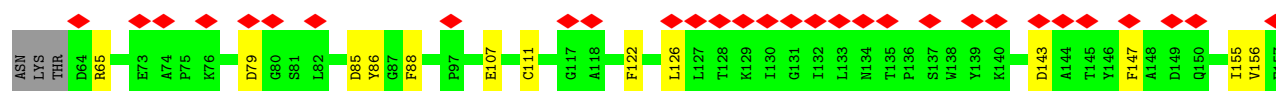




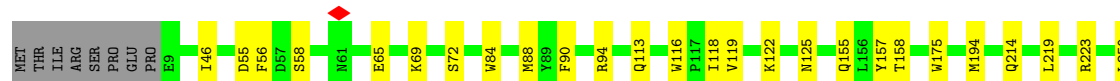
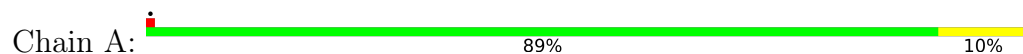
- Molecule 5: Chlorophyll a-b binding protein, chloroplastic



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



- Molecule 6: Photosystem I P700 chlorophyll a apoprotein A1

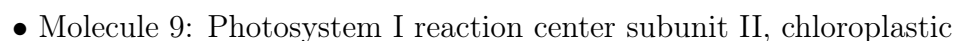


- Molecule 7: Photosystem I P700 chlorophyll a apoprotein A2

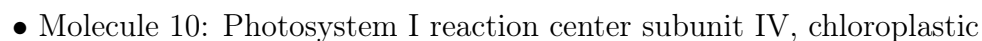
Opinion	Percentage
Doing a good job	87%
Doing a bad job	13%



Satisfaction Level	Percentage
Satisfied	84%
Not Satisfied	15%



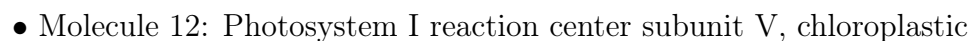
Response	Percentage
Yes	59%
No	9%
Don't know	32%



Response	Percentage
Yes	44%
No	5%
Don't know	52%



Response	Percentage
Yes, the U.S. is a democracy	59%
No, the U.S. is not a democracy	7%
Don't know	35%



Chain G:  54% 9% 37%

MET ALA SER CYS ALA ALA SER MET THR VAL ALA ALA SER SER LEU LEU LEU LYS ALA ASN PHE SER SER GLY LEU ARG ARG GLY THR LYS VAL ASP SER SER ILE ALA ALA MET MET SER ARG SER SER SER PHE SER ALA SER LYS THR ALA ALA ILE LYS SER SER SER SER THR CYS GLU A59

G76 Q84 R85 V83 V95 T100 D103 Q110 E111 V112 K117 G123 F124 T125 I126 W132 T146 Q154 F155


- Molecule 13: Photosystem I reaction center subunit VI, chloroplastic

Chain H:  7% 61% 7% 32%

MET ALA ALA ALA SER THR MET VAL ALA SER GLY LEU ALA GLY SER SER LEU ALA GLN LYS PHE SER ILE ALA PRO LYS SER VAL SER VAL ARG SER PRO SER LYS VAL GLY ALA ILE SER ALA K45 Y46 Q47 E48 F53 Y76 F84 F87 A88 G89 A90 F91

T92 A93 R94 G95 L96 G104 T108 D119 M133 G134 K139

- Molecule 14: Photosystem I reaction center subunit VIII

Chain I:  81% 14% 6%

M1 I9 L13 F18 P19 E34 ILE ILE

- Molecule 15: Photosystem I reaction center subunit IX

Chain J:  95% 5%

M1 E28 R31 L41

- Molecule 16: Photosystem I subunit X

Chain K:  61% 39%

MET ALA ALA MET THR THR MET SER VAL ALA THR VAL ARG GLN PHE GLY LEU LYS THR THR SER PHE SER LYS PRO LEU PRO SER LEU ALA ALA ARG LYS THR ALA GLY LYS ALA THR LEU GLY ALA ARG CYS ASP Y50 D92 V117 A130 LEU

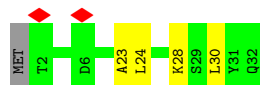
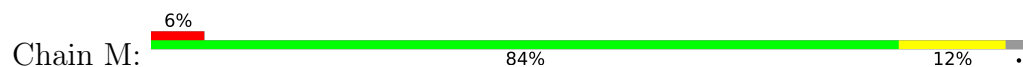
- Molecule 17: PSI subunit V

Chain L:  68% 5% 27%

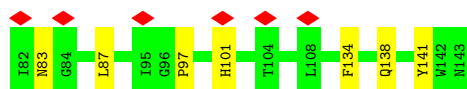
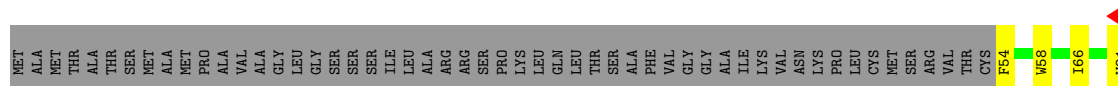
MET ALA ALA MET THR ARG ALA SER GLY LEU LEU ALA MET GLU ARG VAL GLN ARG VAL SER LYS THR THR GLY VAL SER ASN ARG THR PHE LEU GLY ASN ARG GLY LEU ARG ALA THR SER ALA PRO GLN ALA LEU ARG VAL D92 V117 A130 LEU



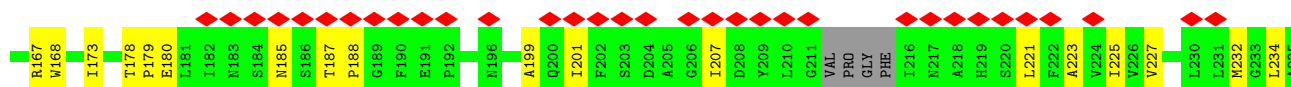
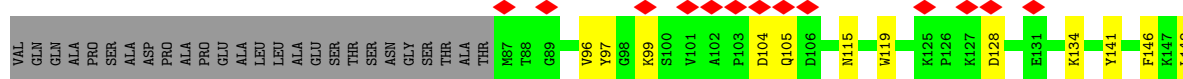
• Molecule 18: Photosystem I reaction center subunit XII



• Molecule 19: Photosystem I subunit O



• 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	144586	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.250	Depositor
Minimum map value	-0.039	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0188	Depositor
Map size (Å)	332.8, 332.8, 332.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, XAT, CLA, LMT, CHL, LHG, LMG, DGD, PQN, SF4, BCR, LUT, 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	U	0.28	0/1708	0.45	0/2327
1	V	0.27	0/1677	0.46	0/2284
1	W	0.28	0/1770	0.47	0/2406
2	1	0.29	0/1527	0.49	0/2088
2	5	0.28	0/1522	0.51	1/2081 (0.0%)
3	2	0.26	0/1676	0.46	0/2296
3	6	0.30	0/1634	0.48	0/2240
4	3	0.28	0/1770	0.47	0/2400
4	7	0.36	1/1738 (0.1%)	0.59	4/2360 (0.2%)
5	4	0.26	0/1650	0.47	0/2255
5	8	0.26	0/1631	0.46	0/2230
6	A	0.28	0/6032	0.46	0/8227
7	B	0.27	0/6064	0.46	0/8274
8	C	0.27	0/605	0.53	0/821
9	D	0.28	0/1142	0.51	0/1546
10	E	0.28	0/518	0.50	0/704
11	F	0.28	0/1277	0.52	0/1725
12	G	0.26	0/758	0.46	0/1034
13	H	0.27	0/753	0.48	0/1013
14	I	0.31	0/273	0.46	0/373
15	J	0.27	0/334	0.48	0/457
16	K	0.26	0/571	0.46	0/773
17	L	0.29	0/1263	0.45	0/1725
18	M	0.28	0/231	0.46	0/312
19	O	0.26	0/738	0.49	0/1009
20	9	0.28	0/1764	0.50	0/2397
All	All	0.28	1/40626 (0.0%)	0.48	5/55357 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	7	183	PRO	CG-CD	-8.08	1.24	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	7	183	PRO	N-CD-CG	-11.22	86.37	103.20
4	7	183	PRO	CA-N-CD	-6.39	102.55	111.50
4	7	192	PRO	CA-N-CD	-5.54	103.75	111.50
4	7	183	PRO	CA-CB-CG	-5.46	93.63	104.00
2	5	156	GLU	CA-CB-CG	5.23	124.90	113.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	U	1659	0	1592	31	0
1	V	1630	0	1562	22	0
1	W	1734	0	1664	20	0
2	1	1478	0	1453	16	0
2	5	1473	0	1448	57	0
3	2	1625	0	1584	22	0
3	6	1583	0	1537	44	0
4	3	1719	0	1685	23	0
4	7	1687	0	1651	47	0
5	4	1600	0	1567	23	0
5	8	1582	0	1553	33	0
6	A	5837	0	5725	67	0
7	B	5850	0	5622	68	0
8	C	595	0	573	10	0
9	D	1114	0	1116	11	0
10	E	507	0	503	4	0
11	F	1251	0	1303	13	0
12	G	740	0	723	13	0
13	H	736	0	721	6	0
14	I	266	0	274	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	J	325	0	341	1	0
16	K	565	0	587	1	0
17	L	1228	0	1238	9	0
18	M	230	0	251	4	0
19	O	711	0	705	10	0
20	9	1713	0	1675	39	0
21	1	103	0	78	2	0
21	2	289	0	210	11	0
21	3	56	0	47	3	0
21	4	182	0	122	8	0
21	5	90	0	61	5	0
21	6	310	0	243	9	0
21	7	46	0	31	3	0
21	8	186	0	128	7	0
21	9	207	0	132	18	0
21	U	319	0	267	12	0
21	V	263	0	168	4	0
21	W	259	0	156	4	0
22	1	645	0	581	11	0
22	2	400	0	322	7	0
22	3	745	0	719	19	0
22	4	532	0	474	15	0
22	5	568	0	442	21	0
22	6	416	0	357	13	0
22	7	626	0	498	20	0
22	8	526	0	448	18	0
22	9	401	0	348	8	0
22	A	2769	0	2877	56	0
22	B	2419	0	2498	52	0
22	F	155	0	137	5	0
22	G	141	0	105	4	0
22	H	38	0	26	0	0
22	J	50	0	39	0	0
22	K	204	0	183	4	0
22	L	190	0	203	3	0
22	O	109	0	55	4	0
22	U	464	0	467	13	0
22	V	387	0	306	9	0
22	W	383	0	308	5	0
23	1	42	0	56	3	0
23	2	42	0	56	4	0
23	3	42	0	56	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	4	42	0	56	3	0
23	5	42	0	56	3	0
23	6	42	0	56	2	0
23	7	42	0	56	2	0
23	8	42	0	56	2	0
23	9	126	0	168	14	0
23	U	84	0	112	8	0
23	V	84	0	112	6	0
23	W	84	0	112	6	0
24	1	44	0	56	5	0
24	2	44	0	56	6	0
24	3	44	0	56	6	0
24	4	44	0	56	11	0
24	5	44	0	56	8	0
24	6	44	0	56	7	0
24	7	44	0	56	3	0
24	8	44	0	56	4	0
24	U	44	0	56	0	0
24	V	44	0	56	0	0
24	W	44	0	56	1	0
25	9	44	0	56	3	0
25	U	44	0	56	3	0
25	V	44	0	56	2	0
25	W	44	0	56	3	0
26	1	49	0	74	2	0
26	2	32	0	34	0	0
26	3	32	0	34	0	0
26	4	38	0	46	3	0
26	5	37	0	44	0	0
26	6	32	0	34	2	0
26	7	34	0	38	0	0
26	8	38	0	46	0	0
26	9	28	0	26	0	0
26	A	78	0	99	0	0
26	B	35	0	40	0	0
26	U	45	0	60	1	0
26	V	42	0	54	0	0
26	W	45	0	60	1	0
27	1	40	0	56	1	0
27	2	40	0	56	5	0
27	3	80	0	112	16	0
27	4	40	0	56	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	6	40	0	56	5	0
27	7	80	0	112	10	0
27	8	40	0	56	7	0
27	A	239	0	333	29	0
27	B	280	0	392	31	0
27	F	40	0	56	3	0
27	G	40	0	56	4	0
27	I	40	0	56	4	0
27	J	40	0	56	4	0
27	K	80	0	112	10	0
27	L	120	0	168	13	0
27	M	40	0	56	5	0
27	O	40	0	56	5	0
28	2	47	0	67	0	0
28	A	34	0	38	0	0
28	G	32	0	34	2	0
28	J	90	0	126	0	0
28	L	44	0	58	0	0
29	A	33	0	46	0	0
29	B	33	0	46	0	0
30	A	8	0	0	0	0
30	C	16	0	0	0	0
31	A	35	0	46	0	0
31	B	31	0	35	0	0
31	G	35	0	46	0	0
31	K	35	0	46	0	0
32	B	66	0	96	0	0
33	A	2	0	0	0	0
All	All	57715	0	56699	925	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (925) 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)
27:L:305:BCR:HC8	27:L:305:BCR:H331	1.56	0.86
6:A:495:THR:HG21	22:A:836:CLA:HMD1	1.56	0.86
4:7:164:ALA:HB2	24:7:619:XAT:H163	1.58	0.85
22:B:813:CLA:HMC1	22:B:813:CLA:HBC2	1.60	0.83
22:B:823:CLA:CBC	27:B:1609:BCR:H343	2.11	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:108:GLU:HB3	2:5:220:LEU:HD21	1.63	0.79
5:8:161:MET:HG3	22:8:609:CLA:HMC3	1.66	0.78
22:7:610:CLA:HMC2	23:7:618:LUT:C31	2.15	0.76
2:5:52:LEU:HD21	21:5:601:CHL:HMA3	1.68	0.76
27:A:856:BCR:H331	27:A:856:BCR:HC8	1.68	0.76
27:3:620:BCR:H383	27:3:620:BCR:H23C	1.68	0.75
22:8:604:CLA:HMB3	24:8:620:XAT:H371	1.65	0.75
7:B:519:VAL:HG11	7:B:593:TYR:CE1	2.21	0.75
22:7:602:CLA:HMC2	24:7:619:XAT:C31	2.17	0.75
6:A:125:ASN:O	11:F:113:ARG:NH2	2.20	0.74
22:B:823:CLA:HBC3	27:B:1609:BCR:H343	1.68	0.74
27:A:851:BCR:H23C	27:A:851:BCR:H403	1.68	0.73
2:5:114:ASN:ND2	2:5:217:THR:O	2.21	0.73
4:7:150:GLU:OE2	4:7:280:ARG:NH1	2.20	0.73
27:L:306:BCR:H321	27:L:306:BCR:HC8	1.71	0.72
21:4:608:CHL:HBB1	21:4:608:CHL:HMB1	1.71	0.71
22:B:815:CLA:HMA1	27:B:845:BCR:H343	1.72	0.71
27:B:801:BCR:H383	27:B:801:BCR:H23C	1.72	0.71
27:F:305:BCR:H383	27:F:305:BCR:H23C	1.72	0.71
20:9:119:TRP:O	21:9:601:CHL:ND	2.24	0.71
2:5:128:GLN:NE2	22:5:604:CLA:OBD	2.23	0.71
1:W:98:GLU:OE2	1:W:214:ILE:HD11	1.91	0.70
22:A:803:CLA:OBD	22:B:802:CLA:HMB3	1.91	0.70
7:B:351:HIS:ND1	22:B:817:CLA:OBD	2.25	0.70
22:B:806:CLA:CBB	22:B:828:CLA:HMC2	2.22	0.70
2:1:195:LYS:NZ	26:1:630:LHG:O5	2.24	0.70
5:8:239:GLN:OE1	22:8:613:CLA:NA	2.25	0.69
7:B:519:VAL:HG11	7:B:593:TYR:CD1	2.28	0.69
2:5:91:LEU:HD12	2:5:169:LYS:CE	2.23	0.69
2:5:91:LEU:HD12	2:5:169:LYS:HE2	1.74	0.68
21:W:609:CHL:HBB1	21:W:609:CHL:HMB1	1.74	0.68
25:9:623:NEX:H192	25:9:623:NEX:H183	1.75	0.68
3:6:116:LEU:CD2	22:6:610:CLA:HMC1	2.24	0.68
2:1:208:ALA:O	2:1:212:ILE:HD12	1.92	0.68
27:B:801:BCR:H381	22:F:301:CLA:HMC2	1.74	0.68
22:4:602:CLA:HMC2	24:4:620:XAT:C31	2.23	0.67
27:B:845:BCR:H383	27:B:845:BCR:H23C	1.75	0.67
27:7:621:BCR:H331	27:7:621:BCR:HC8	1.77	0.67
3:6:225:LYS:HG3	22:6:611:CLA:HMD3	1.76	0.67
4:7:298:VAL:HG13	4:7:302:GLN:NE2	2.10	0.67
4:7:238:LEU:O	4:7:238:LEU:HD12	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:296:THR:HG22	4:3:319:ASN:OD1	1.95	0.66
27:7:620:BCR:H321	27:7:620:BCR:HC8	1.75	0.66
1:W:211:VAL:O	1:W:214:ILE:HG22	1.96	0.66
27:3:620:BCR:H331	27:3:620:BCR:HC8	1.77	0.66
22:4:611:CLA:NC	26:4:630:LHG:O5	2.28	0.66
4:7:174:GLY:O	4:7:175:LEU:HD12	1.96	0.66
1:U:259:THR:O	1:U:259:THR:HG22	1.95	0.65
22:4:604:CLA:C2B	27:4:621:BCR:H323	2.27	0.65
27:M:2001:BCR:H23C	27:M:2001:BCR:H382	1.79	0.65
4:7:221:ALA:HB2	22:7:609:CLA:HMA1	1.78	0.65
27:2:621:BCR:H382	27:2:621:BCR:H23C	1.79	0.65
4:7:213:MET:HG3	22:7:609:CLA:HMC3	1.78	0.65
5:4:133:LEU:HD23	5:4:133:LEU:O	1.97	0.64
2:5:239:ILE:HG21	5:8:155:ILE:HD11	1.80	0.64
22:7:606:CLA:H3A	27:7:620:BCR:C21	2.27	0.64
20:9:199:ALA:N	21:9:607:CHL:O1D	2.31	0.64
4:7:302:GLN:NE2	4:7:303:ASN:OD1	2.30	0.64
22:A:829:CLA:HED1	22:A:830:CLA:H3A	1.80	0.64
22:3:606:CLA:H3A	27:3:620:BCR:C21	2.27	0.64
27:7:621:BCR:H331	27:7:621:BCR:C8	2.28	0.64
27:B:843:BCR:H382	27:B:843:BCR:H23C	1.79	0.64
27:K:205:BCR:H391	22:9:611:CLA:C2	2.28	0.63
6:A:122:LYS:NZ	11:F:130:THR:OG1	2.26	0.63
7:B:40:GLU:OE2	7:B:44:GLN:NE2	2.31	0.63
12:G:146:THR:HG21	28:G:202:LMG:HC91	1.80	0.63
24:5:618:XAT:H28	24:5:618:XAT:H361	1.79	0.63
5:8:186:ASN:OD1	5:8:187:ASN:N	2.31	0.63
1:W:225:PHE:CE1	1:W:225:PHE:CG	2.84	0.62
27:A:856:BCR:H331	27:A:856:BCR:C8	2.29	0.62
27:J:102:BCR:H383	27:J:102:BCR:H23C	1.81	0.62
21:U:607:CHL:HED1	1:W:262:VAL:HG21	1.80	0.62
4:3:192:PRO:HG3	22:A:817:CLA:HMD2	1.81	0.62
3:6:263:THR:HG23	3:6:265:PHE:H	1.65	0.62
22:A:836:CLA:HMD2	22:A:837:CLA:HBB1	1.82	0.62
20:9:236:GLU:HG3	22:9:609:CLA:C4B	2.29	0.62
7:B:656:VAL:HG22	22:B:840:CLA:HMB3	1.80	0.62
6:A:564:LYS:NZ	7:B:673:GLU:OE2	2.32	0.61
22:2:604:CLA:C3B	24:2:620:XAT:H183	2.30	0.61
6:A:399:VAL:HG13	27:A:851:BCR:H343	1.83	0.61
15:J:28:GLU:OE1	15:J:31:ARG:NH1	2.32	0.61
2:5:149:PHE:O	2:5:150:LEU:HD22	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:7:620:BCR:H321	27:7:620:BCR:C8	2.31	0.61
1:U:197:LEU:HD22	20:9:260:LEU:HD21	1.81	0.61
12:G:84:GLN:OE1	12:G:85:ARG:NH1	2.32	0.61
6:A:598:TYR:OH	22:A:801:CLA:HED2	2.01	0.61
22:W:602:CLA:HMC2	23:W:2621:LUT:C31	2.31	0.61
20:9:148:LEU:HD23	23:9:624:LUT:C24	2.31	0.61
6:A:371:MET:SD	6:A:504:SER:HB2	2.40	0.61
6:A:418:THR:HG23	6:A:419:GLN:HE21	1.66	0.61
5:8:65:ARG:NH2	5:8:85:ASP:OD1	2.34	0.60
2:5:87:LYS:HB3	2:5:169:LYS:NZ	2.16	0.60
27:L:306:BCR:H321	27:L:306:BCR:C8	2.32	0.60
27:1:619:BCR:H382	27:1:619:BCR:H23C	1.83	0.60
27:3:620:BCR:H331	27:3:620:BCR:C8	2.30	0.60
22:A:816:CLA:H3A	22:A:816:CLA:O2A	2.01	0.60
27:A:852:BCR:H362	22:A:854:CLA:H2	1.81	0.60
22:B:804:CLA:H3A	18:M:30:LEU:HD13	1.82	0.60
1:U:172:GLU:HG3	21:U:609:CHL:C4B	2.31	0.59
9:D:167:HIS:HB3	9:D:168:PRO:HD3	1.83	0.59
3:6:77:TRP:NE1	3:6:89:ASP:OD2	2.35	0.59
4:7:291:THR:HG21	22:7:613:CLA:HAC2	1.83	0.59
6:A:113:GLN:NE2	22:A:810:CLA:OBD	2.34	0.59
6:A:471:ASP:O	6:A:475:GLN:NE2	2.35	0.59
2:1:57:ARG:NH2	2:1:68:ASP:OD1	2.36	0.59
6:A:735:ILE:HG21	22:A:829:CLA:HMC2	1.83	0.59
27:O:2004:BCR:H383	27:O:2004:BCR:H23C	1.85	0.59
22:V:602:CLA:HMC2	23:V:2621:LUT:C31	2.33	0.59
6:A:403:ALA:HB2	27:A:851:BCR:H323	1.85	0.59
1:V:136:GLN:O	1:V:139:SER:OG	2.21	0.59
2:5:188:GLU:O	2:5:192:LYS:HG3	2.03	0.59
1:U:135:ALA:HB2	21:U:607:CHL:HED2	1.84	0.59
22:B:823:CLA:HBC2	27:B:1609:BCR:H343	1.84	0.59
5:4:112:ARG:NH1	21:4:608:CHL:OBD	2.35	0.59
2:5:108:GLU:CB	2:5:220:LEU:HD21	2.33	0.59
7:B:238:ASP:OD1	7:B:251:GLY:N	2.36	0.59
27:B:848:BCR:H383	27:B:848:BCR:H23C	1.84	0.59
7:B:61:THR:HG23	7:B:142:LEU:HD13	1.85	0.58
2:5:210:GLN:OE1	22:5:613:CLA:C4D	2.51	0.58
4:7:291:THR:HG21	22:7:613:CLA:CAC	2.33	0.58
3:6:216:LEU:O	3:6:220:ARG:HG2	2.04	0.58
21:3:608:CHL:HBB1	21:3:608:CHL:HMB1	1.84	0.58
7:B:696:LYS:NZ	8:C:81:TYR:O	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:112:ARG:NE	5:4:222:GLU:OE2	2.36	0.58
3:6:101:LYS:O	3:6:104:VAL:HG12	2.04	0.58
21:8:607:CHL:HMB3	24:8:620:XAT:H382	1.85	0.58
1:U:237:GLY:O	1:U:241:ASN:ND2	2.32	0.58
4:3:217:GLU:OE1	4:3:220:ARG:NH2	2.36	0.58
7:B:294:ASN:ND2	12:G:110:GLN:O	2.35	0.58
2:5:50:GLU:N	2:5:69:PHE:O	2.37	0.58
2:5:128:GLN:HG2	2:5:129:ALA:H	1.68	0.58
3:6:122:PHE:O	3:6:126:ALA:N	2.32	0.58
1:W:113:LEU:HD22	1:W:239:LEU:HD21	1.86	0.58
3:2:112:ARG:NE	21:2:608:CHL:OBD	2.35	0.58
3:2:160:LEU:HD23	21:2:606:CHL:HMA2	1.86	0.58
22:5:603:CLA:HBC3	24:5:618:XAT:H391	1.86	0.58
12:G:85:ARG:NH2	12:G:123:GLY:O	2.37	0.57
19:O:134:PHE:O	19:O:138:GLN:NE2	2.36	0.57
19:O:97:PRO:O	19:O:101:HIS:ND1	2.37	0.57
7:B:339:ALA:HB2	27:B:847:BCR:H372	1.85	0.57
6:A:371:MET:SD	22:A:828:CLA:HMC2	2.45	0.57
22:U:602:CLA:HMC2	23:U:2621:LUT:C31	2.34	0.57
22:B:824:CLA:H2A	22:B:824:CLA:O1A	2.02	0.57
22:U:604:CLA:CED	22:U:604:CLA:H2A	2.35	0.57
6:A:317:HIS:HB3	6:A:322:ILE:HD11	1.87	0.56
7:B:384:THR:HG21	7:B:583:MET:HG2	1.86	0.56
27:3:621:BCR:H331	27:3:621:BCR:C8	2.35	0.56
3:2:88:PHE:CE2	24:2:620:XAT:H383	2.39	0.56
22:2:610:CLA:H52	23:2:619:LUT:H10	1.87	0.56
5:4:216:LYS:O	5:4:219:ARG:N	2.39	0.56
6:A:320:LYS:NZ	6:A:340:GLU:OE2	2.38	0.56
2:5:108:GLU:HG2	2:5:113:GLY:O	2.04	0.56
2:5:131:TYR:CE2	22:5:604:CLA:HMD2	2.41	0.56
4:7:111:GLN:O	4:7:113:LEU:N	2.38	0.56
9:D:109:GLU:OE2	9:D:124:SER:N	2.39	0.56
2:5:232:HIS:NE2	5:8:147:PHE:O	2.39	0.56
22:8:602:CLA:H2	24:8:620:XAT:H162	1.87	0.56
20:9:232:MET:HE2	21:9:606:CHL:HMB3	1.88	0.56
1:W:259:THR:O	1:W:259:THR:HG22	2.05	0.56
7:B:191:THR:HG23	22:B:815:CLA:HMC3	1.88	0.56
3:2:88:PHE:HE2	24:2:620:XAT:H383	1.71	0.56
6:A:379:THR:HG21	6:A:515:VAL:HB	1.87	0.56
3:6:165:GLU:OE1	3:6:168:ARG:NH2	2.39	0.56
26:4:630:LHG:O5	26:4:630:LHG:O7	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:118:ILE:HG23	6:A:119:VAL:N	2.21	0.55
18:M:23:ALA:HB2	27:M:2001:BCR:H342	1.88	0.55
22:8:603:CLA:HMD2	22:8:609:CLA:CHD	2.35	0.55
22:1:611:CLA:H2A	22:1:611:CLA:HED2	1.88	0.55
22:3:617:CLA:C4B	22:3:617:CLA:C1C	2.84	0.55
2:5:87:LYS:HB3	2:5:169:LYS:HZ1	1.70	0.55
5:8:107:GLU:OE1	22:8:602:CLA:NA	2.39	0.55
26:W:2630:LHG:O3	26:W:2630:LHG:O1	2.18	0.55
22:1:602:CLA:HMC2	24:1:618:XAT:C11	2.36	0.55
3:6:108:LEU:HD22	3:6:196:TYR:OH	2.05	0.55
4:7:189:VAL:O	22:7:607:CLA:NB	2.39	0.55
5:8:235:GLY:O	5:8:239:GLN:N	2.31	0.55
21:8:618:CHL:HAB	27:8:621:BCR:H372	1.87	0.55
17:L:97:ALA:HB2	22:L:303:CLA:HMD1	1.88	0.55
6:A:315:ILE:O	6:A:315:ILE:HG13	2.06	0.55
1:V:92:ALA:O	1:V:96:GLU:OE1	2.25	0.55
27:K:202:BCR:H383	27:K:202:BCR:H23C	1.88	0.55
3:6:163:TRP:O	3:6:167:ARG:HG2	2.06	0.55
22:7:603:CLA:HMD2	22:7:609:CLA:CHD	2.37	0.55
22:2:604:CLA:C2B	24:2:620:XAT:H183	2.37	0.55
6:A:430:HIS:CE1	22:A:832:CLA:ND	2.76	0.54
22:A:822:CLA:HMB2	22:A:826:CLA:HMA3	1.88	0.54
20:9:104:ASP:OD1	20:9:105:GLN:N	2.39	0.54
22:B:825:CLA:HMA1	27:B:847:BCR:H14C	1.89	0.54
11:F:103:GLN:HG2	11:F:138:PHE:CD2	2.42	0.54
17:L:67:GLU:OE1	19:O:54:PHE:N	2.40	0.54
27:B:845:BCR:H383	27:B:845:BCR:C23	2.38	0.54
3:6:167:ARG:HD2	22:8:601:CLA:OBD	2.07	0.54
5:8:190:THR:OG1	5:8:199:GLY:N	2.37	0.54
20:9:97:TYR:CE1	20:9:268:ILE:HD11	2.43	0.54
23:9:624:LUT:H181	23:9:624:LUT:H8	1.90	0.54
6:A:175:TRP:HB2	22:A:812:CLA:HMC3	1.87	0.54
6:A:654:SER:HG	7:B:625:TRP:HZ2	1.54	0.54
22:A:810:CLA:HAB	22:B:833:CLA:HMD2	1.89	0.54
1:V:156:SER:O	1:V:160:ILE:HD12	2.07	0.54
5:8:257:ASP:OD2	5:8:260:HIS:HB2	2.08	0.54
1:U:145:TYR:O	1:U:146:LEU:HB2	2.06	0.54
21:U:606:CHL:HMB2	25:U:2623:NEX:H391	1.89	0.54
22:A:802:CLA:CGA	22:A:802:CLA:H3A	2.38	0.54
12:G:112:VAL:HG23	12:G:112:VAL:O	2.08	0.54
22:A:843:CLA:HMC2	22:B:839:CLA:H11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:852:BCR:C32	27:A:852:BCR:HC8	2.38	0.54
1:U:233:VAL:HG13	1:U:234:THR:HG23	1.90	0.53
22:V:610:CLA:HMC2	23:V:2620:LUT:C31	2.37	0.53
1:V:109:ALA:O	1:V:113:LEU:HD23	2.07	0.53
4:3:126:PHE:HE2	24:3:619:XAT:H383	1.73	0.53
1:W:110:LEU:O	1:W:114:THR:HG23	2.09	0.53
27:O:2004:BCR:H321	27:O:2004:BCR:HC8	1.90	0.53
2:1:138:TRP:NE1	22:1:606:CLA:OBD	2.38	0.53
6:A:683:MET:HB3	22:A:802:CLA:C1C	2.38	0.53
22:A:820:CLA:O1A	22:A:830:CLA:HMD1	2.09	0.53
27:O:2004:BCR:HC8	27:O:2004:BCR:C32	2.38	0.53
4:7:287:LEU:O	4:7:291:THR:HG22	2.08	0.53
4:7:296:THR:HG22	4:7:297:GLY:H	1.74	0.53
7:B:583:MET:SD	7:B:584:LEU:N	2.82	0.53
22:F:304:CLA:C1A	22:F:304:CLA:C4D	2.86	0.53
21:2:608:CHL:HMB3	27:2:621:BCR:C16	2.39	0.53
22:A:827:CLA:CHC	27:A:851:BCR:H342	2.39	0.53
7:B:302:LYS:O	7:B:306:GLU:HG2	2.09	0.53
27:G:205:BCR:H23C	27:G:205:BCR:H382	1.91	0.53
22:B:806:CLA:HBB2	22:B:828:CLA:HMC2	1.91	0.53
3:2:65:ARG:NH2	3:2:85:ASP:OD1	2.42	0.53
4:3:126:PHE:CE2	24:3:619:XAT:H383	2.44	0.53
22:B:813:CLA:HMC1	22:B:813:CLA:CBC	2.36	0.53
3:6:171:ASP:OD2	21:6:608:CHL:HBC1	2.09	0.53
22:U:610:CLA:HMC2	23:U:2620:LUT:C31	2.39	0.53
1:V:127:GLU:O	1:V:136:GLN:NE2	2.41	0.53
13:H:133:MET:SD	13:H:134:GLY:O	2.67	0.53
2:5:131:TYR:C	2:5:133:GLY:H	2.12	0.52
24:5:618:XAT:H361	24:5:618:XAT:C28	2.38	0.52
5:8:263:ILE:N	22:8:613:CLA:O1A	2.42	0.52
20:9:234:LEU:HD23	25:9:623:NEX:H203	1.90	0.52
21:9:607:CHL:HHC	21:9:607:CHL:HBB1	1.90	0.52
27:B:801:BCR:H312	22:B:833:CLA:H61	1.90	0.52
20:9:173:ILE:HG21	23:9:620:LUT:H12	1.92	0.52
20:9:180:GLU:HG3	20:9:302:LEU:HD12	1.91	0.52
3:2:117:GLY:HA2	24:2:620:XAT:H181	1.90	0.52
22:7:609:CLA:HBC1	24:7:619:XAT:C19	2.40	0.52
5:4:263:ILE:HG23	5:4:264:LEU:HD22	1.92	0.52
17:L:125:LEU:HD21	17:L:223:LYS:HA	1.91	0.52
27:7:620:BCR:C23	27:7:620:BCR:H383	2.38	0.52
20:9:99:LYS:NZ	20:9:271:GLU:OE1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:233:VAL:HG11	24:4:620:XAT:H12	1.91	0.52
22:V:602:CLA:H42	22:V:602:CLA:HMB2	1.92	0.52
22:G:201:CLA:HMD1	28:G:202:LMG:O5	2.10	0.52
4:7:264:ASN:OD1	4:7:265:GLU:N	2.36	0.52
3:2:234:VAL:HG11	24:2:620:XAT:H12	1.91	0.52
6:A:90:PHE:CE2	22:A:808:CLA:HMD3	2.45	0.52
6:A:462:LEU:HG	22:B:809:CLA:HMC3	1.92	0.52
22:7:602:CLA:CGA	22:7:602:CLA:H3A	2.40	0.52
5:8:86:TYR:N	22:8:602:CLA:OBD	2.36	0.52
5:4:262:THR:OG1	5:4:265:GLN:OE1	2.26	0.52
6:A:503:THR:HG21	22:A:828:CLA:HAB	1.92	0.52
22:V:613:CLA:CHB	22:V:614:CLA:HMD3	2.40	0.52
22:B:837:CLA:O1A	22:B:838:CLA:HMD1	2.09	0.52
22:6:603:CLA:HMD2	22:6:609:CLA:C1D	2.40	0.52
4:3:283:MET:HE3	22:3:602:CLA:HMC3	1.92	0.51
22:3:603:CLA:HMD2	22:3:609:CLA:CHD	2.40	0.51
1:U:233:VAL:HG13	1:U:234:THR:N	2.24	0.51
5:4:152:THR:O	5:4:156:VAL:HG23	2.10	0.51
7:B:662:MET:HB2	22:B:803:CLA:C1C	2.39	0.51
2:1:186:LEU:HD21	2:1:190:LYS:HE3	1.91	0.51
22:A:837:CLA:HMB1	27:A:851:BCR:H281	1.92	0.51
22:5:602:CLA:HMC2	24:5:618:XAT:C11	2.41	0.51
21:8:608:CHL:O1A	22:8:610:CLA:HMD2	2.11	0.51
22:8:614:CLA:O1D	22:8:614:CLA:H2A	2.10	0.51
20:9:96:VAL:O	20:9:96:VAL:HG22	2.10	0.51
5:4:157:GLU:OE2	21:4:606:CHL:HMB3	2.11	0.51
22:A:801:CLA:HAA1	22:B:802:CLA:HMB1	1.92	0.51
27:B:844:BCR:H23C	27:B:844:BCR:H403	1.92	0.51
27:L:306:BCR:H23C	27:L:306:BCR:C38	2.41	0.51
2:5:128:GLN:HG2	2:5:129:ALA:N	2.25	0.51
23:9:624:LUT:C24	23:9:624:LUT:H372	2.40	0.51
27:4:621:BCR:H402	27:4:621:BCR:H23C	1.93	0.51
18:M:24:LEU:HD11	18:M:28:LYS:HE2	1.92	0.51
2:5:116:VAL:HG12	2:5:116:VAL:O	2.10	0.51
5:8:251:LEU:HD22	23:8:619:LUT:H172	1.92	0.51
13:H:76:TYR:OH	17:L:110:GLU:OE1	2.25	0.51
4:7:156:PHE:CD2	22:7:609:CLA:HMD3	2.45	0.51
1:U:245:HIS:CE1	22:U:614:CLA:NC	2.78	0.51
22:O:2002:CLA:O1D	22:O:2002:CLA:H2A	2.11	0.51
22:3:603:CLA:HMD2	22:3:609:CLA:C1D	2.41	0.51
5:8:88:PHE:HE2	24:8:620:XAT:H173	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:107:LEU:CD2	22:V:610:CLA:HMC1	2.41	0.51
4:3:316:VAL:N	22:3:613:CLA:O1A	2.40	0.51
2:1:71:PHE:HE2	24:1:618:XAT:H183	1.75	0.51
27:3:620:BCR:H383	27:3:620:BCR:C23	2.40	0.51
2:5:65:ALA:N	2:5:68:ASP:OD2	2.42	0.51
5:8:161:MET:CG	22:8:609:CLA:HMC3	2.40	0.51
22:A:803:CLA:CGA	22:A:803:CLA:H3A	2.41	0.50
27:A:849:BCR:H383	27:A:849:BCR:H23C	1.92	0.50
27:A:852:BCR:HC8	27:A:852:BCR:H321	1.94	0.50
9:D:70:THR:HG23	9:D:70:THR:O	2.11	0.50
1:U:127:GLU:N	1:U:127:GLU:OE1	2.43	0.50
1:U:135:ALA:CB	21:U:607:CHL:HED2	2.42	0.50
1:U:222:PHE:CE2	22:U:613:CLA:HMC2	2.46	0.50
17:L:222:VAL:O	17:L:222:VAL:HG13	2.11	0.50
2:5:156:GLU:HG3	22:5:609:CLA:C4B	2.42	0.50
2:1:123:ALA:HB1	12:G:155:PHE:HB2	1.93	0.50
2:5:96:TRP:CD1	22:5:609:CLA:HMD3	2.47	0.50
2:5:240:ILE:HG23	2:5:240:ILE:O	2.11	0.50
1:W:168:MET:HA	1:W:171:VAL:HG22	1.93	0.50
4:3:156:PHE:CD2	22:3:609:CLA:HMD3	2.46	0.50
22:4:610:CLA:HMC2	23:4:619:LUT:C31	2.42	0.50
27:J:102:BCR:H383	27:J:102:BCR:C23	2.41	0.50
27:L:305:BCR:H392	27:L:305:BCR:H23C	1.93	0.50
3:6:234:VAL:HG11	24:6:620:XAT:H12	1.94	0.50
27:7:620:BCR:H383	27:7:620:BCR:H23C	1.94	0.50
20:9:207:ILE:HG21	21:9:606:CHL:HMD2	1.92	0.50
22:3:604:CLA:C2B	24:3:619:XAT:H183	2.42	0.50
5:4:117:GLY:HA2	24:4:620:XAT:H181	1.94	0.50
22:A:827:CLA:H203	27:A:851:BCR:H381	1.93	0.50
20:9:223:ALA:HB3	21:9:605:CHL:HMC	1.93	0.50
1:V:253:ASN:OD1	1:V:255:TRP:N	2.44	0.50
22:3:606:CLA:H3A	27:3:620:BCR:H21C	1.93	0.50
22:A:802:CLA:HBB1	22:A:802:CLA:HMB1	1.94	0.50
27:F:305:BCR:H383	27:F:305:BCR:C23	2.41	0.50
6:A:713:GLN:NE2	10:E:113:VAL:O	2.43	0.50
1:V:168:MET:HA	1:V:171:VAL:HG12	1.93	0.49
6:A:436:SER:OG	7:B:681:ALA:HB2	2.12	0.49
22:B:828:CLA:H191	27:B:845:BCR:H351	1.94	0.49
8:C:32:ASP:OD1	8:C:32:ASP:N	2.44	0.49
22:6:603:CLA:HMC2	24:6:620:XAT:C13	2.41	0.49
22:6:604:CLA:C1B	27:6:621:BCR:H402	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:7:296:THR:HG22	4:7:297:GLY:N	2.27	0.49
3:6:182:PRO:HB2	27:6:621:BCR:H322	1.93	0.49
22:W:604:CLA:HMB3	23:W:2621:LUT:H162	1.94	0.49
9:D:92:ARG:O	9:D:96:VAL:HG22	2.13	0.49
27:3:620:BCR:HC8	27:3:620:BCR:C33	2.43	0.49
6:A:56:PHE:CD2	22:A:806:CLA:HMC2	2.47	0.49
20:9:128:ASP:OD1	20:9:128:ASP:N	2.46	0.49
3:2:231:MET:HE1	21:2:602:CHL:CBB	2.42	0.49
22:3:602:CLA:HMC2	24:3:619:XAT:C31	2.42	0.49
6:A:738:THR:OG1	22:A:801:CLA:HED1	2.12	0.49
2:5:149:PHE:O	2:5:149:PHE:CD1	2.65	0.49
4:7:277:LYS:O	4:7:280:ARG:HB2	2.12	0.49
5:8:122:PHE:O	5:8:126:LEU:N	2.39	0.49
19:O:87:LEU:HD23	19:O:87:LEU:H	1.76	0.49
1:U:83:GLY:O	1:V:90:THR:HG22	2.13	0.49
22:1:610:CLA:HMC2	23:1:617:LUT:C31	2.43	0.49
3:2:129:LYS:HE2	3:2:253:LEU:HD12	1.94	0.49
6:A:582:CYS:O	7:B:669:GLY:N	2.37	0.49
2:5:156:GLU:HG3	22:5:609:CLA:C1B	2.43	0.49
4:7:150:GLU:OE2	4:7:280:ARG:NH2	2.46	0.49
23:9:624:LUT:H181	23:9:624:LUT:C8	2.43	0.49
3:6:225:LYS:HD2	26:6:630:LHG:C23	2.43	0.49
27:2:621:BCR:H11C	27:2:621:BCR:H341	1.68	0.49
22:A:837:CLA:O2D	22:A:837:CLA:H2A	2.13	0.49
20:9:201:ILE:HD12	21:9:606:CHL:CBC	2.42	0.49
21:4:608:CHL:HMB3	27:4:621:BCR:C14	2.42	0.49
22:B:814:CLA:H3A	27:B:845:BCR:H272	1.94	0.49
4:7:154:GLY:N	4:7:283:MET:HE2	2.27	0.49
6:A:214:GLN:O	6:A:219:LEU:HD13	2.12	0.48
3:6:250:ASP:OD1	3:6:251:ASN:N	2.46	0.48
5:8:161:MET:HE2	27:8:621:BCR:H352	1.95	0.48
20:9:168:TRP:CE2	21:9:608:CHL:HED3	2.48	0.48
1:U:152:VAL:HG11	21:U:606:CHL:HMD1	1.96	0.48
5:4:222:GLU:HG3	22:4:610:CLA:C4B	2.44	0.48
22:B:803:CLA:H142	27:I:101:BCR:H271	1.94	0.48
27:K:202:BCR:H23C	27:K:202:BCR:C38	2.43	0.48
22:U:602:CLA:HMC2	23:U:2621:LUT:H31	1.96	0.48
3:2:203:ASP:OD1	3:2:206:GLY:N	2.46	0.48
6:A:503:THR:CG2	22:A:828:CLA:HAB	2.43	0.48
6:A:588:ASP:OD1	6:A:723:ARG:NH1	2.46	0.48
2:5:96:TRP:HD1	22:5:609:CLA:HMD3	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:245:HIS:HE1	22:U:614:CLA:NC	2.10	0.48
1:V:148:ASN:OD1	1:V:151:LEU:HD23	2.14	0.48
2:1:240:ILE:HG13	2:1:240:ILE:O	2.12	0.48
4:3:241:PHE:HD2	4:3:255:ILE:HD11	1.79	0.48
21:3:608:CHL:HMB3	27:3:620:BCR:H16C	1.95	0.48
18:M:23:ALA:HB2	27:M:2001:BCR:C34	2.44	0.48
21:9:608:CHL:HMB3	25:9:623:NEX:C15	2.42	0.48
6:A:503:THR:HB	6:A:507:TRP:HE1	1.77	0.48
3:6:112:ARG:NH1	21:6:608:CHL:OBD	2.46	0.48
20:9:146:PHE:HB2	20:9:148:LEU:CD1	2.44	0.48
7:B:477:LEU:O	7:B:478:LEU:HB2	2.14	0.48
22:8:610:CLA:H2A	22:8:610:CLA:O1D	2.13	0.48
21:U:606:CHL:OMC	23:U:2621:LUT:H163	2.13	0.48
1:V:129:VAL:HG11	1:V:131:PHE:CE1	2.49	0.48
6:A:599:ASN:OD1	22:A:803:CLA:CMC	2.62	0.48
22:A:808:CLA:HMB3	22:A:809:CLA:H3A	1.96	0.48
7:B:25:ILE:HA	22:B:804:CLA:HMD3	1.96	0.48
7:B:450:GLU:OE2	11:F:137:ARG:NE	2.46	0.48
27:F:305:BCR:HC8	27:F:305:BCR:H311	1.96	0.48
6:A:72:SER:HB2	22:A:812:CLA:HMD3	1.95	0.48
27:A:856:BCR:H403	27:A:856:BCR:H23C	1.95	0.48
7:B:175:LEU:HG	22:B:824:CLA:HMD3	1.95	0.48
11:F:102:ARG:NE	11:F:152:GLY:O	2.46	0.48
2:5:101:VAL:HG11	23:5:617:LUT:H12	1.96	0.47
3:6:225:LYS:NZ	26:6:630:LHG:O10	2.21	0.47
20:9:301:PRO:O	23:9:620:LUT:O3	2.32	0.47
22:A:809:CLA:HMC3	22:A:810:CLA:HMD2	1.95	0.47
22:4:602:CLA:HMC2	24:4:620:XAT:H31	1.94	0.47
3:6:246:THR:HG22	3:6:247:GLY:N	2.29	0.47
27:7:621:BCR:HC8	27:7:621:BCR:C33	2.42	0.47
5:8:161:MET:CE	27:8:621:BCR:H352	2.44	0.47
4:3:132:MET:O	4:3:132:MET:HG2	2.13	0.47
2:5:148:GLU:OE1	22:5:606:CLA:C1C	2.61	0.47
21:6:618:CHL:HHC	21:6:618:CHL:HBB1	1.96	0.47
20:9:258:ASP:OD2	20:9:263:SER:OG	2.24	0.47
27:A:851:BCR:H331	27:A:851:BCR:C8	2.43	0.47
2:5:201:LEU:HD22	24:5:618:XAT:C15	2.45	0.47
27:4:621:BCR:H23C	27:4:621:BCR:H393	1.97	0.47
6:A:574:ASP:OD2	6:A:578:ARG:NH1	2.38	0.47
6:A:672:LEU:HD21	7:B:620:LEU:HD22	1.95	0.47
22:B:823:CLA:HAB	22:B:830:CLA:HMD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:6:101:LYS:O	3:6:105:GLN:HG2	2.14	0.47
3:6:137:SER:OG	3:6:140:VAL:HG22	2.15	0.47
3:2:77:TRP:NE1	3:2:89:ASP:OD2	2.40	0.47
22:A:803:CLA:HMB1	22:A:803:CLA:HBB1	1.96	0.47
4:7:239:GLU:N	4:7:239:GLU:OE1	2.46	0.47
22:V:604:CLA:HMB3	23:V:2621:LUT:H162	1.97	0.47
22:A:809:CLA:C4	27:A:852:BCR:H331	2.45	0.47
2:5:51:TRP:O	21:5:601:CHL:ND	2.48	0.47
2:5:131:TYR:CD2	22:5:604:CLA:HMD2	2.50	0.47
2:5:196:ASN:HB3	23:5:617:LUT:H201	1.96	0.47
5:8:168:ARG:NH1	22:8:609:CLA:O1D	2.37	0.47
3:2:148:THR:HG22	3:2:149:ASP:N	2.30	0.47
7:B:125:TYR:O	7:B:130:ARG:NH1	2.45	0.47
7:B:287:ALA:HB2	22:B:819:CLA:HBC2	1.97	0.47
7:B:662:MET:HG3	22:B:803:CLA:NC	2.29	0.47
8:C:29:VAL:HG12	9:D:181:ARG:HB3	1.97	0.47
3:6:115:MET:SD	22:6:610:CLA:HMC3	2.55	0.47
4:7:146:LEU:HD12	22:7:602:CLA:H12	1.97	0.47
21:7:608:CHL:HHC	21:7:608:CHL:HBB1	1.96	0.47
1:U:184:ILE:HG23	1:U:184:ILE:O	2.15	0.47
22:B:839:CLA:H18	27:I:101:BCR:H362	1.95	0.47
27:I:101:BCR:H382	27:I:101:BCR:H23C	1.97	0.47
2:5:57:ARG:NH2	2:5:68:ASP:O	2.47	0.47
21:6:606:CHL:HHC	21:6:606:CHL:HBB1	1.97	0.47
5:4:77:TRP:CD1	5:4:78:LEU:HD12	2.49	0.46
27:G:205:BCR:H11C	27:G:205:BCR:H341	1.76	0.46
14:I:9:ILE:O	14:I:13:LEU:HD13	2.14	0.46
23:9:621:LUT:H11	23:9:621:LUT:H191	1.78	0.46
6:A:672:LEU:HB2	22:A:854:CLA:H42	1.97	0.46
7:B:693:TRP:HE3	22:B:839:CLA:HMD3	1.80	0.46
22:B:812:CLA:CGA	22:B:812:CLA:H3A	2.44	0.46
3:6:234:VAL:HG11	24:6:620:XAT:C12	2.46	0.46
1:V:160:ILE:HD12	1:V:160:ILE:H	1.80	0.46
27:4:621:BCR:H402	27:4:621:BCR:C23	2.45	0.46
22:A:854:CLA:HBA1	22:A:854:CLA:H3A	1.59	0.46
7:B:732:LYS:O	7:B:734:GLY:N	2.47	0.46
3:6:220:ARG:O	3:6:224:ILE:HG12	2.16	0.46
4:7:215:PHE:O	4:7:219:ARG:HG3	2.15	0.46
21:U:607:CHL:HHC	21:U:607:CHL:HBB1	1.98	0.46
21:U:608:CHL:HMB3	25:U:2623:NEX:C35	2.45	0.46
21:1:607:CHL:HHC	21:1:607:CHL:HBB1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:1:611:CLA:H2A	22:1:611:CLA:CED	2.44	0.46
3:2:127:LEU:HB2	3:2:133:LEU:HD12	1.97	0.46
6:A:738:THR:OG1	22:A:801:CLA:CED	2.63	0.46
27:M:2001:BCR:H321	27:M:2001:BCR:HC8	1.97	0.46
19:O:66:ILE:HG22	27:O:2004:BCR:H323	1.97	0.46
3:6:113:TRP:CE2	21:6:608:CHL:HED3	2.50	0.46
1:W:77:TYR:HB2	22:W:602:CLA:HMD1	1.97	0.46
6:A:118:ILE:HG23	6:A:119:VAL:HG22	1.98	0.46
6:A:275:PHE:HE2	6:A:499:ALA:HB2	1.81	0.46
22:G:201:CLA:H3A	22:G:201:CLA:O2A	2.16	0.46
22:O:2002:CLA:H3A	22:O:2002:CLA:H11	1.97	0.46
27:O:2004:BCR:H383	27:O:2004:BCR:C23	2.45	0.46
4:3:145:TRP:NE1	22:3:603:CLA:O1A	2.46	0.46
24:4:620:XAT:H181	24:4:620:XAT:C8	2.46	0.46
7:B:463:ILE:HD12	22:B:836:CLA:O2A	2.15	0.46
13:H:89:GLY:O	13:H:92:THR:OG1	2.31	0.46
7:B:56:ILE:HG21	22:B:806:CLA:HMD2	1.98	0.46
3:6:193:ASP:OD1	3:6:193:ASP:O	2.34	0.46
1:W:174:TYR:O	1:W:178:GLY:N	2.49	0.46
5:4:73:GLU:OE1	5:4:73:GLU:HA	2.16	0.46
27:B:847:BCR:C23	27:B:847:BCR:H383	2.45	0.46
8:C:3:HIS:ND1	8:C:69:LEU:HA	2.31	0.46
8:C:3:HIS:CE1	8:C:76:SER:HG	2.34	0.46
27:L:301:BCR:H24C	22:L:303:CLA:C9	2.45	0.46
2:5:72:ASP:OD1	2:5:75:GLY:N	2.48	0.46
27:7:620:BCR:C23	27:7:620:BCR:C38	2.93	0.46
6:A:599:ASN:OD1	22:A:803:CLA:HMC3	2.16	0.46
27:A:848:BCR:H11C	27:A:848:BCR:H341	1.69	0.46
8:C:70:GLY:O	8:C:72:GLU:N	2.46	0.46
2:5:164:ASP:O	2:5:167:LYS:N	2.49	0.46
1:U:197:LEU:HD12	23:U:2620:LUT:H222	1.98	0.45
27:B:843:BCR:H11C	27:B:843:BCR:H341	1.80	0.45
27:B:844:BCR:H11C	27:B:844:BCR:H341	1.84	0.45
27:B:1609:BCR:H341	27:B:1609:BCR:H11C	1.69	0.45
9:D:166:LEU:O	9:D:169:LYS:HE3	2.16	0.45
20:9:187:THR:HB	20:9:188:PRO:HD3	1.98	0.45
5:4:168:ARG:NH2	22:4:609:CLA:O1D	2.48	0.45
22:4:610:CLA:HBA2	22:4:610:CLA:H3A	1.80	0.45
22:K:204:CLA:HMB2	27:K:205:BCR:C15	2.46	0.45
19:O:81:VAL:HG12	19:O:83:ASN:H	1.81	0.45
20:9:141:TYR:CD2	21:9:601:CHL:HMD3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:611:CLA:HMB1	19:O:66:ILE:HD11	1.98	0.45
5:4:117:GLY:HA2	24:4:620:XAT:C18	2.46	0.45
21:4:618:CHL:HHC	21:4:618:CHL:HBB1	1.97	0.45
6:A:455:HIS:O	6:A:459:MET:HG2	2.15	0.45
12:G:146:THR:HG23	22:G:201:CLA:OBD	2.17	0.45
7:B:53:GLN:HE21	22:B:805:CLA:HMA1	1.81	0.45
9:D:128:LEU:HD21	13:H:53:PHE:HB3	1.98	0.45
3:6:125:GLU:HA	3:6:128:THR:HG22	1.97	0.45
27:6:621:BCR:H11C	27:6:621:BCR:H341	1.73	0.45
5:8:251:LEU:HD13	23:8:619:LUT:H163	1.97	0.45
22:4:601:CLA:CAC	26:4:630:LHG:HC42	2.47	0.45
9:D:75:ASN:OD1	9:D:76:ALA:N	2.50	0.45
13:H:104:GLY:O	13:H:108:THR:OG1	2.27	0.45
22:5:611:CLA:HAB	27:8:621:BCR:H383	1.99	0.45
22:7:602:CLA:CGA	22:7:602:CLA:C3A	2.94	0.45
20:9:207:ILE:O	20:9:207:ILE:HG23	2.17	0.45
2:1:146:ALA:O	2:1:150:LEU:HD13	2.17	0.45
5:4:263:ILE:HG23	5:4:264:LEU:CD2	2.46	0.45
22:4:614:CLA:H3A	22:4:614:CLA:HBA2	1.84	0.45
22:B:837:CLA:H112	22:B:837:CLA:HMC2	1.99	0.45
8:C:4:SER:OG	8:C:6:LYS:NZ	2.50	0.45
21:U:609:CHL:HHC	21:U:609:CHL:HBB1	1.98	0.45
21:W:606:CHL:HMB2	25:W:2623:NEX:H392	1.99	0.45
3:2:112:ARG:NH2	3:2:195:GLY:O	2.39	0.45
4:3:268:LEU:HD21	4:3:272:LYS:HE3	1.99	0.45
7:B:15:ASP:HB3	7:B:20:ARG:HB2	1.99	0.45
7:B:167:TRP:NE1	22:B:813:CLA:HBC3	2.32	0.45
22:F:303:CLA:O2A	22:F:303:CLA:H2A	2.17	0.45
1:U:145:TYR:HD2	1:U:151:LEU:HD13	1.82	0.45
22:U:610:CLA:HMB1	22:U:610:CLA:HBB1	1.98	0.45
21:2:606:CHL:HHC	21:2:606:CHL:HBB1	1.97	0.45
22:4:603:CLA:HMD2	22:4:609:CLA:CHD	2.46	0.45
6:A:223:ARG:NH1	6:A:250:LEU:O	2.49	0.45
22:A:828:CLA:HBB1	22:A:828:CLA:HMB1	1.98	0.45
21:V:609:CHL:HHC	21:V:609:CHL:HBB1	1.99	0.45
1:W:248:ASP:OD1	1:W:251:ALA:HB3	2.17	0.45
2:1:154:PHE:O	2:1:158:GLN:HG2	2.17	0.45
7:B:69:ALA:HB2	7:B:135:LEU:HB2	1.99	0.45
12:G:76:GLY:HA3	12:G:132:TRP:CE2	2.52	0.45
27:L:301:BCR:H392	27:L:301:BCR:H23C	1.98	0.45
21:5:607:CHL:HHC	21:5:607:CHL:HBB1	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:6:139:THR:HG23	3:6:140:VAL:HG13	1.99	0.45
21:8:618:CHL:HHC	21:8:618:CHL:HBB1	1.98	0.45
7:B:203:ARG:NH2	7:B:253:ALA:O	2.47	0.45
22:B:821:CLA:H3A	22:B:822:CLA:H11	1.99	0.45
3:6:203:ASP:OD1	3:6:203:ASP:O	2.35	0.45
5:8:156:VAL:O	5:8:160:LEU:HD13	2.16	0.45
21:V:605:CHL:HHC	21:V:605:CHL:HBB1	1.99	0.44
7:B:2:ALA:O	14:I:34:GLU:HB2	2.16	0.44
17:L:65:VAL:HG13	19:O:58:TRP:HB2	1.98	0.44
5:8:183:ILE:CD1	27:8:621:BCR:H382	2.48	0.44
20:9:299:VAL:HG12	20:9:300:SER:N	2.31	0.44
3:2:109:VAL:HG11	3:2:168:ARG:NH1	2.32	0.44
22:4:604:CLA:C3B	27:4:621:BCR:H323	2.47	0.44
27:A:852:BCR:H371	27:A:852:BCR:H24C	1.81	0.44
27:B:845:BCR:H351	27:B:845:BCR:H15C	1.82	0.44
21:8:607:CHL:HHC	21:8:607:CHL:HBB1	1.99	0.44
21:9:601:CHL:HHC	21:9:601:CHL:HBB1	1.99	0.44
25:W:2623:NEX:H11	25:W:2623:NEX:H191	1.74	0.44
24:4:620:XAT:H181	24:4:620:XAT:H8	1.99	0.44
27:A:856:BCR:HC8	27:A:856:BCR:C33	2.43	0.44
27:K:202:BCR:H331	27:K:202:BCR:C8	2.47	0.44
27:L:301:BCR:H11C	27:L:301:BCR:H341	1.86	0.44
2:5:112:TYR:CE2	2:5:131:TYR:HB2	2.52	0.44
3:6:196:TYR:CE2	3:6:220:ARG:NH2	2.86	0.44
4:7:190:ILE:HD11	22:7:607:CLA:HMC3	2.00	0.44
21:9:605:CHL:HHC	21:9:605:CHL:HBB1	2.00	0.44
25:W:2623:NEX:H31	25:W:2623:NEX:H391	1.82	0.44
4:3:221:ALA:HB2	22:3:609:CLA:HMA1	2.00	0.44
27:4:621:BCR:H11C	27:4:621:BCR:H341	1.86	0.44
27:A:851:BCR:H11C	27:A:851:BCR:H341	1.85	0.44
22:B:822:CLA:HMB3	22:B:841:CLA:C1D	2.47	0.44
21:5:601:CHL:OBD	5:8:167:ARG:NH1	2.50	0.44
22:1:611:CLA:C1D	22:1:612:CLA:HMD2	2.48	0.44
3:2:264:ILE:N	22:2:613:CLA:O1A	2.48	0.44
4:3:312:VAL:HG11	20:9:309:LEU:O	2.17	0.44
7:B:299:HIS:HB3	7:B:304:ILE:HD11	1.98	0.44
10:E:81:ARG:NH2	10:E:127:GLU:OE2	2.51	0.44
22:3:612:CLA:CBB	27:3:621:BCR:H381	2.47	0.44
6:A:495:THR:O	22:A:837:CLA:ND	2.51	0.44
6:A:538:ALA:HB1	22:A:839:CLA:HMB3	1.98	0.44
22:A:845:CLA:HMD3	19:O:141:TYR:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:852:BCR:H382	27:A:852:BCR:H23C	2.00	0.44
7:B:580:VAL:O	7:B:583:MET:HG3	2.17	0.44
7:B:583:MET:O	7:B:587:ILE:HG12	2.17	0.44
2:5:156:GLU:HG3	22:5:609:CLA:C2B	2.48	0.44
21:6:601:CHL:HHC	21:6:601:CHL:HBB1	2.00	0.44
21:6:608:CHL:HHC	21:6:608:CHL:HBB1	1.99	0.44
20:9:148:LEU:HD22	22:9:602:CLA:H12	1.99	0.44
1:W:244:ASP:OD1	1:W:252:ASN:OD1	2.35	0.44
5:4:220:THR:HA	5:4:223:VAL:HG12	2.00	0.44
7:B:430:GLY:HA2	7:B:525:LEU:HD22	2.00	0.44
7:B:459:PHE:CD1	22:F:304:CLA:HMC2	2.53	0.44
7:B:631:LEU:HD22	7:B:724:PHE:HA	1.99	0.44
3:6:229:LEU:HD21	22:6:612:CLA:HBC3	2.00	0.44
27:6:621:BCR:H15C	27:6:621:BCR:H351	1.77	0.44
4:7:270:GLU:N	4:7:270:GLU:OE1	2.51	0.44
20:9:240:ILE:HG21	22:9:609:CLA:CMA	2.48	0.44
3:2:205:LEU:HD12	23:2:619:LUT:H22	1.98	0.44
21:3:608:CHL:HMB2	27:3:621:BCR:HC7	2.00	0.44
5:4:112:ARG:HG3	22:4:610:CLA:C3C	2.48	0.44
21:4:607:CHL:HHC	21:4:607:CHL:HBB1	1.99	0.44
22:A:809:CLA:H92	27:J:102:BCR:H372	1.98	0.44
2:5:91:LEU:HD12	2:5:169:LYS:HE3	1.97	0.44
4:7:156:PHE:CZ	21:7:608:CHL:HED3	2.53	0.44
1:U:168:MET:HA	1:U:171:VAL:HG22	2.00	0.44
3:2:160:LEU:HD11	27:2:621:BCR:C15	2.48	0.44
7:B:395:ILE:HD12	7:B:555:TYR:HD1	1.83	0.44
21:5:601:CHL:HHC	21:5:601:CHL:HBB1	1.99	0.44
5:4:205:LEU:HD12	23:4:619:LUT:H221	1.99	0.43
6:A:46:ILE:HD12	6:A:46:ILE:H	1.83	0.43
7:B:85:ARG:NH2	13:H:139:LYS:O	2.50	0.43
2:5:108:GLU:HB3	2:5:220:LEU:CD2	2.43	0.43
4:7:291:THR:O	4:7:294:ILE:HG22	2.17	0.43
22:9:609:CLA:HHC	22:9:609:CLA:HBB1	1.99	0.43
22:U:603:CLA:HMD1	21:U:609:CHL:O1A	2.17	0.43
1:V:106:MET:HE3	23:V:2620:LUT:C34	2.48	0.43
1:W:145:TYR:CD2	1:W:146:LEU:HD12	2.54	0.43
22:1:606:CLA:HMC2	24:1:618:XAT:H363	2.01	0.43
4:3:255:ILE:HD13	27:3:621:BCR:HC41	2.00	0.43
22:4:613:CLA:HMB3	23:4:619:LUT:H162	1.99	0.43
6:A:55:ASP:OD2	6:A:58:SER:OG	2.30	0.43
6:A:530:ASP:HA	6:A:533:VAL:HG12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:804:CLA:HHC	22:B:806:CLA:OBD	2.18	0.43
8:C:3:HIS:NE2	8:C:76:SER:OG	2.44	0.43
21:6:607:CHL:HHC	21:6:607:CHL:HBB1	1.98	0.43
22:8:603:CLA:HMD2	22:8:609:CLA:C1D	2.48	0.43
6:A:116:TRP:HB3	27:A:856:BCR:H333	1.99	0.43
22:A:803:CLA:C3C	22:B:803:CLA:HMC2	2.48	0.43
7:B:490:GLN:HA	7:B:494:LEU:HB2	2.01	0.43
9:D:189:ARG:NH1	9:D:210:LEU:O	2.51	0.43
3:6:196:TYR:CE2	3:6:220:ARG:CZ	3.02	0.43
22:V:602:CLA:O1A	23:V:2621:LUT:H382	2.18	0.43
21:1:601:CHL:HHC	21:1:601:CHL:HBB1	2.00	0.43
21:2:601:CHL:HHC	21:2:601:CHL:HBB1	1.99	0.43
4:3:286:VAL:HG11	24:3:619:XAT:H12	2.00	0.43
7:B:441:ASP:OD1	7:B:615:TYR:HB2	2.18	0.43
2:5:133:GLY:HA3	2:5:136:VAL:HB	2.00	0.43
3:6:233:ALA:HB2	23:6:619:LUT:H392	2.00	0.43
23:6:619:LUT:H15	23:6:619:LUT:H201	1.85	0.43
4:7:155:ARG:NH1	4:7:275:GLU:OE2	2.52	0.43
4:7:283:MET:SD	22:7:602:CLA:HMC3	2.59	0.43
20:9:260:LEU:HD22	23:9:620:LUT:H222	2.00	0.43
23:U:2620:LUT:H11	23:U:2620:LUT:H191	1.81	0.43
1:W:113:LEU:CD2	1:W:239:LEU:HD21	2.48	0.43
4:3:175:LEU:HD12	4:3:176:ILE:HG23	1.98	0.43
24:4:620:XAT:H35	24:4:620:XAT:H401	1.85	0.43
6:A:622:ASP:OD1	6:A:622:ASP:N	2.48	0.43
22:A:806:CLA:HBB1	22:A:806:CLA:HMB1	1.99	0.43
7:B:605:ASN:OD1	7:B:605:ASN:O	2.36	0.43
2:5:108:GLU:O	2:5:111:GLY:N	2.47	0.43
22:6:610:CLA:CGA	22:6:610:CLA:H3A	2.49	0.43
5:8:143:ASP:OD1	5:8:143:ASP:O	2.36	0.43
1:V:103:ARG:O	1:V:107:LEU:HD23	2.18	0.43
27:3:621:BCR:C23	27:3:621:BCR:H383	2.47	0.43
27:B:843:BCR:H15C	27:B:843:BCR:H351	1.88	0.43
2:5:104:VAL:HG12	2:5:104:VAL:O	2.18	0.43
2:5:212:ILE:HG22	2:5:212:ILE:O	2.18	0.43
2:5:238:VAL:HG11	22:5:613:CLA:HMD1	2.01	0.43
3:6:116:LEU:HD21	22:6:610:CLA:HMC1	2.00	0.43
24:6:620:XAT:H11	24:6:620:XAT:H191	1.93	0.43
21:8:608:CHL:HHC	21:8:608:CHL:HBB1	1.99	0.43
21:9:608:CHL:HHC	21:9:608:CHL:HBB1	2.01	0.43
6:A:155:GLN:HA	6:A:158:THR:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:852:BCR:H20C	27:A:852:BCR:H361	1.69	0.43
7:B:600:THR:HG21	7:B:609:PHE:HB2	2.01	0.43
5:8:65:ARG:NH1	5:8:79:ASP:O	2.50	0.43
2:1:71:PHE:CE2	24:1:618:XAT:H183	2.53	0.43
4:3:263:LYS:HE2	4:3:263:LYS:HA	2.01	0.43
6:A:543:VAL:HG11	6:A:596:TRP:CZ2	2.54	0.43
7:B:21:ILE:O	7:B:25:ILE:HG13	2.19	0.43
19:O:134:PHE:HD1	22:O:2002:CLA:HMD2	1.84	0.43
2:5:156:GLU:HG3	22:5:609:CLA:C3B	2.49	0.43
23:9:624:LUT:H27	23:9:624:LUT:H371	1.74	0.43
3:2:84:GLY:HA3	3:2:224:ILE:HG21	2.01	0.43
4:3:241:PHE:HE1	2:5:82:ASN:OD1	2.01	0.43
4:3:271:LEU:HD23	22:3:610:CLA:H3A	2.01	0.43
6:A:423:LEU:HD13	22:A:825:CLA:C1C	2.49	0.43
27:A:851:BCR:H321	27:A:851:BCR:HC7	1.82	0.43
27:L:305:BCR:H15C	27:L:305:BCR:H351	1.81	0.43
4:7:150:GLU:OE1	22:7:602:CLA:HMA3	2.19	0.43
5:8:170:ALA:HB3	5:8:178:VAL:HG11	1.99	0.43
22:8:604:CLA:C1B	27:8:621:BCR:H323	2.49	0.43
23:V:2620:LUT:H11	23:V:2620:LUT:H191	1.77	0.43
2:1:156:GLU:OE2	22:1:609:CLA:C1C	2.66	0.43
22:4:604:CLA:H3A	22:4:604:CLA:HBA2	1.76	0.43
21:4:606:CHL:HHC	21:4:606:CHL:HBB1	2.00	0.43
27:4:621:BCR:H281	27:4:621:BCR:H403	1.73	0.43
12:G:125:THR:HG22	12:G:126:ILE:N	2.34	0.43
27:L:306:BCR:H23C	27:L:306:BCR:H382	2.01	0.43
24:1:618:XAT:H15	24:1:618:XAT:H201	1.92	0.42
6:A:84:TRP:O	6:A:88:MET:HG2	2.19	0.42
7:B:406:ASN:O	7:B:410:ARG:HG2	2.19	0.42
11:F:150:THR:O	11:F:151:ASP:CG	2.57	0.42
22:O:2002:CLA:H3A	22:O:2002:CLA:HBA2	1.84	0.42
3:6:219:LEU:HD21	22:6:610:CLA:O1A	2.19	0.42
3:6:264:ILE:O	3:6:264:ILE:HG13	2.19	0.42
4:7:191:PRO:N	4:7:192:PRO:HD3	2.34	0.42
23:9:624:LUT:H11	23:9:624:LUT:H191	1.94	0.42
1:U:116:GLU:O	1:U:120:LYS:HG2	2.19	0.42
1:U:215:LYS:NZ	26:U:2630:LHG:O4	2.47	0.42
1:W:202:ASP:HB3	1:W:205:THR:HG22	2.01	0.42
1:W:238:PRO:O	23:W:2620:LUT:O3	2.36	0.42
4:3:238:LEU:H	4:3:238:LEU:HD23	1.83	0.42
6:A:194:MET:HE2	22:A:814:CLA:CHD	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:851:BCR:H331	27:A:851:BCR:HC8	2.02	0.42
7:B:662:MET:HG3	22:B:803:CLA:C4C	2.49	0.42
11:F:112:GLY:HA2	11:F:115:LYS:HE2	2.01	0.42
2:5:141:LEU:HB2	2:5:142:PRO:HD3	2.01	0.42
3:6:137:SER:HG	3:6:140:VAL:HG22	1.84	0.42
4:7:111:GLN:O	4:7:112:SER:C	2.56	0.42
5:8:111:CYS:HB2	5:8:226:GLY:HA3	2.02	0.42
23:1:617:LUT:C8	23:1:617:LUT:H181	2.49	0.42
21:2:606:CHL:HBB2	21:2:607:CHL:CBB	2.49	0.42
27:2:621:BCR:H23C	27:2:621:BCR:C38	2.48	0.42
5:4:82:LEU:HD12	5:4:83:PRO:HD2	2.01	0.42
7:B:60:TRP:NE1	22:B:827:CLA:OBD	2.53	0.42
22:B:840:CLA:HBA1	22:B:840:CLA:H3A	1.91	0.42
27:B:1609:BCR:C33	27:B:1609:BCR:HC8	2.50	0.42
9:D:129:LEU:HD23	9:D:131:LEU:HD21	2.02	0.42
16:K:117:VAL:HA	27:K:205:BCR:H332	2.02	0.42
2:5:191:LEU:O	2:5:194:ILE:HG22	2.18	0.42
4:7:156:PHE:CE1	21:7:608:CHL:HED3	2.55	0.42
22:A:829:CLA:HBB1	22:A:829:CLA:HMB1	2.00	0.42
21:U:606:CHL:HHC	21:U:606:CHL:HBB1	2.00	0.42
2:1:85:ARG:HG3	2:1:85:ARG:HH11	1.83	0.42
2:5:134:ASN:O	2:5:135:PRO:C	2.58	0.42
27:7:620:BCR:H15C	27:7:620:BCR:H351	1.88	0.42
21:8:606:CHL:HHC	21:8:606:CHL:HBB1	2.00	0.42
20:9:115:ASN:OD1	20:9:115:ASN:O	2.38	0.42
27:A:848:BCR:H382	27:A:848:BCR:H23C	2.01	0.42
7:B:276:HIS:HE2	22:B:818:CLA:C2B	2.32	0.42
12:G:146:THR:HG23	22:G:201:CLA:CAD	2.50	0.42
27:I:101:BCR:H402	27:L:301:BCR:H353	2.00	0.42
27:L:305:BCR:H331	27:L:305:BCR:C8	2.33	0.42
24:5:618:XAT:H15	24:5:618:XAT:H201	1.85	0.42
1:U:102:ALA:O	1:U:106:MET:HG3	2.19	0.42
1:U:126:GLY:C	1:U:127:GLU:OE1	2.58	0.42
24:W:2622:XAT:C28	24:W:2622:XAT:H381	2.48	0.42
2:1:94:ALA:O	2:1:98:MET:HG3	2.19	0.42
21:2:601:CHL:HMD2	27:3:620:BCR:H333	2.02	0.42
21:2:618:CHL:HHC	21:2:618:CHL:HBB1	2.01	0.42
6:A:122:LYS:CE	11:F:130:THR:OG1	2.68	0.42
7:B:631:LEU:HD13	7:B:727:ALA:CB	2.49	0.42
27:K:202:BCR:H11C	27:K:202:BCR:H341	1.81	0.42
4:7:106:ILE:HG12	4:7:107:PHE:H	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:9:613:CLA:HMB3	23:9:620:LUT:H162	2.02	0.42
1:U:109:ALA:HA	1:U:224:MET:SD	2.60	0.42
22:V:602:CLA:O1A	22:V:602:CLA:H43	2.20	0.42
22:3:615:CLA:HMD3	22:5:616:CLA:CED	2.50	0.42
7:B:120:VAL:HG21	22:B:808:CLA:HED1	2.01	0.42
27:B:847:BCR:H351	27:B:847:BCR:H15C	1.81	0.42
8:C:3:HIS:HE2	8:C:76:SER:HG	1.57	0.42
11:F:211:ALA:O	11:F:215:MET:HG3	2.19	0.42
27:M:2001:BCR:HC8	27:M:2001:BCR:H311	2.01	0.42
3:6:109:VAL:HG21	22:6:609:CLA:CAD	2.50	0.42
23:U:2621:LUT:H15	23:U:2621:LUT:H201	1.93	0.42
6:A:599:ASN:OD1	22:A:803:CLA:HBC2	2.20	0.42
27:A:851:BCR:HC8	27:A:851:BCR:C33	2.50	0.42
7:B:595:HIS:O	7:B:599:ILE:HG13	2.20	0.42
27:B:843:BCR:H401	12:G:132:TRP:CE2	2.55	0.42
10:E:124:SER:OG	10:E:126:ASP:OD1	2.30	0.42
17:L:125:LEU:HD12	22:L:304:CLA:HHB	2.02	0.42
3:6:156:ILE:O	3:6:160:LEU:HD23	2.20	0.42
21:9:606:CHL:HHC	21:9:606:CHL:HBB1	2.02	0.42
5:4:205:LEU:HD13	5:4:207:TRP:CZ2	2.54	0.42
7:B:279:ALA:HA	22:B:816:CLA:HMC3	2.02	0.42
27:J:102:BCR:H351	27:J:102:BCR:H15C	1.81	0.42
22:K:201:CLA:HBB1	22:K:201:CLA:HMB1	2.02	0.42
27:L:306:BCR:H20C	27:L:306:BCR:H361	1.85	0.42
2:5:240:ILE:O	2:5:240:ILE:CG2	2.67	0.42
1:V:211:VAL:O	1:V:214:ILE:HG22	2.20	0.41
1:V:253:ASN:OD1	1:V:253:ASN:C	2.58	0.41
22:2:611:CLA:O1A	2:5:157:SER:OG	2.28	0.41
22:2:614:CLA:CBB	22:2:614:CLA:HHC	2.50	0.41
4:3:238:LEU:HD22	22:5:603:CLA:CED	2.50	0.41
7:B:548:PRO:HB3	11:F:245:PRO:HG2	2.02	0.41
27:K:202:BCR:C33	27:K:202:BCR:HC8	2.49	0.41
27:6:621:BCR:H20C	27:6:621:BCR:H361	1.82	0.41
5:8:85:ASP:OD1	5:8:85:ASP:C	2.58	0.41
1:V:143:LEU:HD23	21:V:606:CHL:HMD2	2.02	0.41
22:V:613:CLA:O1D	22:V:613:CLA:H2A	2.19	0.41
1:W:152:VAL:HG11	21:W:606:CHL:HMD1	2.02	0.41
3:2:221:THR:HG22	3:2:221:THR:O	2.20	0.41
22:3:612:CLA:CBB	22:3:612:CLA:HHC	2.50	0.41
5:4:138:TRP:HB2	24:4:620:XAT:H3	2.03	0.41
6:A:314:GLY:O	6:A:315:ILE:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B:801:BCR:H371	27:B:801:BCR:H24C	1.92	0.41
17:L:81:PRO:O	17:L:85:SER:HB2	2.19	0.41
4:7:150:GLU:OE2	4:7:280:ARG:CZ	2.68	0.41
4:7:213:MET:O	4:7:217:GLU:HG2	2.21	0.41
1:U:148:ASN:HB2	1:U:151:LEU:HD12	2.02	0.41
22:1:603:CLA:HMD2	22:1:609:CLA:C1D	2.51	0.41
21:2:607:CHL:HHC	21:2:607:CHL:HBB1	2.01	0.41
6:A:118:ILE:HG23	6:A:119:VAL:H	1.85	0.41
27:B:1609:BCR:C23	27:B:1609:BCR:H382	2.49	0.41
2:5:206:GLY:O	2:5:207:PHE:C	2.58	0.41
3:6:181:ASP:OD1	21:6:618:CHL:CHC	2.69	0.41
4:7:302:GLN:OE1	4:7:306:ASP:OD2	2.38	0.41
5:8:183:ILE:HD13	27:8:621:BCR:C38	2.51	0.41
1:V:157:ILE:HG23	1:V:158:LEU:HD22	2.02	0.41
23:W:2621:LUT:H11	23:W:2621:LUT:H191	1.88	0.41
22:3:615:CLA:HMD3	22:5:616:CLA:HED3	2.02	0.41
22:B:806:CLA:HMC2	27:B:844:BCR:H381	2.02	0.41
4:7:209:GLU:OE2	22:7:606:CLA:C3B	2.68	0.41
4:7:298:VAL:CG1	4:7:302:GLN:NE2	2.82	0.41
20:9:148:LEU:N	20:9:148:LEU:HD12	2.36	0.41
1:U:259:THR:O	1:U:259:THR:CG2	2.66	0.41
25:V:2623:NEX:H15	25:V:2623:NEX:H201	1.84	0.41
2:1:152:ILE:O	2:1:156:GLU:CG	2.68	0.41
8:C:24:ASP:O	8:C:44:ARG:HD2	2.20	0.41
3:6:263:THR:HG21	4:7:204:THR:OG1	2.20	0.41
4:7:211:ALA:O	4:7:215:PHE:CD2	2.74	0.41
5:8:107:GLU:HB2	22:8:602:CLA:C1B	2.51	0.41
20:9:207:ILE:HG21	21:9:606:CHL:CMD	2.51	0.41
20:9:232:MET:CE	21:9:606:CHL:HMB3	2.50	0.41
4:3:202:PRO:HB2	22:3:607:CLA:HMA2	2.02	0.41
6:A:395:GLY:O	6:A:399:VAL:HG23	2.20	0.41
22:A:809:CLA:H3A	22:A:809:CLA:HBA2	1.86	0.41
22:A:835:CLA:H2A	22:A:835:CLA:O2D	2.20	0.41
7:B:58:PHE:HA	7:B:61:THR:HG22	2.02	0.41
24:5:618:XAT:H11	24:5:618:XAT:H191	1.86	0.41
3:6:91:LEU:HD22	24:6:620:XAT:H363	2.02	0.41
20:9:227:VAL:HG11	21:9:606:CHL:HED3	2.02	0.41
22:9:612:CLA:CHC	23:9:620:LUT:H203	2.50	0.41
22:U:604:CLA:H2A	22:U:604:CLA:HED3	2.00	0.41
22:U:610:CLA:CGA	22:U:610:CLA:C3A	2.99	0.41
3:2:137:SER:O	3:2:138:TRP:CD1	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B:801:BCR:H331	27:B:801:BCR:C8	2.50	0.41
22:5:610:CLA:HBB1	22:5:612:CLA:H3A	2.02	0.41
23:5:617:LUT:H35	23:5:617:LUT:H401	1.88	0.41
1:U:175:ARG:O	1:U:184:ILE:HD12	2.20	0.41
1:U:211:VAL:O	1:U:214:ILE:HG22	2.21	0.41
1:U:253:ASN:HB2	22:U:614:CLA:HED1	2.02	0.41
25:V:2623:NEX:H11	25:V:2623:NEX:H191	1.77	0.41
2:1:148:GLU:HA	22:1:606:CLA:HMA3	2.02	0.41
22:1:611:CLA:HMC3	27:4:621:BCR:C39	2.51	0.41
23:2:619:LUT:H35	23:2:619:LUT:H401	1.97	0.41
24:3:619:XAT:H35	24:3:619:XAT:H401	1.88	0.41
5:4:108:LEU:O	5:4:112:ARG:HD3	2.20	0.41
22:A:801:CLA:HMB3	22:A:854:CLA:OBD	2.21	0.41
9:D:78:THR:HG23	9:D:126:PRO:HB2	2.02	0.41
22:K:201:CLA:HBC3	22:9:611:CLA:O2A	2.20	0.41
4:7:284:MET:HA	4:7:284:MET:CE	2.51	0.41
20:9:221:LEU:O	20:9:225:ILE:HG12	2.20	0.41
22:U:610:CLA:CGA	22:U:610:CLA:H3A	2.51	0.41
1:V:102:ALA:O	1:V:106:MET:HG3	2.21	0.41
1:V:204:ASP:OD1	1:V:205:THR:N	2.54	0.41
22:W:610:CLA:HMC2	23:W:2620:LUT:C31	2.51	0.41
3:2:177:CYS:O	3:2:178:VAL:HG22	2.21	0.41
22:3:604:CLA:HBB1	22:3:604:CLA:HMB1	2.03	0.41
6:A:674:ALA:HB1	6:A:733:GLY:O	2.21	0.41
7:B:80:ASP:OD2	7:B:83:HIS:HB2	2.21	0.41
22:B:805:CLA:HBA1	22:B:805:CLA:H3A	1.77	0.41
22:B:819:CLA:HMB2	22:B:824:CLA:HMA3	2.03	0.41
11:F:156:LEU:HD22	11:F:167:GLU:HG2	2.02	0.41
12:G:84:GLN:NE2	12:G:88:VAL:HG11	2.35	0.41
27:K:205:BCR:H383	27:K:205:BCR:C23	2.51	0.41
3:6:110:HIS:CE1	22:6:609:CLA:OBD	2.73	0.41
3:6:189:LEU:O	3:6:190:THR:OG1	2.38	0.41
4:7:127:ASP:OD1	22:7:602:CLA:HBA2	2.21	0.41
22:7:612:CLA:HMB1	22:7:612:CLA:HBB1	2.02	0.41
5:8:190:THR:O	5:8:198:GLY:N	2.50	0.41
23:9:621:LUT:H35	23:9:621:LUT:H401	1.97	0.41
25:U:2623:NEX:H15	25:U:2623:NEX:H201	1.91	0.41
1:W:181:LEU:HD13	21:W:608:CHL:CAB	2.50	0.41
1:W:200:ALA:HB1	1:W:206:PHE:CD1	2.56	0.41
27:3:620:BCR:H23C	27:3:620:BCR:C38	2.42	0.41
22:A:841:CLA:HMC3	22:F:301:CLA:C4D	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:95:VAL:HA	12:G:100:THR:HA	2.03	0.41
27:G:205:BCR:H15C	27:G:205:BCR:H351	1.81	0.41
24:5:618:XAT:H381	24:5:618:XAT:H27	1.71	0.41
4:7:304:LEU:O	4:7:308:LEU:HD23	2.21	0.41
1:U:81:THR:HG21	21:V:609:CHL:CBA	2.51	0.40
1:U:197:LEU:HD22	20:9:260:LEU:CD2	2.49	0.40
23:U:2621:LUT:H181	23:U:2621:LUT:C8	2.51	0.40
1:V:114:THR:OG1	1:V:115:PRO:HD3	2.22	0.40
1:W:226:GLY:O	1:W:227:PHE:C	2.57	0.40
23:1:617:LUT:H11	23:1:617:LUT:H191	1.91	0.40
22:2:613:CLA:CHB	22:2:614:CLA:HMD3	2.50	0.40
21:4:606:CHL:CHB	27:4:621:BCR:H342	2.51	0.40
27:A:851:BCR:H20C	27:A:851:BCR:H361	1.97	0.40
27:B:1609:BCR:C33	27:B:1609:BCR:C8	2.99	0.40
27:B:1609:BCR:C8	27:B:1609:BCR:H331	2.51	0.40
10:E:81:ARG:HD2	10:E:84:SER:HB2	2.03	0.40
27:G:205:BCR:H24C	27:G:205:BCR:H371	1.85	0.40
2:5:136:VAL:N	2:5:137:PRO:CD	2.84	0.40
2:5:148:GLU:OE1	22:5:606:CLA:C4B	2.69	0.40
4:7:253:GLY:O	4:7:257:ASN:N	2.49	0.40
5:8:239:GLN:HG3	22:8:613:CLA:C4D	2.51	0.40
20:9:286:ALA:O	20:9:290:LEU:HD13	2.21	0.40
23:9:624:LUT:H8	23:9:624:LUT:C18	2.51	0.40
24:4:620:XAT:H11	24:4:620:XAT:H191	1.94	0.40
6:A:94:ARG:NH2	6:A:157:TYR:CE1	2.89	0.40
6:A:122:LYS:HE2	11:F:130:THR:OG1	2.22	0.40
7:B:15:ASP:OD1	7:B:17:THR:OG1	2.25	0.40
22:6:604:CLA:HMA3	24:6:620:XAT:O3	2.22	0.40
4:7:164:ALA:HB3	4:7:289:TYR:CE2	2.56	0.40
23:7:618:LUT:H11	23:7:618:LUT:H191	1.95	0.40
20:9:167:ARG:NH1	21:9:608:CHL:OBD	2.53	0.40
23:W:2620:LUT:H11	23:W:2620:LUT:H191	1.78	0.40
26:1:630:LHG:C24	27:4:621:BCR:H291	2.52	0.40
6:A:65:GLU:HG3	6:A:69:LYS:NZ	2.37	0.40
6:A:691:TYR:HA	7:B:536:LYS:HZ1	1.86	0.40
27:A:852:BCR:H15C	27:A:852:BCR:H351	1.96	0.40
7:B:246:THR:HG22	7:B:248:GLU:H	1.86	0.40
7:B:415:LYS:NZ	7:B:540:ASP:OD1	2.39	0.40
7:B:652:PHE:O	7:B:656:VAL:HG23	2.20	0.40
14:I:18:PHE:HB3	14:I:19:PRO:HD3	2.04	0.40
27:K:202:BCR:H331	27:K:202:BCR:HC8	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:6:620:XAT:H31	24:6:620:XAT:H391	1.96	0.40
5:8:171:ASP:C	5:8:171:ASP:OD1	2.60	0.40
20:9:178:THR:OG1	20:9:179:PRO:HD3	2.22	0.40
21:2:608:CHL:HHC	21:2:608:CHL:HBB1	2.03	0.40
27:3:620:BCR:C23	27:3:620:BCR:C38	2.98	0.40
27:A:852:BCR:H391	22:B:832:CLA:HMA1	2.02	0.40
7:B:527:LEU:HD12	7:B:586:THR:HG21	2.02	0.40
17:L:69:LEU:HD12	17:L:79:GLU:OE2	2.21	0.40
2:5:108:GLU:CG	2:5:220:LEU:HD21	2.51	0.40
1:V:148:ASN:OD1	1:V:150:SER:N	2.55	0.40
23:2:619:LUT:H11	23:2:619:LUT:H191	1.92	0.40
24:4:620:XAT:H31	24:4:620:XAT:H391	1.90	0.40
27:4:621:BCR:H361	27:4:621:BCR:H20C	1.86	0.40
7:B:229:GLN:O	7:B:229:GLN:HG3	2.21	0.40
11:F:151:ASP:OD1	11:F:151:ASP:C	2.60	0.40
22:K:204:CLA:HHD	22:K:204:CLA:HBC2	2.03	0.40
22:5:602:CLA:H3A	22:5:602:CLA:CGA	2.52	0.40
4:7:133:ASP:HB3	4:7:136:GLY:HA3	2.03	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	U	217/265 (82%)	208 (96%)	9 (4%)	0	100	100
1	V	213/265 (80%)	207 (97%)	6 (3%)	0	100	100
1	W	225/265 (85%)	215 (96%)	9 (4%)	1 (0%)	30	58
2	1	191/245 (78%)	183 (96%)	8 (4%)	0	100	100
2	5	190/245 (78%)	166 (87%)	23 (12%)	1 (0%)	25	53
3	2	209/273 (77%)	200 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	6	203/273 (74%)	190 (94%)	13 (6%)	0	100	100
4	3	220/323 (68%)	213 (97%)	7 (3%)	0	100	100
4	7	217/323 (67%)	203 (94%)	13 (6%)	1 (0%)	25	53
5	4	204/270 (76%)	192 (94%)	12 (6%)	0	100	100
5	8	202/270 (75%)	187 (93%)	15 (7%)	0	100	100
6	A	740/750 (99%)	716 (97%)	23 (3%)	1 (0%)	48	75
7	B	731/734 (100%)	714 (98%)	17 (2%)	0	100	100
8	C	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
9	D	140/210 (67%)	133 (95%)	7 (5%)	0	100	100
10	E	62/132 (47%)	62 (100%)	0	0	100	100
11	F	159/246 (65%)	152 (96%)	6 (4%)	1 (1%)	22	49
12	G	95/155 (61%)	91 (96%)	4 (4%)	0	100	100
13	H	93/139 (67%)	90 (97%)	3 (3%)	0	100	100
14	I	32/36 (89%)	31 (97%)	1 (3%)	0	100	100
15	J	39/41 (95%)	39 (100%)	0	0	100	100
16	K	79/132 (60%)	79 (100%)	0	0	100	100
17	L	161/223 (72%)	155 (96%)	6 (4%)	0	100	100
18	M	29/32 (91%)	29 (100%)	0	0	100	100
19	O	88/143 (62%)	81 (92%)	7 (8%)	0	100	100
20	9	217/311 (70%)	190 (88%)	26 (12%)	1 (0%)	25	53
All	All	5034/6382 (79%)	4800 (95%)	228 (4%)	6 (0%)	50	75

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	A	315	ILE
2	5	135	PRO
4	7	112	SER
11	F	88	ALA
1	W	39	ARG
20	9	185	ASN

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	U	166/203 (82%)	165 (99%)	1 (1%)	84	94
1	V	163/203 (80%)	163 (100%)	0	100	100
1	W	173/203 (85%)	173 (100%)	0	100	100
2	1	148/186 (80%)	148 (100%)	0	100	100
2	5	148/186 (80%)	147 (99%)	1 (1%)	81	93
3	2	167/213 (78%)	167 (100%)	0	100	100
3	6	162/213 (76%)	160 (99%)	2 (1%)	67	87
4	3	174/256 (68%)	174 (100%)	0	100	100
4	7	170/256 (66%)	170 (100%)	0	100	100
5	4	164/210 (78%)	162 (99%)	2 (1%)	67	87
5	8	162/210 (77%)	162 (100%)	0	100	100
6	A	603/611 (99%)	602 (100%)	1 (0%)	92	98
7	B	595/596 (100%)	593 (100%)	2 (0%)	91	97
8	C	67/68 (98%)	67 (100%)	0	100	100
9	D	115/157 (73%)	115 (100%)	0	100	100
10	E	56/105 (53%)	56 (100%)	0	100	100
11	F	132/193 (68%)	132 (100%)	0	100	100
12	G	77/121 (64%)	77 (100%)	0	100	100
13	H	75/103 (73%)	74 (99%)	1 (1%)	65	86
14	I	30/32 (94%)	30 (100%)	0	100	100
15	J	35/35 (100%)	35 (100%)	0	100	100
16	K	58/95 (61%)	58 (100%)	0	100	100
17	L	124/165 (75%)	122 (98%)	2 (2%)	58	82
18	M	26/27 (96%)	26 (100%)	0	100	100
19	O	74/115 (64%)	74 (100%)	0	100	100
20	9	174/243 (72%)	173 (99%)	1 (1%)	84	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4038/5005 (81%)	4025 (100%)	13 (0%)	90 97

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

Mol	Chain	Res	Type
1	U	201	ASP
5	4	65	ARG
5	4	112	ARG
6	A	585	SER
7	B	479	SER
7	B	516	ASP
13	H	119	ASP
17	L	135	ARG
17	L	223	LYS
2	5	85	ARG
3	6	137	SER
3	6	226	ASN
20	9	134	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	U	245	HIS
2	1	140	ASN
6	A	419	GLN
6	A	422	ASN
17	L	94	ASN
4	7	302	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	$\# Z > 2$
1	TPO	W	40	1	8,10,11	1.58	1 (12%)	10,14,16	1.83	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 Torsions and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	W	40	1	-	0/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	W	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(°)
1	W	40	TPO	P-OG1-CB	-5.15	107.66	123.21

There are no chirality outliers.

There are no torsion outliers.

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](#)

366 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
28	LMG	G	202	-	32,32,55	1.21	3 (9%)	40,40,63	1.15	2 (5%)
27	BCR	A	856	-	40,40,41	0.70	0	54,54,56	1.68	13 (24%)
22	CLA	V	613	1	56,64,73	1.65	6 (10%)	64,101,113	1.42	11 (17%)
22	CLA	7	610	4	55,63,73	1.68	5 (9%)	64,101,113	1.36	7 (10%)
22	CLA	V	602	1	59,67,73	1.59	5 (8%)	68,105,113	1.30	9 (13%)
22	CLA	A	833	-	55,63,73	1.63	5 (9%)	64,101,113	1.34	8 (12%)
22	CLA	5	602	2	60,68,73	1.57	6 (10%)	70,107,113	1.29	8 (11%)
22	CLA	B	827	-	56,64,73	1.58	6 (10%)	65,102,113	1.38	7 (10%)
23	LUT	1	617	-	42,43,43	0.74	0	51,60,60	1.58	12 (23%)
27	BCR	B	847	-	41,41,41	0.75	0	56,56,56	2.14	19 (33%)
22	CLA	A	841	-	65,73,73	1.51	6 (9%)	76,113,113	1.21	7 (9%)
22	CLA	U	604	-	52,60,73	1.68	6 (11%)	60,97,113	1.38	8 (13%)
21	CHL	4	606	-	46,54,74	2.29	16 (34%)	49,90,114	3.22	19 (38%)
21	CHL	6	602	3	56,64,74	2.11	15 (26%)	61,102,114	2.99	18 (29%)
22	CLA	2	603	-	46,54,73	1.79	7 (15%)	53,90,113	1.47	7 (13%)
22	CLA	5	609	2	41,49,73	1.99	8 (19%)	47,84,113	1.40	7 (14%)
22	CLA	3	604	-	55,63,73	1.61	6 (10%)	64,101,113	1.35	9 (14%)
22	CLA	A	820	-	65,73,73	1.47	5 (7%)	76,113,113	1.29	8 (10%)
21	CHL	6	607	-	47,55,74	2.29	16 (34%)	50,91,114	3.16	19 (38%)
22	CLA	B	832	-	65,73,73	1.53	6 (9%)	76,113,113	1.30	9 (11%)
22	CLA	U	614	-	42,50,73	1.90	6 (14%)	48,85,113	1.34	7 (14%)
22	CLA	B	814	-	65,73,73	1.51	6 (9%)	76,113,113	1.38	12 (15%)
22	CLA	7	609	4	57,65,73	1.73	8 (14%)	66,103,113	1.28	8 (12%)
31	LMT	A	857	-	36,36,36	0.77	0	47,47,47	1.36	7 (14%)
22	CLA	B	810	-	65,73,73	1.47	7 (10%)	76,113,113	1.30	8 (10%)
22	CLA	4	609	5	45,53,73	1.80	6 (13%)	52,89,113	1.42	9 (17%)
27	BCR	A	851	-	41,41,41	0.80	1 (2%)	56,56,56	2.14	24 (42%)
23	LUT	V	2620	-	42,43,43	0.76	0	51,60,60	1.73	16 (31%)
22	CLA	A	843	-	65,73,73	1.50	7 (10%)	76,113,113	1.27	7 (9%)
22	CLA	1	603	-	55,63,73	1.63	6 (10%)	64,101,113	1.43	9 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	B	839	-	65,73,73	1.49	7 (10%)	76,113,113	1.26	8 (10%)
22	CLA	3	610	4	60,68,73	1.59	7 (11%)	70,107,113	1.27	8 (11%)
22	CLA	B	825	-	65,73,73	1.47	6 (9%)	76,113,113	1.33	8 (10%)
22	CLA	7	606	-	46,54,73	1.78	6 (13%)	53,90,113	1.39	7 (13%)
22	CLA	3	617	-	55,63,73	1.77	10 (18%)	63,98,113	2.10	11 (17%)
23	LUT	4	619	-	42,43,43	0.71	0	51,60,60	1.81	14 (27%)
21	CHL	8	608	-	51,59,74	2.20	15 (29%)	55,96,114	3.11	22 (40%)
27	BCR	A	849	-	41,41,41	0.77	0	56,56,56	2.01	18 (32%)
23	LUT	U	2620	-	42,43,43	0.73	0	51,60,60	1.72	14 (27%)
23	LUT	3	618	-	42,43,43	0.77	1 (2%)	51,60,60	1.60	11 (21%)
22	CLA	A	826	-	65,73,73	1.51	7 (10%)	76,113,113	1.24	8 (10%)
22	CLA	7	612	4	45,53,73	1.83	6 (13%)	52,89,113	1.50	7 (13%)
25	NEX	U	2623	-	38,46,46	1.06	3 (7%)	50,70,70	2.53	17 (34%)
28	LMG	J	104	-	35,35,55	1.14	2 (5%)	43,43,63	1.01	2 (4%)
22	CLA	A	815	-	65,73,73	1.51	8 (12%)	76,113,113	1.25	9 (11%)
23	LUT	W	2620	-	42,43,43	0.79	0	51,60,60	1.67	13 (25%)
23	LUT	9	620	-	42,43,43	0.75	0	51,60,60	1.79	13 (25%)
22	CLA	6	613	3	65,73,73	1.54	6 (9%)	76,113,113	1.22	8 (10%)
23	LUT	6	619	-	42,43,43	0.74	0	51,60,60	1.55	11 (21%)
23	LUT	5	617	-	42,43,43	1.71	8 (19%)	51,60,60	1.76	11 (21%)
22	CLA	8	602	5	60,68,73	1.59	6 (10%)	70,107,113	1.28	9 (12%)
22	CLA	W	602	1	60,68,73	1.56	5 (8%)	70,107,113	1.29	7 (10%)
21	CHL	V	605	1	42,50,74	2.40	16 (38%)	44,85,114	3.45	20 (45%)
22	CLA	F	303	-	45,53,73	1.77	6 (13%)	52,89,113	1.49	8 (15%)
21	CHL	6	618	3	47,55,74	2.26	15 (31%)	50,91,114	3.15	18 (36%)
22	CLA	V	611	26	39,48,73	1.98	6 (15%)	48,83,113	1.50	9 (18%)
30	SF4	C	102	8	0,12,12	-	-	-	-	-
22	CLA	A	806	-	65,73,73	1.49	6 (9%)	76,113,113	1.29	8 (10%)
22	CLA	8	610	5	55,63,73	1.67	6 (10%)	64,101,113	1.31	9 (14%)
22	CLA	5	613	2	50,58,73	1.75	7 (14%)	58,95,113	1.38	10 (17%)
26	LHG	8	630	22	37,37,48	1.07	2 (5%)	40,43,54	1.09	4 (10%)
24	XAT	4	620	-	39,47,47	0.99	1 (2%)	54,74,74	5.03	22 (40%)
22	CLA	1	602	2	65,73,73	1.50	6 (9%)	76,113,113	1.23	8 (10%)
22	CLA	5	614	-	43,51,73	1.83	5 (11%)	49,86,113	1.41	7 (14%)
21	CHL	W	609	1	39,48,74	2.27	13 (33%)	42,82,114	3.38	18 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	A	829	-	60,68,73	1.52	6 (10%)	70,107,113	1.42	8 (11%)
32	DGD	B	850	-	67,67,67	0.89	2 (2%)	81,81,81	0.96	3 (3%)
26	LHG	V	2630	22	41,41,48	1.02	2 (4%)	44,47,54	0.96	2 (4%)
22	CLA	G	204	12	46,54,73	1.81	5 (10%)	53,90,113	1.42	7 (13%)
21	CHL	9	608	-	43,51,74	2.29	15 (34%)	45,86,114	3.24	19 (42%)
22	CLA	B	828	-	65,73,73	1.50	7 (10%)	76,113,113	1.25	7 (9%)
22	CLA	B	812	-	43,52,73	1.78	6 (13%)	48,87,113	1.51	8 (16%)
24	XAT	8	620	-	39,47,47	1.76	6 (15%)	54,74,74	1.94	15 (27%)
22	CLA	A	822	-	65,73,73	1.50	7 (10%)	76,113,113	1.26	8 (10%)
22	CLA	2	604	-	50,58,73	1.70	6 (12%)	58,95,113	1.43	9 (15%)
22	CLA	A	817	-	65,73,73	1.51	5 (7%)	76,113,113	1.33	8 (10%)
21	CHL	8	618	5	43,51,74	2.32	14 (32%)	45,86,114	3.26	19 (42%)
26	LHG	B	851	22	34,34,48	1.11	2 (5%)	37,40,54	1.01	2 (5%)
21	CHL	U	609	1	66,74,74	1.95	15 (22%)	73,114,114	2.73	22 (30%)
22	CLA	B	830	-	45,53,73	1.87	6 (13%)	52,89,113	1.37	7 (13%)
26	LHG	U	2630	22	44,44,48	0.98	2 (4%)	47,50,54	0.96	2 (4%)
22	CLA	9	609	20	45,53,73	2.37	16 (35%)	52,89,113	3.13	21 (40%)
22	CLA	3	603	4	65,73,73	1.54	7 (10%)	76,113,113	1.25	7 (9%)
22	CLA	B	838	-	47,55,73	1.80	8 (17%)	54,91,113	1.41	9 (16%)
21	CHL	2	606	-	46,54,74	2.29	16 (34%)	49,90,114	3.22	20 (40%)
22	CLA	B	802	-	65,73,73	1.48	7 (10%)	76,113,113	1.19	6 (7%)
22	CLA	B	826	-	65,73,73	1.53	6 (9%)	76,113,113	1.24	8 (10%)
23	LUT	W	2621	-	42,43,43	0.76	0	51,60,60	1.66	9 (17%)
24	XAT	V	2622	-	39,47,47	1.06	1 (2%)	54,74,74	5.76	21 (38%)
27	BCR	B	801	-	41,41,41	0.72	0	56,56,56	1.91	17 (30%)
22	CLA	B	815	-	45,53,73	1.81	6 (13%)	52,89,113	1.42	7 (13%)
21	CHL	V	608	-	39,48,74	2.26	13 (33%)	45,83,114	3.30	18 (40%)
26	LHG	5	630	22	36,36,48	1.08	2 (5%)	39,42,54	1.07	3 (7%)
22	CLA	B	833	-	65,73,73	1.50	7 (10%)	76,113,113	1.30	9 (11%)
22	CLA	5	603	-	45,53,73	1.85	6 (13%)	52,89,113	1.43	7 (13%)
21	CHL	6	601	3	66,74,74	1.95	15 (22%)	73,114,114	2.67	21 (28%)
26	LHG	3	630	22	31,31,48	1.16	2 (6%)	34,37,54	1.05	2 (5%)
22	CLA	B	816	-	65,73,73	1.51	6 (9%)	76,113,113	1.28	8 (10%)
22	CLA	6	611	26	45,53,73	1.79	5 (11%)	52,89,113	1.50	8 (15%)
24	XAT	2	620	-	39,47,47	0.91	2 (5%)	54,74,74	2.53	22 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	9	612	20	38,47,73	1.94	8 (21%)	45,81,113	1.41	6 (13%)
26	LHG	A	847	22	30,30,48	1.16	2 (6%)	33,36,54	1.23	3 (9%)
23	LUT	U	2621	-	42,43,43	0.78	0	51,60,60	1.70	11 (21%)
21	CHL	1	601	2	56,64,74	2.11	16 (28%)	61,102,114	2.89	23 (37%)
25	NEX	9	623	-	38,46,46	1.04	2 (5%)	50,70,70	2.21	14 (28%)
21	CHL	V	606	-	37,46,74	2.43	14 (37%)	46,81,114	3.23	19 (41%)
21	CHL	U	608	-	39,48,74	2.27	13 (33%)	45,83,114	3.24	19 (42%)
22	CLA	1	606	-	45,53,73	1.86	7 (15%)	52,89,113	1.41	7 (13%)
22	CLA	B	806	-	65,73,73	1.48	7 (10%)	76,113,113	1.30	8 (10%)
22	CLA	B	805	-	65,73,73	1.49	6 (9%)	76,113,113	1.34	10 (13%)
24	XAT	1	618	-	39,47,47	0.91	1 (2%)	54,74,74	2.52	24 (44%)
22	CLA	A	832	-	55,63,73	1.63	8 (14%)	64,101,113	1.43	7 (10%)
22	CLA	5	606	2	45,53,73	1.85	6 (13%)	52,89,113	1.42	8 (15%)
29	PQN	B	842	-	34,34,34	0.63	1 (2%)	42,45,45	0.89	2 (4%)
22	CLA	1	608	-	45,53,73	1.83	7 (15%)	52,89,113	1.41	8 (15%)
22	CLA	7	615	-	39,48,73	1.94	6 (15%)	44,83,113	1.44	7 (15%)
26	LHG	4	630	22	37,37,48	1.03	2 (5%)	40,43,54	1.21	6 (15%)
22	CLA	A	837	6	65,73,73	1.55	7 (10%)	76,113,113	1.22	6 (7%)
22	CLA	W	614	-	38,47,73	1.99	7 (18%)	47,82,113	1.49	9 (19%)
22	CLA	V	612	1	37,46,73	2.01	7 (18%)	46,81,113	1.67	9 (19%)
22	CLA	2	612	3	45,53,73	1.82	6 (13%)	52,89,113	1.43	6 (11%)
24	XAT	7	619	-	39,47,47	1.22	3 (7%)	54,74,74	6.06	18 (33%)
22	CLA	6	604	-	50,58,73	1.73	6 (12%)	58,95,113	1.42	8 (13%)
22	CLA	7	607	4	45,53,73	1.80	5 (11%)	52,89,113	1.48	6 (11%)
22	CLA	B	821	-	50,58,73	1.77	7 (14%)	58,95,113	1.37	8 (13%)
22	CLA	8	601	5	50,58,73	1.77	7 (14%)	58,95,113	1.37	9 (15%)
22	CLA	3	607	4	50,58,73	1.72	7 (14%)	58,95,113	1.40	9 (15%)
22	CLA	1	611	26	65,73,73	1.53	6 (9%)	76,113,113	1.30	11 (14%)
22	CLA	5	604	-	41,49,73	1.92	7 (17%)	47,84,113	1.43	6 (12%)
21	CHL	V	609	1	39,48,74	2.31	13 (33%)	42,82,114	3.34	19 (45%)
21	CHL	5	601	2	51,59,74	2.21	16 (31%)	55,96,114	3.04	23 (41%)
26	LHG	7	630	22	33,33,48	1.14	2 (6%)	36,39,54	1.08	3 (8%)
22	CLA	O	2003	-	29,35,73	2.68	9 (31%)	28,60,113	1.47	3 (10%)
22	CLA	L	304	-	60,68,73	1.56	6 (10%)	70,107,113	1.30	9 (12%)
22	CLA	U	612	1	65,73,73	1.52	7 (10%)	76,113,113	1.21	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	V	610	1	39,47,73	2.01	6 (15%)	49,82,113	1.50	10 (20%)
23	LUT	9	621	-	42,43,43	0.81	0	51,60,60	1.68	13 (25%)
21	CHL	6	608	-	48,56,74	2.26	15 (31%)	51,92,114	3.19	19 (37%)
22	CLA	V	614	-	45,53,73	1.82	6 (13%)	52,89,113	1.38	8 (15%)
22	CLA	A	807	6	65,73,73	1.48	6 (9%)	76,113,113	1.27	7 (9%)
22	CLA	3	615	-	53,61,73	1.68	6 (11%)	61,98,113	1.42	7 (11%)
22	CLA	B	819	-	60,68,73	1.59	7 (11%)	70,107,113	1.37	10 (14%)
22	CLA	8	603	-	55,63,73	1.66	6 (10%)	64,101,113	1.38	7 (10%)
22	CLA	6	603	-	46,54,73	1.83	6 (13%)	53,90,113	1.46	7 (13%)
22	CLA	5	608	-	50,58,73	1.72	5 (10%)	58,95,113	1.45	9 (15%)
22	CLA	6	612	3	45,53,73	1.86	6 (13%)	52,89,113	1.40	6 (11%)
21	CHL	4	608	-	46,54,74	2.37	15 (32%)	49,90,114	3.15	17 (34%)
22	CLA	A	839	-	60,68,73	1.56	6 (10%)	70,107,113	1.32	8 (11%)
24	XAT	3	619	-	39,47,47	0.87	1 (2%)	54,74,74	2.76	21 (38%)
22	CLA	B	836	-	52,60,73	1.64	6 (11%)	60,97,113	1.44	7 (11%)
27	BCR	L	306	-	41,41,41	0.70	0	56,56,56	2.06	20 (35%)
22	CLA	5	610	2	55,63,73	1.66	6 (10%)	64,101,113	1.28	8 (12%)
26	LHG	A	846	-	46,46,48	0.96	2 (4%)	49,52,54	0.99	3 (6%)
22	CLA	A	823	-	53,62,73	1.60	5 (9%)	60,99,113	1.45	8 (13%)
22	CLA	1	610	2	65,73,73	1.52	6 (9%)	76,113,113	1.25	9 (11%)
22	CLA	4	612	5	45,53,73	1.82	7 (15%)	52,89,113	1.45	7 (13%)
22	CLA	B	829	-	65,73,73	1.51	6 (9%)	76,113,113	1.26	7 (9%)
22	CLA	L	302	17	65,73,73	1.53	7 (10%)	76,113,113	1.25	8 (10%)
22	CLA	A	818	-	65,73,73	1.51	6 (9%)	76,113,113	1.23	7 (9%)
22	CLA	A	821	-	55,63,73	1.64	8 (14%)	64,101,113	1.25	7 (10%)
22	CLA	3	606	-	46,54,73	1.78	6 (13%)	53,90,113	1.44	7 (13%)
22	CLA	K	201	16	42,50,73	1.83	6 (14%)	48,85,113	1.55	8 (16%)
22	CLA	B	809	7	65,73,73	1.51	7 (10%)	76,113,113	1.30	8 (10%)
22	CLA	7	611	26	41,49,73	1.91	6 (14%)	47,84,113	1.40	8 (17%)
21	CHL	8	607	-	46,54,74	2.33	16 (34%)	49,90,114	3.19	19 (38%)
31	LMT	G	206	-	36,36,36	0.65	0	47,47,47	1.26	6 (12%)
28	LMG	2	631	-	47,47,55	0.98	2 (4%)	55,55,63	0.98	4 (7%)
22	CLA	8	613	5	55,63,73	1.67	6 (10%)	64,101,113	1.36	8 (12%)
22	CLA	4	614	-	46,54,73	1.79	6 (13%)	53,90,113	1.39	7 (13%)
22	CLA	A	842	-	55,63,73	1.67	7 (12%)	64,101,113	1.36	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CHL	V	601	1	62,71,74	1.89	14 (22%)	76,111,114	2.67	22 (28%)
22	CLA	W	613	1	60,68,73	1.58	7 (11%)	70,107,113	1.29	8 (11%)
27	BCR	2	621	-	41,41,41	0.77	0	56,56,56	2.08	20 (35%)
22	CLA	3	614	-	45,53,73	1.82	6 (13%)	52,89,113	1.44	8 (15%)
22	CLA	A	809	6	56,64,73	1.61	6 (10%)	65,102,113	1.40	8 (12%)
22	CLA	6	614	-	50,58,73	1.72	6 (12%)	58,95,113	1.44	9 (15%)
22	CLA	1	613	2	50,58,73	1.72	6 (12%)	58,95,113	1.40	8 (13%)
25	NEX	V	2623	-	38,46,46	0.89	1 (2%)	50,70,70	2.56	18 (36%)
27	BCR	A	850	-	41,41,41	0.74	0	56,56,56	1.80	15 (26%)
22	CLA	L	303	-	65,73,73	1.51	8 (12%)	76,113,113	1.26	9 (11%)
21	CHL	6	606	-	46,54,74	2.30	15 (32%)	49,90,114	3.20	19 (38%)
22	CLA	F	301	33	65,73,73	1.50	7 (10%)	76,113,113	1.23	7 (9%)
22	CLA	4	601	5	50,58,73	1.72	5 (10%)	58,95,113	1.42	10 (17%)
22	CLA	6	610	3	60,68,73	1.57	6 (10%)	70,107,113	1.27	8 (11%)
22	CLA	2	610	3	60,68,73	1.57	7 (11%)	70,107,113	1.22	7 (10%)
22	CLA	5	611	26	46,54,73	1.84	7 (15%)	53,90,113	1.39	6 (11%)
22	CLA	B	840	-	65,73,73	1.47	6 (9%)	76,113,113	1.24	8 (10%)
24	XAT	5	618	-	39,47,47	0.88	0	54,74,74	2.70	24 (44%)
22	CLA	F	304	11	41,51,73	1.91	11 (26%)	41,81,113	1.92	7 (17%)
28	LMG	L	307	-	44,44,55	1.00	2 (4%)	52,52,63	0.93	2 (3%)
22	CLA	2	609	3	46,54,73	1.79	6 (13%)	53,90,113	1.44	7 (13%)
21	CHL	4	618	5	43,51,74	2.28	14 (32%)	45,86,114	3.29	20 (44%)
22	CLA	B	822	-	60,68,73	1.58	5 (8%)	70,107,113	1.36	11 (15%)
27	BCR	7	620	-	41,41,41	0.68	0	56,56,56	2.08	20 (35%)
22	CLA	3	602	4	65,73,73	1.51	7 (10%)	76,113,113	1.23	8 (10%)
22	CLA	9	610	20	55,63,73	1.65	8 (14%)	64,101,113	1.29	8 (12%)
22	CLA	A	854	-	60,68,73	1.56	6 (10%)	70,107,113	1.39	7 (10%)
22	CLA	W	603	-	38,47,73	1.97	6 (15%)	43,82,113	1.46	9 (20%)
30	SF4	C	101	8	0,12,12	-	-	-	-	-
22	CLA	B	841	26	65,73,73	1.51	6 (9%)	76,113,113	1.32	9 (11%)
30	SF4	A	853	7,6	0,12,12	-	-	-	-	-
27	BCR	B	844	-	41,41,41	0.70	0	56,56,56	2.02	23 (41%)
27	BCR	M	2001	-	41,41,41	0.65	0	56,56,56	2.15	22 (39%)
22	CLA	1	609	2	65,73,73	1.59	7 (10%)	76,113,113	1.24	9 (11%)
22	CLA	A	803	-	65,73,73	1.51	9 (13%)	76,113,113	1.34	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CHL	W	606	-	37,46,74	2.44	14 (37%)	46,81,114	3.32	20 (43%)
21	CHL	2	608	-	46,54,74	2.35	16 (34%)	49,90,114	3.15	21 (42%)
27	BCR	B	848	-	41,41,41	0.73	0	56,56,56	1.97	17 (30%)
22	CLA	A	835	-	65,73,73	1.51	7 (10%)	76,113,113	1.21	8 (10%)
22	CLA	3	613	4	65,73,73	1.52	6 (9%)	76,113,113	1.32	10 (13%)
22	CLA	V	603	-	60,68,73	1.57	5 (8%)	70,107,113	1.31	7 (10%)
22	CLA	B	804	-	65,73,73	1.51	5 (7%)	76,113,113	1.33	10 (13%)
31	LMT	B	849	-	32,32,36	0.66	0	43,43,47	1.32	7 (16%)
23	LUT	V	2621	-	42,43,43	0.78	0	51,60,60	1.68	11 (21%)
22	CLA	4	603	-	65,73,73	1.51	6 (9%)	76,113,113	1.29	8 (10%)
22	CLA	A	819	-	62,70,73	1.52	7 (11%)	72,109,113	1.32	8 (11%)
22	CLA	B	824	-	65,73,73	1.50	6 (9%)	76,113,113	1.37	8 (10%)
24	XAT	U	2622	-	39,47,47	0.89	0	54,74,74	2.62	16 (29%)
23	LUT	2	619	-	42,43,43	1.60	8 (19%)	51,60,60	1.58	11 (21%)
27	BCR	8	621	-	41,41,41	0.79	0	56,56,56	2.29	19 (33%)
28	LMG	J	103	-	55,55,55	0.87	2 (3%)	63,63,63	1.00	3 (4%)
27	BCR	K	205	-	41,41,41	0.81	1 (2%)	56,56,56	2.36	25 (44%)
22	CLA	8	614	-	45,53,73	1.84	5 (11%)	52,89,113	1.47	9 (17%)
27	BCR	L	305	-	41,41,41	0.70	0	56,56,56	1.98	21 (37%)
22	CLA	4	613	5	55,63,73	1.66	5 (9%)	64,101,113	1.32	9 (14%)
22	CLA	B	807	-	65,73,73	1.49	6 (9%)	76,113,113	1.28	8 (10%)
22	CLA	B	808	-	65,73,73	1.52	8 (12%)	76,113,113	1.18	7 (9%)
22	CLA	U	603	-	65,73,73	1.51	7 (10%)	76,113,113	1.30	7 (9%)
22	CLA	4	602	5	65,73,73	1.51	5 (7%)	76,113,113	1.22	9 (11%)
22	CLA	A	828	-	65,73,73	1.51	7 (10%)	76,113,113	1.33	8 (10%)
22	CLA	U	610	1	65,73,73	1.50	6 (9%)	76,113,113	1.28	10 (13%)
22	CLA	9	602	20	60,68,73	1.57	8 (13%)	70,107,113	1.44	9 (12%)
21	CHL	5	607	2	38,47,74	2.39	15 (39%)	41,81,114	3.34	18 (43%)
22	CLA	1	616	2	45,53,73	1.85	6 (13%)	52,89,113	1.45	7 (13%)
23	LUT	8	619	-	42,43,43	0.75	1 (2%)	51,60,60	1.68	12 (23%)
22	CLA	A	834	-	65,73,73	1.52	6 (9%)	76,113,113	1.23	7 (9%)
22	CLA	A	813	-	55,63,73	1.61	6 (10%)	64,101,113	1.44	7 (10%)
22	CLA	8	604	-	50,58,73	1.74	6 (12%)	58,95,113	1.35	9 (15%)
22	CLA	7	602	4	60,68,73	1.62	5 (8%)	70,107,113	1.42	9 (12%)
22	CLA	A	827	33	65,73,73	1.50	6 (9%)	76,113,113	1.27	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	LHG	6	630	22	31,31,48	1.17	2 (6%)	34,37,54	1.07	2 (5%)
21	CHL	U	601	1	62,71,74	1.89	14 (22%)	76,111,114	2.57	21 (27%)
27	BCR	4	621	-	41,41,41	0.80	0	56,56,56	3.03	16 (28%)
22	CLA	K	206	16	42,50,73	1.87	7 (16%)	48,85,113	1.43	7 (14%)
26	LHG	1	630	22	48,48,48	0.93	2 (4%)	51,54,54	0.95	3 (5%)
22	CLA	A	840	-	50,58,73	1.71	6 (12%)	58,95,113	1.40	7 (12%)
22	CLA	G	203	-	50,58,73	1.72	5 (10%)	58,95,113	1.41	8 (13%)
23	LUT	7	618	-	42,43,43	0.78	0	51,60,60	1.61	10 (19%)
21	CHL	W	601	1	62,71,74	1.89	14 (22%)	76,111,114	2.59	21 (27%)
22	CLA	1	604	-	50,58,73	1.71	5 (10%)	58,95,113	1.41	8 (13%)
22	CLA	W	611	26	39,48,73	1.97	7 (17%)	48,83,113	1.49	8 (16%)
24	XAT	6	620	-	39,47,47	1.23	2 (5%)	54,74,74	6.73	25 (46%)
22	CLA	B	803	-	65,73,73	1.49	8 (12%)	76,113,113	1.29	7 (9%)
22	CLA	O	2002	-	55,63,73	1.68	6 (10%)	64,101,113	1.28	7 (10%)
22	CLA	A	824	-	62,70,73	1.54	6 (9%)	72,109,113	1.29	9 (12%)
22	CLA	5	616	2	46,54,73	1.84	5 (10%)	53,90,113	1.34	6 (11%)
27	BCR	O	2004	-	41,41,41	0.75	0	56,56,56	2.10	18 (32%)
21	CHL	2	602	3	61,69,74	2.04	16 (26%)	67,108,114	2.84	24 (35%)
27	BCR	B	843	-	41,41,41	0.74	0	56,56,56	2.18	22 (39%)
22	CLA	B	835	-	45,53,73	1.77	5 (11%)	52,89,113	1.44	8 (15%)
22	CLA	U	602	1	65,73,73	1.52	6 (9%)	76,113,113	1.24	9 (11%)
22	CLA	K	204	-	65,73,73	1.49	6 (9%)	76,113,113	1.35	8 (10%)
21	CHL	U	605	1	37,46,74	2.44	14 (37%)	46,81,114	3.34	18 (39%)
22	CLA	7	604	-	50,58,73	1.72	5 (10%)	58,95,113	1.42	9 (15%)
27	BCR	3	621	-	41,41,41	0.79	1 (2%)	56,56,56	2.26	19 (33%)
22	CLA	7	614	-	41,49,73	1.89	5 (12%)	47,84,113	1.52	7 (14%)
27	BCR	J	102	-	41,41,41	0.71	0	56,56,56	2.24	17 (30%)
21	CHL	2	607	-	47,55,74	2.30	15 (31%)	50,91,114	3.21	21 (42%)
21	CHL	W	605	1	37,46,74	2.43	14 (37%)	46,81,114	3.31	18 (39%)
22	CLA	B	834	-	65,73,73	1.49	7 (10%)	76,113,113	1.28	7 (9%)
27	BCR	B	1609	-	41,41,41	0.75	0	56,56,56	3.14	26 (46%)
22	CLA	B	820	-	55,63,73	1.63	6 (10%)	64,101,113	1.34	8 (12%)
21	CHL	8	606	-	46,54,74	2.32	16 (34%)	49,90,114	3.17	21 (42%)
22	CLA	4	610	5	61,69,73	1.63	6 (9%)	71,108,113	1.29	7 (9%)
21	CHL	2	618	3	43,51,74	2.31	14 (32%)	45,86,114	3.30	20 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CHL	9	601	20	38,47,74	2.39	14 (36%)	41,81,114	3.31	19 (46%)
22	CLA	V	604	-	50,58,73	1.73	7 (14%)	58,95,113	1.42	9 (15%)
22	CLA	4	611	26	45,53,73	1.86	6 (13%)	52,89,113	1.41	5 (9%)
22	CLA	9	611	26	65,73,73	1.54	7 (10%)	76,113,113	1.24	8 (10%)
21	CHL	3	608	-	56,64,74	2.10	15 (26%)	61,102,114	2.91	19 (31%)
22	CLA	O	2001	-	29,35,73	2.68	9 (31%)	28,60,113	1.53	4 (14%)
27	BCR	F	305	-	41,41,41	0.69	0	56,56,56	2.13	19 (33%)
24	XAT	W	2622	-	39,47,47	0.90	0	54,74,74	2.64	19 (35%)
27	BCR	1	619	-	41,41,41	0.74	0	56,56,56	2.55	27 (48%)
22	CLA	9	613	20	52,60,73	1.72	7 (13%)	60,97,113	1.39	7 (11%)
22	CLA	A	801	-	65,73,73	1.50	7 (10%)	76,113,113	1.55	12 (15%)
21	CHL	W	608	-	39,48,74	2.25	13 (33%)	45,83,114	3.28	19 (42%)
22	CLA	7	617	-	46,54,73	1.80	5 (10%)	53,90,113	1.41	8 (15%)
22	CLA	7	613	4	55,63,73	1.67	7 (12%)	64,101,113	1.31	8 (12%)
22	CLA	A	805	-	65,73,73	1.51	5 (7%)	76,113,113	1.36	9 (11%)
21	CHL	V	607	-	40,48,74	2.34	14 (35%)	47,83,114	3.41	20 (42%)
22	CLA	A	808	-	60,68,73	1.59	6 (10%)	70,107,113	1.28	8 (11%)
22	CLA	B	817	-	65,73,73	1.51	7 (10%)	76,113,113	1.28	7 (9%)
21	CHL	2	601	3	46,54,74	2.31	15 (32%)	49,90,114	3.23	20 (40%)
29	PQN	A	844	-	34,34,34	0.49	0	42,45,45	0.86	3 (7%)
22	CLA	W	610	1	65,73,73	1.54	6 (9%)	76,113,113	1.36	8 (10%)
22	CLA	2	613	3	57,65,73	1.62	7 (12%)	66,103,113	1.41	10 (15%)
26	LHG	9	2630	22	27,27,48	1.30	2 (7%)	30,33,54	0.98	3 (10%)
22	CLA	8	611	26	55,63,73	1.67	6 (10%)	64,101,113	1.24	6 (9%)
27	BCR	6	621	-	41,41,41	0.81	0	56,56,56	2.42	21 (37%)
28	LMG	A	860	-	34,34,55	1.14	2 (5%)	42,42,63	1.10	2 (4%)
22	CLA	6	609	3	55,63,73	1.65	5 (9%)	64,101,113	1.32	9 (14%)
21	CHL	9	607	-	43,51,74	2.31	14 (32%)	45,86,114	3.19	20 (44%)
22	CLA	W	612	1	37,46,73	2.02	7 (18%)	46,81,113	1.56	11 (23%)
22	CLA	A	836	-	57,66,73	1.48	9 (15%)	66,99,113	1.82	12 (18%)
27	BCR	G	205	-	41,41,41	0.76	0	56,56,56	1.92	19 (33%)
22	CLA	B	811	-	61,69,73	1.59	7 (11%)	71,108,113	1.22	8 (11%)
21	CHL	1	607	-	47,55,74	2.31	16 (34%)	50,91,114	3.08	20 (40%)
27	BCR	L	301	-	41,41,41	0.72	0	56,56,56	2.29	19 (33%)
26	LHG	2	630	22	31,31,48	1.17	2 (6%)	34,37,54	1.04	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	3	611	26	55,63,73	1.70	6 (10%)	64,101,113	1.31	7 (10%)
21	CHL	U	607	-	66,74,74	1.94	15 (22%)	73,114,114	2.74	22 (30%)
27	BCR	A	852	-	41,41,41	0.72	0	56,56,56	2.28	24 (42%)
22	CLA	U	611	26	45,53,73	1.86	5 (11%)	52,89,113	1.37	7 (13%)
22	CLA	3	609	4	65,73,73	1.54	7 (10%)	76,113,113	1.37	9 (11%)
22	CLA	U	613	1	65,73,73	1.51	6 (9%)	76,113,113	1.26	8 (10%)
22	CLA	8	609	5	55,63,73	1.64	6 (10%)	64,101,113	1.42	7 (10%)
26	LHG	W	2630	22	44,44,48	0.97	2 (4%)	47,50,54	0.97	2 (4%)
27	BCR	A	848	-	41,41,41	0.78	0	56,56,56	1.93	17 (30%)
22	CLA	A	831	-	65,73,73	1.51	5 (7%)	76,113,113	1.27	8 (10%)
25	NEX	W	2623	-	38,46,46	0.94	1 (2%)	50,70,70	2.78	19 (38%)
22	CLA	B	823	-	45,53,73	1.78	6 (13%)	52,89,113	1.49	8 (15%)
22	CLA	W	604	-	42,50,73	1.85	7 (16%)	48,85,113	1.46	7 (14%)
21	CHL	9	605	-	37,46,74	2.41	14 (37%)	41,80,114	3.44	18 (43%)
22	CLA	J	101	15	50,58,73	1.73	7 (14%)	58,95,113	1.43	8 (13%)
22	CLA	B	813	-	65,73,73	1.50	6 (9%)	76,113,113	1.29	9 (11%)
22	CLA	7	603	4	45,53,73	1.88	6 (13%)	52,89,113	1.38	6 (11%)
21	CHL	4	607	-	47,55,74	2.32	15 (31%)	50,91,114	3.10	20 (40%)
22	CLA	B	837	-	65,73,73	1.50	7 (10%)	76,113,113	1.33	8 (10%)
21	CHL	7	608	-	46,54,74	2.30	15 (32%)	49,90,114	3.22	20 (40%)
27	BCR	B	845	-	41,41,41	0.73	0	56,56,56	2.51	22 (39%)
22	CLA	A	845	26	65,73,73	1.52	6 (9%)	76,113,113	1.21	7 (9%)
22	CLA	A	838	-	55,63,73	1.62	6 (10%)	64,101,113	1.39	7 (10%)
22	CLA	G	201	-	45,53,73	1.84	7 (15%)	52,89,113	1.39	8 (15%)
27	BCR	3	620	-	41,41,41	0.73	0	56,56,56	2.08	19 (33%)
22	CLA	A	804	-	65,73,73	1.50	6 (9%)	76,113,113	1.33	9 (11%)
22	CLA	K	203	-	55,63,73	1.65	6 (10%)	64,101,113	1.33	9 (14%)
22	CLA	2	611	26	45,53,73	1.84	5 (11%)	52,89,113	1.46	7 (13%)
22	CLA	A	814	-	65,73,73	1.50	7 (10%)	76,113,113	1.36	8 (10%)
27	BCR	I	101	-	41,41,41	0.74	0	56,56,56	1.75	11 (19%)
22	CLA	9	603	20	42,50,73	1.95	6 (14%)	48,85,113	1.46	7 (14%)
21	CHL	W	607	-	40,48,74	2.33	14 (35%)	47,83,114	3.38	19 (40%)
21	CHL	U	606	-	46,54,74	2.28	16 (34%)	49,90,114	3.30	19 (38%)
22	CLA	A	812	-	65,73,73	1.49	8 (12%)	76,113,113	1.24	8 (10%)
22	CLA	4	604	-	55,63,73	1.63	6 (10%)	64,101,113	1.42	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	A	810	6	65,73,73	1.52	7 (10%)	76,113,113	1.32	9 (11%)
31	LMT	K	208	-	36,36,36	0.61	0	47,47,47	1.27	6 (12%)
22	CLA	1	612	2	46,54,73	1.79	7 (15%)	53,90,113	1.36	7 (13%)
22	CLA	2	614	-	50,58,73	1.74	7 (14%)	58,95,113	1.39	8 (13%)
22	CLA	B	818	-	64,72,73	1.49	7 (10%)	74,111,113	1.27	8 (10%)
22	CLA	A	830	-	65,73,73	1.51	7 (10%)	76,113,113	1.28	8 (10%)
22	CLA	H	201	-	37,46,73	1.99	6 (16%)	44,80,113	1.42	7 (15%)
22	CLA	5	612	2	46,54,73	1.91	8 (17%)	53,90,113	1.36	6 (11%)
22	CLA	9	604	-	43,51,73	1.88	6 (13%)	49,86,113	1.39	7 (14%)
22	CLA	3	612	4	65,73,73	1.50	7 (10%)	76,113,113	1.24	9 (11%)
22	CLA	A	825	-	65,73,73	1.51	5 (7%)	76,113,113	1.36	8 (10%)
22	CLA	A	802	-	65,73,73	1.51	8 (12%)	76,113,113	1.19	7 (9%)
23	LUT	9	624	-	42,43,43	0.81	0	51,60,60	3.48	25 (49%)
22	CLA	8	612	5	46,54,73	1.82	5 (10%)	53,90,113	1.36	6 (11%)
27	BCR	7	621	-	41,41,41	0.73	0	56,56,56	2.19	21 (37%)
21	CHL	9	606	-	44,52,74	2.25	14 (31%)	46,87,114	3.28	20 (43%)
22	CLA	1	614	-	49,57,73	1.76	5 (10%)	57,94,113	1.34	8 (14%)
27	BCR	K	202	-	41,41,41	0.71	0	56,56,56	2.03	19 (33%)
22	CLA	A	811	-	55,63,73	1.63	7 (12%)	64,101,113	1.31	7 (10%)
22	CLA	B	831	-	65,73,73	1.53	6 (9%)	76,113,113	1.35	9 (11%)
22	CLA	A	816	-	45,53,73	1.77	7 (15%)	52,89,113	1.48	8 (15%)

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
28	LMG	G	202	-	-	9/27/47/70	0/1/1/1
27	BCR	A	856	-	-	1/27/61/63	0/2/2/2
22	CLA	V	613	1	1/1/12/20	13/26/104/115	-
22	CLA	7	610	4	1/1/13/20	8/25/103/115	-
22	CLA	V	602	1	-	7/30/108/115	-
22	CLA	A	833	-	1/1/13/20	8/25/103/115	-
22	CLA	5	602	2	1/1/14/20	14/31/109/115	-
22	CLA	B	827	-	1/1/13/20	12/27/105/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	LUT	1	617	-	-	0/29/67/67	0/2/2/2
27	BCR	B	847	-	-	2/29/63/63	0/2/2/2
22	CLA	A	841	-	1/1/15/20	11/37/115/115	-
22	CLA	U	604	-	1/1/12/20	10/22/100/115	-
21	CHL	4	606	-	3/3/16/26	3/15/113/137	-
21	CHL	6	602	3	3/3/18/26	10/27/125/137	-
22	CLA	2	603	-	1/1/11/20	5/15/93/115	-
22	CLA	5	609	2	1/1/10/20	4/8/86/115	-
22	CLA	3	604	-	1/1/13/20	8/25/103/115	-
22	CLA	A	820	-	1/1/15/20	11/37/115/115	-
21	CHL	6	607	-	3/3/16/26	7/17/115/137	-
22	CLA	B	832	-	-	10/37/115/115	-
22	CLA	U	614	-	1/1/10/20	4/10/88/115	-
22	CLA	B	814	-	1/1/15/20	12/37/115/115	-
22	CLA	7	609	4	1/1/13/20	8/28/106/115	-
31	LMT	A	857	-	-	7/21/61/61	0/2/2/2
22	CLA	B	810	-	1/1/15/20	16/37/115/115	-
22	CLA	4	609	5	1/1/11/20	4/13/91/115	-
27	BCR	A	851	-	-	2/29/63/63	0/2/2/2
23	LUT	V	2620	-	-	1/29/67/67	0/2/2/2
22	CLA	A	843	-	1/1/15/20	14/37/115/115	-
22	CLA	1	603	-	1/1/13/20	9/25/103/115	-
22	CLA	B	839	-	1/1/15/20	9/37/115/115	-
22	CLA	3	610	4	1/1/14/20	8/31/109/115	-
22	CLA	B	825	-	1/1/15/20	10/37/115/115	-
22	CLA	7	606	-	1/1/11/20	7/15/93/115	-
22	CLA	3	617	-	1/1/13/20	13/28/102/115	-
23	LUT	4	619	-	-	0/29/67/67	0/2/2/2
21	CHL	8	608	-	3/3/17/26	7/21/119/137	-
27	BCR	A	849	-	-	4/29/63/63	0/2/2/2
23	LUT	U	2620	-	-	0/29/67/67	0/2/2/2
23	LUT	3	618	-	-	1/29/67/67	0/2/2/2
22	CLA	A	826	-	1/1/15/20	10/37/115/115	-
22	CLA	7	612	4	1/1/11/20	4/13/91/115	-
25	NEX	U	2623	-	-	3/27/83/83	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LMG	J	104	-	-	6/30/50/70	0/1/1/1
22	CLA	A	815	-	1/1/15/20	15/37/115/115	-
23	LUT	W	2620	-	-	2/29/67/67	0/2/2/2
23	LUT	9	620	-	-	2/29/67/67	0/2/2/2
22	CLA	6	613	3	1/1/15/20	12/37/115/115	-
23	LUT	6	619	-	-	2/29/67/67	0/2/2/2
23	LUT	5	617	-	-	14/29/67/67	0/2/2/2
22	CLA	8	602	5	1/1/14/20	8/31/109/115	-
22	CLA	W	602	1	1/1/14/20	5/31/109/115	-
21	CHL	V	605	1	3/3/15/26	2/10/108/137	-
22	CLA	F	303	-	1/1/11/20	2/13/91/115	-
21	CHL	6	618	3	3/3/16/26	10/17/115/137	-
22	CLA	V	611	26	1/1/10/20	2/8/84/115	-
30	SF4	C	102	8	-	-	0/6/5/5
22	CLA	A	806	-	1/1/15/20	17/37/115/115	-
22	CLA	8	610	5	1/1/13/20	6/25/103/115	-
22	CLA	5	613	2	-	9/19/97/115	-
26	LHG	8	630	22	-	9/42/42/53	-
24	XAT	4	620	-	-	3/31/93/93	0/4/4/4
22	CLA	1	602	2	1/1/15/20	14/37/115/115	-
22	CLA	5	614	-	1/1/10/20	4/11/89/115	-
21	CHL	W	609	1	3/3/14/26	1/6/104/137	-
22	CLA	A	829	-	1/1/14/20	11/31/109/115	-
32	DGD	B	850	-	-	16/55/95/95	0/2/2/2
26	LHG	V	2630	22	-	8/46/46/53	-
22	CLA	G	204	12	1/1/11/20	4/15/93/115	-
21	CHL	9	608	-	3/3/15/26	2/12/110/137	-
22	CLA	B	828	-	1/1/15/20	14/37/115/115	-
22	CLA	B	812	-	1/1/11/20	2/13/91/115	-
24	XAT	8	620	-	-	18/31/93/93	0/4/4/4
22	CLA	A	822	-	1/1/15/20	12/37/115/115	-
22	CLA	2	604	-	1/1/12/20	4/19/97/115	-
22	CLA	A	817	-	1/1/15/20	12/37/115/115	-
21	CHL	8	618	5	3/3/15/26	2/12/110/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LHG	B	851	22	-	10/39/39/53	-
21	CHL	U	609	1	3/3/20/26	23/39/137/137	-
22	CLA	B	830	-	1/1/11/20	6/13/91/115	-
26	LHG	U	2630	22	-	11/49/49/53	-
22	CLA	9	609	20	1/1/11/20	4/13/91/115	-
22	CLA	3	603	4	1/1/15/20	7/37/115/115	-
22	CLA	B	838	-	-	5/16/94/115	-
21	CHL	2	606	-	3/3/16/26	4/15/113/137	-
22	CLA	B	802	-	1/1/15/20	8/37/115/115	-
22	CLA	B	826	-	1/1/15/20	9/37/115/115	-
23	LUT	W	2621	-	-	2/29/67/67	0/2/2/2
24	XAT	V	2622	-	-	2/31/93/93	0/4/4/4
27	BCR	B	801	-	-	4/29/63/63	0/2/2/2
22	CLA	B	815	-	1/1/11/20	3/13/91/115	-
21	CHL	V	608	-	3/3/15/26	3/8/104/137	-
26	LHG	5	630	22	-	5/41/41/53	-
22	CLA	B	833	-	1/1/15/20	16/37/115/115	-
22	CLA	5	603	-	1/1/11/20	6/13/91/115	-
21	CHL	6	601	3	3/3/20/26	16/39/137/137	-
26	LHG	3	630	22	-	8/36/36/53	-
22	CLA	B	816	-	1/1/15/20	9/37/115/115	-
22	CLA	6	611	26	1/1/11/20	7/13/91/115	-
24	XAT	2	620	-	-	0/31/93/93	0/4/4/4
22	CLA	9	612	20	1/1/9/20	1/4/82/115	-
26	LHG	A	847	22	-	17/35/35/53	-
23	LUT	U	2621	-	-	1/29/67/67	0/2/2/2
21	CHL	1	601	2	3/3/18/26	11/27/125/137	-
25	NEX	9	623	-	-	2/27/83/83	0/3/3/3
21	CHL	V	606	-	3/3/15/26	2/4/100/137	-
21	CHL	U	608	-	3/3/15/26	3/8/104/137	-
22	CLA	1	606	-	1/1/11/20	6/13/91/115	-
22	CLA	B	806	-	1/1/15/20	14/37/115/115	-
22	CLA	B	805	-	1/1/15/20	11/37/115/115	-
24	XAT	1	618	-	-	0/31/93/93	0/4/4/4
22	CLA	A	832	-	1/1/13/20	5/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	5	606	2	1/1/11/20	2/13/91/115	-
29	PQN	B	842	-	-	6/23/43/43	0/2/2/2
22	CLA	1	608	-	1/1/11/20	5/13/91/115	-
22	CLA	7	615	-	1/1/10/20	2/6/84/115	-
26	LHG	4	630	22	-	20/42/42/53	-
22	CLA	A	837	6	-	17/37/115/115	-
22	CLA	W	614	-	1/1/10/20	2/6/82/115	-
22	CLA	V	612	1	1/1/10/20	2/4/80/115	-
22	CLA	2	612	3	1/1/11/20	8/13/91/115	-
24	XAT	7	619	-	-	6/31/93/93	0/4/4/4
22	CLA	6	604	-	1/1/12/20	4/19/97/115	-
22	CLA	7	607	4	1/1/11/20	3/13/91/115	-
22	CLA	B	821	-	1/1/12/20	5/19/97/115	-
22	CLA	8	601	5	1/1/12/20	5/19/97/115	-
22	CLA	3	607	4	1/1/12/20	8/19/97/115	-
22	CLA	1	611	26	1/1/15/20	16/37/115/115	-
22	CLA	5	604	-	1/1/10/20	5/8/86/115	-
21	CHL	V	609	1	3/3/14/26	2/6/104/137	-
21	CHL	5	601	2	3/3/17/26	7/21/119/137	-
26	LHG	7	630	22	-	11/38/38/53	-
22	CLA	O	2003	-	1/1/5/20	-	-
22	CLA	L	304	-	1/1/14/20	13/31/109/115	-
22	CLA	U	612	1	1/1/15/20	10/37/115/115	-
22	CLA	V	610	1	1/1/10/20	3/6/82/115	-
23	LUT	9	621	-	-	1/29/67/67	0/2/2/2
21	CHL	6	608	-	3/3/16/26	5/18/116/137	-
22	CLA	V	614	-	1/1/11/20	5/13/91/115	-
22	CLA	A	807	6	1/1/15/20	18/37/115/115	-
22	CLA	3	615	-	1/1/12/20	4/23/101/115	-
22	CLA	B	819	-	1/1/14/20	14/31/109/115	-
22	CLA	8	603	-	1/1/13/20	8/25/103/115	-
22	CLA	6	603	-	1/1/11/20	7/15/93/115	-
22	CLA	5	608	-	1/1/12/20	8/19/97/115	-
22	CLA	6	612	3	1/1/11/20	6/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CHL	4	608	-	3/3/16/26	3/15/113/137	-
22	CLA	A	839	-	1/1/14/20	6/31/109/115	-
24	XAT	3	619	-	-	0/31/93/93	0/4/4/4
22	CLA	B	836	-	1/1/12/20	10/22/100/115	-
27	BCR	L	306	-	-	3/29/63/63	0/2/2/2
22	CLA	5	610	2	1/1/13/20	4/25/103/115	-
26	LHG	A	846	-	-	12/51/51/53	-
22	CLA	A	823	-	1/1/13/20	8/25/103/115	-
22	CLA	1	610	2	1/1/15/20	10/37/115/115	-
22	CLA	4	612	5	1/1/11/20	5/13/91/115	-
22	CLA	B	829	-	1/1/15/20	8/37/115/115	-
22	CLA	L	302	17	1/1/15/20	21/37/115/115	-
22	CLA	A	818	-	1/1/15/20	5/37/115/115	-
22	CLA	A	821	-	1/1/13/20	4/25/103/115	-
22	CLA	3	606	-	1/1/11/20	8/15/93/115	-
22	CLA	K	201	16	1/1/10/20	4/10/88/115	-
22	CLA	B	809	7	1/1/15/20	11/37/115/115	-
22	CLA	7	611	26	1/1/10/20	2/8/86/115	-
21	CHL	8	607	-	3/3/16/26	5/15/113/137	-
31	LMT	G	206	-	-	7/21/61/61	0/2/2/2
28	LMG	2	631	-	-	12/42/62/70	0/1/1/1
22	CLA	8	613	5	1/1/13/20	8/25/103/115	-
22	CLA	4	614	-	1/1/11/20	7/15/93/115	-
22	CLA	A	842	-	1/1/13/20	8/25/103/115	-
21	CHL	V	601	1	3/3/20/26	18/35/131/137	-
22	CLA	W	613	1	1/1/14/20	7/31/109/115	-
27	BCR	2	621	-	-	6/29/63/63	0/2/2/2
22	CLA	3	614	-	1/1/11/20	6/13/91/115	-
22	CLA	A	809	6	1/1/13/20	7/27/105/115	-
22	CLA	6	614	-	1/1/12/20	3/19/97/115	-
22	CLA	1	613	2	1/1/12/20	8/19/97/115	-
25	NEX	V	2623	-	-	2/27/83/83	0/3/3/3
27	BCR	A	850	-	-	4/29/63/63	0/2/2/2
22	CLA	L	303	-	1/1/15/20	11/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CHL	6	606	-	3/3/16/26	4/15/113/137	-
22	CLA	F	301	33	1/1/15/20	13/37/115/115	-
22	CLA	4	601	5	1/1/12/20	8/19/97/115	-
22	CLA	6	610	3	1/1/14/20	9/31/109/115	-
22	CLA	2	610	3	1/1/14/20	6/31/109/115	-
22	CLA	5	611	26	1/1/11/20	6/15/93/115	-
22	CLA	B	840	-	1/1/15/20	12/37/115/115	-
24	XAT	5	618	-	-	4/31/93/93	0/4/4/4
22	CLA	F	304	11	1/1/8/20	7/18/73/115	-
28	LMG	L	307	-	-	14/39/59/70	0/1/1/1
22	CLA	2	609	3	1/1/11/20	6/15/93/115	-
21	CHL	4	618	5	3/3/15/26	2/12/110/137	-
22	CLA	B	822	-	1/1/14/20	15/31/109/115	-
27	BCR	7	620	-	-	1/29/63/63	0/2/2/2
22	CLA	3	602	4	1/1/15/20	9/37/115/115	-
22	CLA	9	610	20	1/1/13/20	9/25/103/115	-
22	CLA	A	854	-	1/1/14/20	17/31/109/115	-
22	CLA	W	603	-	1/1/10/20	2/4/82/115	-
30	SF4	C	101	8	-	-	0/6/5/5
22	CLA	B	841	26	1/1/15/20	8/37/115/115	-
30	SF4	A	853	7,6	-	-	0/6/5/5
27	BCR	B	844	-	-	0/29/63/63	0/2/2/2
27	BCR	M	2001	-	-	5/29/63/63	0/2/2/2
22	CLA	1	609	2	1/1/15/20	12/37/115/115	-
22	CLA	A	803	-	1/1/15/20	8/37/115/115	-
21	CHL	W	606	-	3/3/15/26	0/4/100/137	-
21	CHL	2	608	-	3/3/16/26	0/15/113/137	-
27	BCR	B	848	-	-	3/29/63/63	0/2/2/2
22	CLA	A	835	-	1/1/15/20	12/37/115/115	-
22	CLA	3	613	4	1/1/15/20	11/37/115/115	-
22	CLA	V	603	-	1/1/14/20	12/31/109/115	-
22	CLA	B	804	-	1/1/15/20	10/37/115/115	-
31	LMT	B	849	-	-	5/17/57/61	0/2/2/2
23	LUT	V	2621	-	-	2/29/67/67	0/2/2/2
22	CLA	4	603	-	1/1/15/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	819	-	1/1/14/20	9/34/112/115	-
22	CLA	B	824	-	1/1/15/20	9/37/115/115	-
24	XAT	U	2622	-	-	1/31/93/93	0/4/4/4
23	LUT	2	619	-	-	12/29/67/67	0/2/2/2
27	BCR	8	621	-	-	4/29/63/63	0/2/2/2
28	LMG	J	103	-	-	11/50/70/70	0/1/1/1
27	BCR	K	205	-	-	3/29/63/63	0/2/2/2
22	CLA	8	614	-	1/1/11/20	9/13/91/115	-
27	BCR	L	305	-	-	2/29/63/63	0/2/2/2
22	CLA	4	613	5	1/1/13/20	6/25/103/115	-
22	CLA	B	807	-	-	4/37/115/115	-
22	CLA	B	808	-	1/1/15/20	11/37/115/115	-
22	CLA	U	603	-	1/1/15/20	10/37/115/115	-
22	CLA	4	602	5	1/1/15/20	17/37/115/115	-
22	CLA	A	828	-	1/1/15/20	14/37/115/115	-
22	CLA	U	610	1	1/1/15/20	13/37/115/115	-
22	CLA	9	602	20	1/1/14/20	12/31/109/115	-
21	CHL	5	607	2	3/3/14/26	0/4/102/137	-
22	CLA	1	616	2	1/1/11/20	7/13/91/115	-
23	LUT	8	619	-	-	1/29/67/67	0/2/2/2
22	CLA	A	834	-	1/1/15/20	9/37/115/115	-
22	CLA	A	813	-	1/1/13/20	7/25/103/115	-
22	CLA	8	604	-	1/1/12/20	5/19/97/115	-
22	CLA	7	602	4	-	10/31/109/115	-
22	CLA	A	827	33	-	14/37/115/115	-
26	LHG	6	630	22	-	9/36/36/53	-
21	CHL	U	601	1	3/3/20/26	20/35/131/137	-
27	BCR	4	621	-	-	7/29/63/63	0/2/2/2
22	CLA	K	206	16	1/1/10/20	2/10/88/115	-
26	LHG	1	630	22	-	25/53/53/53	-
22	CLA	A	840	-	1/1/12/20	5/19/97/115	-
22	CLA	G	203	-	1/1/12/20	8/19/97/115	-
23	LUT	7	618	-	-	1/29/67/67	0/2/2/2
21	CHL	W	601	1	3/3/20/26	15/35/131/137	-
22	CLA	1	604	-	-	8/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	W	611	26	1/1/10/20	1/8/84/115	-
24	XAT	6	620	-	-	3/31/93/93	0/4/4/4
22	CLA	B	803	-	1/1/15/20	16/37/115/115	-
22	CLA	O	2002	-	1/1/13/20	12/25/103/115	-
22	CLA	A	824	-	1/1/14/20	15/34/112/115	-
22	CLA	5	616	2	1/1/11/20	4/15/93/115	-
27	BCR	O	2004	-	-	5/29/63/63	0/2/2/2
21	CHL	2	602	3	3/3/19/26	10/33/131/137	-
27	BCR	B	843	-	-	5/29/63/63	0/2/2/2
22	CLA	B	835	-	1/1/11/20	2/13/91/115	-
22	CLA	U	602	1	1/1/15/20	10/37/115/115	-
22	CLA	K	204	-	1/1/15/20	16/37/115/115	-
21	CHL	U	605	1	3/3/15/26	0/4/100/137	-
22	CLA	7	604	-	1/1/12/20	8/19/97/115	-
27	BCR	3	621	-	-	0/29/63/63	0/2/2/2
22	CLA	7	614	-	1/1/10/20	3/8/86/115	-
27	BCR	J	102	-	-	2/29/63/63	0/2/2/2
21	CHL	2	607	-	3/3/16/26	3/17/115/137	-
21	CHL	W	605	1	3/3/15/26	0/4/100/137	-
22	CLA	B	834	-	1/1/15/20	13/37/115/115	-
27	BCR	B	1609	-	-	5/29/63/63	0/2/2/2
22	CLA	B	820	-	1/1/13/20	10/25/103/115	-
21	CHL	8	606	-	3/3/16/26	3/15/113/137	-
22	CLA	4	610	5	1/1/14/20	14/33/111/115	-
21	CHL	2	618	3	3/3/15/26	4/12/110/137	-
21	CHL	9	601	20	3/3/14/26	0/4/102/137	-
22	CLA	V	604	-	1/1/12/20	8/19/97/115	-
22	CLA	4	611	26	1/1/11/20	5/13/91/115	-
22	CLA	9	611	26	1/1/15/20	14/37/115/115	-
21	CHL	3	608	-	3/3/18/26	10/27/125/137	-
22	CLA	O	2001	-	1/1/5/20	-	-
27	BCR	F	305	-	-	5/29/63/63	0/2/2/2
24	XAT	W	2622	-	-	1/31/93/93	0/4/4/4
27	BCR	1	619	-	-	6/29/63/63	0/2/2/2
22	CLA	9	613	20	1/1/12/20	3/22/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	801	-	1/1/15/20	12/37/115/115	-
21	CHL	W	608	-	3/3/15/26	1/8/104/137	-
22	CLA	7	617	-	1/1/11/20	7/15/93/115	-
22	CLA	7	613	4	1/1/13/20	9/25/103/115	-
22	CLA	A	805	-	-	17/37/115/115	-
21	CHL	V	607	-	3/3/15/26	0/8/104/137	-
22	CLA	A	808	-	1/1/14/20	6/31/109/115	-
22	CLA	B	817	-	1/1/15/20	16/37/115/115	-
21	CHL	2	601	3	3/3/16/26	5/15/113/137	-
29	PQN	A	844	-	-	7/23/43/43	0/2/2/2
22	CLA	W	610	1	1/1/15/20	19/37/115/115	-
22	CLA	2	613	3	1/1/13/20	12/28/106/115	-
26	LHG	9	2630	22	-	14/32/32/53	-
22	CLA	8	611	26	1/1/13/20	4/25/103/115	-
27	BCR	6	621	-	-	6/29/63/63	0/2/2/2
28	LMG	A	860	-	-	12/29/49/70	0/1/1/1
22	CLA	6	609	3	1/1/13/20	2/25/103/115	-
21	CHL	9	607	-	3/3/15/26	3/12/110/137	-
22	CLA	W	612	1	1/1/10/20	2/4/80/115	-
22	CLA	A	836	-	1/1/14/20	13/36/105/115	-
27	BCR	G	205	-	-	4/29/63/63	0/2/2/2
22	CLA	B	811	-	1/1/14/20	7/33/111/115	-
21	CHL	1	607	-	3/3/16/26	8/17/115/137	-
27	BCR	L	301	-	-	6/29/63/63	0/2/2/2
26	LHG	2	630	22	-	9/36/36/53	-
22	CLA	3	611	26	1/1/13/20	11/25/103/115	-
21	CHL	U	607	-	3/3/20/26	14/39/137/137	-
27	BCR	A	852	-	-	8/29/63/63	0/2/2/2
22	CLA	U	611	26	1/1/11/20	7/13/91/115	-
22	CLA	3	609	4	1/1/15/20	12/37/115/115	-
22	CLA	U	613	1	1/1/15/20	12/37/115/115	-
22	CLA	8	609	5	1/1/13/20	8/25/103/115	-
26	LHG	W	2630	22	-	13/49/49/53	-
27	BCR	A	848	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	831	-	1/1/15/20	10/37/115/115	-
25	NEX	W	2623	-	-	7/27/83/83	0/3/3/3
22	CLA	B	823	-	1/1/11/20	6/13/91/115	-
22	CLA	W	604	-	1/1/10/20	3/10/88/115	-
21	CHL	9	605	-	3/3/14/26	0/2/100/137	-
22	CLA	J	101	15	1/1/12/20	5/19/97/115	-
22	CLA	B	813	-	1/1/15/20	12/37/115/115	-
22	CLA	7	603	4	1/1/11/20	5/13/91/115	-
21	CHL	4	607	-	3/3/16/26	5/17/115/137	-
22	CLA	B	837	-	1/1/15/20	8/37/115/115	-
21	CHL	7	608	-	3/3/16/26	5/15/113/137	-
27	BCR	B	845	-	-	10/29/63/63	0/2/2/2
22	CLA	A	845	26	1/1/15/20	12/37/115/115	-
22	CLA	A	838	-	1/1/13/20	9/25/103/115	-
22	CLA	G	201	-	1/1/11/20	5/13/91/115	-
27	BCR	3	620	-	-	2/29/63/63	0/2/2/2
22	CLA	A	804	-	1/1/15/20	20/37/115/115	-
22	CLA	K	203	-	1/1/13/20	8/25/103/115	-
22	CLA	2	611	26	1/1/11/20	6/13/91/115	-
22	CLA	A	814	-	1/1/15/20	22/37/115/115	-
27	BCR	I	101	-	-	3/29/63/63	0/2/2/2
22	CLA	9	603	20	1/1/10/20	3/10/88/115	-
21	CHL	W	607	-	3/3/15/26	3/8/104/137	-
21	CHL	U	606	-	3/3/16/26	5/15/113/137	-
22	CLA	A	812	-	1/1/15/20	10/37/115/115	-
22	CLA	4	604	-	1/1/13/20	8/25/103/115	-
22	CLA	A	810	6	1/1/15/20	15/37/115/115	-
31	LMT	K	208	-	-	7/21/61/61	0/2/2/2
22	CLA	1	612	2	1/1/11/20	3/15/93/115	-
22	CLA	2	614	-	1/1/12/20	4/19/97/115	-
22	CLA	B	818	-	1/1/14/20	13/36/114/115	-
22	CLA	A	830	-	1/1/15/20	17/37/115/115	-
22	CLA	H	201	-	1/1/9/20	0/2/80/115	-
22	CLA	5	612	2	1/1/11/20	8/15/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	9	604	-	1/1/10/20	3/11/89/115	-
22	CLA	3	612	4	1/1/15/20	16/37/115/115	-
22	CLA	A	825	-	-	18/37/115/115	-
22	CLA	A	802	-	1/1/15/20	8/37/115/115	-
23	LUT	9	624	-	-	3/29/67/67	0/2/2/2
22	CLA	8	612	5	1/1/11/20	7/15/93/115	-
27	BCR	7	621	-	-	1/29/63/63	0/2/2/2
21	CHL	9	606	-	3/3/15/26	1/13/111/137	-
22	CLA	1	614	-	1/1/12/20	10/17/95/115	-
27	BCR	K	202	-	-	4/29/63/63	0/2/2/2
22	CLA	A	811	-	1/1/13/20	8/25/103/115	-
22	CLA	B	831	-	1/1/15/20	15/37/115/115	-
22	CLA	A	816	-	1/1/11/20	5/13/91/115	-

All (2228) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	5	609	CLA	C4B-NB	8.61	1.42	1.35
22	7	609	CLA	C4B-NB	8.58	1.42	1.35
22	5	612	CLA	C4B-NB	8.57	1.42	1.35
22	1	609	CLA	C4B-NB	8.37	1.42	1.35
22	9	603	CLA	C4B-NB	8.35	1.42	1.35
22	4	610	CLA	C4B-NB	8.31	1.42	1.35
22	3	611	CLA	C4B-NB	8.14	1.42	1.35
22	7	602	CLA	C4B-NB	8.09	1.42	1.35
22	6	603	CLA	C4B-NB	8.08	1.42	1.35
22	9	604	CLA	C4B-NB	8.05	1.42	1.35
22	7	610	CLA	C4B-NB	8.02	1.42	1.35
22	8	601	CLA	C4B-NB	8.01	1.42	1.35
22	U	611	CLA	C4B-NB	7.99	1.42	1.35
22	O	2002	CLA	C4B-NB	7.98	1.42	1.35
22	5	611	CLA	C4B-NB	7.97	1.42	1.35
22	5	616	CLA	C4B-NB	7.97	1.42	1.35
22	7	603	CLA	C4B-NB	7.97	1.42	1.35
22	3	609	CLA	C4B-NB	7.96	1.42	1.35
22	A	837	CLA	C4B-NB	7.96	1.42	1.35
22	V	610	CLA	C4B-NB	7.94	1.42	1.35
22	B	830	CLA	C4B-NB	7.93	1.42	1.35
22	U	614	CLA	C4B-NB	7.92	1.42	1.35
22	3	603	CLA	C4B-NB	7.92	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	811	CLA	C4B-NB	7.91	1.42	1.35
22	2	611	CLA	C4B-NB	7.91	1.42	1.35
22	8	612	CLA	C4B-NB	7.91	1.42	1.35
22	4	611	CLA	C4B-NB	7.91	1.42	1.35
22	5	606	CLA	C4B-NB	7.90	1.42	1.35
22	7	613	CLA	C4B-NB	7.89	1.42	1.35
22	F	304	CLA	C4B-NB	7.89	1.42	1.35
22	A	842	CLA	C4B-NB	7.89	1.42	1.35
22	9	613	CLA	C4B-NB	7.88	1.42	1.35
22	5	613	CLA	C4B-NB	7.87	1.42	1.35
22	W	603	CLA	C4B-NB	7.87	1.42	1.35
22	6	612	CLA	C4B-NB	7.86	1.42	1.35
22	8	610	CLA	C4B-NB	7.85	1.42	1.35
22	W	610	CLA	C4B-NB	7.84	1.42	1.35
22	7	611	CLA	C4B-NB	7.84	1.42	1.35
22	6	613	CLA	C4B-NB	7.83	1.42	1.35
22	5	604	CLA	C4B-NB	7.83	1.42	1.35
22	G	201	CLA	C4B-NB	7.83	1.42	1.35
22	B	821	CLA	C4B-NB	7.82	1.42	1.35
22	8	613	CLA	C4B-NB	7.82	1.42	1.35
22	V	613	CLA	C4B-NB	7.81	1.42	1.35
22	7	612	CLA	C4B-NB	7.81	1.42	1.35
22	1	616	CLA	C4B-NB	7.80	1.42	1.35
22	O	2001	CLA	C4B-NB	7.80	1.42	1.35
22	8	614	CLA	C4B-NB	7.80	1.42	1.35
22	8	611	CLA	C4B-NB	7.80	1.42	1.35
22	5	603	CLA	C4B-NB	7.79	1.42	1.35
22	B	838	CLA	C4B-NB	7.79	1.42	1.35
22	G	204	CLA	C4B-NB	7.78	1.42	1.35
22	7	617	CLA	C4B-NB	7.78	1.42	1.35
22	1	606	CLA	C4B-NB	7.78	1.42	1.35
22	5	610	CLA	C4B-NB	7.78	1.42	1.35
22	O	2003	CLA	C4B-NB	7.77	1.42	1.35
22	H	201	CLA	C4B-NB	7.76	1.42	1.35
22	8	603	CLA	C4B-NB	7.76	1.42	1.35
22	B	822	CLA	C4B-NB	7.75	1.42	1.35
22	4	613	CLA	C4B-NB	7.75	1.42	1.35
22	W	611	CLA	C4B-NB	7.74	1.42	1.35
22	6	609	CLA	C4B-NB	7.74	1.42	1.35
22	B	831	CLA	C4B-NB	7.74	1.42	1.35
22	2	614	CLA	C4B-NB	7.74	1.42	1.35
22	3	610	CLA	C4B-NB	7.73	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	3	613	CLA	C4B-NB	7.73	1.42	1.35
22	9	611	CLA	C4B-NB	7.73	1.42	1.35
22	1	611	CLA	C4B-NB	7.73	1.42	1.35
22	B	832	CLA	C4B-NB	7.73	1.42	1.35
22	V	611	CLA	C4B-NB	7.72	1.42	1.35
22	9	612	CLA	C4B-NB	7.72	1.42	1.35
22	U	612	CLA	C4B-NB	7.71	1.42	1.35
22	2	609	CLA	C4B-NB	7.71	1.42	1.35
22	6	604	CLA	C4B-NB	7.70	1.42	1.35
22	A	808	CLA	C4B-NB	7.70	1.42	1.35
22	B	826	CLA	C4B-NB	7.70	1.42	1.35
22	7	614	CLA	C4B-NB	7.70	1.42	1.35
22	4	614	CLA	C4B-NB	7.70	1.42	1.35
22	K	206	CLA	C4B-NB	7.69	1.42	1.35
22	1	614	CLA	C4B-NB	7.68	1.42	1.35
22	5	608	CLA	C4B-NB	7.68	1.42	1.35
22	A	802	CLA	C4B-NB	7.67	1.42	1.35
22	7	615	CLA	C4B-NB	7.67	1.42	1.35
22	A	845	CLA	C4B-NB	7.67	1.42	1.35
22	B	814	CLA	C4B-NB	7.66	1.42	1.35
22	W	612	CLA	C4B-NB	7.66	1.42	1.35
22	2	610	CLA	C4B-NB	7.66	1.42	1.35
22	A	841	CLA	C4B-NB	7.66	1.42	1.35
22	8	602	CLA	C4B-NB	7.66	1.42	1.35
22	B	804	CLA	C4B-NB	7.66	1.42	1.35
22	B	808	CLA	C4B-NB	7.66	1.42	1.35
22	1	610	CLA	C4B-NB	7.65	1.42	1.35
22	8	604	CLA	C4B-NB	7.65	1.42	1.35
22	9	602	CLA	C4B-NB	7.65	1.42	1.35
22	1	608	CLA	C4B-NB	7.65	1.42	1.35
22	V	614	CLA	C4B-NB	7.64	1.42	1.35
22	L	302	CLA	C4B-NB	7.63	1.42	1.35
22	A	805	CLA	C4B-NB	7.63	1.42	1.35
22	6	614	CLA	C4B-NB	7.62	1.42	1.35
22	4	612	CLA	C4B-NB	7.62	1.42	1.35
22	A	834	CLA	C4B-NB	7.62	1.42	1.35
22	3	614	CLA	C4B-NB	7.61	1.42	1.35
22	4	604	CLA	C4B-NB	7.61	1.42	1.35
22	4	602	CLA	C4B-NB	7.61	1.42	1.35
22	5	614	CLA	C4B-NB	7.61	1.42	1.35
22	3	615	CLA	C4B-NB	7.61	1.42	1.35
22	1	613	CLA	C4B-NB	7.61	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	854	CLA	C4B-NB	7.60	1.42	1.35
22	K	203	CLA	C4B-NB	7.60	1.42	1.35
22	A	814	CLA	C4B-NB	7.60	1.42	1.35
22	W	614	CLA	C4B-NB	7.59	1.42	1.35
22	4	601	CLA	C4B-NB	7.59	1.42	1.35
22	A	831	CLA	C4B-NB	7.59	1.42	1.35
22	U	610	CLA	C4B-NB	7.59	1.42	1.35
22	B	816	CLA	C4B-NB	7.59	1.42	1.35
22	U	603	CLA	C4B-NB	7.59	1.42	1.35
22	7	604	CLA	C4B-NB	7.58	1.42	1.35
22	V	603	CLA	C4B-NB	7.58	1.42	1.35
22	A	828	CLA	C4B-NB	7.58	1.42	1.35
22	B	819	CLA	C4B-NB	7.58	1.42	1.35
22	U	602	CLA	C4B-NB	7.58	1.42	1.35
22	B	829	CLA	C4B-NB	7.57	1.42	1.35
22	J	101	CLA	C4B-NB	7.57	1.42	1.35
22	V	602	CLA	C4B-NB	7.57	1.42	1.35
22	U	613	CLA	C4B-NB	7.57	1.42	1.35
22	2	612	CLA	C4B-NB	7.57	1.42	1.35
22	4	603	CLA	C4B-NB	7.57	1.42	1.35
22	A	810	CLA	C4B-NB	7.56	1.42	1.35
22	1	612	CLA	C4B-NB	7.56	1.42	1.35
22	G	203	CLA	C4B-NB	7.56	1.42	1.35
22	W	613	CLA	C4B-NB	7.56	1.42	1.35
22	3	606	CLA	C4B-NB	7.55	1.41	1.35
22	A	826	CLA	C4B-NB	7.55	1.41	1.35
22	2	603	CLA	C4B-NB	7.54	1.41	1.35
22	B	833	CLA	C4B-NB	7.54	1.41	1.35
22	B	841	CLA	C4B-NB	7.54	1.41	1.35
22	V	604	CLA	C4B-NB	7.54	1.41	1.35
22	8	609	CLA	C4B-NB	7.54	1.41	1.35
22	A	803	CLA	C4B-NB	7.54	1.41	1.35
22	F	301	CLA	C4B-NB	7.53	1.41	1.35
22	5	602	CLA	C4B-NB	7.53	1.41	1.35
22	U	604	CLA	C4B-NB	7.53	1.41	1.35
22	A	818	CLA	C4B-NB	7.53	1.41	1.35
22	A	835	CLA	C4B-NB	7.52	1.41	1.35
22	B	824	CLA	C4B-NB	7.52	1.41	1.35
22	9	610	CLA	C4B-NB	7.52	1.41	1.35
22	6	610	CLA	C4B-NB	7.52	1.41	1.35
22	A	843	CLA	C4B-NB	7.52	1.41	1.35
22	1	604	CLA	C4B-NB	7.51	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	820	CLA	C4B-NB	7.51	1.41	1.35
22	A	809	CLA	C4B-NB	7.51	1.41	1.35
22	4	609	CLA	C4B-NB	7.51	1.41	1.35
22	B	837	CLA	C4B-NB	7.50	1.41	1.35
22	A	822	CLA	C4B-NB	7.50	1.41	1.35
22	A	825	CLA	C4B-NB	7.50	1.41	1.35
22	W	604	CLA	C4B-NB	7.49	1.41	1.35
22	B	815	CLA	C4B-NB	7.49	1.41	1.35
22	A	811	CLA	C4B-NB	7.49	1.41	1.35
22	A	813	CLA	C4B-NB	7.49	1.41	1.35
22	L	303	CLA	C4B-NB	7.48	1.41	1.35
22	A	824	CLA	C4B-NB	7.47	1.41	1.35
22	B	813	CLA	C4B-NB	7.47	1.41	1.35
22	7	607	CLA	C4B-NB	7.47	1.41	1.35
22	A	823	CLA	C4B-NB	7.47	1.41	1.35
22	B	809	CLA	C4B-NB	7.47	1.41	1.35
22	1	602	CLA	C4B-NB	7.46	1.41	1.35
22	B	805	CLA	C4B-NB	7.46	1.41	1.35
22	A	815	CLA	C4B-NB	7.45	1.41	1.35
22	7	606	CLA	C4B-NB	7.45	1.41	1.35
22	2	613	CLA	C4B-NB	7.45	1.41	1.35
22	A	840	CLA	C4B-NB	7.45	1.41	1.35
22	3	607	CLA	C4B-NB	7.44	1.41	1.35
22	2	604	CLA	C4B-NB	7.44	1.41	1.35
22	A	833	CLA	C4B-NB	7.43	1.41	1.35
22	A	839	CLA	C4B-NB	7.43	1.41	1.35
22	V	612	CLA	C4B-NB	7.42	1.41	1.35
22	3	602	CLA	C4B-NB	7.42	1.41	1.35
22	B	803	CLA	C4B-NB	7.42	1.41	1.35
22	A	801	CLA	C4B-NB	7.41	1.41	1.35
22	3	612	CLA	C4B-NB	7.41	1.41	1.35
22	A	817	CLA	C4B-NB	7.40	1.41	1.35
22	6	611	CLA	C4B-NB	7.40	1.41	1.35
22	A	821	CLA	C4B-NB	7.39	1.41	1.35
22	1	603	CLA	C4B-NB	7.39	1.41	1.35
22	A	804	CLA	C4B-NB	7.38	1.41	1.35
22	A	806	CLA	C4B-NB	7.38	1.41	1.35
22	B	834	CLA	C4B-NB	7.38	1.41	1.35
22	W	602	CLA	C4B-NB	7.37	1.41	1.35
22	K	204	CLA	C4B-NB	7.36	1.41	1.35
22	A	830	CLA	C4B-NB	7.36	1.41	1.35
22	B	812	CLA	C4B-NB	7.36	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	812	CLA	C4B-NB	7.35	1.41	1.35
22	A	827	CLA	C4B-NB	7.34	1.41	1.35
22	K	201	CLA	C4B-NB	7.34	1.41	1.35
22	B	828	CLA	C4B-NB	7.32	1.41	1.35
22	B	807	CLA	C4B-NB	7.31	1.41	1.35
22	B	817	CLA	C4B-NB	7.31	1.41	1.35
22	3	604	CLA	C4B-NB	7.31	1.41	1.35
22	F	303	CLA	C4B-NB	7.30	1.41	1.35
22	A	832	CLA	C4B-NB	7.30	1.41	1.35
22	B	839	CLA	C4B-NB	7.29	1.41	1.35
22	A	819	CLA	C4B-NB	7.29	1.41	1.35
22	A	807	CLA	C4B-NB	7.28	1.41	1.35
22	B	802	CLA	C4B-NB	7.27	1.41	1.35
22	B	827	CLA	C4B-NB	7.27	1.41	1.35
22	L	304	CLA	C4B-NB	7.26	1.41	1.35
22	B	810	CLA	C4B-NB	7.25	1.41	1.35
22	B	840	CLA	C4B-NB	7.23	1.41	1.35
22	A	829	CLA	C4B-NB	7.21	1.41	1.35
22	A	838	CLA	C4B-NB	7.19	1.41	1.35
22	B	823	CLA	C4B-NB	7.18	1.41	1.35
22	B	836	CLA	C4B-NB	7.18	1.41	1.35
22	B	835	CLA	C4B-NB	7.17	1.41	1.35
22	A	816	CLA	C4B-NB	7.16	1.41	1.35
22	B	818	CLA	C4B-NB	7.16	1.41	1.35
22	B	806	CLA	C4B-NB	7.14	1.41	1.35
22	A	820	CLA	C4B-NB	7.09	1.41	1.35
22	B	825	CLA	C4B-NB	6.98	1.41	1.35
22	A	836	CLA	C4B-C3B	5.73	1.49	1.39
22	3	617	CLA	C4B-C3B	5.53	1.48	1.39
21	2	602	CHL	CHC-C1C	5.48	1.49	1.35
22	O	2003	CLA	C2B-C1B	5.46	1.49	1.39
22	O	2001	CLA	C2B-C1B	5.43	1.49	1.39
21	2	608	CHL	CHC-C1C	5.40	1.48	1.35
21	6	602	CHL	CHC-C1C	5.37	1.48	1.35
22	O	2003	CLA	C3B-C4B	5.36	1.49	1.39
22	O	2001	CLA	C3B-C4B	5.33	1.49	1.39
21	U	606	CHL	CHC-C1C	5.31	1.48	1.35
21	4	608	CHL	C3B-C2B	5.29	1.47	1.40
21	4	607	CHL	O2D-CGD	5.28	1.46	1.33
21	3	608	CHL	C3B-C2B	5.27	1.47	1.40
21	6	608	CHL	O2D-CGD	5.24	1.46	1.33
21	4	606	CHL	O2D-CGD	5.24	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	6	607	CHL	O2D-CGD	5.23	1.46	1.33
21	2	607	CHL	CHC-C1C	5.23	1.48	1.35
21	8	607	CHL	CHC-C1C	5.23	1.48	1.35
21	8	608	CHL	CHC-C1C	5.23	1.48	1.35
21	4	607	CHL	CHC-C1C	5.22	1.48	1.35
21	2	608	CHL	O2D-CGD	5.22	1.45	1.33
21	7	608	CHL	O2D-CGD	5.22	1.45	1.33
21	1	601	CHL	CHC-C1C	5.20	1.48	1.35
21	8	618	CHL	O2D-CGD	5.20	1.45	1.33
21	9	608	CHL	O2D-CGD	5.20	1.45	1.33
21	6	601	CHL	CHC-C1C	5.19	1.48	1.35
21	2	618	CHL	CHC-C1C	5.19	1.48	1.35
21	6	608	CHL	CHC-C1C	5.19	1.48	1.35
21	U	605	CHL	C3C-C2C	5.19	1.46	1.36
21	8	606	CHL	O2D-CGD	5.19	1.45	1.33
21	5	607	CHL	CHC-C1C	5.18	1.48	1.35
21	8	606	CHL	CHC-C1C	5.18	1.48	1.35
21	U	607	CHL	O2D-CGD	5.18	1.45	1.33
21	5	601	CHL	CHC-C1C	5.17	1.48	1.35
21	6	606	CHL	O2D-CGD	5.17	1.45	1.33
21	9	606	CHL	O2D-CGD	5.17	1.45	1.33
21	4	608	CHL	O2D-CGD	5.17	1.45	1.33
21	W	609	CHL	C3B-C2B	5.17	1.47	1.40
21	2	607	CHL	O2D-CGD	5.17	1.45	1.33
21	9	607	CHL	O2D-CGD	5.17	1.45	1.33
21	1	607	CHL	CHC-C1C	5.16	1.48	1.35
21	V	607	CHL	CHC-C1C	5.16	1.48	1.35
21	4	608	CHL	CHC-C1C	5.16	1.48	1.35
21	6	607	CHL	CHC-C1C	5.16	1.48	1.35
21	2	601	CHL	CHC-C1C	5.16	1.48	1.35
21	V	609	CHL	CHC-C1C	5.15	1.48	1.35
21	4	618	CHL	O2D-CGD	5.15	1.45	1.33
21	W	607	CHL	CHC-C1C	5.15	1.48	1.35
21	8	608	CHL	O2D-CGD	5.15	1.45	1.33
21	8	607	CHL	O2D-CGD	5.15	1.45	1.33
21	3	608	CHL	O2D-CGD	5.15	1.45	1.33
21	8	618	CHL	CHC-C1C	5.14	1.48	1.35
22	9	609	CLA	CHC-C1C	5.14	1.48	1.35
21	2	606	CHL	O2D-CGD	5.14	1.45	1.33
22	9	609	CLA	O2D-CGD	5.14	1.45	1.33
21	U	608	CHL	CHC-C1C	5.14	1.48	1.35
21	W	605	CHL	C3C-C2C	5.13	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	9	605	CHL	CHC-C1C	5.13	1.48	1.35
22	3	617	CLA	C2C-C3C	5.12	1.39	1.33
21	U	607	CHL	CHC-C1C	5.12	1.48	1.35
21	6	606	CHL	CHC-C1C	5.12	1.48	1.35
21	1	607	CHL	O2D-CGD	5.11	1.45	1.33
21	V	608	CHL	CHC-C1C	5.11	1.48	1.35
21	6	618	CHL	O2D-CGD	5.11	1.45	1.33
21	W	606	CHL	C3C-C2C	5.11	1.46	1.36
21	2	618	CHL	O2D-CGD	5.11	1.45	1.33
21	9	606	CHL	CHC-C1C	5.11	1.48	1.35
21	V	607	CHL	O2D-CGD	5.10	1.45	1.33
21	U	606	CHL	O2D-CGD	5.10	1.45	1.33
21	V	605	CHL	CHC-C1C	5.10	1.48	1.35
21	4	606	CHL	CHC-C1C	5.10	1.48	1.35
21	1	601	CHL	O2D-CGD	5.09	1.45	1.33
21	2	602	CHL	O2D-CGD	5.09	1.45	1.33
21	9	601	CHL	CHC-C1C	5.09	1.48	1.35
21	W	605	CHL	CHC-C1C	5.08	1.48	1.35
21	6	602	CHL	O2D-CGD	5.08	1.45	1.33
21	U	609	CHL	CHC-C1C	5.08	1.48	1.35
21	W	607	CHL	O2D-CGD	5.08	1.45	1.33
21	9	608	CHL	CHC-C1C	5.08	1.48	1.35
21	U	609	CHL	O2D-CGD	5.08	1.45	1.33
21	7	608	CHL	CHC-C1C	5.07	1.48	1.35
21	W	601	CHL	CHC-C1C	5.06	1.48	1.35
21	V	605	CHL	O2D-CGD	5.06	1.45	1.33
21	U	601	CHL	CHC-C1C	5.06	1.47	1.35
21	6	601	CHL	O2D-CGD	5.06	1.45	1.33
21	V	606	CHL	C3C-C2C	5.05	1.46	1.36
21	5	601	CHL	O2D-CGD	5.05	1.45	1.33
21	2	606	CHL	CHC-C1C	5.04	1.47	1.35
21	U	605	CHL	CHC-C1C	5.03	1.47	1.35
21	W	609	CHL	CHC-C1C	5.02	1.47	1.35
21	V	601	CHL	CHC-C1C	5.01	1.47	1.35
21	2	601	CHL	O2D-CGD	5.01	1.45	1.33
21	3	608	CHL	CHC-C1C	4.99	1.47	1.35
21	6	618	CHL	CHC-C1C	4.95	1.47	1.35
21	V	606	CHL	CHC-C1C	4.93	1.47	1.35
21	W	608	CHL	CHC-C1C	4.93	1.47	1.35
21	W	606	CHL	CHC-C1C	4.93	1.47	1.35
21	9	601	CHL	C3D-C4D	-4.93	1.33	1.44
21	9	607	CHL	C3B-C2B	4.92	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	9	607	CHL	CHC-C1C	4.91	1.47	1.35
21	V	609	CHL	C3B-C2B	4.90	1.47	1.40
21	7	608	CHL	C3D-C4D	-4.90	1.33	1.44
22	9	609	CLA	C3D-C4D	-4.90	1.33	1.44
21	3	608	CHL	C3D-C4D	-4.88	1.33	1.44
21	2	602	CHL	C3D-C4D	-4.88	1.33	1.44
21	W	606	CHL	C3D-C4D	-4.87	1.33	1.44
21	U	609	CHL	C3D-C4D	-4.87	1.33	1.44
22	3	617	CLA	C1C-C2C	-4.87	1.45	1.51
21	W	601	CHL	C3D-C4D	-4.87	1.33	1.44
21	9	608	CHL	C3D-C4D	-4.87	1.33	1.44
21	4	618	CHL	CHC-C1C	4.85	1.47	1.35
21	6	601	CHL	C3B-C2B	4.85	1.47	1.40
21	2	608	CHL	C3D-C4D	-4.84	1.33	1.44
21	U	608	CHL	C3D-C4D	-4.84	1.33	1.44
21	2	601	CHL	C3D-C4D	-4.84	1.33	1.44
21	8	618	CHL	C3B-C2B	4.84	1.47	1.40
21	W	607	CHL	C3D-C4D	-4.83	1.33	1.44
21	V	609	CHL	C3D-C4D	-4.83	1.33	1.44
21	9	606	CHL	C3D-C4D	-4.83	1.33	1.44
21	1	607	CHL	C3D-C4D	-4.83	1.33	1.44
21	2	618	CHL	C3D-C4D	-4.83	1.33	1.44
21	2	607	CHL	C3D-C4D	-4.82	1.33	1.44
21	2	606	CHL	C3D-C4D	-4.81	1.33	1.44
21	8	608	CHL	C3D-C4D	-4.81	1.33	1.44
21	U	609	CHL	C3B-C2B	4.81	1.47	1.40
21	V	605	CHL	C3B-C2B	4.81	1.47	1.40
21	4	606	CHL	C3D-C4D	-4.80	1.33	1.44
21	U	606	CHL	C3D-C4D	-4.80	1.33	1.44
21	4	607	CHL	C3D-C4D	-4.80	1.33	1.44
21	1	601	CHL	C3D-C4D	-4.80	1.33	1.44
21	1	607	CHL	C3B-C2B	4.79	1.47	1.40
21	U	601	CHL	C3D-C4D	-4.79	1.33	1.44
21	5	607	CHL	C3B-C2B	4.79	1.47	1.40
21	8	606	CHL	C3D-C4D	-4.79	1.33	1.44
21	W	605	CHL	C3D-C4D	-4.79	1.33	1.44
21	9	605	CHL	C3D-C4D	-4.79	1.33	1.44
21	U	605	CHL	C3D-C4D	-4.79	1.33	1.44
21	V	607	CHL	C3D-C4D	-4.78	1.33	1.44
21	V	608	CHL	C3D-C4D	-4.78	1.33	1.44
21	4	608	CHL	C3D-C4D	-4.77	1.33	1.44
21	8	618	CHL	C3D-C4D	-4.77	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	6	608	CHL	C3D-C4D	-4.77	1.33	1.44
21	5	607	CHL	C3D-C4D	-4.77	1.33	1.44
21	6	606	CHL	C3D-C4D	-4.77	1.33	1.44
21	6	608	CHL	C3B-C2B	4.77	1.47	1.40
21	W	608	CHL	C3D-C4D	-4.77	1.33	1.44
21	2	618	CHL	C3B-C2B	4.77	1.47	1.40
21	1	601	CHL	C3B-C2B	4.77	1.47	1.40
21	U	607	CHL	C3D-C4D	-4.76	1.33	1.44
21	V	601	CHL	C3D-C4D	-4.76	1.33	1.44
21	W	609	CHL	C3D-C4D	-4.76	1.33	1.44
21	6	618	CHL	C3B-C2B	4.75	1.47	1.40
21	8	608	CHL	C3B-C2B	4.75	1.47	1.40
21	V	605	CHL	C3D-C4D	-4.75	1.33	1.44
21	9	607	CHL	C3D-C4D	-4.75	1.33	1.44
21	5	601	CHL	C3B-C2B	4.75	1.47	1.40
21	8	607	CHL	C3D-C4D	-4.75	1.33	1.44
21	7	608	CHL	C3B-C2B	4.74	1.46	1.40
21	6	618	CHL	C3D-C4D	-4.73	1.33	1.44
21	6	607	CHL	C3D-C4D	-4.73	1.33	1.44
21	V	606	CHL	C3D-C4D	-4.73	1.33	1.44
21	6	601	CHL	C3D-C4D	-4.73	1.33	1.44
21	9	605	CHL	C3B-C2B	4.73	1.46	1.40
21	6	602	CHL	C3D-C4D	-4.72	1.33	1.44
21	5	601	CHL	C3D-C4D	-4.72	1.33	1.44
21	4	607	CHL	C3B-C2B	4.72	1.46	1.40
22	9	609	CLA	C3B-C2B	4.71	1.46	1.40
26	9	2630	LHG	O8-C23	4.69	1.47	1.33
21	W	605	CHL	O2D-CGD	4.68	1.45	1.30
21	4	618	CHL	C3B-C2B	4.68	1.46	1.40
21	V	606	CHL	O2D-CGD	4.68	1.45	1.30
21	4	618	CHL	C3D-C4D	-4.67	1.33	1.44
21	9	601	CHL	C3B-C2B	4.66	1.46	1.40
21	2	607	CHL	C3B-C2B	4.66	1.46	1.40
21	6	607	CHL	C3B-C2B	4.66	1.46	1.40
21	2	601	CHL	C3B-C2B	4.65	1.46	1.40
21	U	605	CHL	O2D-CGD	4.64	1.45	1.30
21	W	606	CHL	O2D-CGD	4.64	1.45	1.30
21	V	601	CHL	O2D-CGD	4.64	1.45	1.30
21	U	607	CHL	C3B-C2B	4.64	1.46	1.40
21	W	601	CHL	O2D-CGD	4.63	1.45	1.30
21	U	601	CHL	O2D-CGD	4.63	1.45	1.30
21	W	608	CHL	O2D-CGD	4.63	1.45	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	V	608	CHL	O2D-CGD	4.62	1.45	1.30
21	1	601	CHL	C2C-C3C	4.62	1.46	1.36
21	8	606	CHL	C3B-C2B	4.62	1.46	1.40
21	U	608	CHL	O2D-CGD	4.61	1.45	1.30
21	6	607	CHL	C2C-C3C	4.61	1.46	1.36
21	U	601	CHL	C3C-C2C	4.61	1.46	1.36
21	1	607	CHL	C2C-C3C	4.61	1.46	1.36
21	V	609	CHL	C2C-C3C	4.60	1.46	1.36
21	9	601	CHL	C2C-C3C	4.59	1.46	1.36
21	5	607	CHL	C2C-C3C	4.59	1.46	1.36
21	6	606	CHL	C3B-C2B	4.58	1.46	1.40
21	8	607	CHL	C2C-C3C	4.58	1.46	1.36
21	2	608	CHL	C2C-C3C	4.57	1.46	1.36
21	6	601	CHL	C2C-C3C	4.56	1.46	1.36
21	9	605	CHL	C2C-C3C	4.56	1.46	1.37
22	9	609	CLA	C3C-C2C	4.56	1.46	1.36
21	8	606	CHL	C2C-C3C	4.55	1.46	1.36
21	U	607	CHL	C2C-C3C	4.55	1.46	1.36
21	8	618	CHL	C2C-C3C	4.55	1.46	1.36
21	9	608	CHL	C2C-C3C	4.54	1.46	1.36
21	V	601	CHL	C3C-C2C	4.53	1.46	1.36
21	6	602	CHL	C2C-C3C	4.53	1.46	1.36
21	4	608	CHL	O2A-CGA	4.53	1.46	1.30
21	2	608	CHL	C3B-C2B	4.53	1.46	1.40
21	V	601	CHL	CHD-C1D	4.52	1.47	1.38
21	2	618	CHL	C2C-C3C	4.52	1.46	1.36
21	2	607	CHL	C2C-C3C	4.52	1.46	1.36
22	O	2001	CLA	CHB-C4A	4.52	1.38	1.34
21	W	601	CHL	C3C-C2C	4.52	1.46	1.36
21	4	606	CHL	O2A-CGA	4.52	1.45	1.30
21	2	602	CHL	O2A-CGA	4.51	1.46	1.33
21	2	608	CHL	O2A-CGA	4.51	1.45	1.30
21	U	606	CHL	C3B-C2B	4.51	1.46	1.40
21	V	605	CHL	C2C-C3C	4.51	1.46	1.36
21	4	607	CHL	C2C-C3C	4.50	1.46	1.36
21	2	601	CHL	O2A-CGA	4.50	1.45	1.30
21	7	608	CHL	O2A-CGA	4.50	1.45	1.30
21	W	607	CHL	C2C-C3C	4.50	1.46	1.37
21	2	601	CHL	C2C-C3C	4.49	1.46	1.36
21	5	601	CHL	C2C-C3C	4.49	1.46	1.36
21	2	606	CHL	C3B-C2B	4.49	1.46	1.40
21	1	607	CHL	CHD-C1D	4.49	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	8	607	CHL	O2A-CGA	4.49	1.45	1.30
21	8	606	CHL	O2A-CGA	4.49	1.45	1.30
21	2	606	CHL	O2A-CGA	4.49	1.45	1.30
21	U	606	CHL	O2A-CGA	4.49	1.45	1.30
21	8	607	CHL	C3B-C2B	4.49	1.46	1.40
21	V	608	CHL	C2C-C3C	4.48	1.46	1.37
22	9	609	CLA	O2A-CGA	4.47	1.45	1.30
24	8	620	XAT	C30-C29	4.47	1.41	1.35
21	6	606	CHL	O2A-CGA	4.46	1.45	1.30
21	V	607	CHL	C2C-C3C	4.46	1.46	1.37
21	9	606	CHL	C2C-C3C	4.46	1.46	1.36
24	8	620	XAT	C14-C13	4.45	1.41	1.35
21	U	605	CHL	CHD-C1D	4.45	1.47	1.38
21	W	606	CHL	CHD-C1D	4.45	1.47	1.38
21	8	618	CHL	CHD-C1D	4.45	1.47	1.38
21	2	602	CHL	C2C-C3C	4.45	1.46	1.36
21	W	608	CHL	C2C-C3C	4.45	1.46	1.37
21	U	608	CHL	C2C-C3C	4.45	1.46	1.37
22	9	609	CLA	CHD-C1D	4.45	1.47	1.38
23	5	617	LUT	C34-C33	4.44	1.41	1.35
21	4	606	CHL	C3B-C2B	4.43	1.46	1.40
21	U	608	CHL	CHD-C1D	4.43	1.47	1.38
21	4	607	CHL	CHD-C1D	4.43	1.47	1.38
21	6	618	CHL	CHD-C1D	4.42	1.47	1.38
24	8	620	XAT	C34-C33	4.42	1.41	1.35
21	5	601	CHL	O2A-CGA	4.42	1.46	1.33
21	V	606	CHL	CHD-C1D	4.42	1.47	1.38
21	4	606	CHL	C2C-C3C	4.41	1.46	1.36
21	W	605	CHL	CHD-C1D	4.41	1.47	1.38
21	9	601	CHL	CHD-C1D	4.41	1.47	1.38
21	U	609	CHL	C2C-C3C	4.41	1.46	1.36
21	U	601	CHL	CHD-C1D	4.40	1.46	1.38
21	6	602	CHL	O2A-CGA	4.40	1.46	1.33
21	4	608	CHL	C2C-C3C	4.40	1.46	1.36
21	W	601	CHL	CHD-C1D	4.39	1.46	1.38
21	W	608	CHL	CHD-C1D	4.38	1.46	1.38
21	V	605	CHL	CHD-C1D	4.38	1.46	1.38
21	4	618	CHL	C2C-C3C	4.38	1.46	1.36
21	4	618	CHL	CHD-C1D	4.38	1.46	1.38
21	W	609	CHL	C2C-C3C	4.38	1.46	1.36
21	8	608	CHL	O2A-CGA	4.38	1.46	1.33
21	6	618	CHL	C2C-C3C	4.38	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4	608	CHL	CHD-C1D	4.38	1.46	1.38
21	V	608	CHL	CHD-C1D	4.37	1.46	1.38
26	6	630	LHG	O8-C23	4.37	1.46	1.33
21	8	606	CHL	CHD-C1D	4.37	1.46	1.38
21	9	608	CHL	C3B-C2B	4.36	1.46	1.40
21	U	609	CHL	O2A-CGA	4.36	1.46	1.33
21	6	606	CHL	C2C-C3C	4.36	1.46	1.36
21	8	607	CHL	CHD-C1D	4.36	1.46	1.38
26	7	630	LHG	O8-C23	4.36	1.46	1.33
21	6	602	CHL	CHD-C1D	4.36	1.46	1.38
21	2	606	CHL	C2C-C3C	4.36	1.46	1.36
21	7	608	CHL	C2C-C3C	4.35	1.46	1.36
21	9	606	CHL	CHD-C1D	4.35	1.46	1.38
21	6	608	CHL	C2C-C3C	4.35	1.46	1.36
21	W	609	CHL	CHD-C1D	4.35	1.46	1.38
28	A	860	LMG	O8-C28	4.34	1.46	1.33
26	5	630	LHG	O8-C23	4.34	1.46	1.33
21	2	602	CHL	C3B-C2B	4.33	1.46	1.40
21	2	607	CHL	CHD-C1D	4.33	1.46	1.38
21	9	607	CHL	C2C-C3C	4.33	1.46	1.36
21	9	608	CHL	CHD-C1D	4.33	1.46	1.38
21	V	601	CHL	O2A-CGA	4.33	1.46	1.33
21	6	607	CHL	CHD-C1D	4.33	1.46	1.38
21	8	608	CHL	C2C-C3C	4.33	1.46	1.36
21	V	607	CHL	CHD-C1D	4.32	1.46	1.38
26	1	630	LHG	O8-C23	4.32	1.46	1.33
21	V	609	CHL	CHD-C1D	4.32	1.46	1.38
21	2	608	CHL	CHD-C1D	4.32	1.46	1.38
21	6	606	CHL	CHD-C1D	4.32	1.46	1.38
21	6	601	CHL	CHD-C1D	4.32	1.46	1.38
21	U	607	CHL	CHD-C1D	4.32	1.46	1.38
28	G	202	LMG	O8-C28	4.32	1.46	1.33
21	5	607	CHL	CHD-C1D	4.31	1.46	1.38
21	W	601	CHL	O2A-CGA	4.31	1.45	1.33
21	1	601	CHL	O2A-CGA	4.31	1.45	1.33
21	9	605	CHL	CHD-C1D	4.31	1.46	1.38
21	U	607	CHL	O2A-CGA	4.31	1.45	1.33
21	3	608	CHL	CHD-C1D	4.31	1.46	1.38
22	O	2003	CLA	CHB-C4A	4.31	1.38	1.34
21	9	606	CHL	C3B-C2B	4.31	1.46	1.40
21	2	601	CHL	CHD-C1D	4.30	1.46	1.38
21	2	618	CHL	CHD-C1D	4.30	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	8	630	LHG	O8-C23	4.30	1.45	1.33
23	5	617	LUT	C14-C13	4.30	1.41	1.35
21	3	608	CHL	C2C-C3C	4.29	1.46	1.36
26	3	630	LHG	O8-C23	4.29	1.45	1.33
21	6	608	CHL	O2A-CGA	4.29	1.45	1.33
28	J	104	LMG	O7-C10	4.29	1.46	1.34
21	6	601	CHL	O2A-CGA	4.29	1.45	1.33
24	8	620	XAT	C10-C9	4.28	1.41	1.35
21	W	607	CHL	CHD-C1D	4.28	1.46	1.38
26	B	851	LHG	O8-C23	4.28	1.45	1.33
28	J	104	LMG	O8-C28	4.27	1.45	1.33
21	4	606	CHL	CHD-C1D	4.27	1.46	1.38
21	U	606	CHL	C2C-C3C	4.27	1.45	1.36
21	2	606	CHL	CHD-C1D	4.27	1.46	1.38
21	5	601	CHL	CHD-C1D	4.27	1.46	1.38
21	9	607	CHL	CHD-C1D	4.27	1.46	1.38
28	2	631	LMG	O8-C28	4.26	1.45	1.33
26	2	630	LHG	O8-C23	4.26	1.45	1.33
21	1	601	CHL	CHD-C1D	4.25	1.46	1.38
32	B	850	DGD	O1G-C1A	4.25	1.45	1.33
26	U	2630	LHG	O8-C23	4.25	1.45	1.33
21	U	601	CHL	O2A-CGA	4.25	1.45	1.33
21	2	602	CHL	CHD-C1D	4.24	1.46	1.38
21	6	602	CHL	C3B-C2B	4.24	1.46	1.40
32	B	850	DGD	O2G-C1B	4.24	1.46	1.34
26	V	2630	LHG	O8-C23	4.23	1.45	1.33
26	A	846	LHG	O8-C23	4.23	1.45	1.33
22	4	610	CLA	C1D-ND	4.22	1.43	1.37
26	2	630	LHG	O7-C7	4.22	1.46	1.34
26	4	630	LHG	O8-C23	4.22	1.45	1.33
23	5	617	LUT	C30-C29	4.21	1.41	1.35
22	7	609	CLA	C1D-ND	4.21	1.43	1.37
26	W	2630	LHG	O8-C23	4.21	1.45	1.33
21	3	608	CHL	O2A-CGA	4.21	1.45	1.33
28	J	103	LMG	O8-C28	4.20	1.45	1.33
21	U	609	CHL	CHD-C1D	4.20	1.46	1.38
28	L	307	LMG	O8-C28	4.20	1.45	1.33
21	7	608	CHL	CHD-C1D	4.20	1.46	1.38
26	V	2630	LHG	O7-C7	4.20	1.46	1.34
26	B	851	LHG	O7-C7	4.20	1.46	1.34
21	6	608	CHL	CHD-C1D	4.20	1.46	1.38
26	6	630	LHG	O7-C7	4.20	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	U	606	CHL	CHD-C1D	4.19	1.46	1.38
28	G	202	LMG	O7-C10	4.18	1.46	1.34
21	8	608	CHL	CHD-C1D	4.17	1.46	1.38
22	A	801	CLA	C1D-ND	4.15	1.42	1.37
22	3	617	CLA	C1D-ND	4.15	1.42	1.37
26	A	847	LHG	O8-C23	4.14	1.45	1.33
21	4	607	CHL	CHD-C4C	4.14	1.48	1.39
23	5	617	LUT	C10-C9	4.14	1.41	1.35
26	7	630	LHG	O7-C7	4.12	1.45	1.34
26	3	630	LHG	O7-C7	4.12	1.45	1.34
22	5	616	CLA	C1D-ND	4.12	1.42	1.37
26	U	2630	LHG	O7-C7	4.11	1.45	1.34
21	W	606	CHL	C3A-C2A	-4.11	1.50	1.54
28	L	307	LMG	O7-C10	4.11	1.45	1.34
26	A	846	LHG	O7-C7	4.11	1.45	1.34
22	9	609	CLA	CHD-C4C	4.10	1.48	1.39
22	5	612	CLA	C1D-ND	4.10	1.42	1.37
26	A	847	LHG	O7-C7	4.10	1.45	1.34
21	U	605	CHL	C3A-C2A	-4.09	1.50	1.54
26	W	2630	LHG	O7-C7	4.09	1.45	1.34
21	9	605	CHL	C3A-C2A	-4.08	1.50	1.54
21	6	602	CHL	CHD-C4C	4.08	1.48	1.39
21	V	601	CHL	CHD-C4C	4.08	1.48	1.39
26	8	630	LHG	O7-C7	4.07	1.45	1.34
21	1	607	CHL	O2A-CGA	4.07	1.46	1.33
21	V	609	CHL	CHD-C4C	4.07	1.48	1.39
21	6	607	CHL	O2A-CGA	4.07	1.46	1.33
21	9	601	CHL	CHD-C4C	4.07	1.48	1.39
21	4	608	CHL	CHD-C4C	4.06	1.48	1.39
28	A	860	LMG	O7-C10	4.06	1.45	1.34
26	9	2630	LHG	O7-C7	4.06	1.45	1.34
22	6	612	CLA	C1D-ND	4.05	1.42	1.37
22	8	602	CLA	C1D-ND	4.05	1.42	1.37
22	3	609	CLA	C1D-ND	4.05	1.42	1.37
24	4	620	XAT	O4-C5	-4.05	1.40	1.46
22	5	609	CLA	C1D-ND	4.05	1.42	1.37
21	2	607	CHL	O2A-CGA	4.05	1.45	1.33
22	1	609	CLA	C1D-ND	4.04	1.42	1.37
22	3	611	CLA	C1D-ND	4.04	1.42	1.37
28	2	631	LMG	O7-C10	4.04	1.45	1.34
22	7	602	CLA	C1D-ND	4.04	1.42	1.37
21	2	608	CHL	CHD-C4C	4.04	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	5	630	LHG	O7-C7	4.03	1.45	1.34
21	9	606	CHL	CHD-C4C	4.03	1.48	1.39
21	V	607	CHL	C3A-C2A	-4.03	1.50	1.54
21	4	607	CHL	O2A-CGA	4.03	1.45	1.33
22	W	610	CLA	C1D-ND	4.02	1.42	1.37
25	9	623	NEX	C7-C8	-4.02	1.25	1.32
22	A	827	CLA	C1D-ND	4.02	1.42	1.37
21	V	606	CHL	C3A-C2A	-4.02	1.50	1.54
21	2	618	CHL	CHD-C4C	4.02	1.48	1.39
21	U	608	CHL	CHD-C4C	4.01	1.48	1.39
21	6	618	CHL	O2A-CGA	4.01	1.45	1.33
22	7	603	CLA	C1D-ND	4.01	1.42	1.37
21	W	609	CHL	CHD-C4C	4.01	1.48	1.39
21	8	618	CHL	CHD-C4C	4.00	1.48	1.39
21	9	601	CHL	C3A-C2A	-4.00	1.50	1.54
21	V	605	CHL	C3A-C2A	-4.00	1.50	1.54
21	2	607	CHL	CHD-C4C	4.00	1.48	1.39
21	8	607	CHL	CHD-C4C	3.99	1.48	1.39
21	1	607	CHL	CHD-C4C	3.99	1.48	1.39
21	6	601	CHL	CHD-C4C	3.98	1.48	1.39
21	W	601	CHL	CHD-C4C	3.98	1.48	1.39
21	W	607	CHL	C3A-C2A	-3.98	1.50	1.54
22	2	603	CLA	C1D-ND	3.98	1.42	1.37
21	9	607	CHL	CHD-C4C	3.98	1.48	1.39
22	1	616	CLA	C1D-ND	3.97	1.42	1.37
21	7	608	CHL	CHD-C4C	3.97	1.48	1.39
21	W	606	CHL	CHD-C4C	3.97	1.48	1.39
21	5	607	CHL	C3A-C2A	-3.97	1.50	1.54
22	2	613	CLA	C1D-ND	3.97	1.42	1.37
21	W	605	CHL	CHD-C4C	3.97	1.48	1.39
22	8	604	CLA	C1D-ND	3.96	1.42	1.37
21	U	609	CHL	CHD-C4C	3.96	1.48	1.39
21	U	601	CHL	CHD-C4C	3.96	1.48	1.39
21	6	618	CHL	CHD-C4C	3.96	1.48	1.39
21	V	605	CHL	CHD-C4C	3.95	1.48	1.39
22	5	603	CLA	C1D-ND	3.95	1.42	1.37
22	4	612	CLA	C1D-ND	3.95	1.42	1.37
21	9	608	CHL	CHD-C4C	3.95	1.48	1.39
22	7	612	CLA	C1D-ND	3.95	1.42	1.37
21	1	601	CHL	CHD-C4C	3.95	1.48	1.39
22	2	609	CLA	C1D-ND	3.94	1.42	1.37
21	2	601	CHL	CHD-C4C	3.94	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	W	608	CHL	CHD-C4C	3.94	1.48	1.39
22	B	821	CLA	C1D-ND	3.94	1.42	1.37
21	6	607	CHL	CHD-C4C	3.94	1.48	1.39
21	5	607	CHL	CHD-C4C	3.94	1.48	1.39
22	1	603	CLA	C1D-ND	3.94	1.42	1.37
26	1	630	LHG	O7-C7	3.94	1.45	1.34
21	2	602	CHL	CHD-C4C	3.94	1.48	1.39
21	6	606	CHL	CHD-C4C	3.93	1.48	1.39
22	8	614	CLA	C1D-ND	3.93	1.42	1.37
21	5	601	CHL	CHD-C4C	3.93	1.48	1.39
21	9	605	CHL	CHD-C4C	3.93	1.48	1.39
22	7	607	CLA	C1D-ND	3.93	1.42	1.37
22	4	603	CLA	C1D-ND	3.92	1.42	1.37
22	G	203	CLA	C1D-ND	3.92	1.42	1.37
21	U	605	CHL	CHD-C4C	3.92	1.48	1.39
22	H	201	CLA	C1D-ND	3.92	1.42	1.37
24	6	620	XAT	O24-C25	-3.92	1.40	1.46
22	7	604	CLA	C1D-ND	3.92	1.42	1.37
22	L	304	CLA	C1D-ND	3.91	1.42	1.37
22	8	603	CLA	C1D-ND	3.91	1.42	1.37
22	U	611	CLA	C1D-ND	3.91	1.42	1.37
22	3	612	CLA	C1D-ND	3.91	1.42	1.37
22	1	611	CLA	C1D-ND	3.91	1.42	1.37
22	4	604	CLA	C1D-ND	3.91	1.42	1.37
22	7	610	CLA	C1D-ND	3.91	1.42	1.37
22	1	614	CLA	C1D-ND	3.91	1.42	1.37
22	A	829	CLA	C1D-ND	3.91	1.42	1.37
22	7	615	CLA	C1D-ND	3.90	1.42	1.37
21	6	608	CHL	CHD-C4C	3.90	1.48	1.39
22	A	838	CLA	C1D-ND	3.90	1.42	1.37
22	U	614	CLA	C1D-ND	3.90	1.42	1.37
21	8	606	CHL	CHD-C4C	3.90	1.48	1.39
21	V	608	CHL	CHD-C4C	3.90	1.48	1.39
22	8	601	CLA	C1D-ND	3.89	1.42	1.37
22	2	614	CLA	C1D-ND	3.89	1.42	1.37
22	K	201	CLA	C1D-ND	3.89	1.42	1.37
21	U	607	CHL	CHD-C4C	3.89	1.48	1.39
22	3	613	CLA	C1D-ND	3.89	1.42	1.37
21	V	606	CHL	CHD-C4C	3.88	1.48	1.39
22	6	614	CLA	C1D-ND	3.88	1.42	1.37
22	4	611	CLA	C1D-ND	3.88	1.42	1.37
22	8	612	CLA	C1D-ND	3.88	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	816	CLA	C1D-ND	3.88	1.42	1.37
21	3	608	CHL	CHD-C4C	3.88	1.48	1.39
22	B	826	CLA	C1D-ND	3.88	1.42	1.37
22	A	845	CLA	C1D-ND	3.87	1.42	1.37
22	B	823	CLA	C1D-ND	3.87	1.42	1.37
21	8	608	CHL	CHD-C4C	3.87	1.48	1.39
22	9	603	CLA	C1D-ND	3.87	1.42	1.37
22	6	604	CLA	C1D-ND	3.87	1.42	1.37
22	V	612	CLA	C1D-ND	3.87	1.42	1.37
22	W	602	CLA	C1D-ND	3.87	1.42	1.37
22	9	611	CLA	C1D-ND	3.86	1.42	1.37
22	5	606	CLA	C1D-ND	3.86	1.42	1.37
22	V	613	CLA	C1D-ND	3.86	1.42	1.37
21	2	606	CHL	CHD-C4C	3.86	1.48	1.39
21	W	607	CHL	CHD-C4C	3.85	1.48	1.39
22	1	604	CLA	C1D-ND	3.85	1.42	1.37
21	V	607	CHL	CHD-C4C	3.85	1.48	1.39
22	V	611	CLA	C1D-ND	3.84	1.42	1.37
22	6	603	CLA	C1D-ND	3.84	1.42	1.37
22	8	613	CLA	C1D-ND	3.84	1.42	1.37
22	V	602	CLA	C1D-ND	3.84	1.42	1.37
22	V	603	CLA	C1D-ND	3.84	1.42	1.37
22	2	611	CLA	C1D-ND	3.84	1.42	1.37
22	5	614	CLA	C1D-ND	3.84	1.42	1.37
21	4	618	CHL	CHD-C4C	3.84	1.48	1.39
22	6	613	CLA	C1D-ND	3.83	1.42	1.37
22	W	604	CLA	C1D-ND	3.83	1.42	1.37
22	5	604	CLA	C1D-ND	3.83	1.42	1.37
22	A	835	CLA	C1D-ND	3.83	1.42	1.37
22	G	204	CLA	C1D-ND	3.83	1.42	1.37
22	F	304	CLA	C1D-ND	3.83	1.43	1.37
22	J	101	CLA	C1D-ND	3.83	1.42	1.37
22	V	604	CLA	C1D-ND	3.83	1.42	1.37
21	W	605	CHL	C3A-C2A	-3.83	1.50	1.54
22	V	610	CLA	C1D-ND	3.83	1.42	1.37
22	5	608	CLA	C1D-ND	3.83	1.42	1.37
22	7	614	CLA	C1D-ND	3.83	1.42	1.37
22	A	818	CLA	C1D-ND	3.82	1.42	1.37
22	4	601	CLA	C1D-ND	3.82	1.42	1.37
22	A	842	CLA	C1D-ND	3.82	1.42	1.37
22	3	614	CLA	C1D-ND	3.82	1.42	1.37
22	9	602	CLA	C1D-ND	3.82	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	K	204	CLA	C1D-ND	3.82	1.42	1.37
22	K	206	CLA	C1D-ND	3.82	1.42	1.37
28	J	103	LMG	O7-C10	3.82	1.45	1.34
22	A	828	CLA	C1D-ND	3.81	1.42	1.37
22	5	610	CLA	C1D-ND	3.81	1.42	1.37
22	2	612	CLA	C1D-ND	3.81	1.42	1.37
22	6	611	CLA	C1D-ND	3.81	1.42	1.37
22	9	610	CLA	C1D-ND	3.81	1.42	1.37
22	6	610	CLA	C1D-ND	3.81	1.42	1.37
21	U	606	CHL	CHD-C4C	3.81	1.47	1.39
22	W	612	CLA	C1D-ND	3.81	1.42	1.37
22	7	617	CLA	C1D-ND	3.81	1.42	1.37
22	G	201	CLA	C1D-ND	3.81	1.42	1.37
22	1	606	CLA	C1D-ND	3.81	1.42	1.37
22	F	303	CLA	C1D-ND	3.81	1.42	1.37
22	V	614	CLA	C1D-ND	3.80	1.42	1.37
22	B	804	CLA	C1D-ND	3.80	1.42	1.37
22	8	609	CLA	C1D-ND	3.80	1.42	1.37
22	3	602	CLA	C1D-ND	3.80	1.42	1.37
22	A	806	CLA	C1D-ND	3.80	1.42	1.37
22	3	607	CLA	C1D-ND	3.80	1.42	1.37
22	A	815	CLA	C1D-ND	3.80	1.42	1.37
22	A	825	CLA	C1D-ND	3.80	1.42	1.37
22	1	610	CLA	C1D-ND	3.80	1.42	1.37
22	4	614	CLA	C1D-ND	3.80	1.42	1.37
22	9	604	CLA	C1D-ND	3.80	1.42	1.37
22	7	611	CLA	C1D-ND	3.79	1.42	1.37
22	A	817	CLA	C1D-ND	3.79	1.42	1.37
22	B	811	CLA	C1D-ND	3.79	1.42	1.37
22	8	611	CLA	C1D-ND	3.79	1.42	1.37
21	9	607	CHL	OBD-CAD	3.78	1.29	1.22
22	B	831	CLA	C1D-ND	3.78	1.42	1.37
22	A	804	CLA	C1D-ND	3.78	1.42	1.37
22	A	809	CLA	C1D-ND	3.78	1.42	1.37
22	O	2002	CLA	C1D-ND	3.78	1.42	1.37
22	U	602	CLA	C1D-ND	3.78	1.42	1.37
22	U	603	CLA	C1D-ND	3.78	1.42	1.37
22	U	604	CLA	C1D-ND	3.77	1.42	1.37
21	6	606	CHL	OBD-CAD	3.77	1.29	1.22
22	B	841	CLA	C1D-ND	3.77	1.42	1.37
22	A	807	CLA	C1D-ND	3.77	1.42	1.37
22	1	612	CLA	C1D-ND	3.77	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	K	203	CLA	C1D-ND	3.77	1.42	1.37
22	L	302	CLA	C1D-ND	3.77	1.42	1.37
22	A	808	CLA	C1D-ND	3.76	1.42	1.37
22	3	610	CLA	C1D-ND	3.76	1.42	1.37
22	B	836	CLA	C1D-ND	3.76	1.42	1.37
21	9	605	CHL	OBD-CAD	3.76	1.29	1.22
22	W	603	CLA	C1D-ND	3.76	1.42	1.37
22	2	610	CLA	C1D-ND	3.76	1.42	1.37
22	B	839	CLA	C1D-ND	3.76	1.42	1.37
22	A	840	CLA	C1D-ND	3.76	1.42	1.37
21	4	606	CHL	CHD-C4C	3.76	1.47	1.39
22	3	603	CLA	C1D-ND	3.75	1.42	1.37
22	3	606	CLA	C1D-ND	3.75	1.42	1.37
22	4	613	CLA	C1D-ND	3.75	1.42	1.37
22	A	816	CLA	C1D-ND	3.75	1.42	1.37
22	5	611	CLA	C1D-ND	3.75	1.42	1.37
22	8	610	CLA	C1D-ND	3.75	1.42	1.37
22	W	613	CLA	C1D-ND	3.75	1.42	1.37
22	U	612	CLA	C1D-ND	3.75	1.42	1.37
22	2	604	CLA	C1D-ND	3.75	1.42	1.37
22	B	829	CLA	C1D-ND	3.75	1.42	1.37
21	U	605	CHL	OBD-CAD	3.75	1.28	1.22
22	A	834	CLA	C1D-ND	3.75	1.42	1.37
26	4	630	LHG	O7-C7	3.74	1.44	1.34
21	W	608	CHL	OBD-CAD	3.74	1.28	1.22
21	4	607	CHL	OBD-CAD	3.74	1.28	1.22
22	9	613	CLA	C1D-ND	3.74	1.42	1.37
22	O	2003	CLA	C4B-CHC	-3.74	1.36	1.43
22	7	613	CLA	C1D-ND	3.74	1.42	1.37
21	8	618	CHL	OBD-CAD	3.74	1.28	1.22
22	A	831	CLA	C1D-ND	3.74	1.42	1.37
22	U	613	CLA	C1D-ND	3.74	1.42	1.37
22	B	832	CLA	C1D-ND	3.74	1.42	1.37
22	7	606	CLA	C1D-ND	3.74	1.42	1.37
22	B	807	CLA	C1D-ND	3.74	1.42	1.37
22	B	806	CLA	C1D-ND	3.73	1.42	1.37
22	W	614	CLA	C1D-ND	3.73	1.42	1.37
21	V	607	CHL	OBD-CAD	3.73	1.28	1.22
22	A	805	CLA	C1D-ND	3.73	1.42	1.37
22	5	613	CLA	C1D-ND	3.73	1.42	1.37
22	4	602	CLA	C1D-ND	3.72	1.42	1.37
22	1	608	CLA	C1D-ND	3.72	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	8	607	CHL	OBD-CAD	3.72	1.28	1.22
22	A	837	CLA	C1D-ND	3.72	1.42	1.37
22	O	2001	CLA	C4B-CHC	-3.72	1.36	1.43
22	B	824	CLA	C1D-ND	3.72	1.42	1.37
22	B	822	CLA	C1D-ND	3.71	1.42	1.37
22	B	819	CLA	C1D-ND	3.71	1.42	1.37
22	A	839	CLA	C1D-ND	3.71	1.42	1.37
22	A	810	CLA	C1D-ND	3.71	1.42	1.37
22	1	613	CLA	C1D-ND	3.71	1.42	1.37
22	4	609	CLA	C1D-ND	3.70	1.42	1.37
22	A	814	CLA	C1D-ND	3.70	1.42	1.37
22	A	826	CLA	C1D-ND	3.70	1.42	1.37
22	1	602	CLA	C1D-ND	3.70	1.42	1.37
22	9	612	CLA	C1D-ND	3.70	1.42	1.37
22	B	803	CLA	C1D-ND	3.70	1.42	1.37
21	U	601	CHL	OBD-CAD	3.70	1.28	1.22
21	2	607	CHL	OBD-CAD	3.70	1.28	1.22
21	4	618	CHL	OBD-CAD	3.70	1.28	1.22
21	V	605	CHL	OBD-CAD	3.70	1.28	1.22
21	1	607	CHL	OBD-CAD	3.70	1.28	1.22
22	B	815	CLA	C1D-ND	3.69	1.42	1.37
22	6	609	CLA	C1D-ND	3.69	1.42	1.37
21	V	608	CHL	OBD-CAD	3.69	1.28	1.22
21	4	608	CHL	OBD-CAD	3.69	1.28	1.22
22	B	809	CLA	C1D-ND	3.69	1.42	1.37
21	9	601	CHL	OBD-CAD	3.69	1.28	1.22
22	A	832	CLA	C1D-ND	3.69	1.42	1.37
21	6	601	CHL	OBD-CAD	3.69	1.28	1.22
21	6	607	CHL	OBD-CAD	3.69	1.28	1.22
21	2	618	CHL	OBD-CAD	3.68	1.28	1.22
22	U	610	CLA	C1D-ND	3.68	1.42	1.37
23	2	619	LUT	C30-C29	3.68	1.40	1.35
21	U	607	CHL	OBD-CAD	3.68	1.28	1.22
22	A	820	CLA	C1D-ND	3.68	1.42	1.37
22	5	602	CLA	C1D-ND	3.68	1.42	1.37
22	B	825	CLA	C1D-ND	3.68	1.42	1.37
21	W	605	CHL	OBD-CAD	3.68	1.28	1.22
23	2	619	LUT	C14-C13	3.67	1.40	1.35
21	5	601	CHL	OBD-CAD	3.67	1.28	1.22
22	9	609	CLA	OBD-CAD	3.67	1.28	1.22
22	A	803	CLA	C1D-ND	3.67	1.42	1.37
21	W	606	CHL	OBD-CAD	3.67	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	W	609	CHL	OBD-CAD	3.67	1.28	1.22
22	B	835	CLA	C1D-ND	3.67	1.42	1.37
22	B	817	CLA	C1D-ND	3.67	1.42	1.37
22	B	818	CLA	C1D-ND	3.67	1.42	1.37
22	3	615	CLA	C1D-ND	3.67	1.42	1.37
22	F	301	CLA	C1D-ND	3.67	1.42	1.37
22	A	824	CLA	C1D-ND	3.66	1.42	1.37
21	6	602	CHL	OBD-CAD	3.66	1.28	1.22
21	V	601	CHL	OBD-CAD	3.66	1.28	1.22
21	U	608	CHL	OBD-CAD	3.66	1.28	1.22
22	3	604	CLA	C1D-ND	3.66	1.42	1.37
22	A	819	CLA	C1D-ND	3.65	1.42	1.37
22	V	610	CLA	CAB-C3B	-3.65	1.44	1.51
21	V	606	CHL	OBD-CAD	3.65	1.28	1.22
21	U	606	CHL	OBD-CAD	3.65	1.28	1.22
21	6	618	CHL	OBD-CAD	3.64	1.28	1.22
22	A	812	CLA	C1D-ND	3.64	1.42	1.37
21	2	606	CHL	OBD-CAD	3.64	1.28	1.22
21	V	609	CHL	OBD-CAD	3.63	1.28	1.22
21	2	601	CHL	OBD-CAD	3.63	1.28	1.22
21	9	608	CHL	OBD-CAD	3.63	1.28	1.22
22	B	834	CLA	C1D-ND	3.63	1.42	1.37
21	W	607	CHL	OBD-CAD	3.63	1.28	1.22
22	A	822	CLA	C1D-ND	3.62	1.42	1.37
22	B	837	CLA	C1D-ND	3.62	1.42	1.37
22	B	827	CLA	C1D-ND	3.61	1.42	1.37
22	A	811	CLA	C1D-ND	3.61	1.42	1.37
22	B	813	CLA	C1D-ND	3.61	1.42	1.37
22	B	838	CLA	C1D-ND	3.61	1.42	1.37
21	8	608	CHL	OBD-CAD	3.61	1.28	1.22
24	V	2622	XAT	O4-C5	-3.61	1.41	1.46
21	U	609	CHL	OBD-CAD	3.61	1.28	1.22
22	A	833	CLA	C1D-ND	3.61	1.42	1.37
25	U	2623	NEX	C7-C8	-3.60	1.26	1.32
24	7	619	XAT	O24-C25	-3.60	1.41	1.46
21	9	606	CHL	OBD-CAD	3.60	1.28	1.22
22	B	814	CLA	C1D-ND	3.60	1.42	1.37
21	3	608	CHL	OBD-CAD	3.60	1.28	1.22
22	B	802	CLA	C1D-ND	3.60	1.42	1.37
22	B	828	CLA	C1D-ND	3.60	1.42	1.37
22	B	805	CLA	C1D-ND	3.59	1.42	1.37
22	W	611	CLA	C1D-ND	3.59	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	813	CLA	C1D-ND	3.59	1.42	1.37
21	2	608	CHL	OBD-CAD	3.59	1.28	1.22
22	A	802	CLA	C1D-ND	3.59	1.42	1.37
22	A	821	CLA	C1D-ND	3.59	1.42	1.37
23	2	619	LUT	C34-C33	3.59	1.40	1.35
21	5	607	CHL	OBD-CAD	3.58	1.28	1.22
21	2	602	CHL	OBD-CAD	3.58	1.28	1.22
21	8	606	CHL	OBD-CAD	3.57	1.28	1.22
21	W	601	CHL	OBD-CAD	3.57	1.28	1.22
21	4	606	CHL	OBD-CAD	3.57	1.28	1.22
22	A	830	CLA	C1D-ND	3.57	1.42	1.37
22	B	833	CLA	C1D-ND	3.57	1.42	1.37
22	W	614	CLA	CAB-C3B	-3.56	1.44	1.51
22	L	303	CLA	C1D-ND	3.55	1.42	1.37
21	1	601	CHL	OBD-CAD	3.54	1.28	1.22
22	B	810	CLA	C1D-ND	3.54	1.42	1.37
22	A	841	CLA	C1D-ND	3.54	1.42	1.37
21	6	608	CHL	OBD-CAD	3.54	1.28	1.22
22	B	820	CLA	C1D-ND	3.54	1.42	1.37
22	W	612	CLA	CAB-C3B	-3.52	1.44	1.51
22	B	808	CLA	C1D-ND	3.52	1.42	1.37
22	A	854	CLA	C1D-ND	3.52	1.42	1.37
22	A	843	CLA	C1D-ND	3.51	1.42	1.37
22	V	611	CLA	CAB-C3B	-3.51	1.44	1.51
22	W	611	CLA	CAB-C3B	-3.49	1.44	1.51
22	V	612	CLA	CAB-C3B	-3.49	1.44	1.51
22	B	830	CLA	C1D-ND	3.49	1.42	1.37
21	7	608	CHL	OBD-CAD	3.48	1.28	1.22
22	B	840	CLA	C1D-ND	3.45	1.42	1.37
24	7	619	XAT	O4-C5	-3.43	1.41	1.46
24	6	620	XAT	O4-C5	-3.42	1.41	1.46
25	W	2623	NEX	C7-C8	-3.38	1.26	1.32
22	A	836	CLA	C1D-ND	3.38	1.41	1.37
22	B	821	CLA	C4D-ND	-3.31	1.33	1.37
22	B	812	CLA	C2D-C1D	3.30	1.48	1.42
23	2	619	LUT	C10-C9	3.29	1.40	1.35
22	1	611	CLA	CHC-C1C	3.27	1.43	1.35
22	7	610	CLA	CHC-C1C	3.26	1.43	1.35
22	4	604	CLA	CHC-C1C	3.25	1.43	1.35
22	O	2003	CLA	C2D-C1D	3.25	1.48	1.42
22	B	830	CLA	C4D-ND	-3.23	1.33	1.37
22	8	601	CLA	C4D-ND	-3.23	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	8	611	CLA	CHC-C1C	3.22	1.43	1.35
22	O	2001	CLA	C2D-C1D	3.21	1.48	1.42
22	8	609	CLA	CHC-C1C	3.20	1.43	1.35
22	V	611	CLA	CHC-C1C	3.20	1.43	1.35
22	B	830	CLA	CHC-C1C	3.20	1.43	1.35
22	A	823	CLA	C2D-C1D	3.20	1.48	1.42
22	L	303	CLA	CHC-C1C	3.19	1.43	1.35
22	3	602	CLA	CHC-C1C	3.18	1.43	1.35
22	B	811	CLA	CHC-C1C	3.18	1.43	1.35
22	A	812	CLA	C4D-ND	-3.18	1.33	1.37
22	B	838	CLA	C4D-ND	-3.17	1.33	1.37
22	B	813	CLA	CHC-C1C	3.17	1.43	1.35
22	A	803	CLA	C4D-ND	-3.17	1.33	1.37
22	9	611	CLA	CHC-C1C	3.17	1.43	1.35
22	A	820	CLA	C4D-ND	-3.17	1.33	1.37
22	A	832	CLA	CHC-C1C	3.16	1.43	1.35
22	A	805	CLA	CHC-C1C	3.16	1.43	1.35
22	8	610	CLA	CHC-C1C	3.16	1.43	1.35
22	6	613	CLA	C4D-ND	-3.16	1.33	1.37
22	A	811	CLA	C4D-ND	-3.16	1.33	1.37
22	A	809	CLA	C4D-ND	-3.15	1.33	1.37
22	9	609	CLA	C1D-C2D	3.15	1.51	1.45
22	A	821	CLA	C4D-ND	-3.15	1.33	1.37
22	B	814	CLA	CHC-C1C	3.15	1.43	1.35
22	A	841	CLA	CHC-C1C	3.15	1.43	1.35
21	9	605	CHL	C1D-C2D	3.14	1.51	1.45
22	B	806	CLA	C4D-ND	-3.14	1.33	1.37
22	A	828	CLA	CHC-C1C	3.14	1.43	1.35
22	7	603	CLA	CHC-C1C	3.14	1.43	1.35
22	B	803	CLA	CHC-C1C	3.14	1.43	1.35
22	B	817	CLA	CHC-C1C	3.14	1.43	1.35
22	6	603	CLA	CHC-C1C	3.14	1.43	1.35
22	3	607	CLA	CHC-C1C	3.13	1.43	1.35
22	B	826	CLA	CHC-C1C	3.13	1.43	1.35
22	3	610	CLA	CHC-C1C	3.13	1.43	1.35
22	A	836	CLA	C4D-ND	-3.13	1.33	1.37
22	B	819	CLA	C4D-ND	-3.13	1.33	1.37
22	V	602	CLA	CHC-C1C	3.13	1.43	1.35
22	7	617	CLA	CHC-C1C	3.13	1.43	1.35
22	A	807	CLA	C4D-ND	-3.13	1.33	1.37
22	1	606	CLA	CHC-C1C	3.13	1.43	1.35
22	W	611	CLA	CHC-C1C	3.13	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	7	611	CLA	CHC-C1C	3.12	1.43	1.35
22	B	835	CLA	C4D-ND	-3.12	1.33	1.37
22	2	611	CLA	CHC-C1C	3.12	1.43	1.35
22	4	614	CLA	CHC-C1C	3.12	1.43	1.35
22	3	615	CLA	CHC-C1C	3.12	1.43	1.35
22	U	602	CLA	CHC-C1C	3.12	1.43	1.35
22	9	604	CLA	CHC-C1C	3.12	1.43	1.35
22	A	843	CLA	CHC-C1C	3.12	1.43	1.35
22	B	823	CLA	CHC-C1C	3.12	1.43	1.35
22	A	833	CLA	C4D-ND	-3.12	1.33	1.37
22	3	602	CLA	C4D-ND	-3.11	1.33	1.37
22	A	814	CLA	CHC-C1C	3.11	1.43	1.35
22	B	837	CLA	CHC-C1C	3.11	1.43	1.35
22	A	818	CLA	C4D-ND	-3.11	1.33	1.37
22	9	610	CLA	CHC-C1C	3.11	1.42	1.35
22	O	2002	CLA	CHC-C1C	3.11	1.42	1.35
22	U	610	CLA	CHC-C1C	3.11	1.42	1.35
22	A	810	CLA	CHC-C1C	3.11	1.42	1.35
22	7	614	CLA	CHC-C1C	3.11	1.42	1.35
22	B	802	CLA	CHC-C1C	3.11	1.42	1.35
22	K	206	CLA	CHC-C1C	3.10	1.42	1.35
22	B	829	CLA	C4D-ND	-3.10	1.33	1.37
22	A	830	CLA	CHC-C1C	3.10	1.42	1.35
22	A	837	CLA	CHC-C1C	3.10	1.42	1.35
21	6	602	CHL	C1D-C2D	3.10	1.51	1.45
22	A	825	CLA	CHC-C1C	3.10	1.42	1.35
22	6	609	CLA	CHC-C1C	3.10	1.42	1.35
22	5	611	CLA	CHC-C1C	3.10	1.42	1.35
22	9	612	CLA	C4D-ND	-3.10	1.33	1.37
22	1	609	CLA	CHC-C1C	3.10	1.42	1.35
22	A	824	CLA	C4D-ND	-3.09	1.33	1.37
22	A	823	CLA	C4D-ND	-3.09	1.33	1.37
22	W	602	CLA	CHC-C1C	3.09	1.42	1.35
22	3	607	CLA	C4D-ND	-3.09	1.33	1.37
22	F	301	CLA	C4D-ND	-3.09	1.33	1.37
22	U	613	CLA	C4D-ND	-3.09	1.33	1.37
22	7	607	CLA	CHC-C1C	3.09	1.42	1.35
22	B	840	CLA	C4D-ND	-3.09	1.33	1.37
21	6	601	CHL	C1D-C2D	3.09	1.51	1.45
22	J	101	CLA	CHC-C1C	3.09	1.42	1.35
22	2	613	CLA	C4D-ND	-3.09	1.33	1.37
21	4	607	CHL	C1D-C2D	3.09	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	6	614	CLA	CHC-C1C	3.09	1.42	1.35
22	7	609	CLA	CHC-C1C	3.08	1.42	1.35
22	B	819	CLA	CHC-C1C	3.08	1.42	1.35
22	5	614	CLA	CHC-C1C	3.08	1.42	1.35
22	A	806	CLA	CHC-C1C	3.08	1.42	1.35
22	8	614	CLA	CHC-C1C	3.08	1.42	1.35
22	B	812	CLA	C4D-ND	-3.08	1.33	1.37
22	A	824	CLA	CHC-C1C	3.08	1.42	1.35
22	2	610	CLA	CHC-C1C	3.08	1.42	1.35
22	A	819	CLA	CHC-C1C	3.08	1.42	1.35
22	B	818	CLA	C4D-ND	-3.08	1.33	1.37
22	9	612	CLA	CHC-C1C	3.07	1.42	1.35
22	A	808	CLA	C4D-ND	-3.07	1.33	1.37
22	B	822	CLA	C4D-ND	-3.07	1.33	1.37
22	B	826	CLA	C4D-ND	-3.07	1.33	1.37
21	8	607	CHL	C1D-C2D	3.07	1.51	1.45
22	1	610	CLA	C4D-ND	-3.07	1.33	1.37
22	A	854	CLA	C4D-ND	-3.07	1.33	1.37
22	A	810	CLA	C4D-ND	-3.07	1.33	1.37
22	A	840	CLA	C4D-ND	-3.07	1.33	1.37
22	5	606	CLA	C4D-ND	-3.07	1.33	1.37
21	2	607	CHL	C1D-C2D	3.07	1.51	1.45
22	V	612	CLA	CHC-C1C	3.07	1.42	1.35
22	4	611	CLA	CHC-C1C	3.07	1.42	1.35
22	A	808	CLA	CHC-C1C	3.07	1.42	1.35
22	3	614	CLA	CHC-C1C	3.07	1.42	1.35
22	7	604	CLA	CHC-C1C	3.07	1.42	1.35
22	5	604	CLA	C4D-ND	-3.07	1.33	1.37
22	A	822	CLA	C4D-ND	-3.07	1.33	1.37
22	5	606	CLA	CHC-C1C	3.07	1.42	1.35
21	V	609	CHL	C1D-C2D	3.07	1.51	1.45
21	W	609	CHL	C1D-C2D	3.07	1.51	1.45
22	W	614	CLA	CHC-C1C	3.07	1.42	1.35
22	1	608	CLA	CHC-C1C	3.07	1.42	1.35
22	B	822	CLA	CHC-C1C	3.07	1.42	1.35
22	B	825	CLA	CHC-C1C	3.07	1.42	1.35
22	V	612	CLA	C4D-ND	-3.07	1.33	1.37
22	A	823	CLA	CHC-C1C	3.07	1.42	1.35
21	W	606	CHL	C1D-C2D	3.07	1.51	1.45
22	2	604	CLA	C4D-ND	-3.07	1.33	1.37
22	7	602	CLA	CHC-C1C	3.06	1.42	1.35
23	2	619	LUT	C8-C9	-3.06	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	602	CLA	C4D-ND	-3.06	1.33	1.37
22	3	606	CLA	CHC-C1C	3.06	1.42	1.35
22	U	611	CLA	CHC-C1C	3.06	1.42	1.35
22	1	613	CLA	C4D-ND	-3.06	1.33	1.37
22	O	2002	CLA	C4D-ND	-3.06	1.33	1.37
22	B	828	CLA	CHC-C1C	3.06	1.42	1.35
22	G	204	CLA	CHC-C1C	3.06	1.42	1.35
22	A	819	CLA	C4D-ND	-3.06	1.33	1.37
21	V	601	CHL	C1D-C2D	3.06	1.51	1.45
22	B	814	CLA	C4D-ND	-3.06	1.33	1.37
21	4	618	CHL	C1D-C2D	3.06	1.51	1.45
22	W	613	CLA	C4D-ND	-3.06	1.33	1.37
22	A	834	CLA	C4D-ND	-3.06	1.33	1.37
22	B	831	CLA	C4D-ND	-3.06	1.33	1.37
22	U	613	CLA	CHC-C1C	3.06	1.42	1.35
22	B	820	CLA	CHC-C1C	3.06	1.42	1.35
22	B	806	CLA	CHC-C1C	3.05	1.42	1.35
22	B	824	CLA	C4D-ND	-3.05	1.33	1.37
22	A	815	CLA	CHC-C1C	3.05	1.42	1.35
21	2	618	CHL	C1D-C2D	3.05	1.51	1.45
22	B	818	CLA	CHC-C1C	3.05	1.42	1.35
22	7	602	CLA	C4D-ND	-3.05	1.33	1.37
22	A	842	CLA	CHC-C1C	3.05	1.42	1.35
22	6	604	CLA	CHC-C1C	3.05	1.42	1.35
22	A	806	CLA	C4D-ND	-3.05	1.33	1.37
22	B	805	CLA	C4D-ND	-3.05	1.33	1.37
22	K	203	CLA	C4D-ND	-3.05	1.33	1.37
22	U	604	CLA	CHC-C1C	3.05	1.42	1.35
22	V	614	CLA	CHC-C1C	3.05	1.42	1.35
22	2	614	CLA	C4D-ND	-3.05	1.33	1.37
22	A	831	CLA	C4D-ND	-3.05	1.33	1.37
22	B	817	CLA	C4D-ND	-3.05	1.33	1.37
22	B	836	CLA	CHC-C1C	3.05	1.42	1.35
22	1	608	CLA	C4D-ND	-3.05	1.33	1.37
22	A	805	CLA	C4D-ND	-3.05	1.33	1.37
22	B	815	CLA	C4D-ND	-3.05	1.33	1.37
22	B	805	CLA	CHC-C1C	3.05	1.42	1.35
22	4	603	CLA	CHC-C1C	3.05	1.42	1.35
22	A	816	CLA	C4D-ND	-3.04	1.33	1.37
22	V	610	CLA	CHC-C1C	3.04	1.42	1.35
22	B	838	CLA	CHC-C1C	3.04	1.42	1.35
22	B	807	CLA	C4D-ND	-3.04	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	L	304	CLA	C4D-ND	-3.04	1.33	1.37
22	B	825	CLA	C4D-ND	-3.04	1.33	1.37
22	B	809	CLA	CHC-C1C	3.04	1.42	1.35
22	W	610	CLA	CHC-C1C	3.04	1.42	1.35
22	B	821	CLA	CHC-C1C	3.04	1.42	1.35
22	4	609	CLA	C4D-ND	-3.04	1.33	1.37
22	A	854	CLA	CHC-C1C	3.04	1.42	1.35
22	B	815	CLA	CHC-C1C	3.04	1.42	1.35
22	B	837	CLA	C4D-ND	-3.04	1.33	1.37
22	L	303	CLA	C4D-ND	-3.04	1.33	1.37
22	1	602	CLA	CHC-C1C	3.04	1.42	1.35
22	B	807	CLA	CHC-C1C	3.04	1.42	1.35
22	A	833	CLA	CHC-C1C	3.04	1.42	1.35
22	A	834	CLA	CHC-C1C	3.04	1.42	1.35
22	G	203	CLA	CHC-C1C	3.04	1.42	1.35
22	1	604	CLA	CHC-C1C	3.04	1.42	1.35
22	3	614	CLA	C4D-ND	-3.04	1.33	1.37
22	V	604	CLA	CHC-C1C	3.03	1.42	1.35
22	5	616	CLA	CHC-C1C	3.03	1.42	1.35
22	9	603	CLA	C4D-ND	-3.03	1.33	1.37
22	3	613	CLA	CHC-C1C	3.03	1.42	1.35
22	K	203	CLA	CHC-C1C	3.03	1.42	1.35
22	4	609	CLA	CHC-C1C	3.03	1.42	1.35
22	B	834	CLA	CHC-C1C	3.03	1.42	1.35
22	7	615	CLA	CHC-C1C	3.03	1.42	1.35
21	W	605	CHL	C1D-C2D	3.03	1.51	1.45
22	A	830	CLA	C4D-ND	-3.03	1.33	1.37
22	3	611	CLA	CHC-C1C	3.03	1.42	1.35
22	V	611	CLA	C4D-ND	-3.03	1.33	1.37
22	A	817	CLA	C4D-ND	-3.03	1.33	1.37
22	5	603	CLA	C4D-ND	-3.03	1.33	1.37
22	4	602	CLA	CHC-C1C	3.03	1.42	1.35
22	5	602	CLA	CHC-C1C	3.03	1.42	1.35
22	A	838	CLA	CHC-C1C	3.03	1.42	1.35
22	A	813	CLA	CHC-C1C	3.03	1.42	1.35
21	5	607	CHL	C1D-C2D	3.03	1.51	1.45
22	A	839	CLA	C4D-ND	-3.03	1.33	1.37
22	5	610	CLA	CHC-C1C	3.03	1.42	1.35
22	A	841	CLA	C4D-ND	-3.03	1.33	1.37
22	4	601	CLA	CHC-C1C	3.02	1.42	1.35
22	A	809	CLA	CHC-C1C	3.02	1.42	1.35
22	4	602	CLA	C4D-ND	-3.02	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	610	CLA	CHC-C1C	3.02	1.42	1.35
22	B	808	CLA	C4D-ND	-3.02	1.33	1.37
22	W	612	CLA	C4D-ND	-3.02	1.33	1.37
22	L	302	CLA	CHC-C1C	3.02	1.42	1.35
22	8	604	CLA	CHC-C1C	3.02	1.42	1.35
22	9	613	CLA	CHC-C1C	3.02	1.42	1.35
22	B	836	CLA	C4D-ND	-3.02	1.33	1.37
22	8	611	CLA	C4D-ND	-3.02	1.33	1.37
22	9	610	CLA	C4D-ND	-3.02	1.33	1.37
22	4	613	CLA	C4D-ND	-3.02	1.33	1.37
22	A	811	CLA	CHC-C1C	3.02	1.42	1.35
22	H	201	CLA	CHC-C1C	3.02	1.42	1.35
22	A	802	CLA	C4D-ND	-3.02	1.33	1.37
22	8	612	CLA	CHC-C1C	3.02	1.42	1.35
22	1	603	CLA	CHC-C1C	3.02	1.42	1.35
22	1	614	CLA	CHC-C1C	3.01	1.42	1.35
22	B	804	CLA	C4D-ND	-3.01	1.33	1.37
22	8	603	CLA	CHC-C1C	3.01	1.42	1.35
22	A	815	CLA	C4D-ND	-3.01	1.33	1.37
22	B	832	CLA	CHC-C1C	3.01	1.42	1.35
22	2	611	CLA	C4D-ND	-3.01	1.33	1.37
22	F	303	CLA	C4D-ND	-3.01	1.33	1.37
22	W	603	CLA	CHC-C1C	3.01	1.42	1.35
22	2	603	CLA	CHC-C1C	3.01	1.42	1.35
21	U	609	CHL	C1D-C2D	3.01	1.51	1.45
22	7	606	CLA	C4D-ND	-3.01	1.33	1.37
22	A	817	CLA	CHC-C1C	3.01	1.42	1.35
22	A	842	CLA	C4D-ND	-3.01	1.33	1.37
22	6	610	CLA	C4D-ND	-3.01	1.33	1.37
22	5	604	CLA	CHC-C1C	3.01	1.42	1.35
21	8	618	CHL	C1D-C2D	3.00	1.51	1.45
22	B	841	CLA	C4D-ND	-3.00	1.33	1.37
22	V	602	CLA	C4D-ND	-3.00	1.33	1.37
22	A	825	CLA	C4D-ND	-3.00	1.33	1.37
22	A	827	CLA	CHC-C1C	3.00	1.42	1.35
22	7	612	CLA	CHC-C1C	3.00	1.42	1.35
21	9	607	CHL	C1D-C2D	3.00	1.51	1.45
22	1	612	CLA	CHC-C1C	3.00	1.42	1.35
22	3	604	CLA	C4D-ND	-3.00	1.33	1.37
22	A	826	CLA	C4D-ND	-3.00	1.33	1.37
22	B	828	CLA	C4D-ND	-3.00	1.33	1.37
22	B	839	CLA	C4D-ND	-3.00	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	7	614	CLA	C4D-ND	-3.00	1.33	1.37
21	V	605	CHL	C1D-C2D	3.00	1.51	1.45
22	7	613	CLA	C4D-ND	-3.00	1.33	1.37
22	B	810	CLA	CHC-C1C	3.00	1.42	1.35
22	7	610	CLA	C4D-ND	-3.00	1.33	1.37
22	B	812	CLA	CHC-C1C	3.00	1.42	1.35
22	A	837	CLA	C4D-ND	-3.00	1.33	1.37
21	2	601	CHL	C1D-C2D	3.00	1.51	1.45
22	2	609	CLA	CHC-C1C	3.00	1.42	1.35
22	B	808	CLA	CHC-C1C	3.00	1.42	1.35
22	B	827	CLA	CHC-C1C	2.99	1.42	1.35
22	F	301	CLA	CHC-C1C	2.99	1.42	1.35
21	2	608	CHL	C1D-C2D	2.99	1.51	1.45
22	9	602	CLA	C4D-ND	-2.99	1.33	1.37
22	B	824	CLA	CHC-C1C	2.99	1.42	1.35
22	B	833	CLA	C4D-ND	-2.99	1.33	1.37
22	6	604	CLA	C4D-ND	-2.99	1.33	1.37
22	G	201	CLA	CHC-C1C	2.99	1.42	1.35
22	A	804	CLA	CHC-C1C	2.99	1.42	1.35
22	B	827	CLA	C4D-ND	-2.99	1.33	1.37
22	6	611	CLA	CHC-C1C	2.99	1.42	1.35
22	7	617	CLA	C4D-ND	-2.99	1.33	1.37
22	8	612	CLA	C4D-ND	-2.99	1.33	1.37
22	A	832	CLA	C4D-ND	-2.99	1.33	1.37
22	8	601	CLA	CHC-C1C	2.99	1.42	1.35
21	4	608	CHL	C1D-C2D	2.99	1.51	1.45
21	U	608	CHL	C1D-C2D	2.99	1.51	1.45
22	B	820	CLA	C4D-ND	-2.98	1.33	1.37
22	A	820	CLA	CHC-C1C	2.98	1.42	1.35
22	A	821	CLA	CHC-C1C	2.98	1.42	1.35
22	4	610	CLA	CHC-C1C	2.98	1.42	1.35
22	K	201	CLA	CHC-C1C	2.98	1.42	1.35
22	7	606	CLA	CHC-C1C	2.98	1.42	1.35
22	3	611	CLA	C4D-ND	-2.98	1.33	1.37
22	5	608	CLA	CHC-C1C	2.98	1.42	1.35
22	5	611	CLA	C4D-ND	-2.98	1.33	1.37
22	4	601	CLA	C4D-ND	-2.98	1.33	1.37
22	4	604	CLA	C4D-ND	-2.98	1.33	1.37
22	9	602	CLA	CHC-C1C	2.98	1.42	1.35
21	U	601	CHL	C1D-C2D	2.98	1.51	1.45
21	U	605	CHL	C1D-C2D	2.98	1.51	1.45
21	W	601	CHL	C1D-C2D	2.98	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	W	604	CLA	CHC-C1C	2.98	1.42	1.35
22	A	813	CLA	C4D-ND	-2.98	1.33	1.37
22	1	613	CLA	CHC-C1C	2.98	1.42	1.35
22	V	614	CLA	C4D-ND	-2.98	1.33	1.37
21	W	608	CHL	C1D-C2D	2.98	1.51	1.45
22	G	201	CLA	C4D-ND	-2.98	1.33	1.37
22	3	606	CLA	C4D-ND	-2.97	1.33	1.37
22	A	812	CLA	CHC-C1C	2.97	1.42	1.35
22	B	816	CLA	CHC-C1C	2.97	1.42	1.35
22	1	614	CLA	C4D-ND	-2.97	1.33	1.37
22	3	603	CLA	CHC-C1C	2.97	1.42	1.35
22	2	614	CLA	CHC-C1C	2.97	1.42	1.35
22	4	612	CLA	C4D-ND	-2.97	1.33	1.37
22	6	611	CLA	C4D-ND	-2.97	1.33	1.37
22	U	610	CLA	C4D-ND	-2.97	1.33	1.37
22	A	822	CLA	CHC-C1C	2.97	1.42	1.35
22	B	813	CLA	C4D-ND	-2.97	1.33	1.37
22	8	610	CLA	C4D-ND	-2.97	1.33	1.37
21	6	618	CHL	C1D-C2D	2.97	1.51	1.45
22	7	615	CLA	C4D-ND	-2.97	1.33	1.37
22	F	303	CLA	CHC-C1C	2.97	1.42	1.35
22	5	603	CLA	CHC-C1C	2.97	1.42	1.35
22	5	602	CLA	C4D-ND	-2.97	1.33	1.37
21	6	607	CHL	C1D-C2D	2.97	1.51	1.45
22	1	616	CLA	CHC-C1C	2.97	1.42	1.35
22	3	612	CLA	C4D-ND	-2.97	1.33	1.37
22	V	613	CLA	C4D-ND	-2.96	1.33	1.37
21	6	606	CHL	C1D-C2D	2.96	1.51	1.45
22	A	839	CLA	CHC-C1C	2.96	1.42	1.35
21	8	606	CHL	C1D-C2D	2.96	1.51	1.45
22	V	603	CLA	CHC-C1C	2.96	1.42	1.35
22	K	204	CLA	CHC-C1C	2.96	1.42	1.35
21	9	606	CHL	C1D-C2D	2.96	1.51	1.45
22	B	810	CLA	C4D-ND	-2.96	1.33	1.37
22	W	610	CLA	C4D-ND	-2.96	1.33	1.37
22	B	839	CLA	CHC-C1C	2.96	1.42	1.35
22	A	845	CLA	CHC-C1C	2.96	1.42	1.35
22	V	604	CLA	C4D-ND	-2.96	1.33	1.37
22	A	843	CLA	C4D-ND	-2.96	1.33	1.37
22	G	203	CLA	C4D-ND	-2.96	1.33	1.37
22	A	828	CLA	C4D-ND	-2.96	1.33	1.37
22	U	614	CLA	CHC-C1C	2.96	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	807	CLA	CHC-C1C	2.96	1.42	1.35
22	B	809	CLA	C4D-ND	-2.96	1.33	1.37
22	B	816	CLA	C4D-ND	-2.96	1.33	1.37
22	4	613	CLA	CHC-C1C	2.96	1.42	1.35
22	8	604	CLA	C4D-ND	-2.95	1.33	1.37
22	2	612	CLA	CHC-C1C	2.95	1.42	1.35
22	5	609	CLA	CHC-C1C	2.95	1.42	1.35
22	4	614	CLA	C4D-ND	-2.95	1.33	1.37
22	A	818	CLA	CHC-C1C	2.95	1.42	1.35
22	A	835	CLA	CHC-C1C	2.95	1.42	1.35
22	B	841	CLA	CHC-C1C	2.95	1.42	1.35
22	U	602	CLA	C4D-ND	-2.95	1.33	1.37
21	1	601	CHL	C1D-C2D	2.95	1.51	1.45
22	A	831	CLA	CHC-C1C	2.95	1.42	1.35
22	B	804	CLA	CHC-C1C	2.94	1.42	1.35
22	W	602	CLA	C4D-ND	-2.94	1.33	1.37
22	A	826	CLA	CHC-C1C	2.94	1.42	1.35
22	A	804	CLA	C4D-ND	-2.94	1.33	1.37
22	B	840	CLA	CHC-C1C	2.94	1.42	1.35
22	A	836	CLA	C4C-C3C	2.94	1.46	1.41
21	2	606	CHL	C1D-C2D	2.94	1.51	1.45
21	W	607	CHL	C1D-C2D	2.94	1.51	1.45
22	W	613	CLA	CHC-C1C	2.94	1.42	1.35
22	6	610	CLA	CHC-C1C	2.94	1.42	1.35
21	V	607	CHL	C1D-C2D	2.94	1.51	1.45
22	J	101	CLA	C4D-ND	-2.94	1.33	1.37
22	O	2001	CLA	C4D-ND	-2.94	1.33	1.37
22	9	613	CLA	C4D-ND	-2.94	1.33	1.37
22	9	604	CLA	C4D-ND	-2.94	1.33	1.37
22	A	836	CLA	C3B-CAB	-2.94	1.44	1.48
22	8	613	CLA	C4D-ND	-2.94	1.33	1.37
21	2	602	CHL	C1D-C2D	2.94	1.51	1.45
22	A	801	CLA	CHC-C1C	2.94	1.42	1.35
22	G	204	CLA	C4D-ND	-2.94	1.33	1.37
22	L	302	CLA	C4D-ND	-2.93	1.33	1.37
22	W	603	CLA	C4D-ND	-2.93	1.33	1.37
22	B	831	CLA	CHC-C1C	2.93	1.42	1.35
22	B	835	CLA	CHC-C1C	2.93	1.42	1.35
22	3	613	CLA	C4D-ND	-2.93	1.33	1.37
22	W	612	CLA	CHC-C1C	2.93	1.42	1.35
22	U	612	CLA	CHC-C1C	2.93	1.42	1.35
22	B	832	CLA	C4D-ND	-2.93	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	814	CLA	C4D-ND	-2.93	1.33	1.37
22	3	604	CLA	CHC-C1C	2.93	1.42	1.35
22	W	611	CLA	C4D-ND	-2.93	1.33	1.37
22	U	611	CLA	C4D-ND	-2.93	1.33	1.37
21	5	601	CHL	C1D-C2D	2.93	1.51	1.45
22	B	834	CLA	C4D-ND	-2.93	1.33	1.37
22	5	614	CLA	C4D-ND	-2.93	1.33	1.37
22	B	829	CLA	CHC-C1C	2.93	1.42	1.35
22	3	615	CLA	C4D-ND	-2.92	1.33	1.37
21	8	608	CHL	C1D-C2D	2.92	1.51	1.45
22	W	604	CLA	C4D-ND	-2.92	1.33	1.37
22	A	829	CLA	CHC-C1C	2.92	1.42	1.35
22	K	204	CLA	C4D-ND	-2.92	1.33	1.37
22	9	603	CLA	CHC-C1C	2.92	1.42	1.35
22	1	606	CLA	C4D-ND	-2.92	1.33	1.37
21	V	608	CHL	C1D-C2D	2.92	1.51	1.45
22	8	602	CLA	CHC-C1C	2.92	1.42	1.35
22	A	845	CLA	C4D-ND	-2.92	1.33	1.37
21	V	606	CHL	C1D-C2D	2.92	1.51	1.45
22	V	610	CLA	C4D-ND	-2.92	1.33	1.37
22	A	816	CLA	CHC-C1C	2.92	1.42	1.35
22	B	823	CLA	C4D-ND	-2.92	1.33	1.37
22	A	827	CLA	C4D-ND	-2.92	1.33	1.37
21	1	607	CHL	C1D-C2D	2.92	1.51	1.45
22	5	612	CLA	C4D-ND	-2.91	1.33	1.37
22	H	201	CLA	C4D-ND	-2.91	1.33	1.37
22	7	604	CLA	C4D-ND	-2.91	1.33	1.37
21	6	608	CHL	C1D-C2D	2.91	1.51	1.45
21	U	606	CHL	C1D-C2D	2.91	1.51	1.45
22	3	603	CLA	C4D-ND	-2.91	1.33	1.37
22	B	802	CLA	C4D-ND	-2.91	1.33	1.37
22	L	304	CLA	CHC-C1C	2.91	1.42	1.35
22	4	612	CLA	CHC-C1C	2.91	1.42	1.35
22	U	603	CLA	CHC-C1C	2.91	1.42	1.35
22	B	833	CLA	CHC-C1C	2.91	1.42	1.35
22	B	803	CLA	C4D-ND	-2.91	1.33	1.37
22	5	612	CLA	CHC-C1C	2.90	1.42	1.35
22	5	610	CLA	C4D-ND	-2.90	1.33	1.37
22	8	602	CLA	C4D-ND	-2.90	1.33	1.37
22	3	612	CLA	CHC-C1C	2.90	1.42	1.35
22	6	603	CLA	C4D-ND	-2.90	1.33	1.37
21	7	608	CHL	C1D-C2D	2.90	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	8	603	CLA	C4D-ND	-2.89	1.33	1.37
22	W	614	CLA	C4D-ND	-2.89	1.33	1.37
22	1	604	CLA	C4D-ND	-2.89	1.33	1.37
21	9	601	CHL	C1D-C2D	2.89	1.51	1.45
22	9	611	CLA	C4D-ND	-2.89	1.33	1.37
22	1	616	CLA	C4D-ND	-2.89	1.33	1.37
21	2	602	CHL	C4B-CHC	2.89	1.49	1.41
22	U	612	CLA	C4D-ND	-2.89	1.33	1.37
22	A	838	CLA	C4D-ND	-2.89	1.33	1.37
21	V	606	CHL	C3D-C2D	2.89	1.47	1.39
22	8	613	CLA	CHC-C1C	2.89	1.42	1.35
22	A	835	CLA	C4D-ND	-2.88	1.33	1.37
22	K	206	CLA	C4D-ND	-2.88	1.33	1.37
22	7	613	CLA	CHC-C1C	2.88	1.42	1.35
22	2	603	CLA	C4D-ND	-2.88	1.33	1.37
22	3	610	CLA	C4D-ND	-2.88	1.33	1.37
22	A	802	CLA	CHC-C1C	2.88	1.42	1.35
22	U	614	CLA	C4D-ND	-2.88	1.33	1.37
22	8	609	CLA	C4D-ND	-2.88	1.33	1.37
21	9	608	CHL	C1D-C2D	2.88	1.51	1.45
22	V	613	CLA	CHC-C1C	2.88	1.42	1.35
22	O	2003	CLA	C4D-ND	-2.87	1.33	1.37
22	B	811	CLA	C4D-ND	-2.87	1.33	1.37
22	2	613	CLA	CHC-C1C	2.87	1.42	1.35
22	2	610	CLA	C4D-ND	-2.87	1.33	1.37
22	8	614	CLA	C4D-ND	-2.87	1.33	1.37
22	A	803	CLA	CHC-C1C	2.86	1.42	1.35
22	A	829	CLA	C4D-ND	-2.86	1.33	1.37
22	7	607	CLA	C4D-ND	-2.86	1.33	1.37
22	1	609	CLA	C4D-ND	-2.86	1.33	1.37
21	U	607	CHL	C1D-C2D	2.86	1.51	1.45
22	4	603	CLA	C4D-ND	-2.86	1.33	1.37
22	V	603	CLA	C4D-ND	-2.86	1.33	1.37
22	5	608	CLA	C4D-ND	-2.86	1.33	1.37
22	3	609	CLA	CHC-C1C	2.86	1.42	1.35
22	1	612	CLA	C4D-ND	-2.86	1.33	1.37
22	3	617	CLA	C3B-CAB	-2.85	1.44	1.48
22	2	609	CLA	C4D-ND	-2.85	1.33	1.37
22	A	840	CLA	CHC-C1C	2.85	1.42	1.35
22	2	604	CLA	CHC-C1C	2.85	1.42	1.35
22	7	611	CLA	C4D-ND	-2.84	1.33	1.37
21	9	607	CHL	C3D-C2D	2.84	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	7	612	CLA	C4D-ND	-2.84	1.33	1.37
22	4	611	CLA	C4D-ND	-2.83	1.33	1.37
21	4	606	CHL	C1D-C2D	2.83	1.50	1.45
22	1	611	CLA	C4D-ND	-2.83	1.33	1.37
22	6	609	CLA	C4D-ND	-2.83	1.33	1.37
21	4	618	CHL	C3D-C2D	2.83	1.46	1.39
22	6	612	CLA	C4D-ND	-2.82	1.33	1.37
22	U	604	CLA	C4D-ND	-2.82	1.33	1.37
22	K	201	CLA	C4D-ND	-2.82	1.33	1.37
22	1	603	CLA	C4D-ND	-2.82	1.33	1.37
22	5	616	CLA	C4D-ND	-2.82	1.33	1.37
22	7	603	CLA	C4D-ND	-2.80	1.33	1.37
22	6	612	CLA	CHC-C1C	2.80	1.42	1.35
22	6	614	CLA	C4D-ND	-2.80	1.33	1.37
22	A	801	CLA	C4D-ND	-2.80	1.33	1.37
21	3	608	CHL	C1D-C2D	2.79	1.50	1.45
22	2	612	CLA	C4D-ND	-2.79	1.33	1.37
22	6	613	CLA	CHC-C1C	2.79	1.42	1.35
22	5	613	CLA	CHC-C1C	2.79	1.42	1.35
21	6	618	CHL	C3D-C2D	2.79	1.46	1.39
22	U	603	CLA	C4D-ND	-2.79	1.33	1.37
21	2	602	CHL	MG-NA	-2.78	1.99	2.06
21	2	602	CHL	C3D-C2D	2.77	1.46	1.39
21	4	607	CHL	C3D-C2D	2.76	1.46	1.39
21	W	605	CHL	C3D-C2D	2.76	1.46	1.39
21	5	607	CHL	C3D-C2D	2.76	1.46	1.39
21	5	601	CHL	C3D-C2D	2.75	1.46	1.39
21	9	607	CHL	MG-NA	-2.74	1.99	2.06
21	4	608	CHL	MG-NA	-2.74	1.99	2.06
22	A	821	CLA	CMB-C2B	-2.74	1.45	1.51
21	6	602	CHL	C3D-C2D	2.73	1.46	1.39
23	2	619	LUT	C28-C29	-2.72	1.40	1.45
21	U	605	CHL	C3D-C2D	2.72	1.46	1.39
22	9	613	CLA	CMB-C2B	-2.72	1.46	1.51
21	4	608	CHL	C3D-C2D	2.71	1.46	1.39
22	B	829	CLA	CMB-C2B	-2.71	1.46	1.51
21	8	618	CHL	C3D-C2D	2.71	1.46	1.39
21	V	607	CHL	C3D-C2D	2.70	1.46	1.39
21	U	607	CHL	C3D-C2D	2.70	1.46	1.39
22	L	302	CLA	CMB-C2B	-2.70	1.46	1.51
21	V	601	CHL	C3D-C2D	2.70	1.46	1.39
21	W	609	CHL	C3D-C2D	2.70	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	8	607	CHL	C3D-C2D	2.70	1.46	1.39
21	6	607	CHL	C3D-C2D	2.69	1.46	1.39
22	A	832	CLA	CMB-C2B	-2.69	1.46	1.51
22	B	830	CLA	CMB-C2B	-2.69	1.46	1.51
21	W	601	CHL	C3D-C2D	2.69	1.46	1.39
21	8	606	CHL	C3D-C2D	2.69	1.46	1.39
21	U	601	CHL	C3D-C2D	2.68	1.46	1.39
22	U	603	CLA	CMB-C2B	-2.68	1.46	1.51
21	2	608	CHL	C4B-CHC	2.68	1.48	1.41
21	U	606	CHL	C4B-CHC	2.67	1.48	1.41
21	4	606	CHL	C3D-C2D	2.67	1.46	1.39
22	W	611	CLA	CMB-C2B	-2.67	1.46	1.51
21	W	608	CHL	C3D-C2D	2.67	1.46	1.39
21	1	607	CHL	C4B-CHC	2.67	1.48	1.41
21	2	607	CHL	C3D-C2D	2.66	1.46	1.39
22	B	808	CLA	CMB-C2B	-2.66	1.46	1.51
21	W	601	CHL	MG-NA	-2.66	1.99	2.06
21	V	605	CHL	C3D-C2D	2.66	1.46	1.39
21	W	606	CHL	C3D-C2D	2.66	1.46	1.39
22	4	610	CLA	C4D-ND	-2.66	1.34	1.37
21	1	607	CHL	C3D-C2D	2.65	1.46	1.39
22	A	802	CLA	CMB-C2B	-2.65	1.46	1.51
22	A	836	CLA	C2C-C3C	2.65	1.39	1.34
21	1	601	CHL	C3D-C2D	2.65	1.46	1.39
21	9	605	CHL	C3D-C2D	2.65	1.46	1.39
21	V	601	CHL	C4C-C3C	2.65	1.49	1.45
21	U	608	CHL	C3D-C2D	2.65	1.46	1.39
22	5	613	CLA	CMB-C2B	-2.65	1.46	1.51
21	6	606	CHL	C3D-C2D	2.64	1.46	1.39
21	2	608	CHL	C3D-C2D	2.64	1.46	1.39
21	W	607	CHL	C3D-C2D	2.64	1.46	1.39
22	3	617	CLA	C4D-ND	-2.64	1.34	1.37
22	V	604	CLA	CMB-C2B	-2.64	1.46	1.51
22	A	822	CLA	CMB-C2B	-2.64	1.46	1.51
22	B	828	CLA	CMB-C2B	-2.64	1.46	1.51
21	2	606	CHL	C3D-C2D	2.64	1.46	1.39
22	O	2001	CLA	CAD-C3D	-2.64	1.45	1.50
22	5	613	CLA	C4D-ND	-2.63	1.34	1.37
22	3	609	CLA	CMB-C2B	-2.63	1.46	1.51
22	B	819	CLA	CMB-C2B	-2.63	1.46	1.51
21	6	618	CHL	C4C-C3C	2.63	1.49	1.45
22	3	617	CLA	CMC-C2C	-2.62	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	618	CHL	C3D-C2D	2.62	1.46	1.39
22	1	604	CLA	CMB-C2B	-2.62	1.46	1.51
22	3	609	CLA	C4D-ND	-2.62	1.34	1.37
21	U	606	CHL	C3D-C2D	2.62	1.46	1.39
21	V	609	CHL	C3D-C2D	2.62	1.46	1.39
21	5	607	CHL	C4B-CHC	2.62	1.48	1.41
21	V	608	CHL	C3D-C2D	2.61	1.46	1.39
23	5	617	LUT	C8-C9	-2.61	1.40	1.45
22	B	809	CLA	CMB-C2B	-2.61	1.46	1.51
22	9	609	CLA	C4C-C3C	2.61	1.49	1.45
21	3	608	CHL	MG-NA	-2.61	2.00	2.06
22	3	615	CLA	CMB-C2B	-2.61	1.46	1.51
21	9	608	CHL	C3D-C2D	2.61	1.46	1.39
22	A	826	CLA	CMB-C2B	-2.60	1.46	1.51
22	5	603	CLA	CMB-C2B	-2.60	1.46	1.51
22	8	613	CLA	CMB-C2B	-2.60	1.46	1.51
22	A	801	CLA	CMB-C2B	-2.60	1.46	1.51
22	F	304	CLA	CHC-C1C	2.59	1.41	1.35
21	2	601	CHL	C3D-C2D	2.59	1.46	1.39
21	2	618	CHL	C4B-CHC	2.59	1.48	1.41
21	V	609	CHL	MG-NA	-2.59	2.00	2.06
21	2	608	CHL	MG-NA	-2.59	2.00	2.06
22	A	811	CLA	CMB-C2B	-2.59	1.46	1.51
21	5	601	CHL	C4B-CHC	2.59	1.48	1.41
21	U	609	CHL	C3D-C2D	2.58	1.46	1.39
22	O	2003	CLA	CAD-C3D	-2.58	1.45	1.50
21	6	607	CHL	C4B-CHC	2.58	1.48	1.41
22	A	831	CLA	CMB-C2B	-2.58	1.46	1.51
21	1	607	CHL	MG-NA	-2.58	2.00	2.06
21	4	618	CHL	C4C-C3C	2.58	1.49	1.45
22	W	604	CLA	CMB-C2B	-2.58	1.46	1.51
22	9	610	CLA	CMB-C2B	-2.58	1.46	1.51
21	8	608	CHL	C3D-C2D	2.58	1.46	1.39
22	6	612	CLA	CMB-C2B	-2.58	1.46	1.51
21	8	607	CHL	C4B-CHC	2.58	1.48	1.41
22	7	613	CLA	CMB-C2B	-2.58	1.46	1.51
22	K	204	CLA	CMB-C2B	-2.57	1.46	1.51
22	B	824	CLA	CMB-C2B	-2.57	1.46	1.51
22	A	837	CLA	CMB-C2B	-2.57	1.46	1.51
22	B	816	CLA	CMB-C2B	-2.57	1.46	1.51
22	8	603	CLA	CMB-C2B	-2.57	1.46	1.51
22	B	811	CLA	CMB-C2B	-2.57	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	601	CHL	MG-NA	-2.57	2.00	2.06
21	2	607	CHL	C4B-CHC	2.57	1.48	1.41
21	6	601	CHL	C3D-C2D	2.57	1.46	1.39
22	4	610	CLA	CMB-C2B	-2.56	1.46	1.51
22	B	835	CLA	CMB-C2B	-2.56	1.46	1.51
22	4	613	CLA	CMB-C2B	-2.56	1.46	1.51
22	B	820	CLA	CMB-C2B	-2.56	1.46	1.51
22	1	613	CLA	CMB-C2B	-2.56	1.46	1.51
21	8	608	CHL	C4B-CHC	2.56	1.48	1.41
21	6	602	CHL	C4C-C3C	2.56	1.49	1.45
21	6	608	CHL	C3D-C2D	2.56	1.46	1.39
21	6	602	CHL	C4B-CHC	2.56	1.48	1.41
22	L	304	CLA	CMB-C2B	-2.55	1.46	1.51
22	B	832	CLA	CMB-C2B	-2.55	1.46	1.51
22	K	206	CLA	CMB-C2B	-2.55	1.46	1.51
22	2	604	CLA	CMB-C2B	-2.55	1.46	1.51
22	B	833	CLA	CMB-C2B	-2.55	1.46	1.51
21	9	601	CHL	C4C-C3C	2.55	1.49	1.45
21	9	607	CHL	C4B-CHC	2.55	1.48	1.41
21	2	601	CHL	C4B-CHC	2.55	1.48	1.41
21	W	609	CHL	C4C-C3C	2.55	1.49	1.45
21	2	607	CHL	MG-NA	-2.55	2.00	2.06
22	A	824	CLA	CMB-C2B	-2.54	1.46	1.51
22	1	603	CLA	CMB-C2B	-2.54	1.46	1.51
22	3	603	CLA	CMB-C2B	-2.54	1.46	1.51
22	A	840	CLA	CMB-C2B	-2.54	1.46	1.51
22	4	601	CLA	CMB-C2B	-2.54	1.46	1.51
22	A	803	CLA	CMB-C2B	-2.54	1.46	1.51
22	A	817	CLA	CMB-C2B	-2.54	1.46	1.51
21	2	606	CHL	C4B-CHC	2.53	1.48	1.41
21	6	601	CHL	C4B-CHC	2.53	1.48	1.41
22	2	611	CLA	CMB-C2B	-2.53	1.46	1.51
22	A	833	CLA	CMB-C2B	-2.53	1.46	1.51
22	3	604	CLA	CMB-C2B	-2.53	1.46	1.51
21	4	607	CHL	C4C-C3C	2.53	1.49	1.45
21	U	609	CHL	MG-NA	-2.53	2.00	2.06
21	4	607	CHL	C4B-CHC	2.53	1.48	1.41
22	B	812	CLA	CMB-C2B	-2.53	1.46	1.51
22	B	830	CLA	C3B-C2B	-2.53	1.36	1.40
22	9	603	CLA	CMB-C2B	-2.53	1.46	1.51
21	U	601	CHL	MG-NA	-2.53	2.00	2.06
21	1	601	CHL	C4B-CHC	2.53	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	842	CLA	CMB-C2B	-2.53	1.46	1.51
22	7	603	CLA	CMB-C2B	-2.53	1.46	1.51
21	8	618	CHL	C4C-C3C	2.53	1.49	1.45
22	W	613	CLA	CMB-C2B	-2.53	1.46	1.51
22	9	609	CLA	C3D-C2D	2.52	1.46	1.39
22	A	835	CLA	CMB-C2B	-2.52	1.46	1.51
21	8	606	CHL	C4B-CHC	2.52	1.48	1.41
22	8	602	CLA	CMB-C2B	-2.52	1.46	1.51
23	2	619	LUT	C12-C13	-2.52	1.40	1.45
22	A	812	CLA	CMB-C2B	-2.52	1.46	1.51
22	B	818	CLA	CMB-C2B	-2.52	1.46	1.51
22	8	610	CLA	CMB-C2B	-2.52	1.46	1.51
22	A	820	CLA	CMB-C2B	-2.52	1.46	1.51
22	2	614	CLA	CMB-C2B	-2.52	1.46	1.51
22	2	603	CLA	CMB-C2B	-2.52	1.46	1.51
22	3	610	CLA	CMB-C2B	-2.51	1.46	1.51
21	6	608	CHL	C4B-CHC	2.51	1.48	1.41
21	9	605	CHL	C4B-CHC	2.51	1.48	1.41
21	V	609	CHL	C4B-CHC	2.51	1.48	1.41
21	V	605	CHL	C4B-CHC	2.51	1.48	1.41
22	A	808	CLA	CMB-C2B	-2.51	1.46	1.51
22	9	609	CLA	C4B-CHC	2.51	1.48	1.41
22	9	604	CLA	CMB-C2B	-2.51	1.46	1.51
21	5	601	CHL	MG-NA	-2.51	2.00	2.06
22	B	815	CLA	CMB-C2B	-2.51	1.46	1.51
22	A	834	CLA	CMB-C2B	-2.50	1.46	1.51
22	B	822	CLA	CMB-C2B	-2.50	1.46	1.51
21	9	606	CHL	C3D-C2D	2.50	1.46	1.39
22	B	817	CLA	CMB-C2B	-2.50	1.46	1.51
22	B	840	CLA	CMB-C2B	-2.50	1.46	1.51
22	1	606	CLA	CMB-C2B	-2.50	1.46	1.51
22	1	609	CLA	CMB-C2B	-2.50	1.46	1.51
22	B	806	CLA	CMB-C2B	-2.50	1.46	1.51
22	B	807	CLA	CMB-C2B	-2.50	1.46	1.51
22	A	805	CLA	CMB-C2B	-2.50	1.46	1.51
22	B	826	CLA	CMB-C2B	-2.50	1.46	1.51
22	B	838	CLA	CMB-C2B	-2.50	1.46	1.51
21	V	609	CHL	C4C-C3C	2.50	1.49	1.45
22	G	203	CLA	CMB-C2B	-2.50	1.46	1.51
21	6	602	CHL	MG-NA	-2.49	2.00	2.06
22	U	604	CLA	CMB-C2B	-2.49	1.46	1.51
21	4	606	CHL	C4B-CHC	2.49	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	2	610	CLA	CMB-C2B	-2.49	1.46	1.51
22	V	613	CLA	CMB-C2B	-2.49	1.46	1.51
22	A	854	CLA	CMB-C2B	-2.49	1.46	1.51
22	6	604	CLA	CMB-C2B	-2.49	1.46	1.51
21	3	608	CHL	C3D-C2D	2.49	1.45	1.39
22	3	607	CLA	CMB-C2B	-2.49	1.46	1.51
21	U	607	CHL	C4C-C3C	2.49	1.49	1.45
22	A	827	CLA	CMB-C2B	-2.49	1.46	1.51
22	V	603	CLA	CMB-C2B	-2.49	1.46	1.51
22	B	810	CLA	CMB-C2B	-2.49	1.46	1.51
22	B	841	CLA	CMB-C2B	-2.49	1.46	1.51
21	U	601	CHL	C4C-C3C	2.49	1.49	1.45
22	J	101	CLA	CMB-C2B	-2.49	1.46	1.51
22	W	603	CLA	CMB-C2B	-2.49	1.46	1.51
22	F	301	CLA	CMB-C2B	-2.49	1.46	1.51
21	U	609	CHL	C4B-CHC	2.49	1.47	1.41
22	W	602	CLA	CMB-C2B	-2.49	1.46	1.51
21	6	606	CHL	C4B-CHC	2.48	1.47	1.41
22	U	612	CLA	CMB-C2B	-2.48	1.46	1.51
21	9	601	CHL	C4B-CHC	2.48	1.47	1.41
21	4	608	CHL	C1B-CHB	2.48	1.47	1.41
21	U	607	CHL	C4B-CHC	2.48	1.47	1.41
21	4	618	CHL	MG-NA	-2.48	2.00	2.06
21	6	601	CHL	MG-NA	-2.48	2.00	2.06
22	A	823	CLA	CMB-C2B	-2.48	1.46	1.51
22	A	841	CLA	CMB-C2B	-2.48	1.46	1.51
21	7	608	CHL	C4B-CHC	2.48	1.47	1.41
22	5	608	CLA	CMB-C2B	-2.48	1.46	1.51
22	A	804	CLA	CMB-C2B	-2.48	1.46	1.51
22	1	602	CLA	CMB-C2B	-2.48	1.46	1.51
22	A	843	CLA	CMB-C2B	-2.48	1.46	1.51
22	K	201	CLA	CMB-C2B	-2.48	1.46	1.51
21	4	607	CHL	MG-NA	-2.48	2.00	2.06
22	3	612	CLA	CMB-C2B	-2.48	1.46	1.51
22	A	836	CLA	CMB-C2B	-2.48	1.46	1.51
22	5	604	CLA	CMB-C2B	-2.48	1.46	1.51
22	A	828	CLA	CMB-C2B	-2.47	1.46	1.51
22	B	834	CLA	CMB-C2B	-2.47	1.46	1.51
22	G	201	CLA	CMB-C2B	-2.47	1.46	1.51
22	L	303	CLA	CMB-C2B	-2.47	1.46	1.51
22	B	831	CLA	CMB-C2B	-2.47	1.46	1.51
22	B	804	CLA	CMB-C2B	-2.47	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	2	613	CLA	CMB-C2B	-2.46	1.46	1.51
22	B	813	CLA	CMB-C2B	-2.46	1.46	1.51
22	A	839	CLA	CMB-C2B	-2.46	1.46	1.51
21	V	606	CHL	C4C-C3C	2.46	1.49	1.44
22	4	602	CLA	CMB-C2B	-2.46	1.46	1.51
22	4	603	CLA	CMB-C2B	-2.46	1.46	1.51
22	H	201	CLA	CMB-C2B	-2.46	1.46	1.51
22	7	611	CLA	CMB-C2B	-2.46	1.46	1.51
22	W	614	CLA	CMB-C2B	-2.46	1.46	1.51
22	5	609	CLA	CMB-C2B	-2.46	1.46	1.51
22	B	821	CLA	CMB-C2B	-2.46	1.46	1.51
21	W	606	CHL	C4C-C3C	2.46	1.49	1.44
22	3	614	CLA	CMB-C2B	-2.46	1.46	1.51
22	1	614	CLA	CMB-C2B	-2.46	1.46	1.51
22	A	845	CLA	CMB-C2B	-2.46	1.46	1.51
22	B	803	CLA	CMB-C2B	-2.46	1.46	1.51
22	2	612	CLA	CMB-C2B	-2.46	1.46	1.51
22	B	805	CLA	CMB-C2B	-2.46	1.46	1.51
22	5	606	CLA	CMB-C2B	-2.46	1.46	1.51
22	8	601	CLA	CMB-C2B	-2.46	1.46	1.51
22	8	611	CLA	CMB-C2B	-2.46	1.46	1.51
22	U	614	CLA	CMB-C2B	-2.45	1.46	1.51
22	6	610	CLA	CMB-C2B	-2.45	1.46	1.51
21	7	608	CHL	C3D-C2D	2.45	1.45	1.39
22	A	813	CLA	CMB-C2B	-2.45	1.46	1.51
22	5	616	CLA	CMB-C2B	-2.45	1.46	1.51
22	A	816	CLA	CMB-C2B	-2.45	1.46	1.51
22	8	609	CLA	CMB-C2B	-2.45	1.46	1.51
21	W	605	CHL	C4C-C3C	2.45	1.49	1.44
22	1	608	CLA	CMB-C2B	-2.45	1.46	1.51
22	A	818	CLA	CMB-C2B	-2.45	1.46	1.51
22	B	837	CLA	CMB-C2B	-2.45	1.46	1.51
22	4	612	CLA	CMB-C2B	-2.44	1.46	1.51
22	3	606	CLA	CMB-C2B	-2.44	1.46	1.51
22	U	602	CLA	CMB-C2B	-2.44	1.46	1.51
22	O	2002	CLA	CMB-C2B	-2.44	1.46	1.51
21	W	608	CHL	C1B-CHB	2.44	1.47	1.41
22	6	609	CLA	CMB-C2B	-2.44	1.46	1.51
21	6	608	CHL	C4C-C3C	2.44	1.49	1.45
22	V	612	CLA	CMB-C2B	-2.44	1.46	1.51
22	3	613	CLA	CMB-C2B	-2.44	1.46	1.51
22	A	819	CLA	CMB-C2B	-2.44	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	F	304	CLA	C3B-C2B	-2.44	1.37	1.40
22	A	825	CLA	CMB-C2B	-2.44	1.46	1.51
21	9	606	CHL	C4C-C3C	2.44	1.49	1.45
21	W	607	CHL	MG-NA	-2.44	2.00	2.06
22	B	839	CLA	CMB-C2B	-2.44	1.46	1.51
22	8	612	CLA	CMB-C2B	-2.44	1.46	1.51
22	9	612	CLA	CMB-C2B	-2.44	1.46	1.51
22	K	203	CLA	CMB-C2B	-2.44	1.46	1.51
22	5	612	CLA	CMB-C2B	-2.43	1.46	1.51
22	7	609	CLA	CMB-C2B	-2.43	1.46	1.51
22	7	602	CLA	CMB-C2B	-2.43	1.46	1.51
22	A	810	CLA	CMB-C2B	-2.43	1.46	1.51
21	V	606	CHL	MG-NA	-2.43	2.00	2.06
22	B	825	CLA	CMB-C2B	-2.43	1.46	1.51
22	6	611	CLA	CMB-C2B	-2.43	1.46	1.51
22	U	611	CLA	CMB-C2B	-2.43	1.46	1.51
21	2	606	CHL	MG-NA	-2.43	2.00	2.06
22	1	610	CLA	CMB-C2B	-2.43	1.46	1.51
22	V	610	CLA	CMB-C2B	-2.43	1.46	1.51
22	A	807	CLA	CMB-C2B	-2.43	1.46	1.51
22	A	809	CLA	CMB-C2B	-2.43	1.46	1.51
22	7	615	CLA	CMB-C2B	-2.43	1.46	1.51
22	2	609	CLA	CMB-C2B	-2.42	1.46	1.51
22	A	830	CLA	CMB-C2B	-2.42	1.46	1.51
21	8	618	CHL	C4B-CHC	2.42	1.47	1.41
22	A	815	CLA	CMB-C2B	-2.42	1.46	1.51
22	7	607	CLA	CMB-C2B	-2.42	1.46	1.51
23	2	619	LUT	C32-C33	-2.42	1.40	1.45
22	U	610	CLA	CMB-C2B	-2.42	1.46	1.51
22	1	616	CLA	CMB-C2B	-2.42	1.46	1.51
22	A	814	CLA	CMB-C2B	-2.42	1.46	1.51
21	W	606	CHL	MG-NA	-2.42	2.00	2.06
22	7	606	CLA	CMB-C2B	-2.42	1.46	1.51
22	8	614	CLA	CMB-C2B	-2.42	1.46	1.51
22	V	611	CLA	CMB-C2B	-2.42	1.46	1.51
22	G	204	CLA	CMB-C2B	-2.42	1.46	1.51
22	6	614	CLA	CMB-C2B	-2.42	1.46	1.51
21	V	601	CHL	MG-NA	-2.41	2.00	2.06
21	8	618	CHL	MG-NA	-2.41	2.00	2.06
22	F	304	CLA	CMB-C2B	-2.41	1.46	1.51
22	3	611	CLA	CMB-C2B	-2.41	1.46	1.51
22	9	611	CLA	CMB-C2B	-2.41	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	5	614	CLA	CMB-C2B	-2.41	1.46	1.51
22	B	814	CLA	CMB-C2B	-2.41	1.46	1.51
21	U	606	CHL	MG-NA	-2.41	2.00	2.06
22	4	614	CLA	CMB-C2B	-2.41	1.46	1.51
21	9	608	CHL	C4B-CHC	2.41	1.47	1.41
22	B	836	CLA	CMB-C2B	-2.41	1.46	1.51
25	V	2623	NEX	C7-C8	-2.41	1.28	1.32
22	5	611	CLA	CMB-C2B	-2.40	1.46	1.51
22	V	614	CLA	CMB-C2B	-2.40	1.46	1.51
22	1	611	CLA	CMB-C2B	-2.40	1.46	1.51
22	5	602	CLA	CMB-C2B	-2.40	1.46	1.51
21	V	607	CHL	MG-NA	-2.40	2.00	2.06
21	9	606	CHL	C4B-CHC	2.40	1.47	1.41
21	7	608	CHL	MG-NA	-2.40	2.00	2.06
21	U	609	CHL	C4C-C3C	2.40	1.49	1.45
22	F	303	CLA	CMB-C2B	-2.40	1.46	1.51
22	1	612	CLA	CMB-C2B	-2.40	1.46	1.51
22	F	304	CLA	C4D-C3D	-2.40	1.47	1.50
21	U	605	CHL	C4C-C3C	2.40	1.49	1.44
22	3	617	CLA	CMB-C2B	-2.40	1.46	1.51
22	9	602	CLA	CMB-C2B	-2.40	1.46	1.51
22	5	610	CLA	CMB-C2B	-2.40	1.46	1.51
22	7	604	CLA	CMB-C2B	-2.40	1.46	1.51
22	4	611	CLA	CMB-C2B	-2.39	1.46	1.51
21	6	618	CHL	MG-NA	-2.39	2.00	2.06
21	4	618	CHL	C1B-CHB	2.39	1.47	1.41
22	3	602	CLA	CMB-C2B	-2.39	1.46	1.51
21	5	607	CHL	MG-NA	-2.39	2.00	2.06
22	A	838	CLA	CMB-C2B	-2.39	1.46	1.51
22	6	613	CLA	CMB-C2B	-2.39	1.46	1.51
21	9	601	CHL	C3D-C2D	2.39	1.45	1.39
22	W	612	CLA	CMB-C2B	-2.39	1.46	1.51
22	B	827	CLA	CMB-C2B	-2.39	1.46	1.51
22	A	806	CLA	CMB-C2B	-2.39	1.46	1.51
22	4	609	CLA	CMB-C2B	-2.38	1.46	1.51
21	8	608	CHL	C4C-C3C	2.38	1.49	1.45
22	B	823	CLA	CMB-C2B	-2.38	1.46	1.51
22	1	606	CLA	C3B-C2B	-2.38	1.37	1.40
21	U	605	CHL	MG-NA	-2.38	2.00	2.06
21	2	618	CHL	MG-NA	-2.38	2.00	2.06
21	9	608	CHL	MG-NA	-2.38	2.00	2.06
22	F	304	CLA	MG-NA	2.38	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	8	608	CHL	MG-NA	-2.38	2.00	2.06
22	U	613	CLA	CMB-C2B	-2.38	1.46	1.51
22	6	603	CLA	CMB-C2B	-2.38	1.46	1.51
21	8	607	CHL	MG-NA	-2.37	2.00	2.06
22	A	829	CLA	CMB-C2B	-2.37	1.46	1.51
21	U	607	CHL	MG-NA	-2.37	2.00	2.06
21	W	605	CHL	MG-NA	-2.37	2.00	2.06
21	6	607	CHL	MG-NA	-2.37	2.00	2.06
22	7	617	CLA	CMB-C2B	-2.37	1.46	1.51
22	3	603	CLA	C3B-C2B	-2.37	1.37	1.40
21	9	607	CHL	C1B-CHB	2.36	1.47	1.41
22	1	611	CLA	CMC-C2C	-2.36	1.45	1.50
22	7	614	CLA	CMB-C2B	-2.36	1.46	1.51
22	5	609	CLA	C4D-ND	-2.36	1.34	1.37
21	7	608	CHL	C4C-C3C	2.36	1.49	1.45
21	U	608	CHL	MG-NA	-2.36	2.00	2.06
22	8	604	CLA	CMB-C2B	-2.35	1.46	1.51
21	W	608	CHL	C4C-C3C	2.35	1.49	1.44
21	W	605	CHL	C4B-CHC	2.35	1.47	1.41
22	9	609	CLA	MG-NA	-2.35	2.00	2.06
22	A	821	CLA	C3B-C2B	-2.35	1.37	1.40
23	5	617	LUT	C12-C13	-2.34	1.40	1.45
21	V	606	CHL	C1B-CHB	2.34	1.47	1.41
22	A	843	CLA	CMD-C2D	-2.34	1.45	1.50
21	W	609	CHL	MG-NA	-2.34	2.00	2.06
21	U	601	CHL	C4B-CHC	2.34	1.47	1.41
22	L	302	CLA	C3B-C2B	-2.34	1.37	1.40
22	7	610	CLA	CMB-C2B	-2.34	1.46	1.51
21	W	601	CHL	C4C-C3C	2.34	1.49	1.45
22	W	610	CLA	CMB-C2B	-2.34	1.46	1.51
21	2	618	CHL	C4C-C3C	2.34	1.49	1.45
21	6	618	CHL	C4B-CHC	2.34	1.47	1.41
21	2	608	CHL	C1B-CHB	2.34	1.47	1.41
22	B	802	CLA	CMB-C2B	-2.34	1.46	1.51
21	4	608	CHL	C4B-CHC	2.34	1.47	1.41
21	4	606	CHL	MG-NA	-2.33	2.00	2.06
22	7	612	CLA	CMB-C2B	-2.33	1.46	1.51
27	K	205	BCR	C30-C25	-2.33	1.50	1.53
21	6	608	CHL	MG-NA	-2.32	2.00	2.06
21	U	608	CHL	C4C-C3C	2.32	1.49	1.44
22	9	602	CLA	CMC-C2C	-2.32	1.45	1.50
21	V	605	CHL	MG-NA	-2.32	2.00	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	842	PQN	C11-C3	-2.31	1.47	1.51
21	9	605	CHL	MG-NA	-2.31	2.00	2.06
21	2	607	CHL	C4C-C3C	2.31	1.49	1.45
21	W	608	CHL	MG-NA	-2.31	2.00	2.06
21	8	607	CHL	C4C-C3C	2.31	1.49	1.45
21	V	609	CHL	C1B-CHB	2.31	1.47	1.41
21	9	608	CHL	C1B-CHB	2.31	1.47	1.41
21	4	618	CHL	C4B-CHC	2.31	1.47	1.41
22	V	602	CLA	CMB-C2B	-2.30	1.46	1.51
21	V	608	CHL	C4C-C3C	2.30	1.49	1.44
21	U	605	CHL	C4B-CHC	2.30	1.47	1.41
21	6	601	CHL	C1B-CHB	2.30	1.47	1.41
21	V	608	CHL	MG-NA	-2.30	2.00	2.06
21	U	601	CHL	C1B-CHB	2.30	1.47	1.41
22	A	835	CLA	C3B-C2B	-2.30	1.37	1.40
21	4	608	CHL	C4C-C3C	2.30	1.49	1.45
21	6	606	CHL	C4C-C3C	2.30	1.49	1.45
21	W	601	CHL	C4B-CHC	2.30	1.47	1.41
22	B	808	CLA	CMD-C2D	-2.30	1.45	1.50
22	5	613	CLA	C3B-C2B	-2.30	1.37	1.40
21	9	601	CHL	C1B-CHB	2.29	1.47	1.41
21	W	607	CHL	C1B-CHB	2.29	1.47	1.41
21	7	608	CHL	C1B-CHB	2.29	1.47	1.41
21	6	608	CHL	C1B-CHB	2.29	1.47	1.41
21	6	601	CHL	C4C-C3C	2.29	1.49	1.45
21	W	609	CHL	C1B-CHB	2.29	1.47	1.41
21	3	608	CHL	C1B-CHB	2.28	1.47	1.41
21	W	607	CHL	C4B-CHC	2.28	1.47	1.41
25	U	2623	NEX	O24-C25	-2.28	1.42	1.46
21	U	605	CHL	C1B-CHB	2.28	1.47	1.41
21	U	609	CHL	C1B-CHB	2.28	1.47	1.41
21	9	608	CHL	C4C-C3C	2.28	1.49	1.45
21	4	607	CHL	C1B-CHB	2.28	1.47	1.41
22	9	610	CLA	C3B-C2B	-2.28	1.37	1.40
21	W	605	CHL	C1B-CHB	2.27	1.47	1.41
21	6	606	CHL	C1B-CHB	2.27	1.47	1.41
21	5	607	CHL	C1B-CHB	2.27	1.47	1.41
21	6	607	CHL	C4C-C3C	2.27	1.49	1.45
21	6	606	CHL	MG-NA	-2.27	2.00	2.06
21	V	606	CHL	C4B-CHC	2.27	1.47	1.41
21	W	606	CHL	C4B-CHC	2.27	1.47	1.41
21	V	608	CHL	C1B-CHB	2.27	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	851	BCR	C1-C6	-2.27	1.50	1.53
21	W	601	CHL	C1B-CHB	2.27	1.47	1.41
21	2	601	CHL	C1B-CHB	2.27	1.47	1.41
22	3	607	CLA	C3B-C2B	-2.27	1.37	1.40
22	A	837	CLA	C3B-C2B	-2.27	1.37	1.40
21	W	606	CHL	C1B-CHB	2.26	1.47	1.41
21	5	607	CHL	C4C-C3C	2.26	1.48	1.45
21	8	606	CHL	C4C-C3C	2.26	1.48	1.45
22	7	609	CLA	C4D-ND	-2.26	1.34	1.37
21	V	605	CHL	C4C-C3C	2.26	1.48	1.45
21	1	607	CHL	C1B-CHB	2.26	1.47	1.41
21	2	607	CHL	C1B-CHB	2.26	1.47	1.41
21	4	606	CHL	C4C-C3C	2.26	1.48	1.45
21	5	601	CHL	C1B-CHB	2.26	1.47	1.41
21	V	601	CHL	C4B-CHC	2.26	1.47	1.41
22	B	808	CLA	C3B-C2B	-2.26	1.37	1.40
21	V	607	CHL	C4B-CHC	2.25	1.47	1.41
21	V	607	CHL	C1B-CHB	2.25	1.47	1.41
21	V	605	CHL	C1B-CHB	2.25	1.47	1.41
22	A	832	CLA	C3B-C2B	-2.25	1.37	1.40
22	B	817	CLA	C3B-CAB	-2.25	1.43	1.47
21	U	607	CHL	C1B-CHB	2.25	1.47	1.41
21	U	608	CHL	C1B-CHB	2.25	1.47	1.41
21	W	609	CHL	C4B-CHC	2.24	1.47	1.41
22	A	821	CLA	CMD-C2D	-2.24	1.46	1.50
21	9	605	CHL	C1B-CHB	2.24	1.47	1.41
21	2	608	CHL	C4C-C3C	2.24	1.48	1.45
21	2	601	CHL	MG-NA	-2.23	2.01	2.06
21	8	618	CHL	C1B-CHB	2.23	1.47	1.41
21	2	618	CHL	C1B-CHB	2.23	1.47	1.41
22	7	611	CLA	CMD-C2D	-2.23	1.46	1.50
22	9	611	CLA	C3B-C2B	-2.23	1.37	1.40
21	U	608	CHL	C4B-CHC	2.23	1.47	1.41
21	8	608	CHL	C1B-CHB	2.23	1.47	1.41
22	B	819	CLA	C3B-C2B	-2.23	1.37	1.40
22	B	838	CLA	C3B-C2B	-2.23	1.37	1.40
21	1	607	CHL	C4C-C3C	2.23	1.48	1.45
22	B	827	CLA	CMD-C2D	-2.23	1.46	1.50
22	5	611	CLA	CMD-C2D	-2.23	1.46	1.50
21	V	608	CHL	C4B-CHC	2.22	1.47	1.41
21	6	602	CHL	C1B-CHB	2.22	1.47	1.41
21	8	606	CHL	MG-NA	-2.22	2.01	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	9	609	CLA	C1B-CHB	2.22	1.47	1.41
22	A	840	CLA	C3B-C2B	-2.22	1.37	1.40
21	6	607	CHL	C1B-CHB	2.22	1.47	1.41
22	B	840	CLA	CMD-C2D	-2.22	1.46	1.50
22	2	612	CLA	C3B-C2B	-2.22	1.37	1.40
22	B	808	CLA	CMC-C2C	-2.21	1.46	1.50
22	W	611	CLA	CMD-C2D	-2.21	1.46	1.50
21	2	602	CHL	C1B-CHB	2.21	1.47	1.41
21	3	608	CHL	C4B-CHC	2.21	1.47	1.41
22	A	854	CLA	CMD-C2D	-2.21	1.46	1.50
22	A	801	CLA	CMD-C2D	-2.21	1.46	1.50
22	1	609	CLA	MG-NC	2.21	2.11	2.06
21	2	602	CHL	C2C-C1C	2.21	1.49	1.44
23	5	617	LUT	C28-C29	-2.21	1.41	1.45
21	V	607	CHL	C4C-C3C	2.20	1.48	1.44
22	7	609	CLA	C3B-C2B	-2.20	1.37	1.40
21	9	601	CHL	MG-NA	-2.20	2.01	2.06
21	6	618	CHL	C1B-CHB	2.20	1.47	1.41
22	B	832	CLA	C3B-C2B	-2.20	1.37	1.40
21	1	601	CHL	C1B-CHB	2.20	1.47	1.41
22	B	838	CLA	CMD-C2D	-2.20	1.46	1.50
21	2	601	CHL	C4C-C3C	2.19	1.48	1.45
22	A	830	CLA	C3B-CAB	-2.19	1.43	1.47
22	2	603	CLA	C3B-C2B	-2.19	1.37	1.40
21	8	607	CHL	C1B-CHB	2.19	1.47	1.41
21	W	607	CHL	C4C-C3C	2.19	1.48	1.44
22	9	609	CLA	C1C-C2C	2.19	1.48	1.44
22	9	603	CLA	C3B-C2B	-2.19	1.37	1.40
22	B	820	CLA	CMD-C2D	-2.19	1.46	1.50
22	6	612	CLA	C3B-C2B	-2.18	1.37	1.40
22	9	612	CLA	CMD-C2D	-2.18	1.46	1.50
22	A	830	CLA	CMD-C2D	-2.18	1.46	1.50
22	A	841	CLA	CMD-C2D	-2.18	1.46	1.50
22	V	614	CLA	CMD-C2D	-2.18	1.46	1.50
21	2	602	CHL	C4C-C3C	2.18	1.48	1.45
21	V	601	CHL	C1B-CHB	2.17	1.47	1.41
22	8	613	CLA	C3B-C2B	-2.17	1.37	1.40
28	G	202	LMG	O1-C1	2.17	1.43	1.40
22	A	810	CLA	C3B-C2B	-2.17	1.37	1.40
22	B	821	CLA	C3B-C2B	-2.17	1.37	1.40
22	7	603	CLA	C3B-C2B	-2.17	1.37	1.40
21	8	606	CHL	C1B-CHB	2.17	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	9	606	CHL	C1B-CHB	2.17	1.47	1.41
22	A	828	CLA	CMC-C2C	-2.17	1.46	1.50
22	1	606	CLA	C3B-CAB	-2.16	1.43	1.47
22	B	809	CLA	CMD-C2D	-2.16	1.46	1.50
22	B	825	CLA	CMD-C2D	-2.16	1.46	1.50
21	2	606	CHL	C1B-CHB	2.16	1.47	1.41
22	A	824	CLA	CMD-C2D	-2.16	1.46	1.50
22	U	602	CLA	C3B-C2B	-2.16	1.37	1.40
22	U	613	CLA	CMD-C2D	-2.16	1.46	1.50
23	3	618	LUT	C22-C21	-2.16	1.52	1.54
21	9	606	CHL	MG-NA	-2.16	2.01	2.06
22	3	610	CLA	C3B-C2B	-2.16	1.37	1.40
24	8	620	XAT	C12-C13	-2.16	1.41	1.45
22	5	612	CLA	CMD-C2D	-2.15	1.46	1.50
21	5	601	CHL	C4C-C3C	2.15	1.48	1.45
22	5	612	CLA	C3B-C2B	-2.15	1.37	1.40
22	A	808	CLA	C3B-C2B	-2.15	1.37	1.40
22	5	611	CLA	C3B-C2B	-2.15	1.37	1.40
22	B	811	CLA	C3B-C2B	-2.15	1.37	1.40
22	B	824	CLA	CMD-C2D	-2.15	1.46	1.50
22	4	604	CLA	CMB-C2B	-2.15	1.47	1.51
24	8	620	XAT	C8-C9	-2.14	1.41	1.45
22	B	802	CLA	CMD-C2D	-2.14	1.46	1.50
22	5	604	CLA	CMD-C2D	-2.14	1.46	1.50
21	U	606	CHL	C1B-CHB	2.14	1.46	1.41
22	7	609	CLA	C1B-NB	2.14	1.37	1.35
24	1	618	XAT	O4-C5	-2.14	1.43	1.46
22	B	814	CLA	CMD-C2D	-2.14	1.46	1.50
22	A	802	CLA	CMD-C2D	-2.14	1.46	1.50
22	3	606	CLA	CMD-C2D	-2.14	1.46	1.50
21	1	601	CHL	C4C-C3C	2.14	1.48	1.45
22	A	845	CLA	CMD-C2D	-2.13	1.46	1.50
22	U	603	CLA	C3B-C2B	-2.13	1.37	1.40
22	4	610	CLA	CMD-C2D	-2.13	1.46	1.50
22	B	817	CLA	C3B-C2B	-2.13	1.37	1.40
22	5	602	CLA	CMD-C2D	-2.13	1.46	1.50
23	5	617	LUT	C32-C33	-2.13	1.41	1.45
22	B	836	CLA	CMD-C2D	-2.12	1.46	1.50
22	L	304	CLA	C3B-C2B	-2.12	1.37	1.40
21	2	606	CHL	C4C-C3C	2.12	1.48	1.45
21	9	605	CHL	C4C-C3C	2.12	1.48	1.44
22	F	304	CLA	C2A-C3A	-2.12	1.54	1.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	809	CLA	C3B-C2B	-2.12	1.37	1.40
22	3	615	CLA	CMD-C2D	-2.12	1.46	1.50
21	W	608	CHL	C4B-CHC	2.12	1.46	1.41
22	1	609	CLA	C3B-C2B	-2.12	1.37	1.40
22	W	614	CLA	CMD-C2D	-2.12	1.46	1.50
21	8	606	CHL	C2C-C1C	2.12	1.49	1.44
22	8	610	CLA	C3B-C2B	-2.12	1.37	1.40
21	6	607	CHL	C2C-C1C	2.12	1.49	1.44
22	B	805	CLA	CMD-C2D	-2.12	1.46	1.50
22	3	617	CLA	C3B-C2B	-2.12	1.37	1.40
22	5	613	CLA	CMD-C2D	-2.12	1.46	1.50
22	9	611	CLA	CMD-C2D	-2.12	1.46	1.50
22	U	612	CLA	C3B-C2B	-2.12	1.37	1.40
22	B	819	CLA	CMD-C2D	-2.12	1.46	1.50
22	B	833	CLA	CMD-C2D	-2.11	1.46	1.50
24	3	619	XAT	O4-C5	-2.11	1.43	1.46
22	1	602	CLA	CMD-C2D	-2.11	1.46	1.50
22	A	803	CLA	C3B-CAB	-2.11	1.43	1.47
22	A	832	CLA	CMD-C2D	-2.11	1.46	1.50
22	F	304	CLA	C4B-CHC	-2.11	1.35	1.41
22	A	836	CLA	CMD-C2D	-2.11	1.46	1.50
22	U	610	CLA	CMD-C2D	-2.11	1.46	1.50
22	V	612	CLA	CMC-C2C	-2.11	1.46	1.50
22	B	818	CLA	C3B-CAB	-2.11	1.43	1.47
22	F	301	CLA	CMD-C2D	-2.11	1.46	1.50
22	7	609	CLA	MG-NC	2.10	2.11	2.06
22	A	835	CLA	CMD-C2D	-2.10	1.46	1.50
22	A	811	CLA	C3B-C2B	-2.10	1.37	1.40
22	3	609	CLA	C3B-C2B	-2.10	1.37	1.40
22	9	613	CLA	C3B-C2B	-2.10	1.37	1.40
22	7	613	CLA	C3B-C2B	-2.10	1.37	1.40
22	3	607	CLA	C3B-CAB	-2.10	1.43	1.47
21	U	606	CHL	C2C-C1C	2.10	1.49	1.44
22	B	806	CLA	C3B-C2B	-2.09	1.37	1.40
21	9	607	CHL	C4C-C3C	2.09	1.48	1.45
22	U	603	CLA	CMD-C2D	-2.09	1.46	1.50
22	1	613	CLA	CMD-C2D	-2.09	1.46	1.50
22	A	813	CLA	CMD-C2D	-2.09	1.46	1.50
21	3	608	CHL	C4C-C3C	2.09	1.48	1.45
21	8	607	CHL	C2C-C1C	2.09	1.49	1.44
22	9	612	CLA	CMC-C2C	-2.09	1.46	1.50
22	2	614	CLA	CMD-C2D	-2.09	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	834	CLA	CMD-C2D	-2.09	1.46	1.50
27	3	621	BCR	C30-C25	-2.09	1.50	1.53
25	U	2623	NEX	C1-C6	-2.09	1.51	1.54
22	H	201	CLA	C3B-C2B	-2.09	1.37	1.40
22	A	812	CLA	CMD-C2D	-2.09	1.46	1.50
22	B	829	CLA	CMD-C2D	-2.09	1.46	1.50
22	A	836	CLA	CAC-C3C	-2.09	1.47	1.51
22	A	834	CLA	CMD-C2D	-2.09	1.46	1.50
22	K	201	CLA	CMD-C2D	-2.09	1.46	1.50
21	5	607	CHL	C2C-C1C	2.09	1.49	1.44
22	A	826	CLA	CMD-C2D	-2.08	1.46	1.50
22	A	819	CLA	C3B-CAB	-2.08	1.43	1.47
22	B	823	CLA	CMD-C2D	-2.08	1.46	1.50
22	A	812	CLA	CMC-C2C	-2.08	1.46	1.50
22	8	602	CLA	C3B-C2B	-2.08	1.37	1.40
22	A	807	CLA	CMD-C2D	-2.08	1.46	1.50
22	B	828	CLA	CMD-C2D	-2.08	1.46	1.50
22	L	303	CLA	CMD-C2D	-2.08	1.46	1.50
22	A	839	CLA	CMD-C2D	-2.08	1.46	1.50
22	A	842	CLA	C3B-C2B	-2.08	1.37	1.40
24	2	620	XAT	O4-C5	-2.08	1.43	1.46
22	7	606	CLA	C3B-CAB	-2.08	1.43	1.47
22	2	610	CLA	CMD-C2D	-2.08	1.46	1.50
22	B	807	CLA	CMD-C2D	-2.08	1.46	1.50
22	V	604	CLA	C3B-C2B	-2.08	1.37	1.40
22	A	838	CLA	CMD-C2D	-2.08	1.46	1.50
22	W	612	CLA	CMC-C2C	-2.07	1.46	1.50
22	4	609	CLA	CMD-C2D	-2.07	1.46	1.50
21	4	606	CHL	C1B-CHB	2.07	1.46	1.41
22	3	609	CLA	CMD-C2D	-2.07	1.46	1.50
22	9	602	CLA	CMD-C2D	-2.07	1.46	1.50
22	6	603	CLA	CMD-C2D	-2.07	1.46	1.50
22	B	806	CLA	C3B-CAB	-2.07	1.43	1.47
22	A	802	CLA	C3B-C2B	-2.07	1.37	1.40
22	8	604	CLA	C3B-C2B	-2.07	1.37	1.40
22	A	829	CLA	CMD-C2D	-2.07	1.46	1.50
22	B	803	CLA	C3B-C2B	-2.07	1.37	1.40
22	L	303	CLA	C3B-C2B	-2.07	1.37	1.40
22	9	613	CLA	CMD-C2D	-2.07	1.46	1.50
22	1	612	CLA	CMD-C2D	-2.07	1.46	1.50
22	A	826	CLA	C3B-C2B	-2.07	1.37	1.40
22	5	612	CLA	CMC-C2C	-2.07	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	7	619	XAT	C8-C9	2.06	1.50	1.45
22	A	815	CLA	C3B-CAB	-2.06	1.43	1.47
22	U	614	CLA	C3B-C2B	-2.06	1.37	1.40
22	4	604	CLA	CMD-C2D	-2.06	1.46	1.50
22	A	806	CLA	CMD-C2D	-2.06	1.46	1.50
22	A	803	CLA	CMD-C2D	-2.06	1.46	1.50
22	B	837	CLA	CMD-C2D	-2.06	1.46	1.50
22	L	303	CLA	C3B-CAB	-2.06	1.43	1.47
22	V	613	CLA	C3B-C2B	-2.06	1.37	1.40
22	A	804	CLA	C3B-C2B	-2.06	1.37	1.40
22	4	611	CLA	CMD-C2D	-2.06	1.46	1.50
22	W	603	CLA	C3B-C2B	-2.06	1.37	1.40
22	A	812	CLA	C3B-C2B	-2.06	1.37	1.40
22	3	603	CLA	CMD-C2D	-2.06	1.46	1.50
22	A	822	CLA	CMD-C2D	-2.06	1.46	1.50
22	J	101	CLA	C3B-C2B	-2.06	1.37	1.40
22	5	609	CLA	C3B-C2B	-2.06	1.37	1.40
22	B	810	CLA	CMD-C2D	-2.06	1.46	1.50
22	B	811	CLA	CMD-C2D	-2.06	1.46	1.50
22	A	801	CLA	C3B-C2B	-2.05	1.37	1.40
22	A	822	CLA	C3B-C2B	-2.05	1.37	1.40
23	8	619	LUT	C22-C21	-2.05	1.52	1.54
22	1	610	CLA	C3B-C2B	-2.05	1.37	1.40
22	1	616	CLA	C3B-C2B	-2.05	1.37	1.40
22	2	613	CLA	C3B-C2B	-2.05	1.37	1.40
22	3	613	CLA	CMD-C2D	-2.05	1.46	1.50
22	B	838	CLA	C3B-CAB	-2.05	1.43	1.47
22	O	2003	CLA	C3C-C2C	2.05	1.39	1.35
22	W	613	CLA	C3B-C2B	-2.05	1.37	1.40
22	B	833	CLA	C3B-C2B	-2.05	1.37	1.40
22	A	814	CLA	CMC-C2C	-2.05	1.46	1.50
22	2	604	CLA	C3B-C2B	-2.05	1.37	1.40
22	F	304	CLA	MG-NC	2.05	2.11	2.06
22	A	818	CLA	CMD-C2D	-2.05	1.46	1.50
22	B	818	CLA	CMD-C2D	-2.05	1.46	1.50
21	V	605	CHL	C2C-C1C	2.05	1.49	1.44
21	1	607	CHL	C2C-C1C	2.05	1.49	1.44
22	9	604	CLA	C3B-C2B	-2.05	1.37	1.40
22	6	614	CLA	CMD-C2D	-2.05	1.46	1.50
22	8	601	CLA	CMD-C2D	-2.05	1.46	1.50
22	1	603	CLA	C3B-C2B	-2.05	1.37	1.40
22	G	201	CLA	C3B-C2B	-2.05	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	K	203	CLA	C3B-C2B	-2.05	1.37	1.40
22	8	611	CLA	C3B-C2B	-2.05	1.37	1.40
22	2	614	CLA	C3B-C2B	-2.05	1.37	1.40
22	5	609	CLA	C1B-NB	2.04	1.37	1.35
25	9	623	NEX	O24-C25	-2.04	1.43	1.46
22	3	611	CLA	C3B-C2B	-2.04	1.37	1.40
21	4	606	CHL	C2C-C1C	2.04	1.49	1.44
22	6	613	CLA	C4B-CHC	-2.04	1.35	1.41
22	B	841	CLA	CMD-C2D	-2.04	1.46	1.50
22	7	613	CLA	CMD-C2D	-2.04	1.46	1.50
22	A	811	CLA	CMD-C2D	-2.04	1.46	1.50
22	3	612	CLA	C3B-C2B	-2.04	1.37	1.40
22	9	612	CLA	C3B-C2B	-2.04	1.37	1.40
22	3	602	CLA	C3B-CAB	-2.04	1.43	1.47
22	K	206	CLA	C3B-C2B	-2.04	1.37	1.40
22	O	2001	CLA	C3C-C2C	2.04	1.39	1.35
22	8	609	CLA	CMC-C2C	-2.04	1.46	1.50
22	F	301	CLA	CMC-C2C	-2.04	1.46	1.50
22	A	815	CLA	CMD-C2D	-2.04	1.46	1.50
22	B	839	CLA	CMD-C2D	-2.04	1.46	1.50
22	K	204	CLA	CMD-C2D	-2.04	1.46	1.50
22	5	603	CLA	C3B-C2B	-2.04	1.37	1.40
22	W	613	CLA	CMD-C2D	-2.04	1.46	1.50
22	A	803	CLA	CMC-C2C	-2.04	1.46	1.50
22	1	612	CLA	C3B-C2B	-2.04	1.37	1.40
22	A	816	CLA	CMD-C2D	-2.04	1.46	1.50
21	5	601	CHL	C2C-C1C	2.04	1.48	1.44
22	4	612	CLA	CMC-C2C	-2.04	1.46	1.50
22	3	602	CLA	CMD-C2D	-2.04	1.46	1.50
22	B	802	CLA	CMC-C2C	-2.03	1.46	1.50
22	B	803	CLA	CMD-C2D	-2.03	1.46	1.50
22	A	803	CLA	C3B-C2B	-2.03	1.37	1.40
22	B	837	CLA	C3B-C2B	-2.03	1.37	1.40
22	3	614	CLA	CMD-C2D	-2.03	1.46	1.50
22	A	809	CLA	CMD-C2D	-2.03	1.46	1.50
22	7	612	CLA	CMC-C2C	-2.03	1.46	1.50
22	A	837	CLA	CMD-C2D	-2.03	1.46	1.50
22	B	839	CLA	C3B-CAB	-2.03	1.43	1.47
22	A	828	CLA	CMD-C2D	-2.03	1.46	1.50
22	B	812	CLA	C3B-C2B	-2.03	1.37	1.40
22	W	610	CLA	CMD-C2D	-2.03	1.46	1.50
22	F	303	CLA	CMD-C2D	-2.03	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	601	CHL	C2C-C1C	2.03	1.48	1.44
22	9	610	CLA	C3B-CAB	-2.03	1.43	1.47
22	9	610	CLA	CMD-C2D	-2.03	1.46	1.50
22	8	603	CLA	CMD-C2D	-2.03	1.46	1.50
22	A	832	CLA	CMC-C2C	-2.03	1.46	1.50
22	K	206	CLA	CMD-C2D	-2.03	1.46	1.50
22	4	612	CLA	C3B-C2B	-2.03	1.37	1.40
22	A	821	CLA	C3B-CAB	-2.03	1.43	1.47
22	O	2002	CLA	CMD-C2D	-2.03	1.46	1.50
22	B	826	CLA	CMD-C2D	-2.03	1.46	1.50
22	A	810	CLA	C3B-CAB	-2.02	1.43	1.47
22	J	101	CLA	CMD-C2D	-2.02	1.46	1.50
22	2	610	CLA	C3B-C2B	-2.02	1.37	1.40
22	A	842	CLA	CMD-C2D	-2.02	1.46	1.50
22	2	609	CLA	C3B-C2B	-2.02	1.37	1.40
22	6	610	CLA	C3B-C2B	-2.02	1.37	1.40
22	A	802	CLA	CMC-C2C	-2.02	1.46	1.50
22	1	608	CLA	CMD-C2D	-2.02	1.46	1.50
22	B	813	CLA	CMD-C2D	-2.02	1.46	1.50
22	V	604	CLA	CMD-C2D	-2.02	1.46	1.50
22	4	603	CLA	CMD-C2D	-2.02	1.46	1.50
22	5	609	CLA	MG-NA	2.02	2.11	2.06
22	B	828	CLA	C3B-CAB	-2.02	1.43	1.47
22	2	603	CLA	CMD-C2D	-2.02	1.46	1.50
22	4	614	CLA	CMD-C2D	-2.02	1.46	1.50
22	B	821	CLA	CMD-C2D	-2.02	1.46	1.50
22	W	604	CLA	C3B-C2B	-2.02	1.37	1.40
21	U	606	CHL	C4C-C3C	2.02	1.48	1.45
22	7	615	CLA	C3B-C2B	-2.02	1.37	1.40
22	5	606	CLA	CMC-C2C	-2.02	1.46	1.50
22	3	612	CLA	CMD-C2D	-2.01	1.46	1.50
22	9	602	CLA	C3B-CAB	-2.01	1.43	1.47
22	2	613	CLA	CMD-C2D	-2.01	1.46	1.50
22	B	803	CLA	CMC-C2C	-2.01	1.46	1.50
22	A	819	CLA	CMD-C2D	-2.01	1.46	1.50
22	G	201	CLA	CMD-C2D	-2.01	1.46	1.50
22	A	814	CLA	CMD-C2D	-2.01	1.46	1.50
22	B	815	CLA	CMD-C2D	-2.01	1.46	1.50
22	B	816	CLA	CMD-C2D	-2.01	1.46	1.50
22	6	604	CLA	CMD-C2D	-2.01	1.46	1.50
22	W	604	CLA	CMD-C2D	-2.01	1.46	1.50
22	A	816	CLA	C3B-CAB	-2.01	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	U	612	CLA	CMC-C2C	-2.01	1.46	1.50
22	A	815	CLA	C3B-C2B	-2.01	1.37	1.40
22	3	604	CLA	CMD-C2D	-2.01	1.46	1.50
22	3	610	CLA	CMD-C2D	-2.01	1.46	1.50
22	A	843	CLA	CMC-C2C	-2.01	1.46	1.50
22	L	302	CLA	CMD-C2D	-2.01	1.46	1.50
22	B	834	CLA	C3B-CAB	-2.01	1.43	1.47
22	A	827	CLA	C3B-C2B	-2.01	1.37	1.40
21	9	608	CHL	C2C-C1C	2.01	1.48	1.44
22	8	601	CLA	CMC-C2C	-2.01	1.46	1.50
22	5	604	CLA	C3B-C2B	-2.01	1.37	1.40
22	B	831	CLA	CMD-C2D	-2.01	1.46	1.50
21	2	606	CHL	C2C-C1C	2.01	1.48	1.44
22	F	304	CLA	CMD-C2D	-2.00	1.46	1.50
22	3	617	CLA	C4C-NC	2.00	1.40	1.37
22	5	610	CLA	C3B-C2B	-2.00	1.37	1.40
24	2	620	XAT	O24-C25	-2.00	1.43	1.46
22	U	604	CLA	CMD-C2D	-2.00	1.46	1.50
21	2	608	CHL	C2C-C1C	2.00	1.48	1.44
22	B	810	CLA	C3B-CAB	-2.00	1.43	1.47
22	1	608	CLA	C3B-C2B	-2.00	1.37	1.40

All (3987) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	V	2622	XAT	O4-C5-C4	-29.06	91.55	113.38
24	4	620	XAT	O4-C5-C4	-27.98	92.37	113.38
24	6	620	XAT	O4-C5-C4	-26.00	93.85	113.38
24	7	619	XAT	O24-C25-C24	-25.27	94.40	113.38
24	6	620	XAT	O24-C25-C24	-22.02	96.84	113.38
24	7	619	XAT	O4-C5-C4	-21.43	97.29	113.38
24	7	619	XAT	O4-C5-C18	-20.33	90.69	115.06
24	6	620	XAT	O4-C5-C18	-18.63	92.74	115.06
24	6	620	XAT	O24-C25-C38	-18.60	92.77	115.06
24	7	619	XAT	O24-C25-C38	-17.52	94.06	115.06
24	4	620	XAT	O4-C5-C18	-17.24	94.41	115.06
24	V	2622	XAT	O4-C5-C18	-16.18	95.67	115.06
23	9	624	LUT	C37-C21-C36	-14.07	87.15	107.89
24	V	2622	XAT	C17-C1-C16	-13.85	86.95	107.37
24	6	620	XAT	C37-C21-C36	-13.44	87.54	107.37
22	3	617	CLA	C1C-C2C-C3C	-12.59	105.61	110.89
24	6	620	XAT	C37-C21-C22	-12.46	87.34	108.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	V	2622	XAT	C17-C1-C2	-12.35	87.52	108.98
27	B	1609	BCR	C40-C30-C25	-12.32	90.31	110.30
25	U	2623	NEX	O24-C25-C24	12.24	122.58	113.38
27	4	621	BCR	C40-C30-C25	-11.75	91.23	110.30
24	U	2622	XAT	O4-C5-C4	11.36	121.91	113.38
24	3	619	XAT	O4-C5-C4	10.71	121.42	113.38
25	V	2623	NEX	O24-C25-C24	10.43	121.22	113.38
24	W	2622	XAT	O4-C5-C4	10.36	121.17	113.38
24	2	620	XAT	O4-C5-C4	10.20	121.04	113.38
27	4	621	BCR	C39-C30-C25	9.89	126.34	110.30
23	9	624	LUT	C37-C21-C22	-9.55	91.35	109.44
24	V	2622	XAT	O24-C25-C24	9.36	120.41	113.38
22	9	609	CLA	CMD-C2D-C1D	9.15	140.84	124.71
21	9	605	CHL	C1D-ND-C4D	-9.09	99.88	106.33
21	U	606	CHL	C1D-ND-C4D	-9.04	99.91	106.33
23	9	624	LUT	C37-C21-C26	-8.94	96.00	109.55
21	6	602	CHL	C1D-ND-C4D	-8.94	99.99	106.33
25	9	623	NEX	O24-C25-C24	8.92	120.08	113.38
21	V	605	CHL	C1D-ND-C4D	-8.84	100.05	106.33
21	U	609	CHL	C1D-ND-C4D	-8.84	100.05	106.33
21	2	606	CHL	C1D-ND-C4D	-8.84	100.06	106.33
21	7	608	CHL	CMD-C2D-C1D	8.83	140.28	124.71
21	6	606	CHL	C1D-ND-C4D	-8.83	100.06	106.33
21	6	608	CHL	C1D-ND-C4D	-8.79	100.09	106.33
21	2	601	CHL	CMD-C2D-C1D	8.79	140.20	124.71
21	9	601	CHL	CMD-C2D-C1D	8.77	140.17	124.71
21	U	609	CHL	CMD-C2D-C1D	8.75	140.14	124.71
21	9	606	CHL	CMD-C2D-C1D	8.75	140.13	124.71
21	V	609	CHL	C1D-ND-C4D	-8.74	100.12	106.33
21	2	602	CHL	C1D-ND-C4D	-8.74	100.13	106.33
21	9	605	CHL	CMD-C2D-C1D	8.73	140.09	124.71
24	V	2622	XAT	C16-C1-C2	8.72	124.13	108.98
21	W	609	CHL	C1D-ND-C4D	-8.69	100.16	106.33
21	7	608	CHL	C1D-ND-C4D	-8.68	100.17	106.33
21	2	607	CHL	CMD-C2D-C1D	8.67	139.99	124.71
21	8	607	CHL	C1D-ND-C4D	-8.66	100.19	106.33
22	9	609	CLA	C1D-ND-C4D	-8.65	100.19	106.33
21	8	608	CHL	C1D-ND-C4D	-8.64	100.20	106.33
21	V	607	CHL	C1D-ND-C4D	-8.64	100.20	106.33
21	5	607	CHL	C1D-ND-C4D	-8.63	100.20	106.33
21	2	618	CHL	CMD-C2D-C1D	8.62	139.91	124.71
21	4	606	CHL	C1D-ND-C4D	-8.62	100.21	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	6	601	CHL	C1D-ND-C4D	-8.61	100.22	106.33
21	V	609	CHL	CMD-C2D-C1D	8.61	139.88	124.71
21	6	607	CHL	C1D-ND-C4D	-8.60	100.23	106.33
21	2	607	CHL	C1D-ND-C4D	-8.58	100.24	106.33
21	W	607	CHL	C1D-ND-C4D	-8.54	100.27	106.33
21	U	607	CHL	C1D-ND-C4D	-8.53	100.27	106.33
21	6	601	CHL	CMD-C2D-C1D	8.52	139.74	124.71
21	W	608	CHL	C1D-ND-C4D	-8.52	100.28	106.33
21	2	601	CHL	C1D-ND-C4D	-8.52	100.28	106.33
21	9	608	CHL	C1D-ND-C4D	-8.52	100.28	106.33
21	3	608	CHL	CMD-C2D-C1D	8.52	139.72	124.71
21	W	601	CHL	C1D-ND-C4D	-8.51	100.29	106.33
21	W	606	CHL	CMD-C2D-C1D	8.51	139.71	124.71
21	8	608	CHL	CMD-C2D-C1D	8.51	139.71	124.71
21	U	606	CHL	CMD-C2D-C1D	8.49	139.68	124.71
21	2	618	CHL	C1D-ND-C4D	-8.49	100.31	106.33
21	8	607	CHL	CMD-C2D-C1D	8.49	139.67	124.71
21	U	605	CHL	C1D-ND-C4D	-8.48	100.31	106.33
21	5	601	CHL	C1D-ND-C4D	-8.47	100.32	106.33
21	4	607	CHL	CMD-C2D-C1D	8.46	139.62	124.71
21	6	608	CHL	CMD-C2D-C1D	8.45	139.60	124.71
21	9	606	CHL	C1D-ND-C4D	-8.44	100.34	106.33
21	8	618	CHL	C1D-ND-C4D	-8.44	100.34	106.33
21	4	607	CHL	C1D-ND-C4D	-8.44	100.34	106.33
21	8	606	CHL	C1D-ND-C4D	-8.42	100.35	106.33
21	2	608	CHL	CMD-C2D-C1D	8.41	139.54	124.71
21	9	601	CHL	C1D-ND-C4D	-8.40	100.37	106.33
21	1	601	CHL	CMD-C2D-C1D	8.40	139.51	124.71
21	W	607	CHL	CMD-C2D-C1D	8.39	139.50	124.71
21	W	606	CHL	C1D-ND-C4D	-8.39	100.38	106.33
21	V	601	CHL	CMD-C2D-C1D	8.37	139.47	124.71
21	4	618	CHL	C1D-ND-C4D	-8.37	100.39	106.33
21	V	608	CHL	CMD-C2D-C1D	8.37	139.46	124.71
21	W	609	CHL	CMD-C2D-C1D	8.36	139.46	124.71
21	W	608	CHL	CMD-C2D-C1D	8.36	139.45	124.71
21	4	608	CHL	CMD-C2D-C1D	8.36	139.45	124.71
21	8	606	CHL	CMD-C2D-C1D	8.35	139.43	124.71
21	W	601	CHL	CMD-C2D-C1D	8.34	139.41	124.71
21	4	606	CHL	CMD-C2D-C1D	8.34	139.41	124.71
21	9	607	CHL	C1D-ND-C4D	-8.34	100.41	106.33
21	W	605	CHL	C1D-ND-C4D	-8.33	100.41	106.33
21	U	605	CHL	CMD-C2D-C1D	8.33	139.40	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	2	606	CHL	CMD-C2D-C1D	8.33	139.40	124.71
21	2	608	CHL	C1D-ND-C4D	-8.33	100.42	106.33
21	1	607	CHL	CMD-C2D-C1D	8.33	139.39	124.71
21	W	605	CHL	CMD-C2D-C1D	8.33	139.39	124.71
21	V	608	CHL	C1D-ND-C4D	-8.32	100.42	106.33
21	U	601	CHL	CMD-C2D-C1D	8.32	139.38	124.71
21	6	618	CHL	C1D-ND-C4D	-8.32	100.43	106.33
21	V	605	CHL	CMD-C2D-C1D	8.31	139.36	124.71
21	6	607	CHL	CMD-C2D-C1D	8.30	139.35	124.71
21	6	606	CHL	CMD-C2D-C1D	8.28	139.30	124.71
21	8	618	CHL	CMD-C2D-C1D	8.27	139.28	124.71
21	U	601	CHL	C1D-ND-C4D	-8.26	100.47	106.33
21	V	607	CHL	CMD-C2D-C1D	8.26	139.27	124.71
21	1	601	CHL	C1D-ND-C4D	-8.26	100.47	106.33
21	6	602	CHL	CMD-C2D-C1D	8.26	139.26	124.71
21	4	608	CHL	C1D-ND-C4D	-8.25	100.47	106.33
21	U	608	CHL	CMD-C2D-C1D	8.22	139.21	124.71
21	9	608	CHL	CMD-C2D-C1D	8.18	139.14	124.71
21	U	607	CHL	CMD-C2D-C1D	8.17	139.12	124.71
21	V	606	CHL	C1D-ND-C4D	-8.16	100.53	106.33
21	5	607	CHL	CMD-C2D-C1D	8.16	139.10	124.71
24	6	620	XAT	C36-C21-C22	8.14	123.13	108.98
21	V	601	CHL	C1D-ND-C4D	-8.14	100.55	106.33
21	1	607	CHL	C1D-ND-C4D	-8.13	100.56	106.33
21	U	608	CHL	C1D-ND-C4D	-8.13	100.56	106.33
21	6	618	CHL	CMD-C2D-C1D	8.10	138.99	124.71
21	5	601	CHL	CMD-C2D-C1D	8.10	138.98	124.71
21	2	602	CHL	CMD-C2D-C1D	7.99	138.80	124.71
24	3	619	XAT	C18-C5-C6	-7.90	109.02	122.26
21	6	608	CHL	C2C-C3C-C4C	-7.90	100.86	106.49
21	4	618	CHL	CMD-C2D-C1D	7.90	138.64	124.71
21	9	607	CHL	CMD-C2D-C1D	7.87	138.58	124.71
21	3	608	CHL	C1D-ND-C4D	-7.83	100.77	106.33
21	8	608	CHL	C2C-C3C-C4C	-7.76	100.96	106.49
22	F	304	CLA	C4D-ND-C1D	-7.74	103.37	112.85
21	6	602	CHL	C2C-C3C-C4C	-7.74	100.97	106.49
21	U	607	CHL	C2C-C3C-C4C	-7.71	101.00	106.49
21	4	606	CHL	C2C-C3C-C4C	-7.69	101.01	106.49
21	V	606	CHL	CMD-C2D-C1D	7.67	138.24	124.71
21	4	618	CHL	C2C-C3C-C4C	-7.66	101.03	106.49
21	2	602	CHL	C2C-C3C-C4C	-7.62	101.06	106.49
27	3	621	BCR	C38-C26-C25	-7.52	116.08	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	U	606	CHL	C2C-C3C-C4C	-7.51	101.13	106.49
21	2	608	CHL	C2C-C3C-C4C	-7.46	101.17	106.49
21	2	607	CHL	C2C-C3C-C4C	-7.40	101.21	106.49
21	2	601	CHL	C2C-C3C-C4C	-7.39	101.22	106.49
23	9	624	LUT	C36-C21-C26	7.39	120.75	109.55
21	6	618	CHL	C2C-C3C-C4C	-7.38	101.23	106.49
27	B	1609	BCR	C39-C30-C25	7.33	122.19	110.30
27	L	301	BCR	C37-C22-C21	-7.33	112.66	122.92
24	W	2622	XAT	O24-C25-C24	7.32	118.88	113.38
21	6	607	CHL	C2C-C3C-C4C	-7.30	101.29	106.49
21	5	607	CHL	C2C-C3C-C4C	-7.29	101.30	106.49
27	6	621	BCR	C7-C8-C9	-7.28	115.23	126.23
27	8	621	BCR	C7-C8-C9	-7.26	115.27	126.23
21	2	618	CHL	C2C-C3C-C4C	-7.26	101.32	106.49
21	6	606	CHL	C2C-C3C-C4C	-7.25	101.32	106.49
21	V	607	CHL	C2C-C3C-C4C	-7.24	101.11	106.49
21	8	607	CHL	C2C-C3C-C4C	-7.23	101.34	106.49
21	6	601	CHL	C2C-C3C-C4C	-7.22	101.34	106.49
21	W	609	CHL	C2C-C3C-C4C	-7.21	101.35	106.49
21	V	605	CHL	C2C-C3C-C4C	-7.21	101.35	106.49
21	W	607	CHL	C2C-C3C-C4C	-7.20	101.14	106.49
21	8	618	CHL	C2C-C3C-C4C	-7.19	101.36	106.49
21	U	609	CHL	C2C-C3C-C4C	-7.19	101.36	106.49
21	1	607	CHL	C2C-C3C-C4C	-7.19	101.36	106.49
21	9	608	CHL	C2C-C3C-C4C	-7.18	101.37	106.49
21	V	609	CHL	C2C-C3C-C4C	-7.17	101.38	106.49
21	1	601	CHL	C2C-C3C-C4C	-7.13	101.41	106.49
21	U	606	CHL	C2D-C1D-ND	7.12	115.35	110.10
21	2	606	CHL	C2C-C3C-C4C	-7.12	101.42	106.49
21	U	608	CHL	C2C-C3C-C4C	-7.10	101.22	106.49
21	9	606	CHL	C2C-C3C-C4C	-7.10	101.43	106.49
21	8	606	CHL	C2C-C3C-C4C	-7.10	101.43	106.49
21	4	608	CHL	C2C-C3C-C4C	-7.09	101.43	106.49
21	5	601	CHL	C2C-C3C-C4C	-7.09	101.43	106.49
21	9	601	CHL	C2C-C3C-C4C	-7.09	101.43	106.49
21	7	608	CHL	C2C-C3C-C4C	-7.09	101.44	106.49
21	V	608	CHL	C2C-C3C-C4C	-7.04	101.26	106.49
27	B	1609	BCR	C40-C30-C39	-7.04	86.93	108.53
21	9	605	CHL	C2C-C3C-C4C	-7.03	101.27	106.49
24	U	2622	XAT	O24-C25-C24	7.03	118.66	113.38
24	2	620	XAT	O24-C25-C24	7.02	118.66	113.38
21	6	602	CHL	C2D-C1D-ND	6.99	115.26	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	4	607	CHL	C2C-C3C-C4C	-6.96	101.53	106.49
21	W	608	CHL	C2C-C3C-C4C	-6.95	101.33	106.49
21	6	608	CHL	C2D-C1D-ND	6.90	115.19	110.10
21	V	601	CHL	C1B-C2B-C3B	-6.88	100.52	106.92
21	2	606	CHL	C2D-C1D-ND	6.87	115.17	110.10
21	9	605	CHL	C2D-C1D-ND	6.86	115.16	110.10
24	5	618	XAT	O4-C5-C4	6.85	118.53	113.38
21	8	608	CHL	C2D-C1D-ND	6.83	115.14	110.10
21	4	618	CHL	C2D-C1D-ND	6.83	115.14	110.10
27	1	619	BCR	C27-C26-C25	-6.79	112.87	122.73
21	5	601	CHL	C2D-C1D-ND	6.79	115.11	110.10
21	W	605	CHL	C1B-C2B-C3B	-6.79	100.61	106.92
21	V	607	CHL	C2D-C1D-ND	6.77	115.09	110.10
21	V	605	CHL	C2D-C1D-ND	6.77	115.09	110.10
21	U	605	CHL	C4C-C3C-C2C	-6.76	100.87	107.07
21	U	601	CHL	C1B-C2B-C3B	-6.75	100.64	106.92
21	W	607	CHL	C1B-C2B-C3B	-6.74	100.65	106.92
21	U	605	CHL	C1B-C2B-C3B	-6.74	100.65	106.92
21	4	606	CHL	C2D-C1D-ND	6.74	115.07	110.10
21	6	606	CHL	C2D-C1D-ND	6.73	115.06	110.10
21	V	607	CHL	C1B-C2B-C3B	-6.72	100.67	106.92
21	W	605	CHL	C4C-C3C-C2C	-6.71	100.91	107.07
21	2	602	CHL	C2D-C1D-ND	6.71	115.05	110.10
21	W	607	CHL	C2D-C1D-ND	6.70	115.04	110.10
21	W	609	CHL	C2D-C1D-ND	6.70	115.04	110.10
21	V	608	CHL	C1B-C2B-C3B	-6.69	100.70	106.92
21	U	609	CHL	C2D-C1D-ND	6.69	115.03	110.10
21	V	606	CHL	C4C-C3C-C2C	-6.69	100.94	107.07
21	6	607	CHL	C2D-C1D-ND	6.68	115.03	110.10
21	3	608	CHL	C2C-C3C-C4C	-6.68	101.73	106.49
21	U	607	CHL	C2D-C1D-ND	6.67	115.02	110.10
21	2	607	CHL	C2D-C1D-ND	6.67	115.02	110.10
21	2	601	CHL	C2D-C1D-ND	6.66	115.01	110.10
21	V	609	CHL	C2D-C1D-ND	6.65	115.01	110.10
21	6	601	CHL	C2D-C1D-ND	6.65	115.00	110.10
21	W	601	CHL	C1B-C2B-C3B	-6.65	100.73	106.92
21	8	607	CHL	C2D-C1D-ND	6.64	114.99	110.10
21	W	606	CHL	C4C-C3C-C2C	-6.63	100.99	107.07
21	9	607	CHL	C2D-C1D-ND	6.63	114.99	110.10
21	5	607	CHL	C2D-C1D-ND	6.62	114.98	110.10
24	4	620	XAT	O24-C25-C24	6.62	118.36	113.38
21	9	605	CHL	CHD-C1D-ND	-6.59	118.40	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	U	605	CHL	C2D-C1D-ND	6.59	114.96	110.10
21	7	608	CHL	C2D-C1D-ND	6.59	114.96	110.10
21	W	601	CHL	C2D-C1D-ND	6.58	114.95	110.10
27	K	205	BCR	C33-C5-C6	-6.57	117.14	124.53
25	W	2623	NEX	C35-C34-C33	-6.56	117.95	127.31
21	V	608	CHL	C2D-C1D-ND	6.56	114.94	110.10
21	6	618	CHL	C2D-C1D-ND	6.54	114.93	110.10
21	9	606	CHL	C2D-C1D-ND	6.54	114.92	110.10
21	8	606	CHL	C2D-C1D-ND	6.52	114.91	110.10
21	W	606	CHL	C1B-C2B-C3B	-6.52	100.85	106.92
21	V	605	CHL	O2D-CGD-CBD	6.50	122.83	111.27
21	4	608	CHL	C2D-C1D-ND	6.50	114.90	110.10
21	U	601	CHL	C2D-C1D-ND	6.50	114.89	110.10
21	V	606	CHL	C2D-C1D-ND	6.50	114.89	110.10
21	W	608	CHL	C2D-C1D-ND	6.50	114.89	110.10
21	2	608	CHL	C2D-C1D-ND	6.48	114.88	110.10
21	2	618	CHL	C2D-C1D-ND	6.48	114.88	110.10
27	A	852	BCR	C32-C1-C6	6.47	120.80	110.30
21	1	601	CHL	C2D-C1D-ND	6.46	114.86	110.10
21	8	618	CHL	C2D-C1D-ND	6.45	114.86	110.10
21	V	609	CHL	CHD-C1D-ND	-6.43	118.54	124.45
21	W	605	CHL	C2D-C1D-ND	6.43	114.84	110.10
21	2	607	CHL	CHD-C1D-ND	-6.42	118.55	124.45
21	V	606	CHL	C1B-C2B-C3B	-6.42	100.95	106.92
21	9	608	CHL	C2D-C1D-ND	6.39	114.81	110.10
21	4	607	CHL	C2D-C1D-ND	6.38	114.81	110.10
27	L	301	BCR	C23-C24-C25	-6.38	109.28	127.20
21	2	602	CHL	CHD-C1D-ND	-6.36	118.61	124.45
27	7	621	BCR	C28-C27-C26	-6.36	102.73	114.08
21	W	606	CHL	CHD-C1D-ND	-6.35	118.61	124.45
21	9	607	CHL	CHD-C1D-ND	-6.35	118.62	124.45
21	4	607	CHL	CHD-C1D-ND	-6.35	118.62	124.45
21	U	608	CHL	C1B-C2B-C3B	-6.34	101.02	106.92
21	W	601	CHL	CHD-C1D-ND	-6.34	118.63	124.45
21	6	601	CHL	CHD-C1D-ND	-6.32	118.64	124.45
21	4	618	CHL	CHD-C1D-ND	-6.31	118.65	124.45
21	8	607	CHL	CHD-C1D-ND	-6.29	118.67	124.45
21	V	601	CHL	C2D-C1D-ND	6.29	114.74	110.10
21	U	605	CHL	CHD-C1D-ND	-6.28	118.69	124.45
21	U	606	CHL	CHD-C1D-ND	-6.27	118.69	124.45
21	W	606	CHL	C2D-C1D-ND	6.27	114.72	110.10
27	B	845	BCR	C37-C22-C21	-6.26	114.15	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	W	605	CHL	CHD-C1D-ND	-6.26	118.70	124.45
22	9	609	CLA	CHD-C1D-ND	-6.26	118.70	124.45
21	9	607	CHL	C2C-C3C-C4C	-6.26	102.03	106.49
21	6	602	CHL	CHD-C1D-ND	-6.25	118.71	124.45
25	W	2623	NEX	O24-C25-C24	6.25	118.08	113.38
21	4	608	CHL	CHD-C1D-ND	-6.25	118.71	124.45
22	A	832	CLA	C4A-NA-C1A	6.25	109.51	106.71
21	U	609	CHL	CHD-C1D-ND	-6.24	118.72	124.45
21	U	608	CHL	C2D-C1D-ND	6.22	114.69	110.10
21	1	601	CHL	CHD-C1D-ND	-6.22	118.74	124.45
21	W	608	CHL	C1B-C2B-C3B	-6.21	101.14	106.92
22	9	609	CLA	C2D-C1D-ND	6.21	114.68	110.10
25	W	2623	NEX	C31-C30-C29	-6.19	118.47	127.31
21	1	607	CHL	C2D-C1D-ND	6.19	114.66	110.10
21	V	607	CHL	CHD-C1D-ND	-6.19	118.77	124.45
21	2	608	CHL	CHD-C1D-ND	-6.18	118.77	124.45
21	3	608	CHL	C2D-C1D-ND	6.18	114.66	110.10
27	4	621	BCR	C24-C23-C22	-6.18	116.90	126.23
24	1	618	XAT	O24-C25-C24	6.15	118.00	113.38
21	8	606	CHL	CHD-C1D-ND	-6.15	118.80	124.45
21	5	601	CHL	CHD-C1D-ND	-6.15	118.81	124.45
21	W	609	CHL	CHD-C1D-ND	-6.14	118.81	124.45
21	V	606	CHL	CHD-C1D-ND	-6.14	118.81	124.45
27	6	621	BCR	C33-C5-C6	-6.13	117.64	124.53
23	9	624	LUT	C36-C21-C22	6.13	121.05	109.44
21	W	607	CHL	CHD-C1D-ND	-6.13	118.82	124.45
21	5	607	CHL	CHD-C1D-ND	-6.13	118.82	124.45
21	2	606	CHL	CHD-C1D-ND	-6.12	118.83	124.45
21	2	601	CHL	CHD-C1D-ND	-6.12	118.83	124.45
21	V	601	CHL	CHD-C1D-ND	-6.11	118.84	124.45
21	8	618	CHL	CHD-C1D-ND	-6.11	118.84	124.45
21	V	605	CHL	CHD-C1D-ND	-6.11	118.84	124.45
21	W	608	CHL	CHD-C1D-ND	-6.10	118.85	124.45
21	U	601	CHL	CHD-C1D-ND	-6.09	118.86	124.45
21	V	608	CHL	CHD-C1D-ND	-6.08	118.86	124.45
21	6	607	CHL	CHD-C1D-ND	-6.08	118.87	124.45
21	6	606	CHL	CHD-C1D-ND	-6.06	118.88	124.45
21	7	608	CHL	CHD-C1D-ND	-6.05	118.89	124.45
24	1	618	XAT	C38-C25-C26	-6.05	112.12	122.26
21	U	608	CHL	CHD-C1D-ND	-6.05	118.90	124.45
27	B	1609	BCR	C3-C4-C5	-6.03	103.30	114.08
21	1	607	CHL	CHD-C1D-ND	-6.03	118.91	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	W	2623	NEX	C38-C25-C26	-6.03	112.16	122.26
22	B	809	CLA	C4A-NA-C1A	6.02	109.41	106.71
22	V	612	CLA	C4A-NA-C1A	6.02	109.41	106.71
21	2	618	CHL	CHD-C1D-ND	-5.99	118.95	124.45
22	B	825	CLA	C4A-NA-C1A	5.98	109.40	106.71
21	9	608	CHL	CHD-C1D-ND	-5.97	118.96	124.45
21	U	607	CHL	CHD-C1D-ND	-5.95	118.99	124.45
21	8	608	CHL	CHD-C1D-ND	-5.94	118.99	124.45
21	9	606	CHL	CHD-C1D-ND	-5.94	119.00	124.45
27	8	621	BCR	C24-C23-C22	-5.94	117.27	126.23
21	6	618	CHL	CHD-C1D-ND	-5.92	119.01	124.45
24	5	618	XAT	O24-C25-C38	5.90	122.12	115.06
21	4	606	CHL	CHD-C1D-ND	-5.90	119.03	124.45
21	6	608	CHL	CHD-C1D-ND	-5.89	119.05	124.45
24	5	618	XAT	C18-C5-C6	-5.88	112.40	122.26
27	4	621	BCR	C40-C30-C39	-5.85	90.56	108.53
24	1	618	XAT	C18-C5-C6	-5.79	112.55	122.26
27	K	202	BCR	C3-C4-C5	-5.79	103.75	114.08
22	K	204	CLA	C4A-NA-C1A	5.78	109.31	106.71
22	7	602	CLA	C4A-NA-C1A	5.77	109.30	106.71
21	3	608	CHL	CHD-C1D-ND	-5.77	119.15	124.45
22	4	604	CLA	C4A-NA-C1A	5.77	109.30	106.71
27	B	845	BCR	C3-C4-C5	-5.76	103.79	114.08
22	U	603	CLA	C4A-NA-C1A	5.74	109.29	106.71
27	J	102	BCR	C3-C4-C5	-5.74	103.83	114.08
21	V	607	CHL	O2D-CGD-CBD	5.73	121.45	111.27
21	9	601	CHL	CHD-C1D-ND	-5.71	119.21	124.45
25	W	2623	NEX	O24-C25-C38	5.71	121.89	115.06
22	A	836	CLA	CAC-C3C-C4C	5.70	125.17	117.97
22	3	606	CLA	C4A-NA-C1A	5.67	109.26	106.71
27	K	205	BCR	C38-C26-C25	-5.65	118.19	124.53
21	9	601	CHL	C2D-C1D-ND	5.64	114.26	110.10
22	J	101	CLA	C4A-NA-C1A	5.63	109.24	106.71
27	K	205	BCR	C8-C7-C6	-5.63	111.40	127.20
22	7	607	CLA	C4A-NA-C1A	5.62	109.23	106.71
22	8	609	CLA	C4A-NA-C1A	5.62	109.23	106.71
27	6	621	BCR	C24-C23-C22	-5.58	117.80	126.23
25	W	2623	NEX	C15-C14-C13	-5.57	119.36	127.31
22	2	603	CLA	C4A-NA-C1A	5.57	109.21	106.71
22	3	615	CLA	C4A-NA-C1A	5.56	109.21	106.71
25	V	2623	NEX	C38-C25-C26	-5.56	112.94	122.26
27	3	620	BCR	C28-C27-C26	-5.55	104.16	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	J	102	BCR	C8-C7-C6	-5.54	111.64	127.20
22	8	613	CLA	C4A-NA-C1A	5.51	109.19	106.71
21	9	605	CHL	C3D-C4D-ND	5.51	119.16	110.24
27	A	851	BCR	C28-C27-C26	-5.51	104.23	114.08
24	U	2622	XAT	C38-C25-C26	-5.51	113.03	122.26
24	W	2622	XAT	C18-C5-C6	-5.50	113.04	122.26
22	A	836	CLA	C4A-NA-C1A	5.49	109.17	106.71
27	B	845	BCR	C15-C14-C13	-5.49	119.48	127.31
22	A	836	CLA	C2C-C3C-C4C	-5.48	107.53	119.42
27	7	620	BCR	C23-C24-C25	-5.48	111.82	127.20
27	O	2004	BCR	C32-C1-C6	5.48	119.18	110.30
21	2	602	CHL	C3D-C4D-ND	5.47	119.09	110.24
22	A	814	CLA	C4A-NA-C1A	5.45	109.16	106.71
24	4	620	XAT	C38-C25-C26	-5.45	113.13	122.26
22	6	611	CLA	C4A-NA-C1A	5.44	109.15	106.71
21	6	618	CHL	O2D-CGD-CBD	5.44	120.93	111.27
25	9	623	NEX	C38-C25-C26	-5.44	113.15	122.26
22	1	603	CLA	C4A-NA-C1A	5.43	109.15	106.71
21	9	601	CHL	C3D-C4D-ND	5.43	119.02	110.24
21	U	609	CHL	C3D-C4D-ND	5.42	119.01	110.24
21	5	607	CHL	C3D-C4D-ND	5.41	118.98	110.24
24	W	2622	XAT	C38-C25-C26	-5.40	113.20	122.26
22	A	828	CLA	C4A-NA-C1A	5.40	109.14	106.71
22	B	826	CLA	C4A-NA-C1A	5.40	109.13	106.71
21	U	606	CHL	O2D-CGD-CBD	5.39	120.85	111.27
21	V	609	CHL	C3D-C4D-ND	5.39	118.95	110.24
21	8	607	CHL	C3D-C4D-ND	5.38	118.95	110.24
21	V	605	CHL	C3D-C4D-ND	5.38	118.94	110.24
22	9	609	CLA	C3D-C4D-ND	5.38	118.94	110.24
21	2	601	CHL	O2D-CGD-CBD	5.38	120.83	111.27
21	4	607	CHL	C3D-C4D-ND	5.38	118.94	110.24
21	6	606	CHL	C3D-C4D-ND	5.38	118.94	110.24
21	6	602	CHL	C3D-C4D-ND	5.37	118.93	110.24
21	U	606	CHL	C3D-C4D-ND	5.37	118.92	110.24
21	2	606	CHL	C3D-C4D-ND	5.35	118.90	110.24
21	9	608	CHL	C3D-C4D-ND	5.35	118.89	110.24
21	2	607	CHL	O2D-CGD-CBD	5.35	120.77	111.27
22	B	810	CLA	C4A-NA-C1A	5.34	109.11	106.71
22	7	612	CLA	C4A-NA-C1A	5.34	109.11	106.71
21	W	609	CHL	C3D-C4D-ND	5.33	118.87	110.24
22	1	611	CLA	C4A-NA-C1A	5.33	109.10	106.71
22	9	609	CLA	O2D-CGD-CBD	5.33	120.74	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	W	601	CHL	C3D-C4D-ND	5.33	118.86	110.24
21	W	606	CHL	C3D-C4D-ND	5.32	118.85	110.24
27	B	847	BCR	C28-C27-C26	-5.32	104.57	114.08
21	V	607	CHL	C3D-C4D-ND	5.32	118.85	110.24
22	B	840	CLA	C4A-NA-C1A	5.32	109.10	106.71
27	K	205	BCR	C7-C8-C9	-5.32	118.20	126.23
22	K	201	CLA	C4A-NA-C1A	5.31	109.09	106.71
22	B	832	CLA	C4A-NA-C1A	5.30	109.09	106.71
21	8	618	CHL	C3D-C4D-ND	5.30	118.82	110.24
21	W	608	CHL	C3D-C4D-ND	5.30	118.81	110.24
27	7	621	BCR	C3-C4-C5	-5.30	104.61	114.08
21	9	607	CHL	C3D-C4D-ND	5.30	118.81	110.24
21	2	607	CHL	C3D-C4D-ND	5.29	118.80	110.24
27	F	305	BCR	C28-C27-C26	-5.29	104.63	114.08
24	U	2622	XAT	C18-C5-C6	-5.29	113.39	122.26
21	W	605	CHL	C3D-C4D-ND	5.29	118.79	110.24
21	U	605	CHL	C3D-C4D-ND	5.29	118.79	110.24
21	6	606	CHL	O2D-CGD-CBD	5.28	120.65	111.27
22	A	834	CLA	C4A-NA-C1A	5.28	109.08	106.71
22	A	806	CLA	C4A-NA-C1A	5.27	109.08	106.71
22	8	603	CLA	C4A-NA-C1A	5.27	109.08	106.71
27	J	102	BCR	C28-C27-C26	-5.27	104.66	114.08
21	V	608	CHL	C3C-C4C-NC	5.27	116.33	110.57
21	6	608	CHL	CAC-C3C-C4C	5.27	131.64	124.81
21	4	618	CHL	C3D-C4D-ND	5.26	118.75	110.24
21	6	607	CHL	C3D-C4D-ND	5.26	118.75	110.24
21	V	606	CHL	C3D-C4D-ND	5.26	118.75	110.24
21	W	607	CHL	C3D-C4D-ND	5.24	118.72	110.24
21	U	607	CHL	C3D-C4D-ND	5.24	118.71	110.24
21	6	608	CHL	C3D-C4D-ND	5.23	118.70	110.24
22	B	824	CLA	C4A-NA-C1A	5.22	109.05	106.71
21	2	618	CHL	C3D-C4D-ND	5.22	118.68	110.24
21	4	606	CHL	C3D-C4D-ND	5.22	118.68	110.24
21	8	606	CHL	C3D-C4D-ND	5.22	118.68	110.24
22	4	603	CLA	C4A-NA-C1A	5.22	109.05	106.71
22	B	841	CLA	C4A-NA-C1A	5.22	109.05	106.71
21	6	618	CHL	C3D-C4D-ND	5.21	118.67	110.24
21	6	601	CHL	C3D-C4D-ND	5.21	118.66	110.24
21	W	607	CHL	C3C-C4C-NC	5.20	116.25	110.57
21	7	608	CHL	C3D-C4D-ND	5.20	118.66	110.24
22	A	803	CLA	C4A-NA-C1A	5.20	109.05	106.71
21	5	601	CHL	C3D-C4D-ND	5.20	118.65	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	U	608	CHL	C3D-C4D-ND	5.19	118.64	110.24
21	U	605	CHL	C3C-C4C-NC	5.19	116.24	110.57
21	4	618	CHL	CAC-C3C-C4C	5.18	131.53	124.81
21	5	601	CHL	O2D-CGD-CBD	5.18	120.47	111.27
21	9	607	CHL	O2D-CGD-CBD	5.17	120.46	111.27
21	V	601	CHL	C3D-C4D-ND	5.17	118.60	110.24
21	1	601	CHL	O2D-CGD-CBD	5.16	120.45	111.27
21	W	607	CHL	O2D-CGD-CBD	5.16	120.44	111.27
21	V	607	CHL	C3C-C4C-NC	5.16	116.21	110.57
22	B	817	CLA	C4A-NA-C1A	5.16	109.03	106.71
22	B	829	CLA	C4A-NA-C1A	5.16	109.03	106.71
21	9	606	CHL	O2D-CGD-CBD	5.16	120.44	111.27
21	8	606	CHL	O2D-CGD-CBD	5.16	120.44	111.27
22	A	813	CLA	C4A-NA-C1A	5.16	109.03	106.71
21	V	606	CHL	C3C-C4C-NC	5.16	116.20	110.57
21	2	608	CHL	C3D-C4D-ND	5.16	118.58	110.24
21	2	601	CHL	C3D-C4D-ND	5.15	118.58	110.24
27	4	621	BCR	C7-C8-C9	-5.15	118.45	126.23
21	1	607	CHL	C3D-C4D-ND	5.15	118.56	110.24
22	A	854	CLA	C4A-NA-C1A	5.14	109.02	106.71
21	8	608	CHL	C3D-C4D-ND	5.14	118.56	110.24
27	M	2001	BCR	C11-C10-C9	-5.14	119.98	127.31
21	1	601	CHL	C3D-C4D-ND	5.13	118.54	110.24
24	3	619	XAT	O24-C25-C24	5.13	117.24	113.38
22	A	807	CLA	C4A-NA-C1A	5.12	109.01	106.71
22	6	603	CLA	C4A-NA-C1A	5.12	109.01	106.71
21	4	608	CHL	C3D-C4D-ND	5.12	118.52	110.24
25	W	2623	NEX	C11-C10-C9	-5.12	120.01	127.31
25	W	2623	NEX	C27-C28-C29	-5.11	117.59	125.53
23	5	617	LUT	C15-C35-C34	5.11	133.95	123.47
21	V	608	CHL	C3D-C4D-ND	5.11	118.50	110.24
24	1	618	XAT	O4-C5-C18	5.11	121.18	115.06
22	5	608	CLA	C4A-NA-C1A	5.11	109.00	106.71
21	U	601	CHL	C3D-C4D-ND	5.11	118.50	110.24
22	A	816	CLA	C4A-NA-C1A	5.11	109.00	106.71
22	9	602	CLA	C4A-NA-C1A	5.10	109.00	106.71
22	B	807	CLA	C4A-NA-C1A	5.10	109.00	106.71
21	W	605	CHL	C3C-C4C-NC	5.10	116.14	110.57
22	B	820	CLA	C4A-NA-C1A	5.09	109.00	106.71
27	8	621	BCR	C33-C5-C6	-5.09	118.81	124.53
21	4	606	CHL	C3C-C4C-NC	5.08	116.27	110.57
21	U	606	CHL	C3D-C2D-C1D	-5.08	98.90	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	840	CLA	C4A-NA-C1A	5.08	108.99	106.71
22	V	603	CLA	C4A-NA-C1A	5.08	108.99	106.71
27	L	301	BCR	C3-C4-C5	-5.08	105.01	114.08
21	8	608	CHL	C3D-C2D-C1D	-5.08	98.91	105.83
22	B	827	CLA	C4A-NA-C1A	5.07	108.99	106.71
27	A	852	BCR	C31-C1-C6	-5.07	102.08	110.30
21	9	606	CHL	C3D-C4D-ND	5.07	118.43	110.24
21	6	607	CHL	O2D-CGD-CBD	5.06	120.27	111.27
21	6	602	CHL	C3D-C2D-C1D	-5.05	98.94	105.83
27	M	2001	BCR	C28-C27-C26	-5.05	105.06	114.08
22	A	833	CLA	C4A-NA-C1A	5.04	108.97	106.71
21	2	606	CHL	C3D-C2D-C1D	-5.04	98.96	105.83
22	U	613	CLA	C4A-NA-C1A	5.03	108.97	106.71
27	L	305	BCR	C28-C27-C26	-5.03	105.09	114.08
21	W	608	CHL	C3C-C4C-NC	5.02	116.06	110.57
27	B	1609	BCR	C40-C30-C29	-5.02	88.81	108.91
21	4	618	CHL	C3D-C2D-C1D	-5.02	98.98	105.83
22	A	825	CLA	C4A-NA-C1A	5.02	108.96	106.71
22	8	604	CLA	C4A-NA-C1A	5.02	108.96	106.71
21	U	608	CHL	C3C-C4C-NC	5.02	116.05	110.57
21	2	601	CHL	C3D-C2D-C1D	-5.02	98.98	105.83
21	6	602	CHL	O2D-CGD-CBD	5.02	120.18	111.27
21	U	606	CHL	C3C-C4C-NC	5.01	116.19	110.57
21	2	607	CHL	C3D-C2D-C1D	-5.01	98.99	105.83
21	6	608	CHL	C3D-C2D-C1D	-5.01	98.99	105.83
22	A	826	CLA	C4A-NA-C1A	5.00	108.96	106.71
21	U	609	CHL	O2D-CGD-CBD	5.00	120.16	111.27
22	6	604	CLA	C4A-NA-C1A	5.00	108.95	106.71
21	W	607	CHL	C3D-C2D-C1D	-4.99	99.02	105.83
27	2	621	BCR	C11-C10-C9	-4.99	120.19	127.31
21	8	618	CHL	O2D-CGD-CBD	4.99	120.14	111.27
22	B	813	CLA	C4A-NA-C1A	4.99	108.95	106.71
24	2	620	XAT	C38-C25-C26	-4.99	113.90	122.26
21	W	606	CHL	C3C-C4C-NC	4.98	116.01	110.57
21	2	606	CHL	O2D-CGD-CBD	4.98	120.12	111.27
21	9	605	CHL	C3D-C2D-C1D	-4.98	99.03	105.83
22	4	601	CLA	C4A-NA-C1A	4.98	108.94	106.71
22	F	303	CLA	C4A-NA-C1A	4.98	108.94	106.71
22	1	616	CLA	C4A-NA-C1A	4.97	108.94	106.71
22	A	842	CLA	C4A-NA-C1A	4.97	108.94	106.71
27	B	848	BCR	C24-C23-C22	-4.97	118.73	126.23
21	6	601	CHL	C3D-C2D-C1D	-4.96	99.06	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	5	601	CHL	C3D-C2D-C1D	-4.96	99.06	105.83
21	V	607	CHL	C3D-C2D-C1D	-4.96	99.06	105.83
21	U	609	CHL	C3D-C2D-C1D	-4.96	99.07	105.83
21	9	606	CHL	C3D-C2D-C1D	-4.96	99.07	105.83
22	A	804	CLA	C4A-NA-C1A	4.95	108.93	106.71
27	7	620	BCR	C28-C27-C26	-4.95	105.24	114.08
22	1	613	CLA	C4A-NA-C1A	4.95	108.93	106.71
22	A	837	CLA	C4A-NA-C1A	4.95	108.93	106.71
21	W	609	CHL	C3D-C2D-C1D	-4.95	99.08	105.83
22	G	204	CLA	C4A-NA-C1A	4.94	108.93	106.71
22	9	609	CLA	CAC-C3C-C4C	4.94	131.22	124.81
22	3	614	CLA	C4A-NA-C1A	4.94	108.93	106.71
22	A	823	CLA	C4A-NA-C1A	4.94	108.93	106.71
22	1	606	CLA	C4A-NA-C1A	4.94	108.92	106.71
21	U	605	CHL	C3D-C2D-C1D	-4.93	99.10	105.83
24	5	618	XAT	C38-C25-C26	-4.93	113.99	122.26
22	A	819	CLA	C4A-NA-C1A	4.93	108.92	106.71
22	6	614	CLA	C4A-NA-C1A	4.93	108.92	106.71
21	9	605	CHL	C3C-C4C-NC	4.93	115.95	110.57
21	U	601	CHL	C3D-C2D-C1D	-4.93	99.10	105.83
21	8	607	CHL	O2D-CGD-CBD	4.93	120.03	111.27
21	6	607	CHL	C3C-C4C-NC	4.92	116.09	110.57
22	A	805	CLA	C4A-NA-C1A	4.92	108.92	106.71
21	6	618	CHL	CAC-C3C-C4C	4.92	131.19	124.81
22	2	611	CLA	C4A-NA-C1A	4.92	108.92	106.71
21	7	608	CHL	C3D-C2D-C1D	-4.92	99.12	105.83
21	6	618	CHL	C3D-C2D-C1D	-4.92	99.12	105.83
21	W	601	CHL	C3D-C2D-C1D	-4.91	99.13	105.83
21	2	601	CHL	C3C-C4C-NC	4.91	116.08	110.57
21	4	606	CHL	C3D-C2D-C1D	-4.91	99.13	105.83
21	U	607	CHL	C3C-C4C-NC	4.91	116.08	110.57
22	B	808	CLA	C4A-NA-C1A	4.91	108.91	106.71
23	8	619	LUT	C17-C1-C6	-4.91	102.34	110.30
21	V	609	CHL	C3D-C2D-C1D	-4.90	99.14	105.83
21	V	608	CHL	C3D-C2D-C1D	-4.90	99.14	105.83
21	9	607	CHL	C3D-C2D-C1D	-4.90	99.14	105.83
21	2	602	CHL	C3D-C2D-C1D	-4.90	99.15	105.83
24	5	618	XAT	O4-C5-C18	4.90	120.92	115.06
21	2	608	CHL	C3D-C2D-C1D	-4.89	99.15	105.83
21	W	605	CHL	C3D-C2D-C1D	-4.89	99.15	105.83
21	5	607	CHL	C3C-C4C-NC	4.89	116.06	110.57
21	8	606	CHL	C3C-C4C-NC	4.89	116.06	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	4	606	CHL	O2D-CGD-CBD	4.89	119.95	111.27
21	2	618	CHL	O2D-CGD-CBD	4.89	119.95	111.27
21	6	608	CHL	C3C-C4C-NC	4.89	116.05	110.57
21	5	607	CHL	C3D-C2D-C1D	-4.88	99.16	105.83
27	I	101	BCR	C33-C5-C6	-4.88	119.04	124.53
21	V	605	CHL	C3D-C2D-C1D	-4.88	99.17	105.83
21	1	601	CHL	C3D-C2D-C1D	-4.88	99.17	105.83
22	L	302	CLA	C4A-NA-C1A	4.88	108.90	106.71
21	W	609	CHL	CAC-C3C-C4C	4.88	131.14	124.81
21	6	607	CHL	C3D-C2D-C1D	-4.88	99.17	105.83
21	8	607	CHL	C3D-C2D-C1D	-4.88	99.17	105.83
22	U	604	CLA	C4A-NA-C1A	4.87	108.90	106.71
22	O	2001	CLA	C4A-NA-C1A	4.87	108.90	106.71
21	2	618	CHL	C3D-C2D-C1D	-4.87	99.18	105.83
22	A	808	CLA	C4A-NA-C1A	4.87	108.89	106.71
21	4	608	CHL	C3D-C2D-C1D	-4.86	99.19	105.83
22	1	604	CLA	C4A-NA-C1A	4.86	108.89	106.71
21	6	606	CHL	C3D-C2D-C1D	-4.86	99.19	105.83
27	F	305	BCR	C35-C13-C14	-4.86	116.11	122.92
22	A	843	CLA	C4A-NA-C1A	4.86	108.89	106.71
21	3	608	CHL	C3D-C2D-C1D	-4.86	99.20	105.83
27	7	621	BCR	C38-C26-C25	-4.86	119.07	124.53
21	8	608	CHL	C3C-C4C-NC	4.86	116.02	110.57
21	4	618	CHL	O2D-CGD-CBD	4.85	119.89	111.27
21	V	601	CHL	C3D-C2D-C1D	-4.85	99.21	105.83
21	6	606	CHL	C3C-C4C-NC	4.85	116.01	110.57
21	U	607	CHL	O2D-CGD-CBD	4.85	119.88	111.27
22	A	824	CLA	C4A-NA-C1A	4.84	108.88	106.71
22	7	606	CLA	C4A-NA-C1A	4.84	108.88	106.71
21	W	608	CHL	C3D-C2D-C1D	-4.84	99.23	105.83
21	8	606	CHL	C3D-C2D-C1D	-4.84	99.23	105.83
22	7	610	CLA	C4A-NA-C1A	4.84	108.88	106.71
22	A	822	CLA	C4A-NA-C1A	4.83	108.88	106.71
21	U	607	CHL	C3D-C2D-C1D	-4.83	99.24	105.83
21	8	608	CHL	CAC-C3C-C4C	4.83	131.07	124.81
21	3	608	CHL	C3D-C4D-ND	4.82	118.04	110.24
21	W	606	CHL	C3D-C2D-C1D	-4.82	99.25	105.83
21	V	605	CHL	C3C-C4C-NC	4.82	115.98	110.57
23	4	619	LUT	C17-C1-C6	-4.82	102.48	110.30
22	B	806	CLA	C4A-NA-C1A	4.82	108.87	106.71
27	O	2004	BCR	C20-C21-C22	-4.82	120.43	127.31
21	V	606	CHL	C3D-C2D-C1D	-4.82	99.26	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	831	CLA	C4A-NA-C1A	4.81	108.87	106.71
21	9	608	CHL	C3C-C4C-NC	4.81	115.97	110.57
27	1	619	BCR	C28-C27-C26	-4.81	105.49	114.08
27	B	845	BCR	C35-C13-C12	-4.80	110.51	118.08
21	V	601	CHL	CAC-C3C-C4C	4.80	131.04	124.81
22	A	839	CLA	C4A-NA-C1A	4.80	108.86	106.71
27	6	621	BCR	C11-C10-C9	-4.79	120.47	127.31
21	2	606	CHL	C3C-C4C-NC	4.79	115.94	110.57
21	4	607	CHL	C3D-C2D-C1D	-4.79	99.30	105.83
22	B	805	CLA	C4A-NA-C1A	4.78	108.86	106.71
22	B	836	CLA	C4A-NA-C1A	4.78	108.85	106.71
21	8	618	CHL	C3D-C2D-C1D	-4.77	99.32	105.83
22	U	602	CLA	C4A-NA-C1A	4.77	108.85	106.71
27	B	847	BCR	C23-C24-C25	-4.77	113.80	127.20
21	U	601	CHL	C3C-C4C-NC	4.77	115.92	110.57
22	A	801	CLA	O2D-CGD-CBD	4.77	119.75	111.27
21	U	608	CHL	C3D-C2D-C1D	-4.77	99.33	105.83
21	4	618	CHL	C3C-C4C-NC	4.76	115.91	110.57
22	B	823	CLA	C4A-NA-C1A	4.76	108.85	106.71
22	8	601	CLA	C4A-NA-C1A	4.76	108.84	106.71
27	O	2004	BCR	C24-C23-C22	-4.76	119.05	126.23
21	1	607	CHL	C3D-C2D-C1D	-4.76	99.34	105.83
21	5	601	CHL	C3C-C4C-NC	4.75	115.90	110.57
21	7	608	CHL	CAC-C3C-C4C	4.75	130.97	124.81
22	9	609	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
22	K	206	CLA	C4A-NA-C1A	4.74	108.84	106.71
21	4	608	CHL	CAC-C3C-C4C	4.73	130.95	124.81
21	8	607	CHL	C3C-C4C-NC	4.73	115.88	110.57
21	W	609	CHL	C3C-C4C-NC	4.73	115.88	110.57
21	9	606	CHL	C3C-C4C-NC	4.73	115.87	110.57
22	2	604	CLA	C4A-NA-C1A	4.72	108.83	106.71
22	B	816	CLA	C4A-NA-C1A	4.72	108.83	106.71
21	6	601	CHL	C3C-C4C-NC	4.72	115.86	110.57
22	3	617	CLA	CMB-C2B-C3B	4.72	130.79	125.30
21	2	602	CHL	C3C-C4C-NC	4.72	115.86	110.57
27	1	619	BCR	C37-C22-C23	4.72	125.51	118.08
22	B	812	CLA	C4A-NA-C1A	4.70	108.82	106.71
22	9	613	CLA	C4A-NA-C1A	4.69	108.82	106.71
21	9	608	CHL	C3D-C2D-C1D	-4.69	99.43	105.83
25	U	2623	NEX	C38-C25-C26	-4.69	114.40	122.26
21	W	601	CHL	C3C-C4C-NC	4.69	115.83	110.57
27	B	847	BCR	C38-C26-C25	-4.69	119.26	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1	602	CLA	C4A-NA-C1A	4.69	108.81	106.71
24	V	2622	XAT	C38-C25-C26	-4.69	114.41	122.26
27	B	801	BCR	C28-C27-C26	-4.68	105.72	114.08
22	3	613	CLA	C4A-NA-C1A	4.68	108.81	106.71
27	O	2004	BCR	C38-C26-C25	-4.67	119.28	124.53
27	8	621	BCR	C3-C4-C5	-4.67	105.74	114.08
22	4	612	CLA	C4A-NA-C1A	4.66	108.80	106.71
21	7	608	CHL	C3C-C4C-NC	4.66	115.79	110.57
21	2	602	CHL	O2D-CGD-CBD	4.65	119.54	111.27
21	6	602	CHL	CAC-C3C-C4C	4.65	130.85	124.81
21	2	607	CHL	C3C-C4C-NC	4.65	115.79	110.57
22	W	604	CLA	C4A-NA-C1A	4.65	108.80	106.71
21	9	601	CHL	C3C-C4C-NC	4.64	115.78	110.57
21	2	618	CHL	C3C-C4C-NC	4.64	115.78	110.57
25	W	2623	NEX	C5-C6-C1	4.64	124.30	119.70
21	1	601	CHL	C3C-C4C-NC	4.64	115.77	110.57
22	4	614	CLA	C4A-NA-C1A	4.62	108.78	106.71
22	A	836	CLA	CMB-C2B-C3B	4.62	130.67	125.30
22	B	834	CLA	C4A-NA-C1A	4.62	108.78	106.71
22	B	804	CLA	C4A-NA-C1A	4.62	108.78	106.71
22	B	839	CLA	C4A-NA-C1A	4.61	108.78	106.71
21	1	607	CHL	C3C-C4C-NC	4.61	115.74	110.57
21	V	601	CHL	C4-C3-C5	4.61	123.02	115.27
23	3	618	LUT	C8-C7-C6	-4.60	114.29	127.20
22	O	2003	CLA	C4A-NA-C1A	4.60	108.77	106.71
22	6	613	CLA	C4A-NA-C1A	4.60	108.77	106.71
21	U	609	CHL	CAC-C3C-C4C	4.59	130.77	124.81
22	G	203	CLA	C4A-NA-C1A	4.59	108.77	106.71
22	5	614	CLA	C4A-NA-C1A	4.59	108.77	106.71
21	V	601	CHL	C3C-C4C-NC	4.58	115.71	110.57
22	B	833	CLA	C4A-NA-C1A	4.58	108.76	106.71
21	U	609	CHL	C3C-C4C-NC	4.58	115.70	110.57
21	6	602	CHL	C3C-C4C-NC	4.57	115.70	110.57
22	A	854	CLA	CMB-C2B-C1B	-4.57	121.44	128.46
24	3	619	XAT	C38-C25-C26	-4.57	114.60	122.26
21	3	608	CHL	C3C-C4C-NC	4.57	115.69	110.57
21	8	618	CHL	C3C-C4C-NC	4.57	115.69	110.57
22	5	606	CLA	C4A-NA-C1A	4.56	108.76	106.71
22	A	827	CLA	C4A-NA-C1A	4.56	108.76	106.71
22	4	613	CLA	C4A-NA-C1A	4.56	108.76	106.71
22	B	836	CLA	CMB-C2B-C1B	-4.55	121.46	128.46
22	A	813	CLA	CMB-C2B-C1B	-4.55	121.47	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	6	618	CHL	C3C-C4C-NC	4.55	115.67	110.57
22	2	614	CLA	C4A-NA-C1A	4.54	108.75	106.71
22	A	812	CLA	C4A-NA-C1A	4.54	108.75	106.71
22	7	613	CLA	C4A-NA-C1A	4.54	108.75	106.71
21	U	607	CHL	CAC-C3C-C4C	4.53	130.69	124.81
22	F	301	CLA	C4A-NA-C1A	4.53	108.74	106.71
21	V	609	CHL	C3C-C4C-NC	4.53	115.65	110.57
22	7	614	CLA	C4A-NA-C1A	4.52	108.74	106.71
21	2	608	CHL	C3C-C4C-NC	4.52	115.64	110.57
27	6	621	BCR	C20-C21-C22	-4.52	120.86	127.31
27	3	620	BCR	C31-C1-C6	-4.52	102.97	110.30
22	5	602	CLA	C4A-NA-C1A	4.52	108.74	106.71
22	L	304	CLA	C4A-NA-C1A	4.51	108.73	106.71
22	4	611	CLA	C4A-NA-C1A	4.51	108.73	106.71
22	A	841	CLA	C4A-NA-C1A	4.51	108.73	106.71
24	5	618	XAT	O24-C25-C24	4.51	116.77	113.38
24	8	620	XAT	C35-C15-C14	4.50	132.70	123.47
22	3	609	CLA	O2D-CGD-CBD	4.50	119.26	111.27
27	A	849	BCR	C7-C8-C9	-4.49	119.45	126.23
22	B	819	CLA	C4A-NA-C1A	4.49	108.72	106.71
21	4	608	CHL	C3C-C4C-NC	4.49	115.60	110.57
21	V	601	CHL	C2C-C1C-NC	4.49	114.18	109.97
21	V	606	CHL	C2C-C1C-NC	4.49	114.17	109.97
22	7	615	CLA	C4A-NA-C1A	4.49	108.72	106.71
22	9	609	CLA	C3C-C4C-NC	4.48	115.60	110.57
21	3	608	CHL	CMB-C2B-C3B	4.48	133.06	124.68
21	U	606	CHL	CHD-C4C-C3C	-4.48	118.26	124.84
27	A	856	BCR	C28-C27-C26	-4.47	106.09	114.08
22	A	818	CLA	C4A-NA-C1A	4.47	108.72	106.71
22	W	613	CLA	C4A-NA-C1A	4.47	108.72	106.71
22	A	835	CLA	C4A-NA-C1A	4.46	108.71	106.71
21	1	607	CHL	O2D-CGD-CBD	4.46	119.20	111.27
21	9	608	CHL	O2D-CGD-CBD	4.46	119.19	111.27
21	U	605	CHL	C2C-C1C-NC	4.46	114.15	109.97
27	A	850	BCR	C7-C8-C9	-4.46	119.50	126.23
21	3	608	CHL	CAC-C3C-C4C	4.46	130.59	124.81
22	A	829	CLA	C4A-NA-C1A	4.46	108.71	106.71
27	B	844	BCR	C33-C5-C6	-4.45	119.53	124.53
22	B	802	CLA	C4A-NA-C1A	4.45	108.71	106.71
22	A	823	CLA	CMB-C2B-C1B	-4.44	121.63	128.46
22	B	830	CLA	C4A-NA-C1A	4.44	108.70	106.71
27	B	801	BCR	C20-C21-C22	-4.43	120.98	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	9	607	CHL	C3C-C4C-NC	4.43	115.54	110.57
22	B	837	CLA	C4A-NA-C1A	4.43	108.70	106.71
21	W	606	CHL	C2C-C1C-NC	4.43	114.12	109.97
21	4	607	CHL	O2D-CGD-CBD	4.42	119.13	111.27
27	1	619	BCR	C30-C25-C26	-4.42	116.39	122.61
27	B	843	BCR	C28-C27-C26	-4.42	106.19	114.08
22	3	604	CLA	C4A-NA-C1A	4.41	108.69	106.71
22	V	604	CLA	C4A-NA-C1A	4.41	108.69	106.71
27	3	621	BCR	C8-C7-C6	-4.40	114.84	127.20
27	A	849	BCR	C38-C26-C25	-4.40	119.59	124.53
22	V	614	CLA	C4A-NA-C1A	4.40	108.68	106.71
22	8	612	CLA	C4A-NA-C1A	4.40	108.68	106.71
27	4	621	BCR	C29-C30-C25	4.40	117.25	110.48
27	A	851	BCR	C30-C25-C24	4.40	128.21	115.78
24	V	2622	XAT	C17-C1-C6	-4.39	98.18	110.05
22	7	604	CLA	C4A-NA-C1A	4.39	108.68	106.71
22	9	603	CLA	C4A-NA-C1A	4.39	108.68	106.71
27	A	848	BCR	C11-C10-C9	-4.39	121.05	127.31
22	2	613	CLA	C4A-NA-C1A	4.38	108.68	106.71
32	B	850	DGD	O2G-C1B-C2B	4.38	120.95	111.50
22	B	818	CLA	C4A-NA-C1A	4.38	108.67	106.71
27	B	1609	BCR	C11-C10-C9	-4.38	121.07	127.31
22	3	607	CLA	C4A-NA-C1A	4.37	108.67	106.71
24	3	619	XAT	O24-C25-C38	4.37	120.29	115.06
27	A	850	BCR	C24-C23-C22	-4.37	119.64	126.23
21	2	608	CHL	CAC-C3C-C4C	4.37	130.48	124.81
21	4	607	CHL	CAC-C3C-C4C	4.36	130.47	124.81
22	5	613	CLA	C4A-NA-C1A	4.35	108.66	106.71
22	3	603	CLA	C4A-NA-C1A	4.35	108.66	106.71
22	H	201	CLA	C4A-NA-C1A	4.35	108.66	106.71
27	L	306	BCR	C20-C21-C22	-4.34	121.11	127.31
21	W	605	CHL	C2C-C1C-NC	4.34	114.04	109.97
24	8	620	XAT	C39-C29-C30	-4.34	116.84	122.92
23	V	2620	LUT	C17-C1-C6	-4.34	103.27	110.30
21	6	601	CHL	O2D-CGD-CBD	4.33	118.97	111.27
21	9	606	CHL	CAC-C3C-C4C	4.33	130.43	124.81
27	7	620	BCR	C3-C4-C5	-4.32	106.36	114.08
21	U	601	CHL	C2C-C1C-NC	4.32	114.02	109.97
22	B	815	CLA	C4A-NA-C1A	4.31	108.64	106.71
21	8	608	CHL	O2D-CGD-CBD	4.31	118.92	111.27
26	A	847	LHG	O7-C7-C8	4.30	120.77	111.50
21	8	618	CHL	CAC-C3C-C4C	4.30	130.39	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	850	BCR	C38-C26-C25	-4.30	119.70	124.53
27	A	851	BCR	C34-C9-C8	4.30	124.85	118.08
22	W	602	CLA	C4A-NA-C1A	4.30	108.64	106.71
22	A	829	CLA	CMB-C2B-C1B	-4.30	121.86	128.46
27	A	852	BCR	C34-C9-C10	-4.30	116.90	122.92
23	9	620	LUT	C17-C1-C6	-4.29	103.34	110.30
22	A	817	CLA	CMB-C2B-C1B	-4.29	121.87	128.46
22	B	811	CLA	C4A-NA-C1A	4.28	108.63	106.71
27	A	849	BCR	C20-C21-C22	-4.28	121.20	127.31
22	A	810	CLA	C4A-NA-C1A	4.28	108.63	106.71
22	B	819	CLA	C4-C3-C5	4.28	122.47	115.27
22	7	617	CLA	C4A-NA-C1A	4.28	108.63	106.71
21	4	607	CHL	C3C-C4C-NC	4.27	115.36	110.57
27	M	2001	BCR	C27-C26-C25	-4.27	116.53	122.73
27	6	621	BCR	C38-C26-C25	-4.27	119.73	124.53
22	A	820	CLA	CMB-C2B-C1B	-4.27	121.90	128.46
21	W	601	CHL	C2C-C1C-NC	4.27	113.97	109.97
22	V	611	CLA	C4A-NA-C1A	4.27	108.62	106.71
27	4	621	BCR	C11-C10-C9	-4.26	121.22	127.31
22	L	303	CLA	C4A-NA-C1A	4.26	108.62	106.71
21	U	601	CHL	CAC-C3C-C4C	4.26	130.34	124.81
22	A	811	CLA	C4A-NA-C1A	4.26	108.62	106.71
21	2	618	CHL	CAC-C3C-C4C	4.26	130.33	124.81
22	A	838	CLA	C4A-NA-C1A	4.26	108.62	106.71
22	5	603	CLA	C4A-NA-C1A	4.26	108.62	106.71
22	F	304	CLA	C4D-C3D-CAD	-4.25	109.18	121.60
27	3	621	BCR	C33-C5-C6	4.25	129.30	124.53
22	1	608	CLA	C4A-NA-C1A	4.25	108.61	106.71
28	2	631	LMG	O7-C10-C11	4.24	120.64	111.50
22	B	814	CLA	C4A-NA-C1A	4.24	108.61	106.71
27	B	845	BCR	C24-C23-C22	-4.24	119.83	126.23
27	G	205	BCR	C11-C10-C9	-4.24	121.26	127.31
23	5	617	LUT	C39-C29-C30	-4.23	116.99	122.92
21	9	601	CHL	C3D-C2D-C1D	-4.23	100.06	105.83
27	I	101	BCR	C24-C23-C22	-4.23	119.84	126.23
27	B	845	BCR	C15-C16-C17	-4.23	114.81	123.47
22	1	610	CLA	C4A-NA-C1A	4.22	108.60	106.71
23	5	617	LUT	C19-C9-C10	-4.22	117.01	122.92
22	3	609	CLA	O2D-CGD-O1D	-4.22	115.59	123.84
22	B	803	CLA	C4A-NA-C1A	4.22	108.60	106.71
22	9	604	CLA	C4A-NA-C1A	4.21	108.60	106.71
21	9	601	CHL	CAC-C3C-C4C	4.21	130.27	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3	609	CLA	C4A-NA-C1A	4.21	108.60	106.71
23	7	618	LUT	C17-C1-C6	-4.20	103.49	110.30
21	3	608	CHL	C4-C3-C5	4.20	122.33	115.27
22	O	2002	CLA	C4A-NA-C1A	4.20	108.59	106.71
22	A	809	CLA	C4A-NA-C1A	4.19	108.59	106.71
28	A	860	LMG	O7-C10-C11	4.19	120.53	111.50
21	4	606	CHL	CHD-C4C-C3C	-4.18	118.69	124.84
22	V	602	CLA	C4A-NA-C1A	4.18	108.59	106.71
22	A	821	CLA	C4A-NA-C1A	4.18	108.59	106.71
27	1	619	BCR	C16-C17-C18	-4.18	121.35	127.31
27	I	101	BCR	C38-C26-C25	-4.17	119.84	124.53
27	B	843	BCR	C20-C21-C22	-4.17	121.35	127.31
21	2	602	CHL	CHD-C4C-C3C	-4.17	118.71	124.84
24	1	618	XAT	C26-C27-C28	-4.17	117.18	125.99
21	8	606	CHL	CHD-C4C-C3C	-4.17	118.72	124.84
21	6	606	CHL	CHD-C4C-C3C	-4.16	118.72	124.84
24	8	620	XAT	C19-C9-C10	-4.16	117.10	122.92
22	3	612	CLA	C4A-NA-C1A	4.15	108.57	106.71
22	A	809	CLA	CMB-C2B-C1B	-4.15	122.08	128.46
21	2	606	CHL	CHD-C4C-C3C	-4.15	118.74	124.84
23	2	619	LUT	C19-C9-C10	-4.15	117.11	122.92
22	W	603	CLA	C4A-NA-C1A	4.15	108.57	106.71
22	8	602	CLA	C4A-NA-C1A	4.15	108.57	106.71
21	V	607	CHL	CHD-C4C-C3C	-4.15	118.50	124.98
22	A	805	CLA	CMB-C2B-C1B	-4.14	122.09	128.46
21	W	607	CHL	CHD-C4C-C3C	-4.14	118.51	124.98
21	7	608	CHL	O2D-CGD-CBD	4.14	118.63	111.27
27	4	621	BCR	C20-C21-C22	-4.14	121.40	127.31
21	6	607	CHL	CHD-C4C-C3C	-4.14	118.76	124.84
22	3	610	CLA	C4A-NA-C1A	4.14	108.57	106.71
27	4	621	BCR	C33-C5-C6	-4.13	119.89	124.53
27	K	205	BCR	C3-C4-C5	-4.13	106.70	114.08
27	3	621	BCR	C23-C24-C25	-4.13	115.61	127.20
23	V	2620	LUT	C11-C10-C9	-4.13	121.42	127.31
22	4	610	CLA	CMB-C2B-C1B	-4.13	122.12	128.46
27	L	306	BCR	C7-C8-C9	-4.12	120.01	126.23
22	B	838	CLA	C4A-NA-C1A	4.11	108.56	106.71
27	B	845	BCR	C28-C27-C26	-4.11	106.73	114.08
21	V	609	CHL	CAC-C3C-C4C	4.11	130.14	124.81
22	B	824	CLA	CMB-C2B-C1B	-4.11	122.15	128.46
24	4	620	XAT	C35-C34-C33	-4.11	121.45	127.31
23	W	2620	LUT	C11-C10-C9	-4.10	121.45	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	3	620	BCR	C37-C22-C23	4.10	124.54	118.08
22	A	838	CLA	CMB-C2B-C1B	-4.10	122.16	128.46
27	3	620	BCR	C7-C8-C9	-4.10	120.04	126.23
27	2	621	BCR	C30-C25-C26	-4.10	116.84	122.61
23	8	619	LUT	C3-C4-C5	-4.10	103.69	111.85
21	U	607	CHL	C4-C3-C5	4.09	122.16	115.27
22	B	835	CLA	C4A-NA-C1A	4.09	108.55	106.71
21	V	605	CHL	CHD-C4C-C3C	-4.09	118.83	124.84
22	W	610	CLA	CMB-C2B-C1B	-4.08	122.19	128.46
27	B	843	BCR	C37-C22-C23	4.08	124.51	118.08
27	A	849	BCR	C33-C5-C6	-4.08	119.95	124.53
22	B	828	CLA	C4A-NA-C1A	4.08	108.54	106.71
21	9	605	CHL	CHD-C4C-C3C	-4.07	118.62	124.98
22	5	616	CLA	C4A-NA-C1A	4.07	108.53	106.71
24	1	618	XAT	O24-C25-C38	4.07	119.93	115.06
22	A	815	CLA	C4A-NA-C1A	4.06	108.53	106.71
27	L	301	BCR	C37-C22-C23	4.06	124.47	118.08
22	A	854	CLA	CMB-C2B-C3B	4.06	132.27	124.68
27	1	619	BCR	C11-C10-C9	-4.06	121.52	127.31
27	B	1609	BCR	C30-C25-C26	-4.06	116.90	122.61
22	A	819	CLA	CMB-C2B-C1B	-4.06	122.23	128.46
22	4	609	CLA	C4A-NA-C1A	4.05	108.53	106.71
21	5	607	CHL	CHD-C4C-C3C	-4.05	118.88	124.84
22	A	828	CLA	CMB-C2B-C1B	-4.05	122.25	128.46
22	3	602	CLA	C4A-NA-C1A	4.05	108.53	106.71
27	J	102	BCR	C32-C1-C6	-4.05	103.74	110.30
21	W	609	CHL	C3B-C4B-NB	4.05	114.44	109.21
23	W	2620	LUT	C17-C1-C6	-4.04	103.74	110.30
27	O	2004	BCR	C31-C1-C6	-4.04	103.74	110.30
22	9	613	CLA	CMB-C2B-C1B	-4.04	122.26	128.46
22	2	610	CLA	C4A-NA-C1A	4.03	108.52	106.71
27	F	305	BCR	C7-C8-C9	-4.03	120.14	126.23
22	B	805	CLA	CMB-C2B-C1B	-4.03	122.28	128.46
21	8	607	CHL	CHD-C4C-C3C	-4.02	118.93	124.84
22	W	611	CLA	CMB-C2B-C1B	-4.02	122.29	128.46
22	B	836	CLA	CMB-C2B-C3B	4.02	132.20	124.68
23	4	619	LUT	C7-C8-C9	-4.02	120.16	126.23
23	W	2621	LUT	C17-C1-C6	-4.01	103.79	110.30
21	2	601	CHL	CHD-C4C-C3C	-4.01	118.94	124.84
22	7	603	CLA	C4A-NA-C1A	4.01	108.51	106.71
25	V	2623	NEX	C11-C10-C9	-4.01	121.59	127.31
27	K	202	BCR	C20-C21-C22	-4.01	121.59	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	7	609	CLA	C1D-ND-C4D	-4.01	103.49	106.33
22	A	831	CLA	C4A-NA-C1A	4.01	108.51	106.71
27	3	621	BCR	C20-C21-C22	-4.01	121.59	127.31
21	V	608	CHL	CHD-C4C-C3C	-4.01	118.72	124.98
27	L	306	BCR	C30-C25-C26	-4.01	116.97	122.61
23	9	620	LUT	C3-C4-C5	-4.00	103.88	111.85
24	6	620	XAT	C15-C14-C13	-4.00	121.60	127.31
27	2	621	BCR	C27-C26-C25	-4.00	116.92	122.73
21	U	601	CHL	C4C-C3C-C2C	-4.00	101.07	106.90
23	1	617	LUT	C17-C1-C6	-3.99	103.82	110.30
21	2	602	CHL	CAC-C3C-C4C	3.99	129.99	124.81
22	9	612	CLA	C4A-NA-C1A	3.99	108.50	106.71
22	9	609	CLA	C2C-C1C-NC	3.98	113.70	109.97
22	A	817	CLA	C4A-NA-C1A	3.98	108.50	106.71
22	A	801	CLA	O2D-CGD-O1D	-3.98	116.06	123.84
21	2	607	CHL	CAC-C3C-C4C	3.98	129.97	124.81
23	V	2621	LUT	C17-C1-C6	-3.98	103.84	110.30
27	B	845	BCR	C12-C13-C14	3.98	125.04	118.94
22	A	831	CLA	CMB-C2B-C1B	-3.98	122.35	128.46
22	U	611	CLA	C4A-NA-C1A	3.97	108.49	106.71
23	U	2620	LUT	C17-C1-C6	-3.97	103.86	110.30
27	B	843	BCR	C11-C10-C9	-3.97	121.64	127.31
25	9	623	NEX	C26-C27-C28	-3.97	117.60	125.99
24	5	618	XAT	C35-C34-C33	-3.97	121.65	127.31
27	3	620	BCR	C3-C4-C5	-3.97	107.00	114.08
27	G	205	BCR	C38-C26-C25	-3.96	120.08	124.53
22	9	602	CLA	CMB-C2B-C1B	-3.96	122.37	128.46
22	F	303	CLA	CMB-C2B-C1B	-3.96	122.38	128.46
24	U	2622	XAT	O24-C25-C38	3.96	119.80	115.06
24	V	2622	XAT	O24-C25-C38	3.96	119.80	115.06
21	8	608	CHL	CHD-C4C-C3C	-3.96	119.02	124.84
22	A	830	CLA	CMB-C2B-C1B	-3.95	122.39	128.46
27	K	202	BCR	C37-C22-C23	3.95	124.30	118.08
22	A	845	CLA	C4A-NA-C1A	3.95	108.48	106.71
23	2	619	LUT	C35-C15-C14	3.95	131.56	123.47
22	7	612	CLA	CMB-C2B-C1B	-3.95	122.40	128.46
22	9	611	CLA	C4A-NA-C1A	3.94	108.48	106.71
21	5	601	CHL	CHD-C4C-C3C	-3.94	119.05	124.84
21	6	601	CHL	CHD-C4C-C3C	-3.94	119.05	124.84
22	1	614	CLA	C4A-NA-C1A	3.93	108.47	106.71
21	6	606	CHL	CAC-C3C-C4C	3.93	129.91	124.81
21	W	601	CHL	CAC-C3C-C4C	3.93	129.91	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	9	608	CHL	CHD-C4C-C3C	-3.93	119.06	124.84
28	J	104	LMG	O7-C10-C11	3.93	119.96	111.50
22	4	602	CLA	C4A-NA-C1A	3.93	108.47	106.71
21	2	608	CHL	O2D-CGD-CBD	3.92	118.24	111.27
22	8	603	CLA	CMB-C2B-C1B	-3.92	122.44	128.46
22	A	803	CLA	CMB-C2B-C1B	-3.92	122.44	128.46
27	J	102	BCR	C38-C26-C25	-3.91	120.13	124.53
21	1	601	CHL	CHD-C4C-C3C	-3.91	119.09	124.84
21	V	601	CHL	C4C-C3C-C2C	-3.91	101.20	106.90
22	B	837	CLA	CMB-C2B-C1B	-3.91	122.45	128.46
22	A	829	CLA	O2D-CGD-O1D	-3.90	116.21	123.84
27	M	2001	BCR	C37-C22-C23	3.90	124.22	118.08
21	W	601	CHL	C4C-C3C-C2C	-3.90	101.22	106.90
22	B	813	CLA	CMB-C2B-C1B	-3.89	122.48	128.46
27	B	848	BCR	C28-C27-C26	-3.89	107.13	114.08
27	8	621	BCR	C16-C17-C18	-3.89	121.76	127.31
27	B	845	BCR	C38-C26-C25	-3.89	120.17	124.53
23	7	618	LUT	C7-C8-C9	-3.88	120.37	126.23
21	3	608	CHL	CHD-C4C-C3C	-3.88	119.14	124.84
22	A	814	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
22	3	615	CLA	CMB-C2B-C1B	-3.87	122.52	128.46
26	A	846	LHG	O7-C7-C8	3.86	119.83	111.50
22	8	614	CLA	C4A-NA-C1A	3.86	108.44	106.71
27	F	305	BCR	C33-C5-C6	-3.86	120.19	124.53
21	1	607	CHL	CHD-C4C-C3C	-3.86	119.17	124.84
22	W	602	CLA	CMB-C2B-C1B	-3.86	122.53	128.46
21	6	608	CHL	CHD-C4C-C3C	-3.86	119.17	124.84
21	W	608	CHL	CHD-C4C-C3C	-3.86	118.95	124.98
25	V	2623	NEX	C17-C1-C6	-3.85	107.02	110.47
21	U	605	CHL	CHD-C4C-C3C	-3.85	118.97	124.98
21	3	608	CHL	O2D-CGD-CBD	3.85	118.10	111.27
22	6	604	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
21	2	607	CHL	CHD-C4C-C3C	-3.84	119.20	124.84
22	5	604	CLA	C4A-NA-C1A	3.84	108.43	106.71
22	A	804	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
27	B	801	BCR	C16-C17-C18	-3.84	121.84	127.31
22	B	829	CLA	CMB-C2B-C1B	-3.83	122.57	128.46
22	1	609	CLA	C4A-NA-C1A	3.83	108.43	106.71
22	A	802	CLA	CMB-C2B-C1B	-3.83	122.57	128.46
27	L	306	BCR	C33-C5-C6	-3.83	120.23	124.53
27	B	847	BCR	C3-C4-C5	-3.82	107.25	114.08
21	U	608	CHL	CHD-C4C-C3C	-3.82	119.01	124.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	3	630	LHG	O7-C7-C8	3.82	119.73	111.50
22	A	822	CLA	CMB-C2B-C1B	-3.82	122.59	128.46
24	5	618	XAT	C31-C30-C29	-3.81	121.87	127.31
22	9	609	CLA	C4C-C3C-C2C	-3.81	101.34	106.90
22	A	836	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
21	9	607	CHL	CHD-C4C-C3C	-3.81	119.24	124.84
21	4	606	CHL	CAC-C3C-C4C	3.81	129.75	124.81
21	4	608	CHL	C3B-C4B-NB	3.81	114.13	109.21
22	6	609	CLA	CMB-C2B-C1B	-3.80	122.62	128.46
27	F	305	BCR	C3-C4-C5	-3.80	107.29	114.08
22	7	610	CLA	CMB-C2B-C1B	-3.80	122.63	128.46
27	J	102	BCR	C11-C10-C9	-3.79	121.89	127.31
27	A	852	BCR	C24-C23-C22	-3.79	120.50	126.23
22	A	820	CLA	C4A-NA-C1A	3.79	108.41	106.71
24	1	618	XAT	O4-C5-C4	3.79	116.23	113.38
22	B	828	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
22	B	816	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
22	V	604	CLA	CMB-C2B-C1B	-3.78	122.65	128.46
22	A	823	CLA	CMB-C2B-C3B	3.78	131.76	124.68
22	6	614	CLA	CMB-C2B-C1B	-3.78	122.65	128.46
22	B	814	CLA	CMB-C2B-C1B	-3.78	122.66	128.46
27	A	848	BCR	C38-C26-C25	-3.78	120.29	124.53
27	A	848	BCR	C7-C8-C9	-3.78	120.53	126.23
24	W	2622	XAT	O24-C25-C38	3.77	119.58	115.06
23	3	618	LUT	C7-C8-C9	-3.77	120.53	126.23
22	6	603	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
21	2	602	CHL	O2A-CGA-CBA	3.77	123.75	111.91
21	7	608	CHL	CHD-C4C-C3C	-3.77	119.30	124.84
21	W	605	CHL	CHD-C4C-C3C	-3.77	119.09	124.98
23	9	621	LUT	C3-C4-C5	-3.77	104.34	111.85
22	7	614	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
21	W	601	CHL	CHD-C4C-C3C	-3.77	119.30	124.84
21	9	608	CHL	CAC-C3C-C4C	3.77	129.70	124.81
22	A	839	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
27	7	620	BCR	C11-C10-C9	-3.77	121.94	127.31
22	3	602	CLA	CMB-C2B-C1B	-3.77	122.68	128.46
22	4	604	CLA	CMB-C2B-C1B	-3.77	122.68	128.46
22	A	813	CLA	CMB-C2B-C3B	3.76	131.72	124.68
27	3	621	BCR	C28-C27-C26	-3.76	107.36	114.08
23	U	2621	LUT	C7-C8-C9	-3.76	120.55	126.23
22	9	604	CLA	CMB-C2B-C1B	-3.76	122.68	128.46
27	B	1609	BCR	C24-C23-C22	-3.76	120.55	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	W	610	CLA	C4-C3-C5	3.76	121.59	115.27
27	K	205	BCR	C20-C21-C22	-3.76	121.95	127.31
21	3	608	CHL	C3B-C4B-NB	3.76	114.07	109.21
27	1	619	BCR	C23-C22-C21	-3.75	113.18	118.94
28	J	103	LMG	O7-C10-C11	3.75	119.59	111.50
22	K	203	CLA	C4A-NA-C1A	3.75	108.39	106.71
22	3	617	CLA	CMB-C2B-C1B	-3.75	122.70	128.46
21	V	606	CHL	CHD-C4C-C3C	-3.75	119.12	124.98
22	8	614	CLA	CMB-C2B-C1B	-3.75	122.70	128.46
23	V	2621	LUT	C11-C10-C9	-3.75	121.96	127.31
22	B	835	CLA	CMB-C2B-C1B	-3.75	122.71	128.46
21	U	607	CHL	CHD-C4C-C3C	-3.74	119.34	124.84
25	V	2623	NEX	C26-C27-C28	-3.74	118.08	125.99
22	B	807	CLA	CMB-C2B-C1B	-3.74	122.71	128.46
22	B	827	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
24	3	619	XAT	C26-C27-C28	-3.74	118.09	125.99
28	G	202	LMG	O7-C10-C11	3.74	119.56	111.50
27	B	1609	BCR	C23-C24-C25	-3.73	116.72	127.20
22	B	804	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
22	A	827	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
22	7	617	CLA	CMB-C2B-C1B	-3.73	122.74	128.46
25	V	2623	NEX	C2-C1-C6	3.72	112.83	109.21
27	2	621	BCR	C33-C5-C6	-3.72	120.35	124.53
27	B	845	BCR	C36-C18-C19	3.72	123.94	118.08
21	U	606	CHL	CAC-C3C-C4C	3.72	129.64	124.81
21	2	601	CHL	CAC-C3C-C4C	3.72	129.63	124.81
25	9	623	NEX	C39-C29-C30	-3.72	117.72	122.92
27	B	843	BCR	C24-C23-C22	-3.71	120.62	126.23
27	G	205	BCR	C15-C14-C13	-3.71	122.01	127.31
22	2	611	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
27	B	844	BCR	C38-C26-C25	-3.71	120.36	124.53
21	1	607	CHL	CAC-C3C-C4C	3.71	129.62	124.81
24	8	620	XAT	C12-C13-C14	3.71	124.63	118.94
21	9	606	CHL	CHD-C4C-C3C	-3.71	119.39	124.84
23	4	619	LUT	C3-C4-C5	-3.71	104.47	111.85
21	6	608	CHL	O2D-CGD-CBD	3.71	117.85	111.27
22	U	612	CLA	C4A-NA-C1A	3.71	108.37	106.71
27	A	848	BCR	C16-C17-C18	-3.70	122.02	127.31
27	J	102	BCR	C15-C14-C13	-3.70	122.03	127.31
21	4	608	CHL	O2D-CGD-CBD	3.70	117.84	111.27
22	B	839	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
22	8	610	CLA	CMB-C2B-C1B	-3.70	122.78	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	U	609	CHL	CHD-C4C-C3C	-3.70	119.41	124.84
22	A	829	CLA	CMB-C2B-C3B	3.70	131.59	124.68
26	7	630	LHG	O7-C7-C8	3.70	119.47	111.50
27	B	1609	BCR	C29-C30-C25	3.69	116.17	110.48
24	4	620	XAT	O24-C25-C38	3.69	119.48	115.06
22	5	606	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
22	U	610	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
23	2	619	LUT	C39-C29-C30	-3.69	117.75	122.92
22	A	825	CLA	C4-C3-C5	3.69	121.47	115.27
24	5	618	XAT	C15-C14-C13	-3.68	122.05	127.31
21	U	601	CHL	CHD-C4C-C3C	-3.68	119.42	124.84
27	4	621	BCR	C40-C30-C29	-3.68	94.17	108.91
22	B	822	CLA	C4A-NA-C1A	3.68	108.36	106.71
27	M	2001	BCR	C33-C5-C6	-3.68	120.40	124.53
23	5	617	LUT	C32-C33-C34	3.68	124.59	118.94
26	1	630	LHG	O7-C7-C8	3.68	119.43	111.50
22	A	838	CLA	CMB-C2B-C3B	3.68	131.56	124.68
22	A	820	CLA	CMB-C2B-C3B	3.67	131.55	124.68
22	W	604	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
24	4	620	XAT	C5-C4-C3	-3.67	105.48	112.75
27	B	848	BCR	C32-C1-C6	-3.67	104.34	110.30
24	3	619	XAT	C35-C15-C14	-3.67	115.95	123.47
24	6	620	XAT	O24-C25-C26	-3.67	55.92	58.96
23	V	2620	LUT	C7-C8-C9	-3.67	120.69	126.23
27	B	848	BCR	C11-C10-C9	-3.67	122.08	127.31
24	3	619	XAT	C35-C34-C33	-3.67	122.08	127.31
27	L	305	BCR	C35-C13-C12	3.66	123.85	118.08
22	8	609	CLA	CMB-C2B-C1B	-3.66	122.83	128.46
23	7	618	LUT	C3-C4-C5	-3.66	104.56	111.85
22	B	834	CLA	CMB-C2B-C1B	-3.66	122.83	128.46
23	9	621	LUT	C11-C10-C9	-3.66	122.09	127.31
22	W	614	CLA	C4A-NA-C1A	3.66	108.35	106.71
27	1	619	BCR	C36-C18-C19	3.66	123.84	118.08
22	L	302	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
22	G	201	CLA	C4A-NA-C1A	3.66	108.35	106.71
21	2	608	CHL	CHD-C4C-C3C	-3.66	119.47	124.84
21	2	618	CHL	CHD-C4C-C3C	-3.65	119.47	124.84
22	7	604	CLA	CMB-C2B-C1B	-3.65	122.85	128.46
27	2	621	BCR	C20-C21-C22	-3.65	122.10	127.31
25	U	2623	NEX	C26-C27-C28	-3.65	118.28	125.99
27	1	619	BCR	C7-C8-C9	-3.65	120.72	126.23
26	8	630	LHG	O7-C7-C8	3.65	119.36	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	851	LHG	O7-C7-C8	3.64	119.36	111.50
21	4	608	CHL	CHD-C4C-C3C	-3.64	119.48	124.84
21	6	601	CHL	CAC-C3C-C4C	3.64	129.54	124.81
24	8	620	XAT	C15-C35-C34	3.64	130.94	123.47
27	K	202	BCR	C37-C22-C21	-3.64	117.82	122.92
22	2	604	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
21	W	609	CHL	CHD-C4C-C3C	-3.64	119.49	124.84
22	U	604	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
24	8	620	XAT	C20-C13-C14	-3.64	117.83	122.92
22	B	803	CLA	CMB-C2B-C1B	-3.64	122.88	128.46
26	5	630	LHG	O7-C7-C8	3.63	119.33	111.50
22	W	612	CLA	CAB-C3B-C4B	-3.63	122.89	128.46
23	5	617	LUT	C40-C33-C34	-3.63	117.84	122.92
22	6	610	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
27	7	620	BCR	C37-C22-C23	3.62	123.79	118.08
21	W	606	CHL	CHD-C4C-C3C	-3.62	119.33	124.98
27	L	306	BCR	C37-C22-C21	-3.62	117.86	122.92
27	F	305	BCR	C20-C21-C22	-3.62	122.15	127.31
22	2	609	CLA	O2D-CGD-O1D	-3.61	116.77	123.84
22	A	807	CLA	CMB-C2B-C1B	-3.61	122.91	128.46
22	5	609	CLA	C1D-ND-C4D	-3.61	103.77	106.33
22	A	819	CLA	CMB-C2B-C3B	3.61	131.43	124.68
21	2	606	CHL	CAC-C3C-C4C	3.60	129.49	124.81
22	W	612	CLA	C4A-NA-C1A	3.60	108.33	106.71
22	7	607	CLA	CMB-C2B-C1B	-3.60	122.93	128.46
22	W	610	CLA	CMB-C2B-C3B	3.60	131.41	124.68
22	O	2002	CLA	CMB-C2B-C1B	-3.60	122.93	128.46
23	U	2620	LUT	C11-C10-C9	-3.60	122.18	127.31
22	A	824	CLA	CMB-C2B-C1B	-3.60	122.94	128.46
23	W	2620	LUT	C7-C8-C9	-3.60	120.80	126.23
21	V	609	CHL	CHD-C4C-C3C	-3.60	119.55	124.84
27	3	621	BCR	C16-C17-C18	-3.60	122.18	127.31
26	2	630	LHG	O7-C7-C8	3.59	119.25	111.50
21	8	607	CHL	CAC-C3C-C4C	3.59	129.47	124.81
22	A	811	CLA	CMB-C2B-C1B	-3.59	122.94	128.46
22	3	604	CLA	CMB-C2B-C1B	-3.59	122.95	128.46
24	7	619	XAT	O4-C5-C6	-3.59	55.99	58.96
24	6	620	XAT	C37-C21-C26	-3.58	100.37	110.05
27	2	621	BCR	C24-C23-C22	-3.58	120.82	126.23
22	4	613	CLA	CMB-C2B-C1B	-3.58	122.95	128.46
22	A	830	CLA	CMB-C2B-C3B	3.58	131.38	124.68
22	B	831	CLA	CMB-C2B-C1B	-3.58	122.96	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	G	201	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
22	3	613	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
23	9	621	LUT	C17-C1-C6	-3.58	104.49	110.30
27	7	621	BCR	C32-C1-C6	-3.58	104.50	110.30
25	9	623	NEX	O24-C25-C38	3.58	119.34	115.06
22	9	610	CLA	C4A-NA-C1A	3.58	108.31	106.71
27	B	847	BCR	C38-C26-C27	3.58	120.48	113.62
22	V	612	CLA	CAB-C3B-C4B	-3.57	122.97	128.46
21	6	602	CHL	CHD-C4C-C3C	-3.57	119.59	124.84
27	B	844	BCR	C30-C25-C24	3.57	125.87	115.78
24	8	620	XAT	C28-C29-C30	3.57	124.42	118.94
22	V	611	CLA	CAB-C3B-C4B	-3.57	122.98	128.46
27	B	847	BCR	C15-C14-C13	-3.57	122.22	127.31
22	W	613	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
26	U	2630	LHG	O7-C7-C8	3.56	119.18	111.50
22	2	614	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
22	F	301	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
24	6	620	XAT	C36-C21-C26	3.56	119.65	110.05
27	B	1609	BCR	C34-C9-C10	-3.56	117.94	122.92
22	W	611	CLA	C4A-NA-C1A	3.56	108.31	106.71
22	9	612	CLA	CMB-C2B-C1B	-3.56	123.00	128.46
22	5	610	CLA	CMB-C2B-C1B	-3.55	123.00	128.46
22	7	602	CLA	CMB-C2B-C1B	-3.55	123.00	128.46
22	B	821	CLA	C4A-NA-C1A	3.55	108.30	106.71
27	B	845	BCR	C10-C11-C12	-3.55	112.14	123.22
22	A	803	CLA	CMB-C2B-C3B	3.55	131.32	124.68
22	A	817	CLA	CMB-C2B-C3B	3.54	131.31	124.68
22	W	614	CLA	CAB-C3B-C4B	-3.54	123.02	128.46
27	7	621	BCR	C37-C22-C23	3.54	123.66	118.08
27	J	102	BCR	C20-C21-C22	-3.54	122.25	127.31
23	V	2621	LUT	C3-C4-C5	-3.54	104.80	111.85
22	A	815	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
25	V	2623	NEX	C4-C3-C2	-3.54	103.94	110.77
22	3	610	CLA	CMB-C2B-C1B	-3.54	123.03	128.46
22	4	614	CLA	CMB-C2B-C1B	-3.54	123.03	128.46
22	A	833	CLA	CMB-C2B-C1B	-3.54	123.03	128.46
27	L	306	BCR	C3-C4-C5	-3.54	107.76	114.08
21	9	601	CHL	CHD-C4C-C3C	-3.54	119.64	124.84
22	U	613	CLA	CMB-C2B-C1B	-3.54	123.03	128.46
22	5	614	CLA	CMB-C2B-C1B	-3.53	123.03	128.46
22	L	303	CLA	CMB-C2B-C1B	-3.53	123.03	128.46
26	W	2630	LHG	O7-C7-C8	3.53	119.12	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1	604	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
27	B	843	BCR	C37-C22-C21	-3.53	117.98	122.92
27	L	306	BCR	C27-C26-C25	-3.53	117.61	122.73
27	A	848	BCR	C24-C23-C22	-3.53	120.91	126.23
21	5	601	CHL	CAC-C3C-C4C	3.53	129.38	124.81
22	8	611	CLA	CMB-C2B-C1B	-3.52	123.05	128.46
24	1	618	XAT	C28-C29-C30	-3.52	113.53	118.94
22	A	809	CLA	O2D-CGD-O1D	-3.52	116.95	123.84
23	6	619	LUT	C15-C14-C13	-3.52	122.29	127.31
22	B	820	CLA	CMB-C2B-C1B	-3.52	123.05	128.46
24	8	620	XAT	C40-C33-C34	-3.52	117.99	122.92
22	V	611	CLA	CMB-C2B-C1B	-3.52	123.06	128.46
27	K	202	BCR	C32-C1-C6	-3.52	104.59	110.30
22	A	845	CLA	CMB-C2B-C1B	-3.52	123.06	128.46
27	B	845	BCR	C33-C5-C6	-3.52	120.58	124.53
22	K	203	CLA	CMB-C2B-C1B	-3.51	123.06	128.46
22	G	203	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
22	2	613	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
22	4	604	CLA	CMB-C2B-C3B	3.51	131.24	124.68
22	V	613	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
22	8	611	CLA	C4A-NA-C1A	3.50	108.28	106.71
22	5	604	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
22	A	832	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
22	4	610	CLA	C1D-ND-C4D	-3.50	103.85	106.33
22	A	809	CLA	CMB-C2B-C3B	3.50	131.22	124.68
22	5	611	CLA	C4A-NA-C1A	3.49	108.28	106.71
22	V	610	CLA	C4A-NA-C1A	3.49	108.28	106.71
22	9	609	CLA	CHD-C4C-C3C	-3.49	119.71	124.84
27	3	620	BCR	C2-C1-C6	3.49	115.85	110.48
27	M	2001	BCR	C29-C30-C25	3.49	115.85	110.48
21	9	605	CHL	C2A-C1A-CHA	-3.48	117.77	123.85
27	A	852	BCR	C20-C21-C22	-3.48	122.34	127.31
22	B	815	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
22	5	611	CLA	O2D-CGD-O1D	-3.48	117.03	123.84
22	2	612	CLA	C4A-NA-C1A	3.48	108.27	106.71
23	V	2620	LUT	C3-C4-C5	-3.48	104.92	111.85
22	4	611	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
22	K	201	CLA	CMB-C2B-C1B	-3.48	123.12	128.46
27	1	619	BCR	C24-C23-C22	-3.48	120.98	126.23
21	8	618	CHL	CHD-C4C-C3C	-3.48	119.73	124.84
27	A	849	BCR	C11-C10-C9	-3.47	122.35	127.31
27	B	843	BCR	C1-C6-C5	-3.47	117.72	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	4	620	XAT	C11-C10-C9	-3.47	122.35	127.31
24	5	618	XAT	C28-C29-C30	-3.47	113.61	118.94
22	3	611	CLA	O2D-CGD-O1D	-3.47	117.05	123.84
27	B	1609	BCR	C38-C26-C25	-3.47	120.63	124.53
22	G	204	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
22	K	203	CLA	O2D-CGD-O1D	-3.47	117.05	123.84
27	L	305	BCR	C15-C14-C13	-3.47	122.36	127.31
22	A	801	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
27	B	1609	BCR	C4-C5-C6	-3.47	117.70	122.73
22	B	825	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
22	W	611	CLA	CAB-C3B-C4B	-3.47	123.14	128.46
22	U	612	CLA	CMB-C2B-C1B	-3.47	123.14	128.46
22	5	612	CLA	CMB-C2B-C1B	-3.47	123.14	128.46
27	K	202	BCR	C11-C10-C9	-3.46	122.36	127.31
22	A	825	CLA	CHD-C1D-ND	-3.46	121.27	124.45
27	A	849	BCR	C37-C22-C23	3.46	123.53	118.08
23	W	2620	LUT	C3-C4-C5	-3.46	104.97	111.85
26	6	630	LHG	O7-C7-C8	3.46	118.95	111.50
22	5	602	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
22	B	824	CLA	CMB-C2B-C3B	3.46	131.14	124.68
27	L	305	BCR	C24-C23-C22	-3.46	121.01	126.23
27	L	301	BCR	C16-C17-C18	-3.46	122.38	127.31
22	9	602	CLA	CMB-C2B-C3B	3.45	131.14	124.68
22	6	612	CLA	C4A-NA-C1A	3.45	108.26	106.71
26	V	2630	LHG	O7-C7-C8	3.45	118.94	111.50
21	W	609	CHL	CHB-C4A-NA	3.45	129.28	124.51
22	3	612	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
24	4	620	XAT	C6-C7-C8	-3.45	118.70	125.99
21	9	601	CHL	C2A-C1A-CHA	-3.45	117.83	123.85
27	B	847	BCR	C8-C7-C6	-3.45	117.52	127.20
22	U	610	CLA	C4A-NA-C1A	3.45	108.26	106.71
22	B	822	CLA	O2D-CGD-O1D	-3.45	117.10	123.84
22	2	612	CLA	CMB-C2B-C1B	-3.45	123.17	128.46
24	2	620	XAT	O24-C25-C38	3.45	119.18	115.06
27	A	848	BCR	C34-C9-C10	-3.44	118.10	122.92
22	F	303	CLA	CMB-C2B-C3B	3.44	131.12	124.68
22	1	602	CLA	CMB-C2B-C1B	-3.44	123.17	128.46
22	A	818	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
21	6	618	CHL	CHD-C4C-C3C	-3.44	119.78	124.84
22	5	608	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
27	M	2001	BCR	C3-C4-C5	-3.44	107.94	114.08
22	2	603	CLA	CMB-C2B-C1B	-3.44	123.18	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	805	CLA	CMB-C2B-C3B	3.43	131.10	124.68
22	V	613	CLA	C4A-NA-C1A	3.43	108.25	106.71
26	4	630	LHG	O7-C7-C8	3.43	118.89	111.50
22	6	610	CLA	C4A-NA-C1A	3.43	108.25	106.71
22	4	610	CLA	CMB-C2B-C3B	3.43	131.09	124.68
22	1	610	CLA	CMB-C2B-C1B	-3.43	123.20	128.46
22	3	602	CLA	CMB-C2B-C3B	3.43	131.09	124.68
22	8	602	CLA	CMB-C2B-C1B	-3.43	123.20	128.46
27	1	619	BCR	C38-C26-C25	3.42	128.37	124.53
23	U	2621	LUT	C11-C10-C9	-3.42	122.43	127.31
27	8	621	BCR	C11-C10-C9	-3.42	122.43	127.31
21	4	607	CHL	CHD-C4C-C3C	-3.42	119.81	124.84
22	8	601	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
22	B	805	CLA	CMB-C2B-C3B	3.42	131.07	124.68
22	V	614	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
22	B	841	CLA	CMB-C2B-C1B	-3.42	123.22	128.46
22	6	611	CLA	CMB-C2B-C1B	-3.42	123.22	128.46
21	9	601	CHL	CMD-C2D-C3D	-3.41	119.76	127.61
22	W	602	CLA	CMB-C2B-C3B	3.41	131.06	124.68
22	A	828	CLA	CMB-C2B-C3B	3.41	131.06	124.68
23	1	617	LUT	C8-C7-C6	-3.41	117.62	127.20
22	1	611	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
22	B	818	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
22	7	611	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
22	3	603	CLA	CMB-C2B-C1B	-3.41	123.23	128.46
22	1	612	CLA	C4A-NA-C1A	3.41	108.24	106.71
22	B	822	CLA	C4-C3-C5	3.41	121.00	115.27
22	3	614	CLA	CMB-C2B-C1B	-3.41	123.23	128.46
22	W	603	CLA	CMB-C2B-C1B	-3.41	123.23	128.46
22	4	609	CLA	CMB-C2B-C1B	-3.41	123.23	128.46
23	5	617	LUT	C20-C13-C14	-3.41	118.15	122.92
27	I	101	BCR	C20-C21-C22	-3.40	122.45	127.31
22	W	610	CLA	C4A-NA-C1A	3.40	108.24	106.71
22	A	829	CLA	O2D-CGD-CBD	3.40	117.31	111.27
22	4	612	CLA	CMB-C2B-C1B	-3.40	123.23	128.46
27	A	848	BCR	C20-C21-C22	-3.40	122.45	127.31
22	7	612	CLA	CMB-C2B-C3B	3.40	131.04	124.68
27	1	619	BCR	C3-C4-C5	-3.40	108.00	114.08
22	U	611	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
27	L	306	BCR	C38-C26-C25	3.40	128.34	124.53
27	B	844	BCR	C11-C10-C9	-3.40	122.46	127.31
23	1	617	LUT	C7-C8-C9	-3.40	121.10	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	810	CLA	CMB-C2B-C1B	-3.40	123.25	128.46
27	L	301	BCR	C38-C26-C25	-3.39	120.72	124.53
24	7	619	XAT	O24-C25-C26	-3.39	56.15	58.96
22	9	609	CLA	CMD-C2D-C3D	-3.39	119.81	127.61
23	U	2621	LUT	C17-C1-C6	-3.39	104.80	110.30
27	B	848	BCR	C34-C9-C8	3.39	123.42	118.08
22	A	843	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
27	G	205	BCR	C30-C25-C26	-3.39	117.84	122.61
22	A	841	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
22	5	611	CLA	CMB-C2B-C1B	-3.38	123.26	128.46
24	1	618	XAT	C18-C5-C4	3.38	118.09	114.28
22	B	837	CLA	CMB-C2B-C3B	3.38	131.00	124.68
22	W	614	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
22	1	614	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
22	B	832	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
27	A	850	BCR	C20-C21-C22	-3.38	122.49	127.31
27	B	843	BCR	C15-C14-C13	-3.38	122.49	127.31
21	6	607	CHL	CAC-C3C-C4C	3.38	129.19	124.81
22	1	608	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
23	9	621	LUT	C1-C6-C5	-3.37	117.86	122.61
27	8	621	BCR	C36-C18-C19	3.37	123.39	118.08
24	V	2622	XAT	C16-C1-C6	3.37	119.15	110.05
27	G	205	BCR	C24-C23-C22	-3.37	121.14	126.23
22	B	822	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
24	6	620	XAT	O4-C5-C6	-3.37	56.17	58.96
22	8	612	CLA	CMB-C2B-C1B	-3.37	123.29	128.46
21	5	607	CHL	CAC-C3C-C4C	3.37	129.18	124.81
22	B	805	CLA	O2D-CGD-O1D	-3.37	117.25	123.84
25	V	2623	NEX	C39-C29-C30	-3.37	118.21	122.92
21	V	608	CHL	CHB-C4A-NA	3.36	129.16	124.51
27	B	801	BCR	C37-C22-C23	3.36	123.38	118.08
22	V	603	CLA	CMB-C2B-C1B	-3.36	123.29	128.46
27	B	801	BCR	C37-C22-C21	-3.36	118.21	122.92
23	U	2621	LUT	C19-C9-C8	3.36	123.37	118.08
23	U	2621	LUT	C1-C6-C5	-3.36	117.88	122.61
22	B	813	CLA	CMB-C2B-C3B	3.36	130.97	124.68
22	B	807	CLA	O2D-CGD-O1D	-3.36	117.27	123.84
21	V	605	CHL	CAC-C3C-C4C	3.36	129.17	124.81
22	B	823	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
22	6	609	CLA	C4A-NA-C1A	3.35	108.21	106.71
27	A	849	BCR	C3-C4-C5	-3.35	108.09	114.08
22	2	610	CLA	CMB-C2B-C1B	-3.35	123.31	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	5	617	LUT	C12-C13-C14	3.35	124.08	118.94
22	A	801	CLA	C1D-ND-C4D	-3.35	103.96	106.33
22	2	609	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
21	W	608	CHL	C2A-C1A-CHA	-3.34	118.01	123.86
22	3	611	CLA	C4A-NA-C1A	3.34	108.21	106.71
22	B	819	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
24	5	618	XAT	C11-C10-C9	-3.34	122.54	127.31
25	U	2623	NEX	C27-C28-C29	-3.34	120.35	125.53
22	B	806	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
22	A	812	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
21	W	606	CHL	CHB-C4A-NA	3.34	129.13	124.51
24	5	618	XAT	C39-C29-C28	3.34	123.34	118.08
22	1	603	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
22	3	607	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
24	2	620	XAT	C18-C5-C6	-3.34	116.67	122.26
27	7	621	BCR	C23-C24-C25	-3.34	117.83	127.20
22	4	602	CLA	CMB-C2B-C1B	-3.33	123.34	128.46
27	B	1609	BCR	C20-C21-C22	-3.33	122.55	127.31
22	B	821	CLA	CMB-C2B-C1B	-3.33	123.34	128.46
22	A	808	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
24	7	619	XAT	C16-C1-C2	-3.33	103.20	108.98
22	V	610	CLA	CAB-C3B-C4B	-3.33	123.35	128.46
22	1	616	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
21	V	601	CHL	CHD-C4C-C3C	-3.32	119.95	124.84
22	5	603	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
22	B	810	CLA	O2D-CGD-O1D	-3.32	117.34	123.84
22	A	830	CLA	C1B-CHB-C4A	-3.32	123.54	130.12
27	F	305	BCR	C37-C22-C23	3.32	123.31	118.08
27	A	849	BCR	C36-C18-C19	3.32	123.31	118.08
22	B	812	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
27	6	621	BCR	C33-C5-C4	3.32	119.99	113.62
22	B	839	CLA	CMB-C2B-C3B	3.31	130.88	124.68
22	U	614	CLA	CMB-C2B-C1B	-3.31	123.37	128.46
24	W	2622	XAT	O4-C5-C18	3.31	119.03	115.06
27	B	847	BCR	C20-C21-C22	-3.31	122.58	127.31
22	7	602	CLA	O2D-CGD-O1D	-3.31	117.36	123.84
22	W	612	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
27	3	620	BCR	C1-C6-C5	-3.31	117.95	122.61
27	3	621	BCR	C11-C10-C9	-3.31	122.58	127.31
23	2	619	LUT	C40-C33-C34	-3.31	118.29	122.92
22	A	820	CLA	O2D-CGD-O1D	-3.31	117.37	123.84
22	3	606	CLA	CMB-C2B-C1B	-3.31	123.38	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	838	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
22	1	613	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
22	B	833	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
21	4	618	CHL	CHD-C4C-C3C	-3.30	119.98	124.84
21	W	606	CHL	C2A-C1A-CHA	-3.30	118.09	123.85
27	B	843	BCR	C27-C26-C25	-3.30	117.94	122.73
22	8	610	CLA	C4A-NA-C1A	3.30	108.19	106.71
21	6	602	CHL	CHB-C4A-NA	3.30	129.08	124.51
23	2	619	LUT	C20-C13-C14	-3.30	118.30	122.92
27	7	621	BCR	C38-C26-C27	3.30	119.96	113.62
22	B	831	CLA	C4-C3-C5	3.30	120.82	115.27
22	A	805	CLA	O2D-CGD-O1D	-3.30	117.39	123.84
22	1	609	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
22	K	206	CLA	CMB-C2B-C1B	-3.30	123.40	128.46
22	L	304	CLA	CMB-C2B-C1B	-3.30	123.40	128.46
23	U	2620	LUT	C3-C4-C5	-3.30	105.29	111.85
23	9	621	LUT	C19-C9-C8	3.30	123.27	118.08
22	A	831	CLA	CMB-C2B-C3B	3.29	130.84	124.68
27	B	843	BCR	C36-C18-C19	3.29	123.27	118.08
24	V	2622	XAT	O4-C5-C6	-3.29	56.23	58.96
22	A	825	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
25	U	2623	NEX	C39-C29-C30	-3.29	118.32	122.92
22	A	804	CLA	CMB-C2B-C3B	3.29	130.83	124.68
22	3	611	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
27	A	852	BCR	C30-C25-C26	-3.29	117.98	122.61
27	A	852	BCR	C38-C26-C25	-3.28	120.84	124.53
22	B	827	CLA	CMB-C2B-C3B	3.28	130.82	124.68
22	5	616	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
22	6	612	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
22	A	816	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
22	B	808	CLA	O2D-CGD-O1D	-3.28	117.43	123.84
22	4	603	CLA	CMB-C2B-C1B	-3.28	123.43	128.46
27	6	621	BCR	C15-C14-C13	-3.28	122.63	127.31
21	V	605	CHL	C2A-C1A-CHA	-3.28	118.13	123.85
21	4	608	CHL	CHB-C4A-NA	3.27	129.04	124.51
27	B	848	BCR	C8-C7-C6	-3.27	118.01	127.20
27	8	621	BCR	C8-C7-C6	-3.27	118.02	127.20
27	7	621	BCR	C4-C5-C6	-3.27	117.98	122.73
23	W	2621	LUT	C3-C4-C5	-3.27	105.34	111.85
22	6	609	CLA	CMB-C2B-C3B	3.27	130.79	124.68
22	7	609	CLA	C1B-CHB-C4A	-3.26	123.65	130.12
23	9	620	LUT	C11-C10-C9	-3.26	122.65	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	848	BCR	C20-C21-C22	-3.26	122.65	127.31
22	B	814	CLA	CMB-C2B-C3B	3.26	130.78	124.68
22	B	803	CLA	C1B-CHB-C4A	-3.26	123.66	130.12
22	A	804	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
23	9	621	LUT	C36-C21-C26	3.26	114.48	109.55
22	A	806	CLA	CMB-C2B-C1B	-3.26	123.45	128.46
21	U	601	CHL	CHB-C4A-NA	3.26	129.02	124.51
27	B	845	BCR	C23-C22-C21	3.26	123.94	118.94
22	3	609	CLA	CMB-C2B-C1B	-3.26	123.46	128.46
22	1	612	CLA	CMB-C2B-C1B	-3.26	123.46	128.46
22	7	613	CLA	CMB-C2B-C1B	-3.25	123.46	128.46
28	L	307	LMG	O7-C10-C11	3.25	118.51	111.50
22	7	610	CLA	CMB-C2B-C3B	3.25	130.76	124.68
27	G	205	BCR	C15-C16-C17	-3.25	116.82	123.47
27	3	621	BCR	C38-C26-C27	3.25	119.85	113.62
27	2	621	BCR	C7-C8-C9	-3.25	121.33	126.23
22	J	101	CLA	CMB-C2B-C1B	-3.25	123.48	128.46
27	B	843	BCR	C34-C9-C8	3.25	123.19	118.08
27	B	801	BCR	C36-C18-C19	3.24	123.19	118.08
22	A	814	CLA	CMB-C2B-C3B	3.24	130.74	124.68
22	A	826	CLA	CMB-C2B-C1B	-3.24	123.49	128.46
21	U	605	CHL	C2A-C1A-CHA	-3.24	118.20	123.85
23	6	619	LUT	C15-C35-C34	-3.24	116.84	123.47
22	9	610	CLA	CMB-C2B-C1B	-3.24	123.49	128.46
22	B	810	CLA	CMB-C2B-C1B	-3.24	123.49	128.46
22	B	826	CLA	CMB-C2B-C1B	-3.24	123.49	128.46
22	B	817	CLA	CMB-C2B-C1B	-3.23	123.50	128.46
22	4	610	CLA	C1B-CHB-C4A	-3.23	123.72	130.12
27	A	848	BCR	C30-C25-C26	-3.23	118.07	122.61
22	A	824	CLA	O2D-CGD-O1D	-3.23	117.53	123.84
22	V	612	CLA	CMB-C2B-C1B	-3.23	123.51	128.46
24	1	618	XAT	C6-C7-C8	-3.22	119.18	125.99
22	V	602	CLA	CMB-C2B-C1B	-3.22	123.51	128.46
22	7	614	CLA	CMB-C2B-C3B	3.22	130.71	124.68
27	K	202	BCR	C34-C9-C8	3.22	123.15	118.08
21	6	618	CHL	C3B-C4B-NB	3.22	113.37	109.21
22	8	614	CLA	CMB-C2B-C3B	3.22	130.70	124.68
27	M	2001	BCR	C20-C21-C22	-3.22	122.72	127.31
24	5	618	XAT	C31-C32-C33	-3.22	117.38	126.42
22	9	610	CLA	C1B-CHB-C4A	-3.22	123.75	130.12
22	V	602	CLA	O2D-CGD-O1D	-3.22	117.55	123.84
21	8	606	CHL	CAC-C3C-C4C	3.22	128.98	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3	615	CLA	CMB-C2B-C3B	3.22	130.69	124.68
27	A	851	BCR	C30-C25-C26	-3.21	118.08	122.61
21	V	601	CHL	O2A-CGA-CBA	3.21	122.00	111.91
27	B	844	BCR	C1-C6-C7	3.21	124.87	115.78
22	7	603	CLA	CMB-C2B-C1B	-3.21	123.52	128.46
27	7	620	BCR	C33-C5-C6	-3.21	120.92	124.53
22	V	613	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
22	K	204	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
27	B	843	BCR	C29-C30-C25	3.21	115.42	110.48
24	7	619	XAT	C39-C29-C28	3.21	123.14	118.08
27	L	301	BCR	C16-C15-C14	-3.21	116.90	123.47
21	V	605	CHL	C3B-C4B-NB	3.21	113.36	109.21
21	W	607	CHL	CHB-C4A-NA	3.21	128.95	124.51
21	9	606	CHL	C3B-C4B-NB	3.21	113.36	109.21
21	9	606	CHL	CHB-C4A-NA	3.21	128.94	124.51
27	A	851	BCR	C24-C25-C26	-3.21	113.70	121.46
21	1	601	CHL	CAC-C3C-C4C	3.20	128.97	124.81
27	A	851	BCR	C38-C26-C27	3.20	119.77	113.62
22	4	601	CLA	CMB-C2B-C1B	-3.20	123.54	128.46
23	9	620	LUT	C19-C9-C8	3.20	123.12	118.08
27	L	305	BCR	C36-C18-C19	3.20	123.12	118.08
24	6	620	XAT	C27-C28-C29	-3.20	120.56	125.53
23	3	618	LUT	C17-C1-C6	-3.20	105.11	110.30
22	U	610	CLA	CMB-C2B-C3B	3.20	130.66	124.68
22	9	609	CLA	C2A-C1A-CHA	-3.20	118.27	123.86
23	6	619	LUT	C7-C8-C9	-3.20	121.40	126.23
27	B	801	BCR	C24-C23-C22	-3.20	121.40	126.23
27	A	849	BCR	C16-C17-C18	-3.20	122.75	127.31
22	2	609	CLA	C1B-CHB-C4A	-3.20	123.79	130.12
22	A	834	CLA	O2D-CGD-O1D	-3.20	117.59	123.84
22	B	828	CLA	CMB-C2B-C3B	3.20	130.66	124.68
21	3	608	CHL	CHB-C4A-NA	3.19	128.93	124.51
22	A	803	CLA	O2D-CGD-O1D	-3.19	117.59	123.84
22	7	611	CLA	O2D-CGD-O1D	-3.19	117.59	123.84
22	B	835	CLA	CMB-C2B-C3B	3.19	130.65	124.68
22	B	818	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
22	B	831	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
22	A	835	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
27	A	852	BCR	C7-C8-C9	-3.19	121.42	126.23
22	B	804	CLA	CMB-C2B-C3B	3.19	130.64	124.68
22	A	854	CLA	C1B-CHB-C4A	-3.19	123.81	130.12
22	A	815	CLA	CMB-C2B-C3B	3.19	130.64	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	W	608	CHL	CHB-C4A-NA	3.19	128.92	124.51
27	L	301	BCR	C11-C10-C9	-3.19	122.76	127.31
22	A	842	CLA	CMB-C2B-C1B	-3.18	123.57	128.46
21	W	605	CHL	C2A-C1A-CHA	-3.18	118.30	123.85
22	B	838	CLA	C1B-CHB-C4A	-3.18	123.81	130.12
22	B	802	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
22	3	611	CLA	C1B-CHB-C4A	-3.18	123.81	130.12
24	8	620	XAT	C32-C33-C34	3.18	123.82	118.94
22	V	613	CLA	C1B-CHB-C4A	-3.18	123.82	130.12
22	5	612	CLA	C1B-CHB-C4A	-3.18	123.82	130.12
24	2	620	XAT	C35-C15-C14	-3.18	116.97	123.47
27	B	847	BCR	C11-C10-C9	-3.18	122.78	127.31
23	W	2621	LUT	C7-C8-C9	-3.18	121.44	126.23
22	A	802	CLA	C1B-CHB-C4A	-3.17	123.83	130.12
22	B	816	CLA	O2D-CGD-O1D	-3.17	117.63	123.84
27	K	202	BCR	C28-C27-C26	-3.17	108.41	114.08
22	5	610	CLA	C1B-CHB-C4A	-3.17	123.84	130.12
24	2	620	XAT	C6-C7-C8	-3.17	119.29	125.99
22	A	801	CLA	C4A-NA-C1A	3.17	108.13	106.71
21	U	608	CHL	CHB-C4A-NA	3.17	128.90	124.51
27	8	621	BCR	C30-C25-C24	3.17	124.74	115.78
22	8	610	CLA	C1B-CHB-C4A	-3.17	123.84	130.12
22	V	604	CLA	CMB-C2B-C3B	3.17	130.60	124.68
22	6	614	CLA	CMB-C2B-C3B	3.17	130.60	124.68
22	B	811	CLA	CMB-C2B-C1B	-3.16	123.60	128.46
21	7	608	CHL	C3B-C4B-NB	3.16	113.30	109.21
21	9	601	CHL	C3B-C4B-NB	3.16	113.30	109.21
21	U	605	CHL	CHB-C4A-NA	3.16	128.89	124.51
22	5	610	CLA	C4A-NA-C1A	3.16	108.13	106.71
22	A	845	CLA	O2D-CGD-O1D	-3.16	117.65	123.84
27	K	205	BCR	C16-C17-C18	-3.16	122.80	127.31
22	5	613	CLA	CMB-C2B-C1B	-3.16	123.60	128.46
22	6	603	CLA	CMB-C2B-C3B	3.16	130.59	124.68
21	V	605	CHL	CHB-C4A-NA	3.16	128.88	124.51
26	8	630	LHG	O8-C23-C24	3.16	121.82	111.91
22	7	617	CLA	CMB-C2B-C3B	3.16	130.59	124.68
24	5	618	XAT	C6-C7-C8	-3.16	119.31	125.99
22	A	831	CLA	C1B-CHB-C4A	-3.16	123.86	130.12
22	B	834	CLA	CMB-C2B-C3B	3.16	130.58	124.68
22	L	303	CLA	O2D-CGD-O1D	-3.16	117.67	123.84
22	8	602	CLA	O2D-CGD-O1D	-3.16	117.67	123.84
22	3	607	CLA	O2D-CGD-O1D	-3.15	117.67	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	V	607	CHL	CHB-C4A-NA	3.15	128.87	124.51
27	G	205	BCR	C33-C5-C6	-3.15	120.99	124.53
22	A	802	CLA	CMB-C2B-C3B	3.15	130.58	124.68
22	9	603	CLA	CMB-C2B-C1B	-3.15	123.62	128.46
23	9	621	LUT	C7-C8-C9	-3.15	121.47	126.23
22	9	609	CLA	CHB-C4A-NA	3.15	128.87	124.51
22	G	201	CLA	CMB-C2B-C3B	3.15	130.57	124.68
24	6	620	XAT	C19-C9-C8	3.15	123.04	118.08
22	8	609	CLA	CMB-C2B-C3B	3.15	130.57	124.68
21	4	618	CHL	C3B-C4B-NB	3.15	113.28	109.21
22	B	833	CLA	C4-C3-C5	3.15	120.56	115.27
24	2	620	XAT	C26-C27-C28	-3.15	119.34	125.99
22	A	827	CLA	CMB-C2B-C3B	3.15	130.56	124.68
22	O	2003	CLA	C3A-C4A-CHB	-3.14	120.06	123.91
21	6	607	CHL	CHB-C4A-NA	3.14	128.86	124.51
22	B	834	CLA	O2D-CGD-O1D	-3.14	117.69	123.84
27	B	1609	BCR	C39-C30-C29	3.14	121.48	108.91
21	V	607	CHL	C2A-C1A-CHA	-3.14	118.37	123.85
21	9	605	CHL	C3B-C4B-NB	3.14	113.27	109.21
22	B	816	CLA	CMB-C2B-C3B	3.14	130.55	124.68
22	7	604	CLA	CMB-C2B-C3B	3.14	130.55	124.68
22	8	614	CLA	C1B-CHB-C4A	-3.14	123.90	130.12
23	W	2621	LUT	C19-C9-C8	3.14	123.02	118.08
22	A	807	CLA	CMB-C2B-C3B	3.14	130.55	124.68
23	4	619	LUT	C36-C21-C26	3.14	114.29	109.55
22	A	840	CLA	O2D-CGD-O1D	-3.13	117.71	123.84
22	B	807	CLA	CMB-C2B-C3B	3.13	130.54	124.68
22	8	613	CLA	CMB-C2B-C1B	-3.13	123.65	128.46
22	B	825	CLA	CMB-C2B-C3B	3.13	130.54	124.68
22	B	837	CLA	C1B-CHB-C4A	-3.13	123.92	130.12
24	U	2622	XAT	C26-C27-C28	-3.13	119.38	125.99
22	B	804	CLA	C1B-CHB-C4A	-3.13	123.92	130.12
22	1	611	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
27	A	850	BCR	C33-C5-C6	-3.13	121.02	124.53
22	U	614	CLA	C4A-NA-C1A	3.13	108.11	106.71
27	2	621	BCR	C32-C1-C6	-3.13	105.23	110.30
22	L	303	CLA	CMB-C2B-C3B	3.13	130.53	124.68
22	A	842	CLA	O2D-CGD-O1D	-3.13	117.73	123.84
27	B	847	BCR	C15-C16-C17	-3.13	117.07	123.47
22	5	612	CLA	C4A-NA-C1A	3.13	108.11	106.71
22	8	611	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
22	A	839	CLA	CMB-C2B-C3B	3.12	130.52	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	8	610	CLA	CMB-C2B-C3B	3.12	130.52	124.68
27	J	102	BCR	C38-C26-C27	3.12	119.62	113.62
22	6	610	CLA	CMB-C2B-C3B	3.12	130.52	124.68
22	2	609	CLA	O2D-CGD-CBD	3.12	116.81	111.27
22	B	824	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
22	6	610	CLA	C1B-CHB-C4A	-3.12	123.94	130.12
22	A	827	CLA	CHD-C1D-ND	-3.12	121.59	124.45
21	V	606	CHL	CAC-C3C-C4C	3.12	129.78	125.04
27	O	2004	BCR	C1-C6-C7	3.11	124.59	115.78
24	7	619	XAT	C15-C14-C13	-3.11	122.87	127.31
21	6	608	CHL	C3B-C4B-NB	3.11	113.23	109.21
22	5	610	CLA	CMB-C2B-C3B	3.11	130.50	124.68
22	B	804	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
21	U	607	CHL	C3B-C4B-NB	3.11	113.23	109.21
27	B	848	BCR	C37-C22-C23	3.11	122.98	118.08
21	U	608	CHL	CAC-C3C-C4C	3.11	129.77	125.04
27	A	851	BCR	C11-C10-C9	-3.11	122.88	127.31
22	A	815	CLA	C1B-CHB-C4A	-3.11	123.97	130.12
22	1	603	CLA	O2D-CGD-O1D	-3.11	117.77	123.84
23	U	2620	LUT	C36-C21-C26	3.10	114.25	109.55
22	B	803	CLA	CMB-C2B-C3B	3.10	130.48	124.68
25	U	2623	NEX	C15-C14-C13	-3.10	122.88	127.31
22	A	839	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
22	1	608	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
22	A	816	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
21	W	605	CHL	CHB-C4A-NA	3.10	128.80	124.51
21	9	607	CHL	C1C-C2C-C3C	-3.10	104.65	107.11
22	U	603	CLA	CMB-C2B-C1B	-3.10	123.70	128.46
21	6	601	CHL	CHB-C4A-NA	3.10	128.80	124.51
27	B	848	BCR	C16-C17-C18	-3.10	122.89	127.31
22	2	612	CLA	CMB-C2B-C3B	3.10	130.47	124.68
27	F	305	BCR	C11-C10-C9	-3.10	122.89	127.31
22	6	613	CLA	CMB-C2B-C1B	-3.10	123.70	128.46
22	A	802	CLA	C4A-NA-C1A	3.10	108.10	106.71
22	1	612	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
22	5	613	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
27	1	619	BCR	C16-C15-C14	-3.09	117.14	123.47
22	F	304	CLA	CMB-C2B-C1B	-3.09	123.71	128.46
21	W	601	CHL	CHB-C4A-NA	3.09	128.79	124.51
24	4	620	XAT	O4-C5-C6	-3.09	56.40	58.96
22	B	813	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
27	A	852	BCR	C36-C18-C17	-3.09	118.60	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	V	610	CLA	CMB-C2B-C1B	-3.09	123.72	128.46
22	A	810	CLA	CMB-C2B-C3B	3.09	130.45	124.68
21	W	606	CHL	CAC-C3C-C4C	3.08	129.74	125.04
21	W	608	CHL	CAC-C3C-C4C	3.08	129.74	125.04
21	U	607	CHL	CHB-C4A-NA	3.08	128.78	124.51
22	A	820	CLA	C1B-CHB-C4A	-3.08	124.01	130.12
22	U	604	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
22	3	609	CLA	C1B-CHB-C4A	-3.08	124.02	130.12
24	4	620	XAT	C31-C30-C29	-3.08	122.91	127.31
22	3	604	CLA	CMB-C2B-C3B	3.08	130.44	124.68
21	6	606	CHL	C3B-C4B-NB	3.08	113.19	109.21
23	1	617	LUT	C3-C4-C5	-3.08	105.72	111.85
22	B	837	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
21	6	618	CHL	CHB-C4A-NA	3.08	128.77	124.51
22	9	609	CLA	C3B-C4B-NB	3.08	113.19	109.21
22	V	610	CLA	C1B-CHB-C4A	-3.08	124.02	130.12
22	A	810	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
22	3	603	CLA	C1B-CHB-C4A	-3.08	124.03	130.12
21	2	618	CHL	CHB-C4A-NA	3.08	128.76	124.51
22	A	829	CLA	C1B-CHB-C4A	-3.08	124.03	130.12
22	A	845	CLA	CMB-C2B-C3B	3.08	130.43	124.68
23	9	624	LUT	C39-C29-C28	3.07	122.92	118.08
21	V	609	CHL	C3B-C4B-NB	3.07	113.18	109.21
22	A	801	CLA	C1B-CHB-C4A	-3.07	124.03	130.12
27	A	856	BCR	C23-C22-C21	-3.07	117.97	124.81
22	B	818	CLA	CMB-C2B-C3B	3.07	130.43	124.68
27	1	619	BCR	C20-C21-C22	-3.07	122.92	127.31
22	W	610	CLA	C1B-CHB-C4A	-3.07	124.03	130.12
24	7	619	XAT	C18-C5-C4	-3.07	110.83	114.28
22	B	809	CLA	CMB-C2B-C1B	-3.07	123.75	128.46
22	A	822	CLA	CMB-C2B-C3B	3.07	130.42	124.68
23	U	2621	LUT	C3-C4-C5	-3.07	105.74	111.85
21	9	608	CHL	C3B-C4B-NB	3.07	113.18	109.21
22	W	611	CLA	CMB-C2B-C3B	3.07	130.69	124.69
22	B	802	CLA	C1B-CHB-C4A	-3.06	124.05	130.12
22	A	830	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
22	2	604	CLA	CMB-C2B-C3B	3.06	130.41	124.68
21	6	602	CHL	C3B-C4B-NB	3.06	113.17	109.21
27	K	205	BCR	C33-C5-C4	3.06	119.50	113.62
22	8	603	CLA	CMB-C2B-C3B	3.06	130.41	124.68
22	B	812	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
21	U	607	CHL	C4-C3-C2	-3.06	115.82	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	V	610	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
22	A	833	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
24	V	2622	XAT	C31-C30-C29	-3.06	122.94	127.31
21	8	608	CHL	CHB-C4A-NA	3.06	128.74	124.51
31	A	857	LMT	C1'-C2'-C3'	-3.06	103.62	110.00
22	2	611	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
22	7	607	CLA	CMB-C2B-C3B	3.06	130.40	124.68
21	5	601	CHL	C1-C2-C3	-3.06	121.80	126.75
27	A	848	BCR	C16-C15-C14	-3.06	117.21	123.47
24	1	618	XAT	C32-C33-C34	-3.06	114.25	118.94
21	5	607	CHL	C2A-C1A-CHA	-3.05	118.52	123.85
22	3	617	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
22	U	610	CLA	C1B-CHB-C4A	-3.05	124.07	130.12
21	6	601	CHL	C3B-C4B-NB	3.05	113.16	109.21
24	4	620	XAT	C27-C28-C29	-3.05	120.80	125.53
22	B	820	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
27	B	847	BCR	C24-C23-C22	-3.05	121.62	126.23
21	W	605	CHL	CAC-C3C-C4C	3.05	129.69	125.04
21	7	608	CHL	CMD-C2D-C3D	-3.05	120.60	127.61
27	2	621	BCR	C15-C14-C13	-3.05	122.96	127.31
22	A	814	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
24	4	620	XAT	C39-C29-C28	3.05	122.88	118.08
22	6	609	CLA	C1B-CHB-C4A	-3.05	124.08	130.12
21	6	606	CHL	C2A-C1A-CHA	-3.05	118.53	123.86
21	6	608	CHL	CHB-C4A-NA	3.05	128.73	124.51
23	U	2620	LUT	C7-C8-C9	-3.05	121.63	126.23
22	B	823	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
22	4	609	CLA	C1B-CHB-C4A	-3.05	124.08	130.12
22	A	821	CLA	CMB-C2B-C1B	-3.05	123.78	128.46
21	V	601	CHL	CHB-C4A-NA	3.05	128.72	124.51
21	4	606	CHL	CHB-C4A-NA	3.05	128.72	124.51
22	2	611	CLA	CMB-C2B-C3B	3.05	130.38	124.68
21	7	608	CHL	CHB-C4A-NA	3.05	128.72	124.51
21	W	607	CHL	C2A-C1A-CHA	-3.05	118.54	123.85
22	A	801	CLA	CGD-CBD-CAD	3.05	120.60	110.73
22	A	835	CLA	CMB-C2B-C1B	-3.04	123.78	128.46
22	B	829	CLA	CMB-C2B-C3B	3.04	130.37	124.68
22	B	814	CLA	C1B-CHB-C4A	-3.04	124.09	130.12
22	B	815	CLA	CMB-C2B-C3B	3.04	130.37	124.68
22	5	604	CLA	C1B-CHB-C4A	-3.04	124.09	130.12
22	A	828	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
22	2	612	CLA	O2D-CGD-O1D	-3.04	117.89	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	9	611	CLA	C1B-CHB-C4A	-3.04	124.10	130.12
21	6	601	CHL	O2A-CGA-CBA	3.04	121.45	111.91
22	U	604	CLA	CMB-C2B-C3B	3.04	130.36	124.68
22	K	203	CLA	CMB-C2B-C3B	3.04	130.36	124.68
22	7	606	CLA	CMB-C2B-C1B	-3.04	123.79	128.46
27	3	620	BCR	C29-C30-C25	3.04	115.16	110.48
22	F	304	CLA	C1B-CHB-C4A	-3.04	124.10	130.12
22	4	609	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
27	7	620	BCR	C15-C14-C13	-3.04	122.98	127.31
22	3	612	CLA	CMB-C2B-C3B	3.03	130.35	124.68
27	A	849	BCR	C38-C26-C27	3.03	119.44	113.62
27	J	102	BCR	C34-C9-C8	3.03	122.85	118.08
31	K	208	LMT	C1'-O5'-C5'	-3.03	107.74	113.69
22	9	603	CLA	C1B-CHB-C4A	-3.03	124.11	130.12
22	A	808	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
21	U	606	CHL	C2A-C1A-CHA	-3.03	118.56	123.86
22	2	612	CLA	C1B-CHB-C4A	-3.03	124.12	130.12
27	B	848	BCR	C7-C8-C9	-3.03	121.66	126.23
22	5	604	CLA	CMB-C2B-C3B	3.03	130.34	124.68
22	W	610	CLA	C4-C3-C2	-3.03	115.91	123.68
22	B	803	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
22	9	611	CLA	CAA-C2A-C3A	-3.03	104.49	112.78
24	1	618	XAT	C39-C29-C28	3.03	122.85	118.08
21	5	607	CHL	C3B-C4B-NB	3.03	113.12	109.21
22	A	811	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
22	A	843	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
22	W	604	CLA	CMB-C2B-C3B	3.03	130.34	124.68
22	A	812	CLA	O2D-CGD-O1D	-3.02	117.92	123.84
22	B	831	CLA	C1B-CHB-C4A	-3.02	124.13	130.12
27	8	621	BCR	C33-C5-C4	3.02	119.42	113.62
21	2	602	CHL	C4A-NA-C1A	-3.02	105.35	106.71
21	V	606	CHL	CHB-C4A-NA	3.02	128.69	124.51
22	A	826	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
22	A	833	CLA	CMB-C2B-C3B	3.02	130.33	124.68
22	9	613	CLA	CMB-C2B-C3B	3.02	130.33	124.68
24	4	620	XAT	C35-C15-C14	-3.02	117.28	123.47
22	A	831	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
22	1	610	CLA	C1B-CHB-C4A	-3.02	124.14	130.12
25	9	623	NEX	C15-C35-C34	-3.02	117.29	123.47
27	G	205	BCR	C36-C18-C19	3.02	122.83	118.08
21	8	608	CHL	C3B-C4B-NB	3.02	113.11	109.21
27	B	801	BCR	C32-C1-C6	-3.02	105.40	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	U	2621	LUT	C36-C21-C26	3.02	114.12	109.55
22	G	204	CLA	CMB-C2B-C3B	3.02	130.32	124.68
22	B	814	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
27	A	851	BCR	C33-C5-C6	-3.02	121.14	124.53
22	4	612	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
22	A	810	CLA	C1B-CHB-C4A	-3.02	124.14	130.12
22	5	608	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
25	W	2623	NEX	C26-C27-C28	-3.01	119.62	125.99
21	W	609	CHL	CMB-C2B-C3B	3.01	130.32	124.68
27	8	621	BCR	C38-C26-C25	-3.01	121.14	124.53
22	A	822	CLA	C1B-CHB-C4A	-3.01	124.15	130.12
23	V	2621	LUT	C7-C8-C9	-3.01	121.68	126.23
22	5	606	CLA	CMB-C2B-C3B	3.01	130.32	124.68
27	A	850	BCR	C11-C10-C9	-3.01	123.01	127.31
23	5	617	LUT	C35-C15-C14	3.01	129.64	123.47
22	B	826	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
24	4	620	XAT	C38-C25-C24	3.01	117.67	114.28
24	7	619	XAT	C26-C27-C28	-3.01	119.63	125.99
22	U	614	CLA	C1B-CHB-C4A	-3.01	124.16	130.12
22	3	613	CLA	CMB-C2B-C3B	3.01	130.31	124.68
27	B	844	BCR	C30-C25-C26	-3.01	118.38	122.61
22	W	604	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
21	V	608	CHL	CAC-C3C-C4C	3.01	129.62	125.04
24	5	618	XAT	C24-C23-C22	-3.01	104.97	110.77
21	W	607	CHL	CAC-C3C-C4C	3.01	129.62	125.04
22	1	614	CLA	C1B-CHB-C4A	-3.01	124.16	130.12
22	8	602	CLA	C1B-CHB-C4A	-3.01	124.17	130.12
27	B	843	BCR	C7-C8-C9	-3.00	121.69	126.23
22	1	610	CLA	CMB-C2B-C3B	3.00	130.30	124.68
22	A	812	CLA	C1B-CHB-C4A	-3.00	124.17	130.12
22	5	613	CLA	C1B-CHB-C4A	-3.00	124.17	130.12
21	2	601	CHL	CHB-C4A-NA	3.00	128.66	124.51
22	7	617	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
22	V	604	CLA	C1B-CHB-C4A	-3.00	124.17	130.12
22	3	602	CLA	C1B-CHB-C4A	-3.00	124.18	130.12
22	B	818	CLA	C1B-CHB-C4A	-3.00	124.18	130.12
22	6	604	CLA	CMB-C2B-C3B	3.00	130.29	124.68
22	2	613	CLA	C1B-CHB-C4A	-3.00	124.18	130.12
22	9	609	CLA	CMC-C2C-C1C	3.00	129.60	125.04
22	9	604	CLA	CMB-C2B-C3B	3.00	130.29	124.68
22	B	821	CLA	C1B-CHB-C4A	-3.00	124.18	130.12
21	8	608	CHL	C1-C2-C3	-3.00	121.90	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	6	621	BCR	C3-C4-C5	-3.00	108.72	114.08
27	A	850	BCR	C30-C25-C26	-3.00	118.39	122.61
25	U	2623	NEX	C2-C1-C6	3.00	112.12	109.21
23	U	2620	LUT	C8-C7-C6	-2.99	118.79	127.20
22	V	613	CLA	C1-C2-C3	-2.99	120.87	126.04
22	4	601	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
22	2	613	CLA	CMB-C2B-C3B	2.99	130.28	124.68
22	8	611	CLA	CMB-C2B-C3B	2.99	130.28	124.68
22	G	203	CLA	CMB-C2B-C3B	2.99	130.27	124.68
21	8	607	CHL	CHB-C4A-NA	2.99	128.65	124.51
22	A	817	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
27	L	301	BCR	C39-C30-C25	2.99	115.15	110.30
22	A	821	CLA	C1B-CHB-C4A	-2.99	124.20	130.12
22	5	609	CLA	C1B-CHB-C4A	-2.99	124.20	130.12
27	L	306	BCR	C37-C22-C23	2.99	122.78	118.08
27	3	621	BCR	C32-C1-C6	-2.99	105.45	110.30
22	7	615	CLA	CMB-C2B-C1B	-2.99	123.87	128.46
21	U	609	CHL	C3B-C4B-NB	2.99	113.07	109.21
21	6	607	CHL	C3B-C4B-NB	2.99	113.07	109.21
21	8	618	CHL	C3B-C4B-NB	2.99	113.07	109.21
22	B	806	CLA	CMB-C2B-C3B	2.99	130.26	124.68
22	O	2002	CLA	CMB-C2B-C3B	2.99	130.26	124.68
22	5	614	CLA	CMB-C2B-C3B	2.99	130.26	124.68
22	8	614	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
22	B	828	CLA	C1B-CHB-C4A	-2.98	124.21	130.12
22	B	830	CLA	C1B-CHB-C4A	-2.98	124.21	130.12
22	O	2002	CLA	C1B-CHB-C4A	-2.98	124.21	130.12
22	3	607	CLA	CMB-C2B-C3B	2.98	130.26	124.68
22	3	615	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
22	W	602	CLA	C1B-CHB-C4A	-2.98	124.21	130.12
22	A	823	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
21	U	606	CHL	CHB-C4A-NA	2.98	128.63	124.51
22	V	604	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
22	B	831	CLA	CMB-C2B-C3B	2.98	130.25	124.68
24	3	619	XAT	C18-C5-C4	2.98	117.63	114.28
22	A	835	CLA	C1B-CHB-C4A	-2.98	124.22	130.12
22	B	827	CLA	C1B-CHB-C4A	-2.98	124.22	130.12
24	W	2622	XAT	C26-C27-C28	-2.98	119.70	125.99
22	3	610	CLA	CMB-C2B-C3B	2.98	130.25	124.68
22	B	824	CLA	C4-C3-C5	2.98	120.28	115.27
24	1	618	XAT	C15-C14-C13	-2.98	123.06	127.31
21	2	601	CHL	C3B-C4B-NB	2.98	113.06	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	832	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
22	6	611	CLA	CMB-C2B-C3B	2.98	130.25	124.68
27	A	852	BCR	C16-C17-C18	-2.98	123.06	127.31
27	M	2001	BCR	C8-C9-C10	2.97	123.51	118.94
22	A	813	CLA	O2D-CGD-O1D	-2.97	118.02	123.84
22	A	824	CLA	CMB-C2B-C3B	2.97	130.24	124.68
25	V	2623	NEX	C15-C14-C13	-2.97	123.07	127.31
27	I	101	BCR	C8-C7-C6	-2.97	118.85	127.20
27	B	844	BCR	C28-C27-C26	-2.97	108.77	114.08
22	V	613	CLA	CMB-C2B-C3B	2.97	130.24	124.68
22	4	613	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
22	A	806	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
22	K	201	CLA	CMB-C2B-C3B	2.97	130.24	124.68
22	B	840	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
22	B	819	CLA	C1B-CHB-C4A	-2.97	124.23	130.12
21	2	607	CHL	CHB-C4A-NA	2.97	128.62	124.51
27	A	851	BCR	C15-C14-C13	-2.97	123.07	127.31
21	2	606	CHL	CHB-C4A-NA	2.97	128.62	124.51
21	8	618	CHL	CHB-C4A-NA	2.97	128.62	124.51
22	B	829	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
21	V	608	CHL	C2A-C1A-CHA	-2.97	118.67	123.86
22	B	815	CLA	C1B-CHB-C4A	-2.97	124.23	130.12
22	3	613	CLA	CAA-C2A-C3A	-2.97	104.65	112.78
22	4	612	CLA	CMB-C2B-C3B	2.97	130.23	124.68
27	A	851	BCR	C7-C8-C9	-2.97	121.75	126.23
22	9	612	CLA	CMB-C2B-C3B	2.97	130.23	124.68
22	7	611	CLA	C4A-NA-C1A	2.97	108.04	106.71
23	5	617	LUT	C8-C9-C10	2.97	123.49	118.94
22	U	611	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
22	5	611	CLA	C1B-CHB-C4A	-2.97	124.24	130.12
27	K	205	BCR	C38-C26-C27	2.97	119.31	113.62
22	G	201	CLA	C1B-CHB-C4A	-2.97	124.24	130.12
22	K	203	CLA	C1B-CHB-C4A	-2.97	124.24	130.12
22	L	302	CLA	C1B-CHB-C4A	-2.97	124.24	130.12
21	4	607	CHL	C3B-C4B-NB	2.97	113.05	109.21
21	U	609	CHL	CMD-C2D-C3D	-2.97	120.79	127.61
22	5	611	CLA	CMB-C2B-C3B	2.97	130.23	124.68
23	9	624	LUT	C22-C23-C24	2.96	115.11	111.74
22	1	613	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
22	5	609	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
22	6	609	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
22	L	303	CLA	C1B-CHB-C4A	-2.96	124.25	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	8	606	CHL	C3B-C4B-NB	2.96	113.04	109.21
21	4	606	CHL	C3B-C4B-NB	2.96	113.04	109.21
27	K	205	BCR	C37-C22-C23	2.96	122.74	118.08
22	F	301	CLA	CMB-C2B-C3B	2.96	130.22	124.68
22	B	838	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
22	7	610	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
22	B	817	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
21	9	606	CHL	CMD-C2D-C3D	-2.96	120.80	127.61
27	B	843	BCR	C16-C17-C18	-2.96	123.08	127.31
22	B	812	CLA	CMB-C2B-C3B	2.96	130.22	124.68
22	U	613	CLA	CMB-C2B-C3B	2.96	130.21	124.68
27	6	621	BCR	C35-C13-C12	2.96	122.74	118.08
21	9	605	CHL	CHB-C4A-NA	2.96	128.60	124.51
21	U	607	CHL	C2A-C1A-CHA	-2.96	118.69	123.86
21	2	606	CHL	C2A-C1A-CHA	-2.96	118.69	123.86
21	U	606	CHL	CMB-C2B-C3B	2.96	130.21	124.68
23	9	620	LUT	C36-C21-C26	2.96	114.03	109.55
22	3	617	CLA	C1B-CHB-C4A	-2.96	124.26	130.12
27	4	621	BCR	C15-C16-C17	-2.96	117.42	123.47
22	O	2001	CLA	C3A-C4A-CHB	-2.96	120.29	123.91
22	3	613	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
21	2	601	CHL	CMD-C2D-C3D	-2.95	120.82	127.61
21	V	607	CHL	CAC-C3C-C4C	2.95	129.54	125.04
22	5	608	CLA	CMB-C2B-C3B	2.95	130.20	124.68
27	A	851	BCR	C38-C26-C25	-2.95	121.21	124.53
27	A	849	BCR	C24-C23-C22	-2.95	121.77	126.23
22	B	814	CLA	C1-C2-C3	-2.95	120.94	126.04
22	U	612	CLA	CMB-C2B-C3B	2.95	130.20	124.68
22	B	841	CLA	CMB-C2B-C3B	2.95	130.20	124.68
27	B	848	BCR	C29-C30-C25	2.95	115.02	110.48
22	U	612	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
27	7	621	BCR	C30-C25-C26	-2.95	118.46	122.61
22	A	845	CLA	C1B-CHB-C4A	-2.95	124.28	130.12
21	U	609	CHL	CMB-C2B-C3B	2.95	130.20	124.68
27	8	621	BCR	C15-C14-C13	-2.95	123.10	127.31
22	A	818	CLA	CMB-C2B-C3B	2.95	130.19	124.68
22	A	818	CLA	C1B-CHB-C4A	-2.95	124.28	130.12
21	U	605	CHL	CAC-C3C-C4C	2.95	129.53	125.04
22	6	612	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
27	F	305	BCR	C16-C17-C18	-2.95	123.10	127.31
22	K	206	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
22	5	608	CLA	C1-C2-C3	-2.95	121.98	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	5	614	CLA	C1B-CHB-C4A	-2.95	124.28	130.12
22	4	609	CLA	CMB-C2B-C3B	2.94	130.19	124.68
22	L	304	CLA	C1B-CHB-C4A	-2.94	124.29	130.12
22	4	611	CLA	CMB-C2B-C3B	2.94	130.19	124.68
22	8	602	CLA	CMB-C2B-C3B	2.94	130.19	124.68
22	3	611	CLA	O2D-CGD-CBD	2.94	116.50	111.27
27	7	621	BCR	C20-C21-C22	-2.94	123.11	127.31
22	V	602	CLA	CMB-C2B-C3B	2.94	130.18	124.68
21	6	602	CHL	O2A-CGA-CBA	2.94	121.14	111.91
22	3	610	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
22	B	841	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
22	9	602	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
22	A	816	CLA	CMB-C2B-C3B	2.94	130.18	124.68
21	V	606	CHL	C2A-C1A-CHA	-2.94	118.72	123.85
23	V	2621	LUT	C19-C9-C8	2.94	122.71	118.08
22	2	610	CLA	CMB-C2B-C3B	2.94	130.18	124.68
22	1	602	CLA	CMB-C2B-C3B	2.94	130.18	124.68
22	4	611	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
22	W	612	CLA	CMA-C3A-C2A	-2.94	109.24	116.10
22	2	610	CLA	C1B-CHB-C4A	-2.94	124.30	130.12
22	V	603	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
27	3	620	BCR	C16-C17-C18	-2.94	123.12	127.31
22	V	614	CLA	CMB-C2B-C3B	2.93	130.17	124.68
22	W	613	CLA	CMB-C2B-C3B	2.93	130.17	124.68
27	4	621	BCR	C36-C18-C19	2.93	122.70	118.08
22	4	610	CLA	C4A-NA-C1A	2.93	108.03	106.71
21	9	605	CHL	CMD-C2D-C3D	-2.93	120.87	127.61
22	4	614	CLA	CMB-C2B-C3B	2.93	130.16	124.68
22	B	829	CLA	C1B-CHB-C4A	-2.93	124.31	130.12
23	5	617	LUT	C28-C29-C30	2.93	123.44	118.94
21	U	607	CHL	CMB-C2B-C3B	2.93	130.16	124.68
22	1	611	CLA	CMB-C2B-C3B	2.93	130.16	124.68
22	3	614	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
21	9	601	CHL	CHB-C4A-NA	2.93	128.56	124.51
27	A	850	BCR	C38-C26-C27	2.93	119.24	113.62
24	8	620	XAT	C8-C9-C10	2.93	123.43	118.94
21	5	601	CHL	CHB-C4A-NA	2.93	128.56	124.51
22	7	604	CLA	C1B-CHB-C4A	-2.93	124.32	130.12
27	1	619	BCR	C21-C20-C19	-2.92	114.09	123.22
22	B	817	CLA	CMB-C2B-C3B	2.92	130.15	124.68
27	I	101	BCR	C30-C25-C26	-2.92	118.50	122.61
22	7	602	CLA	CMB-C2B-C3B	2.92	130.14	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	837	CLA	CMB-C2B-C1B	-2.92	123.97	128.46
22	A	817	CLA	C1B-CHB-C4A	-2.92	124.33	130.12
22	7	614	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
26	7	630	LHG	O8-C23-C24	2.92	121.07	111.91
21	8	606	CHL	CHB-C4A-NA	2.92	128.55	124.51
22	8	610	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
22	3	607	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
22	A	803	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
22	B	840	CLA	CMB-C2B-C1B	-2.92	123.98	128.46
22	6	604	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
21	2	618	CHL	CMD-C2D-C3D	-2.92	120.90	127.61
22	B	822	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
22	A	830	CLA	C4A-NA-C1A	2.92	108.02	106.71
22	2	614	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
22	B	832	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
21	9	607	CHL	CAC-C3C-C4C	2.92	128.59	124.81
21	1	601	CHL	C3B-C4B-NB	2.92	112.98	109.21
27	1	619	BCR	C33-C5-C4	2.92	119.22	113.62
22	3	604	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
23	9	624	LUT	C38-C25-C24	-2.91	117.32	123.56
22	8	611	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
21	U	609	CHL	C2A-C1A-CHA	-2.91	118.77	123.86
22	3	613	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
22	4	614	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
22	L	303	CLA	CHD-C1D-ND	-2.91	121.78	124.45
22	4	602	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
22	B	834	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
22	9	611	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
23	2	619	LUT	C12-C13-C14	2.91	123.41	118.94
22	2	604	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
22	G	204	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
22	9	613	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
22	6	613	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
22	8	613	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
27	1	619	BCR	C11-C12-C13	-2.91	118.24	126.42
22	2	609	CLA	CMB-C2B-C3B	2.91	130.12	124.68
22	4	613	CLA	CMB-C2B-C3B	2.91	130.12	124.68
22	B	812	CLA	C1B-CHB-C4A	-2.91	124.36	130.12
27	L	306	BCR	C11-C10-C9	-2.91	123.16	127.31
22	4	602	CLA	CMB-C2B-C3B	2.91	130.12	124.68
27	B	1609	BCR	C30-C25-C24	2.91	124.00	115.78
22	H	201	CLA	CMB-C2B-C1B	-2.91	124.00	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	4	604	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
22	B	838	CLA	CMB-C2B-C3B	2.90	130.11	124.68
22	5	602	CLA	CMB-C2B-C3B	2.90	130.11	124.68
27	B	844	BCR	C7-C8-C9	-2.90	121.85	126.23
21	W	609	CHL	C2A-C1A-CHA	-2.90	118.78	123.86
22	A	840	CLA	CMB-C2B-C1B	-2.90	124.00	128.46
24	3	619	XAT	C6-C7-C8	-2.90	119.86	125.99
22	W	612	CLA	C1B-CHB-C4A	-2.90	124.37	130.12
27	B	844	BCR	C15-C16-C17	-2.90	117.53	123.47
22	1	604	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
22	F	301	CLA	C1B-CHB-C4A	-2.90	124.37	130.12
22	7	611	CLA	CMB-C2B-C3B	2.90	130.11	124.68
22	1	616	CLA	CMB-C2B-C3B	2.90	130.10	124.68
21	2	606	CHL	C3B-C4B-NB	2.90	112.96	109.21
21	4	618	CHL	CHB-C4A-NA	2.90	128.52	124.51
27	J	102	BCR	C37-C22-C23	2.90	122.65	118.08
22	1	614	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
22	U	603	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
22	B	839	CLA	C1B-CHB-C4A	-2.90	124.38	130.12
24	7	619	XAT	C15-C35-C34	-2.90	117.54	123.47
22	A	837	CLA	C1B-CHB-C4A	-2.90	124.38	130.12
22	9	610	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
22	A	832	CLA	CMB-C2B-C3B	2.90	130.10	124.68
22	V	602	CLA	C1B-CHB-C4A	-2.90	124.38	130.12
27	G	205	BCR	C7-C8-C9	-2.90	121.86	126.23
22	B	825	CLA	O2D-CGD-O1D	-2.90	118.18	123.84
27	1	619	BCR	C40-C30-C25	-2.89	105.60	110.30
22	A	821	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
21	W	601	CHL	O2A-CGA-CBA	2.89	120.99	111.91
22	1	609	CLA	C1B-CHB-C4A	-2.89	124.39	130.12
22	U	611	CLA	CMB-C2B-C3B	2.89	130.09	124.68
27	A	848	BCR	C32-C1-C6	-2.89	105.61	110.30
22	B	820	CLA	CMB-C2B-C3B	2.89	130.09	124.68
27	1	619	BCR	C33-C5-C6	-2.89	121.28	124.53
22	V	612	CLA	CAB-C3B-C2B	2.89	130.35	124.69
22	1	616	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
22	2	613	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
21	2	607	CHL	C3B-C4B-NB	2.89	112.94	109.21
27	B	1609	BCR	C2-C1-C6	2.89	114.93	110.48
21	7	608	CHL	C2A-C1A-CHA	-2.89	118.81	123.86
22	A	822	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
22	1	612	CLA	CMB-C2B-C3B	2.89	130.08	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1	606	CLA	C1B-CHB-C4A	-2.89	124.40	130.12
22	A	809	CLA	C1B-CHB-C4A	-2.89	124.40	130.12
22	A	825	CLA	O2D-CGD-O1D	-2.89	118.20	123.84
23	6	619	LUT	C32-C33-C34	-2.88	114.51	118.94
31	A	857	LMT	C1'-O5'-C5'	-2.88	108.03	113.69
21	V	609	CHL	CMD-C2D-C3D	-2.88	120.98	127.61
21	U	607	CHL	O2A-CGA-CBA	2.88	120.96	111.91
22	A	812	CLA	CMB-C2B-C3B	2.88	130.07	124.68
22	U	614	CLA	CMB-C2B-C3B	2.88	130.07	124.68
22	A	819	CLA	C1B-CHB-C4A	-2.88	124.41	130.12
27	J	102	BCR	C4-C5-C6	-2.88	118.55	122.73
22	1	608	CLA	CMB-C2B-C3B	2.88	130.07	124.68
24	8	620	XAT	C27-C28-C29	2.88	130.00	125.53
22	G	201	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
22	8	613	CLA	C1B-CHB-C4A	-2.88	124.41	130.12
22	8	612	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
22	2	613	CLA	CAA-C2A-C3A	-2.88	104.89	112.78
26	4	630	LHG	O8-C23-C24	2.88	120.95	111.91
21	6	602	CHL	OMC-CMC-C2C	-2.88	119.17	125.69
22	3	611	CLA	CMB-C2B-C3B	2.88	130.07	124.68
21	9	607	CHL	CHB-C4A-NA	2.88	128.49	124.51
22	F	301	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
22	A	827	CLA	C1B-CHB-C4A	-2.88	124.42	130.12
22	A	840	CLA	C1B-CHB-C4A	-2.88	124.42	130.12
22	B	806	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
22	B	810	CLA	CMB-C2B-C3B	2.88	130.06	124.68
21	5	601	CHL	C3B-C4B-NB	2.88	112.93	109.21
22	4	611	CLA	C1B-CHB-C4A	-2.88	124.42	130.12
22	B	833	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
22	L	304	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
24	U	2622	XAT	O4-C5-C18	2.88	118.50	115.06
24	8	620	XAT	C38-C25-C26	-2.88	117.44	122.26
22	A	811	CLA	C1B-CHB-C4A	-2.87	124.42	130.12
22	B	835	CLA	C1B-CHB-C4A	-2.87	124.42	130.12
22	1	610	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
22	5	610	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
22	U	602	CLA	C1B-CHB-C4A	-2.87	124.43	130.12
22	A	816	CLA	C1B-CHB-C4A	-2.87	124.43	130.12
22	4	613	CLA	C1B-CHB-C4A	-2.87	124.43	130.12
22	5	616	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
27	3	620	BCR	C11-C10-C9	-2.87	123.21	127.31
22	W	611	CLA	O2D-CGD-O1D	-2.87	117.57	124.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	836	CLA	C1B-CHB-C4A	-2.87	124.43	130.12
21	1	607	CHL	CHB-C4A-NA	2.87	128.48	124.51
27	4	621	BCR	C30-C25-C26	-2.87	118.57	122.61
22	A	841	CLA	CMB-C2B-C3B	2.87	130.05	124.68
22	A	805	CLA	C1B-CHB-C4A	-2.87	124.43	130.12
22	1	612	CLA	C1B-CHB-C4A	-2.87	124.44	130.12
22	2	611	CLA	C1B-CHB-C4A	-2.87	124.44	130.12
22	3	604	CLA	C1B-CHB-C4A	-2.87	124.44	130.12
21	5	607	CHL	CHB-C4A-NA	2.87	128.48	124.51
21	2	607	CHL	CMD-C2D-C3D	-2.87	121.02	127.61
22	B	830	CLA	CHD-C1D-ND	-2.87	121.82	124.45
27	A	851	BCR	C15-C16-C17	-2.87	117.60	123.47
22	4	603	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
22	2	603	CLA	C1B-CHB-C4A	-2.87	124.44	130.12
22	A	842	CLA	CHD-C1D-ND	-2.87	121.82	124.45
27	L	305	BCR	C11-C10-C9	-2.87	123.22	127.31
22	7	611	CLA	C1B-CHB-C4A	-2.86	124.44	130.12
22	7	615	CLA	C1B-CHB-C4A	-2.86	124.44	130.12
27	A	849	BCR	C37-C22-C21	-2.86	118.91	122.92
22	6	611	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
24	4	620	XAT	C15-C14-C13	-2.86	123.22	127.31
22	B	823	CLA	CMB-C2B-C3B	2.86	130.03	124.68
21	W	606	CHL	CMD-C2D-C3D	-2.86	121.03	127.61
23	W	2621	LUT	C15-C14-C13	-2.86	123.23	127.31
27	K	202	BCR	C7-C8-C9	-2.86	121.91	126.23
22	U	602	CLA	C4-C3-C5	2.86	120.08	115.27
22	L	302	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
22	1	614	CLA	CMB-C2B-C3B	2.86	130.03	124.68
22	A	801	CLA	CMB-C2B-C3B	2.86	130.03	124.68
22	K	204	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
22	L	302	CLA	CMB-C2B-C3B	2.86	130.03	124.68
21	2	602	CHL	CHB-C4A-NA	2.86	128.47	124.51
22	5	616	CLA	CMB-C2B-C3B	2.86	130.03	124.68
22	6	612	CLA	C1B-CHB-C4A	-2.86	124.46	130.12
22	7	604	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
22	W	604	CLA	C1B-CHB-C4A	-2.86	124.46	130.12
22	G	204	CLA	C1B-CHB-C4A	-2.86	124.46	130.12
24	2	620	XAT	O4-C5-C18	2.86	118.48	115.06
28	A	860	LMG	O8-C28-C29	2.86	120.88	111.91
22	H	201	CLA	C1B-CHB-C4A	-2.86	124.46	130.12
23	8	619	LUT	C7-C8-C9	-2.86	121.92	126.23
22	U	611	CLA	C1B-CHB-C4A	-2.86	124.46	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	1	601	CHL	CHB-C4A-NA	2.86	128.46	124.51
22	8	612	CLA	CMB-C2B-C3B	2.86	130.02	124.68
27	B	844	BCR	C37-C22-C23	2.85	122.58	118.08
22	A	819	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
23	9	624	LUT	C7-C8-C9	-2.85	121.92	126.23
27	B	1609	BCR	C33-C5-C4	2.85	119.10	113.62
27	A	852	BCR	C3-C4-C5	-2.85	108.98	114.08
22	6	613	CLA	C1B-CHB-C4A	-2.85	124.47	130.12
24	6	620	XAT	C18-C5-C6	-2.85	117.48	122.26
22	B	821	CLA	CMB-C2B-C3B	2.85	130.01	124.68
22	F	303	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
22	5	614	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
22	4	603	CLA	C1B-CHB-C4A	-2.85	124.47	130.12
31	G	206	LMT	C1'-C2'-C3'	-2.85	104.06	110.00
27	B	848	BCR	C16-C15-C14	-2.85	117.64	123.47
22	A	815	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
22	1	613	CLA	C1B-CHB-C4A	-2.85	124.47	130.12
27	A	856	BCR	C7-C8-C9	-2.85	121.93	126.23
22	A	818	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
27	2	621	BCR	C8-C7-C6	-2.85	119.21	127.20
24	4	620	XAT	C8-C9-C10	-2.85	114.58	118.94
22	B	833	CLA	CMB-C2B-C3B	2.84	130.00	124.68
22	V	603	CLA	CMB-C2B-C3B	2.84	130.00	124.68
22	J	101	CLA	CMB-C2B-C3B	2.84	130.00	124.68
21	4	607	CHL	CHB-C4A-NA	2.84	128.44	124.51
22	4	602	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
22	9	602	CLA	C4-C3-C5	2.84	120.05	115.27
21	V	609	CHL	CMB-C2B-C3B	2.84	129.99	124.68
22	4	613	CLA	CHD-C1D-ND	-2.84	121.84	124.45
27	J	102	BCR	C15-C16-C17	-2.84	117.65	123.47
25	U	2623	NEX	C38-C25-C24	2.84	117.48	114.28
21	3	608	CHL	CMD-C2D-C3D	-2.84	121.08	127.61
21	4	607	CHL	CMD-C2D-C3D	-2.84	121.08	127.61
28	J	103	LMG	O8-C28-C29	2.84	120.81	111.91
22	B	830	CLA	CMB-C2B-C1B	-2.84	124.10	128.46
22	B	806	CLA	C1B-CHB-C4A	-2.84	124.50	130.12
21	V	601	CHL	CAA-C2A-C3A	2.84	120.54	112.78
27	B	844	BCR	C3-C4-C5	-2.84	109.01	114.08
22	2	614	CLA	CMB-C2B-C3B	2.84	129.98	124.68
21	V	609	CHL	CHB-C4A-NA	2.83	128.43	124.51
24	6	620	XAT	C6-C7-C8	-2.83	120.00	125.99
21	U	609	CHL	O2A-CGA-CBA	2.83	120.80	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	7	619	XAT	C31-C30-C29	-2.83	123.27	127.31
22	3	612	CLA	C1B-CHB-C4A	-2.83	124.51	130.12
24	W	2622	XAT	C35-C34-C33	-2.83	123.27	127.31
22	2	603	CLA	CMB-C2B-C3B	2.83	129.98	124.68
22	B	823	CLA	C1B-CHB-C4A	-2.83	124.51	130.12
21	2	618	CHL	C3B-C4B-NB	2.83	112.87	109.21
24	3	619	XAT	O4-C5-C18	2.83	118.45	115.06
21	V	605	CHL	O2D-CGD-O1D	-2.83	118.30	123.84
22	8	604	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
23	9	620	LUT	C35-C15-C14	-2.83	117.68	123.47
22	B	815	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
27	A	851	BCR	C37-C22-C23	2.83	122.53	118.08
25	9	623	NEX	C15-C14-C13	-2.83	123.27	127.31
23	9	621	LUT	C19-C9-C10	-2.83	118.96	122.92
22	5	616	CLA	C1B-CHB-C4A	-2.83	124.52	130.12
24	6	620	XAT	C11-C10-C9	-2.83	123.27	127.31
21	5	601	CHL	O2A-CGA-CBA	2.83	120.78	111.91
22	V	602	CLA	CHD-C1D-ND	-2.83	121.86	124.45
22	W	614	CLA	C1B-CHB-C4A	-2.83	124.52	130.12
22	B	822	CLA	CMB-C2B-C3B	2.83	129.97	124.68
22	W	613	CLA	C1B-CHB-C4A	-2.83	124.52	130.12
22	U	604	CLA	C1B-CHB-C4A	-2.83	124.52	130.12
21	5	601	CHL	O2D-CGD-O1D	-2.83	118.31	123.84
25	V	2623	NEX	O24-C25-C38	2.83	118.44	115.06
22	5	611	CLA	O2D-CGD-CBD	2.82	116.29	111.27
24	W	2622	XAT	C31-C30-C29	-2.82	123.28	127.31
22	B	817	CLA	C1B-CHB-C4A	-2.82	124.53	130.12
27	L	305	BCR	C16-C17-C18	-2.82	123.29	127.31
22	B	830	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
22	3	606	CLA	CMB-C2B-C3B	2.82	129.95	124.68
22	1	606	CLA	CMB-C2B-C1B	-2.82	124.13	128.46
22	5	603	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
22	V	611	CLA	C1B-CHB-C4A	-2.82	124.54	130.12
22	V	614	CLA	C1B-CHB-C4A	-2.82	124.54	130.12
27	8	621	BCR	C36-C18-C17	-2.82	118.98	122.92
21	9	608	CHL	CHB-C4A-NA	2.82	128.41	124.51
22	A	833	CLA	C1B-CHB-C4A	-2.82	124.54	130.12
22	A	811	CLA	CMB-C2B-C3B	2.81	129.94	124.68
22	5	606	CLA	C1B-CHB-C4A	-2.81	124.54	130.12
22	W	612	CLA	CAB-C3B-C2B	2.81	130.20	124.69
22	3	603	CLA	CMB-C2B-C3B	2.81	129.94	124.68
22	8	612	CLA	C1B-CHB-C4A	-2.81	124.55	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	843	CLA	CMB-C2B-C3B	2.81	129.94	124.68
22	F	304	CLA	CMB-C2B-C3B	2.81	129.94	124.68
22	A	838	CLA	C1B-CHB-C4A	-2.81	124.55	130.12
21	V	601	CHL	C2A-C1A-CHA	-2.81	118.94	123.86
22	W	611	CLA	CAB-C3B-C2B	2.81	130.19	124.69
22	A	825	CLA	CMB-C2B-C3B	2.81	129.94	124.68
21	8	607	CHL	CMD-C2D-C3D	-2.81	121.16	127.61
21	6	607	CHL	C2A-C1A-CHA	-2.81	118.95	123.86
22	B	826	CLA	CMB-C2B-C3B	2.81	129.93	124.68
22	5	612	CLA	O2D-CGD-O1D	-2.80	118.35	123.84
24	1	618	XAT	C4-C3-C2	-2.80	105.36	110.77
28	J	104	LMG	O8-C28-C29	2.80	120.71	111.91
21	1	601	CHL	O2A-CGA-CBA	2.80	120.71	111.91
22	A	841	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
24	2	620	XAT	C8-C9-C10	-2.80	114.64	118.94
22	A	808	CLA	CMB-C2B-C3B	2.80	129.92	124.68
22	7	606	CLA	CMB-C2B-C3B	2.80	129.92	124.68
22	A	834	CLA	C1B-CHB-C4A	-2.80	124.57	130.12
22	B	841	CLA	C1B-CHB-C4A	-2.80	124.57	130.12
22	7	617	CLA	C1B-CHB-C4A	-2.80	124.57	130.12
27	K	205	BCR	C1-C6-C7	2.80	123.71	115.78
27	K	205	BCR	C23-C24-C25	-2.80	119.33	127.20
27	K	202	BCR	C24-C23-C22	-2.80	122.00	126.23
22	3	606	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
25	V	2623	NEX	C15-C35-C34	-2.80	117.74	123.47
22	B	811	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
23	V	2621	LUT	C15-C14-C13	-2.80	123.31	127.31
22	W	603	CLA	CMB-C2B-C3B	2.80	129.92	124.68
27	A	848	BCR	C35-C13-C12	2.80	122.49	118.08
22	U	602	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
22	V	611	CLA	CMB-C2B-C3B	2.80	130.17	124.69
22	1	603	CLA	CMB-C2B-C3B	2.80	129.91	124.68
22	5	612	CLA	CMB-C2B-C3B	2.80	129.91	124.68
27	2	621	BCR	C40-C30-C25	-2.80	105.76	110.30
22	5	608	CLA	C1B-CHB-C4A	-2.80	124.58	130.12
22	8	601	CLA	C1B-CHB-C4A	-2.80	124.58	130.12
24	W	2622	XAT	C35-C15-C14	-2.80	117.75	123.47
22	8	609	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
22	B	835	CLA	CHD-C1D-ND	-2.80	121.88	124.45
27	B	847	BCR	C29-C30-C25	2.80	114.78	110.48
22	7	614	CLA	C1B-CHB-C4A	-2.80	124.58	130.12
22	A	808	CLA	C1B-CHB-C4A	-2.80	124.58	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	842	CLA	C1B-CHB-C4A	-2.80	124.58	130.12
22	6	612	CLA	CMB-C2B-C3B	2.79	129.91	124.68
22	U	612	CLA	C1B-CHB-C4A	-2.79	124.58	130.12
22	3	610	CLA	C1B-CHB-C4A	-2.79	124.58	130.12
22	A	813	CLA	C1B-CHB-C4A	-2.79	124.58	130.12
22	1	604	CLA	CMB-C2B-C3B	2.79	129.91	124.68
22	8	601	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
21	U	601	CHL	C1-C2-C3	-2.79	121.21	126.04
22	W	611	CLA	C1B-CHB-C4A	-2.79	124.58	130.12
22	1	608	CLA	C1B-CHB-C4A	-2.79	124.59	130.12
22	9	604	CLA	C1B-CHB-C4A	-2.79	124.59	130.12
22	4	603	CLA	CMB-C2B-C3B	2.79	129.90	124.68
22	7	609	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
21	2	608	CHL	CHB-C4A-NA	2.79	128.37	124.51
22	G	203	CLA	C1B-CHB-C4A	-2.79	124.59	130.12
27	O	2004	BCR	C2-C1-C6	2.79	114.78	110.48
22	V	612	CLA	C1B-CHB-C4A	-2.79	124.59	130.12
22	2	603	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
27	L	306	BCR	C28-C27-C26	-2.79	109.10	114.08
22	8	601	CLA	CMB-C2B-C3B	2.79	129.90	124.68
22	7	606	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
21	6	601	CHL	CMD-C2D-C3D	-2.79	121.20	127.61
22	B	816	CLA	C1B-CHB-C4A	-2.79	124.60	130.12
22	A	838	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
27	B	801	BCR	C29-C30-C25	2.79	114.77	110.48
27	7	620	BCR	C40-C30-C25	-2.79	105.78	110.30
22	A	806	CLA	CMB-C2B-C3B	2.79	129.89	124.68
24	4	620	XAT	C26-C27-C28	-2.79	120.10	125.99
27	2	621	BCR	C34-C9-C10	-2.78	119.02	122.92
24	6	620	XAT	C8-C9-C10	-2.78	114.67	118.94
22	A	823	CLA	C1B-CHB-C4A	-2.78	124.60	130.12
27	A	851	BCR	C24-C23-C22	-2.78	122.03	126.23
22	A	826	CLA	C1B-CHB-C4A	-2.78	124.61	130.12
22	A	832	CLA	C1B-CHB-C4A	-2.78	124.61	130.12
27	A	848	BCR	C34-C9-C8	2.78	122.46	118.08
22	7	613	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
21	9	607	CHL	C3B-C4B-NB	2.78	112.81	109.21
27	3	621	BCR	C37-C22-C23	2.78	122.46	118.08
22	B	837	CLA	CHD-C1D-ND	-2.78	121.90	124.45
21	8	607	CHL	C3B-C4B-NB	2.78	112.80	109.21
22	1	613	CLA	CMB-C2B-C3B	2.78	129.88	124.68
25	U	2623	NEX	C19-C9-C10	-2.78	119.03	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	827	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
21	U	608	CHL	CMB-C2B-C3B	2.78	130.13	124.69
22	2	614	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
21	9	607	CHL	CMB-C2B-C3B	2.78	129.88	124.68
22	W	603	CLA	C1B-CHB-C4A	-2.78	124.62	130.12
22	4	614	CLA	C1B-CHB-C4A	-2.78	124.62	130.12
21	6	602	CHL	C2A-C1A-CHA	-2.78	119.00	123.86
25	9	623	NEX	C11-C10-C9	-2.78	123.35	127.31
22	B	808	CLA	C1B-CHB-C4A	-2.77	124.62	130.12
24	7	619	XAT	C8-C9-C10	2.77	123.19	118.94
27	3	620	BCR	C23-C22-C21	-2.77	114.69	118.94
22	9	612	CLA	C1B-CHB-C4A	-2.77	124.63	130.12
22	8	609	CLA	C1B-CHB-C4A	-2.77	124.63	130.12
22	U	613	CLA	C1B-CHB-C4A	-2.77	124.63	130.12
22	7	612	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
22	6	614	CLA	C1B-CHB-C4A	-2.77	124.63	130.12
22	1	616	CLA	C1B-CHB-C4A	-2.77	124.64	130.12
22	B	833	CLA	C1B-CHB-C4A	-2.77	124.64	130.12
22	A	805	CLA	CHD-C1D-ND	-2.77	121.91	124.45
24	1	618	XAT	C15-C35-C34	-2.76	117.81	123.47
27	F	305	BCR	C36-C18-C19	2.76	122.43	118.08
21	2	618	CHL	O2D-CGD-O1D	-2.76	118.43	123.84
22	K	201	CLA	O2D-CGD-O1D	-2.76	118.43	123.84
25	W	2623	NEX	C11-C12-C13	-2.76	118.65	126.42
23	9	624	LUT	C40-C33-C32	2.76	122.43	118.08
27	I	101	BCR	C7-C8-C9	-2.76	122.06	126.23
22	9	602	CLA	C1B-CHB-C4A	-2.76	124.65	130.12
27	A	851	BCR	C8-C9-C10	-2.76	114.70	118.94
21	9	608	CHL	C2A-C1A-CHA	-2.76	119.03	123.86
22	9	610	CLA	CMB-C2B-C3B	2.76	129.84	124.68
22	6	614	CLA	C1-C2-C3	-2.76	122.28	126.75
22	A	843	CLA	C1B-CHB-C4A	-2.76	124.65	130.12
22	5	603	CLA	C1B-CHB-C4A	-2.76	124.65	130.12
22	L	304	CLA	CMB-C2B-C3B	2.76	129.84	124.68
22	5	602	CLA	C1B-CHB-C4A	-2.76	124.65	130.12
22	2	604	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
21	1	607	CHL	CMD-C2D-C3D	-2.76	121.27	127.61
22	3	609	CLA	CMB-C2B-C3B	2.76	129.84	124.68
22	A	827	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
22	F	303	CLA	C1B-CHB-C4A	-2.76	124.66	130.12
22	G	203	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
22	K	206	CLA	C1B-CHB-C4A	-2.76	124.66	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	7	610	CLA	C1B-CHB-C4A	-2.76	124.66	130.12
23	2	619	LUT	C32-C33-C34	2.76	123.17	118.94
22	7	612	CLA	C1B-CHB-C4A	-2.76	124.66	130.12
21	W	601	CHL	C1-C2-C3	-2.76	121.28	126.04
22	3	614	CLA	CMB-C2B-C3B	2.75	129.83	124.68
22	1	611	CLA	C1B-CHB-C4A	-2.75	124.66	130.12
21	6	618	CHL	O2D-CGD-O1D	-2.75	118.45	123.84
22	6	611	CLA	C1B-CHB-C4A	-2.75	124.67	130.12
21	U	608	CHL	C2A-C1A-CHA	-2.75	119.05	123.86
27	M	2001	BCR	C30-C25-C26	-2.75	118.74	122.61
24	V	2622	XAT	C11-C10-C9	-2.75	123.38	127.31
22	B	828	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
22	2	612	CLA	CHB-C4A-NA	2.75	128.31	124.51
27	K	202	BCR	C36-C18-C19	2.75	122.41	118.08
22	A	854	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
27	A	852	BCR	C19-C18-C17	2.75	123.16	118.94
22	K	206	CLA	CMB-C2B-C3B	2.75	129.82	124.68
22	A	806	CLA	C1B-CHB-C4A	-2.75	124.67	130.12
22	A	801	CLA	C4D-C3D-CAD	-2.75	104.86	108.10
22	B	809	CLA	C1B-CHB-C4A	-2.75	124.67	130.12
22	A	818	CLA	CHD-C1D-ND	-2.75	121.93	124.45
21	1	607	CHL	C3B-C4B-NB	2.75	112.76	109.21
22	6	603	CLA	C1B-CHB-C4A	-2.75	124.68	130.12
27	A	856	BCR	C21-C20-C19	-2.75	117.81	124.67
23	U	2620	LUT	C19-C9-C8	2.75	122.40	118.08
22	1	606	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
23	V	2620	LUT	C19-C9-C8	2.74	122.40	118.08
22	B	806	CLA	CHD-C1D-ND	-2.74	121.93	124.45
22	5	609	CLA	CMB-C2B-C1B	-2.74	124.25	128.46
22	W	602	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
21	V	605	CHL	O1D-CGD-CBD	-2.74	118.87	124.48
27	6	621	BCR	C35-C13-C14	-2.74	119.08	122.92
22	7	613	CLA	C1B-CHB-C4A	-2.74	124.69	130.12
22	7	606	CLA	C1B-CHB-C4A	-2.74	124.69	130.12
22	B	819	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
22	V	611	CLA	O2D-CGD-O1D	-2.74	117.86	124.09
22	B	836	CLA	C1B-CHB-C4A	-2.74	124.69	130.12
22	4	601	CLA	C1B-CHB-C4A	-2.74	124.69	130.12
22	8	603	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
21	2	608	CHL	CMD-C2D-C3D	-2.74	121.31	127.61
27	7	621	BCR	C34-C9-C8	2.74	122.39	118.08
24	V	2622	XAT	C27-C28-C29	-2.74	121.28	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	801	BCR	C16-C15-C14	-2.74	117.86	123.47
22	W	614	CLA	CMB-C2B-C3B	2.74	130.05	124.69
22	4	601	CLA	CMB-C2B-C3B	2.74	129.80	124.68
21	1	601	CHL	CMD-C2D-C3D	-2.74	121.31	127.61
22	6	603	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
22	U	614	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
22	B	835	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
22	3	614	CLA	C1B-CHB-C4A	-2.74	124.69	130.12
27	G	205	BCR	C28-C27-C26	-2.74	109.19	114.08
27	2	621	BCR	C16-C17-C18	-2.74	123.40	127.31
24	5	618	XAT	C7-C8-C9	-2.74	121.28	125.53
22	7	603	CLA	C1B-CHB-C4A	-2.74	124.70	130.12
23	7	618	LUT	C18-C5-C4	2.74	119.42	114.36
21	V	601	CHL	CMD-C2D-C3D	-2.74	121.32	127.61
27	F	305	BCR	C29-C30-C25	2.74	114.69	110.48
22	1	609	CLA	C4-C3-C5	2.74	119.87	115.27
27	B	1609	BCR	C32-C1-C6	-2.73	105.86	110.30
22	A	802	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
22	V	611	CLA	CAB-C3B-C2B	2.73	130.04	124.69
21	W	608	CHL	CMD-C2D-C3D	-2.73	121.33	127.61
22	A	810	CLA	C4-C3-C5	2.73	119.87	115.27
24	W	2622	XAT	C7-C8-C9	-2.73	121.29	125.53
22	B	820	CLA	C1B-CHB-C4A	-2.73	124.71	130.12
22	7	602	CLA	C1B-CHB-C4A	-2.73	124.71	130.12
22	1	602	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
27	4	621	BCR	C30-C25-C24	2.73	123.50	115.78
21	8	607	CHL	C2A-C1A-CHA	-2.73	119.08	123.86
22	4	612	CLA	C1B-CHB-C4A	-2.73	124.71	130.12
21	U	609	CHL	CHB-C4A-NA	2.73	128.29	124.51
27	7	621	BCR	C11-C10-C9	-2.73	123.42	127.31
21	W	601	CHL	C2A-C1A-CHA	-2.73	119.09	123.86
22	B	840	CLA	C1B-CHB-C4A	-2.73	124.71	130.12
22	6	604	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
21	8	606	CHL	CMD-C2D-C3D	-2.73	121.34	127.61
22	A	826	CLA	CMB-C2B-C3B	2.73	129.78	124.68
22	A	825	CLA	C1B-CHB-C4A	-2.73	124.72	130.12
22	A	834	CLA	CMB-C2B-C1B	-2.73	124.28	128.46
24	1	618	XAT	C30-C31-C32	-2.73	114.71	123.22
22	A	804	CLA	C1B-CHB-C4A	-2.72	124.72	130.12
25	U	2623	NEX	C11-C10-C9	-2.72	123.42	127.31
27	J	102	BCR	C37-C22-C21	-2.72	119.11	122.92
22	3	606	CLA	C1B-CHB-C4A	-2.72	124.72	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	7	607	CLA	C1B-CHB-C4A	-2.72	124.72	130.12
21	1	601	CHL	CMB-C2B-C3B	2.72	129.77	124.68
27	L	306	BCR	C15-C14-C13	-2.72	123.43	127.31
27	6	621	BCR	C16-C17-C18	-2.72	123.43	127.31
22	3	615	CLA	C1B-CHB-C4A	-2.72	124.73	130.12
22	9	602	CLA	C4-C3-C2	-2.72	116.70	123.68
22	A	809	CLA	CHD-C1D-ND	-2.72	121.96	124.45
21	4	608	CHL	CMD-C2D-C3D	-2.72	121.36	127.61
22	9	604	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
22	B	809	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
22	W	614	CLA	CAB-C3B-C2B	2.72	130.01	124.69
21	U	601	CHL	O2A-CGA-CBA	2.72	120.43	111.91
27	A	852	BCR	C1-C6-C7	2.72	123.46	115.78
22	J	101	CLA	C1B-CHB-C4A	-2.72	124.74	130.12
22	9	613	CLA	C1B-CHB-C4A	-2.72	124.74	130.12
22	3	607	CLA	CHD-C1D-ND	-2.71	121.96	124.45
27	B	845	BCR	C33-C5-C4	2.71	118.83	113.62
22	B	811	CLA	C1B-CHB-C4A	-2.71	124.74	130.12
23	7	618	LUT	C18-C5-C6	-2.71	121.48	124.53
21	8	608	CHL	O2A-CGA-CBA	2.71	120.42	111.91
22	A	836	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
22	8	603	CLA	C1B-CHB-C4A	-2.71	124.75	130.12
21	8	606	CHL	C2A-C1A-CHA	-2.71	119.12	123.86
22	B	832	CLA	C1B-CHB-C4A	-2.71	124.75	130.12
22	1	609	CLA	CMB-C2B-C3B	2.71	129.75	124.68
22	K	201	CLA	C1B-CHB-C4A	-2.71	124.75	130.12
21	6	608	CHL	C2A-C1A-CHA	-2.71	119.12	123.86
22	1	604	CLA	C1B-CHB-C4A	-2.71	124.75	130.12
21	8	608	CHL	CMD-C2D-C3D	-2.71	121.39	127.61
22	B	805	CLA	CHD-C1D-ND	-2.71	121.97	124.45
22	L	302	CLA	CHD-C1D-ND	-2.71	121.97	124.45
24	6	620	XAT	C20-C13-C12	2.71	122.34	118.08
21	V	608	CHL	CMD-C2D-C3D	-2.70	121.39	127.61
21	8	606	CHL	CMB-C2B-C3B	2.70	129.74	124.68
27	B	844	BCR	C38-C26-C27	2.70	118.81	113.62
24	W	2622	XAT	C11-C10-C9	-2.70	123.45	127.31
21	8	618	CHL	CMD-C2D-C3D	-2.70	121.40	127.61
22	B	806	CLA	C1-C2-C3	-2.70	121.37	126.04
21	2	618	CHL	CMB-C2B-C3B	2.70	129.73	124.68
22	V	612	CLA	CMB-C2B-C3B	2.70	129.97	124.69
23	9	624	LUT	C28-C29-C30	-2.70	114.80	118.94
27	L	301	BCR	C7-C8-C9	-2.70	122.16	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	8	604	CLA	C1B-CHB-C4A	-2.70	124.77	130.12
21	6	608	CHL	CMD-C2D-C3D	-2.70	121.41	127.61
32	B	850	DGD	O1G-C1A-C2A	2.70	120.37	111.91
22	A	807	CLA	C1B-CHB-C4A	-2.70	124.77	130.12
22	B	824	CLA	C1B-CHB-C4A	-2.70	124.78	130.12
25	V	2623	NEX	C27-C28-C29	-2.70	121.34	125.53
22	3	602	CLA	O2D-CGD-O1D	-2.70	118.57	123.84
24	6	620	XAT	C26-C27-C28	-2.70	120.29	125.99
22	4	604	CLA	C1B-CHB-C4A	-2.70	124.78	130.12
25	V	2623	NEX	C5-C6-C1	2.69	122.37	119.70
24	4	620	XAT	C19-C9-C8	2.69	122.32	118.08
24	3	619	XAT	C12-C13-C14	-2.69	114.81	118.94
24	3	619	XAT	C20-C13-C12	2.69	122.32	118.08
26	V	2630	LHG	O8-C23-C24	2.69	120.36	111.91
22	W	612	CLA	CMB-C2B-C3B	2.69	129.96	124.69
27	B	844	BCR	C34-C9-C8	2.69	122.32	118.08
27	O	2004	BCR	C36-C18-C19	2.69	122.32	118.08
22	V	603	CLA	C1B-CHB-C4A	-2.69	124.78	130.12
22	B	821	CLA	CHD-C1D-ND	-2.69	121.98	124.45
21	2	601	CHL	O2D-CGD-O1D	-2.69	118.58	123.84
27	3	621	BCR	C4-C5-C6	-2.69	118.82	122.73
21	U	606	CHL	CMD-C2D-C3D	-2.69	121.42	127.61
25	V	2623	NEX	C20-C13-C12	2.69	122.32	118.08
23	9	624	LUT	C32-C33-C34	-2.69	114.81	118.94
22	W	613	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
27	7	620	BCR	C34-C9-C8	2.69	122.31	118.08
22	B	807	CLA	CHD-C1D-ND	-2.69	121.98	124.45
22	B	810	CLA	C1B-CHB-C4A	-2.69	124.79	130.12
22	B	821	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
26	6	630	LHG	O8-C23-C24	2.69	120.34	111.91
22	B	803	CLA	CHB-C4A-NA	2.69	128.23	124.51
26	U	2630	LHG	O8-C23-C24	2.69	120.34	111.91
22	O	2002	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
21	9	608	CHL	CMD-C2D-C3D	-2.69	121.44	127.61
27	B	844	BCR	C15-C14-C13	-2.69	123.48	127.31
22	A	803	CLA	O2A-CGA-O1A	-2.68	116.82	123.59
21	6	608	CHL	OMC-CMC-C2C	-2.68	119.62	125.69
27	B	845	BCR	C40-C30-C25	-2.68	105.95	110.30
24	W	2622	XAT	C25-C24-C23	2.68	118.06	112.75
25	V	2623	NEX	C31-C30-C29	-2.68	123.48	127.31
26	A	847	LHG	O8-C23-C24	2.68	120.33	111.91
27	L	301	BCR	C35-C13-C12	2.68	122.30	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	G	203	CLA	C1-C2-C3	-2.68	122.41	126.75
22	A	801	CLA	CBA-CAA-C2A	-2.68	105.95	113.86
22	K	204	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
21	4	608	CHL	CMB-C2B-C3B	2.68	129.69	124.68
21	4	606	CHL	CMD-C2D-C3D	-2.68	121.45	127.61
26	5	630	LHG	O8-C23-C24	2.68	120.31	111.91
23	9	620	LUT	C7-C8-C9	-2.68	122.19	126.23
27	A	852	BCR	C16-C15-C14	-2.68	117.99	123.47
22	1	602	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
22	B	813	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
21	9	605	CHL	CAC-C3C-C4C	2.68	129.12	125.04
27	B	847	BCR	C34-C9-C8	2.68	122.30	118.08
21	W	601	CHL	CMD-C2D-C3D	-2.68	121.46	127.61
21	W	605	CHL	CMD-C2D-C3D	-2.68	121.46	127.61
22	J	101	CLA	O2D-CGD-O1D	-2.68	118.61	123.84
24	1	618	XAT	C38-C25-C24	2.68	117.29	114.28
27	B	847	BCR	C40-C30-C25	-2.68	105.96	110.30
22	A	806	CLA	CHD-C1D-ND	-2.67	122.00	124.45
23	2	619	LUT	C15-C35-C34	2.67	128.95	123.47
27	A	850	BCR	C16-C17-C18	-2.67	123.49	127.31
21	3	608	CHL	O2A-CGA-CBA	2.67	120.30	111.91
21	W	609	CHL	CMD-C2D-C3D	-2.67	121.46	127.61
22	2	614	CLA	CHD-C1D-ND	-2.67	122.00	124.45
22	6	610	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
27	B	847	BCR	C33-C5-C6	-2.67	121.53	124.53
21	1	601	CHL	O2D-CGD-O1D	-2.67	118.61	123.84
23	U	2620	LUT	C22-C23-C24	2.67	114.78	111.74
21	U	608	CHL	CMD-C2D-C3D	-2.67	121.47	127.61
27	M	2001	BCR	C37-C22-C21	-2.67	119.18	122.92
23	W	2621	LUT	C11-C10-C9	-2.67	123.50	127.31
22	H	201	CLA	CBD-CHA-C1A	2.67	131.71	127.43
27	A	849	BCR	C15-C14-C13	-2.67	123.50	127.31
22	U	613	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
21	V	605	CHL	CMD-C2D-C3D	-2.67	121.48	127.61
21	6	607	CHL	CMD-C2D-C3D	-2.67	121.48	127.61
21	W	607	CHL	CMD-C2D-C3D	-2.67	121.48	127.61
22	U	610	CLA	O2A-CGA-O1A	-2.67	116.87	123.59
28	G	202	LMG	O8-C28-C29	2.67	120.27	111.91
27	B	847	BCR	C36-C18-C19	2.66	122.28	118.08
22	5	606	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
22	7	607	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
22	2	609	CLA	C4A-NA-C1A	2.66	107.90	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	839	CLA	C1B-CHB-C4A	-2.66	124.84	130.12
27	F	305	BCR	C1-C6-C7	2.66	123.31	115.78
21	8	618	CHL	CMB-C2B-C3B	2.66	129.66	124.68
23	4	619	LUT	C8-C7-C6	-2.66	119.72	127.20
27	L	305	BCR	C19-C18-C17	-2.66	114.86	118.94
22	B	819	CLA	CMB-C2B-C3B	2.66	129.66	124.68
21	8	608	CHL	OMC-CMC-C2C	-2.66	119.67	125.69
31	G	206	LMT	C1B-O1B-C4'	-2.66	111.38	117.96
26	3	630	LHG	O8-C23-C24	2.66	120.25	111.91
22	3	612	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
22	7	617	CLA	CHD-C1D-ND	-2.66	122.01	124.45
22	A	824	CLA	C1B-CHB-C4A	-2.66	124.85	130.12
21	U	605	CHL	CMD-C2D-C3D	-2.66	121.50	127.61
21	6	606	CHL	CMD-C2D-C3D	-2.66	121.50	127.61
27	B	801	BCR	C36-C18-C17	-2.66	119.20	122.92
21	U	606	CHL	OMC-CMC-C2C	-2.66	119.68	125.69
22	K	203	CLA	CHD-C1D-ND	-2.65	122.02	124.45
22	K	204	CLA	C4-C3-C5	2.65	119.73	115.27
22	B	832	CLA	CMB-C2B-C3B	2.65	129.64	124.68
24	8	620	XAT	C37-C21-C22	-2.65	104.38	108.98
21	6	606	CHL	CHB-C4A-NA	2.65	128.18	124.51
21	U	601	CHL	CMD-C2D-C3D	-2.65	121.52	127.61
24	3	619	XAT	C24-C23-C22	-2.65	105.65	110.77
27	K	202	BCR	C2-C1-C6	2.65	114.56	110.48
22	V	602	CLA	O2D-CGD-CBD	2.65	115.98	111.27
27	8	621	BCR	C30-C25-C26	-2.65	118.88	122.61
22	V	614	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
27	A	856	BCR	C30-C25-C24	2.65	123.27	115.78
21	V	601	CHL	CMB-C2B-C3B	2.65	129.87	124.69
23	9	624	LUT	C19-C9-C8	2.65	122.25	118.08
22	9	609	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
26	W	2630	LHG	O8-C23-C24	2.65	120.21	111.91
27	B	845	BCR	C21-C20-C19	-2.65	114.96	123.22
23	6	619	LUT	C28-C29-C30	-2.65	114.88	118.94
22	1	603	CLA	C1B-CHB-C4A	-2.65	124.88	130.12
23	4	619	LUT	C16-C1-C6	2.64	114.59	110.30
22	3	603	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
26	9	2630	LHG	C9-C8-C7	-2.64	104.01	113.62
22	3	614	CLA	CHD-C1D-ND	-2.64	122.03	124.45
22	B	814	CLA	CHD-C1D-ND	-2.64	122.03	124.45
27	K	205	BCR	C28-C27-C26	-2.64	109.36	114.08
23	W	2621	LUT	C1-C6-C5	-2.64	118.89	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	3	621	BCR	C36-C18-C17	-2.64	119.22	122.92
23	U	2621	LUT	C19-C9-C10	-2.64	119.22	122.92
27	1	619	BCR	C15-C14-C13	-2.64	123.54	127.31
22	A	837	CLA	CHD-C1D-ND	-2.64	122.03	124.45
22	7	604	CLA	CHD-C1D-ND	-2.64	122.03	124.45
22	B	839	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
22	A	837	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
27	A	850	BCR	C28-C27-C26	-2.64	109.37	114.08
22	1	610	CLA	C1-C2-C3	-2.64	121.48	126.04
23	9	624	LUT	C20-C13-C12	2.64	122.23	118.08
23	9	620	LUT	C28-C29-C30	-2.64	114.90	118.94
21	1	601	CHL	C1-C2-C3	-2.63	121.49	126.04
21	6	618	CHL	CMB-C2B-C3B	2.63	129.60	124.68
22	5	603	CLA	CMB-C2B-C3B	2.63	129.60	124.68
27	L	306	BCR	C1-C6-C5	-2.63	118.91	122.61
23	6	619	LUT	C11-C10-C9	-2.63	123.55	127.31
21	1	607	CHL	CMB-C2B-C3B	2.63	129.60	124.68
22	9	611	CLA	CHB-C4A-NA	2.63	128.15	124.51
23	1	617	LUT	C11-C10-C9	-2.63	123.56	127.31
22	A	815	CLA	CHB-C4A-NA	2.63	128.15	124.51
22	1	604	CLA	CHD-C1D-ND	-2.63	122.04	124.45
21	2	608	CHL	C3B-C4B-NB	2.63	112.61	109.21
27	B	845	BCR	C38-C26-C27	2.63	118.67	113.62
22	7	602	CLA	O2D-CGD-CBD	2.63	115.94	111.27
27	7	620	BCR	C20-C21-C22	-2.63	123.56	127.31
22	B	807	CLA	C1B-CHB-C4A	-2.63	124.91	130.12
22	A	839	CLA	CHD-C1D-ND	-2.63	122.04	124.45
22	5	602	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
22	B	814	CLA	CHB-C4A-NA	2.63	128.15	124.51
27	L	305	BCR	C8-C9-C10	-2.63	114.91	118.94
27	B	801	BCR	C7-C8-C9	-2.63	122.27	126.23
22	5	613	CLA	C1-C2-C3	-2.63	122.50	126.75
22	1	609	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
27	L	306	BCR	C8-C7-C6	-2.63	119.83	127.20
22	7	610	CLA	CHD-C1D-ND	-2.63	122.04	124.45
22	7	604	CLA	C1-C2-C3	-2.63	122.50	126.75
22	7	607	CLA	CHD-C1D-ND	-2.62	122.04	124.45
27	O	2004	BCR	C1-C6-C5	-2.62	118.92	122.61
22	B	812	CLA	CHD-C1D-ND	-2.62	121.98	124.52
22	4	614	CLA	CHD-C1D-ND	-2.62	122.04	124.45
22	U	610	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
26	1	630	LHG	O8-C23-C24	2.62	120.13	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	9	624	LUT	C35-C34-C33	-2.62	123.57	127.31
22	7	615	CLA	O2D-CGD-O1D	-2.62	118.14	124.09
22	K	203	CLA	O2D-CGD-CBD	2.62	115.92	111.27
22	A	814	CLA	C1B-CHB-C4A	-2.62	124.93	130.12
27	6	621	BCR	C23-C24-C25	-2.62	119.85	127.20
22	K	204	CLA	CMB-C2B-C3B	2.62	129.58	124.68
22	7	615	CLA	CMB-C2B-C3B	2.62	129.57	124.68
22	W	614	CLA	O2D-CGD-O1D	-2.62	118.15	124.09
23	1	617	LUT	C36-C21-C26	2.62	113.51	109.55
27	A	849	BCR	C28-C27-C26	-2.62	109.41	114.08
22	B	836	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
23	U	2621	LUT	C15-C14-C13	-2.61	123.58	127.31
27	7	621	BCR	C1-C6-C5	-2.61	118.93	122.61
22	U	610	CLA	C1-C2-C3	-2.61	121.52	126.04
22	B	809	CLA	CMB-C2B-C3B	2.61	129.57	124.68
23	9	624	LUT	C15-C14-C13	-2.61	123.58	127.31
21	U	606	CHL	C3B-C4B-NB	2.61	112.59	109.21
27	1	619	BCR	C19-C18-C17	-2.61	114.93	118.94
27	G	205	BCR	C3-C4-C5	-2.61	109.42	114.08
27	1	619	BCR	C38-C26-C27	2.61	118.63	113.62
22	7	603	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
22	B	834	CLA	CHD-C1D-ND	-2.61	122.06	124.45
22	V	613	CLA	CAA-C2A-C3A	-2.61	105.64	112.78
24	V	2622	XAT	C18-C5-C6	-2.61	117.89	122.26
25	U	2623	NEX	C35-C15-C14	-2.61	118.13	123.47
21	V	607	CHL	O2D-CGD-O1D	-2.61	118.74	123.84
27	3	620	BCR	C27-C26-C25	-2.61	118.94	122.73
27	M	2001	BCR	C15-C16-C17	-2.61	118.13	123.47
22	A	817	CLA	CAA-C2A-C3A	-2.61	105.64	112.78
27	1	619	BCR	C1-C6-C5	-2.61	118.94	122.61
27	1	619	BCR	C29-C30-C25	2.60	114.49	110.48
23	7	618	LUT	C11-C10-C9	-2.60	123.59	127.31
31	A	857	LMT	C1-O1'-C1'	-2.60	109.52	113.84
27	K	205	BCR	C24-C23-C22	-2.60	122.30	126.23
22	9	603	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
22	A	835	CLA	CHD-C1D-ND	-2.60	122.06	124.45
23	9	624	LUT	C11-C10-C9	-2.60	123.60	127.31
27	L	305	BCR	C20-C21-C22	-2.60	123.60	127.31
27	O	2004	BCR	C37-C22-C21	-2.60	119.28	122.92
22	A	836	CLA	CHD-C1D-ND	-2.60	122.07	124.45
22	B	827	CLA	CHB-C4A-NA	2.60	128.10	124.51
22	2	613	CLA	C1-C2-C3	-2.60	121.55	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	8	604	CLA	C1-C2-C3	-2.60	122.55	126.75
27	G	205	BCR	C33-C5-C4	2.60	118.61	113.62
25	U	2623	NEX	C31-C30-C29	-2.60	123.60	127.31
21	U	607	CHL	CMD-C2D-C3D	-2.60	121.64	127.61
21	2	606	CHL	CMD-C2D-C3D	-2.60	121.64	127.61
22	W	612	CLA	O2D-CGD-O1D	-2.59	118.20	124.09
22	7	603	CLA	CMB-C2B-C3B	2.59	129.53	124.68
22	B	821	CLA	C1-C2-C3	-2.59	122.56	126.75
31	G	206	LMT	C1'-O5'-C5'	-2.59	108.60	113.69
22	U	602	CLA	CMB-C2B-C1B	-2.59	124.48	128.46
21	8	618	CHL	C2A-C1A-CHA	-2.59	119.33	123.86
25	W	2623	NEX	C2-C1-C6	2.59	111.72	109.21
22	7	602	CLA	CHD-C1D-ND	-2.59	122.08	124.45
27	B	845	BCR	C34-C9-C10	-2.59	119.30	122.92
22	6	614	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
27	K	205	BCR	C36-C18-C19	2.59	122.15	118.08
22	7	602	CLA	C1-C2-C3	-2.58	121.57	126.04
27	G	205	BCR	C38-C26-C27	2.58	118.58	113.62
21	V	607	CHL	CMD-C2D-C3D	-2.58	121.67	127.61
22	G	204	CLA	CHD-C1D-ND	-2.58	122.08	124.45
27	6	621	BCR	C30-C25-C26	-2.58	118.98	122.61
22	1	612	CLA	CHB-C4A-NA	2.58	128.08	124.51
22	B	804	CLA	CHB-C4A-NA	2.58	128.08	124.51
27	B	1609	BCR	C8-C7-C6	-2.58	119.96	127.20
27	4	621	BCR	C11-C12-C13	-2.58	119.17	126.42
22	9	604	CLA	CHD-C1D-ND	-2.58	122.08	124.45
22	B	825	CLA	C1B-CHB-C4A	-2.58	125.01	130.12
27	3	620	BCR	C23-C24-C25	-2.58	119.96	127.20
22	1	609	CLA	C1D-ND-C4D	-2.58	104.50	106.33
22	V	612	CLA	O2D-CGD-O1D	-2.58	118.24	124.09
24	5	618	XAT	C20-C13-C12	2.57	122.13	118.08
21	U	606	CHL	O2D-CGD-O1D	-2.57	118.81	123.84
22	B	805	CLA	C1B-CHB-C4A	-2.57	125.02	130.12
23	4	619	LUT	C35-C34-C33	-2.57	123.64	127.31
23	2	619	LUT	C8-C9-C10	2.57	122.89	118.94
21	5	607	CHL	CMB-C2B-C3B	2.57	129.49	124.68
27	O	2004	BCR	C15-C14-C13	-2.57	123.64	127.31
22	A	811	CLA	CHD-C1D-ND	-2.57	122.09	124.45
22	B	832	CLA	CHD-C1D-ND	-2.57	122.09	124.45
27	8	621	BCR	C15-C16-C17	-2.57	118.21	123.47
22	A	808	CLA	CHD-C1D-ND	-2.57	122.09	124.45
21	V	605	CHL	CMB-C2B-C3B	2.57	129.49	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	6	608	CHL	O2A-CGA-CBA	2.57	119.97	111.91
21	U	609	CHL	O2D-CGD-O1D	-2.57	118.81	123.84
25	U	2623	NEX	C20-C13-C12	2.57	122.12	118.08
22	A	828	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
21	2	607	CHL	C2A-C1A-CHA	-2.57	119.37	123.86
22	W	610	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
22	6	611	CLA	CHD-C1D-ND	-2.57	122.09	124.45
27	F	305	BCR	C16-C15-C14	-2.57	118.22	123.47
21	V	609	CHL	C2A-C1A-CHA	-2.57	119.37	123.86
22	3	613	CLA	CHB-C4A-NA	2.57	128.06	124.51
22	A	814	CLA	CHB-C4A-NA	2.57	128.06	124.51
24	W	2622	XAT	C6-C7-C8	-2.57	120.57	125.99
27	B	845	BCR	C19-C18-C17	-2.56	115.01	118.94
27	K	202	BCR	C11-C12-C13	-2.56	119.21	126.42
22	7	613	CLA	CMB-C2B-C3B	2.56	129.47	124.68
21	8	608	CHL	CMB-C2B-C3B	2.56	129.47	124.68
22	9	613	CLA	CHD-C1D-ND	-2.56	122.10	124.45
24	U	2622	XAT	C31-C30-C29	-2.56	123.66	127.31
22	2	613	CLA	CHB-C4A-NA	2.56	128.05	124.51
24	7	619	XAT	C31-C32-C33	-2.56	119.22	126.42
22	A	835	CLA	CMB-C2B-C3B	2.56	129.47	124.68
21	6	606	CHL	O2D-CGD-O1D	-2.56	118.83	123.84
27	A	851	BCR	C27-C26-C25	-2.56	119.02	122.73
21	4	606	CHL	C2A-C1A-CHA	-2.56	119.39	123.86
21	4	606	CHL	OMC-CMC-C2C	-2.56	119.90	125.69
22	V	610	CLA	CMB-C2B-C3B	2.56	129.70	124.69
27	A	852	BCR	C35-C13-C12	2.56	122.11	118.08
22	B	817	CLA	CHD-C1D-ND	-2.56	122.10	124.45
22	8	613	CLA	CHD-C1D-ND	-2.56	122.10	124.45
27	A	852	BCR	C20-C19-C18	-2.56	119.23	126.42
27	L	301	BCR	C23-C22-C21	2.56	122.86	118.94
21	5	607	CHL	CMD-C2D-C3D	-2.56	121.73	127.61
22	B	826	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
27	3	620	BCR	C40-C30-C25	-2.56	106.15	110.30
27	K	205	BCR	C16-C15-C14	-2.56	118.24	123.47
22	B	831	CLA	CHD-C1D-ND	-2.55	122.11	124.45
31	A	857	LMT	O3B-C3B-C4B	-2.55	104.44	110.35
21	U	601	CHL	CMB-C2B-C3B	2.55	129.69	124.69
21	6	607	CHL	CMB-C2B-C3B	2.55	129.46	124.68
27	2	621	BCR	C38-C26-C25	2.55	127.39	124.53
23	9	620	LUT	C39-C29-C28	2.55	122.10	118.08
23	4	619	LUT	C35-C15-C14	-2.55	118.25	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	L	305	BCR	C30-C25-C24	2.55	123.00	115.78
27	B	844	BCR	C31-C1-C6	2.55	114.44	110.30
24	1	618	XAT	C19-C9-C8	2.55	122.09	118.08
22	3	602	CLA	CHD-C1D-ND	-2.55	122.11	124.45
22	A	841	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
27	2	621	BCR	C34-C9-C8	2.55	122.09	118.08
22	U	612	CLA	CHB-C4A-NA	2.55	128.03	124.51
22	A	816	CLA	CHD-C1D-ND	-2.55	122.11	124.45
27	G	205	BCR	C1-C6-C5	-2.54	119.03	122.61
22	7	614	CLA	CHD-C1D-ND	-2.54	122.12	124.45
22	B	807	CLA	O2D-CGD-CBD	2.54	115.78	111.27
31	B	849	LMT	C1'-C2'-C3'	-2.54	104.71	110.00
22	B	802	CLA	CMB-C2B-C1B	-2.54	124.56	128.46
21	U	601	CHL	C4-C3-C5	2.54	119.54	115.27
27	3	621	BCR	C34-C9-C8	2.54	122.08	118.08
22	1	608	CLA	CHD-C1D-ND	-2.54	122.12	124.45
22	8	609	CLA	CHD-C1D-ND	-2.54	122.12	124.45
22	B	814	CLA	O2A-CGA-O1A	-2.54	117.19	123.59
27	M	2001	BCR	C15-C14-C13	-2.54	123.69	127.31
27	G	205	BCR	C34-C9-C8	2.54	122.07	118.08
27	7	620	BCR	C30-C25-C26	-2.53	119.04	122.61
27	3	620	BCR	C4-C5-C6	-2.53	119.05	122.73
27	A	852	BCR	C28-C27-C26	-2.53	109.55	114.08
27	7	621	BCR	C16-C17-C18	-2.53	123.70	127.31
22	B	815	CLA	CHD-C1D-ND	-2.53	122.13	124.45
25	W	2623	NEX	C19-C9-C10	-2.53	119.38	122.92
22	A	833	CLA	CHD-C1D-ND	-2.53	122.13	124.45
21	6	602	CHL	CMD-C2D-C3D	-2.53	121.79	127.61
22	7	606	CLA	CHD-C1D-ND	-2.53	122.13	124.45
28	J	103	LMG	C8-O7-C10	-2.53	111.56	117.79
21	9	605	CHL	CMB-C2B-C3B	2.53	129.41	124.68
21	2	601	CHL	C2A-C1A-CHA	-2.53	119.44	123.86
22	3	615	CLA	CHD-C1D-ND	-2.53	122.13	124.45
27	O	2004	BCR	C3-C4-C5	-2.53	109.56	114.08
24	5	618	XAT	C19-C9-C8	2.53	122.06	118.08
22	3	613	CLA	CHD-C1D-ND	-2.53	122.13	124.45
22	A	807	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
22	A	842	CLA	CMB-C2B-C3B	2.53	129.40	124.68
27	O	2004	BCR	C11-C10-C9	-2.52	123.71	127.31
22	A	810	CLA	CHD-C1D-ND	-2.52	122.13	124.45
22	A	813	CLA	CHD-C1D-ND	-2.52	122.13	124.45
22	6	609	CLA	CHD-C1D-ND	-2.52	122.14	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	3	618	LUT	C21-C26-C27	-2.52	109.51	112.70
22	5	604	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
31	B	849	LMT	C1'-O5'-C5'	-2.52	108.74	113.69
27	L	305	BCR	C3-C4-C5	-2.52	109.58	114.08
22	9	609	CLA	CMB-C2B-C3B	2.52	129.39	124.68
22	U	603	CLA	CHB-C4A-NA	2.52	128.00	124.51
21	8	608	CHL	C2A-C1A-CHA	-2.52	119.45	123.86
27	B	848	BCR	C34-C9-C10	-2.52	119.40	122.92
22	1	606	CLA	CMB-C2B-C3B	2.52	129.39	124.68
22	1	613	CLA	CHD-C1D-ND	-2.52	122.14	124.45
27	A	852	BCR	C38-C26-C27	2.52	118.45	113.62
21	1	607	CHL	O2D-CGD-O1D	-2.52	118.92	123.84
27	A	856	BCR	C29-C30-C25	2.52	114.35	110.48
22	2	604	CLA	C1-C2-C3	-2.51	122.68	126.75
22	A	828	CLA	CHD-C1D-ND	-2.51	122.14	124.45
22	A	821	CLA	CMB-C2B-C3B	2.51	129.38	124.68
21	4	607	CHL	CMB-C2B-C3B	2.51	129.38	124.68
26	4	630	LHG	O4-P-O6	2.51	119.42	107.75
22	3	613	CLA	O2A-CGA-O1A	-2.51	117.25	123.59
23	3	618	LUT	C3-C4-C5	-2.51	106.85	111.85
22	6	604	CLA	CHD-C1D-ND	-2.51	122.15	124.45
21	4	607	CHL	C2A-C1A-CHA	-2.51	119.47	123.86
21	2	601	CHL	CMB-C2B-C3B	2.51	129.37	124.68
22	7	603	CLA	CHD-C1D-ND	-2.51	122.15	124.45
22	B	811	CLA	CMB-C2B-C3B	2.51	129.37	124.68
22	5	604	CLA	CHD-C1D-ND	-2.51	122.15	124.45
24	7	619	XAT	C17-C1-C16	2.51	111.07	107.37
22	6	613	CLA	CMB-C2B-C3B	2.51	129.37	124.68
27	K	202	BCR	C4-C5-C6	-2.50	119.10	122.73
22	5	606	CLA	CHD-C1D-ND	-2.50	122.15	124.45
21	1	601	CHL	C4-C3-C5	2.50	119.48	115.27
22	B	808	CLA	CMB-C2B-C1B	-2.50	124.62	128.46
27	L	301	BCR	C4-C5-C6	-2.50	119.10	122.73
21	W	605	CHL	CMB-C2B-C3B	2.50	129.59	124.69
22	4	601	CLA	C1-C2-C3	-2.50	122.70	126.75
21	6	601	CHL	CMB-C2B-C3B	2.50	129.36	124.68
24	2	620	XAT	C35-C34-C33	-2.50	123.74	127.31
22	6	613	CLA	CHD-C1D-ND	-2.50	122.16	124.45
22	8	614	CLA	CHD-C1D-ND	-2.50	122.16	124.45
21	W	606	CHL	CMB-C2B-C3B	2.50	129.58	124.69
27	7	621	BCR	C15-C14-C13	-2.50	123.75	127.31
22	3	617	CLA	CHB-C4A-NA	2.50	127.97	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	V	604	CLA	C1-C2-C3	-2.50	122.71	126.75
22	9	603	CLA	CMB-C2B-C3B	2.50	129.35	124.68
31	A	857	LMT	O5'-C1'-C2'	-2.50	105.06	110.35
22	1	604	CLA	C1-C2-C3	-2.50	122.71	126.75
27	B	844	BCR	C33-C5-C4	2.49	118.41	113.62
24	V	2622	XAT	C35-C34-C33	-2.49	123.75	127.31
21	6	618	CHL	CMD-C2D-C3D	-2.49	121.88	127.61
27	O	2004	BCR	C38-C26-C27	2.49	118.40	113.62
27	B	847	BCR	C37-C22-C23	2.49	122.00	118.08
22	A	831	CLA	CHD-C1D-ND	-2.49	122.17	124.45
24	5	618	XAT	C35-C15-C14	-2.49	118.37	123.47
27	A	856	BCR	C11-C10-C9	-2.49	123.76	127.31
22	W	613	CLA	C1-C2-C3	-2.49	121.74	126.04
22	8	614	CLA	CHB-C4A-NA	2.49	127.95	124.51
22	W	603	CLA	O2D-CGD-O1D	-2.48	118.45	124.09
22	A	814	CLA	CHD-C1D-ND	-2.48	122.17	124.45
27	B	844	BCR	C19-C18-C17	-2.48	115.13	118.94
22	B	837	CLA	CHB-C4A-NA	2.48	127.95	124.51
27	A	848	BCR	C38-C26-C27	2.48	118.39	113.62
24	U	2622	XAT	C11-C10-C9	-2.48	123.77	127.31
22	B	816	CLA	O2D-CGD-CBD	2.48	115.68	111.27
22	O	2001	CLA	CHD-C1D-ND	-2.48	122.12	124.52
23	8	619	LUT	C11-C10-C9	-2.48	123.77	127.31
22	B	822	CLA	CHD-C1D-ND	-2.48	122.17	124.45
27	O	2004	BCR	C16-C17-C18	-2.48	123.77	127.31
23	V	2620	LUT	C1-C6-C5	-2.48	119.12	122.61
27	8	621	BCR	C20-C21-C22	-2.48	123.77	127.31
22	2	613	CLA	CHD-C1D-ND	-2.48	122.18	124.45
22	B	810	CLA	CHB-C4A-NA	2.48	127.94	124.51
22	B	841	CLA	C1-C2-C3	-2.48	121.76	126.04
23	V	2620	LUT	C31-C30-C29	-2.48	123.78	127.31
22	W	602	CLA	CHD-C1D-ND	-2.48	122.18	124.45
22	L	303	CLA	O2A-CGA-O1A	-2.48	117.34	123.59
22	H	201	CLA	CMB-C2B-C3B	2.48	129.31	124.68
21	6	601	CHL	O2D-CGD-O1D	-2.48	119.00	123.84
23	6	619	LUT	C40-C33-C32	2.48	121.98	118.08
27	2	621	BCR	C36-C18-C19	2.48	121.98	118.08
31	G	206	LMT	O3B-C3B-C4B	-2.48	104.63	110.35
27	A	856	BCR	C2-C1-C6	2.47	114.29	110.48
21	2	602	CHL	OMC-CMC-C2C	-2.47	120.10	125.69
21	6	608	CHL	CMB-C2B-C3B	2.47	129.30	124.68
21	V	608	CHL	CMB-C2B-C3B	2.47	129.52	124.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	M	2001	BCR	C36-C18-C19	2.47	121.97	118.08
21	6	618	CHL	C2A-C1A-CHA	-2.47	119.54	123.86
22	U	610	CLA	CAA-C2A-C1A	-2.47	103.88	111.97
21	7	608	CHL	CMB-C2B-C3B	2.47	129.30	124.68
22	9	610	CLA	CHD-C1D-ND	-2.47	122.19	124.45
21	U	608	CHL	OMC-CMC-C2C	-2.47	120.11	125.69
27	7	620	BCR	C7-C8-C9	-2.47	122.51	126.23
28	2	631	LMG	O8-C28-C29	2.47	119.65	111.91
22	4	609	CLA	CHD-C1D-ND	-2.47	122.19	124.45
27	6	621	BCR	C31-C1-C6	2.46	114.30	110.30
22	8	604	CLA	CHB-C4A-NA	2.46	127.92	124.51
22	5	612	CLA	CHB-C4A-NA	2.46	127.92	124.51
27	K	205	BCR	C32-C1-C6	-2.46	106.30	110.30
25	V	2623	NEX	C28-C29-C30	2.46	122.72	118.94
21	3	608	CHL	C1C-C2C-C3C	-2.46	105.16	107.11
21	V	607	CHL	CMB-C2B-C3B	2.46	129.51	124.69
22	4	604	CLA	CHB-C4A-NA	2.46	127.92	124.51
21	5	601	CHL	CMB-C2B-C3B	2.46	129.28	124.68
27	K	202	BCR	C16-C17-C18	-2.46	123.80	127.31
22	A	840	CLA	CMB-C2B-C3B	2.46	129.28	124.68
21	5	601	CHL	CMD-C2D-C3D	-2.46	121.96	127.61
24	6	620	XAT	C38-C25-C24	-2.46	111.51	114.28
22	A	840	CLA	CHD-C1D-ND	-2.46	122.19	124.45
22	B	823	CLA	CHD-C1D-ND	-2.46	122.19	124.45
21	2	606	CHL	OMC-CMC-C2C	-2.46	120.13	125.69
27	B	1609	BCR	C8-C9-C10	2.46	122.71	118.94
27	L	305	BCR	C7-C8-C9	-2.46	122.52	126.23
22	1	603	CLA	CHB-C4A-NA	2.46	127.91	124.51
27	3	621	BCR	C30-C25-C24	2.46	122.73	115.78
22	A	822	CLA	CHD-C1D-ND	-2.46	122.20	124.45
22	U	602	CLA	CHB-C4A-NA	2.46	127.91	124.51
22	9	611	CLA	CHD-C1D-ND	-2.45	122.20	124.45
29	B	842	PQN	C11-C12-C13	-2.45	122.71	126.79
22	J	101	CLA	CHB-C4A-NA	2.45	127.91	124.51
22	U	603	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
22	U	613	CLA	C1-C2-C3	-2.45	121.80	126.04
21	W	607	CHL	OMC-CMC-C2C	-2.45	120.14	125.69
21	U	605	CHL	CMB-C2B-C3B	2.45	129.49	124.69
22	B	839	CLA	CHD-C1D-ND	-2.45	122.20	124.45
22	F	303	CLA	CHD-C1D-ND	-2.45	122.20	124.45
22	5	613	CLA	CMB-C2B-C3B	2.45	129.27	124.68
22	7	609	CLA	O2D-CGD-CBD	2.45	115.62	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	2	613	CLA	O2A-CGA-O1A	-2.45	117.41	123.59
21	2	608	CHL	OMC-CMC-C2C	-2.45	120.14	125.69
21	V	608	CHL	OMC-CMC-C2C	-2.45	120.15	125.69
22	4	602	CLA	CHB-C4A-NA	2.45	127.90	124.51
27	K	205	BCR	C37-C22-C21	-2.45	119.49	122.92
22	B	833	CLA	CHD-C1D-ND	-2.45	122.20	124.45
27	A	852	BCR	C1-C6-C5	-2.45	119.17	122.61
23	W	2621	LUT	C18-C5-C4	2.45	118.89	114.36
22	A	807	CLA	CHD-C1D-ND	-2.45	122.20	124.45
22	B	813	CLA	CHD-C1D-ND	-2.45	122.20	124.45
22	5	614	CLA	CHD-C1D-ND	-2.45	122.20	124.45
27	A	849	BCR	C33-C5-C4	2.45	118.32	113.62
22	A	823	CLA	CHD-C1D-ND	-2.45	122.15	124.52
21	6	608	CHL	CED-O2D-CGD	2.45	121.47	115.94
27	L	301	BCR	C34-C9-C8	2.45	121.93	118.08
22	U	604	CLA	CHD-C1D-ND	-2.45	122.21	124.45
21	2	602	CHL	C4-C3-C5	2.44	119.38	115.27
27	M	2001	BCR	C1-C6-C7	2.44	122.69	115.78
22	A	820	CLA	O2D-CGD-CBD	2.44	115.61	111.27
22	4	604	CLA	CHD-C1D-ND	-2.44	122.21	124.45
21	9	607	CHL	O2D-CGD-O1D	-2.44	119.06	123.84
21	W	607	CHL	CMB-C2B-C3B	2.44	129.47	124.69
22	B	825	CLA	CHB-C4A-NA	2.44	127.89	124.51
21	2	607	CHL	O2D-CGD-O1D	-2.44	119.06	123.84
27	O	2004	BCR	C7-C8-C9	-2.44	122.54	126.23
25	9	623	NEX	C5-C4-C3	2.44	114.64	111.75
22	A	820	CLA	CHD-C1D-ND	-2.44	122.21	124.45
22	5	609	CLA	CMB-C2B-C3B	2.44	129.25	124.68
22	8	613	CLA	CMB-C2B-C3B	2.44	129.25	124.68
27	A	856	BCR	C15-C16-C17	-2.44	118.47	123.47
22	A	839	CLA	C1-C2-C3	-2.44	121.82	126.04
31	K	208	LMT	C1'-C2'-C3'	-2.44	104.91	110.00
22	V	602	CLA	O2A-CGA-O1A	-2.44	117.43	123.59
22	A	834	CLA	CHD-C1D-ND	-2.44	122.21	124.45
31	B	849	LMT	O3B-C3B-C4B	-2.44	104.71	110.35
22	B	840	CLA	CMB-C2B-C3B	2.44	129.24	124.68
22	A	807	CLA	CHB-C4A-NA	2.44	127.89	124.51
22	A	804	CLA	CHB-C4A-NA	2.44	127.88	124.51
23	6	619	LUT	C30-C31-C32	-2.44	115.61	123.22
22	A	804	CLA	O2D-CGD-CBD	2.44	115.60	111.27
24	V	2622	XAT	C35-C15-C14	-2.44	118.48	123.47
24	1	618	XAT	C8-C9-C10	-2.44	115.20	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	816	CLA	O2A-CGA-O1A	-2.43	117.23	123.30
24	7	619	XAT	C6-C7-C8	-2.43	120.85	125.99
22	V	610	CLA	CAB-C3B-C2B	2.43	129.45	124.69
31	K	208	LMT	C4B-C3B-C2B	-2.43	106.58	110.82
27	F	305	BCR	C12-C13-C14	2.43	122.67	118.94
23	V	2621	LUT	C36-C21-C26	2.43	113.23	109.55
22	8	602	CLA	CHB-C4A-NA	2.43	127.87	124.51
27	B	845	BCR	C37-C22-C23	2.43	121.91	118.08
22	4	612	CLA	CHB-C4A-NA	2.43	127.87	124.51
22	A	829	CLA	CHB-C4A-NA	2.43	127.87	124.51
22	B	840	CLA	CHB-C4A-NA	2.43	127.87	124.51
26	4	630	LHG	P-O6-C4	-2.43	107.45	121.68
22	8	604	CLA	CHD-C1D-ND	-2.43	122.22	124.45
27	3	620	BCR	C20-C21-C22	-2.43	123.85	127.31
22	W	602	CLA	CHB-C4A-NA	2.43	127.87	124.51
22	B	834	CLA	CHB-C4A-NA	2.43	127.87	124.51
27	M	2001	BCR	C24-C23-C22	-2.42	122.57	126.23
22	7	604	CLA	CHB-C4A-NA	2.42	127.86	124.51
21	8	606	CHL	C1C-C2C-C3C	-2.42	105.19	107.11
22	B	813	CLA	CHB-C4A-NA	2.42	127.86	124.51
22	2	610	CLA	C1-C2-C3	-2.42	121.86	126.04
21	6	607	CHL	O2D-CGD-O1D	-2.42	119.11	123.84
24	2	620	XAT	C20-C13-C12	2.42	121.89	118.08
21	6	606	CHL	OMC-CMC-C2C	-2.42	120.21	125.69
22	K	204	CLA	CHB-C4A-NA	2.42	127.86	124.51
27	B	844	BCR	C7-C6-C5	-2.42	115.60	121.46
26	B	851	LHG	O8-C23-C24	2.42	119.50	111.91
22	8	604	CLA	CMB-C2B-C1B	-2.42	124.75	128.46
21	2	602	CHL	CMD-C2D-C3D	-2.42	122.05	127.61
22	9	611	CLA	CMB-C2B-C1B	-2.42	124.75	128.46
22	3	612	CLA	O2A-CGA-O1A	-2.42	117.49	123.59
21	5	601	CHL	C2A-C1A-CHA	-2.42	119.63	123.86
22	6	610	CLA	O2A-CGA-O1A	-2.42	117.50	123.59
22	V	610	CLA	CHD-C1D-ND	-2.42	122.23	124.45
22	5	613	CLA	CHD-C1D-ND	-2.42	122.23	124.45
22	9	603	CLA	CHB-C4A-NA	2.42	127.85	124.51
21	2	602	CHL	C2A-C3A-C4A	-2.41	97.97	101.87
22	B	809	CLA	CHD-C1D-ND	-2.41	122.24	124.45
22	7	615	CLA	CHD-C1D-ND	-2.41	122.24	124.45
22	4	610	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
22	A	815	CLA	CHD-C1D-ND	-2.41	122.24	124.45
22	8	612	CLA	CHB-C4A-NA	2.41	127.85	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	846	LHG	O8-C23-C24	2.41	119.48	111.91
23	9	624	LUT	C16-C1-C6	-2.41	106.39	110.30
27	A	852	BCR	C2-C1-C6	2.41	114.19	110.48
22	B	838	CLA	CHD-C1D-ND	-2.41	122.24	124.45
21	2	608	CHL	CED-O2D-CGD	2.41	121.38	115.94
22	K	204	CLA	CHD-C1D-ND	-2.41	122.24	124.45
22	U	603	CLA	CMB-C2B-C3B	2.41	129.18	124.68
21	4	608	CHL	OMC-CMC-C2C	-2.41	120.25	125.69
21	2	608	CHL	C4A-NA-C1A	-2.41	105.62	106.71
24	U	2622	XAT	C6-C7-C8	-2.41	120.91	125.99
22	B	829	CLA	CHD-C1D-ND	-2.41	122.24	124.45
22	7	609	CLA	CMB-C2B-C1B	-2.40	124.77	128.46
24	3	619	XAT	C4-C3-C2	-2.40	106.14	110.77
27	6	621	BCR	C40-C30-C25	2.40	114.19	110.30
27	3	621	BCR	C16-C15-C14	-2.40	118.56	123.47
21	6	601	CHL	C2A-C1A-CHA	-2.40	119.67	123.86
22	V	611	CLA	CHD-C1D-ND	-2.40	122.25	124.45
22	K	206	CLA	CHD-C1D-ND	-2.40	122.25	124.45
22	2	610	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
23	W	2620	LUT	C36-C21-C26	2.40	113.18	109.55
22	1	616	CLA	CHD-C1D-ND	-2.40	122.25	124.45
27	8	621	BCR	C39-C30-C25	2.40	114.19	110.30
23	9	624	LUT	C30-C31-C32	-2.39	115.74	123.22
22	B	803	CLA	O2A-CGA-O1A	-2.39	117.55	123.59
21	9	601	CHL	C1C-C2C-C3C	-2.39	105.21	107.11
22	2	603	CLA	CHB-C4A-NA	2.39	127.82	124.51
27	I	101	BCR	C11-C10-C9	-2.39	123.89	127.31
22	L	304	CLA	CHD-C1D-ND	-2.39	122.26	124.45
22	B	836	CLA	CHB-C4A-NA	2.39	127.82	124.51
24	3	619	XAT	C38-C25-C24	2.39	116.97	114.28
22	H	201	CLA	CHD-C1D-ND	-2.39	122.26	124.45
27	L	305	BCR	C16-C15-C14	-2.39	118.58	123.47
22	A	814	CLA	C4-C3-C5	2.39	119.29	115.27
22	B	819	CLA	CHD-C1D-ND	-2.39	122.26	124.45
21	U	601	CHL	C2A-C1A-CHA	-2.39	119.68	123.86
21	2	618	CHL	C2A-C1A-CHA	-2.39	119.68	123.86
31	K	208	LMT	O2'-C2'-C3'	-2.39	104.83	110.35
24	8	620	XAT	O24-C25-C24	-2.39	111.59	113.38
22	B	802	CLA	CMB-C2B-C3B	2.39	129.15	124.68
22	A	819	CLA	O2A-CGA-O1A	-2.39	117.57	123.59
22	B	841	CLA	CHD-C1D-ND	-2.39	122.26	124.45
31	B	849	LMT	C1-O1'-C1'	-2.39	109.88	113.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	845	BCR	C1-C6-C5	-2.39	119.25	122.61
31	K	208	LMT	O3B-C3B-C4B	-2.39	104.83	110.35
22	L	303	CLA	O2D-CGD-CBD	2.38	115.50	111.27
24	6	620	XAT	C35-C34-C33	-2.38	123.91	127.31
26	8	630	LHG	C5-O7-C7	-2.38	111.93	117.79
23	8	619	LUT	C28-C29-C30	-2.38	115.29	118.94
24	2	620	XAT	C12-C13-C14	-2.38	115.29	118.94
22	7	612	CLA	CHB-C4A-NA	2.38	127.81	124.51
22	8	610	CLA	CHB-C4A-NA	2.38	127.81	124.51
22	O	2003	CLA	CHD-C1D-ND	-2.38	122.22	124.52
22	B	818	CLA	CHD-C1D-ND	-2.38	122.27	124.45
22	A	838	CLA	CHB-C4A-NA	2.38	127.80	124.51
22	L	304	CLA	CHB-C4A-NA	2.38	127.80	124.51
22	9	612	CLA	CBD-CHA-C1A	2.38	131.24	127.43
27	B	847	BCR	C37-C22-C21	-2.38	119.59	122.92
22	8	613	CLA	CHB-C4A-NA	2.38	127.80	124.51
21	W	607	CHL	O2D-CGD-O1D	-2.38	119.19	123.84
21	6	602	CHL	O2D-CGD-O1D	-2.38	119.19	123.84
27	F	305	BCR	C37-C22-C21	-2.38	119.59	122.92
24	6	620	XAT	C35-C15-C14	-2.38	118.60	123.47
24	2	620	XAT	C4-C3-C2	-2.38	106.18	110.77
22	A	805	CLA	O2A-CGA-O1A	-2.38	117.59	123.59
22	2	604	CLA	CHD-C1D-ND	-2.38	122.27	124.45
22	A	819	CLA	CHB-C4A-NA	2.38	127.80	124.51
22	6	612	CLA	CHB-C4A-NA	2.38	127.80	124.51
24	U	2622	XAT	C7-C8-C9	-2.37	121.85	125.53
21	7	608	CHL	CED-O2D-CGD	2.37	121.31	115.94
22	V	603	CLA	CHB-C4A-NA	2.37	127.80	124.51
22	A	831	CLA	CHB-C4A-NA	2.37	127.79	124.51
22	3	612	CLA	CHB-C4A-NA	2.37	127.79	124.51
22	A	809	CLA	O2D-CGD-CBD	2.37	115.48	111.27
22	B	802	CLA	CHB-C4A-NA	2.37	127.79	124.51
24	1	618	XAT	C24-C23-C22	-2.37	106.20	110.77
22	A	841	CLA	CHD-C1D-ND	-2.37	122.28	124.45
22	5	608	CLA	CHD-C1D-ND	-2.37	122.28	124.45
22	K	201	CLA	CAA-C2A-C3A	-2.37	108.34	114.26
21	2	606	CHL	O2D-CGD-O1D	-2.37	119.21	123.84
24	7	619	XAT	C38-C25-C26	-2.37	118.29	122.26
21	2	607	CHL	CMB-C2B-C3B	2.37	129.11	124.68
21	6	606	CHL	CMB-C2B-C3B	2.37	129.11	124.68
27	A	848	BCR	C37-C22-C21	-2.37	119.61	122.92
22	8	601	CLA	C1-C2-C3	-2.37	122.92	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	W	604	CLA	CHD-C1D-ND	-2.37	122.28	124.45
22	W	603	CLA	CHD-C1D-ND	-2.37	122.28	124.45
23	W	2620	LUT	C31-C30-C29	-2.36	123.94	127.31
22	B	825	CLA	CHD-C1D-ND	-2.36	122.28	124.45
22	7	615	CLA	CHB-C4A-NA	2.36	127.78	124.51
21	2	602	CHL	CMB-C2B-C3B	2.36	129.10	124.68
22	3	617	CLA	C1-C2-C3	-2.36	121.96	126.04
22	B	804	CLA	CHD-C1D-ND	-2.36	122.28	124.45
21	9	606	CHL	O2D-CGD-O1D	-2.36	119.22	123.84
27	B	844	BCR	C24-C23-C22	-2.36	122.67	126.23
21	8	606	CHL	O2D-CGD-O1D	-2.36	119.22	123.84
21	V	607	CHL	OMC-CMC-C2C	-2.36	120.35	125.69
22	3	609	CLA	C1D-ND-C4D	-2.36	104.66	106.33
22	B	811	CLA	CHD-C1D-ND	-2.36	122.29	124.45
22	B	817	CLA	CHB-C4A-NA	2.36	127.77	124.51
27	B	844	BCR	C24-C25-C26	-2.36	115.75	121.46
27	L	306	BCR	C24-C23-C22	-2.36	122.67	126.23
22	A	813	CLA	CHB-C4A-NA	2.36	127.77	124.51
21	1	601	CHL	C2A-C1A-CHA	-2.36	119.74	123.86
22	B	822	CLA	O2A-CGA-O1A	-2.36	117.64	123.59
22	A	826	CLA	CHB-C4A-NA	2.36	127.77	124.51
22	F	304	CLA	CHB-C4A-NA	2.36	127.77	124.51
22	V	604	CLA	CHD-C1D-ND	-2.36	122.29	124.45
22	B	841	CLA	CHB-C4A-NA	2.36	127.77	124.51
27	7	620	BCR	C33-C5-C4	2.35	118.14	113.62
27	L	305	BCR	C37-C22-C23	2.35	121.79	118.08
22	B	814	CLA	CAA-C2A-C3A	-2.35	106.33	112.78
27	2	621	BCR	C1-C6-C5	-2.35	119.30	122.61
22	G	203	CLA	CHB-C4A-NA	2.35	127.77	124.51
21	1	607	CHL	OMC-CMC-C2C	-2.35	120.37	125.69
27	A	849	BCR	C30-C25-C26	-2.35	119.30	122.61
21	2	606	CHL	CMB-C2B-C3B	2.35	129.08	124.68
21	W	609	CHL	OMC-CMC-C2C	-2.35	120.37	125.69
27	3	621	BCR	C36-C18-C19	2.35	121.78	118.08
22	K	201	CLA	CHB-C4A-NA	2.35	127.76	124.51
22	W	614	CLA	CHB-C4A-NA	2.35	127.76	124.51
22	U	602	CLA	CMB-C2B-C3B	2.35	129.07	124.68
22	A	816	CLA	CHB-C4A-NA	2.35	127.76	124.51
23	4	619	LUT	C31-C30-C29	-2.35	123.96	127.31
22	A	837	CLA	CMB-C2B-C3B	2.35	129.07	124.68
21	8	607	CHL	O2D-CGD-O1D	-2.35	119.25	123.84
27	1	619	BCR	C4-C5-C6	-2.35	119.32	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	851	BCR	C35-C13-C12	2.35	121.77	118.08
27	A	848	BCR	C33-C5-C6	-2.34	121.89	124.53
27	A	856	BCR	C22-C23-C24	-2.34	118.82	124.67
27	3	621	BCR	C15-C14-C13	-2.34	123.96	127.31
23	8	619	LUT	C15-C35-C34	-2.34	118.67	123.47
21	V	608	CHL	C1C-C2C-C3C	-2.34	105.25	107.11
27	B	844	BCR	C36-C18-C19	2.34	121.77	118.08
22	1	611	CLA	CHD-C1D-ND	-2.34	122.30	124.45
24	3	619	XAT	C10-C11-C12	-2.34	115.91	123.22
22	3	617	CLA	C1D-ND-C4D	-2.34	104.67	106.33
27	L	305	BCR	C15-C16-C17	-2.34	118.68	123.47
24	1	618	XAT	C40-C33-C32	2.34	121.77	118.08
22	B	827	CLA	CHD-C1D-ND	-2.34	122.30	124.45
23	4	619	LUT	C22-C23-C24	2.34	114.41	111.74
22	1	610	CLA	CHD-C1D-ND	-2.34	122.30	124.45
22	4	609	CLA	CHB-C4A-NA	2.34	127.75	124.51
22	B	831	CLA	CHB-C4A-NA	2.34	127.75	124.51
23	3	618	LUT	C15-C14-C13	-2.34	123.97	127.31
21	9	608	CHL	C1C-C2C-C3C	-2.34	105.26	107.11
27	M	2001	BCR	C34-C9-C8	-2.34	114.39	118.08
22	3	602	CLA	CHB-C4A-NA	2.34	127.75	124.51
23	9	620	LUT	C35-C34-C33	-2.34	123.97	127.31
22	B	830	CLA	CHB-C4A-NA	2.34	127.75	124.51
21	3	608	CHL	OMC-CMC-C2C	-2.34	120.40	125.69
23	3	618	LUT	C35-C34-C33	-2.34	123.97	127.31
22	B	821	CLA	CHB-C4A-NA	2.34	127.74	124.51
21	U	607	CHL	O2D-CGD-O1D	-2.34	119.27	123.84
25	W	2623	NEX	C25-C24-C23	-2.34	108.13	112.75
21	W	601	CHL	CMB-C2B-C3B	2.34	129.26	124.69
22	A	806	CLA	CHB-C4A-NA	2.34	127.74	124.51
31	B	849	LMT	O2'-C2'-C3'	-2.33	104.95	110.35
27	B	843	BCR	C35-C13-C12	2.33	121.75	118.08
22	V	604	CLA	CHB-C4A-NA	2.33	127.74	124.51
22	B	805	CLA	O2D-CGD-CBD	2.33	115.41	111.27
22	F	304	CLA	CHD-C1D-ND	-2.33	122.33	124.45
24	V	2622	XAT	C7-C8-C9	-2.33	121.91	125.53
22	6	610	CLA	CHB-C4A-NA	2.33	127.73	124.51
21	2	602	CHL	O2A-CGA-O1A	-2.33	117.71	123.59
27	B	843	BCR	C33-C5-C6	-2.33	121.91	124.53
24	5	618	XAT	C4-C3-C2	-2.33	106.27	110.77
25	W	2623	NEX	C38-C25-C24	2.33	116.90	114.28
22	4	602	CLA	CHD-C1D-ND	-2.33	122.31	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	827	CLA	CHB-C4A-NA	2.33	127.73	124.51
22	G	201	CLA	CHD-C1D-ND	-2.33	122.31	124.45
21	8	618	CHL	O2D-CGD-O1D	-2.33	119.29	123.84
21	9	605	CHL	OMC-CMC-C2C	-2.33	120.43	125.69
25	W	2623	NEX	O24-C25-C26	-2.33	57.03	58.96
21	W	608	CHL	C1C-C2C-C3C	-2.33	105.27	107.11
22	W	604	CLA	CHB-C4A-NA	2.32	127.73	124.51
22	B	822	CLA	CHB-C4A-NA	2.32	127.73	124.51
27	7	620	BCR	C27-C26-C25	-2.32	119.36	122.73
23	W	2620	LUT	C35-C34-C33	-2.32	123.99	127.31
22	A	809	CLA	CHB-C4A-NA	2.32	127.72	124.51
22	3	606	CLA	CHD-C1D-ND	-2.32	122.32	124.45
22	A	834	CLA	CHB-C4A-NA	2.32	127.72	124.51
22	U	610	CLA	CHD-C1D-ND	-2.32	122.32	124.45
22	4	603	CLA	CHB-C4A-NA	2.32	127.72	124.51
22	A	821	CLA	CHB-C4A-NA	2.32	127.72	124.51
22	5	614	CLA	CHB-C4A-NA	2.32	127.72	124.51
21	W	608	CHL	OMC-CMC-C2C	-2.32	120.44	125.69
22	5	608	CLA	O2A-CGA-O1A	-2.32	117.74	123.59
22	U	614	CLA	CHD-C1D-ND	-2.32	122.32	124.45
31	B	849	LMT	C1B-O1B-C4'	-2.32	112.22	117.96
22	O	2002	CLA	CHD-C1D-ND	-2.32	122.32	124.45
21	9	607	CHL	CMD-C2D-C3D	-2.32	122.28	127.61
22	A	835	CLA	O2D-CGD-CBD	2.32	115.39	111.27
24	V	2622	XAT	C26-C27-C28	-2.32	121.09	125.99
27	I	101	BCR	C15-C16-C17	-2.32	118.73	123.47
27	B	843	BCR	C16-C15-C14	-2.32	118.73	123.47
22	V	613	CLA	CHB-C4A-NA	2.32	127.71	124.51
27	A	852	BCR	C12-C13-C14	-2.31	115.39	118.94
27	A	856	BCR	C24-C25-C26	-2.31	115.86	121.46
22	U	602	CLA	CHD-C1D-ND	-2.31	122.33	124.45
27	K	205	BCR	C15-C14-C13	-2.31	124.01	127.31
22	A	817	CLA	CHB-C4A-NA	2.31	127.71	124.51
27	B	843	BCR	C19-C18-C17	-2.31	115.39	118.94
21	6	601	CHL	C4-C3-C5	2.31	119.16	115.27
21	1	607	CHL	O2A-CGA-CBA	2.31	121.37	112.23
24	2	620	XAT	C38-C25-C24	2.31	116.88	114.28
22	B	804	CLA	C1-C2-C3	-2.31	122.04	126.04
27	7	620	BCR	C1-C6-C7	2.31	122.32	115.78
23	9	620	LUT	C8-C7-C6	-2.31	120.71	127.20
27	A	852	BCR	C8-C9-C10	2.31	122.49	118.94
21	9	606	CHL	C2A-C1A-CHA	-2.31	119.82	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	9	611	CLA	CMB-C2B-C3B	2.31	129.00	124.68
22	A	830	CLA	CHB-C4A-NA	2.31	127.70	124.51
22	5	613	CLA	CHB-C4A-NA	2.31	127.70	124.51
22	B	839	CLA	CHB-C4A-NA	2.31	127.70	124.51
21	4	606	CHL	O2A-CGA-CBA	2.31	121.45	114.03
22	B	820	CLA	CHB-C4A-NA	2.31	127.70	124.51
22	5	602	CLA	C1-C2-C3	-2.31	122.05	126.04
22	8	609	CLA	CHB-C4A-NA	2.31	127.70	124.51
27	A	850	BCR	C32-C1-C6	-2.31	106.56	110.30
22	9	603	CLA	CHD-C1D-ND	-2.31	122.33	124.45
22	3	607	CLA	CHB-C4A-NA	2.31	127.70	124.51
27	K	202	BCR	C29-C30-C25	2.30	114.03	110.48
31	A	857	LMT	C1B-O1B-C4'	-2.30	112.26	117.96
23	9	624	LUT	C8-C9-C10	-2.30	115.41	118.94
22	A	801	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
22	L	303	CLA	CHB-C4A-NA	2.30	127.70	124.51
22	B	838	CLA	CHB-C4A-NA	2.30	127.69	124.51
26	2	630	LHG	O8-C23-C24	2.30	119.13	111.91
23	V	2621	LUT	C31-C30-C29	-2.30	124.03	127.31
27	L	305	BCR	C29-C30-C25	2.30	114.02	110.48
22	U	603	CLA	CHD-C1D-ND	-2.30	122.34	124.45
22	W	613	CLA	CHD-C1D-ND	-2.30	122.34	124.45
22	B	812	CLA	CHB-C4A-NA	2.30	127.69	124.51
27	L	301	BCR	C36-C18-C19	2.30	121.70	118.08
27	B	844	BCR	C1-C6-C5	-2.30	119.38	122.61
22	1	602	CLA	CHD-C1D-ND	-2.30	122.34	124.45
22	5	602	CLA	CHD-C1D-ND	-2.30	122.34	124.45
27	7	621	BCR	C36-C18-C19	2.30	121.70	118.08
22	7	609	CLA	C1-C2-C3	-2.30	122.07	126.04
21	W	601	CHL	O2D-CGD-O1D	-2.30	118.87	124.09
21	9	607	CHL	C2A-C1A-CHA	-2.30	119.84	123.86
23	4	619	LUT	C1-C6-C5	-2.30	119.38	122.61
22	A	819	CLA	CHD-C1D-ND	-2.30	122.34	124.45
22	6	614	CLA	CHD-C1D-ND	-2.30	122.34	124.45
22	W	614	CLA	CHD-C1D-ND	-2.30	122.34	124.45
22	B	838	CLA	CAA-C2A-C3A	-2.30	106.49	112.78
22	6	603	CLA	CHB-C4A-NA	2.30	127.69	124.51
22	9	610	CLA	CHB-C4A-NA	2.30	127.69	124.51
22	3	612	CLA	CHD-C1D-ND	-2.29	122.34	124.45
23	7	618	LUT	C8-C7-C6	-2.29	120.76	127.20
21	V	605	CHL	C1C-C2C-C3C	-2.29	105.29	107.11
28	2	631	LMG	C8-O7-C10	-2.29	112.14	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	7	614	CLA	CHB-C4A-NA	2.29	127.68	124.51
22	A	823	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
21	U	608	CHL	C4B-C3B-C2B	-2.29	104.79	106.92
22	O	2002	CLA	CHB-C4A-NA	2.29	127.68	124.51
22	V	613	CLA	CHD-C1D-ND	-2.29	122.35	124.45
22	V	612	CLA	CHD-C1D-ND	-2.29	122.35	124.45
22	F	301	CLA	C1-C2-C3	-2.29	122.08	126.04
22	U	604	CLA	CHB-C4A-NA	2.29	127.68	124.51
22	1	610	CLA	CHB-C4A-NA	2.29	127.68	124.51
24	U	2622	XAT	C35-C15-C14	-2.29	118.79	123.47
23	W	2620	LUT	C19-C9-C8	2.29	121.68	118.08
21	V	607	CHL	O1D-CGD-CBD	-2.29	119.80	124.48
22	2	604	CLA	CHB-C4A-NA	2.29	127.67	124.51
22	B	818	CLA	CHB-C4A-NA	2.29	127.67	124.51
22	7	613	CLA	C1-C2-C3	-2.29	122.09	126.04
22	1	613	CLA	C1-C2-C3	-2.29	123.05	126.75
21	9	606	CHL	C1C-C2C-C3C	-2.29	105.30	107.11
22	A	804	CLA	CHD-C1D-ND	-2.29	122.35	124.45
22	G	203	CLA	CHD-C1D-ND	-2.28	122.36	124.45
27	6	621	BCR	C8-C7-C6	-2.28	120.79	127.20
27	G	205	BCR	C32-C1-C6	-2.28	106.60	110.30
22	6	613	CLA	CHB-C4A-NA	2.28	127.67	124.51
27	6	621	BCR	C39-C30-C25	-2.28	106.60	110.30
27	A	856	BCR	C15-C14-C13	-2.28	124.06	127.31
27	L	306	BCR	C40-C30-C25	-2.28	106.60	110.30
21	W	609	CHL	CBD-CHA-C1A	2.28	131.08	127.43
21	W	606	CHL	O2D-CGD-O1D	-2.28	118.91	124.09
23	2	619	LUT	C39-C29-C28	2.28	121.67	118.08
22	K	201	CLA	CHD-C1D-ND	-2.28	122.36	124.45
22	6	611	CLA	CHB-C4A-NA	2.28	127.66	124.51
27	M	2001	BCR	C8-C7-C6	-2.28	120.81	127.20
21	2	618	CHL	OMC-CMC-C2C	-2.28	120.54	125.69
22	B	836	CLA	CHD-C1D-ND	-2.28	122.36	124.45
27	A	849	BCR	C15-C16-C17	-2.28	118.81	123.47
24	4	620	XAT	C24-C23-C22	-2.28	106.38	110.77
22	7	613	CLA	CHD-C1D-ND	-2.28	122.36	124.45
31	A	857	LMT	O2'-C2'-C3'	-2.28	105.09	110.35
22	V	614	CLA	CHB-C4A-NA	2.27	127.66	124.51
22	3	609	CLA	CHB-C4A-NA	2.27	127.66	124.51
22	A	820	CLA	CHB-C4A-NA	2.27	127.66	124.51
22	8	603	CLA	CHB-C4A-NA	2.27	127.66	124.51
21	4	618	CHL	CMD-C2D-C3D	-2.27	122.39	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	V	609	CHL	OMC-CMC-C2C	-2.27	120.55	125.69
21	V	606	CHL	CMB-C2B-C3B	2.27	129.14	124.69
23	4	619	LUT	C15-C14-C13	-2.27	124.07	127.31
21	6	607	CHL	C1C-C2C-C3C	-2.27	105.31	107.11
27	L	305	BCR	C34-C9-C10	2.27	126.10	122.92
22	A	829	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
22	A	845	CLA	CHB-C4A-NA	2.27	127.65	124.51
21	V	601	CHL	CHC-C1C-C2C	-2.27	120.44	126.72
27	B	1609	BCR	C15-C14-C13	-2.27	124.07	127.31
24	8	620	XAT	C10-C11-C12	2.27	130.30	123.22
27	4	621	BCR	C20-C19-C18	-2.27	120.04	126.42
22	2	609	CLA	CHB-C4A-NA	2.27	127.65	124.51
22	A	832	CLA	CHB-C4A-NA	2.27	127.65	124.51
22	1	603	CLA	O2A-CGA-O1A	-2.27	117.87	123.59
22	4	601	CLA	O2A-CGA-O1A	-2.27	117.87	123.59
23	8	619	LUT	C39-C29-C28	2.27	121.65	118.08
24	6	620	XAT	C7-C8-C9	-2.27	122.01	125.53
22	5	610	CLA	O2A-CGA-O1A	-2.27	117.87	123.59
22	B	812	CLA	O2A-CGA-O1A	-2.27	117.65	123.30
21	9	608	CHL	OMC-CMC-C2C	-2.27	120.56	125.69
22	8	610	CLA	CHD-C1D-ND	-2.27	122.37	124.45
22	A	835	CLA	CHB-C4A-NA	2.26	127.64	124.51
27	K	205	BCR	C35-C13-C12	2.26	121.64	118.08
22	1	606	CLA	CHD-C1D-ND	-2.26	122.38	124.45
22	5	603	CLA	CHB-C4A-NA	2.26	127.64	124.51
27	A	850	BCR	C16-C15-C14	-2.26	118.84	123.47
21	V	609	CHL	CBD-CHA-C1A	2.26	131.05	127.43
22	1	611	CLA	CHB-C4A-NA	2.26	127.64	124.51
27	3	620	BCR	C30-C25-C26	-2.26	119.43	122.61
22	2	611	CLA	CHB-C4A-NA	2.26	127.64	124.51
21	4	606	CHL	O2D-CGD-O1D	-2.26	119.42	123.84
22	A	843	CLA	CHB-C4A-NA	2.26	127.64	124.51
21	1	601	CHL	C1B-CHB-C4A	-2.26	125.64	130.12
22	A	822	CLA	CHB-C4A-NA	2.26	127.64	124.51
27	A	852	BCR	C11-C10-C9	-2.26	124.09	127.31
23	9	621	LUT	C38-C25-C24	-2.26	118.73	123.56
21	8	607	CHL	CMB-C2B-C3B	2.26	128.90	124.68
27	2	621	BCR	C3-C4-C5	-2.26	110.05	114.08
22	3	607	CLA	O2A-CGA-O1A	-2.26	117.90	123.59
23	8	619	LUT	C8-C7-C6	-2.26	120.87	127.20
21	4	608	CHL	CED-O2D-CGD	2.25	121.04	115.94
27	7	620	BCR	C29-C30-C25	2.25	113.95	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	812	CLA	CHD-C1D-ND	-2.25	122.38	124.45
21	V	606	CHL	O2D-CGD-O1D	-2.25	118.97	124.09
22	A	827	CLA	O1D-CGD-CBD	2.25	129.09	124.48
27	K	202	BCR	C15-C14-C13	-2.25	124.09	127.31
22	A	805	CLA	O2D-CGD-CBD	2.25	115.27	111.27
22	B	815	CLA	CHB-C4A-NA	2.25	127.63	124.51
31	G	206	LMT	O2'-C2'-C3'	-2.25	105.14	110.35
23	9	624	LUT	C15-C35-C34	-2.25	118.86	123.47
27	A	851	BCR	C23-C22-C21	-2.25	115.49	118.94
22	W	610	CLA	C6-C5-C3	2.25	119.36	113.45
27	J	102	BCR	C30-C25-C26	-2.25	119.44	122.61
22	3	606	CLA	CHB-C4A-NA	2.25	127.62	124.51
23	9	624	LUT	C35-C15-C14	-2.25	118.87	123.47
27	A	851	BCR	C31-C1-C6	-2.25	106.65	110.30
27	L	306	BCR	C31-C1-C6	2.25	113.94	110.30
22	3	615	CLA	CHB-C4A-NA	2.25	127.62	124.51
22	V	613	CLA	O2D-CGD-CBD	2.25	115.26	111.27
27	B	848	BCR	C15-C14-C13	-2.25	124.11	127.31
22	B	823	CLA	CHB-C4A-NA	2.24	127.61	124.51
27	L	306	BCR	C15-C16-C17	-2.24	118.88	123.47
21	4	607	CHL	CED-O2D-CGD	2.24	121.01	115.94
22	A	832	CLA	CHD-C1D-ND	-2.24	122.39	124.45
22	6	604	CLA	CHB-C4A-NA	2.24	127.61	124.51
23	9	624	LUT	C12-C13-C14	-2.24	115.50	118.94
21	U	605	CHL	O2D-CGD-O1D	-2.24	119.00	124.09
22	U	614	CLA	CHB-C4A-NA	2.24	127.61	124.51
22	1	611	CLA	O2D-CGD-CBD	2.24	115.25	111.27
22	W	612	CLA	CHD-C1D-ND	-2.24	122.39	124.45
22	F	303	CLA	CHB-C4A-NA	2.24	127.61	124.51
21	V	605	CHL	OMC-CMC-C2C	-2.24	120.62	125.69
22	4	602	CLA	C1-C2-C3	-2.24	122.17	126.04
21	8	606	CHL	OMC-CMC-C2C	-2.24	120.62	125.69
21	2	606	CHL	C1C-C2C-C3C	-2.24	105.34	107.11
27	K	205	BCR	C7-C6-C5	-2.24	116.04	121.46
24	U	2622	XAT	C15-C14-C13	-2.24	124.11	127.31
22	B	822	CLA	O2D-CGD-CBD	2.24	115.25	111.27
22	B	819	CLA	CHB-C4A-NA	2.24	127.61	124.51
21	U	609	CHL	OMC-CMC-C2C	-2.24	120.63	125.69
22	B	814	CLA	CAA-CBA-CGA	-2.24	106.71	113.25
22	B	810	CLA	CAA-C2A-C3A	-2.24	106.65	112.78
21	9	601	CHL	CMB-C2B-C3B	2.24	128.86	124.68
22	5	602	CLA	CHB-C4A-NA	2.24	127.60	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	5	607	CHL	OMC-CMC-C2C	-2.24	120.63	125.69
22	A	826	CLA	O2A-CGA-O1A	-2.24	117.95	123.59
23	V	2620	LUT	C21-C26-C27	-2.23	109.88	112.70
27	L	306	BCR	C1-C6-C7	2.23	122.10	115.78
27	J	102	BCR	C2-C1-C6	2.23	113.92	110.48
25	V	2623	NEX	C19-C9-C10	-2.23	119.79	122.92
22	B	828	CLA	CHD-C1D-ND	-2.23	122.40	124.45
27	A	852	BCR	C15-C14-C13	-2.23	124.12	127.31
24	2	620	XAT	C10-C11-C12	-2.23	116.25	123.22
21	9	601	CHL	OMC-CMC-C2C	-2.23	120.64	125.69
22	B	816	CLA	CHB-C4A-NA	2.23	127.60	124.51
22	9	602	CLA	CHB-C4A-NA	2.23	127.60	124.51
27	B	1609	BCR	C16-C17-C18	-2.23	124.13	127.31
22	A	810	CLA	CHB-C4A-NA	2.23	127.59	124.51
21	8	618	CHL	C1C-C2C-C3C	-2.23	105.34	107.11
23	4	619	LUT	C11-C10-C9	-2.23	124.13	127.31
22	U	613	CLA	CHB-C4A-NA	2.23	127.59	124.51
27	M	2001	BCR	C19-C18-C17	-2.23	115.52	118.94
21	9	607	CHL	OMC-CMC-C2C	-2.23	120.65	125.69
21	5	601	CHL	C1C-C2C-C3C	-2.23	105.35	107.11
24	5	618	XAT	C37-C21-C26	-2.23	104.03	110.05
22	3	603	CLA	CHD-C1D-ND	-2.23	122.41	124.45
22	A	812	CLA	CHB-C4A-NA	2.23	127.59	124.51
21	1	601	CHL	OMC-CMC-C2C	-2.23	120.66	125.69
24	V	2622	XAT	C6-C7-C8	-2.23	121.29	125.99
22	A	808	CLA	CHB-C4A-NA	2.23	127.59	124.51
21	4	618	CHL	CMB-C2B-C3B	2.23	128.84	124.68
21	7	608	CHL	OMC-CMC-C2C	-2.22	120.66	125.69
24	V	2622	XAT	C15-C14-C13	-2.22	124.14	127.31
23	9	621	LUT	C35-C15-C14	-2.22	118.92	123.47
21	5	607	CHL	C1C-C2C-C3C	-2.22	105.35	107.11
21	V	606	CHL	CMD-C2D-C3D	-2.22	122.50	127.61
21	5	601	CHL	OMC-CMC-C2C	-2.22	120.66	125.69
27	A	851	BCR	C20-C21-C22	-2.22	124.14	127.31
27	M	2001	BCR	C16-C17-C18	-2.22	124.14	127.31
22	5	610	CLA	CHB-C4A-NA	2.22	127.58	124.51
27	B	843	BCR	C15-C16-C17	-2.22	118.93	123.47
22	B	829	CLA	CHB-C4A-NA	2.22	127.58	124.51
22	1	614	CLA	CHD-C1D-ND	-2.22	122.42	124.45
22	3	614	CLA	CHB-C4A-NA	2.22	127.58	124.51
21	9	606	CHL	OMC-CMC-C2C	-2.22	120.67	125.69
27	A	851	BCR	C12-C13-C14	-2.22	115.54	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	1	607	CHL	C1B-CHB-C4A	-2.22	125.72	130.12
25	9	623	NEX	C31-C30-C29	-2.22	124.14	127.31
22	A	834	CLA	CMB-C2B-C3B	2.22	128.83	124.68
22	B	806	CLA	CHB-C4A-NA	2.22	127.58	124.51
21	U	609	CHL	C4-C3-C5	2.22	119.00	115.27
22	6	603	CLA	CHD-C1D-ND	-2.22	122.42	124.45
22	8	611	CLA	CHD-C1D-ND	-2.22	122.42	124.45
22	8	602	CLA	O2D-CGD-CBD	2.22	115.21	111.27
21	2	607	CHL	OMC-CMC-C2C	-2.22	120.68	125.69
22	V	602	CLA	CHB-C4A-NA	2.22	127.58	124.51
22	2	610	CLA	CHB-C4A-NA	2.22	127.58	124.51
22	L	302	CLA	CHB-C4A-NA	2.22	127.58	124.51
29	A	844	PQN	C11-C12-C13	-2.21	123.11	126.79
21	W	605	CHL	O2D-CGD-O1D	-2.21	119.06	124.09
22	4	602	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
21	4	607	CHL	OMC-CMC-C2C	-2.21	120.68	125.69
21	7	608	CHL	C1C-C2C-C3C	-2.21	105.36	107.11
22	G	201	CLA	O2A-CGA-O1A	-2.21	117.78	123.30
23	V	2621	LUT	C1-C6-C5	-2.21	119.50	122.61
21	8	607	CHL	OMC-CMC-C2C	-2.21	120.69	125.69
27	A	850	BCR	C15-C14-C13	-2.21	124.15	127.31
22	A	815	CLA	CAA-C2A-C3A	-2.21	106.72	112.78
22	U	610	CLA	CHB-C4A-NA	2.21	127.57	124.51
24	U	2622	XAT	C35-C34-C33	-2.21	124.16	127.31
21	2	602	CHL	O2D-CGD-O1D	-2.21	119.52	123.84
22	B	830	CLA	CMB-C2B-C3B	2.21	128.81	124.68
23	9	621	LUT	C35-C34-C33	-2.21	124.16	127.31
25	V	2623	NEX	C35-C34-C33	-2.21	124.16	127.31
27	K	202	BCR	C15-C16-C17	-2.21	118.95	123.47
22	B	826	CLA	CHB-C4A-NA	2.21	127.56	124.51
22	7	606	CLA	CHB-C4A-NA	2.21	127.56	124.51
22	A	840	CLA	CHB-C4A-NA	2.21	127.56	124.51
22	2	604	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
23	7	618	LUT	C38-C25-C24	-2.20	118.84	123.56
22	J	101	CLA	CHD-C1D-ND	-2.20	122.43	124.45
23	U	2620	LUT	C19-C9-C10	-2.20	119.83	122.92
22	3	617	CLA	CMC-C2C-C1C	2.20	125.25	118.85
21	W	608	CHL	CMB-C2B-C1B	2.20	131.85	128.46
21	W	608	CHL	O2D-CGD-O1D	-2.20	119.09	124.09
27	6	621	BCR	C34-C9-C10	-2.20	119.84	122.92
21	6	607	CHL	OMC-CMC-C2C	-2.20	120.71	125.69
22	5	609	CLA	CMA-C3A-C2A	-2.20	110.96	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	L	305	BCR	C24-C25-C26	-2.20	116.13	121.46
23	2	619	LUT	C7-C8-C9	-2.20	122.91	126.23
24	4	620	XAT	C28-C29-C30	-2.20	115.57	118.94
27	7	621	BCR	C30-C25-C24	2.20	122.00	115.78
22	9	602	CLA	CHD-C1D-ND	-2.20	122.43	124.45
23	V	2620	LUT	C36-C21-C26	2.20	112.88	109.55
24	W	2622	XAT	C15-C14-C13	-2.20	124.17	127.31
21	2	601	CHL	OMC-CMC-C2C	-2.20	120.72	125.69
27	L	301	BCR	C2-C1-C6	2.20	113.86	110.48
22	6	614	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
21	V	609	CHL	C1C-C2C-C3C	-2.20	105.37	107.11
22	3	604	CLA	CHB-C4A-NA	2.20	127.55	124.51
22	U	611	CLA	CHB-C4A-NA	2.20	127.55	124.51
22	K	206	CLA	CHB-C4A-NA	2.20	127.55	124.51
27	L	305	BCR	C12-C13-C14	-2.20	115.57	118.94
22	3	613	CLA	O2D-CGD-CBD	2.20	115.17	111.27
22	H	201	CLA	CHB-C4A-NA	2.19	127.55	124.51
26	1	630	LHG	C5-O7-C7	-2.19	112.39	117.79
22	A	815	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
22	A	823	CLA	CHB-C4A-NA	2.19	127.54	124.51
27	L	301	BCR	C33-C5-C4	2.19	117.83	113.62
23	W	2620	LUT	C19-C9-C10	-2.19	119.85	122.92
24	4	620	XAT	C30-C31-C32	-2.19	116.38	123.22
22	4	601	CLA	CHD-C1D-ND	-2.19	122.44	124.45
25	9	623	NEX	C24-C23-C22	-2.19	106.54	110.77
23	V	2620	LUT	C8-C7-C6	-2.19	121.05	127.20
21	U	608	CHL	O2D-CGD-O1D	-2.19	119.12	124.09
21	V	601	CHL	O2D-CGD-O1D	-2.19	119.12	124.09
21	5	601	CHL	C1B-CHB-C4A	-2.19	125.78	130.12
22	V	610	CLA	CMA-C3A-C2A	-2.19	110.99	116.10
22	2	614	CLA	CHB-C4A-NA	2.19	127.54	124.51
22	B	825	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
23	6	619	LUT	C38-C25-C24	-2.19	118.88	123.56
27	F	305	BCR	C7-C6-C5	-2.19	116.16	121.46
22	B	809	CLA	CHB-C4A-NA	2.19	127.54	124.51
27	3	621	BCR	C3-C4-C5	-2.19	110.17	114.08
22	7	612	CLA	CHD-C1D-ND	-2.19	122.44	124.45
22	B	818	CLA	O2D-CGD-CBD	2.19	115.15	111.27
22	A	817	CLA	CHD-C1D-ND	-2.19	122.45	124.45
26	5	630	LHG	C5-O7-C7	-2.18	112.41	117.79
23	3	618	LUT	C11-C10-C9	-2.18	124.19	127.31
23	5	617	LUT	C30-C31-C32	2.18	130.03	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1	604	CLA	CHB-C4A-NA	2.18	127.53	124.51
24	5	618	XAT	C15-C35-C34	-2.18	119.00	123.47
27	1	619	BCR	C12-C13-C14	-2.18	115.59	118.94
26	9	2630	LHG	O7-C7-C8	2.18	116.20	111.50
23	9	621	LUT	C31-C30-C29	-2.18	124.20	127.31
21	4	618	CHL	C2A-C1A-CHA	-2.18	120.04	123.86
26	A	846	LHG	C5-O7-C7	-2.18	112.42	117.79
23	W	2620	LUT	C1-C6-C5	-2.18	119.54	122.61
22	A	828	CLA	CHB-C4A-NA	2.18	127.53	124.51
22	3	604	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
22	A	842	CLA	CHB-C4A-NA	2.18	127.53	124.51
24	3	619	XAT	C39-C29-C28	2.18	121.51	118.08
27	7	620	BCR	C8-C7-C6	-2.18	121.08	127.20
22	A	802	CLA	CHD-C1D-ND	-2.18	122.45	124.45
21	2	602	CHL	C1B-CHB-C4A	-2.18	125.81	130.12
27	A	851	BCR	C40-C30-C25	2.18	113.83	110.30
21	2	602	CHL	C3B-C4B-NB	2.18	112.02	109.21
22	A	824	CLA	CHD-C1D-ND	-2.18	122.45	124.45
27	A	851	BCR	C36-C18-C19	2.18	121.50	118.08
21	5	601	CHL	C5-C3-C4	2.18	119.41	114.60
22	A	828	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
23	V	2620	LUT	C11-C12-C13	-2.17	120.31	126.42
22	6	613	CLA	C1-C2-C3	-2.17	122.28	126.04
27	G	205	BCR	C21-C20-C19	-2.17	116.43	123.22
21	U	609	CHL	C1B-CHB-C4A	-2.17	125.81	130.12
21	8	608	CHL	C5-C3-C4	2.17	119.40	114.60
22	U	604	CLA	O2D-CGD-CBD	2.17	115.13	111.27
22	A	842	CLA	C7-C6-C5	-2.17	107.46	113.36
27	A	848	BCR	C36-C18-C19	2.17	121.50	118.08
22	1	614	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
27	7	620	BCR	C37-C22-C21	-2.17	119.88	122.92
21	9	601	CHL	CBD-CHA-C1A	2.17	130.91	127.43
21	V	601	CHL	C1-C2-C3	-2.17	122.29	126.04
21	W	609	CHL	C1C-C2C-C3C	-2.17	105.39	107.11
24	2	620	XAT	C19-C9-C8	2.17	121.50	118.08
22	7	617	CLA	CHB-C4A-NA	2.17	127.51	124.51
21	6	601	CHL	OMC-CMC-C2C	-2.17	120.78	125.69
27	A	850	BCR	C1-C6-C5	-2.17	119.56	122.61
22	2	611	CLA	CHD-C1D-ND	-2.17	122.46	124.45
22	5	609	CLA	CHB-C4A-NA	2.17	127.51	124.51
22	J	101	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
22	B	840	CLA	CHD-C1D-ND	-2.17	122.46	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	5	608	CLA	CHB-C4A-NA	2.17	127.51	124.51
23	3	618	LUT	C31-C30-C29	-2.17	124.22	127.31
23	1	617	LUT	C38-C25-C24	-2.16	118.93	123.56
24	W	2622	XAT	C12-C13-C14	-2.16	115.62	118.94
22	W	612	CLA	CHB-C4A-NA	2.16	127.50	124.51
22	B	813	CLA	O2D-CGD-CBD	2.16	115.11	111.27
27	B	848	BCR	C33-C5-C6	-2.16	122.10	124.53
27	7	620	BCR	C16-C17-C18	-2.16	124.22	127.31
22	7	604	CLA	O2A-CGA-O1A	-2.16	118.13	123.59
22	3	609	CLA	C4-C3-C5	2.16	118.91	115.27
22	W	603	CLA	CMA-C3A-C2A	-2.16	111.05	116.10
27	8	621	BCR	C11-C12-C13	-2.16	120.35	126.42
22	3	604	CLA	CHD-C1D-ND	-2.16	122.47	124.45
22	K	203	CLA	CHB-C4A-NA	2.16	127.50	124.51
22	B	832	CLA	C4-C3-C5	2.16	118.90	115.27
22	8	610	CLA	C1-C2-C3	-2.16	122.31	126.04
27	L	305	BCR	C2-C3-C4	-2.16	106.56	111.38
22	A	830	CLA	O2D-CGD-CBD	2.16	115.10	111.27
22	2	614	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
23	V	2620	LUT	C19-C9-C10	-2.16	119.90	122.92
27	A	848	BCR	C28-C27-C26	-2.16	110.22	114.08
23	1	617	LUT	C31-C30-C29	-2.16	124.23	127.31
27	A	849	BCR	C36-C18-C17	-2.16	119.90	122.92
22	3	602	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
22	B	822	CLA	C1-C2-C3	-2.15	122.32	126.04
21	U	607	CHL	CAA-C2A-C3A	2.15	118.67	112.78
21	1	601	CHL	C1C-C2C-C3C	-2.15	105.41	107.11
21	8	607	CHL	C1C-C2C-C3C	-2.15	105.41	107.11
23	W	2621	LUT	C38-C25-C24	-2.15	118.95	123.56
23	8	619	LUT	C36-C21-C26	2.15	112.81	109.55
21	1	607	CHL	C1C-C2C-C3C	-2.15	105.41	107.11
24	W	2622	XAT	O4-C5-C6	-2.15	57.18	58.96
22	A	824	CLA	O2D-CGD-CBD	2.15	115.09	111.27
21	W	601	CHL	C4-C3-C5	2.15	118.89	115.27
22	A	806	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
22	B	820	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
24	2	620	XAT	C27-C28-C29	-2.15	122.19	125.53
22	A	836	CLA	CAC-C3C-C2C	2.15	127.30	123.22
27	G	205	BCR	C19-C18-C17	-2.15	115.64	118.94
22	3	610	CLA	CHB-C4A-NA	2.15	127.48	124.51
23	W	2620	LUT	C35-C15-C14	-2.15	119.07	123.47
22	3	617	CLA	O2A-CGA-O1A	-2.15	118.17	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	7	611	CLA	CHD-C1D-ND	-2.15	122.48	124.45
23	U	2620	LUT	C35-C34-C33	-2.15	124.25	127.31
22	O	2001	CLA	CHB-C4A-NA	2.15	127.62	124.34
27	L	301	BCR	C28-C27-C26	-2.15	110.25	114.08
25	W	2623	NEX	C35-C15-C14	-2.15	119.08	123.47
22	2	603	CLA	CHD-C1D-ND	-2.14	122.48	124.45
27	B	1609	BCR	C1-C6-C5	-2.14	119.59	122.61
23	V	2621	LUT	C18-C5-C4	2.14	118.33	114.36
21	4	618	CHL	OMC-CMC-C2C	-2.14	120.84	125.69
21	9	601	CHL	C4D-C3D-CAD	2.14	110.62	108.10
21	W	606	CHL	CHC-C1C-C2C	-2.14	120.80	126.72
22	B	808	CLA	CHB-C4A-NA	2.14	127.47	124.51
22	1	611	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
22	A	818	CLA	CHB-C4A-NA	2.14	127.47	124.51
23	7	618	LUT	C40-C33-C32	2.14	121.45	118.08
22	A	838	CLA	CHD-C1D-ND	-2.14	122.49	124.45
27	B	801	BCR	C38-C26-C27	2.14	117.72	113.62
23	3	618	LUT	C1-C6-C5	-2.14	119.60	122.61
31	K	208	LMT	C1B-O1B-C4'	-2.14	112.67	117.96
22	9	613	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
22	6	609	CLA	CHB-C4A-NA	2.14	127.47	124.51
22	B	808	CLA	CHD-C1D-ND	-2.13	122.49	124.45
22	1	608	CLA	CHB-C4A-NA	2.13	127.46	124.51
26	4	630	LHG	O8-C23-O10	-2.13	118.21	123.59
21	6	601	CHL	C1C-C2C-C3C	-2.13	105.42	107.11
24	3	619	XAT	C28-C29-C30	-2.13	115.67	118.94
22	B	826	CLA	O2D-CGD-CBD	2.13	115.06	111.27
22	B	824	CLA	CHB-C4A-NA	2.13	127.46	124.51
22	V	603	CLA	CHD-C1D-ND	-2.13	122.50	124.45
24	2	620	XAT	C15-C35-C34	-2.13	119.11	123.47
27	B	843	BCR	C33-C5-C4	2.13	117.71	113.62
22	8	613	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
22	8	604	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
22	8	601	CLA	CHD-C1D-ND	-2.13	122.50	124.45
22	8	603	CLA	CHD-C1D-ND	-2.13	122.50	124.45
22	A	812	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
29	B	842	PQN	C11-C3-C4	-2.13	116.22	118.50
21	V	606	CHL	CHC-C1C-C2C	-2.13	120.84	126.72
22	B	832	CLA	O2D-CGD-CBD	2.13	115.05	111.27
27	6	621	BCR	C37-C22-C21	-2.13	119.94	122.92
27	8	621	BCR	C24-C25-C26	-2.12	116.31	121.46
22	1	616	CLA	CHB-C4A-NA	2.12	127.45	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	819	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
24	U	2622	XAT	O4-C5-C6	-2.12	57.20	58.96
22	4	603	CLA	CHD-C1D-ND	-2.12	122.50	124.45
23	U	2620	LUT	C31-C30-C29	-2.12	124.28	127.31
27	B	801	BCR	C11-C10-C9	-2.12	124.28	127.31
22	B	833	CLA	CHB-C4A-NA	2.12	127.45	124.51
25	9	623	NEX	C16-C1-C6	2.12	112.37	110.47
21	U	605	CHL	CHC-C1C-C2C	-2.12	120.85	126.72
21	8	618	CHL	OMC-CMC-C2C	-2.12	120.89	125.69
27	B	1609	BCR	C35-C13-C12	2.12	121.42	118.08
23	1	617	LUT	C35-C15-C14	-2.12	119.13	123.47
22	B	819	CLA	C6-C5-C3	2.12	119.02	113.45
27	7	621	BCR	C8-C7-C6	-2.12	121.25	127.20
22	B	835	CLA	O2A-CGA-O1A	-2.12	118.01	123.30
21	U	601	CHL	CHC-C1C-C2C	-2.12	120.86	126.72
22	A	802	CLA	CHB-C4A-NA	2.12	127.44	124.51
22	B	811	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
23	W	2620	LUT	C38-C25-C24	-2.12	119.03	123.56
22	U	613	CLA	CHD-C1D-ND	-2.12	122.51	124.45
27	3	620	BCR	C15-C14-C13	-2.12	124.29	127.31
22	B	840	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
22	1	611	CLA	CAC-C3C-C4C	2.12	127.56	124.81
27	7	621	BCR	C2-C1-C6	2.12	113.74	110.48
22	1	610	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
22	V	611	CLA	CHB-C4A-NA	2.12	127.44	124.51
22	B	814	CLA	CBA-CAA-C2A	2.12	120.11	113.86
22	F	301	CLA	CHB-C4A-NA	2.12	127.44	124.51
22	4	614	CLA	CHB-C4A-NA	2.11	127.44	124.51
22	A	836	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
27	A	851	BCR	C19-C18-C17	-2.11	115.70	118.94
32	B	850	DGD	O3E-C3E-C4E	-2.11	105.46	110.35
22	B	835	CLA	CHB-C4A-NA	2.11	127.44	124.51
23	W	2620	LUT	C11-C12-C13	-2.11	120.48	126.42
27	K	205	BCR	C30-C25-C26	-2.11	119.64	122.61
22	4	610	CLA	CHB-C4A-NA	2.11	127.43	124.51
27	L	301	BCR	C38-C26-C27	2.11	117.67	113.62
31	G	206	LMT	C4B-C3B-C2B	-2.11	107.14	110.82
22	A	836	CLA	CHB-C4A-NA	2.11	127.43	124.51
25	9	623	NEX	C28-C29-C30	2.11	122.18	118.94
22	F	303	CLA	O2A-CGA-O1A	-2.11	118.03	123.30
22	A	805	CLA	CHB-C4A-NA	2.11	127.43	124.51
27	B	848	BCR	C36-C18-C19	2.11	121.40	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1	602	CLA	CHB-C4A-NA	2.11	127.43	124.51
21	2	607	CHL	O1D-CGD-CBD	-2.11	120.17	124.48
21	9	605	CHL	C1C-C2C-C3C	-2.11	105.44	107.11
22	A	830	CLA	CHD-C1D-ND	-2.11	122.52	124.45
22	W	603	CLA	CHB-C4A-NA	2.11	127.43	124.51
22	4	613	CLA	CHB-C4A-NA	2.11	127.43	124.51
25	U	2623	NEX	C35-C34-C33	-2.11	124.30	127.31
22	1	608	CLA	O2A-CGA-O1A	-2.11	118.05	123.30
27	J	102	BCR	C34-C9-C10	-2.11	119.97	122.92
22	V	613	CLA	C5-C3-C2	2.11	125.38	121.12
22	B	805	CLA	C5-C3-C2	2.11	125.38	121.12
22	V	610	CLA	CHB-C4A-NA	2.11	127.42	124.51
22	A	803	CLA	CHD-C1D-ND	-2.11	122.52	124.45
21	4	606	CHL	CED-O2D-CGD	2.11	120.70	115.94
26	4	630	LHG	O7-C7-O9	-2.11	118.61	123.70
22	A	808	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
23	1	617	LUT	C1-C6-C5	-2.10	119.65	122.61
21	4	618	CHL	O2D-CGD-O1D	-2.10	119.72	123.84
27	F	305	BCR	C27-C26-C25	-2.10	119.68	122.73
27	O	2004	BCR	C7-C6-C5	-2.10	116.37	121.46
22	6	609	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
22	U	602	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
28	L	307	LMG	O8-C28-C29	2.10	118.50	111.91
22	5	616	CLA	CHB-C4A-NA	2.10	127.42	124.51
26	9	2630	LHG	C6-O8-C23	2.10	124.90	117.12
31	B	849	LMT	C4B-C3B-C2B	-2.10	107.15	110.82
22	B	811	CLA	CHB-C4A-NA	2.10	127.42	124.51
22	G	201	CLA	CHB-C4A-NA	2.10	127.42	124.51
21	2	602	CHL	CED-O2D-CGD	2.10	120.69	115.94
21	2	608	CHL	O2A-CGA-CBA	2.10	120.78	114.03
22	8	604	CLA	CMB-C2B-C3B	2.10	128.61	124.68
22	4	613	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
22	7	602	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
22	1	614	CLA	CHB-C4A-NA	2.10	127.41	124.51
23	8	619	LUT	C15-C14-C13	-2.10	124.32	127.31
21	W	601	CHL	CHC-C1C-C2C	-2.10	120.92	126.72
22	B	832	CLA	CHB-C4A-NA	2.10	127.41	124.51
22	B	810	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
27	B	1609	BCR	C12-C13-C14	-2.10	115.72	118.94
23	6	619	LUT	C39-C29-C28	2.10	121.38	118.08
22	1	613	CLA	CHB-C4A-NA	2.10	127.41	124.51
27	3	620	BCR	C36-C18-C19	2.10	121.38	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	7	618	LUT	C35-C34-C33	-2.10	124.32	127.31
22	6	614	CLA	CHB-C4A-NA	2.09	127.41	124.51
22	B	824	CLA	CHD-C1D-ND	-2.09	122.53	124.45
22	8	601	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
22	A	826	CLA	CHD-C1D-ND	-2.09	122.53	124.45
22	3	614	CLA	O2A-CGA-O1A	-2.09	118.08	123.30
24	1	618	XAT	O4-C5-C6	-2.09	57.23	58.96
21	U	601	CHL	O2D-CGD-O1D	-2.09	119.34	124.09
23	9	621	LUT	C15-C14-C13	-2.09	124.33	127.31
23	V	2620	LUT	C16-C1-C6	2.09	113.69	110.30
27	F	305	BCR	C38-C26-C27	2.09	117.63	113.62
22	4	601	CLA	O2D-CGD-CBD	2.09	114.98	111.27
22	B	820	CLA	CHD-C1D-ND	-2.09	122.53	124.45
22	A	839	CLA	CHB-C4A-NA	2.09	127.40	124.51
27	B	843	BCR	C3-C4-C5	-2.09	110.35	114.08
21	9	608	CHL	CED-O2D-CGD	2.09	120.66	115.94
22	A	833	CLA	CHB-C4A-NA	2.09	127.40	124.51
22	V	612	CLA	CMA-C3A-C2A	-2.09	111.23	116.10
22	A	824	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
22	6	610	CLA	CHD-C1D-ND	-2.09	122.54	124.45
22	B	838	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
22	1	609	CLA	C4-C3-C2	-2.09	118.33	123.68
23	U	2620	LUT	C35-C15-C14	-2.09	119.20	123.47
21	7	608	CHL	CBC-CAC-C3C	-2.09	106.68	112.43
22	3	607	CLA	O2D-CGD-CBD	2.08	114.97	111.27
22	V	604	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
27	B	847	BCR	C8-C9-C10	-2.08	115.74	118.94
24	1	618	XAT	C35-C34-C33	-2.08	124.34	127.31
21	V	608	CHL	O2D-CGD-O1D	-2.08	119.36	124.09
22	7	610	CLA	CHB-C4A-NA	2.08	127.39	124.51
22	A	821	CLA	CHD-C1D-ND	-2.08	122.54	124.45
22	3	611	CLA	CHB-C4A-NA	2.08	127.39	124.51
22	3	603	CLA	CHB-C4A-NA	2.08	127.39	124.51
22	A	825	CLA	CHB-C4A-NA	2.08	127.39	124.51
24	2	620	XAT	C15-C14-C13	-2.08	124.34	127.31
22	U	611	CLA	CHD-C1D-ND	-2.08	122.54	124.45
22	G	204	CLA	CHB-C4A-NA	2.08	127.38	124.51
29	A	844	PQN	C21-C20-C18	-2.08	109.21	115.92
23	9	620	LUT	C18-C5-C4	2.08	118.20	114.36
22	1	609	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
22	V	614	CLA	CHD-C1D-ND	-2.08	122.55	124.45
22	4	603	CLA	O2A-CGA-O1A	-2.08	118.35	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	837	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
25	U	2623	NEX	C28-C29-C30	2.07	122.12	118.94
22	B	808	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
21	W	605	CHL	CHC-C1C-C2C	-2.07	120.99	126.72
22	B	804	CLA	O2D-CGD-CBD	2.07	114.95	111.27
23	V	2621	LUT	C19-C9-C10	-2.07	120.02	122.92
21	4	607	CHL	C1B-CHB-C4A	-2.07	126.02	130.12
23	V	2620	LUT	C15-C14-C13	-2.07	124.36	127.31
27	B	801	BCR	C34-C9-C8	2.07	121.34	118.08
22	B	826	CLA	CHD-C1D-ND	-2.07	122.55	124.45
27	B	843	BCR	C11-C12-C13	-2.07	120.61	126.42
21	9	607	CHL	C1B-CHB-C4A	-2.07	126.02	130.12
22	7	613	CLA	CHB-C4A-NA	2.07	127.37	124.51
21	8	606	CHL	O2A-CGA-CBA	2.07	120.67	114.03
22	B	823	CLA	CAC-C3C-C4C	2.07	127.49	124.81
22	V	614	CLA	O2A-CGA-O1A	-2.07	118.15	123.30
22	9	604	CLA	CHB-C4A-NA	2.07	127.37	124.51
22	9	612	CLA	CHB-C4A-NA	2.07	127.37	124.51
22	4	612	CLA	CHD-C1D-ND	-2.07	122.56	124.45
23	4	619	LUT	C39-C29-C28	2.07	121.33	118.08
22	A	822	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
21	2	607	CHL	C1B-CHB-C4A	-2.06	126.03	130.12
27	M	2001	BCR	C33-C5-C4	2.06	117.58	113.62
22	4	613	CLA	O2D-CGD-CBD	2.06	114.94	111.27
21	5	607	CHL	CBD-CHA-C1A	2.06	130.73	127.43
22	1	606	CLA	CHB-C4A-NA	2.06	127.37	124.51
22	B	805	CLA	CAA-C2A-C1A	-2.06	105.22	111.97
22	A	824	CLA	CHB-C4A-NA	2.06	127.36	124.51
22	L	302	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
21	2	608	CHL	C2A-C3A-C4A	-2.06	98.54	101.87
25	9	623	NEX	C10-C11-C12	-2.06	116.78	123.22
23	1	617	LUT	C39-C29-C28	2.06	121.32	118.08
21	W	606	CHL	C4B-C3B-C2B	-2.06	105.00	106.92
22	1	603	CLA	O2D-CGD-CBD	2.06	114.93	111.27
21	6	618	CHL	C1C-C2C-C3C	-2.06	105.48	107.11
25	U	2623	NEX	C12-C13-C14	-2.06	115.78	118.94
22	1	603	CLA	CHD-C1D-ND	-2.06	122.56	124.45
23	U	2620	LUT	C39-C29-C28	2.06	121.32	118.08
21	W	608	CHL	C4B-C3B-C2B	-2.06	105.01	106.92
27	B	848	BCR	C10-C11-C12	-2.06	116.80	123.22
22	A	831	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
22	4	601	CLA	CHB-C4A-NA	2.06	127.36	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	K	205	BCR	C1-C6-C5	-2.06	119.72	122.61
22	4	609	CLA	O2A-CGA-O1A	-2.05	118.18	123.30
27	1	619	BCR	C15-C16-C17	-2.05	119.27	123.47
22	3	610	CLA	CHD-C1D-ND	-2.05	122.57	124.45
23	9	624	LUT	C31-C30-C29	-2.05	124.38	127.31
26	8	630	LHG	O8-C23-O10	-2.05	118.41	123.59
29	A	844	PQN	C17-C16-C15	-2.05	107.78	113.36
22	B	805	CLA	CHB-C4A-NA	2.05	127.35	124.51
23	1	617	LUT	C16-C1-C6	2.05	113.63	110.30
27	6	621	BCR	C38-C26-C27	2.05	117.56	113.62
24	U	2622	XAT	C39-C29-C28	2.05	121.31	118.08
22	8	602	CLA	CHD-C1D-ND	-2.05	122.57	124.45
24	1	618	XAT	C11-C10-C9	-2.05	124.38	127.31
22	A	810	CLA	O2D-CGD-CBD	2.05	114.91	111.27
28	2	631	LMG	O7-C10-O9	-2.05	118.75	123.70
21	9	606	CHL	CMB-C2B-C3B	2.05	128.51	124.68
24	2	620	XAT	O4-C5-C6	-2.05	57.26	58.96
22	B	831	CLA	O2D-CGD-CBD	2.05	114.91	111.27
27	K	205	BCR	C36-C18-C17	-2.05	120.05	122.92
22	7	609	CLA	CAC-C3C-C4C	2.05	127.47	124.81
22	5	610	CLA	CHD-C1D-ND	-2.05	122.57	124.45
22	3	612	CLA	C1-C2-C3	-2.05	122.50	126.04
27	2	621	BCR	C24-C25-C26	2.05	126.42	121.46
21	2	618	CHL	C4D-CHA-C1A	-2.05	118.76	121.25
27	A	856	BCR	C8-C9-C10	-2.04	115.80	118.94
22	K	203	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
27	B	801	BCR	C33-C5-C6	-2.04	122.23	124.53
21	9	608	CHL	CMB-C2B-C3B	2.04	128.50	124.68
22	A	811	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
23	8	619	LUT	C38-C25-C24	-2.04	119.19	123.56
27	I	101	BCR	C16-C15-C14	-2.04	119.29	123.47
22	5	606	CLA	CHB-C4A-NA	2.04	127.34	124.51
22	B	813	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
22	W	612	CLA	CAA-C2A-C3A	-2.04	111.33	116.10
21	2	606	CHL	C1B-CHB-C4A	-2.04	126.07	130.12
21	9	605	CHL	CBD-CHA-C1A	2.04	130.70	127.43
26	A	847	LHG	C5-O7-C7	-2.04	112.77	117.79
23	V	2620	LUT	C15-C35-C34	-2.04	119.29	123.47
22	6	604	CLA	C1-C2-C3	-2.04	123.45	126.75
27	K	205	BCR	C11-C10-C9	-2.04	124.40	127.31
21	2	608	CHL	C1B-CHB-C4A	-2.04	126.08	130.12
22	7	609	CLA	CMB-C2B-C3B	2.04	128.49	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	9	610	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
27	B	845	BCR	C29-C30-C25	2.04	113.62	110.48
27	A	850	BCR	C20-C19-C18	-2.04	120.69	126.42
22	B	839	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
24	6	620	XAT	C15-C35-C34	-2.04	119.30	123.47
27	7	621	BCR	C16-C15-C14	-2.04	119.30	123.47
23	U	2620	LUT	C38-C25-C24	-2.04	119.20	123.56
21	U	607	CHL	OMC-CMC-C2C	-2.04	121.08	125.69
22	B	809	CLA	C4-C3-C2	-2.04	118.46	123.68
27	L	306	BCR	C16-C17-C18	-2.04	124.41	127.31
22	A	833	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
22	8	614	CLA	CAA-C2A-C3A	-2.04	107.20	112.78
21	8	608	CHL	O2D-CGD-O1D	-2.03	119.86	123.84
22	L	304	CLA	C1-C2-C3	-2.03	122.53	126.04
21	2	618	CHL	C1C-C2C-C3C	-2.03	105.50	107.11
27	M	2001	BCR	C31-C1-C6	2.03	113.60	110.30
22	8	610	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
22	1	602	CLA	C1-C2-C3	-2.03	122.53	126.04
25	W	2623	NEX	C30-C31-C32	-2.03	116.87	123.22
23	3	618	LUT	C36-C21-C26	2.03	112.62	109.55
27	2	621	BCR	C15-C16-C17	-2.03	119.31	123.47
23	9	620	LUT	C30-C31-C32	-2.03	116.88	123.22
22	5	603	CLA	O2A-CGA-O1A	-2.03	118.23	123.30
21	V	609	CHL	C1B-CHB-C4A	-2.03	126.09	130.12
22	L	304	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
22	A	854	CLA	CHD-C1D-ND	-2.03	122.59	124.45
22	B	816	CLA	CHD-C1D-ND	-2.03	122.59	124.45
21	4	607	CHL	C1C-C2C-C3C	-2.03	105.50	107.11
26	7	630	LHG	O8-C23-O10	-2.03	118.47	123.59
27	I	101	BCR	C28-C27-C26	-2.03	110.45	114.08
22	A	801	CLA	CHA-C4D-ND	2.03	136.75	132.50
22	A	845	CLA	CHD-C1D-ND	-2.03	122.59	124.45
24	3	619	XAT	C19-C9-C8	2.03	121.27	118.08
21	8	608	CHL	CED-O2D-CGD	2.03	120.53	115.94
21	W	606	CHL	C1B-CHB-C4A	-2.03	126.10	130.12
27	B	844	BCR	C20-C21-C22	-2.03	124.42	127.31
27	O	2004	BCR	C15-C16-C17	-2.03	119.32	123.47
27	F	305	BCR	C15-C14-C13	-2.03	124.42	127.31
23	V	2620	LUT	C38-C25-C24	-2.03	119.22	123.56
21	8	606	CHL	O1D-CGD-CBD	-2.03	120.34	124.48
21	9	606	CHL	O1D-CGD-CBD	-2.03	120.34	124.48
22	W	603	CLA	CAA-C2A-C3A	-2.03	111.37	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	U	609	CHL	C1C-C2C-C3C	-2.03	105.51	107.11
25	U	2623	NEX	C24-C23-C22	-2.03	106.86	110.77
22	7	617	CLA	O2D-CGD-CBD	2.02	114.87	111.27
24	2	620	XAT	C36-C21-C22	-2.02	105.47	108.98
22	9	609	CLA	C1B-CHB-C4A	-2.02	126.11	130.12
22	3	604	CLA	O2D-CGD-CBD	2.02	114.86	111.27
21	2	601	CHL	C1C-C2C-C3C	-2.02	105.51	107.11
22	3	617	CLA	CHD-C1D-ND	-2.02	122.59	124.45
22	5	613	CLA	O2D-CGD-CBD	2.02	114.86	111.27
24	W	2622	XAT	C27-C28-C29	-2.02	122.39	125.53
21	U	606	CHL	O1D-CGD-CBD	-2.02	120.35	124.48
22	1	612	CLA	O2D-CGD-CBD	2.02	114.86	111.27
22	3	610	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
22	A	836	CLA	CHD-C4C-NC	2.02	125.98	122.91
22	A	804	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
23	6	619	LUT	C20-C13-C12	2.02	121.26	118.08
24	5	618	XAT	O4-C5-C6	-2.02	57.29	58.96
22	9	609	CLA	C4D-CHA-C1A	-2.02	118.79	121.25
21	W	607	CHL	O1D-CGD-CBD	-2.02	120.35	124.48
22	W	613	CLA	CHB-C4A-NA	2.02	127.30	124.51
21	2	607	CHL	O2A-CGA-CBA	2.02	120.21	112.23
22	4	609	CLA	O2D-CGD-CBD	2.02	114.85	111.27
22	6	609	CLA	O2D-CGD-CBD	2.02	114.85	111.27
22	8	614	CLA	O2A-CGA-O1A	-2.02	118.27	123.30
27	7	620	BCR	C35-C13-C12	2.02	121.26	118.08
25	W	2623	NEX	C31-C32-C33	-2.02	120.75	126.42
22	7	611	CLA	CHB-C4A-NA	2.02	127.30	124.51
22	4	604	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
22	B	804	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
22	B	841	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
22	5	606	CLA	O2A-CGA-O1A	-2.02	118.28	123.30
23	9	624	LUT	C21-C26-C27	-2.02	110.15	112.70
23	U	2621	LUT	C35-C15-C14	-2.02	119.35	123.47
24	5	618	XAT	C11-C12-C13	-2.02	120.75	126.42
22	1	611	CLA	C1-C2-C3	-2.01	122.56	126.04
27	7	621	BCR	C23-C22-C21	-2.01	115.85	118.94
22	7	611	CLA	O2D-CGD-CBD	2.01	114.85	111.27
21	4	618	CHL	C1B-CHB-C4A	-2.01	126.13	130.12
22	A	841	CLA	CHB-C4A-NA	2.01	127.30	124.51
21	2	608	CHL	C4D-CHA-C1A	-2.01	118.80	121.25
22	U	612	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
22	A	854	CLA	O2D-CGD-CBD	2.01	114.84	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	V	606	CHL	C1B-CHB-C4A	-2.01	126.13	130.12
22	8	602	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
22	B	833	CLA	O2D-CGD-CBD	2.01	114.84	111.27
22	A	843	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
21	V	607	CHL	C4B-C3B-C2B	-2.01	105.05	106.92
22	5	613	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
27	K	202	BCR	C24-C25-C26	2.01	126.33	121.46
24	3	619	XAT	O24-C25-C26	-2.01	57.30	58.96
23	8	619	LUT	C35-C34-C33	-2.01	124.45	127.31
21	U	608	CHL	C1B-CHB-C4A	-2.01	126.14	130.12
24	W	2622	XAT	C20-C13-C12	2.01	121.24	118.08
22	B	828	CLA	CHB-C4A-NA	2.01	127.29	124.51
21	4	618	CHL	O1D-CGD-CBD	-2.01	120.38	124.48
21	2	601	CHL	O2A-CGA-O1A	-2.01	118.30	123.30
22	6	611	CLA	O2A-CGA-O1A	-2.01	118.30	123.30
27	B	801	BCR	C27-C26-C25	-2.00	119.82	122.73
22	8	601	CLA	CHB-C4A-NA	2.00	127.28	124.51
21	6	606	CHL	C1C-C2C-C3C	-2.00	105.52	107.11
27	G	205	BCR	C40-C30-C25	-2.00	107.05	110.30
23	U	2621	LUT	C31-C30-C29	-2.00	124.45	127.31
22	W	611	CLA	CHB-C4A-NA	2.00	127.28	124.51
22	B	807	CLA	CHB-C4A-NA	2.00	127.28	124.51

All (357) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	U	601	CHL	NC
21	U	601	CHL	NA
21	U	601	CHL	ND
21	U	605	CHL	NC
21	U	605	CHL	NA
21	U	605	CHL	ND
21	U	606	CHL	NC
21	U	606	CHL	NA
21	U	606	CHL	ND
21	U	607	CHL	NC
21	U	607	CHL	NA
21	U	607	CHL	ND
21	U	608	CHL	NC
21	U	608	CHL	NA
21	U	608	CHL	ND
21	U	609	CHL	NC

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Mol	Chain	Res	Type	Atom
21	U	609	CHL	NA
21	U	609	CHL	ND
21	V	601	CHL	NC
21	V	601	CHL	NA
21	V	601	CHL	ND
21	V	605	CHL	NC
21	V	605	CHL	NA
21	V	605	CHL	ND
21	V	606	CHL	NC
21	V	606	CHL	NA
21	V	606	CHL	ND
21	V	607	CHL	NC
21	V	607	CHL	NA
21	V	607	CHL	ND
21	V	608	CHL	NC
21	V	608	CHL	NA
21	V	608	CHL	ND
21	V	609	CHL	NC
21	V	609	CHL	NA
21	V	609	CHL	ND
21	W	601	CHL	NC
21	W	601	CHL	NA
21	W	601	CHL	ND
21	W	605	CHL	NC
21	W	605	CHL	NA
21	W	605	CHL	ND
21	W	606	CHL	NC
21	W	606	CHL	NA
21	W	606	CHL	ND
21	W	607	CHL	NC
21	W	607	CHL	NA
21	W	607	CHL	ND
21	W	608	CHL	NC
21	W	608	CHL	NA
21	W	608	CHL	ND
21	W	609	CHL	NC
21	W	609	CHL	NA
21	W	609	CHL	ND
21	1	601	CHL	NC
21	1	601	CHL	NA
21	1	601	CHL	ND
21	1	607	CHL	NC

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Mol	Chain	Res	Type	Atom
21	1	607	CHL	NA
21	1	607	CHL	ND
21	2	601	CHL	NC
21	2	601	CHL	NA
21	2	601	CHL	ND
21	2	602	CHL	NC
21	2	602	CHL	NA
21	2	602	CHL	ND
21	2	606	CHL	NC
21	2	606	CHL	NA
21	2	606	CHL	ND
21	2	607	CHL	NC
21	2	607	CHL	NA
21	2	607	CHL	ND
21	2	608	CHL	NC
21	2	608	CHL	NA
21	2	608	CHL	ND
21	2	618	CHL	NC
21	2	618	CHL	NA
21	2	618	CHL	ND
21	3	608	CHL	NC
21	3	608	CHL	NA
21	3	608	CHL	ND
21	4	606	CHL	NC
21	4	606	CHL	NA
21	4	606	CHL	ND
21	4	607	CHL	NC
21	4	607	CHL	NA
21	4	607	CHL	ND
21	4	608	CHL	NC
21	4	608	CHL	NA
21	4	608	CHL	ND
21	4	618	CHL	NC
21	4	618	CHL	NA
21	4	618	CHL	ND
21	5	601	CHL	NC
21	5	601	CHL	NA
21	5	601	CHL	ND
21	5	607	CHL	NC
21	5	607	CHL	NA
21	5	607	CHL	ND
21	6	601	CHL	NC

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Mol	Chain	Res	Type	Atom
21	6	601	CHL	NA
21	6	601	CHL	ND
21	6	602	CHL	NC
21	6	602	CHL	NA
21	6	602	CHL	ND
21	6	606	CHL	NC
21	6	606	CHL	NA
21	6	606	CHL	ND
21	6	607	CHL	NC
21	6	607	CHL	NA
21	6	607	CHL	ND
21	6	608	CHL	NC
21	6	608	CHL	NA
21	6	608	CHL	ND
21	6	618	CHL	NC
21	6	618	CHL	NA
21	6	618	CHL	ND
21	7	608	CHL	NC
21	7	608	CHL	NA
21	7	608	CHL	ND
21	8	606	CHL	NC
21	8	606	CHL	NA
21	8	606	CHL	ND
21	8	607	CHL	NC
21	8	607	CHL	NA
21	8	607	CHL	ND
21	8	608	CHL	NC
21	8	608	CHL	NA
21	8	608	CHL	ND
21	8	618	CHL	NC
21	8	618	CHL	NA
21	8	618	CHL	ND
21	9	601	CHL	NC
21	9	601	CHL	NA
21	9	601	CHL	ND
21	9	605	CHL	NC
21	9	605	CHL	NA
21	9	605	CHL	ND
21	9	606	CHL	NC
21	9	606	CHL	NA
21	9	606	CHL	ND
21	9	607	CHL	NC

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Mol	Chain	Res	Type	Atom
21	9	607	CHL	NA
21	9	607	CHL	ND
21	9	608	CHL	NC
21	9	608	CHL	NA
21	9	608	CHL	ND
22	U	602	CLA	ND
22	U	603	CLA	ND
22	U	604	CLA	ND
22	U	610	CLA	ND
22	U	611	CLA	ND
22	U	612	CLA	ND
22	U	613	CLA	ND
22	U	614	CLA	ND
22	V	603	CLA	ND
22	V	604	CLA	ND
22	V	610	CLA	ND
22	V	611	CLA	ND
22	V	612	CLA	ND
22	V	613	CLA	ND
22	V	614	CLA	ND
22	W	602	CLA	ND
22	W	603	CLA	ND
22	W	604	CLA	ND
22	W	610	CLA	ND
22	W	611	CLA	ND
22	W	612	CLA	ND
22	W	613	CLA	ND
22	W	614	CLA	ND
22	1	602	CLA	ND
22	1	603	CLA	ND
22	1	606	CLA	ND
22	1	608	CLA	ND
22	1	609	CLA	ND
22	1	610	CLA	ND
22	1	611	CLA	ND
22	1	612	CLA	ND
22	1	613	CLA	ND
22	1	614	CLA	ND
22	1	616	CLA	ND
22	2	603	CLA	ND
22	2	604	CLA	ND
22	2	609	CLA	ND

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Mol	Chain	Res	Type	Atom
22	2	610	CLA	ND
22	2	611	CLA	ND
22	2	612	CLA	ND
22	2	613	CLA	ND
22	2	614	CLA	ND
22	3	602	CLA	ND
22	3	603	CLA	ND
22	3	604	CLA	ND
22	3	606	CLA	ND
22	3	607	CLA	ND
22	3	609	CLA	ND
22	3	610	CLA	ND
22	3	611	CLA	ND
22	3	612	CLA	ND
22	3	613	CLA	ND
22	3	614	CLA	ND
22	3	615	CLA	ND
22	3	617	CLA	ND
22	4	601	CLA	ND
22	4	602	CLA	ND
22	4	603	CLA	ND
22	4	604	CLA	ND
22	4	609	CLA	ND
22	4	610	CLA	ND
22	4	611	CLA	ND
22	4	612	CLA	ND
22	4	613	CLA	ND
22	4	614	CLA	ND
22	A	801	CLA	ND
22	A	802	CLA	ND
22	A	803	CLA	ND
22	A	804	CLA	ND
22	A	806	CLA	ND
22	A	807	CLA	ND
22	A	808	CLA	ND
22	A	809	CLA	ND
22	A	810	CLA	ND
22	A	811	CLA	ND
22	A	812	CLA	ND
22	A	813	CLA	ND
22	A	814	CLA	ND
22	A	815	CLA	ND

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Mol	Chain	Res	Type	Atom
22	A	816	CLA	ND
22	A	817	CLA	ND
22	A	818	CLA	ND
22	A	819	CLA	ND
22	A	820	CLA	ND
22	A	821	CLA	ND
22	A	822	CLA	ND
22	A	823	CLA	ND
22	A	824	CLA	ND
22	A	826	CLA	ND
22	A	828	CLA	ND
22	A	829	CLA	ND
22	A	830	CLA	ND
22	A	831	CLA	ND
22	A	832	CLA	ND
22	A	833	CLA	ND
22	A	834	CLA	ND
22	A	835	CLA	ND
22	A	836	CLA	ND
22	A	838	CLA	ND
22	A	839	CLA	ND
22	A	840	CLA	ND
22	A	841	CLA	ND
22	A	842	CLA	ND
22	A	843	CLA	ND
22	A	845	CLA	ND
22	A	854	CLA	ND
22	B	802	CLA	ND
22	B	803	CLA	ND
22	B	804	CLA	ND
22	B	805	CLA	ND
22	B	806	CLA	ND
22	B	808	CLA	ND
22	B	809	CLA	ND
22	B	810	CLA	ND
22	B	811	CLA	ND
22	B	812	CLA	ND
22	B	813	CLA	ND
22	B	814	CLA	ND
22	B	815	CLA	ND
22	B	816	CLA	ND
22	B	817	CLA	ND

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Mol	Chain	Res	Type	Atom
22	B	818	CLA	ND
22	B	819	CLA	ND
22	B	820	CLA	ND
22	B	821	CLA	ND
22	B	822	CLA	ND
22	B	823	CLA	ND
22	B	824	CLA	ND
22	B	825	CLA	ND
22	B	826	CLA	ND
22	B	827	CLA	ND
22	B	828	CLA	ND
22	B	829	CLA	ND
22	B	830	CLA	ND
22	B	831	CLA	ND
22	B	833	CLA	ND
22	B	834	CLA	ND
22	B	835	CLA	ND
22	B	836	CLA	ND
22	B	837	CLA	ND
22	B	839	CLA	ND
22	B	840	CLA	ND
22	B	841	CLA	ND
22	F	301	CLA	ND
22	F	303	CLA	ND
22	F	304	CLA	ND
22	G	201	CLA	ND
22	G	203	CLA	ND
22	G	204	CLA	ND
22	H	201	CLA	ND
22	J	101	CLA	ND
22	K	201	CLA	ND
22	K	203	CLA	ND
22	K	204	CLA	ND
22	K	206	CLA	ND
22	L	302	CLA	ND
22	L	303	CLA	ND
22	L	304	CLA	ND
22	O	2001	CLA	ND
22	O	2002	CLA	ND
22	O	2003	CLA	ND
22	5	602	CLA	ND
22	5	603	CLA	ND

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Mol	Chain	Res	Type	Atom
22	5	604	CLA	ND
22	5	606	CLA	ND
22	5	608	CLA	ND
22	5	609	CLA	ND
22	5	610	CLA	ND
22	5	611	CLA	ND
22	5	612	CLA	ND
22	5	614	CLA	ND
22	5	616	CLA	ND
22	6	603	CLA	ND
22	6	604	CLA	ND
22	6	609	CLA	ND
22	6	610	CLA	ND
22	6	611	CLA	ND
22	6	612	CLA	ND
22	6	613	CLA	ND
22	6	614	CLA	ND
22	7	603	CLA	ND
22	7	604	CLA	ND
22	7	606	CLA	ND
22	7	607	CLA	ND
22	7	609	CLA	ND
22	7	610	CLA	ND
22	7	611	CLA	ND
22	7	612	CLA	ND
22	7	613	CLA	ND
22	7	614	CLA	ND
22	7	615	CLA	ND
22	7	617	CLA	ND
22	8	601	CLA	ND
22	8	602	CLA	ND
22	8	603	CLA	ND
22	8	604	CLA	ND
22	8	609	CLA	ND
22	8	610	CLA	ND
22	8	611	CLA	ND
22	8	612	CLA	ND
22	8	613	CLA	ND
22	8	614	CLA	ND
22	9	602	CLA	ND
22	9	603	CLA	ND
22	9	604	CLA	ND

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Mol	Chain	Res	Type	Atom
22	9	609	CLA	ND
22	9	610	CLA	ND
22	9	611	CLA	ND
22	9	612	CLA	ND
22	9	613	CLA	ND

All (2687) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	U	601	CHL	CAD-CBD-CGD-O2D
21	U	607	CHL	C1A-C2A-CAA-CBA
21	U	607	CHL	C3A-C2A-CAA-CBA
21	U	608	CHL	CHA-CBD-CGD-O2D
21	U	609	CHL	C1A-C2A-CAA-CBA
21	U	609	CHL	CHA-CBD-CGD-O1D
21	U	609	CHL	CHA-CBD-CGD-O2D
21	V	601	CHL	C1A-C2A-CAA-CBA
21	V	601	CHL	C3A-C2A-CAA-CBA
21	V	601	CHL	CAD-CBD-CGD-O2D
21	V	601	CHL	C4-C3-C5-C6
21	V	605	CHL	CHA-CBD-CGD-O2D
21	V	608	CHL	C1A-C2A-CAA-CBA
21	W	608	CHL	C1A-C2A-CAA-CBA
21	W	609	CHL	C1A-C2A-CAA-CBA
21	1	601	CHL	CHA-CBD-CGD-O1D
21	1	601	CHL	CHA-CBD-CGD-O2D
21	1	601	CHL	CAD-CBD-CGD-O1D
21	1	601	CHL	CAD-CBD-CGD-O2D
21	1	607	CHL	C1A-C2A-CAA-CBA
21	1	607	CHL	C3A-C2A-CAA-CBA
21	1	607	CHL	CAD-CBD-CGD-O1D
21	1	607	CHL	CAD-CBD-CGD-O2D
21	2	601	CHL	CHA-CBD-CGD-O1D
21	2	601	CHL	CHA-CBD-CGD-O2D
21	2	601	CHL	CAD-CBD-CGD-O1D
21	2	607	CHL	CHA-CBD-CGD-O1D
21	2	607	CHL	CHA-CBD-CGD-O2D
21	2	618	CHL	CAD-CBD-CGD-O1D
21	2	618	CHL	CAD-CBD-CGD-O2D
21	3	608	CHL	C1A-C2A-CAA-CBA
21	3	608	CHL	C2-C3-C5-C6
21	3	608	CHL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
21	4	606	CHL	CHA-CBD-CGD-O1D
21	4	606	CHL	CHA-CBD-CGD-O2D
21	4	607	CHL	CHA-CBD-CGD-O1D
21	4	607	CHL	CHA-CBD-CGD-O2D
21	5	601	CHL	CHA-CBD-CGD-O1D
21	5	601	CHL	CHA-CBD-CGD-O2D
21	5	601	CHL	CAD-CBD-CGD-O1D
21	5	601	CHL	CAD-CBD-CGD-O2D
21	6	601	CHL	CHA-CBD-CGD-O1D
21	6	601	CHL	CHA-CBD-CGD-O2D
21	6	601	CHL	CAD-CBD-CGD-O1D
21	6	601	CHL	CAD-CBD-CGD-O2D
21	6	607	CHL	CHA-CBD-CGD-O1D
21	6	607	CHL	CHA-CBD-CGD-O2D
21	6	608	CHL	CHA-CBD-CGD-O1D
21	6	608	CHL	CHA-CBD-CGD-O2D
21	7	608	CHL	CHA-CBD-CGD-O1D
21	7	608	CHL	CHA-CBD-CGD-O2D
21	8	606	CHL	CHA-CBD-CGD-O1D
21	8	606	CHL	CHA-CBD-CGD-O2D
21	8	607	CHL	CHA-CBD-CGD-O1D
21	8	607	CHL	CHA-CBD-CGD-O2D
21	8	608	CHL	CHA-CBD-CGD-O1D
21	8	608	CHL	CHA-CBD-CGD-O2D
21	8	618	CHL	CHA-CBD-CGD-O1D
21	8	618	CHL	CHA-CBD-CGD-O2D
21	9	607	CHL	C1A-C2A-CAA-CBA
22	U	602	CLA	C4-C3-C5-C6
22	U	610	CLA	C3A-C2A-CAA-CBA
22	U	611	CLA	CHA-CBD-CGD-O1D
22	U	611	CLA	CBD-CGD-O2D-CED
22	U	612	CLA	CBD-CGD-O2D-CED
22	U	612	CLA	C14-C13-C15-C16
22	V	611	CLA	C1A-C2A-CAA-CBA
22	V	613	CLA	CHA-CBD-CGD-O1D
22	V	613	CLA	CHA-CBD-CGD-O2D
22	V	614	CLA	C1A-C2A-CAA-CBA
22	V	614	CLA	C3A-C2A-CAA-CBA
22	W	610	CLA	C2-C3-C5-C6
22	W	610	CLA	C4-C3-C5-C6
22	W	610	CLA	C6-C7-C8-C9
22	W	610	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
22	1	602	CLA	C1A-C2A-CAA-CBA
22	1	602	CLA	C3A-C2A-CAA-CBA
22	1	604	CLA	C1A-C2A-CAA-CBA
22	1	604	CLA	C3A-C2A-CAA-CBA
22	1	606	CLA	CHA-CBD-CGD-O1D
22	1	606	CLA	CHA-CBD-CGD-O2D
22	1	606	CLA	CBD-CGD-O2D-CED
22	1	608	CLA	C1A-C2A-CAA-CBA
22	1	609	CLA	C1A-C2A-CAA-CBA
22	1	609	CLA	C3A-C2A-CAA-CBA
22	1	609	CLA	C2-C3-C5-C6
22	1	609	CLA	C4-C3-C5-C6
22	1	610	CLA	CBD-CGD-O2D-CED
22	1	611	CLA	C1A-C2A-CAA-CBA
22	1	611	CLA	C3A-C2A-CAA-CBA
22	1	614	CLA	C1A-C2A-CAA-CBA
22	1	614	CLA	C2A-CAA-CBA-CGA
22	1	616	CLA	CHA-CBD-CGD-O1D
22	2	609	CLA	C1A-C2A-CAA-CBA
22	2	609	CLA	C3A-C2A-CAA-CBA
22	2	612	CLA	C1A-C2A-CAA-CBA
22	2	612	CLA	C3A-C2A-CAA-CBA
22	2	613	CLA	CHA-CBD-CGD-O1D
22	3	602	CLA	C1A-C2A-CAA-CBA
22	3	602	CLA	C3A-C2A-CAA-CBA
22	3	604	CLA	C2A-CAA-CBA-CGA
22	3	606	CLA	C1A-C2A-CAA-CBA
22	3	606	CLA	C3A-C2A-CAA-CBA
22	3	607	CLA	C1A-C2A-CAA-CBA
22	3	607	CLA	C3A-C2A-CAA-CBA
22	3	609	CLA	C1A-C2A-CAA-CBA
22	3	609	CLA	C3A-C2A-CAA-CBA
22	3	609	CLA	C4-C3-C5-C6
22	3	610	CLA	C1A-C2A-CAA-CBA
22	3	611	CLA	C1A-C2A-CAA-CBA
22	3	611	CLA	C3A-C2A-CAA-CBA
22	3	617	CLA	C1A-C2A-CAA-CBA
22	3	617	CLA	C3A-C2A-CAA-CBA
22	4	601	CLA	CHA-CBD-CGD-O1D
22	4	601	CLA	CHA-CBD-CGD-O2D
22	4	602	CLA	C3A-C2A-CAA-CBA
22	4	603	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	4	604	CLA	C1A-C2A-CAA-CBA
22	4	609	CLA	C1A-C2A-CAA-CBA
22	4	609	CLA	C3A-C2A-CAA-CBA
22	4	610	CLA	C3A-C2A-CAA-CBA
22	4	614	CLA	C1A-C2A-CAA-CBA
22	4	614	CLA	C3A-C2A-CAA-CBA
22	4	614	CLA	CBA-CGA-O2A-C1
22	4	614	CLA	O1A-CGA-O2A-C1
22	A	801	CLA	CAD-CBD-CGD-O1D
22	A	801	CLA	CAD-CBD-CGD-O2D
22	A	805	CLA	C1A-C2A-CAA-CBA
22	A	805	CLA	C3A-C2A-CAA-CBA
22	A	806	CLA	CHA-CBD-CGD-O1D
22	A	806	CLA	CHA-CBD-CGD-O2D
22	A	806	CLA	CAD-CBD-CGD-O1D
22	A	809	CLA	C1A-C2A-CAA-CBA
22	A	809	CLA	C3A-C2A-CAA-CBA
22	A	811	CLA	C1A-C2A-CAA-CBA
22	A	811	CLA	C3A-C2A-CAA-CBA
22	A	811	CLA	CBD-CGD-O2D-CED
22	A	813	CLA	C1A-C2A-CAA-CBA
22	A	815	CLA	C1A-C2A-CAA-CBA
22	A	817	CLA	C1A-C2A-CAA-CBA
22	A	819	CLA	C1A-C2A-CAA-CBA
22	A	819	CLA	C3A-C2A-CAA-CBA
22	A	820	CLA	C3A-C2A-CAA-CBA
22	A	821	CLA	C1A-C2A-CAA-CBA
22	A	821	CLA	C3A-C2A-CAA-CBA
22	A	824	CLA	CHA-CBD-CGD-O1D
22	A	824	CLA	CHA-CBD-CGD-O2D
22	A	825	CLA	CHA-CBD-CGD-O1D
22	A	825	CLA	CHA-CBD-CGD-O2D
22	A	828	CLA	CHA-CBD-CGD-O1D
22	A	828	CLA	CHA-CBD-CGD-O2D
22	A	830	CLA	C1A-C2A-CAA-CBA
22	A	831	CLA	C1A-C2A-CAA-CBA
22	A	833	CLA	C1A-C2A-CAA-CBA
22	A	833	CLA	C3A-C2A-CAA-CBA
22	A	834	CLA	C1A-C2A-CAA-CBA
22	A	834	CLA	C3A-C2A-CAA-CBA
22	A	835	CLA	C1A-C2A-CAA-CBA
22	A	835	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	A	841	CLA	CHA-CBD-CGD-O1D
22	A	841	CLA	CHA-CBD-CGD-O2D
22	A	842	CLA	C1A-C2A-CAA-CBA
22	A	843	CLA	C1A-C2A-CAA-CBA
22	A	843	CLA	C3A-C2A-CAA-CBA
22	A	845	CLA	CBD-CGD-O2D-CED
22	A	854	CLA	C1A-C2A-CAA-CBA
22	A	854	CLA	C3A-C2A-CAA-CBA
22	B	802	CLA	CBD-CGD-O2D-CED
22	B	803	CLA	CHA-CBD-CGD-O1D
22	B	803	CLA	CHA-CBD-CGD-O2D
22	B	803	CLA	CBD-CGD-O2D-CED
22	B	804	CLA	C1A-C2A-CAA-CBA
22	B	805	CLA	C3A-C2A-CAA-CBA
22	B	805	CLA	CHA-CBD-CGD-O1D
22	B	805	CLA	CHA-CBD-CGD-O2D
22	B	806	CLA	CBD-CGD-O2D-CED
22	B	808	CLA	C1A-C2A-CAA-CBA
22	B	812	CLA	C1A-C2A-CAA-CBA
22	B	812	CLA	C3A-C2A-CAA-CBA
22	B	813	CLA	C3A-C2A-CAA-CBA
22	B	816	CLA	CHA-CBD-CGD-O1D
22	B	816	CLA	CHA-CBD-CGD-O2D
22	B	817	CLA	C2A-CAA-CBA-CGA
22	B	818	CLA	C3A-C2A-CAA-CBA
22	B	819	CLA	O2A-C1-C2-C3
22	B	822	CLA	C2A-CAA-CBA-CGA
22	B	824	CLA	C2-C3-C5-C6
22	B	824	CLA	C4-C3-C5-C6
22	B	827	CLA	C1A-C2A-CAA-CBA
22	B	827	CLA	C3A-C2A-CAA-CBA
22	B	828	CLA	C1A-C2A-CAA-CBA
22	B	831	CLA	C1A-C2A-CAA-CBA
22	B	831	CLA	C4-C3-C5-C6
22	B	833	CLA	C1A-C2A-CAA-CBA
22	B	833	CLA	C2-C3-C5-C6
22	B	833	CLA	C4-C3-C5-C6
22	B	835	CLA	CBD-CGD-O2D-CED
22	B	836	CLA	C1A-C2A-CAA-CBA
22	B	836	CLA	C3A-C2A-CAA-CBA
22	B	836	CLA	C2A-CAA-CBA-CGA
22	B	837	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	B	838	CLA	C1A-C2A-CAA-CBA
22	B	840	CLA	C1A-C2A-CAA-CBA
22	B	840	CLA	C3A-C2A-CAA-CBA
22	G	201	CLA	CBD-CGD-O2D-CED
22	K	201	CLA	C1A-C2A-CAA-CBA
22	K	201	CLA	C3A-C2A-CAA-CBA
22	K	204	CLA	C2A-CAA-CBA-CGA
22	K	204	CLA	C2-C3-C5-C6
22	K	204	CLA	C4-C3-C5-C6
22	L	302	CLA	CHA-CBD-CGD-O1D
22	L	302	CLA	CHA-CBD-CGD-O2D
22	L	302	CLA	CAD-CBD-CGD-O1D
22	L	302	CLA	C11-C12-C13-C14
22	L	304	CLA	C1A-C2A-CAA-CBA
22	L	304	CLA	C2A-CAA-CBA-CGA
22	O	2002	CLA	C3A-C2A-CAA-CBA
22	O	2002	CLA	CAD-CBD-CGD-O1D
22	O	2002	CLA	CAD-CBD-CGD-O2D
22	5	603	CLA	CBD-CGD-O2D-CED
22	5	608	CLA	CHA-CBD-CGD-O1D
22	5	608	CLA	CHA-CBD-CGD-O2D
22	5	610	CLA	C1A-C2A-CAA-CBA
22	5	611	CLA	CHA-CBD-CGD-O1D
22	5	611	CLA	CHA-CBD-CGD-O2D
22	5	611	CLA	CAD-CBD-CGD-O1D
22	5	612	CLA	CBD-CGD-O2D-CED
22	5	613	CLA	C1A-C2A-CAA-CBA
22	5	613	CLA	C3A-C2A-CAA-CBA
22	5	613	CLA	CHA-CBD-CGD-O1D
22	5	614	CLA	CBD-CGD-O2D-CED
22	6	603	CLA	CBD-CGD-O2D-CED
22	6	610	CLA	C1A-C2A-CAA-CBA
22	6	610	CLA	C3A-C2A-CAA-CBA
22	6	613	CLA	CHA-CBD-CGD-O1D
22	6	613	CLA	CHA-CBD-CGD-O2D
22	7	603	CLA	C1A-C2A-CAA-CBA
22	7	603	CLA	C3A-C2A-CAA-CBA
22	7	604	CLA	CHA-CBD-CGD-O1D
22	7	604	CLA	CHA-CBD-CGD-O2D
22	7	604	CLA	CBD-CGD-O2D-CED
22	7	606	CLA	C1A-C2A-CAA-CBA
22	7	609	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	7	609	CLA	C3A-C2A-CAA-CBA
22	7	610	CLA	C1A-C2A-CAA-CBA
22	7	610	CLA	C3A-C2A-CAA-CBA
22	7	610	CLA	CBD-CGD-O2D-CED
22	7	614	CLA	CBD-CGD-O2D-CED
22	7	617	CLA	C1A-C2A-CAA-CBA
22	7	617	CLA	C3A-C2A-CAA-CBA
22	7	617	CLA	CBA-CGA-O2A-C1
22	7	617	CLA	O1A-CGA-O2A-C1
22	8	602	CLA	CHA-CBD-CGD-O2D
22	8	603	CLA	C2A-CAA-CBA-CGA
22	8	612	CLA	CHA-CBD-CGD-O1D
22	8	612	CLA	CHA-CBD-CGD-O2D
22	8	613	CLA	CHA-CBD-CGD-O1D
22	8	613	CLA	CHA-CBD-CGD-O2D
22	8	614	CLA	C1A-C2A-CAA-CBA
22	8	614	CLA	CAD-CBD-CGD-O1D
22	8	614	CLA	CAD-CBD-CGD-O2D
22	8	614	CLA	CBD-CGD-O2D-CED
22	9	604	CLA	CBD-CGD-O2D-CED
22	9	610	CLA	C1A-C2A-CAA-CBA
22	9	612	CLA	C1A-C2A-CAA-CBA
23	2	619	LUT	C7-C8-C9-C10
23	2	619	LUT	C7-C8-C9-C19
23	2	619	LUT	C11-C12-C13-C20
23	2	619	LUT	C28-C29-C30-C31
23	2	619	LUT	C39-C29-C30-C31
23	2	619	LUT	C30-C31-C32-C33
23	5	617	LUT	C6-C7-C8-C9
23	5	617	LUT	C26-C27-C28-C29
24	U	2622	XAT	O4-C6-C7-C8
24	V	2622	XAT	C25-C26-C27-C28
24	V	2622	XAT	O24-C26-C27-C28
24	4	620	XAT	C1-C6-C7-C8
24	4	620	XAT	C5-C6-C7-C8
24	4	620	XAT	O4-C6-C7-C8
24	5	618	XAT	C21-C26-C27-C28
24	5	618	XAT	C25-C26-C27-C28
24	5	618	XAT	C31-C32-C33-C34
24	5	618	XAT	C31-C32-C33-C40
24	6	620	XAT	C21-C26-C27-C28
24	6	620	XAT	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
24	6	620	XAT	O24-C26-C27-C28
24	7	619	XAT	C1-C6-C7-C8
24	7	619	XAT	C5-C6-C7-C8
24	7	619	XAT	O4-C6-C7-C8
24	8	620	XAT	C6-C7-C8-C9
24	8	620	XAT	C31-C32-C33-C34
24	8	620	XAT	C31-C32-C33-C40
25	U	2623	NEX	O24-C26-C27-C28
25	W	2623	NEX	C13-C14-C15-C35
25	W	2623	NEX	C27-C28-C29-C30
25	W	2623	NEX	C27-C28-C29-C39
25	W	2623	NEX	C31-C32-C33-C34
25	W	2623	NEX	C31-C32-C33-C40
26	U	2630	LHG	C4-O6-P-O5
26	V	2630	LHG	C4-O6-P-O5
26	W	2630	LHG	C3-O3-P-O6
26	W	2630	LHG	C4-O6-P-O5
26	1	630	LHG	O1-C1-C2-C3
26	1	630	LHG	C4-O6-P-O5
26	2	630	LHG	C4-O6-P-O4
26	4	630	LHG	O1-C1-C2-O2
26	4	630	LHG	O1-C1-C2-C3
26	4	630	LHG	O9-C7-O7-C5
26	A	847	LHG	C3-O3-P-O6
26	A	847	LHG	O6-C4-C5-O7
26	B	851	LHG	C4-O6-P-O4
26	5	630	LHG	C3-O3-P-O6
26	5	630	LHG	C4-O6-P-O5
26	6	630	LHG	C4-O6-P-O3
26	6	630	LHG	C4-O6-P-O4
26	6	630	LHG	C4-O6-P-O5
26	7	630	LHG	C3-O3-P-O4
26	7	630	LHG	C3-O3-P-O5
26	8	630	LHG	C3-O3-P-O6
26	8	630	LHG	C4-O6-P-O5
27	1	619	BCR	C5-C6-C7-C8
27	4	621	BCR	C7-C8-C9-C10
27	4	621	BCR	C7-C8-C9-C34
27	4	621	BCR	C21-C22-C23-C24
27	4	621	BCR	C37-C22-C23-C24
27	A	848	BCR	C23-C24-C25-C26
27	A	849	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
27	A	850	BCR	C23-C24-C25-C26
27	A	852	BCR	C5-C6-C7-C8
27	A	852	BCR	C23-C24-C25-C26
27	A	852	BCR	C23-C24-C25-C30
27	B	801	BCR	C23-C24-C25-C26
27	B	843	BCR	C23-C24-C25-C26
27	B	843	BCR	C23-C24-C25-C30
27	B	845	BCR	C7-C8-C9-C10
27	B	845	BCR	C7-C8-C9-C34
27	B	845	BCR	C11-C12-C13-C14
27	B	847	BCR	C21-C22-C23-C24
27	B	848	BCR	C23-C24-C25-C26
27	B	848	BCR	C23-C24-C25-C30
27	B	1609	BCR	C7-C8-C9-C10
27	B	1609	BCR	C7-C8-C9-C34
27	G	205	BCR	C5-C6-C7-C8
27	G	205	BCR	C23-C24-C25-C26
27	G	205	BCR	C23-C24-C25-C30
27	K	202	BCR	C23-C24-C25-C26
27	L	305	BCR	C1-C6-C7-C8
27	L	305	BCR	C5-C6-C7-C8
27	M	2001	BCR	C7-C8-C9-C10
27	M	2001	BCR	C7-C8-C9-C34
27	M	2001	BCR	C23-C24-C25-C26
27	6	621	BCR	C7-C8-C9-C10
27	6	621	BCR	C7-C8-C9-C34
27	6	621	BCR	C21-C22-C23-C24
27	6	621	BCR	C37-C22-C23-C24
27	8	621	BCR	C7-C8-C9-C10
27	8	621	BCR	C7-C8-C9-C34
27	8	621	BCR	C21-C22-C23-C24
27	8	621	BCR	C37-C22-C23-C24
28	A	860	LMG	O6-C1-O1-C7
28	A	860	LMG	C11-C10-O7-C8
28	G	202	LMG	O6-C1-O1-C7
28	J	103	LMG	C11-C10-O7-C8
31	A	857	LMT	C2-C1-O1'-C1'
31	K	208	LMT	O5'-C1'-O1'-C1
22	B	813	CLA	C4C-C3C-CAC-CBC
22	U	614	CLA	O1D-CGD-O2D-CED
22	V	603	CLA	O1D-CGD-O2D-CED
22	7	614	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	8	604	CLA	O1D-CGD-O2D-CED
22	B	813	CLA	C2C-C3C-CAC-CBC
22	4	603	CLA	O1D-CGD-O2D-CED
22	A	827	CLA	O1D-CGD-O2D-CED
22	B	802	CLA	O1D-CGD-O2D-CED
22	B	803	CLA	O1D-CGD-O2D-CED
22	5	603	CLA	O1D-CGD-O2D-CED
22	6	603	CLA	O1D-CGD-O2D-CED
21	4	608	CHL	CBD-CGD-O2D-CED
22	U	604	CLA	CBD-CGD-O2D-CED
22	U	614	CLA	CBD-CGD-O2D-CED
22	V	603	CLA	CBD-CGD-O2D-CED
22	W	604	CLA	CBD-CGD-O2D-CED
22	1	614	CLA	CBD-CGD-O2D-CED
22	3	602	CLA	CBD-CGD-O2D-CED
22	3	610	CLA	CBD-CGD-O2D-CED
22	4	602	CLA	CBD-CGD-O2D-CED
22	4	604	CLA	CBD-CGD-O2D-CED
22	4	614	CLA	CBD-CGD-O2D-CED
22	A	812	CLA	CBD-CGD-O2D-CED
22	A	827	CLA	CBD-CGD-O2D-CED
22	A	834	CLA	CBD-CGD-O2D-CED
22	A	854	CLA	CBD-CGD-O2D-CED
22	B	824	CLA	CBD-CGD-O2D-CED
22	B	827	CLA	CBD-CGD-O2D-CED
22	B	830	CLA	CBD-CGD-O2D-CED
22	F	301	CLA	CBD-CGD-O2D-CED
22	G	203	CLA	CBD-CGD-O2D-CED
22	K	204	CLA	CBD-CGD-O2D-CED
22	5	604	CLA	CBD-CGD-O2D-CED
22	5	610	CLA	CBD-CGD-O2D-CED
22	6	604	CLA	CBD-CGD-O2D-CED
22	8	604	CLA	CBD-CGD-O2D-CED
22	8	610	CLA	CBD-CGD-O2D-CED
22	9	602	CLA	CBD-CGD-O2D-CED
22	9	609	CLA	CBD-CGD-O2D-CED
22	1	614	CLA	O1A-CGA-O2A-C1
22	2	604	CLA	O1A-CGA-O2A-C1
22	3	607	CLA	O1A-CGA-O2A-C1
22	3	612	CLA	O1A-CGA-O2A-C1
22	A	803	CLA	O1A-CGA-O2A-C1
22	A	806	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	B	803	CLA	O1A-CGA-O2A-C1
22	B	810	CLA	O1A-CGA-O2A-C1
22	B	813	CLA	O1A-CGA-O2A-C1
22	B	814	CLA	O1A-CGA-O2A-C1
22	L	303	CLA	O1A-CGA-O2A-C1
22	6	609	CLA	O1A-CGA-O2A-C1
22	8	613	CLA	O1A-CGA-O2A-C1
22	3	606	CLA	O1A-CGA-O2A-C1
22	3	606	CLA	CBA-CGA-O2A-C1
22	F	304	CLA	CBD-CGD-O2D-CED
22	U	612	CLA	O1D-CGD-O2D-CED
22	1	606	CLA	O1D-CGD-O2D-CED
22	A	845	CLA	O1D-CGD-O2D-CED
22	B	806	CLA	O1D-CGD-O2D-CED
22	G	201	CLA	O1D-CGD-O2D-CED
22	5	612	CLA	O1D-CGD-O2D-CED
22	9	604	CLA	O1D-CGD-O2D-CED
22	3	607	CLA	CBA-CGA-O2A-C1
22	3	612	CLA	CBA-CGA-O2A-C1
22	A	803	CLA	CBA-CGA-O2A-C1
22	A	806	CLA	CBA-CGA-O2A-C1
22	A	821	CLA	CBA-CGA-O2A-C1
22	B	803	CLA	CBA-CGA-O2A-C1
22	B	810	CLA	CBA-CGA-O2A-C1
22	B	813	CLA	CBA-CGA-O2A-C1
22	L	303	CLA	CBA-CGA-O2A-C1
22	6	609	CLA	CBA-CGA-O2A-C1
22	8	613	CLA	CBA-CGA-O2A-C1
21	3	608	CHL	CBD-CGD-O2D-CED
22	U	603	CLA	CBD-CGD-O2D-CED
22	U	610	CLA	CBD-CGD-O2D-CED
22	V	614	CLA	CBD-CGD-O2D-CED
22	1	604	CLA	CBD-CGD-O2D-CED
22	1	608	CLA	CBD-CGD-O2D-CED
22	1	611	CLA	CBD-CGD-O2D-CED
22	3	603	CLA	CBD-CGD-O2D-CED
22	4	610	CLA	CBD-CGD-O2D-CED
22	4	611	CLA	CBD-CGD-O2D-CED
22	A	801	CLA	CBD-CGD-O2D-CED
22	A	810	CLA	CBD-CGD-O2D-CED
22	A	824	CLA	CBD-CGD-O2D-CED
22	A	837	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	A	840	CLA	CBD-CGD-O2D-CED
22	B	808	CLA	CBD-CGD-O2D-CED
22	B	809	CLA	CBD-CGD-O2D-CED
22	B	814	CLA	CBD-CGD-O2D-CED
22	B	822	CLA	CBD-CGD-O2D-CED
22	B	836	CLA	CBD-CGD-O2D-CED
22	B	840	CLA	CBD-CGD-O2D-CED
22	K	206	CLA	CBD-CGD-O2D-CED
22	6	610	CLA	CBD-CGD-O2D-CED
22	6	611	CLA	CBD-CGD-O2D-CED
22	7	602	CLA	CBD-CGD-O2D-CED
22	7	606	CLA	CBD-CGD-O2D-CED
22	8	611	CLA	CBD-CGD-O2D-CED
22	9	610	CLA	CBD-CGD-O2D-CED
22	1	603	CLA	O1A-CGA-O2A-C1
22	1	613	CLA	O1A-CGA-O2A-C1
22	2	614	CLA	O1A-CGA-O2A-C1
22	3	604	CLA	O1A-CGA-O2A-C1
22	4	601	CLA	O1A-CGA-O2A-C1
22	4	603	CLA	O1A-CGA-O2A-C1
22	4	604	CLA	O1A-CGA-O2A-C1
22	4	613	CLA	O1A-CGA-O2A-C1
22	A	805	CLA	O1A-CGA-O2A-C1
22	A	821	CLA	O1A-CGA-O2A-C1
22	A	829	CLA	O1A-CGA-O2A-C1
22	A	833	CLA	O1A-CGA-O2A-C1
22	A	843	CLA	O1A-CGA-O2A-C1
22	A	845	CLA	O1A-CGA-O2A-C1
22	B	806	CLA	O1A-CGA-O2A-C1
22	B	839	CLA	O1A-CGA-O2A-C1
22	B	841	CLA	O1A-CGA-O2A-C1
22	J	101	CLA	O1A-CGA-O2A-C1
22	O	2002	CLA	O1A-CGA-O2A-C1
22	5	608	CLA	O1A-CGA-O2A-C1
28	A	860	LMG	O10-C28-O8-C9
22	F	304	CLA	O1D-CGD-O2D-CED
22	U	611	CLA	O1D-CGD-O2D-CED
22	A	811	CLA	O1D-CGD-O2D-CED
22	B	835	CLA	O1D-CGD-O2D-CED
22	7	604	CLA	O1D-CGD-O2D-CED
22	1	610	CLA	O1D-CGD-O2D-CED
22	5	614	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	7	610	CLA	O1D-CGD-O2D-CED
22	8	614	CLA	O1D-CGD-O2D-CED
22	A	815	CLA	CBD-CGD-O2D-CED
22	B	820	CLA	CBD-CGD-O2D-CED
22	B	829	CLA	CBD-CGD-O2D-CED
22	O	2002	CLA	CBD-CGD-O2D-CED
22	7	611	CLA	CBD-CGD-O2D-CED
22	W	604	CLA	O1D-CGD-O2D-CED
22	4	602	CLA	O1D-CGD-O2D-CED
22	4	604	CLA	O1D-CGD-O2D-CED
22	A	812	CLA	O1D-CGD-O2D-CED
22	A	804	CLA	O1A-CGA-O2A-C1
22	5	611	CLA	O1A-CGA-O2A-C1
21	U	609	CHL	C3-C5-C6-C7
22	U	602	CLA	C3-C5-C6-C7
22	V	613	CLA	C3-C5-C6-C7
22	3	604	CLA	C3-C5-C6-C7
22	A	807	CLA	C3-C5-C6-C7
22	A	809	CLA	C3-C5-C6-C7
22	A	811	CLA	C3-C5-C6-C7
22	A	820	CLA	C3-C5-C6-C7
22	A	822	CLA	C3-C5-C6-C7
22	A	823	CLA	C3-C5-C6-C7
22	A	824	CLA	C3-C5-C6-C7
22	A	833	CLA	C3-C5-C6-C7
22	A	837	CLA	C3-C5-C6-C7
22	A	838	CLA	C3-C5-C6-C7
22	B	834	CLA	C3-C5-C6-C7
22	K	204	CLA	C3-C5-C6-C7
22	7	610	CLA	C3-C5-C6-C7
22	1	603	CLA	CBA-CGA-O2A-C1
22	1	614	CLA	CBA-CGA-O2A-C1
22	2	604	CLA	CBA-CGA-O2A-C1
22	3	604	CLA	CBA-CGA-O2A-C1
22	A	805	CLA	CBA-CGA-O2A-C1
22	A	843	CLA	CBA-CGA-O2A-C1
22	A	854	CLA	CBA-CGA-O2A-C1
22	B	814	CLA	CBA-CGA-O2A-C1
22	B	836	CLA	CBA-CGA-O2A-C1
22	B	839	CLA	CBA-CGA-O2A-C1
22	5	608	CLA	CBA-CGA-O2A-C1
22	8	603	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
28	A	860	LMG	C29-C28-O8-C9
26	4	630	LHG	C8-C7-O7-C5
22	U	604	CLA	O1D-CGD-O2D-CED
22	A	834	CLA	O1D-CGD-O2D-CED
22	G	203	CLA	O1D-CGD-O2D-CED
22	B	833	CLA	CBD-CGD-O2D-CED
22	5	611	CLA	CBA-CGA-O2A-C1
22	6	603	CLA	CBA-CGA-O2A-C1
22	9	602	CLA	C4-C3-C5-C6
22	U	602	CLA	C2-C3-C5-C6
22	3	609	CLA	C2-C3-C5-C6
22	B	831	CLA	C2-C3-C5-C6
22	9	602	CLA	C2-C3-C5-C6
22	V	610	CLA	CBD-CGD-O2D-CED
22	2	603	CLA	CBD-CGD-O2D-CED
22	9	613	CLA	CBD-CGD-O2D-CED
21	U	606	CHL	C2A-CAA-CBA-CGA
21	U	609	CHL	C2A-CAA-CBA-CGA
21	1	601	CHL	C2A-CAA-CBA-CGA
21	2	607	CHL	C2A-CAA-CBA-CGA
21	4	607	CHL	C2A-CAA-CBA-CGA
21	5	601	CHL	C2A-CAA-CBA-CGA
21	6	602	CHL	C2A-CAA-CBA-CGA
21	6	608	CHL	C2A-CAA-CBA-CGA
21	7	608	CHL	C2A-CAA-CBA-CGA
22	4	601	CLA	C2A-CAA-CBA-CGA
22	A	811	CLA	C2A-CAA-CBA-CGA
22	A	845	CLA	C2A-CAA-CBA-CGA
22	A	854	CLA	C2A-CAA-CBA-CGA
22	B	804	CLA	C2A-CAA-CBA-CGA
22	B	809	CLA	C2A-CAA-CBA-CGA
22	B	825	CLA	C2A-CAA-CBA-CGA
22	L	302	CLA	C2A-CAA-CBA-CGA
22	6	611	CLA	C2A-CAA-CBA-CGA
22	3	617	CLA	O1A-CGA-O2A-C1
22	F	301	CLA	O1A-CGA-O2A-C1
22	L	304	CLA	O1A-CGA-O2A-C1
22	A	843	CLA	C3-C5-C6-C7
22	B	827	CLA	C3-C5-C6-C7
22	F	301	CLA	C3-C5-C6-C7
22	L	303	CLA	C3-C5-C6-C7
22	7	602	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
22	U	604	CLA	CBA-CGA-O2A-C1
22	U	612	CLA	CBA-CGA-O2A-C1
22	V	603	CLA	CBA-CGA-O2A-C1
22	1	602	CLA	CBA-CGA-O2A-C1
22	1	613	CLA	CBA-CGA-O2A-C1
22	2	614	CLA	CBA-CGA-O2A-C1
22	3	602	CLA	CBA-CGA-O2A-C1
22	3	603	CLA	CBA-CGA-O2A-C1
22	4	601	CLA	CBA-CGA-O2A-C1
22	4	603	CLA	CBA-CGA-O2A-C1
22	4	604	CLA	CBA-CGA-O2A-C1
22	4	613	CLA	CBA-CGA-O2A-C1
22	A	804	CLA	CBA-CGA-O2A-C1
22	A	829	CLA	CBA-CGA-O2A-C1
22	A	833	CLA	CBA-CGA-O2A-C1
22	A	836	CLA	CBA-CGA-O2A-C1
22	A	845	CLA	CBA-CGA-O2A-C1
22	B	806	CLA	CBA-CGA-O2A-C1
22	B	820	CLA	CBA-CGA-O2A-C1
22	B	826	CLA	CBA-CGA-O2A-C1
22	B	841	CLA	CBA-CGA-O2A-C1
22	F	301	CLA	CBA-CGA-O2A-C1
22	J	101	CLA	CBA-CGA-O2A-C1
22	O	2002	CLA	CBA-CGA-O2A-C1
22	8	609	CLA	CBA-CGA-O2A-C1
21	4	608	CHL	O1D-CGD-O2D-CED
21	6	602	CHL	CBD-CGD-O2D-CED
22	W	610	CLA	CBD-CGD-O2D-CED
22	B	823	CLA	CBD-CGD-O2D-CED
22	F	303	CLA	CBD-CGD-O2D-CED
22	1	614	CLA	O1D-CGD-O2D-CED
22	B	827	CLA	O1D-CGD-O2D-CED
22	F	301	CLA	O1D-CGD-O2D-CED
22	K	204	CLA	O1D-CGD-O2D-CED
22	5	604	CLA	O1D-CGD-O2D-CED
22	9	602	CLA	O1D-CGD-O2D-CED
22	9	609	CLA	O1D-CGD-O2D-CED
28	A	860	LMG	O9-C10-O7-C8
28	J	103	LMG	O9-C10-O7-C8
22	U	604	CLA	O1A-CGA-O2A-C1
22	V	603	CLA	O1A-CGA-O2A-C1
22	1	602	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	3	602	CLA	O1A-CGA-O2A-C1
22	A	836	CLA	O1A-CGA-O2A-C1
22	A	854	CLA	O1A-CGA-O2A-C1
22	B	820	CLA	O1A-CGA-O2A-C1
22	7	604	CLA	O1A-CGA-O2A-C1
22	8	603	CLA	O1A-CGA-O2A-C1
22	8	609	CLA	O1A-CGA-O2A-C1
21	W	607	CHL	CBD-CGD-O2D-CED
22	U	613	CLA	CBD-CGD-O2D-CED
22	1	616	CLA	CBD-CGD-O2D-CED
22	2	613	CLA	CBD-CGD-O2D-CED
22	3	606	CLA	CBD-CGD-O2D-CED
22	4	613	CLA	CBD-CGD-O2D-CED
22	A	802	CLA	CBD-CGD-O2D-CED
22	A	838	CLA	CBD-CGD-O2D-CED
22	J	101	CLA	CBD-CGD-O2D-CED
22	7	612	CLA	CBD-CGD-O2D-CED
22	8	613	CLA	CBD-CGD-O2D-CED
22	9	603	CLA	CBD-CGD-O2D-CED
22	9	611	CLA	CBD-CGD-O2D-CED
22	6	604	CLA	O1D-CGD-O2D-CED
22	W	610	CLA	C3-C5-C6-C7
22	A	854	CLA	C3-C5-C6-C7
22	3	615	CLA	CBA-CGA-O2A-C1
22	B	811	CLA	CBA-CGA-O2A-C1
22	L	302	CLA	CBA-CGA-O2A-C1
22	L	304	CLA	CBA-CGA-O2A-C1
22	7	604	CLA	CBA-CGA-O2A-C1
28	J	104	LMG	C29-C28-O8-C9
22	B	811	CLA	O1A-CGA-O2A-C1
22	B	836	CLA	O1A-CGA-O2A-C1
22	B	824	CLA	O1D-CGD-O2D-CED
22	5	610	CLA	O1D-CGD-O2D-CED
28	2	631	LMG	C11-C10-O7-C8
22	1	612	CLA	CBA-CGA-O2A-C1
22	5	612	CLA	CBA-CGA-O2A-C1
21	6	607	CHL	CBD-CGD-O2D-CED
22	V	613	CLA	CBD-CGD-O2D-CED
22	2	612	CLA	CBD-CGD-O2D-CED
22	4	601	CLA	CBD-CGD-O2D-CED
22	L	304	CLA	CBD-CGD-O2D-CED
22	5	602	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	5	608	CLA	CBD-CGD-O2D-CED
22	3	602	CLA	O1D-CGD-O2D-CED
22	3	610	CLA	O1D-CGD-O2D-CED
31	B	849	LMT	O5'-C5'-C6'-O6'
22	A	820	CLA	CBD-CGD-O2D-CED
22	8	602	CLA	CBD-CGD-O2D-CED
22	L	302	CLA	C3-C5-C6-C7
22	3	617	CLA	CBA-CGA-O2A-C1
22	8	604	CLA	CBA-CGA-O2A-C1
22	A	854	CLA	O1D-CGD-O2D-CED
22	8	610	CLA	O1D-CGD-O2D-CED
31	G	206	LMT	O5B-C5B-C6B-O6B
22	3	603	CLA	O1A-CGA-O2A-C1
22	B	826	CLA	O1A-CGA-O2A-C1
22	L	302	CLA	O1A-CGA-O2A-C1
22	A	825	CLA	C4-C3-C5-C6
22	B	819	CLA	C4-C3-C5-C6
31	B	849	LMT	C4'-C5'-C6'-O6'
21	V	601	CHL	C2-C3-C5-C6
22	A	825	CLA	C2-C3-C5-C6
22	B	819	CLA	C2-C3-C5-C6
22	B	806	CLA	C2A-CAA-CBA-CGA
22	G	203	CLA	C2A-CAA-CBA-CGA
22	U	612	CLA	O1A-CGA-O2A-C1
22	3	615	CLA	O1A-CGA-O2A-C1
28	L	307	LMG	O6-C1-O1-C7
22	4	614	CLA	O1D-CGD-O2D-CED
22	B	830	CLA	O1D-CGD-O2D-CED
22	6	603	CLA	O1A-CGA-O2A-C1
22	A	827	CLA	C3-C5-C6-C7
22	B	817	CLA	CBA-CGA-O2A-C1
22	B	840	CLA	CBA-CGA-O2A-C1
22	5	616	CLA	CBD-CGD-O2D-CED
22	A	837	CLA	O1D-CGD-O2D-CED
22	U	603	CLA	O1D-CGD-O2D-CED
22	V	614	CLA	O1D-CGD-O2D-CED
22	B	840	CLA	O1D-CGD-O2D-CED
28	J	104	LMG	O10-C28-O8-C9
31	G	206	LMT	C4B-C5B-C6B-O6B
22	1	611	CLA	O1D-CGD-O2D-CED
22	3	603	CLA	O1D-CGD-O2D-CED
22	4	611	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	B	809	CLA	O1D-CGD-O2D-CED
22	B	814	CLA	O1D-CGD-O2D-CED
22	1	613	CLA	CBD-CGD-O2D-CED
26	9	2630	LHG	C1-C2-C3-O3
22	B	817	CLA	O1A-CGA-O2A-C1
22	B	818	CLA	O1A-CGA-O2A-C1
22	B	840	CLA	O1A-CGA-O2A-C1
22	8	604	CLA	O1A-CGA-O2A-C1
22	7	606	CLA	O1D-CGD-O2D-CED
22	8	611	CLA	O1D-CGD-O2D-CED
21	U	601	CHL	CBA-CGA-O2A-C1
22	V	602	CLA	CBA-CGA-O2A-C1
22	V	604	CLA	CBA-CGA-O2A-C1
22	4	602	CLA	CBA-CGA-O2A-C1
22	A	807	CLA	CBA-CGA-O2A-C1
22	A	812	CLA	CBA-CGA-O2A-C1
22	A	840	CLA	CBA-CGA-O2A-C1
22	B	805	CLA	CBA-CGA-O2A-C1
22	B	818	CLA	CBA-CGA-O2A-C1
22	B	819	CLA	CBA-CGA-O2A-C1
22	B	828	CLA	CBA-CGA-O2A-C1
22	5	613	CLA	CBA-CGA-O2A-C1
22	7	609	CLA	CBA-CGA-O2A-C1
22	8	611	CLA	CBA-CGA-O2A-C1
22	2	611	CLA	CBD-CGD-O2D-CED
22	3	614	CLA	CBD-CGD-O2D-CED
22	B	832	CLA	CBD-CGD-O2D-CED
22	5	612	CLA	O1A-CGA-O2A-C1
22	1	612	CLA	O1A-CGA-O2A-C1
26	1	630	LHG	C30-C31-C32-C33
21	U	609	CHL	C8-C10-C11-C12
21	6	601	CHL	C8-C10-C11-C12
22	1	611	CLA	C8-C10-C11-C12
22	A	830	CLA	C8-C10-C11-C12
22	B	817	CLA	C5-C6-C7-C8
22	B	840	CLA	C15-C16-C17-C18
26	9	2630	LHG	O2-C2-C3-O3
31	K	208	LMT	C2'-C1'-O1'-C1
22	A	840	CLA	O1A-CGA-O2A-C1
22	B	805	CLA	O1A-CGA-O2A-C1
22	7	609	CLA	O1A-CGA-O2A-C1
22	B	809	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
21	U	607	CHL	C14-C13-C15-C16
21	U	609	CHL	C11-C10-C8-C9
21	U	609	CHL	C11-C12-C13-C14
21	6	601	CHL	C11-C12-C13-C14
22	U	603	CLA	C11-C10-C8-C9
22	A	828	CLA	C14-C13-C15-C16
22	A	845	CLA	C11-C10-C8-C9
22	B	831	CLA	C6-C7-C8-C9
22	6	610	CLA	C6-C7-C8-C9
22	B	836	CLA	O1D-CGD-O2D-CED
22	6	611	CLA	O1D-CGD-O2D-CED
22	7	602	CLA	O1D-CGD-O2D-CED
22	A	825	CLA	CBD-CGD-O2D-CED
22	B	807	CLA	C15-C16-C17-C18
22	B	832	CLA	C15-C16-C17-C18
22	L	302	CLA	C5-C6-C7-C8
23	5	617	LUT	C11-C12-C13-C20
23	5	617	LUT	C27-C28-C29-C39
24	7	619	XAT	C7-C8-C9-C19
24	8	620	XAT	C7-C8-C9-C19
27	B	845	BCR	C11-C12-C13-C35
27	B	847	BCR	C37-C22-C23-C24
23	5	617	LUT	C27-C28-C29-C30
24	7	619	XAT	C7-C8-C9-C10
24	8	620	XAT	C7-C8-C9-C10
32	B	850	DGD	C1B-C2B-C3B-C4B
21	U	601	CHL	O1A-CGA-O2A-C1
22	4	602	CLA	O1A-CGA-O2A-C1
22	A	812	CLA	O1A-CGA-O2A-C1
22	B	828	CLA	O1A-CGA-O2A-C1
22	3	603	CLA	C13-C15-C16-C17
22	A	828	CLA	C8-C10-C11-C12
22	B	803	CLA	C10-C11-C12-C13
22	B	811	CLA	C5-C6-C7-C8
22	A	824	CLA	O1D-CGD-O2D-CED
22	6	610	CLA	O1D-CGD-O2D-CED
22	5	613	CLA	CBD-CGD-O2D-CED
22	A	830	CLA	CBA-CGA-O2A-C1
26	7	630	LHG	C24-C23-O8-C6
22	1	610	CLA	C5-C6-C7-C8
22	1	610	CLA	C15-C16-C17-C18
22	4	602	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
22	A	803	CLA	C10-C11-C12-C13
22	A	819	CLA	C8-C10-C11-C12
22	B	804	CLA	C13-C15-C16-C17
22	B	837	CLA	C5-C6-C7-C8
22	B	840	CLA	C8-C10-C11-C12
22	6	613	CLA	C5-C6-C7-C8
29	A	844	PQN	C20-C21-C22-C23
29	A	844	PQN	C23-C25-C26-C27
28	A	860	LMG	C10-C11-C12-C13
31	K	208	LMT	C4'-C5'-C6'-O6'
31	K	208	LMT	O5B-C5B-C6B-O6B
21	U	601	CHL	C13-C15-C16-C17
22	W	613	CLA	C8-C10-C11-C12
22	1	610	CLA	C13-C15-C16-C17
22	A	802	CLA	C15-C16-C17-C18
22	A	820	CLA	C13-C15-C16-C17
22	A	828	CLA	C13-C15-C16-C17
22	A	829	CLA	C8-C10-C11-C12
22	B	808	CLA	C5-C6-C7-C8
22	B	822	CLA	C5-C6-C7-C8
22	B	828	CLA	C10-C11-C12-C13
22	K	203	CLA	C5-C6-C7-C8
22	U	610	CLA	O1D-CGD-O2D-CED
22	1	604	CLA	O1D-CGD-O2D-CED
26	1	630	LHG	C23-C24-C25-C26
26	7	630	LHG	C7-C8-C9-C10
26	9	2630	LHG	C7-C8-C9-C10
22	4	610	CLA	O1D-CGD-O2D-CED
22	A	840	CLA	O1D-CGD-O2D-CED
22	B	808	CLA	O1D-CGD-O2D-CED
22	W	610	CLA	C8-C10-C11-C12
22	4	604	CLA	C5-C6-C7-C8
22	A	804	CLA	C13-C15-C16-C17
22	A	810	CLA	C15-C16-C17-C18
22	B	813	CLA	C13-C15-C16-C17
22	B	828	CLA	C5-C6-C7-C8
22	F	301	CLA	C10-C11-C12-C13
22	9	611	CLA	C15-C16-C17-C18
22	B	822	CLA	O1D-CGD-O2D-CED
22	9	610	CLA	O1D-CGD-O2D-CED
28	2	631	LMG	O9-C10-O7-C8
22	5	608	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
21	W	601	CHL	C8-C10-C11-C12
22	U	610	CLA	C5-C6-C7-C8
22	1	611	CLA	C10-C11-C12-C13
22	A	806	CLA	C15-C16-C17-C18
22	B	816	CLA	C13-C15-C16-C17
22	K	204	CLA	C8-C10-C11-C12
22	V	604	CLA	CBD-CGD-O2D-CED
31	A	857	LMT	O1'-C1-C2-C3
26	1	630	LHG	C11-C12-C13-C14
22	A	845	CLA	C5-C6-C7-C8
21	V	601	CHL	C6-C7-C8-C10
22	1	602	CLA	C6-C7-C8-C10
22	3	617	CLA	C11-C10-C8-C7
22	A	803	CLA	C11-C10-C8-C7
22	A	822	CLA	C11-C12-C13-C15
22	A	825	CLA	C6-C7-C8-C10
22	B	810	CLA	C11-C12-C13-C15
22	B	818	CLA	C11-C10-C8-C7
22	A	815	CLA	C3-C5-C6-C7
22	B	825	CLA	C3-C5-C6-C7
22	V	604	CLA	O1A-CGA-O2A-C1
22	B	819	CLA	O1A-CGA-O2A-C1
22	8	611	CLA	O1A-CGA-O2A-C1
21	6	607	CHL	C2A-CAA-CBA-CGA
21	6	618	CHL	C2A-CAA-CBA-CGA
22	A	807	CLA	C2A-CAA-CBA-CGA
22	A	823	CLA	C2A-CAA-CBA-CGA
22	A	825	CLA	C2A-CAA-CBA-CGA
22	B	824	CLA	C2A-CAA-CBA-CGA
22	G	204	CLA	C2A-CAA-CBA-CGA
22	9	611	CLA	C2A-CAA-CBA-CGA
21	3	608	CHL	O1D-CGD-O2D-CED
22	1	608	CLA	O1D-CGD-O2D-CED
22	A	810	CLA	O1D-CGD-O2D-CED
22	B	820	CLA	O1D-CGD-O2D-CED
22	B	829	CLA	O1D-CGD-O2D-CED
22	K	206	CLA	O1D-CGD-O2D-CED
22	O	2002	CLA	O1D-CGD-O2D-CED
21	6	601	CHL	C13-C15-C16-C17
22	A	807	CLA	O1A-CGA-O2A-C1
22	A	839	CLA	CBD-CGD-O2D-CED
22	A	836	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
23	2	619	LUT	C10-C11-C12-C13
23	5	617	LUT	C10-C11-C12-C13
23	5	617	LUT	C30-C31-C32-C33
24	8	620	XAT	C10-C11-C12-C13
31	K	208	LMT	O5'-C5'-C6'-O6'
22	1	610	CLA	C8-C10-C11-C12
22	A	803	CLA	C8-C10-C11-C12
22	A	805	CLA	C5-C6-C7-C8
22	B	806	CLA	C8-C10-C11-C12
22	B	828	CLA	C13-C15-C16-C17
22	9	602	CLA	C8-C10-C11-C12
22	A	801	CLA	CBA-CGA-O2A-C1
22	7	611	CLA	O1D-CGD-O2D-CED
22	V	602	CLA	O1A-CGA-O2A-C1
22	A	830	CLA	O1A-CGA-O2A-C1
22	5	613	CLA	O1A-CGA-O2A-C1
22	G	204	CLA	CBA-CGA-O2A-C1
22	7	606	CLA	CBA-CGA-O2A-C1
21	U	607	CHL	C8-C10-C11-C12
21	U	609	CHL	C13-C15-C16-C17
22	V	603	CLA	C5-C6-C7-C8
22	2	610	CLA	C10-C11-C12-C13
22	A	815	CLA	C10-C11-C12-C13
22	B	824	CLA	C5-C6-C7-C8
22	A	815	CLA	O1D-CGD-O2D-CED
22	A	836	CLA	CBD-CGD-O2D-CED
22	L	302	CLA	CBD-CGD-O2D-CED
22	3	609	CLA	C15-C16-C17-C18
22	A	804	CLA	C15-C16-C17-C18
22	A	806	CLA	C10-C11-C12-C13
22	A	841	CLA	C13-C15-C16-C17
22	B	810	CLA	C8-C10-C11-C12
22	B	837	CLA	C15-C16-C17-C18
26	U	2630	LHG	C4-O6-P-O3
26	V	2630	LHG	C4-O6-P-O3
26	W	2630	LHG	C4-O6-P-O3
26	2	630	LHG	C4-O6-P-O3
26	3	630	LHG	C4-O6-P-O3
26	B	851	LHG	C4-O6-P-O3
26	7	630	LHG	C3-O3-P-O6
26	7	630	LHG	C4-O6-P-O3
26	9	2630	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
22	4	610	CLA	CBA-CGA-O2A-C1
22	A	842	CLA	CBA-CGA-O2A-C1
22	U	603	CLA	C8-C10-C11-C12
22	4	603	CLA	C15-C16-C17-C18
22	A	814	CLA	C15-C16-C17-C18
22	A	835	CLA	C15-C16-C17-C18
22	B	833	CLA	O1D-CGD-O2D-CED
22	9	613	CLA	O1D-CGD-O2D-CED
21	U	601	CHL	C8-C10-C11-C12
21	W	601	CHL	C2A-CAA-CBA-CGA
21	2	602	CHL	C2A-CAA-CBA-CGA
21	3	608	CHL	C2A-CAA-CBA-CGA
22	3	612	CLA	C2A-CAA-CBA-CGA
22	3	615	CLA	C2A-CAA-CBA-CGA
22	A	809	CLA	C2A-CAA-CBA-CGA
22	B	827	CLA	C2A-CAA-CBA-CGA
22	5	608	CLA	C2A-CAA-CBA-CGA
22	L	304	CLA	C11-C12-C13-C15
22	4	610	CLA	C3-C5-C6-C7
22	U	610	CLA	CBA-CGA-O2A-C1
22	A	813	CLA	CBA-CGA-O2A-C1
22	A	841	CLA	CBA-CGA-O2A-C1
26	1	630	LHG	C24-C23-O8-C6
22	V	613	CLA	CAA-CBA-CGA-O2A
22	2	603	CLA	O1D-CGD-O2D-CED
22	A	828	CLA	C5-C6-C7-C8
23	2	619	LUT	C20-C13-C14-C15
23	5	617	LUT	C20-C13-C14-C15
23	5	617	LUT	C39-C29-C30-C31
24	8	620	XAT	C11-C10-C9-C19
24	8	620	XAT	C40-C33-C34-C35
26	U	2630	LHG	C14-C15-C16-C17
22	A	801	CLA	O1A-CGA-O2A-C1
22	A	801	CLA	O1D-CGD-O2D-CED
22	W	613	CLA	C11-C12-C13-C14
22	6	613	CLA	C16-C17-C18-C20
22	A	817	CLA	CBA-CGA-O2A-C1
22	A	831	CLA	CBA-CGA-O2A-C1
22	A	832	CLA	CBA-CGA-O2A-C1
26	A	846	LHG	C13-C14-C15-C16
31	G	206	LMT	C5-C6-C7-C8
22	V	610	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	U	607	CHL	CBD-CGD-O2D-CED
22	3	613	CLA	CBD-CGD-O2D-CED
22	A	813	CLA	CBD-CGD-O2D-CED
22	A	822	CLA	CBD-CGD-O2D-CED
28	L	307	LMG	C16-C17-C18-C19
22	W	610	CLA	O1D-CGD-O2D-CED
22	B	823	CLA	O1D-CGD-O2D-CED
22	F	303	CLA	O1D-CGD-O2D-CED
22	A	842	CLA	O1A-CGA-O2A-C1
26	7	630	LHG	O10-C23-O8-C6
26	1	630	LHG	C33-C34-C35-C36
28	2	631	LMG	C29-C30-C31-C32
22	B	813	CLA	C5-C6-C7-C8
26	1	630	LHG	C32-C33-C34-C35
28	2	631	LMG	C23-C24-C25-C26
32	B	850	DGD	C7A-C8A-C9A-CAA
22	3	606	CLA	O1D-CGD-O2D-CED
23	2	619	LUT	C12-C13-C14-C15
23	5	617	LUT	C12-C13-C14-C15
23	5	617	LUT	C28-C29-C30-C31
24	8	620	XAT	C11-C10-C9-C8
24	8	620	XAT	C32-C33-C34-C35
22	B	838	CLA	CBA-CGA-O2A-C1
26	4	630	LHG	C9-C10-C11-C12
21	U	609	CHL	C16-C17-C18-C20
22	1	603	CLA	C6-C7-C8-C10
22	A	818	CLA	C16-C17-C18-C20
22	A	823	CLA	C6-C7-C8-C9
22	A	825	CLA	C16-C17-C18-C20
22	A	837	CLA	C16-C17-C18-C19
22	B	820	CLA	C6-C7-C8-C10
22	8	603	CLA	C6-C7-C8-C10
22	8	609	CLA	C6-C7-C8-C10
22	A	838	CLA	O1D-CGD-O2D-CED
22	V	613	CLA	C4-C3-C5-C6
22	2	613	CLA	C4-C3-C5-C6
22	6	613	CLA	C4-C3-C5-C6
22	8	609	CLA	C4-C3-C5-C6
21	U	607	CHL	C11-C10-C8-C9
22	V	613	CLA	C11-C10-C8-C9
22	1	611	CLA	C11-C12-C13-C14
22	A	804	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	A	805	CLA	C6-C7-C8-C9
22	A	824	CLA	C6-C7-C8-C9
22	A	827	CLA	C14-C13-C15-C16
22	A	828	CLA	C11-C12-C13-C14
22	B	803	CLA	C11-C12-C13-C14
22	B	810	CLA	C14-C13-C15-C16
22	B	818	CLA	C6-C7-C8-C9
22	B	833	CLA	C14-C13-C15-C16
22	6	613	CLA	C11-C10-C8-C9
22	7	602	CLA	C6-C7-C8-C9
22	2	613	CLA	O1D-CGD-O2D-CED
22	A	802	CLA	O1D-CGD-O2D-CED
22	A	824	CLA	C13-C15-C16-C17
26	A	846	LHG	C23-C24-C25-C26
26	A	847	LHG	C11-C10-C9-C8
28	A	860	LMG	C29-C30-C31-C32
32	B	850	DGD	C8B-C9B-CAB-CBB
21	V	601	CHL	C13-C15-C16-C17
22	A	815	CLA	C15-C16-C17-C18
22	F	304	CLA	CBA-CGA-O2A-C1
22	1	616	CLA	C2A-CAA-CBA-CGA
22	2	609	CLA	C2A-CAA-CBA-CGA
22	A	808	CLA	C2A-CAA-CBA-CGA
27	2	621	BCR	C21-C22-C23-C24
27	L	306	BCR	C7-C8-C9-C10
22	B	833	CLA	C3-C5-C6-C7
22	6	613	CLA	C3-C5-C6-C7
29	B	842	PQN	C15-C16-C17-C18
28	L	307	LMG	C12-C13-C14-C15
26	4	630	LHG	C7-C8-C9-C10
26	2	630	LHG	C11-C10-C9-C8
26	3	630	LHG	C11-C10-C9-C8
32	B	850	DGD	CAA-CBA-CCA-CDA
22	W	613	CLA	C11-C12-C13-C15
22	2	610	CLA	C11-C12-C13-C15
22	A	804	CLA	C16-C17-C18-C20
22	L	304	CLA	C11-C12-C13-C14
22	6	613	CLA	C16-C17-C18-C19
21	6	601	CHL	C5-C6-C7-C8
22	B	826	CLA	C13-C15-C16-C17
22	L	303	CLA	C8-C10-C11-C12
22	9	611	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
22	6	612	CLA	CBD-CGD-O2D-CED
21	W	607	CHL	O1D-CGD-O2D-CED
21	6	602	CHL	O1D-CGD-O2D-CED
22	4	613	CLA	O1D-CGD-O2D-CED
22	8	613	CLA	O1D-CGD-O2D-CED
21	V	601	CHL	C15-C16-C17-C18
22	2	610	CLA	C5-C6-C7-C8
22	U	610	CLA	O1A-CGA-O2A-C1
28	2	631	LMG	C19-C20-C21-C22
22	A	822	CLA	CBA-CGA-O2A-C1
22	B	825	CLA	CBA-CGA-O2A-C1
22	K	203	CLA	CBA-CGA-O2A-C1
26	U	2630	LHG	C15-C16-C17-C18
22	7	612	CLA	O1D-CGD-O2D-CED
22	9	603	CLA	O1D-CGD-O2D-CED
21	U	606	CHL	C3A-C2A-CAA-CBA
21	6	606	CHL	C3A-C2A-CAA-CBA
21	6	618	CHL	C3A-C2A-CAA-CBA
22	V	603	CLA	C3A-C2A-CAA-CBA
22	3	610	CLA	C3A-C2A-CAA-CBA
22	3	612	CLA	C3A-C2A-CAA-CBA
22	A	804	CLA	C3A-C2A-CAA-CBA
22	A	810	CLA	C3A-C2A-CAA-CBA
22	A	813	CLA	C3A-C2A-CAA-CBA
22	A	831	CLA	C3A-C2A-CAA-CBA
22	B	809	CLA	C3A-C2A-CAA-CBA
22	B	810	CLA	C3A-C2A-CAA-CBA
22	B	821	CLA	C3A-C2A-CAA-CBA
22	B	822	CLA	C3A-C2A-CAA-CBA
22	B	828	CLA	C3A-C2A-CAA-CBA
22	B	830	CLA	C3A-C2A-CAA-CBA
22	B	831	CLA	C3A-C2A-CAA-CBA
22	B	833	CLA	C3A-C2A-CAA-CBA
22	B	837	CLA	C3A-C2A-CAA-CBA
22	G	203	CLA	C3A-C2A-CAA-CBA
22	K	203	CLA	C3A-C2A-CAA-CBA
22	K	204	CLA	C3A-C2A-CAA-CBA
22	5	603	CLA	C3A-C2A-CAA-CBA
22	5	610	CLA	C3A-C2A-CAA-CBA
22	5	612	CLA	C3A-C2A-CAA-CBA
22	5	616	CLA	C3A-C2A-CAA-CBA
22	7	606	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	8	603	CLA	C3A-C2A-CAA-CBA
22	9	610	CLA	C3A-C2A-CAA-CBA
21	3	608	CHL	C5-C6-C7-C8
22	4	603	CLA	C5-C6-C7-C8
28	L	307	LMG	C11-C12-C13-C14
22	1	616	CLA	O1D-CGD-O2D-CED
22	4	610	CLA	O1A-CGA-O2A-C1
26	1	630	LHG	O10-C23-O8-C6
21	V	601	CHL	C16-C17-C18-C19
22	A	825	CLA	C16-C17-C18-C19
22	A	845	CLA	C16-C17-C18-C20
22	L	302	CLA	C16-C17-C18-C20
22	8	603	CLA	C6-C7-C8-C9
26	1	630	LHG	C28-C29-C30-C31
22	J	101	CLA	O1D-CGD-O2D-CED
22	A	841	CLA	CBD-CGD-O2D-CED
26	W	2630	LHG	C9-C10-C11-C12
26	1	630	LHG	C14-C15-C16-C17
31	K	208	LMT	C2-C3-C4-C5
22	9	611	CLA	O1D-CGD-O2D-CED
22	U	613	CLA	C3-C5-C6-C7
22	B	805	CLA	C3-C5-C6-C7
26	4	630	LHG	C26-C27-C28-C29
22	3	617	CLA	C4-C3-C5-C6
22	A	807	CLA	C4-C3-C5-C6
22	A	854	CLA	C4-C3-C5-C6
22	B	804	CLA	C4-C3-C5-C6
22	B	820	CLA	C4-C3-C5-C6
22	L	302	CLA	C4-C3-C5-C6
31	A	857	LMT	O5B-C1B-O1B-C4'
22	A	824	CLA	CBA-CGA-O2A-C1
22	9	602	CLA	CBA-CGA-O2A-C1
22	U	613	CLA	C2-C3-C5-C6
22	V	613	CLA	C2-C3-C5-C6
22	3	617	CLA	C2-C3-C5-C6
22	A	826	CLA	C2-C3-C5-C6
22	A	854	CLA	C2-C3-C5-C6
22	B	820	CLA	C2-C3-C5-C6
22	B	836	CLA	C2-C3-C5-C6
22	6	613	CLA	C2-C3-C5-C6
28	G	202	LMG	C11-C10-O7-C8
22	K	203	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
26	1	630	LHG	O1-C1-C2-O2
22	1	609	CLA	C15-C16-C17-C18
26	4	630	LHG	C13-C14-C15-C16
22	5	602	CLA	O1D-CGD-O2D-CED
22	A	838	CLA	C6-C7-C8-C10
26	2	630	LHG	O2-C2-C3-O3
22	3	611	CLA	C5-C6-C7-C8
22	A	815	CLA	C5-C6-C7-C8
22	A	813	CLA	O1A-CGA-O2A-C1
22	A	831	CLA	O1A-CGA-O2A-C1
22	A	832	CLA	O1A-CGA-O2A-C1
22	A	841	CLA	O1A-CGA-O2A-C1
26	3	630	LHG	C23-C24-C25-C26
22	4	602	CLA	C10-C11-C12-C13
28	G	202	LMG	O9-C10-O7-C8
22	3	604	CLA	C2-C1-O2A-CGA
22	3	612	CLA	C2-C1-O2A-CGA
22	A	817	CLA	C2-C1-O2A-CGA
22	B	810	CLA	C2-C1-O2A-CGA
22	B	814	CLA	C2-C1-O2A-CGA
22	4	603	CLA	C10-C11-C12-C13
22	A	823	CLA	C5-C6-C7-C8
22	A	817	CLA	O1A-CGA-O2A-C1
22	A	837	CLA	C16-C17-C18-C20
22	A	829	CLA	C3-C5-C6-C7
22	B	807	CLA	C3-C5-C6-C7
23	U	2621	LUT	C5-C6-C7-C8
23	V	2620	LUT	C5-C6-C7-C8
23	V	2621	LUT	C5-C6-C7-C8
23	W	2620	LUT	C5-C6-C7-C8
23	W	2621	LUT	C1-C6-C7-C8
23	W	2621	LUT	C5-C6-C7-C8
23	6	619	LUT	C5-C6-C7-C8
23	7	618	LUT	C5-C6-C7-C8
23	8	619	LUT	C5-C6-C7-C8
23	9	620	LUT	C5-C6-C7-C8
23	9	621	LUT	C5-C6-C7-C8
23	9	624	LUT	C1-C6-C7-C8
23	9	624	LUT	C5-C6-C7-C8
27	1	619	BCR	C1-C6-C7-C8
27	1	619	BCR	C23-C24-C25-C26
27	2	621	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
27	4	621	BCR	C5-C6-C7-C8
27	4	621	BCR	C23-C24-C25-C26
27	A	848	BCR	C1-C6-C7-C8
27	A	848	BCR	C5-C6-C7-C8
27	A	848	BCR	C23-C24-C25-C30
27	A	849	BCR	C1-C6-C7-C8
27	A	849	BCR	C5-C6-C7-C8
27	A	849	BCR	C23-C24-C25-C30
27	A	850	BCR	C5-C6-C7-C8
27	A	850	BCR	C23-C24-C25-C30
27	A	851	BCR	C5-C6-C7-C8
27	A	852	BCR	C1-C6-C7-C8
27	B	801	BCR	C1-C6-C7-C8
27	B	801	BCR	C5-C6-C7-C8
27	B	801	BCR	C23-C24-C25-C30
27	B	843	BCR	C1-C6-C7-C8
27	B	843	BCR	C5-C6-C7-C8
27	B	845	BCR	C1-C6-C7-C8
27	B	845	BCR	C5-C6-C7-C8
27	B	845	BCR	C23-C24-C25-C26
27	B	1609	BCR	C5-C6-C7-C8
27	F	305	BCR	C23-C24-C25-C26
27	G	205	BCR	C1-C6-C7-C8
27	I	101	BCR	C23-C24-C25-C26
27	I	101	BCR	C23-C24-C25-C30
27	J	102	BCR	C23-C24-C25-C26
27	J	102	BCR	C23-C24-C25-C30
27	K	202	BCR	C5-C6-C7-C8
27	K	202	BCR	C23-C24-C25-C30
27	K	205	BCR	C23-C24-C25-C26
27	L	301	BCR	C5-C6-C7-C8
27	L	301	BCR	C23-C24-C25-C26
27	L	301	BCR	C23-C24-C25-C30
27	M	2001	BCR	C23-C24-C25-C30
27	O	2004	BCR	C1-C6-C7-C8
27	O	2004	BCR	C5-C6-C7-C8
27	O	2004	BCR	C23-C24-C25-C26
27	O	2004	BCR	C23-C24-C25-C30
27	6	621	BCR	C5-C6-C7-C8
27	6	621	BCR	C23-C24-C25-C26
27	7	621	BCR	C23-C24-C25-C26
21	9	606	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
22	A	820	CLA	CBA-CGA-O2A-C1
21	V	601	CHL	C8-C10-C11-C12
22	B	819	CLA	C8-C10-C11-C12
22	K	204	CLA	C5-C6-C7-C8
22	U	613	CLA	O1D-CGD-O2D-CED
22	A	822	CLA	O1A-CGA-O2A-C1
22	B	838	CLA	O1A-CGA-O2A-C1
26	9	2630	LHG	C9-C10-C11-C12
31	A	857	LMT	C4-C5-C6-C7
21	2	602	CHL	C4-C3-C5-C6
22	A	826	CLA	C4-C3-C5-C6
22	A	843	CLA	C4-C3-C5-C6
22	L	304	CLA	C4-C3-C5-C6
21	U	607	CHL	C11-C10-C8-C7
21	U	607	CHL	C12-C13-C15-C16
21	W	601	CHL	C6-C7-C8-C10
21	6	601	CHL	C11-C12-C13-C15
22	V	613	CLA	C11-C10-C8-C7
22	W	602	CLA	C11-C10-C8-C7
22	2	613	CLA	C2-C3-C5-C6
22	A	804	CLA	C6-C7-C8-C10
22	A	805	CLA	C6-C7-C8-C10
22	A	805	CLA	C12-C13-C15-C16
22	A	807	CLA	C2-C3-C5-C6
22	A	810	CLA	C11-C10-C8-C7
22	A	812	CLA	C12-C13-C15-C16
22	A	827	CLA	C11-C10-C8-C7
22	A	827	CLA	C12-C13-C15-C16
22	A	828	CLA	C12-C13-C15-C16
22	A	835	CLA	C2-C3-C5-C6
22	A	843	CLA	C2-C3-C5-C6
22	A	854	CLA	C6-C7-C8-C10
22	B	803	CLA	C11-C12-C13-C15
22	B	810	CLA	C6-C7-C8-C10
22	B	810	CLA	C12-C13-C15-C16
22	B	814	CLA	C2-C3-C5-C6
22	B	818	CLA	C6-C7-C8-C10
22	B	833	CLA	C12-C13-C15-C16
22	B	841	CLA	C12-C13-C15-C16
22	L	302	CLA	C2-C3-C5-C6
22	L	302	CLA	C6-C7-C8-C10
22	L	304	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	6	610	CLA	C11-C10-C8-C7
22	6	613	CLA	C11-C10-C8-C7
22	7	602	CLA	C6-C7-C8-C10
22	8	609	CLA	C2-C3-C5-C6
22	9	602	CLA	C6-C7-C8-C10
29	A	844	PQN	C21-C22-C23-C25
22	3	615	CLA	C3-C5-C6-C7
22	A	824	CLA	O1A-CGA-O2A-C1
22	B	825	CLA	O1A-CGA-O2A-C1
22	K	203	CLA	O1A-CGA-O2A-C1
22	9	602	CLA	O1A-CGA-O2A-C1
21	6	601	CHL	C15-C16-C17-C18
22	B	814	CLA	C8-C10-C11-C12
22	B	817	CLA	C13-C15-C16-C17
22	1	603	CLA	C6-C7-C8-C9
22	A	823	CLA	C6-C7-C8-C10
22	B	826	CLA	C16-C17-C18-C19
22	5	608	CLA	O1D-CGD-O2D-CED
22	A	825	CLA	CBA-CGA-O2A-C1
22	U	604	CLA	C2A-CAA-CBA-CGA
22	3	617	CLA	C2A-CAA-CBA-CGA
22	A	806	CLA	C2A-CAA-CBA-CGA
22	A	824	CLA	C2A-CAA-CBA-CGA
22	F	301	CLA	C2A-CAA-CBA-CGA
22	B	818	CLA	C5-C6-C7-C8
31	A	857	LMT	C2B-C1B-O1B-C4'
31	A	857	LMT	C6-C7-C8-C9
22	4	601	CLA	O1D-CGD-O2D-CED
22	2	612	CLA	O1D-CGD-O2D-CED
32	B	850	DGD	O6D-C5D-C6D-O5D
22	L	304	CLA	O1D-CGD-O2D-CED
22	A	814	CLA	CBA-CGA-O2A-C1
22	A	834	CLA	CBA-CGA-O2A-C1
22	U	610	CLA	C16-C17-C18-C19
22	A	833	CLA	C6-C7-C8-C9
22	B	820	CLA	C6-C7-C8-C9
22	5	602	CLA	C11-C12-C13-C15
31	K	208	LMT	C4B-C5B-C6B-O6B
21	U	607	CHL	C13-C15-C16-C17
22	W	610	CLA	C13-C15-C16-C17
22	A	801	CLA	C5-C6-C7-C8
22	A	834	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
31	G	206	LMT	C1-C2-C3-C4
22	V	613	CLA	O1D-CGD-O2D-CED
26	A	846	LHG	C8-C7-O7-C5
26	A	847	LHG	C8-C7-O7-C5
26	9	2630	LHG	C8-C7-O7-C5
22	A	814	CLA	CBD-CGD-O2D-CED
31	G	206	LMT	C2-C3-C4-C5
31	G	206	LMT	C2'-C1'-O1'-C1
21	U	601	CHL	C5-C6-C7-C8
26	1	630	LHG	C27-C28-C29-C30
28	L	307	LMG	C32-C33-C34-C35
22	A	804	CLA	CBD-CGD-O2D-CED
22	A	820	CLA	O1A-CGA-O2A-C1
21	U	609	CHL	C16-C17-C18-C19
22	A	818	CLA	C16-C17-C18-C19
22	8	609	CLA	C6-C7-C8-C9
22	3	603	CLA	C15-C16-C17-C18
22	B	814	CLA	C15-C16-C17-C18
21	6	607	CHL	O1D-CGD-O2D-CED
22	U	613	CLA	C4-C3-C5-C6
22	A	835	CLA	C4-C3-C5-C6
22	B	814	CLA	C4-C3-C5-C6
22	B	822	CLA	C4-C3-C5-C6
22	B	836	CLA	C4-C3-C5-C6
21	4	607	CHL	CBA-CGA-O2A-C1
21	6	607	CHL	CBA-CGA-O2A-C1
21	2	602	CHL	C2-C3-C5-C6
22	B	804	CLA	C2-C3-C5-C6
22	B	809	CLA	C2-C3-C5-C6
22	B	822	CLA	C2-C3-C5-C6
21	V	601	CHL	C6-C7-C8-C9
22	W	602	CLA	C11-C10-C8-C9
22	1	602	CLA	C6-C7-C8-C9
22	1	609	CLA	C6-C7-C8-C9
22	1	611	CLA	C11-C10-C8-C9
22	3	613	CLA	C11-C12-C13-C14
22	3	617	CLA	C11-C10-C8-C9
22	A	803	CLA	C11-C10-C8-C9
22	A	805	CLA	C14-C13-C15-C16
22	A	810	CLA	C11-C10-C8-C9
22	A	810	CLA	C11-C12-C13-C14
22	A	812	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	A	817	CLA	C14-C13-C15-C16
22	A	825	CLA	C6-C7-C8-C9
22	A	827	CLA	C6-C7-C8-C9
22	A	827	CLA	C11-C10-C8-C9
22	A	836	CLA	C11-C10-C8-C9
22	A	839	CLA	C6-C7-C8-C9
22	B	810	CLA	C6-C7-C8-C9
22	B	810	CLA	C11-C12-C13-C14
22	B	832	CLA	C14-C13-C15-C16
22	L	302	CLA	C6-C7-C8-C9
22	6	610	CLA	C11-C10-C8-C9
29	B	842	PQN	C16-C17-C18-C19
22	B	816	CLA	C3-C5-C6-C7
21	1	607	CHL	C2A-CAA-CBA-CGA
21	8	607	CHL	C2A-CAA-CBA-CGA
22	3	611	CLA	C2A-CAA-CBA-CGA
22	B	808	CLA	C2A-CAA-CBA-CGA
22	B	831	CLA	C2A-CAA-CBA-CGA
22	6	612	CLA	C2A-CAA-CBA-CGA
22	A	820	CLA	O1D-CGD-O2D-CED
22	5	616	CLA	O1D-CGD-O2D-CED
29	B	842	PQN	C20-C21-C22-C23
21	6	618	CHL	CBA-CGA-O2A-C1
21	U	606	CHL	C1A-C2A-CAA-CBA
21	6	606	CHL	C1A-C2A-CAA-CBA
21	6	618	CHL	C1A-C2A-CAA-CBA
22	U	610	CLA	C1A-C2A-CAA-CBA
22	V	602	CLA	C1A-C2A-CAA-CBA
22	V	603	CLA	C1A-C2A-CAA-CBA
22	V	604	CLA	C1A-C2A-CAA-CBA
22	1	613	CLA	C1A-C2A-CAA-CBA
22	2	611	CLA	C1A-C2A-CAA-CBA
22	2	614	CLA	C1A-C2A-CAA-CBA
22	3	604	CLA	C1A-C2A-CAA-CBA
22	3	612	CLA	C1A-C2A-CAA-CBA
22	4	602	CLA	C1A-C2A-CAA-CBA
22	4	610	CLA	C1A-C2A-CAA-CBA
22	A	804	CLA	C1A-C2A-CAA-CBA
22	A	810	CLA	C1A-C2A-CAA-CBA
22	A	812	CLA	C1A-C2A-CAA-CBA
22	A	820	CLA	C1A-C2A-CAA-CBA
22	B	805	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	B	810	CLA	C1A-C2A-CAA-CBA
22	B	813	CLA	C1A-C2A-CAA-CBA
22	B	814	CLA	C1A-C2A-CAA-CBA
22	B	818	CLA	C1A-C2A-CAA-CBA
22	B	821	CLA	C1A-C2A-CAA-CBA
22	B	822	CLA	C1A-C2A-CAA-CBA
22	B	830	CLA	C1A-C2A-CAA-CBA
22	B	834	CLA	C1A-C2A-CAA-CBA
22	B	839	CLA	C1A-C2A-CAA-CBA
22	G	203	CLA	C1A-C2A-CAA-CBA
22	K	203	CLA	C1A-C2A-CAA-CBA
22	K	204	CLA	C1A-C2A-CAA-CBA
22	L	303	CLA	C1A-C2A-CAA-CBA
22	O	2002	CLA	C1A-C2A-CAA-CBA
22	5	603	CLA	C1A-C2A-CAA-CBA
22	5	612	CLA	C1A-C2A-CAA-CBA
22	5	616	CLA	C1A-C2A-CAA-CBA
22	8	603	CLA	C1A-C2A-CAA-CBA
22	A	833	CLA	C6-C7-C8-C10
22	A	838	CLA	C6-C7-C8-C9
22	5	602	CLA	C11-C12-C13-C14
22	8	610	CLA	C6-C7-C8-C10
26	A	846	LHG	O9-C7-O7-C5
26	A	847	LHG	O9-C7-O7-C5
26	9	2630	LHG	O9-C7-O7-C5
26	1	630	LHG	C8-C7-O7-C5
22	1	613	CLA	O1D-CGD-O2D-CED
22	8	602	CLA	O1D-CGD-O2D-CED
22	B	837	CLA	C10-C11-C12-C13
22	F	301	CLA	C15-C16-C17-C18
26	V	2630	LHG	C3-O3-P-O6
22	3	614	CLA	O1D-CGD-O2D-CED
21	2	602	CHL	C8-C10-C11-C12
22	2	611	CLA	O1D-CGD-O2D-CED
32	B	850	DGD	C4D-C5D-C6D-O5D
32	B	850	DGD	CCA-CDA-CEA-CFA
22	K	204	CLA	C10-C11-C12-C13
22	U	604	CLA	C3-C5-C6-C7
22	2	610	CLA	C11-C12-C13-C14
22	B	832	CLA	C3-C5-C6-C7
22	A	829	CLA	C10-C11-C12-C13
26	4	630	LHG	C24-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
22	V	611	CLA	C3A-C2A-CAA-CBA
22	B	834	CLA	C15-C16-C17-C18
22	7	606	CLA	O1A-CGA-O2A-C1
32	B	850	DGD	C6B-C7B-C8B-C9B
26	8	630	LHG	C8-C7-O7-C5
22	A	825	CLA	O1A-CGA-O2A-C1
21	6	601	CHL	C2A-CAA-CBA-CGA
22	2	604	CLA	C2A-CAA-CBA-CGA
22	B	814	CLA	C2A-CAA-CBA-CGA
21	V	601	CHL	C16-C17-C18-C20
22	B	813	CLA	C16-C17-C18-C19
21	W	601	CHL	C3-C5-C6-C7
26	1	630	LHG	C4-C5-C6-O8
26	4	630	LHG	C4-C5-C6-O8
26	A	847	LHG	C4-C5-C6-O8
26	B	851	LHG	C4-C5-C6-O8
28	G	202	LMG	O1-C7-C8-C9
28	J	104	LMG	O1-C7-C8-C9
22	B	832	CLA	O1D-CGD-O2D-CED
22	A	807	CLA	C15-C16-C17-C18
22	B	832	CLA	C13-C15-C16-C17
28	L	307	LMG	C8-C7-O1-C1
26	A	846	LHG	C16-C17-C18-C19
22	7	609	CLA	CBD-CGD-O2D-CED
21	U	601	CHL	C15-C16-C17-C18
21	U	607	CHL	C5-C6-C7-C8
22	A	804	CLA	C8-C10-C11-C12
22	B	825	CLA	C10-C11-C12-C13
26	3	630	LHG	C9-C10-C11-C12
26	9	2630	LHG	C23-C24-C25-C26
22	A	814	CLA	O1A-CGA-O2A-C1
22	A	817	CLA	C3-C5-C6-C7
22	B	834	CLA	C13-C15-C16-C17
22	B	809	CLA	C13-C15-C16-C17
22	5	613	CLA	O1D-CGD-O2D-CED
28	2	631	LMG	O6-C5-C6-O5
22	A	837	CLA	C4-C3-C5-C6
22	B	827	CLA	C4-C3-C5-C6
22	A	828	CLA	C2-C3-C5-C6
21	1	601	CHL	C6-C7-C8-C9
22	B	826	CLA	C16-C17-C18-C20
22	W	610	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	A	808	CLA	CBA-CGA-O2A-C1
22	A	826	CLA	CBA-CGA-O2A-C1
22	9	610	CLA	CBA-CGA-O2A-C1
22	7	613	CLA	CBD-CGD-O2D-CED
22	B	834	CLA	C8-C10-C11-C12
22	G	204	CLA	O1A-CGA-O2A-C1
21	8	608	CHL	C2A-CAA-CBA-CGA
22	4	603	CLA	C2A-CAA-CBA-CGA
22	4	612	CLA	C2A-CAA-CBA-CGA
22	2	604	CLA	C2-C1-O2A-CGA
22	A	803	CLA	C2-C1-O2A-CGA
22	5	602	CLA	C2-C1-O2A-CGA
22	A	826	CLA	C3-C5-C6-C7
26	1	630	LHG	C24-C25-C26-C27
22	A	825	CLA	O1D-CGD-O2D-CED
21	U	609	CHL	CBA-CGA-O2A-C1
22	3	610	CLA	CBA-CGA-O2A-C1
22	A	834	CLA	O1A-CGA-O2A-C1
22	9	610	CLA	O1A-CGA-O2A-C1
26	2	630	LHG	O6-C4-C5-O7
22	8	610	CLA	C6-C7-C8-C9
26	4	630	LHG	C11-C12-C13-C14
22	B	839	CLA	C5-C6-C7-C8
22	B	840	CLA	C10-C11-C12-C13
22	A	808	CLA	O1A-CGA-O2A-C1
26	4	630	LHG	O10-C23-O8-C6
22	A	818	CLA	C13-C15-C16-C17
21	2	602	CHL	CAA-CBA-CGA-O2A
28	L	307	LMG	O7-C8-C9-O8
22	B	828	CLA	C15-C16-C17-C18
22	A	823	CLA	C4-C3-C5-C6
22	A	828	CLA	C4-C3-C5-C6
22	A	830	CLA	C4-C3-C5-C6
22	A	836	CLA	C8-C10-C11-C12
21	U	601	CHL	C11-C12-C13-C15
21	U	609	CHL	C6-C7-C8-C10
21	U	609	CHL	C11-C12-C13-C15
21	U	609	CHL	C12-C13-C15-C16
21	W	601	CHL	C12-C13-C15-C16
22	1	609	CLA	C6-C7-C8-C10
22	1	611	CLA	C11-C10-C8-C7
22	3	609	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	3	613	CLA	C11-C12-C13-C15
22	A	801	CLA	C11-C10-C8-C7
22	A	802	CLA	C12-C13-C15-C16
22	A	810	CLA	C11-C12-C13-C15
22	A	814	CLA	C11-C12-C13-C15
22	A	817	CLA	C12-C13-C15-C16
22	A	827	CLA	C6-C7-C8-C10
22	A	836	CLA	C11-C10-C8-C7
22	A	837	CLA	C2-C3-C5-C6
22	A	839	CLA	C6-C7-C8-C10
22	A	843	CLA	C12-C13-C15-C16
22	B	808	CLA	C11-C10-C8-C7
22	B	811	CLA	C11-C12-C13-C15
22	B	816	CLA	C6-C7-C8-C10
22	B	817	CLA	C11-C12-C13-C15
22	B	818	CLA	C12-C13-C15-C16
22	B	827	CLA	C2-C3-C5-C6
22	B	831	CLA	C6-C7-C8-C10
22	B	832	CLA	C12-C13-C15-C16
22	B	840	CLA	C11-C12-C13-C15
22	B	841	CLA	C11-C10-C8-C7
22	6	610	CLA	C6-C7-C8-C10
29	B	842	PQN	C16-C17-C18-C20
21	U	601	CHL	C11-C10-C8-C9
21	U	601	CHL	C11-C12-C13-C14
21	U	609	CHL	C6-C7-C8-C9
21	U	609	CHL	C14-C13-C15-C16
21	W	601	CHL	C14-C13-C15-C16
22	3	609	CLA	C14-C13-C15-C16
22	A	801	CLA	C11-C10-C8-C9
22	A	805	CLA	C11-C10-C8-C9
22	A	806	CLA	C14-C13-C15-C16
22	A	814	CLA	C11-C12-C13-C14
22	A	825	CLA	C11-C12-C13-C14
22	A	826	CLA	C11-C10-C8-C9
22	A	843	CLA	C14-C13-C15-C16
22	B	811	CLA	C11-C12-C13-C14
22	B	816	CLA	C6-C7-C8-C9
22	B	817	CLA	C11-C12-C13-C14
22	B	818	CLA	C14-C13-C15-C16
22	B	829	CLA	C14-C13-C15-C16
22	B	831	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
22	B	834	CLA	C11-C10-C8-C9
22	B	840	CLA	C11-C12-C13-C14
22	B	841	CLA	C11-C10-C8-C9
22	B	841	CLA	C14-C13-C15-C16
29	A	844	PQN	C21-C22-C23-C24
22	L	302	CLA	O1D-CGD-O2D-CED
22	B	822	CLA	CBA-CGA-O2A-C1
22	A	814	CLA	C2A-CAA-CBA-CGA
22	8	613	CLA	C2A-CAA-CBA-CGA
22	5	609	CLA	CBD-CGD-O2D-CED
24	8	620	XAT	C27-C28-C29-C39
27	K	205	BCR	C7-C8-C9-C34
21	W	601	CHL	C16-C17-C18-C19
22	B	813	CLA	C16-C17-C18-C20
22	V	604	CLA	O1D-CGD-O2D-CED
23	2	619	LUT	C11-C12-C13-C14
24	8	620	XAT	C27-C28-C29-C30
27	1	619	BCR	C21-C22-C23-C24
27	K	205	BCR	C7-C8-C9-C10
22	A	807	CLA	C8-C10-C11-C12
22	A	828	CLA	C15-C16-C17-C18
22	B	820	CLA	C5-C6-C7-C8
22	A	835	CLA	CBA-CGA-O2A-C1
26	6	630	LHG	C24-C23-O8-C6
26	2	630	LHG	O6-C4-C5-C6
26	A	847	LHG	O6-C4-C5-C6
22	V	603	CLA	C3-C5-C6-C7
22	A	839	CLA	O1D-CGD-O2D-CED
22	4	603	CLA	C4-C3-C5-C6
22	A	823	CLA	C2-C3-C5-C6
22	A	830	CLA	C2-C3-C5-C6
22	W	610	CLA	O1A-CGA-O2A-C1
22	A	826	CLA	O1A-CGA-O2A-C1
22	F	304	CLA	O1A-CGA-O2A-C1
22	7	602	CLA	C11-C12-C13-C14
22	J	101	CLA	C2A-CAA-CBA-CGA
21	3	608	CHL	CBA-CGA-O2A-C1
22	B	827	CLA	CBA-CGA-O2A-C1
22	8	610	CLA	CBA-CGA-O2A-C1
28	L	307	LMG	C29-C28-O8-C9
26	2	630	LHG	C2-C3-O3-P
22	A	813	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	U	609	CHL	C3A-C2A-CAA-CBA
22	1	608	CLA	C3A-C2A-CAA-CBA
22	1	614	CLA	C3A-C2A-CAA-CBA
22	4	604	CLA	C3A-C2A-CAA-CBA
22	A	817	CLA	C3A-C2A-CAA-CBA
22	A	830	CLA	C3A-C2A-CAA-CBA
22	A	842	CLA	C3A-C2A-CAA-CBA
22	B	808	CLA	C3A-C2A-CAA-CBA
22	B	814	CLA	C3A-C2A-CAA-CBA
23	5	617	LUT	C9-C10-C11-C12
24	8	620	XAT	C9-C10-C11-C12
22	1	610	CLA	CBA-CGA-O2A-C1
22	A	836	CLA	O1D-CGD-O2D-CED
22	6	612	CLA	O1D-CGD-O2D-CED
26	U	2630	LHG	C23-C24-C25-C26
22	3	610	CLA	O1A-CGA-O2A-C1
22	9	613	CLA	O2A-C1-C2-C3
22	A	841	CLA	O1D-CGD-O2D-CED
22	9	611	CLA	C3-C5-C6-C7
22	A	814	CLA	C4-C3-C5-C6
21	1	601	CHL	C6-C7-C8-C10
22	U	610	CLA	C16-C17-C18-C20
22	A	822	CLA	O1D-CGD-O2D-CED
22	3	606	CLA	C2A-CAA-CBA-CGA
22	A	832	CLA	C2A-CAA-CBA-CGA
22	L	303	CLA	C2A-CAA-CBA-CGA
22	8	601	CLA	C2A-CAA-CBA-CGA
22	8	614	CLA	C2A-CAA-CBA-CGA
22	3	610	CLA	C8-C10-C11-C12
22	B	832	CLA	C5-C6-C7-C8
26	4	630	LHG	O6-C4-C5-O7
22	7	610	CLA	CBA-CGA-O2A-C1
21	U	609	CHL	O1A-CGA-O2A-C1
32	B	850	DGD	C1A-C2A-C3A-C4A
21	W	601	CHL	C16-C17-C18-C20
26	4	630	LHG	C11-C10-C9-C8
22	B	822	CLA	O1A-CGA-O2A-C1
26	4	630	LHG	O7-C5-C6-O8
26	7	630	LHG	O7-C5-C6-O8
22	B	819	CLA	C5-C6-C7-C8
22	A	804	CLA	C16-C17-C18-C19
22	A	841	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
26	A	847	LHG	C1-C2-C3-O3
26	1	630	LHG	O9-C7-O7-C5
26	8	630	LHG	O9-C7-O7-C5
21	8	608	CHL	C2-C1-O2A-CGA
22	A	832	CLA	C2-C1-O2A-CGA
22	4	603	CLA	C2-C3-C5-C6
21	V	609	CHL	C2C-C3C-CAC-CBC
21	V	601	CHL	C11-C12-C13-C14
22	U	603	CLA	C14-C13-C15-C16
22	4	610	CLA	C6-C7-C8-C9
22	A	807	CLA	C11-C12-C13-C14
22	A	831	CLA	C6-C7-C8-C9
22	A	831	CLA	C11-C12-C13-C14
22	A	836	CLA	C6-C7-C8-C9
22	A	837	CLA	C6-C7-C8-C9
22	B	819	CLA	C6-C7-C8-C9
22	B	828	CLA	C11-C10-C8-C9
32	B	850	DGD	C4A-C5A-C6A-C7A
31	B	849	LMT	O5B-C5B-C6B-O6B
22	1	611	CLA	C5-C6-C7-C8
21	4	606	CHL	C2A-CAA-CBA-CGA
22	4	613	CLA	C2A-CAA-CBA-CGA
22	A	845	CLA	C16-C17-C18-C19
22	L	302	CLA	C16-C17-C18-C19
22	3	609	CLA	C3-C5-C6-C7
22	A	814	CLA	C3-C5-C6-C7
23	V	2621	LUT	C1-C6-C7-C8
23	6	619	LUT	C1-C6-C7-C8
27	2	621	BCR	C5-C6-C7-C8
27	3	620	BCR	C23-C24-C25-C26
27	A	850	BCR	C1-C6-C7-C8
27	F	305	BCR	C23-C24-C25-C30
27	K	202	BCR	C1-C6-C7-C8
27	L	301	BCR	C1-C6-C7-C8
22	1	610	CLA	C10-C11-C12-C13
22	B	807	CLA	C8-C10-C11-C12
23	5	617	LUT	C11-C12-C13-C14
27	B	848	BCR	C21-C22-C23-C24
27	B	1609	BCR	C21-C22-C23-C24
22	B	805	CLA	C15-C16-C17-C18
22	U	602	CLA	C15-C16-C17-C18
22	2	613	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
22	3	613	CLA	O1D-CGD-O2D-CED
22	U	603	CLA	C11-C10-C8-C7
22	U	612	CLA	C12-C13-C15-C16
22	V	603	CLA	C11-C10-C8-C7
22	W	610	CLA	C11-C10-C8-C7
22	W	610	CLA	C12-C13-C15-C16
22	1	602	CLA	C11-C10-C8-C7
22	1	609	CLA	C11-C12-C13-C15
22	1	611	CLA	C11-C12-C13-C15
22	3	612	CLA	C11-C10-C8-C7
22	3	617	CLA	C6-C7-C8-C10
22	A	805	CLA	C11-C10-C8-C7
22	A	807	CLA	C11-C12-C13-C15
22	A	822	CLA	C11-C10-C8-C7
22	A	825	CLA	C11-C12-C13-C15
22	A	826	CLA	C11-C10-C8-C7
22	A	828	CLA	C11-C10-C8-C7
22	A	830	CLA	C12-C13-C15-C16
22	A	831	CLA	C11-C12-C13-C15
22	A	837	CLA	C6-C7-C8-C10
22	A	854	CLA	C11-C10-C8-C7
22	B	806	CLA	C6-C7-C8-C10
22	B	819	CLA	C6-C7-C8-C10
22	B	826	CLA	C12-C13-C15-C16
22	B	827	CLA	C6-C7-C8-C10
22	B	829	CLA	C12-C13-C15-C16
22	B	831	CLA	C11-C12-C13-C15
22	B	834	CLA	C11-C10-C8-C7
22	B	837	CLA	C6-C7-C8-C10
22	B	839	CLA	C6-C7-C8-C10
22	L	302	CLA	C11-C12-C13-C15
22	5	602	CLA	C11-C10-C8-C7
22	9	611	CLA	C11-C12-C13-C15
29	A	844	PQN	C17-C18-C20-C21
21	U	601	CHL	C3-C5-C6-C7
22	U	610	CLA	C8-C10-C11-C12
22	A	805	CLA	C10-C11-C12-C13
24	8	620	XAT	C29-C30-C31-C32
25	W	2623	NEX	C33-C34-C35-C15
22	6	604	CLA	CBA-CGA-O2A-C1
21	6	602	CHL	C5-C6-C7-C8
22	U	612	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
22	B	822	CLA	CAA-CBA-CGA-O2A
22	A	835	CLA	O1A-CGA-O2A-C1
21	2	601	CHL	C2A-CAA-CBA-CGA
26	V	2630	LHG	C23-C24-C25-C26
22	A	832	CLA	C3-C5-C6-C7
26	1	630	LHG	C18-C19-C20-C21
21	6	608	CHL	CBA-CGA-O2A-C1
22	5	602	CLA	CBA-CGA-O2A-C1
22	4	610	CLA	C12-C13-C15-C16
22	2	613	CLA	C5-C6-C7-C8
22	B	813	CLA	C10-C11-C12-C13
21	2	601	CHL	CAD-CBD-CGD-O2D
22	W	602	CLA	CAD-CBD-CGD-O2D
22	W	604	CLA	CAD-CBD-CGD-O2D
22	1	608	CLA	CAD-CBD-CGD-O2D
22	1	610	CLA	CAD-CBD-CGD-O2D
22	1	614	CLA	CAD-CBD-CGD-O2D
22	2	603	CLA	CAD-CBD-CGD-O2D
22	2	610	CLA	CAD-CBD-CGD-O2D
22	2	611	CLA	CAD-CBD-CGD-O2D
22	3	602	CLA	CAD-CBD-CGD-O2D
22	3	606	CLA	CAD-CBD-CGD-O2D
22	3	607	CLA	CAD-CBD-CGD-O2D
22	3	611	CLA	CAD-CBD-CGD-O2D
22	4	610	CLA	CAD-CBD-CGD-O2D
22	4	611	CLA	CAD-CBD-CGD-O2D
22	A	806	CLA	CAD-CBD-CGD-O2D
22	A	807	CLA	CAD-CBD-CGD-O2D
22	A	809	CLA	CAD-CBD-CGD-O2D
22	A	823	CLA	CAD-CBD-CGD-O2D
22	A	838	CLA	CAD-CBD-CGD-O2D
22	B	802	CLA	CAD-CBD-CGD-O2D
22	B	804	CLA	CAD-CBD-CGD-O2D
22	B	820	CLA	CAD-CBD-CGD-O2D
22	B	821	CLA	CAD-CBD-CGD-O2D
22	B	831	CLA	CAD-CBD-CGD-O2D
22	B	839	CLA	CAD-CBD-CGD-O2D
22	G	203	CLA	CAD-CBD-CGD-O2D
22	5	602	CLA	CAD-CBD-CGD-O2D
22	6	612	CLA	CAD-CBD-CGD-O2D
22	7	607	CLA	CAD-CBD-CGD-O2D
22	7	617	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	9	611	CLA	CAD-CBD-CGD-O2D
22	A	854	CLA	C8-C10-C11-C12
22	B	816	CLA	CBD-CGD-O2D-CED
22	G	203	CLA	CBA-CGA-O2A-C1
28	J	103	LMG	C29-C28-O8-C9
22	3	611	CLA	C6-C7-C8-C10
22	7	602	CLA	C11-C12-C13-C15
26	U	2630	LHG	C4-C5-C6-O8
26	4	630	LHG	C5-C4-O6-P
26	A	847	LHG	C2-C3-O3-P
22	5	602	CLA	O1A-CGA-O2A-C1
22	6	604	CLA	O1A-CGA-O2A-C1
22	B	803	CLA	C15-C16-C17-C18
22	A	826	CLA	CAA-CBA-CGA-O2A
22	3	603	CLA	C2A-CAA-CBA-CGA
24	8	620	XAT	C14-C15-C35-C34
22	B	806	CLA	C16-C17-C18-C19
22	A	814	CLA	O1D-CGD-O2D-CED
21	V	605	CHL	CHA-CBD-CGD-O1D
21	2	618	CHL	CHA-CBD-CGD-O1D
21	6	618	CHL	CHA-CBD-CGD-O1D
21	6	618	CHL	CHA-CBD-CGD-O2D
21	9	607	CHL	CHA-CBD-CGD-O1D
22	U	604	CLA	CHA-CBD-CGD-O1D
22	U	604	CLA	CHA-CBD-CGD-O2D
22	U	611	CLA	CHA-CBD-CGD-O2D
22	U	612	CLA	CHA-CBD-CGD-O1D
22	U	612	CLA	CHA-CBD-CGD-O2D
22	V	603	CLA	CHA-CBD-CGD-O1D
22	V	603	CLA	CHA-CBD-CGD-O2D
22	1	603	CLA	CHA-CBD-CGD-O1D
22	1	603	CLA	CHA-CBD-CGD-O2D
22	1	611	CLA	CHA-CBD-CGD-O1D
22	1	611	CLA	CHA-CBD-CGD-O2D
22	1	616	CLA	CHA-CBD-CGD-O2D
22	2	612	CLA	CHA-CBD-CGD-O1D
22	2	612	CLA	CHA-CBD-CGD-O2D
22	2	613	CLA	CHA-CBD-CGD-O2D
22	4	602	CLA	CHA-CBD-CGD-O1D
22	4	612	CLA	CHA-CBD-CGD-O1D
22	4	612	CLA	CHA-CBD-CGD-O2D
22	A	815	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	A	815	CLA	CHA-CBD-CGD-O2D
22	A	837	CLA	CHA-CBD-CGD-O1D
22	A	845	CLA	CHA-CBD-CGD-O1D
22	A	845	CLA	CHA-CBD-CGD-O2D
22	B	822	CLA	CHA-CBD-CGD-O1D
22	B	822	CLA	CHA-CBD-CGD-O2D
22	B	833	CLA	CHA-CBD-CGD-O1D
22	5	613	CLA	CHA-CBD-CGD-O2D
22	8	601	CLA	CHA-CBD-CGD-O1D
22	8	602	CLA	CHA-CBD-CGD-O1D
22	1	610	CLA	O1A-CGA-O2A-C1
22	B	827	CLA	O1A-CGA-O2A-C1
22	7	610	CLA	O1A-CGA-O2A-C1
22	8	610	CLA	O1A-CGA-O2A-C1
26	6	630	LHG	O10-C23-O8-C6
26	U	2630	LHG	O7-C5-C6-O8
26	B	851	LHG	O7-C5-C6-O8
28	J	104	LMG	O1-C7-C8-O7
21	3	608	CHL	O1A-CGA-O2A-C1
28	L	307	LMG	O10-C28-O8-C9
32	B	850	DGD	CDA-CEA-CFA-CGA
22	F	304	CLA	OBD-CAD-CBD-CGD
22	A	801	CLA	C3-C5-C6-C7
22	A	836	CLA	C3-C5-C6-C7
22	A	804	CLA	O1D-CGD-O2D-CED
22	7	609	CLA	O1D-CGD-O2D-CED
22	1	609	CLA	C13-C15-C16-C17
22	U	602	CLA	C6-C7-C8-C9
22	U	610	CLA	C11-C12-C13-C14
22	V	603	CLA	C11-C10-C8-C9
22	4	610	CLA	C11-C10-C8-C9
22	A	802	CLA	C11-C10-C8-C9
22	A	817	CLA	C11-C10-C8-C9
22	A	819	CLA	C14-C13-C15-C16
22	B	806	CLA	C11-C12-C13-C14
22	B	827	CLA	C6-C7-C8-C9
22	B	839	CLA	C6-C7-C8-C9
21	6	608	CHL	O1A-CGA-O2A-C1
22	G	203	CLA	O1A-CGA-O2A-C1
31	B	849	LMT	C4-C5-C6-C7
22	A	816	CLA	CBD-CGD-O2D-CED
26	9	2630	LHG	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
27	2	621	BCR	C37-C22-C23-C24
27	L	306	BCR	C7-C8-C9-C34
27	O	2004	BCR	C21-C22-C23-C24
22	W	613	CLA	C3-C5-C6-C7
21	2	606	CHL	C1A-C2A-CAA-CBA
22	W	603	CLA	CHA-CBD-CGD-O2D
22	A	840	CLA	C1A-C2A-CAA-CBA
22	B	809	CLA	C1A-C2A-CAA-CBA
22	B	806	CLA	C16-C17-C18-C20
22	A	842	CLA	C2-C1-O2A-CGA
26	5	630	LHG	C26-C27-C28-C29
25	W	2623	NEX	C29-C30-C31-C32
26	2	630	LHG	C3-O3-P-O6
26	A	846	LHG	C3-O3-P-O6
26	B	851	LHG	C3-O3-P-O6
26	9	2630	LHG	C24-C25-C26-C27
22	5	609	CLA	O1D-CGD-O2D-CED
22	2	603	CLA	CBA-CGA-O2A-C1
26	U	2630	LHG	C4-O6-P-O4
26	V	2630	LHG	C3-O3-P-O4
26	V	2630	LHG	C4-O6-P-O4
26	W	2630	LHG	C3-O3-P-O4
26	W	2630	LHG	C4-O6-P-O4
26	3	630	LHG	C4-O6-P-O5
26	5	630	LHG	C3-O3-P-O4
26	7	630	LHG	C4-O6-P-O4
26	8	630	LHG	C3-O3-P-O4
26	9	2630	LHG	C3-O3-P-O4
22	A	829	CLA	C11-C12-C13-C14
22	4	603	CLA	C13-C15-C16-C17
22	3	611	CLA	CBA-CGA-O2A-C1
22	A	837	CLA	CBA-CGA-O2A-C1
22	7	609	CLA	C8-C10-C11-C12
22	B	834	CLA	C5-C6-C7-C8
22	B	837	CLA	C8-C10-C11-C12
22	A	831	CLA	C2A-CAA-CBA-CGA
22	3	611	CLA	C3-C5-C6-C7
26	A	846	LHG	C10-C11-C12-C13
21	6	602	CHL	CAD-CBD-CGD-O1D
21	6	618	CHL	CAD-CBD-CGD-O1D
22	U	611	CLA	CAD-CBD-CGD-O1D
22	V	613	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	4	601	CLA	CAD-CBD-CGD-O1D
22	4	602	CLA	CAD-CBD-CGD-O1D
22	A	815	CLA	CAD-CBD-CGD-O1D
22	A	824	CLA	CAD-CBD-CGD-O1D
22	A	845	CLA	CAD-CBD-CGD-O1D
22	B	805	CLA	CAD-CBD-CGD-O1D
22	B	822	CLA	CAD-CBD-CGD-O1D
22	5	613	CLA	CAD-CBD-CGD-O1D
22	6	614	CLA	CAD-CBD-CGD-O1D
22	7	604	CLA	CAD-CBD-CGD-O1D
22	7	614	CLA	CAD-CBD-CGD-O1D
22	8	601	CLA	CAD-CBD-CGD-O1D
22	7	606	CLA	CAA-CBA-CGA-O2A
22	3	613	CLA	C15-C16-C17-C18
22	A	831	CLA	C8-C10-C11-C12
22	8	613	CLA	C5-C6-C7-C8
22	B	831	CLA	O1A-CGA-O2A-C1
21	1	601	CHL	C5-C6-C7-C8
21	U	607	CHL	O1D-CGD-O2D-CED
26	W	2630	LHG	C15-C16-C17-C18
22	B	831	CLA	CBA-CGA-O2A-C1
22	7	613	CLA	O1D-CGD-O2D-CED
22	8	612	CLA	CBA-CGA-O2A-C1
21	4	607	CHL	O1A-CGA-O2A-C1
21	U	601	CHL	C16-C17-C18-C20
22	O	2002	CLA	C4-C3-C5-C6
21	U	608	CHL	CHA-CBD-CGD-O1D
21	V	601	CHL	C11-C12-C13-C15
21	V	601	CHL	C12-C13-C15-C16
22	U	602	CLA	C6-C7-C8-C10
22	U	610	CLA	C11-C12-C13-C15
22	W	612	CLA	CAD-CBD-CGD-O2D
22	A	802	CLA	C11-C10-C8-C7
22	A	807	CLA	C11-C10-C8-C7
22	A	814	CLA	C6-C7-C8-C10
22	A	815	CLA	C3A-C2A-CAA-CBA
22	A	817	CLA	C11-C10-C8-C7
22	A	819	CLA	C12-C13-C15-C16
22	A	843	CLA	C11-C10-C8-C7
22	B	805	CLA	C6-C7-C8-C10
22	B	806	CLA	C11-C12-C13-C15
22	F	301	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	L	303	CLA	C11-C12-C13-C15
22	L	304	CLA	C3A-C2A-CAA-CBA
22	7	615	CLA	CAD-CBD-CGD-O2D
23	9	624	LUT	C25-C26-C27-C28
26	1	630	LHG	C16-C17-C18-C19
22	3	613	CLA	CAA-CBA-CGA-O2A
22	1	603	CLA	C5-C6-C7-C8
22	A	827	CLA	C13-C15-C16-C17
22	B	813	CLA	C8-C10-C11-C12
22	L	303	CLA	C10-C11-C12-C13
22	2	610	CLA	C8-C10-C11-C12
22	A	837	CLA	C10-C11-C12-C13
21	6	607	CHL	O1A-CGA-O2A-C1
22	4	602	CLA	C2A-CAA-CBA-CGA
22	A	822	CLA	C2A-CAA-CBA-CGA
22	A	830	CLA	C2A-CAA-CBA-CGA
22	9	602	CLA	C11-C12-C13-C15
21	U	601	CHL	CAD-CBD-CGD-O1D
21	V	601	CHL	CAD-CBD-CGD-O1D
21	V	608	CHL	CAD-CBD-CGD-O1D
22	V	612	CLA	CAD-CBD-CGD-O1D
22	W	612	CLA	CAD-CBD-CGD-O1D
22	W	614	CLA	CAD-CBD-CGD-O1D
22	7	615	CLA	CAD-CBD-CGD-O1D
28	L	307	LMG	C7-C8-C9-O8
26	W	2630	LHG	O7-C5-C6-O8
26	A	847	LHG	O7-C5-C6-O8
28	G	202	LMG	O1-C7-C8-O7
28	L	307	LMG	C29-C30-C31-C32
22	A	825	CLA	C10-C11-C12-C13
22	V	602	CLA	C11-C12-C13-C14
22	A	837	CLA	O1A-CGA-O2A-C1
22	3	611	CLA	C6-C7-C8-C9
21	W	601	CHL	C10-C11-C12-C13
28	J	103	LMG	C37-C38-C39-C40
22	3	611	CLA	O1A-CGA-O2A-C1
28	J	103	LMG	O10-C28-O8-C9
21	6	618	CHL	CBD-CGD-O2D-CED
21	2	602	CHL	CBA-CGA-O2A-C1
22	A	814	CLA	C2-C3-C5-C6
22	B	833	CLA	CAA-CBA-CGA-O2A
22	W	610	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
22	W	610	CLA	C14-C13-C15-C16
22	1	602	CLA	C11-C10-C8-C9
22	3	612	CLA	C11-C10-C8-C9
22	3	617	CLA	C6-C7-C8-C9
22	A	812	CLA	C11-C10-C8-C9
22	A	828	CLA	C11-C10-C8-C9
22	A	830	CLA	C14-C13-C15-C16
22	A	854	CLA	C11-C10-C8-C9
22	B	808	CLA	C14-C13-C15-C16
22	B	810	CLA	C11-C10-C8-C9
22	B	818	CLA	C11-C10-C8-C9
22	B	826	CLA	C14-C13-C15-C16
22	B	833	CLA	C6-C7-C8-C9
22	B	837	CLA	C6-C7-C8-C9
22	5	602	CLA	C11-C10-C8-C9
22	9	611	CLA	C11-C10-C8-C9
29	A	844	PQN	C16-C17-C18-C19
29	A	844	PQN	C19-C18-C20-C21
21	2	602	CHL	O1A-CGA-O2A-C1
22	K	203	CLA	CBD-CGD-O2D-CED
21	6	618	CHL	O1A-CGA-O2A-C1
28	L	307	LMG	C14-C15-C16-C17
27	1	619	BCR	C37-C22-C23-C24
22	A	833	CLA	C5-C6-C7-C8
22	B	816	CLA	O1D-CGD-O2D-CED
21	1	607	CHL	CAA-CBA-CGA-O2A
22	A	810	CLA	C8-C10-C11-C12
22	V	613	CLA	C2A-CAA-CBA-CGA
22	3	612	CLA	C4-C3-C5-C6
22	A	810	CLA	C4-C3-C5-C6
22	7	613	CLA	C4-C3-C5-C6
26	9	2630	LHG	O7-C7-C8-C9
22	U	613	CLA	C15-C16-C17-C18
28	G	202	LMG	O6-C5-C6-O5
22	B	825	CLA	C5-C6-C7-C8
22	U	602	CLA	O1A-CGA-O2A-C1
26	W	2630	LHG	C23-C24-C25-C26
28	L	307	LMG	O8-C28-C29-C30
28	A	860	LMG	C9-C8-O7-C10
22	W	613	CLA	C2A-CAA-CBA-CGA
22	1	604	CLA	C2A-CAA-CBA-CGA
22	2	613	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
22	B	828	CLA	C2A-CAA-CBA-CGA
22	6	613	CLA	C2A-CAA-CBA-CGA
22	A	801	CLA	C2-C1-O2A-CGA
22	A	804	CLA	C2-C1-O2A-CGA
22	A	806	CLA	C2-C1-O2A-CGA
28	J	103	LMG	C36-C37-C38-C39
22	A	816	CLA	O1D-CGD-O2D-CED
22	B	804	CLA	C3-C5-C6-C7
22	U	613	CLA	C8-C10-C11-C12
22	A	805	CLA	C8-C10-C11-C12
22	A	817	CLA	C8-C10-C11-C12
26	7	630	LHG	C25-C26-C27-C28
28	J	103	LMG	C29-C30-C31-C32
27	L	306	BCR	C5-C6-C7-C8
22	O	2002	CLA	C2-C3-C5-C6
22	A	807	CLA	C10-C11-C12-C13
22	U	602	CLA	CBA-CGA-O2A-C1
22	B	831	CLA	CAA-CBA-CGA-O2A
22	A	802	CLA	C8-C10-C11-C12
22	A	829	CLA	C11-C12-C13-C15
22	V	604	CLA	C2A-CAA-CBA-CGA
28	A	860	LMG	C2-C1-O1-C7
26	1	630	LHG	O7-C5-C6-O8
22	K	201	CLA	CBD-CGD-O2D-CED
26	U	2630	LHG	C3-O3-P-O6
26	1	630	LHG	C3-O3-P-O6
26	1	630	LHG	C4-O6-P-O3
26	3	630	LHG	C3-O3-P-O6
26	A	846	LHG	C4-O6-P-O3
26	A	847	LHG	C4-O6-P-O3
26	5	630	LHG	C4-O6-P-O3
26	6	630	LHG	C3-O3-P-O6
26	8	630	LHG	C4-O6-P-O3
26	9	2630	LHG	C4-O6-P-O3
32	B	850	DGD	C7B-C8B-C9B-CAB
21	U	601	CHL	C16-C17-C18-C19
22	W	602	CLA	C11-C12-C13-C15
26	W	2630	LHG	C4-C5-C6-O8
21	U	601	CHL	C11-C10-C8-C7
22	W	610	CLA	C11-C12-C13-C15
22	A	804	CLA	C12-C13-C15-C16
22	A	806	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	A	812	CLA	C11-C10-C8-C7
22	B	833	CLA	C6-C7-C8-C10
22	1	609	CLA	C11-C12-C13-C14
22	A	802	CLA	C14-C13-C15-C16
22	A	806	CLA	C11-C12-C13-C14
22	A	822	CLA	C11-C10-C8-C9
22	A	843	CLA	C11-C10-C8-C9
22	B	808	CLA	C11-C10-C8-C9
22	B	817	CLA	C11-C10-C8-C9
22	F	301	CLA	C14-C13-C15-C16
22	L	303	CLA	C11-C12-C13-C14
28	J	103	LMG	C13-C14-C15-C16
22	W	610	CLA	C15-C16-C17-C18
21	V	609	CHL	C4C-C3C-CAC-CBC
22	A	808	CLA	C5-C6-C7-C8
22	A	837	CLA	C5-C6-C7-C8
31	G	206	LMT	C6-C7-C8-C9
28	J	103	LMG	C39-C40-C41-C42
22	K	203	CLA	O1D-CGD-O2D-CED
29	B	842	PQN	C14-C13-C15-C16
26	A	846	LHG	C7-C8-C9-C10
22	7	613	CLA	C2-C3-C5-C6
22	A	841	CLA	C16-C17-C18-C20
21	6	601	CHL	CBA-CGA-O2A-C1
22	A	819	CLA	CBA-CGA-O2A-C1
22	A	839	CLA	CBA-CGA-O2A-C1
22	B	809	CLA	CBA-CGA-O2A-C1
22	B	829	CLA	CBA-CGA-O2A-C1
22	8	602	CLA	CBA-CGA-O2A-C1
28	2	631	LMG	C29-C28-O8-C9
21	6	601	CHL	O1A-CGA-O2A-C1
22	B	809	CLA	O1A-CGA-O2A-C1
22	K	201	CLA	O1D-CGD-O2D-CED
22	U	613	CLA	C10-C11-C12-C13
22	A	814	CLA	C5-C6-C7-C8
22	A	819	CLA	O1A-CGA-O2A-C1
22	U	613	CLA	C2A-CAA-CBA-CGA
22	3	613	CLA	C2A-CAA-CBA-CGA
31	B	849	LMT	O5'-C1'-O1'-C1
23	5	617	LUT	C29-C30-C31-C32
24	8	620	XAT	C33-C34-C35-C15
32	B	850	DGD	C3A-C4A-C5A-C6A

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Mol	Chain	Res	Type	Atoms
22	W	602	CLA	C3-C5-C6-C7
22	B	819	CLA	C3-C5-C6-C7
22	B	829	CLA	O1A-CGA-O2A-C1
22	B	803	CLA	C2C-C3C-CAC-CBC
22	V	602	CLA	C5-C6-C7-C8
22	F	301	CLA	C13-C15-C16-C17
22	A	830	CLA	C3-C5-C6-C7
32	B	850	DGD	C2A-C3A-C4A-C5A
29	B	842	PQN	C12-C13-C15-C16
22	B	838	CLA	C2C-C3C-CAC-CBC
22	U	610	CLA	C10-C11-C12-C13
22	3	609	CLA	C8-C10-C11-C12
22	6	613	CLA	C8-C10-C11-C12
26	A	847	LHG	O2-C2-C3-O3
22	W	610	CLA	C2-C1-O2A-CGA
22	A	805	CLA	C2-C1-O2A-CGA
22	A	837	CLA	C2-C1-O2A-CGA
22	L	303	CLA	C2-C1-O2A-CGA
22	B	817	CLA	C8-C10-C11-C12
22	B	834	CLA	C10-C11-C12-C13
22	8	602	CLA	C11-C12-C13-C15
28	G	202	LMG	C2-C1-O1-C7
22	U	611	CLA	CAA-CBA-CGA-O1A
22	U	602	CLA	C2A-CAA-CBA-CGA
22	3	607	CLA	C2A-CAA-CBA-CGA
22	A	803	CLA	C2A-CAA-CBA-CGA
22	B	834	CLA	C2A-CAA-CBA-CGA
26	B	851	LHG	C10-C11-C12-C13
22	1	603	CLA	CBD-CGD-O2D-CED
21	2	606	CHL	C3A-C2A-CAA-CBA
22	A	826	CLA	C3A-C2A-CAA-CBA
22	B	803	CLA	C3A-C2A-CAA-CBA
22	B	804	CLA	C3A-C2A-CAA-CBA
22	B	825	CLA	C3A-C2A-CAA-CBA
22	8	614	CLA	C3A-C2A-CAA-CBA
22	9	611	CLA	C3A-C2A-CAA-CBA
22	B	817	CLA	C16-C17-C18-C20
22	7	613	CLA	C6-C7-C8-C9
22	A	822	CLA	C13-C15-C16-C17
21	W	601	CHL	C6-C7-C8-C9
22	U	603	CLA	C6-C7-C8-C9
22	3	612	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	A	807	CLA	C11-C10-C8-C9
22	A	808	CLA	C6-C7-C8-C9
22	A	820	CLA	C11-C12-C13-C14
22	A	825	CLA	C11-C10-C8-C9
22	A	854	CLA	C6-C7-C8-C9
22	9	602	CLA	C11-C12-C13-C14
22	9	610	CLA	C5-C6-C7-C8
26	1	630	LHG	C15-C16-C17-C18
25	U	2623	NEX	C39-C29-C30-C31
25	V	2623	NEX	C39-C29-C30-C31
25	9	623	NEX	C39-C29-C30-C31
26	7	630	LHG	C4-C5-C6-O8
27	A	852	BCR	C11-C10-C9-C34
27	A	852	BCR	C16-C17-C18-C36
27	B	845	BCR	C20-C21-C22-C37
27	F	305	BCR	C35-C13-C14-C15
27	L	301	BCR	C20-C21-C22-C37
26	4	630	LHG	C10-C11-C12-C13
22	1	609	CLA	O2A-C1-C2-C3
22	A	805	CLA	O2A-C1-C2-C3
22	A	810	CLA	O2A-C1-C2-C3
22	B	804	CLA	O2A-C1-C2-C3
22	8	601	CLA	O2A-C1-C2-C3
21	2	606	CHL	CAA-CBA-CGA-O2A
22	7	612	CLA	CAA-CBA-CGA-O1A
22	7	612	CLA	CAA-CBA-CGA-O2A
22	8	602	CLA	O1A-CGA-O2A-C1
28	A	860	LMG	C7-C8-O7-C10
21	6	602	CHL	C1A-C2A-CAA-CBA
22	3	613	CLA	C1A-C2A-CAA-CBA
22	B	803	CLA	C1A-C2A-CAA-CBA
22	B	825	CLA	C1A-C2A-CAA-CBA
21	6	601	CHL	C12-C13-C15-C16
22	4	610	CLA	C6-C7-C8-C10
22	A	830	CLA	C11-C10-C8-C7
22	A	843	CLA	C11-C12-C13-C15
22	B	824	CLA	C6-C7-C8-C10
22	B	810	CLA	O1D-CGD-O2D-CED
22	7	602	CLA	C10-C11-C12-C13
21	2	606	CHL	CAA-CBA-CGA-O1A
22	A	839	CLA	O1A-CGA-O2A-C1
28	2	631	LMG	O10-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
22	4	609	CLA	CAA-CBA-CGA-O1A
26	A	846	LHG	C24-C25-C26-C27
22	A	854	CLA	C11-C12-C13-C15
22	B	807	CLA	C2A-CAA-CBA-CGA
22	6	603	CLA	C2A-CAA-CBA-CGA
22	8	612	CLA	C2A-CAA-CBA-CGA
22	A	814	CLA	C13-C15-C16-C17
22	A	822	CLA	C5-C6-C7-C8
22	8	609	CLA	C2C-C3C-CAC-CBC
22	A	837	CLA	C13-C15-C16-C17
26	3	630	LHG	C26-C27-C28-C29
26	4	630	LHG	O6-C4-C5-C6
22	1	603	CLA	O1D-CGD-O2D-CED
22	W	613	CLA	C4-C3-C5-C6
22	W	613	CLA	C2-C3-C5-C6
22	3	612	CLA	C2-C3-C5-C6
21	U	609	CHL	C2C-C3C-CAC-CBC
22	K	204	CLA	C2C-C3C-CAC-CBC
25	U	2623	NEX	C28-C29-C30-C31
25	V	2623	NEX	C28-C29-C30-C31
25	9	623	NEX	C28-C29-C30-C31
27	A	852	BCR	C11-C10-C9-C8
27	A	852	BCR	C16-C17-C18-C19
27	B	845	BCR	C20-C21-C22-C23
27	F	305	BCR	C12-C13-C14-C15
27	L	301	BCR	C20-C21-C22-C23
26	V	2630	LHG	C11-C10-C9-C8
26	V	2630	LHG	O7-C5-C6-O8
21	2	602	CHL	CAA-CBA-CGA-O1A
23	2	619	LUT	C33-C34-C35-C15
22	9	611	CLA	C8-C10-C11-C12
26	B	851	LHG	C9-C10-C11-C12
22	4	602	CLA	C15-C16-C17-C18
22	A	825	CLA	C5-C6-C7-C8
22	U	611	CLA	CAA-CBA-CGA-O2A
21	5	601	CHL	C2-C1-O2A-CGA
21	6	602	CHL	C2-C1-O2A-CGA
22	4	602	CLA	C2-C1-O2A-CGA
22	B	819	CLA	C2-C1-O2A-CGA
22	B	829	CLA	C2-C1-O2A-CGA
22	B	839	CLA	C2-C1-O2A-CGA
22	7	617	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
28	A	860	LMG	C11-C12-C13-C14
22	4	610	CLA	C11-C12-C13-C14
22	A	804	CLA	C6-C7-C8-C9
22	A	822	CLA	C11-C12-C13-C14
22	A	829	CLA	C6-C7-C8-C9
22	B	833	CLA	O1A-CGA-O2A-C1
26	1	630	LHG	C19-C20-C21-C22
26	W	2630	LHG	C5-C4-O6-P
22	A	819	CLA	CAA-CBA-CGA-O2A
22	U	612	CLA	C2A-CAA-CBA-CGA
22	7	603	CLA	C2A-CAA-CBA-CGA
22	B	802	CLA	O1A-CGA-O2A-C1
27	1	619	BCR	C23-C24-C25-C30
27	2	621	BCR	C23-C24-C25-C30
27	4	621	BCR	C23-C24-C25-C30
27	A	851	BCR	C1-C6-C7-C8
27	A	856	BCR	C5-C6-C7-C8
27	B	1609	BCR	C1-C6-C7-C8
27	M	2001	BCR	C5-C6-C7-C8
22	9	609	CLA	C2C-C3C-CAC-CBC
22	1	611	CLA	CAA-CBA-CGA-O2A
22	A	817	CLA	CAA-CBA-CGA-O2A
26	8	630	LHG	C10-C11-C12-C13
22	A	835	CLA	O1D-CGD-O2D-CED
22	8	614	CLA	CAA-CBA-CGA-O2A
22	3	602	CLA	C8-C10-C11-C12
22	B	802	CLA	CBA-CGA-O2A-C1
21	U	607	CHL	C4-C3-C5-C6
21	6	601	CHL	C4-C3-C5-C6
22	B	832	CLA	C4-C3-C5-C6
22	W	611	CLA	C1A-C2A-CAA-CBA
22	A	841	CLA	C16-C17-C18-C19
22	5	602	CLA	C10-C11-C12-C13
22	A	804	CLA	C5-C6-C7-C8
22	4	611	CLA	CAA-CBA-CGA-O2A
22	6	611	CLA	CAA-CBA-CGA-O2A
22	5	614	CLA	C2A-CAA-CBA-CGA
28	L	307	LMG	C30-C31-C32-C33
22	1	606	CLA	CAA-CBA-CGA-O2A
26	B	851	LHG	C13-C14-C15-C16
22	B	808	CLA	CAA-CBA-CGA-O2A
22	B	833	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
26	U	2630	LHG	C29-C30-C31-C32
22	B	828	CLA	C3-C5-C6-C7
22	4	609	CLA	CAA-CBA-CGA-O2A
22	6	611	CLA	CAA-CBA-CGA-O1A
22	3	612	CLA	C5-C6-C7-C8
22	F	301	CLA	C4-C3-C5-C6
22	3	612	CLA	C6-C7-C8-C10
22	A	828	CLA	C11-C12-C13-C15
22	A	829	CLA	C6-C7-C8-C10
22	B	817	CLA	C11-C10-C8-C7
22	9	611	CLA	C11-C10-C8-C7
21	7	608	CHL	CAA-CBA-CGA-O2A
21	8	607	CHL	CAA-CBA-CGA-O2A
22	B	815	CLA	CAA-CBA-CGA-O2A
26	B	851	LHG	C24-C23-O8-C6
26	A	847	LHG	O1-C1-C2-O2
22	7	617	CLA	CBD-CGD-O2D-CED
26	A	847	LHG	C24-C23-O8-C6
22	K	204	CLA	C15-C16-C17-C18
22	5	606	CLA	CAA-CBA-CGA-O2A
22	7	607	CLA	CAA-CBA-CGA-O2A
21	6	602	CHL	CAA-CBA-CGA-O2A
22	5	612	CLA	C2A-CAA-CBA-CGA
22	B	817	CLA	C15-C16-C17-C18
22	L	302	CLA	C10-C11-C12-C13
22	B	817	CLA	C16-C17-C18-C19
22	B	819	CLA	C11-C12-C13-C15
22	B	825	CLA	C16-C17-C18-C20
22	4	612	CLA	CAA-CBA-CGA-O1A
22	6	612	CLA	CAA-CBA-CGA-O2A
22	A	809	CLA	CBA-CGA-O2A-C1
23	2	619	LUT	C40-C33-C34-C35
24	8	620	XAT	C20-C13-C14-C15
21	U	601	CHL	CAA-CBA-CGA-O2A
22	V	602	CLA	CAA-CBA-CGA-O2A
22	A	814	CLA	CAA-CBA-CGA-O2A
22	9	610	CLA	CAA-CBA-CGA-O2A
22	3	613	CLA	C4-C3-C5-C6
22	B	831	CLA	C15-C16-C17-C18
22	7	603	CLA	CAA-CBA-CGA-O2A
22	A	809	CLA	O1A-CGA-O2A-C1
22	B	821	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	A	810	CLA	C2-C3-C5-C6
22	B	832	CLA	C2-C3-C5-C6
22	A	814	CLA	C16-C17-C18-C20
21	W	601	CHL	CBA-CGA-O2A-C1
26	4	630	LHG	C24-C25-C26-C27
21	V	601	CHL	C14-C13-C15-C16
22	1	602	CLA	C11-C12-C13-C14
22	A	804	CLA	C11-C12-C13-C14
22	A	814	CLA	C6-C7-C8-C9
22	A	843	CLA	C11-C12-C13-C14
22	B	805	CLA	C6-C7-C8-C9
22	B	806	CLA	C6-C7-C8-C9
22	K	204	CLA	C14-C13-C15-C16
22	9	611	CLA	C11-C12-C13-C14
22	1	616	CLA	CAA-CBA-CGA-O2A
21	6	602	CHL	C3A-C2A-CAA-CBA
22	A	806	CLA	C3A-C2A-CAA-CBA
21	W	601	CHL	O1A-CGA-O2A-C1
22	8	612	CLA	CAA-CBA-CGA-O2A
26	6	630	LHG	O8-C23-C24-C25
21	2	602	CHL	CAD-CBD-CGD-O2D
22	V	604	CLA	CAD-CBD-CGD-O2D
22	V	610	CLA	CAD-CBD-CGD-O2D
22	V	614	CLA	CAD-CBD-CGD-O2D
22	2	609	CLA	CAD-CBD-CGD-O2D
22	2	614	CLA	CAD-CBD-CGD-O2D
22	3	610	CLA	CAD-CBD-CGD-O2D
22	3	614	CLA	CAD-CBD-CGD-O2D
22	4	614	CLA	CAD-CBD-CGD-O2D
22	A	813	CLA	CAD-CBD-CGD-O2D
22	A	814	CLA	CAD-CBD-CGD-O2D
22	A	827	CLA	CAD-CBD-CGD-O2D
22	A	842	CLA	CAD-CBD-CGD-O2D
22	B	829	CLA	CAD-CBD-CGD-O2D
22	B	833	CLA	CAD-CBD-CGD-O2D
22	B	834	CLA	CAD-CBD-CGD-O2D
22	B	836	CLA	CAD-CBD-CGD-O2D
22	B	841	CLA	CAD-CBD-CGD-O2D
22	G	201	CLA	CAD-CBD-CGD-O2D
22	K	204	CLA	CAD-CBD-CGD-O2D
22	5	611	CLA	CAD-CBD-CGD-O2D
22	5	614	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	7	610	CLA	CAD-CBD-CGD-O2D
21	U	609	CHL	C4C-C3C-CAC-CBC
22	B	831	CLA	C10-C11-C12-C13
26	3	630	LHG	O9-C7-O7-C5
22	A	831	CLA	C2-C1-O2A-CGA
22	A	835	CLA	C2-C1-O2A-CGA
21	6	606	CHL	CAA-CBA-CGA-O2A
26	4	630	LHG	C27-C28-C29-C30
22	2	609	CLA	CAA-CBA-CGA-O2A
22	3	604	CLA	CAA-CBA-CGA-O2A
22	L	304	CLA	CAA-CBA-CGA-O2A
22	B	815	CLA	CAA-CBA-CGA-O1A
22	3	613	CLA	C2-C3-C5-C6
26	8	630	LHG	O7-C7-C8-C9
26	A	847	LHG	C10-C11-C12-C13
21	1	601	CHL	O1A-CGA-O2A-C1
23	3	618	LUT	C7-C8-C9-C10
27	2	621	BCR	C7-C8-C9-C10
27	3	620	BCR	C7-C8-C9-C10
24	W	2622	XAT	O4-C6-C7-C8
24	7	619	XAT	O24-C26-C27-C28
21	U	606	CHL	CAA-CBA-CGA-O2A
21	8	607	CHL	CAA-CBA-CGA-O1A
22	2	611	CLA	CAA-CBA-CGA-O2A
22	8	614	CLA	CAA-CBA-CGA-O1A
22	A	835	CLA	CBD-CGD-O2D-CED
22	4	603	CLA	CAA-CBA-CGA-O2A
22	B	834	CLA	CAA-CBA-CGA-O2A
22	6	603	CLA	CAA-CBA-CGA-O2A
22	B	818	CLA	C15-C16-C17-C18
22	6	612	CLA	CAA-CBA-CGA-O1A
21	U	601	CHL	O2A-C1-C2-C3
21	W	601	CHL	O2A-C1-C2-C3
21	1	601	CHL	O2A-C1-C2-C3
21	5	601	CHL	O2A-C1-C2-C3
21	8	608	CHL	O2A-C1-C2-C3
22	U	602	CLA	O2A-C1-C2-C3
22	1	611	CLA	O2A-C1-C2-C3
22	4	604	CLA	O2A-C1-C2-C3
22	A	814	CLA	O2A-C1-C2-C3
22	A	830	CLA	O2A-C1-C2-C3
22	B	817	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
22	B	824	CLA	O2A-C1-C2-C3
22	B	841	CLA	O2A-C1-C2-C3
21	1	601	CHL	CBA-CGA-O2A-C1
22	5	602	CLA	C2A-CAA-CBA-CGA
22	A	824	CLA	C10-C11-C12-C13
22	B	817	CLA	C10-C11-C12-C13
22	3	607	CLA	CAA-CBA-CGA-O2A
22	A	836	CLA	CAA-CBA-CGA-O2A
28	2	631	LMG	O8-C28-C29-C30
32	B	850	DGD	O1G-C1A-C2A-C3A
21	U	606	CHL	CAA-CBA-CGA-O1A
21	6	606	CHL	CAA-CBA-CGA-O1A
22	2	611	CLA	CAA-CBA-CGA-O1A
22	4	611	CLA	CAA-CBA-CGA-O1A
28	J	103	LMG	C22-C23-C24-C25
21	6	618	CHL	O1D-CGD-O2D-CED
22	U	603	CLA	C16-C17-C18-C20
22	8	602	CLA	C11-C12-C13-C14
31	A	857	LMT	C9-C10-C11-C12
22	2	603	CLA	O1A-CGA-O2A-C1
28	J	103	LMG	C38-C39-C40-C41
21	1	607	CHL	CHA-CBD-CGD-O1D
21	1	607	CHL	CHA-CBD-CGD-O2D
21	2	602	CHL	CHA-CBD-CGD-O2D
21	2	618	CHL	CHA-CBD-CGD-O2D
21	4	618	CHL	CHA-CBD-CGD-O2D
21	9	607	CHL	CHA-CBD-CGD-O2D
21	9	608	CHL	CHA-CBD-CGD-O1D
21	9	608	CHL	CHA-CBD-CGD-O2D
22	U	613	CLA	CHA-CBD-CGD-O1D
22	U	613	CLA	CHA-CBD-CGD-O2D
22	U	614	CLA	CHA-CBD-CGD-O1D
22	1	602	CLA	CHA-CBD-CGD-O1D
22	1	602	CLA	CHA-CBD-CGD-O2D
22	3	602	CLA	CHA-CBD-CGD-O2D
22	3	612	CLA	CHA-CBD-CGD-O1D
22	3	612	CLA	CHA-CBD-CGD-O2D
22	3	617	CLA	CHA-CBD-CGD-O1D
22	3	617	CLA	CHA-CBD-CGD-O2D
22	4	602	CLA	CHA-CBD-CGD-O2D
22	A	801	CLA	CHA-CBD-CGD-O1D
22	A	804	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	A	804	CLA	CHA-CBD-CGD-O2D
22	A	829	CLA	CHA-CBD-CGD-O1D
22	A	835	CLA	CHA-CBD-CGD-O1D
22	A	835	CLA	CHA-CBD-CGD-O2D
22	A	837	CLA	CHA-CBD-CGD-O2D
22	A	843	CLA	CHA-CBD-CGD-O2D
22	B	819	CLA	CHA-CBD-CGD-O1D
22	B	819	CLA	CHA-CBD-CGD-O2D
22	B	823	CLA	CHA-CBD-CGD-O1D
22	B	823	CLA	CHA-CBD-CGD-O2D
22	B	826	CLA	CHA-CBD-CGD-O1D
22	B	826	CLA	CHA-CBD-CGD-O2D
22	B	830	CLA	CHA-CBD-CGD-O1D
22	O	2002	CLA	CHA-CBD-CGD-O1D
22	O	2002	CLA	CHA-CBD-CGD-O2D
22	5	604	CLA	CHA-CBD-CGD-O1D
22	5	604	CLA	CHA-CBD-CGD-O2D
22	5	609	CLA	CHA-CBD-CGD-O1D
22	5	609	CLA	CHA-CBD-CGD-O2D
22	6	611	CLA	CHA-CBD-CGD-O1D
22	6	611	CLA	CHA-CBD-CGD-O2D
22	7	602	CLA	CHA-CBD-CGD-O1D
22	7	602	CLA	CHA-CBD-CGD-O2D
22	7	613	CLA	CHA-CBD-CGD-O1D
22	7	613	CLA	CHA-CBD-CGD-O2D
22	8	601	CLA	CHA-CBD-CGD-O2D
22	8	603	CLA	CHA-CBD-CGD-O2D
22	8	604	CLA	CHA-CBD-CGD-O2D
22	1	606	CLA	CAA-CBA-CGA-O1A
22	1	616	CLA	CAA-CBA-CGA-O1A
22	U	604	CLA	CAA-CBA-CGA-O2A
22	L	302	CLA	CAA-CBA-CGA-O2A
22	B	810	CLA	C2-C3-C5-C6
22	9	609	CLA	C4C-C3C-CAC-CBC
22	5	603	CLA	CAA-CBA-CGA-O2A
22	U	603	CLA	C10-C11-C12-C13
22	B	804	CLA	C15-C16-C17-C18
22	8	612	CLA	O1A-CGA-O2A-C1
22	1	614	CLA	CAA-CBA-CGA-O2A
22	A	807	CLA	CAA-CBA-CGA-O2A
22	A	824	CLA	CAA-CBA-CGA-O2A
28	G	202	LMG	O8-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
26	A	847	LHG	O10-C23-O8-C6
22	A	818	CLA	C15-C16-C17-C18
22	A	827	CLA	C5-C6-C7-C8
21	7	608	CHL	CAA-CBA-CGA-O1A
22	3	614	CLA	CAA-CBA-CGA-O1A
21	U	609	CHL	CAA-CBA-CGA-O2A
22	A	830	CLA	CAA-CBA-CGA-O2A
28	2	631	LMG	C31-C32-C33-C34
22	A	811	CLA	CBA-CGA-O2A-C1
22	A	834	CLA	C3-C5-C6-C7
22	B	818	CLA	C3-C5-C6-C7
22	3	609	CLA	CAA-CBA-CGA-O2A
22	A	806	CLA	CAA-CBA-CGA-O2A
22	A	842	CLA	CAA-CBA-CGA-O2A
22	A	841	CLA	C8-C10-C11-C12
21	U	601	CHL	C12-C13-C15-C16
22	3	612	CLA	C12-C13-C15-C16
22	A	836	CLA	C6-C7-C8-C10
28	A	860	LMG	C12-C13-C14-C15
26	W	2630	LHG	O9-C7-O7-C5
22	G	204	CLA	O1D-CGD-O2D-CED
22	B	802	CLA	CAA-CBA-CGA-O2A
22	5	602	CLA	CAA-CBA-CGA-O2A
22	A	816	CLA	CAA-CBA-CGA-O2A
22	A	830	CLA	C11-C10-C8-C9
22	B	811	CLA	C11-C10-C8-C9
22	F	301	CLA	C11-C10-C8-C9
22	9	602	CLA	C6-C7-C8-C9
22	4	612	CLA	CAA-CBA-CGA-O2A
22	5	606	CLA	CAA-CBA-CGA-O1A
22	B	821	CLA	CBA-CGA-O2A-C1
22	6	614	CLA	CBA-CGA-O2A-C1
22	4	602	CLA	CAA-CBA-CGA-O2A
22	4	603	CLA	CAA-CBA-CGA-O1A
22	A	854	CLA	C11-C12-C13-C14
22	A	810	CLA	O1A-CGA-O2A-C1
22	7	603	CLA	CAA-CBA-CGA-O1A
22	7	607	CLA	CAA-CBA-CGA-O1A
22	A	818	CLA	C2A-CAA-CBA-CGA
22	7	613	CLA	C2A-CAA-CBA-CGA
22	3	604	CLA	CAA-CBA-CGA-O1A
28	J	104	LMG	O7-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
21	U	607	CHL	C10-C11-C12-C13
21	6	602	CHL	CAA-CBA-CGA-O1A
22	6	603	CLA	CAA-CBA-CGA-O1A
22	A	814	CLA	C16-C17-C18-C19
22	7	613	CLA	C6-C7-C8-C10
22	A	815	CLA	C4-C3-C5-C6
26	A	847	LHG	O1-C1-C2-C3
21	8	608	CHL	CAA-CBA-CGA-O2A
22	1	609	CLA	C10-C11-C12-C13
27	B	843	BCR	C11-C12-C13-C14
27	I	101	BCR	C21-C22-C23-C24
22	1	604	CLA	CBA-CGA-O2A-C1
21	V	601	CHL	C10-C11-C12-C13
21	V	606	CHL	CHA-CBD-CGD-O2D
21	4	608	CHL	C1A-C2A-CAA-CBA
21	6	601	CHL	C1A-C2A-CAA-CBA
21	8	606	CHL	C1A-C2A-CAA-CBA
22	2	613	CLA	C1A-C2A-CAA-CBA
22	A	806	CLA	C1A-C2A-CAA-CBA
22	A	826	CLA	C1A-C2A-CAA-CBA
22	A	838	CLA	C1A-C2A-CAA-CBA
22	B	815	CLA	C1A-C2A-CAA-CBA
22	G	201	CLA	C1A-C2A-CAA-CBA
22	9	604	CLA	C1A-C2A-CAA-CBA
26	2	630	LHG	C1-C2-C3-O3
21	U	601	CHL	CAA-CBA-CGA-O1A
22	V	602	CLA	CAA-CBA-CGA-O1A
22	A	807	CLA	C5-C6-C7-C8
22	5	603	CLA	CAA-CBA-CGA-O1A
22	U	603	CLA	C2-C1-O2A-CGA
22	A	807	CLA	C2-C1-O2A-CGA
22	B	828	CLA	C2-C1-O2A-CGA
22	7	604	CLA	C2-C1-O2A-CGA
22	A	827	CLA	CBA-CGA-O2A-C1
22	A	814	CLA	CAA-CBA-CGA-O1A
22	A	836	CLA	CAA-CBA-CGA-O1A
22	B	834	CLA	CAA-CBA-CGA-O1A
22	9	610	CLA	CAA-CBA-CGA-O1A
26	8	630	LHG	O9-C7-C8-C9
22	7	609	CLA	CAA-CBA-CGA-O2A
28	G	202	LMG	O10-C28-C29-C30
22	1	602	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
26	6	630	LHG	C3-O3-P-O5
26	9	2630	LHG	C4-O6-P-O5
22	B	840	CLA	C4C-C3C-CAC-CBC
22	3	607	CLA	CAA-CBA-CGA-O1A
22	4	602	CLA	CAA-CBA-CGA-O1A
22	A	824	CLA	CAA-CBA-CGA-O1A
22	A	830	CLA	CAA-CBA-CGA-O1A
22	L	302	CLA	CAA-CBA-CGA-O1A
22	L	304	CLA	CAA-CBA-CGA-O1A
26	6	630	LHG	O10-C23-C24-C25
28	J	104	LMG	O9-C10-C11-C12
32	B	850	DGD	O1A-C1A-C2A-C3A
22	1	604	CLA	O1A-CGA-O2A-C1
22	3	614	CLA	CAA-CBA-CGA-O2A
23	W	2620	LUT	C1-C6-C7-C8
23	9	620	LUT	C1-C6-C7-C8
27	B	845	BCR	C23-C24-C25-C30
27	F	305	BCR	C5-C6-C7-C8
27	7	620	BCR	C5-C6-C7-C8
22	1	611	CLA	C15-C16-C17-C18
22	8	612	CLA	CAA-CBA-CGA-O1A
22	A	811	CLA	O1A-CGA-O2A-C1
22	A	827	CLA	O1A-CGA-O2A-C1
22	5	612	CLA	CAA-CBA-CGA-O2A
22	B	803	CLA	C8-C10-C11-C12
22	9	611	CLA	C10-C11-C12-C13
22	A	810	CLA	CBA-CGA-O2A-C1
22	U	604	CLA	CAA-CBA-CGA-O1A
22	1	614	CLA	CAA-CBA-CGA-O1A
22	2	609	CLA	CAA-CBA-CGA-O1A
22	2	613	CLA	CAA-CBA-CGA-O1A
22	A	807	CLA	CAA-CBA-CGA-O1A
22	5	602	CLA	CAA-CBA-CGA-O1A
28	2	631	LMG	O10-C28-C29-C30
22	A	824	CLA	C5-C6-C7-C8
22	V	604	CLA	CAA-CBA-CGA-O2A
22	8	609	CLA	CAA-CBA-CGA-O2A
22	4	613	CLA	C5-C6-C7-C8
22	L	303	CLA	C15-C16-C17-C18
26	U	2630	LHG	C7-C8-C9-C10
21	U	609	CHL	CAA-CBA-CGA-O1A
22	B	822	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
22	1	602	CLA	C4-C3-C5-C6
22	B	817	CLA	C4-C3-C5-C6
22	A	816	CLA	CAA-CBA-CGA-O1A
21	W	607	CHL	CAD-CBD-CGD-O1D
21	4	618	CHL	CAD-CBD-CGD-O1D
22	U	613	CLA	CAD-CBD-CGD-O1D
22	U	614	CLA	CAD-CBD-CGD-O1D
22	A	814	CLA	CAD-CBD-CGD-O1D
22	A	819	CLA	CAD-CBD-CGD-O1D
22	A	829	CLA	CAD-CBD-CGD-O1D
22	B	823	CLA	CAD-CBD-CGD-O1D
22	B	830	CLA	CAD-CBD-CGD-O1D
22	K	204	CLA	CAD-CBD-CGD-O1D
22	5	604	CLA	CAD-CBD-CGD-O1D
22	9	602	CLA	CAD-CBD-CGD-O1D
22	6	614	CLA	O1A-CGA-O2A-C1
22	B	828	CLA	CAA-CBA-CGA-O2A
21	U	601	CHL	C14-C13-C15-C16
22	4	602	CLA	C14-C13-C15-C16
22	A	805	CLA	C11-C12-C13-C14
22	A	815	CLA	C6-C7-C8-C9
22	A	820	CLA	C11-C10-C8-C9
22	B	824	CLA	C6-C7-C8-C9
22	B	802	CLA	C5-C6-C7-C8
21	W	601	CHL	CAA-CBA-CGA-O2A
22	1	613	CLA	CAA-CBA-CGA-O2A
26	W	2630	LHG	C16-C17-C18-C19
22	3	613	CLA	C10-C11-C12-C13
22	A	834	CLA	C13-C15-C16-C17
22	B	802	CLA	C8-C10-C11-C12
26	B	851	LHG	O10-C23-O8-C6
22	A	816	CLA	C2A-CAA-CBA-CGA
22	1	604	CLA	CAA-CBA-CGA-O2A
22	1	612	CLA	CAA-CBA-CGA-O2A
26	A	846	LHG	O8-C23-C24-C25
22	A	812	CLA	C15-C16-C17-C18
26	1	630	LHG	C7-C8-C9-C10
21	8	608	CHL	CAA-CBA-CGA-O1A
22	B	810	CLA	C4-C3-C5-C6
21	U	607	CHL	C2-C3-C5-C6
21	U	608	CHL	CAD-CBD-CGD-O2D
21	V	606	CHL	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
21	V	608	CHL	CAD-CBD-CGD-O2D
21	3	608	CHL	C3A-C2A-CAA-CBA
22	V	612	CLA	CAD-CBD-CGD-O2D
22	V	613	CLA	C3A-C2A-CAA-CBA
22	W	603	CLA	CHA-CBD-CGD-O1D
22	W	614	CLA	CAD-CBD-CGD-O2D
22	1	613	CLA	C3A-C2A-CAA-CBA
22	2	613	CLA	C3A-C2A-CAA-CBA
22	3	609	CLA	C11-C12-C13-C15
22	4	610	CLA	C11-C10-C8-C7
22	A	805	CLA	C11-C12-C13-C15
22	A	808	CLA	C6-C7-C8-C10
22	A	815	CLA	C6-C7-C8-C10
22	A	820	CLA	C11-C10-C8-C7
22	A	838	CLA	C3A-C2A-CAA-CBA
22	B	808	CLA	C12-C13-C15-C16
22	B	809	CLA	C11-C10-C8-C7
22	B	811	CLA	C11-C10-C8-C7
22	B	816	CLA	C11-C12-C13-C15
22	B	838	CLA	C3A-C2A-CAA-CBA
22	G	201	CLA	C3A-C2A-CAA-CBA
22	9	603	CLA	C3A-C2A-CAA-CBA
22	3	609	CLA	CAA-CBA-CGA-O1A
22	A	806	CLA	CAA-CBA-CGA-O1A
22	B	823	CLA	CAA-CBA-CGA-O2A
22	B	839	CLA	CAA-CBA-CGA-O2A
22	F	304	CLA	CAA-CBA-CGA-O2A
22	1	602	CLA	C15-C16-C17-C18
28	2	631	LMG	C17-C18-C19-C20
22	B	806	CLA	C10-C11-C12-C13
24	8	620	XAT	C11-C12-C13-C14
22	1	613	CLA	CAA-CBA-CGA-O1A
22	B	828	CLA	CAA-CBA-CGA-O1A
22	3	611	CLA	CAA-CBA-CGA-O2A
22	B	803	CLA	CAA-CBA-CGA-O2A
22	B	825	CLA	CAA-CBA-CGA-O2A
22	6	610	CLA	CAA-CBA-CGA-O2A
22	W	610	CLA	C10-C11-C12-C13
22	A	842	CLA	CAA-CBA-CGA-O1A
22	B	803	CLA	CAA-CBA-CGA-O1A
22	F	304	CLA	CAA-CBA-CGA-O1A
22	A	838	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	A	815	CLA	CAA-CBA-CGA-O2A
22	A	830	CLA	C13-C15-C16-C17
22	B	806	CLA	C5-C6-C7-C8
26	A	846	LHG	O10-C23-C24-C25
22	3	614	CLA	C2A-CAA-CBA-CGA
22	2	612	CLA	CAA-CBA-CGA-O2A
21	W	601	CHL	CAA-CBA-CGA-O1A
22	2	612	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

259 monomers are involved in 569 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	G	202	LMG	2	0
27	A	856	BCR	5	0
22	V	613	CLA	2	0
22	7	610	CLA	1	0
22	V	602	CLA	4	0
22	5	602	CLA	2	0
22	B	827	CLA	1	0
23	1	617	LUT	3	0
27	B	847	BCR	4	0
22	A	841	CLA	1	0
22	U	604	CLA	2	0
21	4	606	CHL	3	0
22	5	609	CLA	6	0
22	3	604	CLA	2	0
22	A	820	CLA	1	0
21	6	607	CHL	1	0
22	B	832	CLA	1	0
22	U	614	CLA	3	0
22	B	814	CLA	1	0
22	7	609	CLA	5	0
22	4	609	CLA	2	0
27	A	851	BCR	12	0
23	V	2620	LUT	3	0
22	A	843	CLA	1	0
22	1	603	CLA	1	0
22	B	839	CLA	3	0
22	3	610	CLA	1	0
22	B	825	CLA	1	0
22	7	606	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	3	617	CLA	1	0
23	4	619	LUT	3	0
21	8	608	CHL	2	0
27	A	849	BCR	1	0
23	U	2620	LUT	3	0
22	A	826	CLA	1	0
22	7	612	CLA	1	0
25	U	2623	NEX	3	0
23	W	2620	LUT	3	0
23	9	620	LUT	5	0
23	6	619	LUT	2	0
23	5	617	LUT	3	0
22	8	602	CLA	4	0
22	W	602	CLA	2	0
21	V	605	CHL	1	0
22	F	303	CLA	1	0
21	6	618	CHL	2	0
22	A	806	CLA	2	0
22	8	610	CLA	2	0
22	5	613	CLA	2	0
24	4	620	XAT	11	0
22	1	602	CLA	1	0
21	W	609	CHL	1	0
22	A	829	CLA	3	0
21	9	608	CHL	4	0
22	B	828	CLA	3	0
22	B	812	CLA	1	0
24	8	620	XAT	4	0
22	A	822	CLA	1	0
22	2	604	CLA	2	0
22	A	817	CLA	1	0
21	8	618	CHL	2	0
21	U	609	CHL	3	0
22	B	830	CLA	1	0
26	U	2630	LHG	1	0
22	9	609	CLA	3	0
22	3	603	CLA	3	0
22	B	838	CLA	1	0
21	2	606	CHL	3	0
22	B	802	CLA	2	0
23	W	2621	LUT	3	0
27	B	801	BCR	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	815	CLA	2	0
22	B	833	CLA	2	0
22	5	603	CLA	2	0
21	6	601	CHL	1	0
22	B	816	CLA	1	0
22	6	611	CLA	1	0
24	2	620	XAT	6	0
22	9	612	CLA	1	0
23	U	2621	LUT	5	0
21	1	601	CHL	1	0
25	9	623	NEX	3	0
21	V	606	CHL	1	0
21	U	608	CHL	1	0
22	1	606	CLA	3	0
22	B	806	CLA	5	0
22	B	805	CLA	2	0
24	1	618	XAT	5	0
22	A	832	CLA	1	0
22	5	606	CLA	2	0
26	4	630	LHG	3	0
22	A	837	CLA	4	0
24	7	619	XAT	3	0
22	6	604	CLA	2	0
22	7	607	CLA	2	0
22	B	821	CLA	1	0
22	8	601	CLA	1	0
22	3	607	CLA	1	0
22	1	611	CLA	4	0
22	5	604	CLA	3	0
21	V	609	CHL	2	0
21	5	601	CHL	4	0
22	L	304	CLA	1	0
22	V	610	CLA	2	0
23	9	621	LUT	2	0
21	6	608	CHL	4	0
22	V	614	CLA	1	0
22	3	615	CLA	2	0
22	B	819	CLA	2	0
22	8	603	CLA	2	0
22	6	603	CLA	2	0
22	6	612	CLA	1	0
21	4	608	CHL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	839	CLA	1	0
24	3	619	XAT	6	0
22	B	836	CLA	1	0
27	L	306	BCR	5	0
22	5	610	CLA	1	0
22	1	610	CLA	1	0
22	3	606	CLA	2	0
22	K	201	CLA	2	0
22	B	809	CLA	1	0
21	8	607	CHL	2	0
22	8	613	CLA	3	0
22	4	614	CLA	1	0
27	2	621	BCR	5	0
22	A	809	CLA	5	0
25	V	2623	NEX	2	0
22	L	303	CLA	2	0
21	6	606	CHL	1	0
22	F	301	CLA	2	0
22	4	601	CLA	1	0
22	6	610	CLA	5	0
22	2	610	CLA	1	0
22	5	611	CLA	1	0
22	B	840	CLA	2	0
24	5	618	XAT	8	0
22	F	304	CLA	2	0
21	4	618	CHL	1	0
22	B	822	CLA	2	0
27	7	620	BCR	7	0
22	3	602	CLA	2	0
22	A	854	CLA	4	0
22	B	841	CLA	1	0
27	B	844	BCR	3	0
27	M	2001	BCR	5	0
22	1	609	CLA	2	0
22	A	803	CLA	7	0
21	W	606	CHL	2	0
21	2	608	CHL	3	0
27	B	848	BCR	1	0
22	A	835	CLA	1	0
22	3	613	CLA	1	0
22	B	804	CLA	3	0
23	V	2621	LUT	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	4	603	CLA	1	0
22	B	824	CLA	3	0
23	2	619	LUT	4	0
27	8	621	BCR	7	0
27	K	205	BCR	4	0
22	8	614	CLA	1	0
27	L	305	BCR	4	0
22	4	613	CLA	1	0
22	B	808	CLA	1	0
22	U	603	CLA	1	0
22	4	602	CLA	2	0
22	A	828	CLA	4	0
22	U	610	CLA	4	0
22	9	602	CLA	1	0
21	5	607	CHL	1	0
23	8	619	LUT	2	0
22	8	604	CLA	2	0
22	7	602	CLA	7	0
22	A	827	CLA	2	0
26	6	630	LHG	2	0
27	4	621	BCR	12	0
26	1	630	LHG	2	0
23	7	618	LUT	2	0
22	W	611	CLA	1	0
24	6	620	XAT	7	0
22	B	803	CLA	5	0
22	O	2002	CLA	4	0
22	5	616	CLA	2	0
27	O	2004	BCR	5	0
21	2	602	CHL	1	0
27	B	843	BCR	4	0
22	U	602	CLA	2	0
22	K	204	CLA	2	0
27	3	621	BCR	5	0
27	J	102	BCR	4	0
21	2	607	CHL	2	0
27	B	1609	BCR	8	0
21	8	606	CHL	1	0
22	4	610	CLA	4	0
21	2	618	CHL	1	0
21	9	601	CHL	3	0
22	V	604	CLA	1	0

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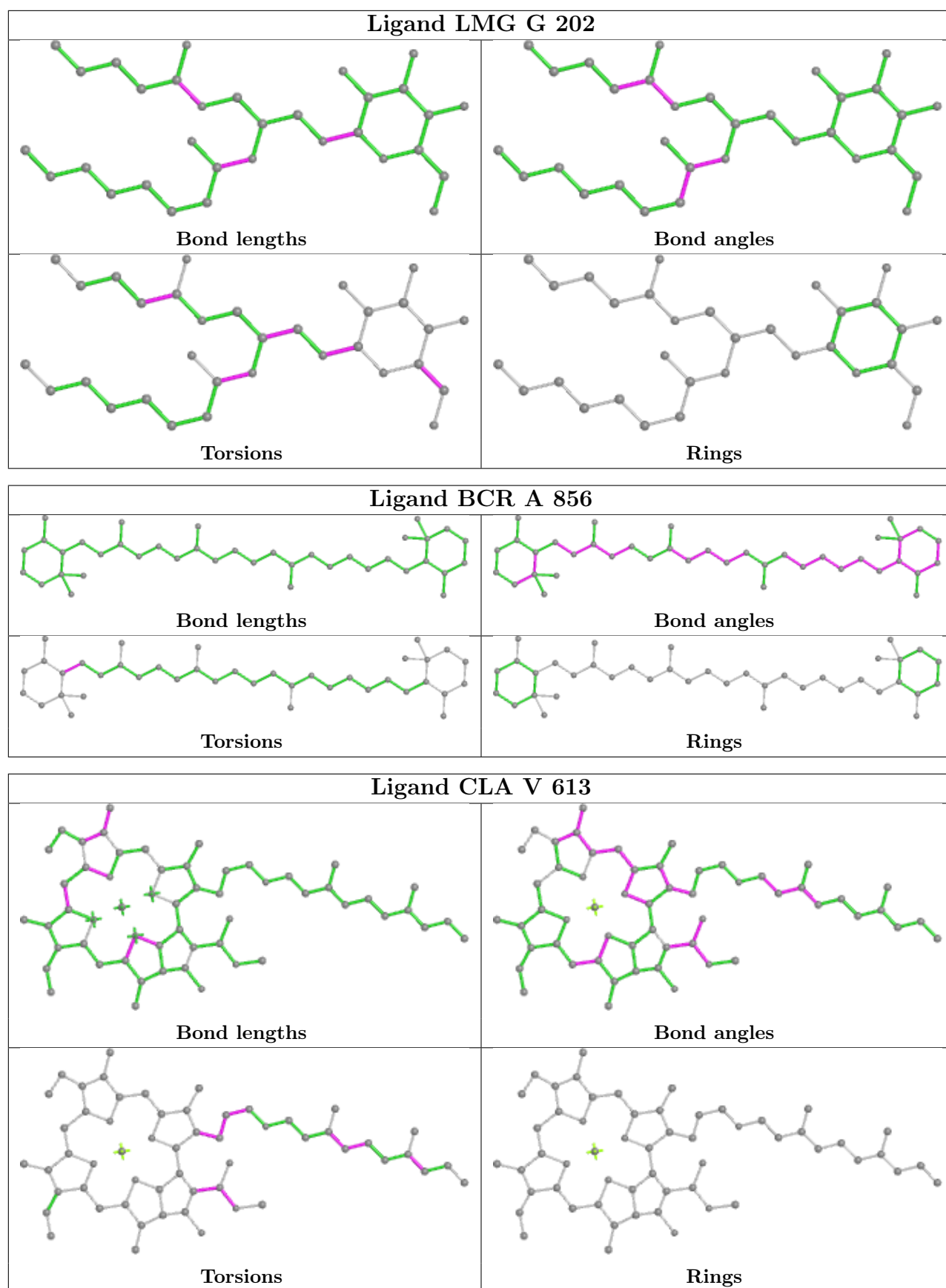
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	4	611	CLA	1	0
22	9	611	CLA	2	0
21	3	608	CHL	3	0
27	F	305	BCR	3	0
24	W	2622	XAT	1	0
27	1	619	BCR	1	0
22	9	613	CLA	1	0
22	A	801	CLA	5	0
21	W	608	CHL	1	0
22	7	613	CLA	2	0
22	A	808	CLA	2	0
22	B	817	CLA	1	0
21	2	601	CHL	2	0
22	W	610	CLA	1	0
22	2	613	CLA	2	0
27	6	621	BCR	5	0
22	6	609	CLA	3	0
21	9	607	CHL	2	0
22	A	836	CLA	2	0
27	G	205	BCR	4	0
21	1	607	CHL	1	0
27	L	301	BCR	4	0
21	U	607	CHL	4	0
27	A	852	BCR	9	0
22	3	609	CLA	4	0
22	U	613	CLA	1	0
22	8	609	CLA	5	0
26	W	2630	LHG	1	0
27	A	848	BCR	2	0
25	W	2623	NEX	3	0
22	B	823	CLA	4	0
22	W	604	CLA	1	0
21	9	605	CHL	2	0
22	B	813	CLA	3	0
22	7	603	CLA	1	0
21	4	607	CHL	1	0
22	B	837	CLA	2	0
21	7	608	CHL	3	0
27	B	845	BCR	6	0
22	A	845	CLA	1	0
22	G	201	CLA	4	0
27	3	620	BCR	11	0

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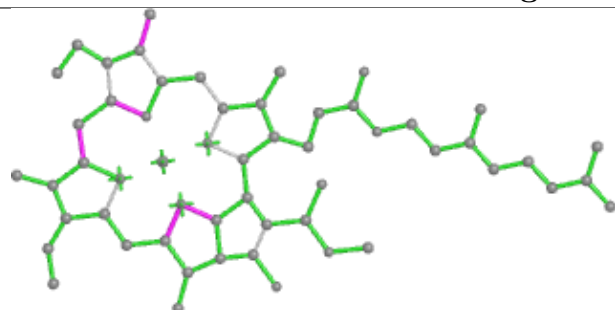
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	2	611	CLA	1	0
22	A	814	CLA	1	0
27	I	101	BCR	4	0
21	U	606	CHL	4	0
22	A	812	CLA	2	0
22	4	604	CLA	3	0
22	A	810	CLA	3	0
22	1	612	CLA	1	0
22	2	614	CLA	2	0
22	B	818	CLA	1	0
22	A	830	CLA	2	0
22	5	612	CLA	1	0
22	3	612	CLA	2	0
22	A	825	CLA	1	0
22	A	802	CLA	3	0
23	9	624	LUT	7	0
27	7	621	BCR	3	0
21	9	606	CHL	7	0
27	K	202	BCR	6	0
22	A	816	CLA	1	0

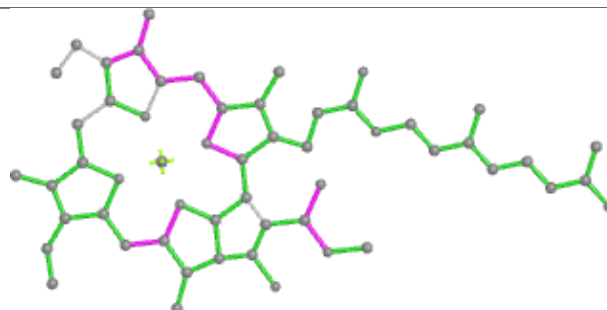
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



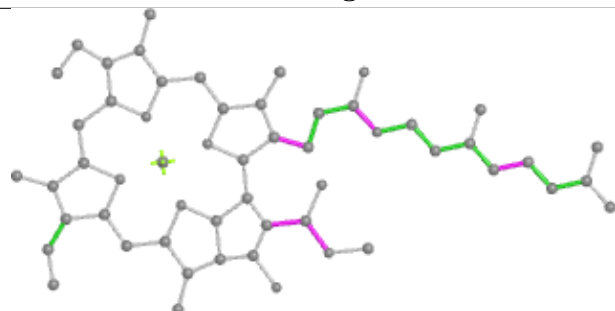
Ligand CLA 7 610



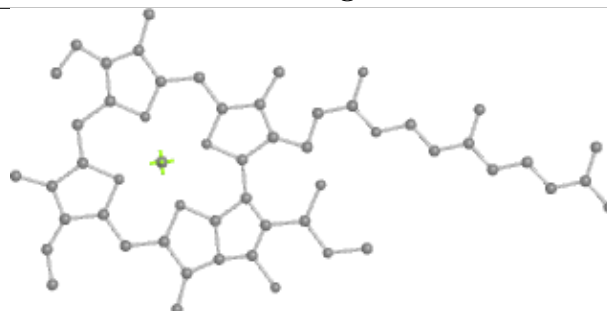
Bond lengths



Bond angles

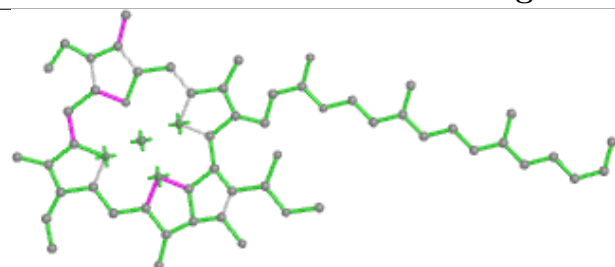


Torsions

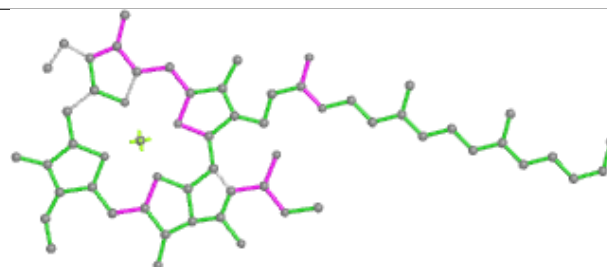


Rings

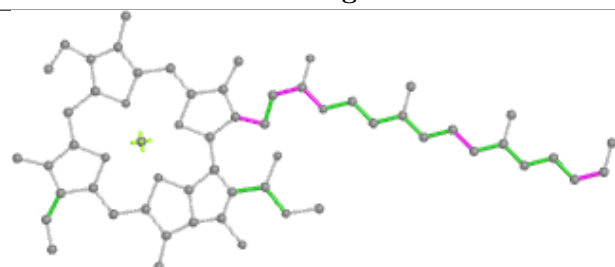
Ligand CLA V 602



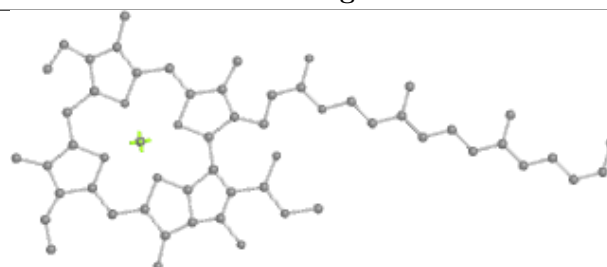
Bond lengths



Bond angles

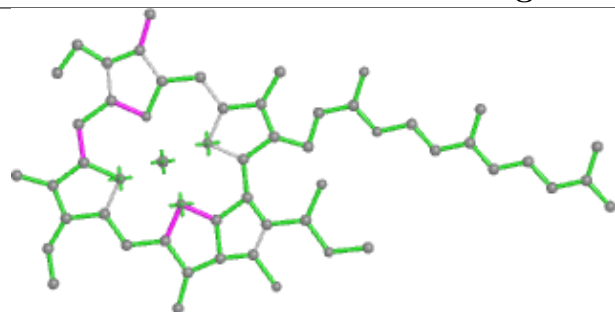


Torsions

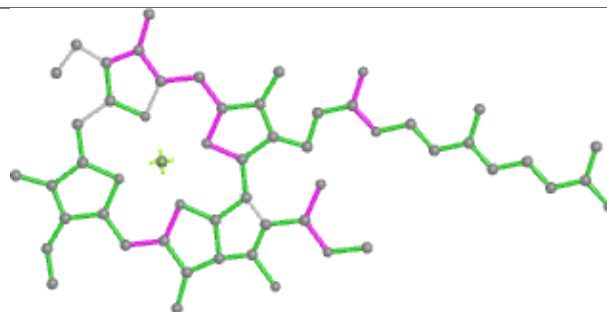


Rings

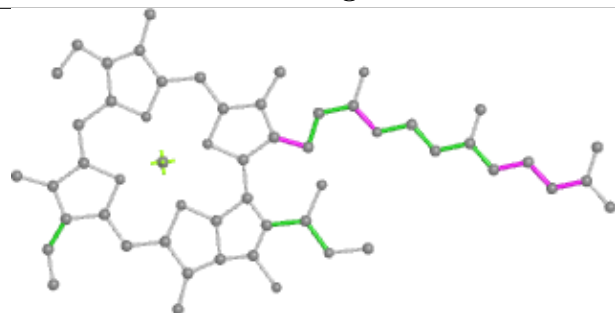
Ligand CLA A 833



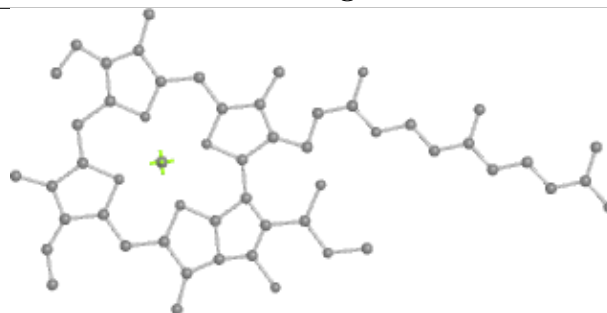
Bond lengths



Bond angles

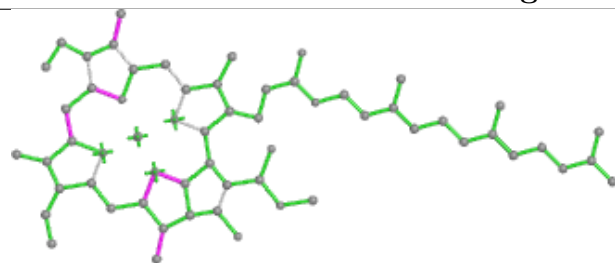


Torsions

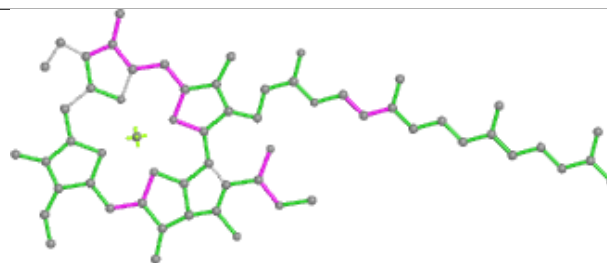


Rings

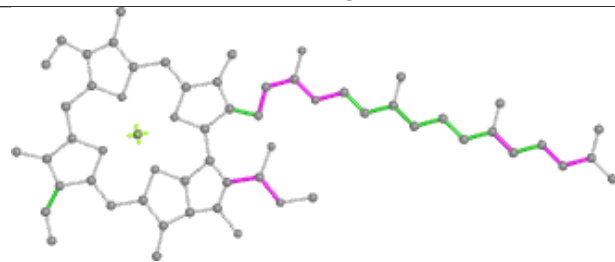
Ligand CLA 5 602



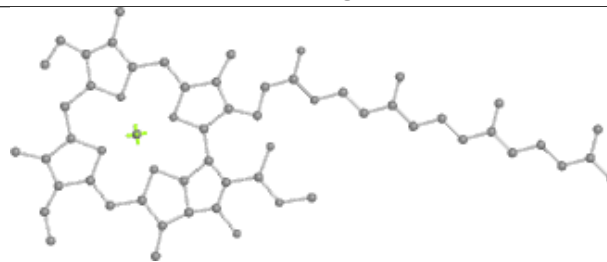
Bond lengths



Bond angles

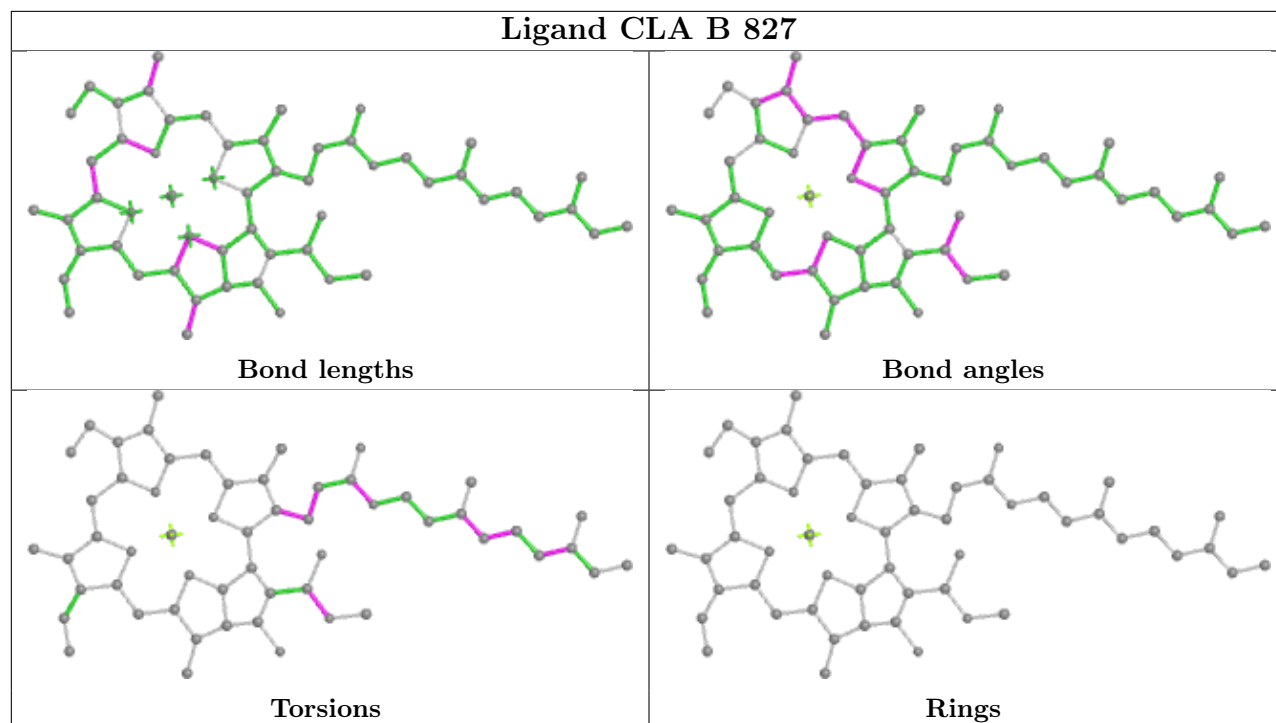


Torsions

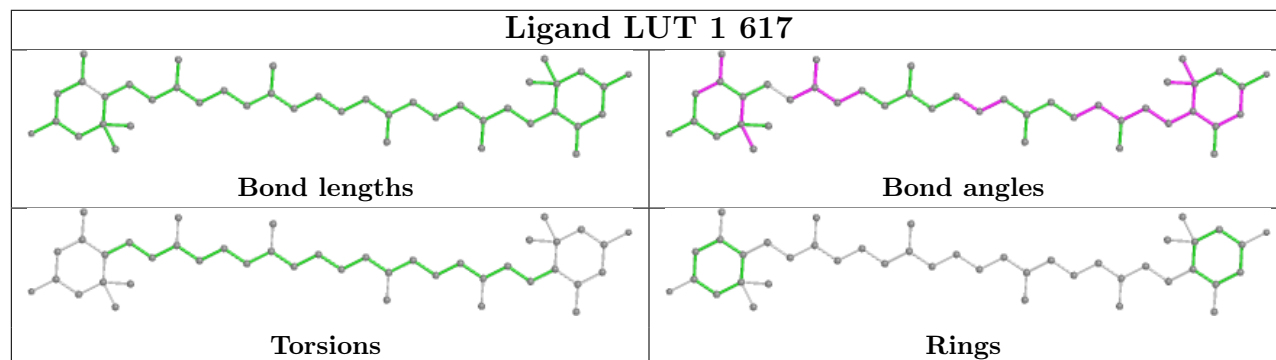


Rings

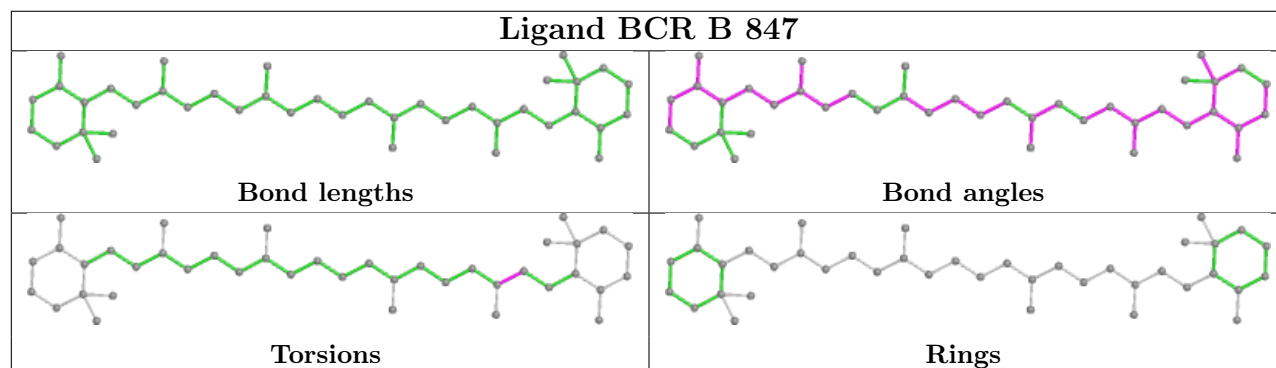
Ligand CLA B 827



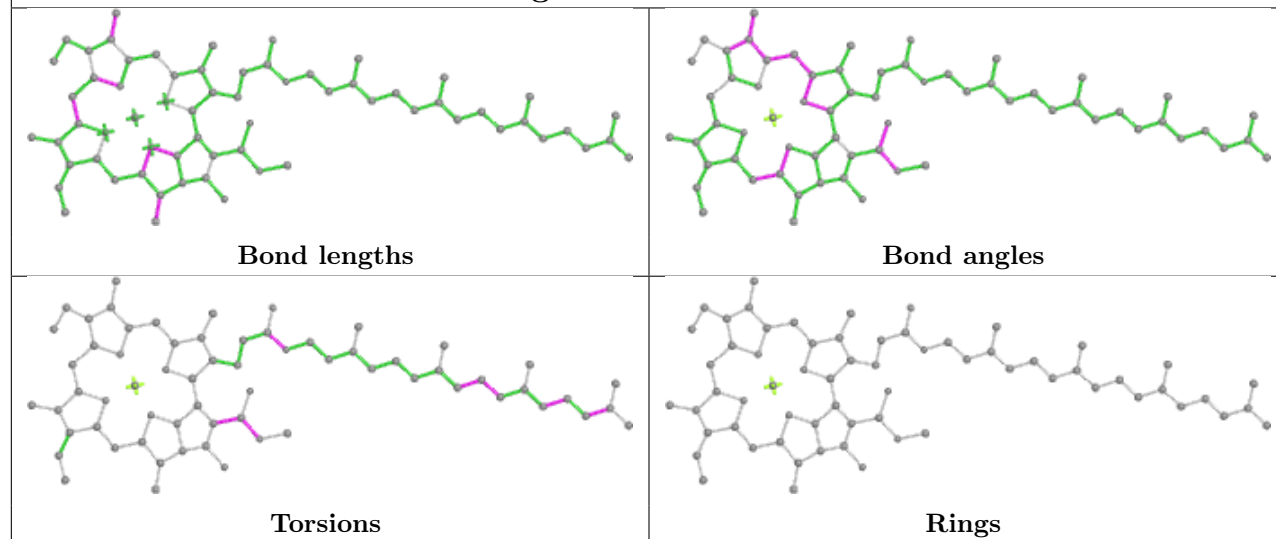
Ligand LUT 1 617



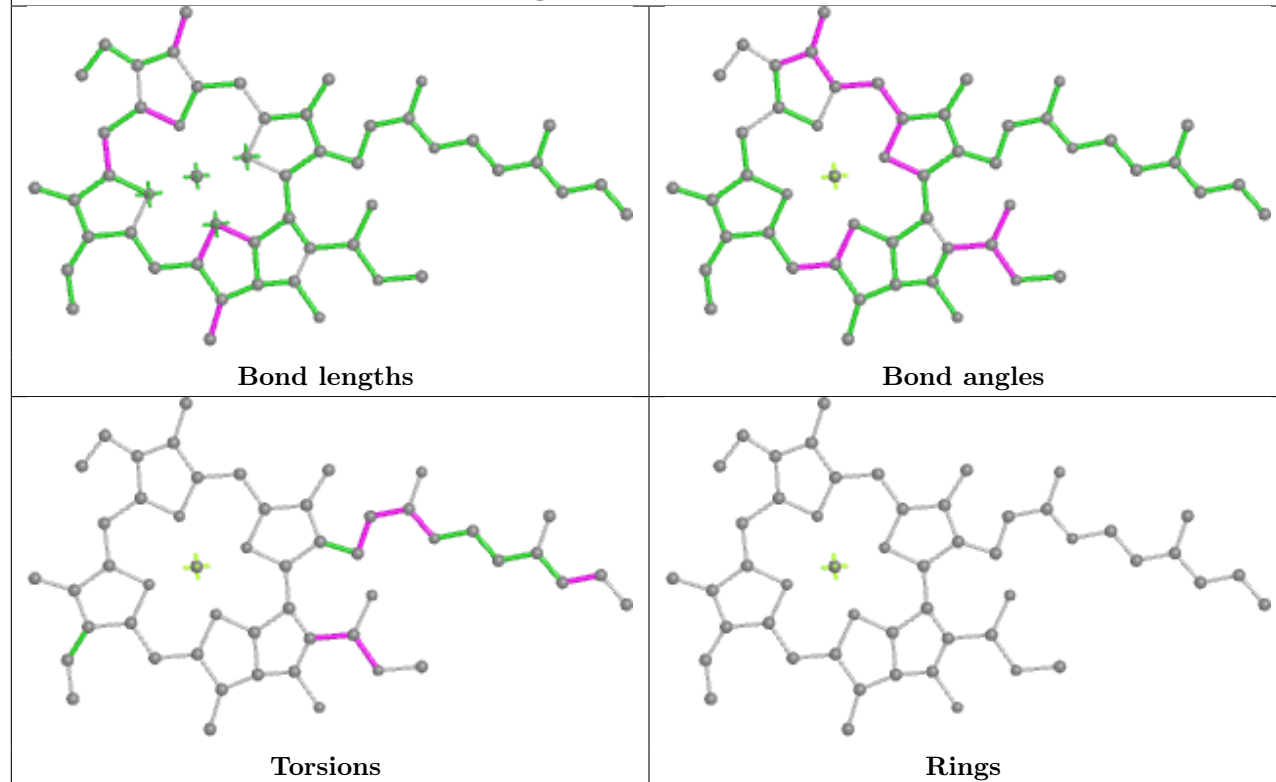
Ligand BCR B 847



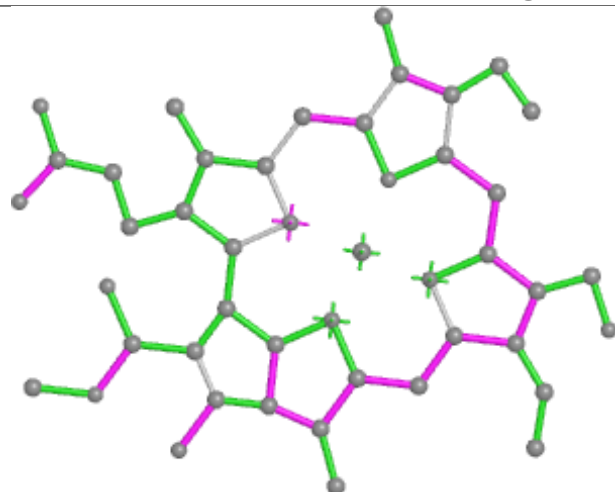
Ligand CLA A 841



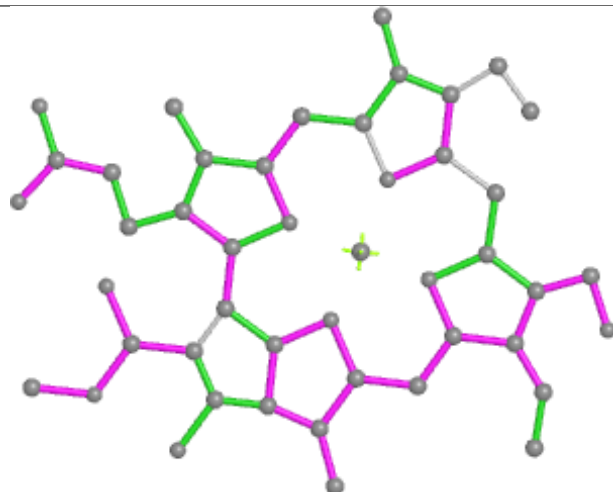
Ligand CLA U 604



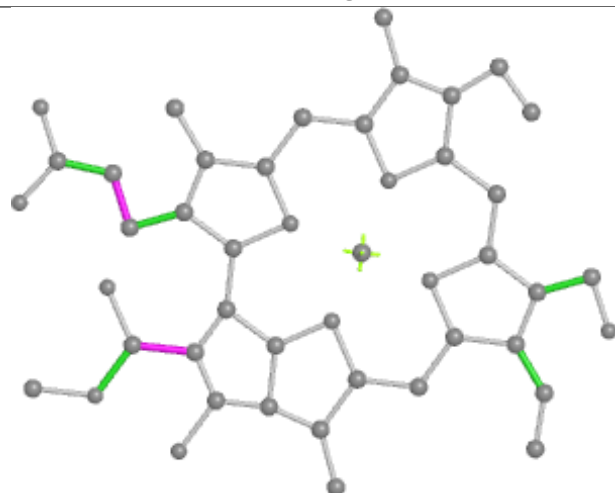
Ligand CHL 4 606



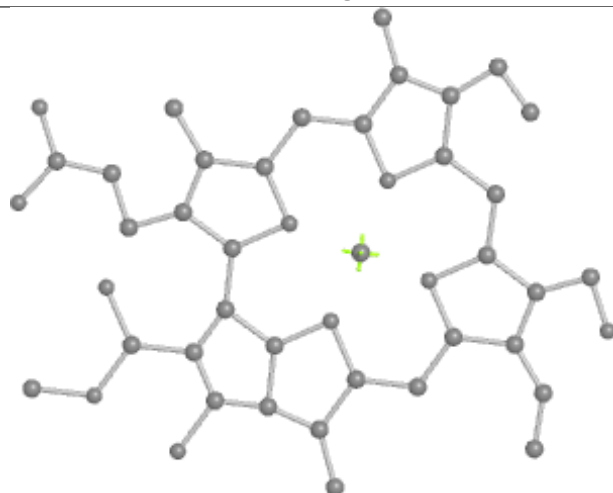
Bond lengths



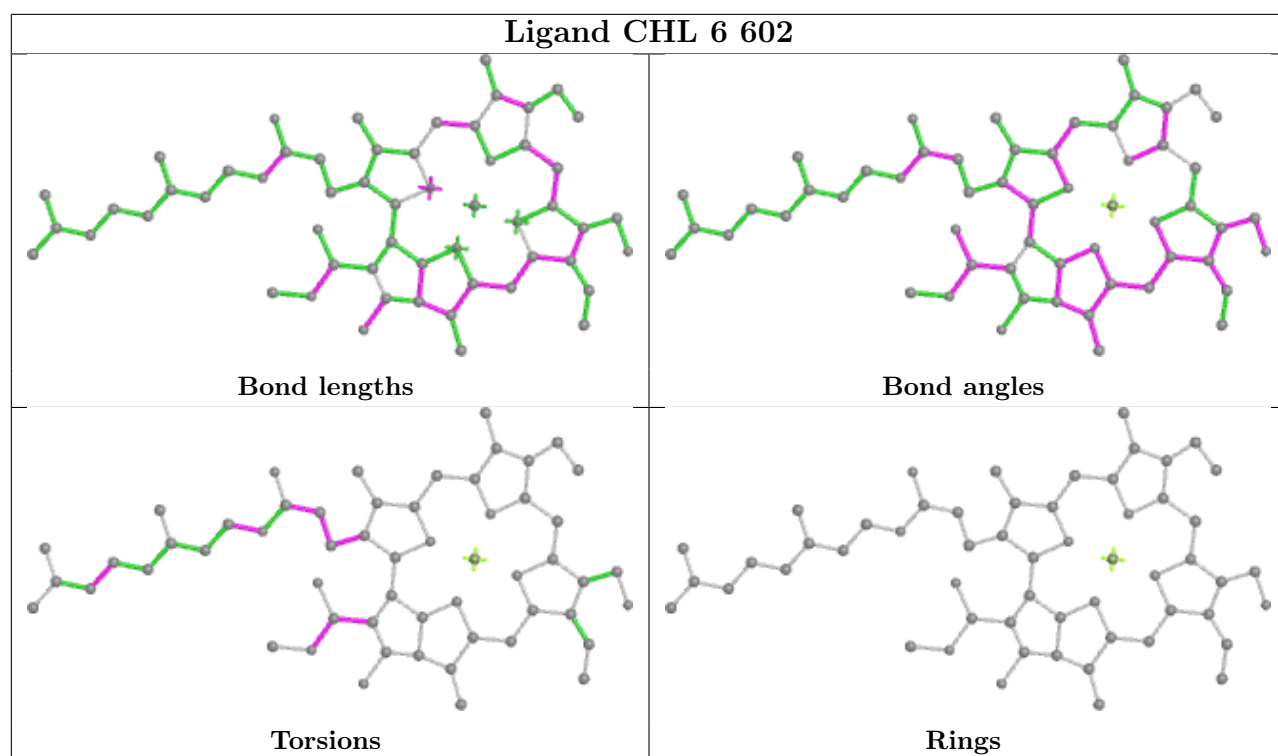
Bond angles



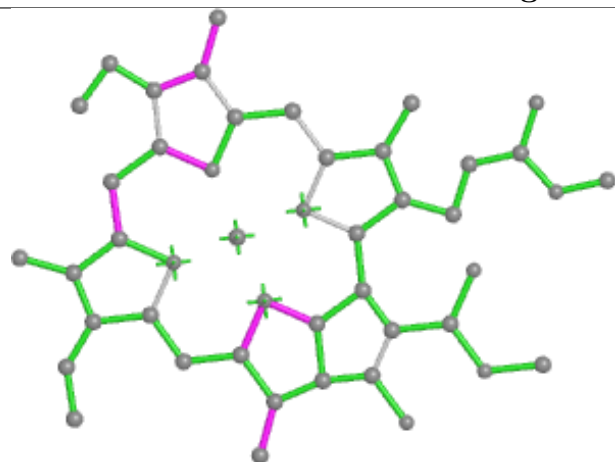
Torsions



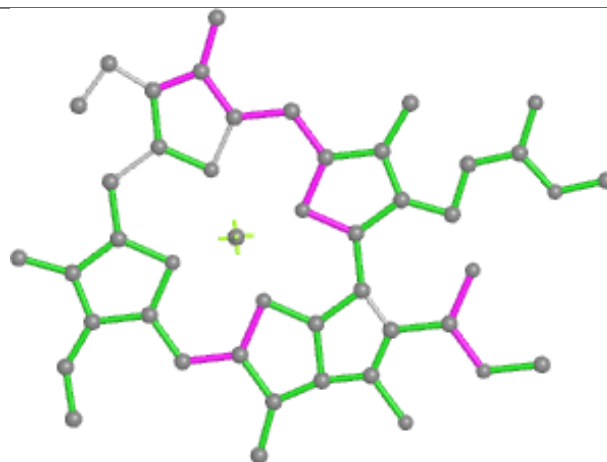
Rings



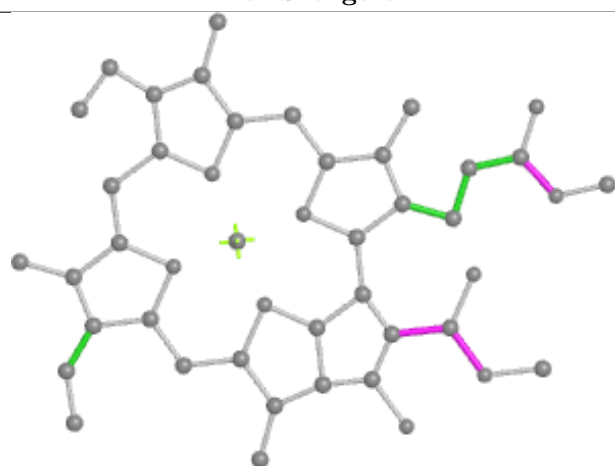
Ligand CLA 2 603



Bond lengths



Bond angles

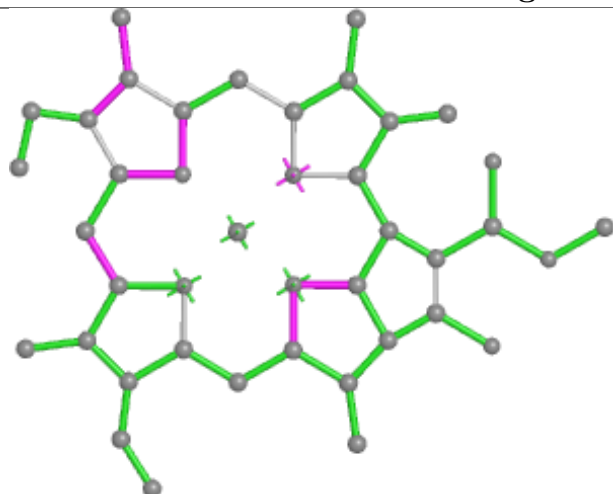


Torsions

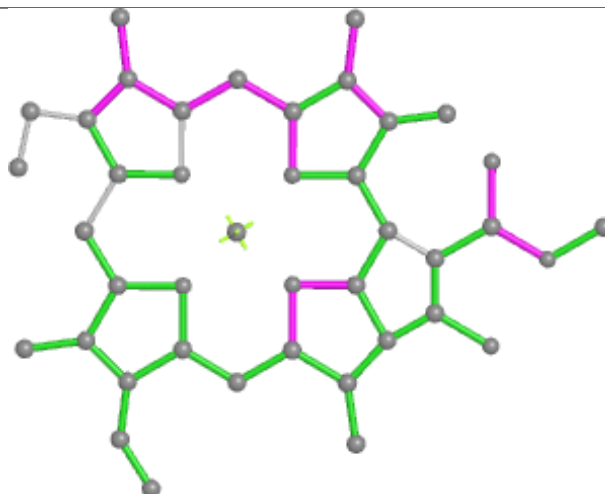


Rings

Ligand CLA 5 609



Bond lengths



Bond angles

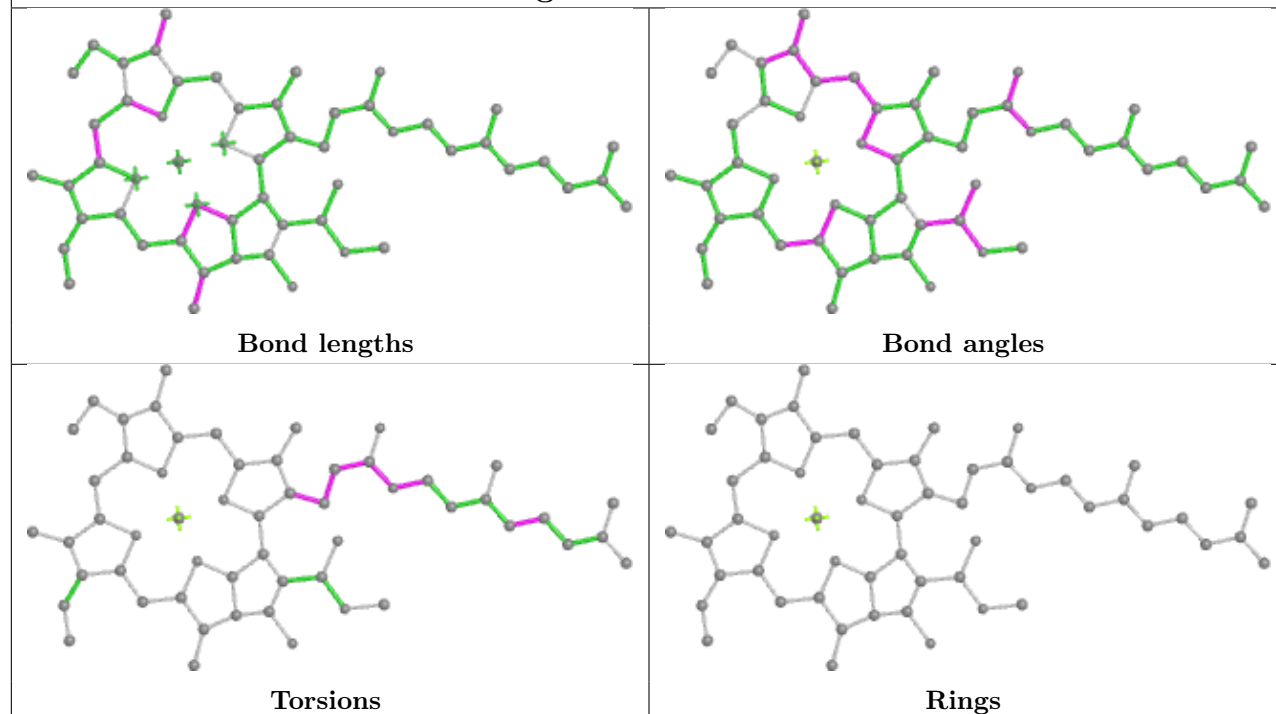


Torsions

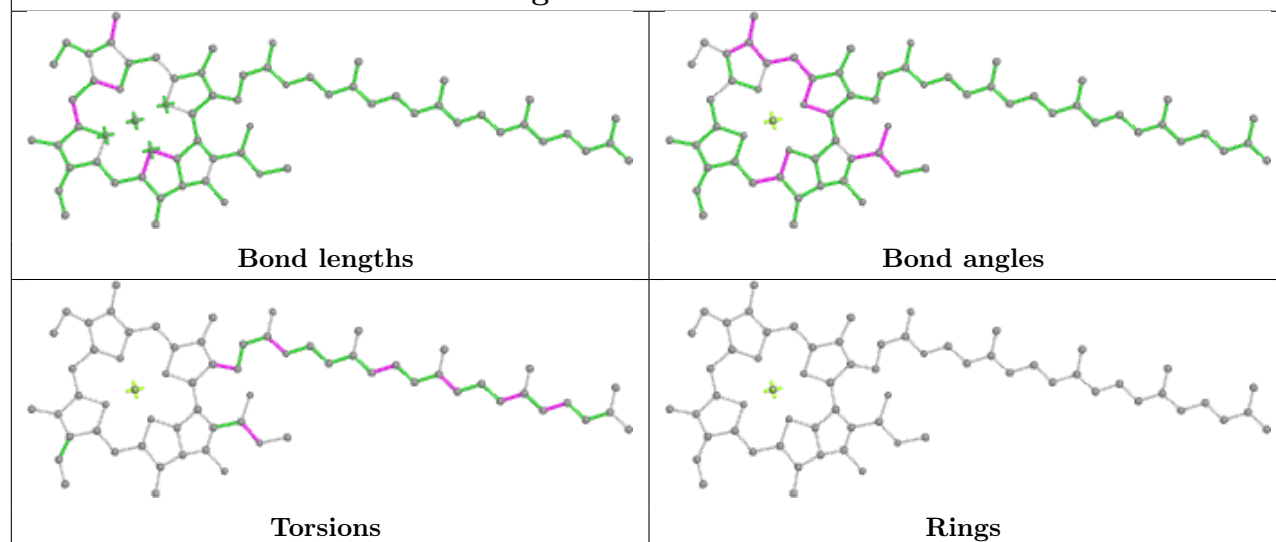


Rings

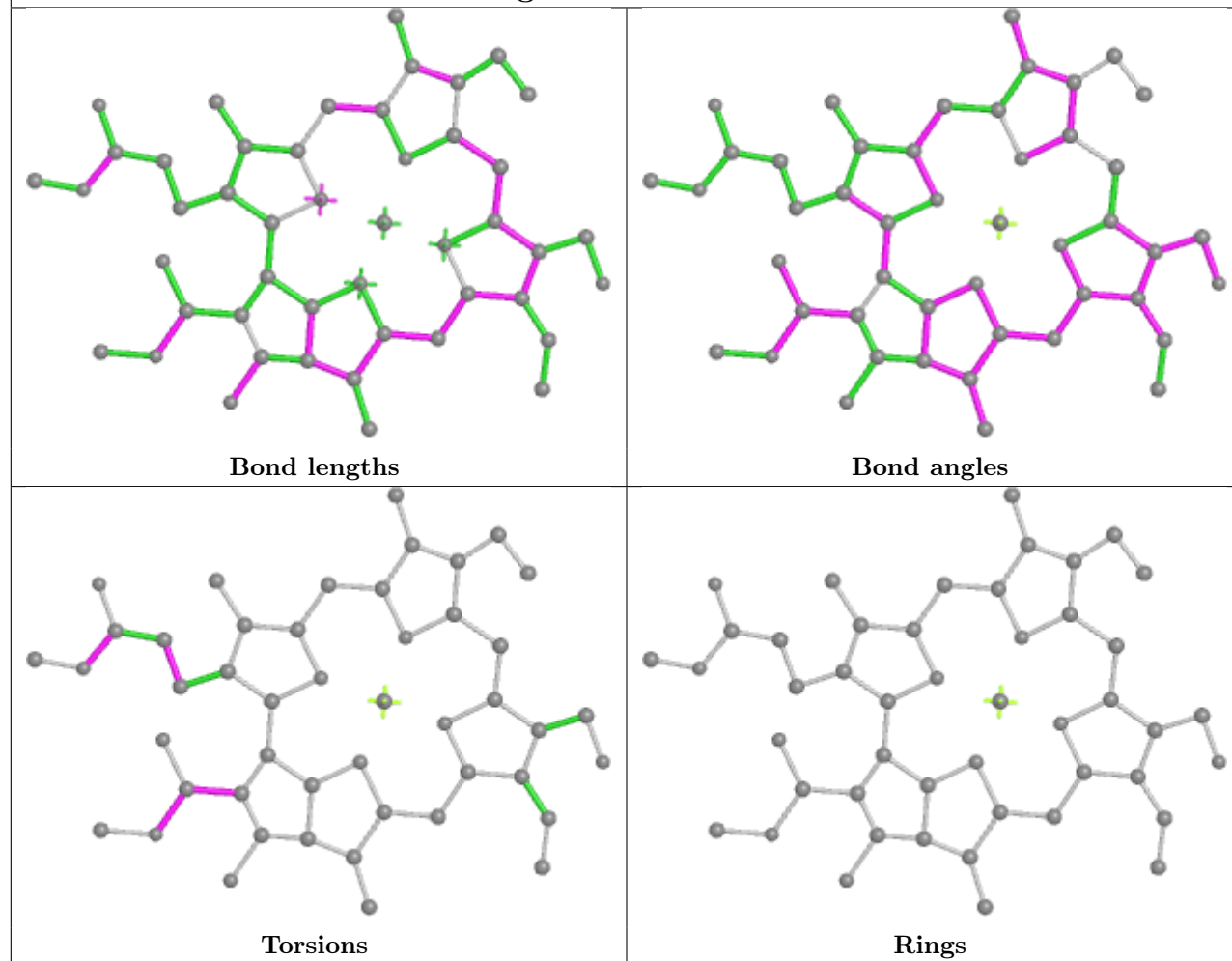
Ligand CLA 3 604



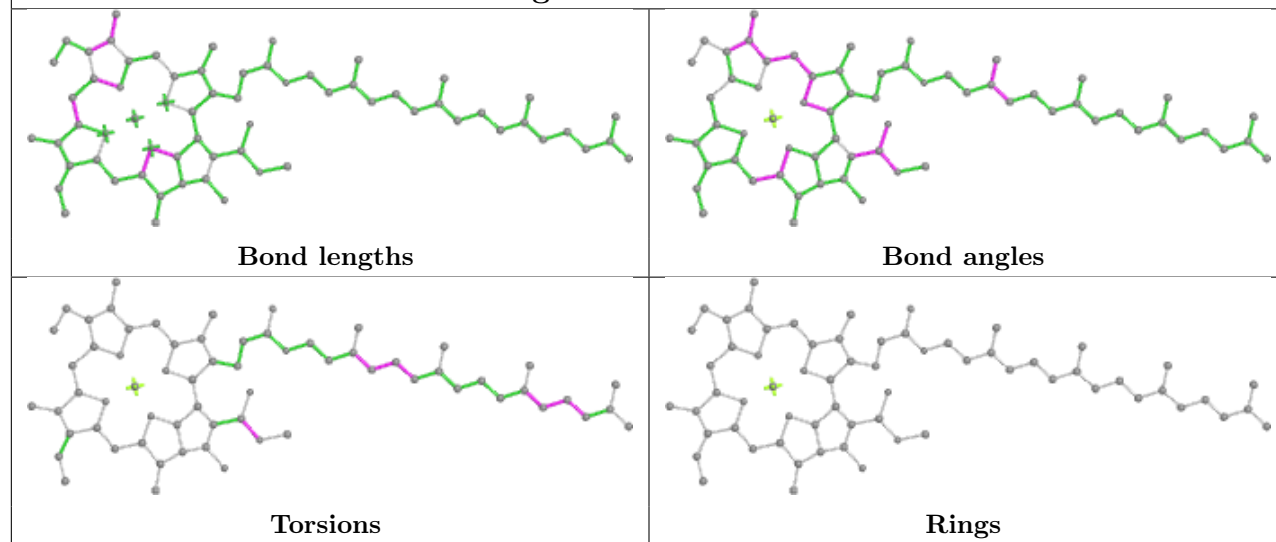
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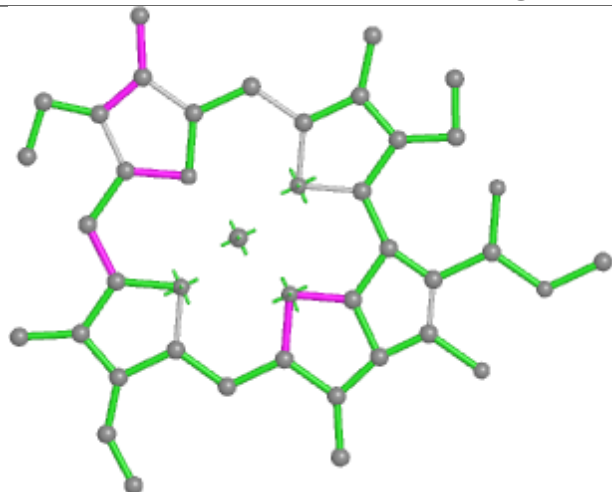
Ligand CHL 6 607



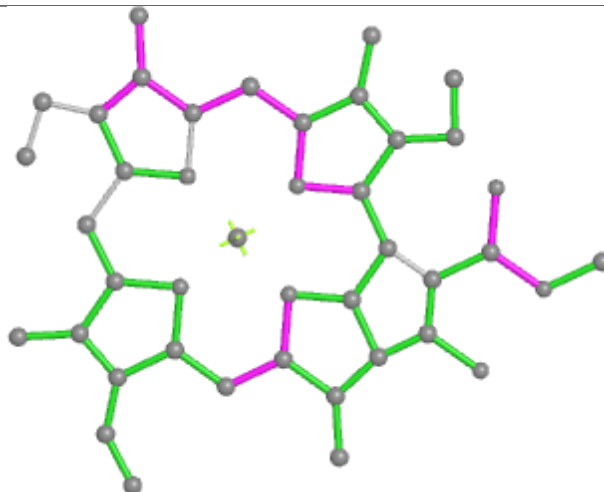
Ligand CLA B 832



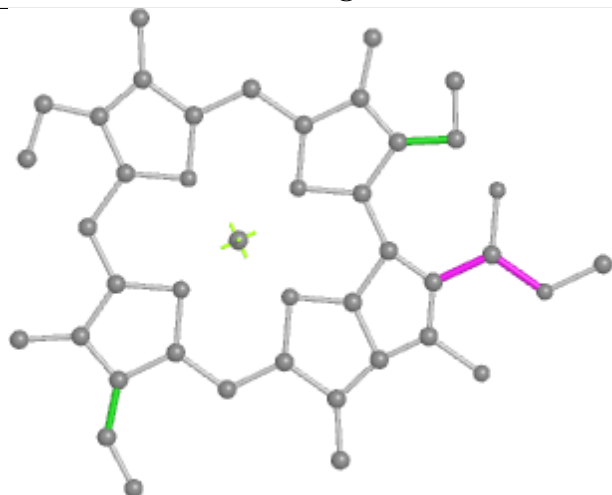
Ligand CLA U 614



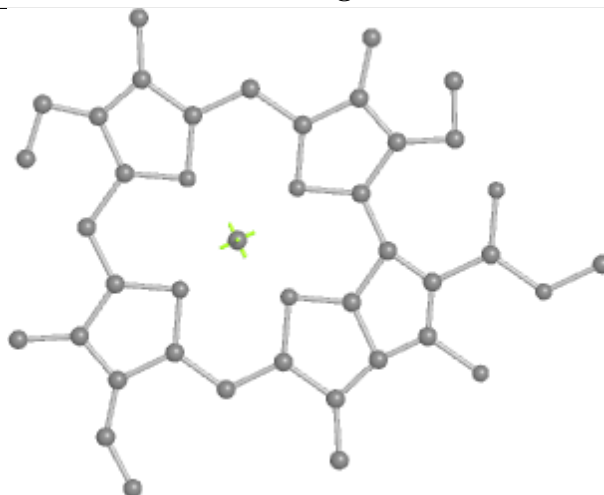
Bond lengths



Bond angles

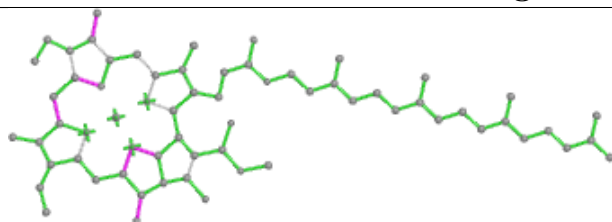


Torsions

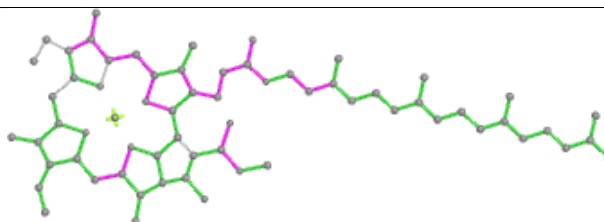


Rings

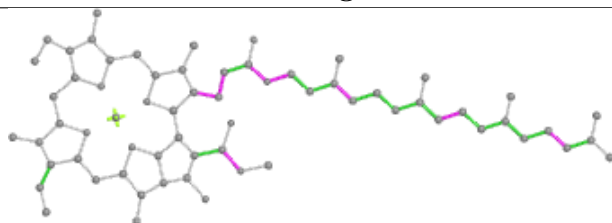
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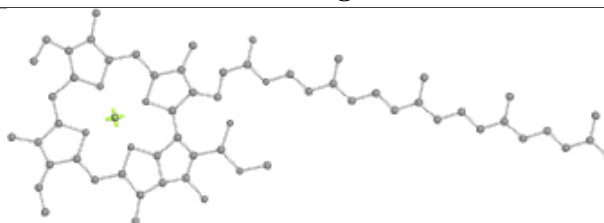
Bond lengths



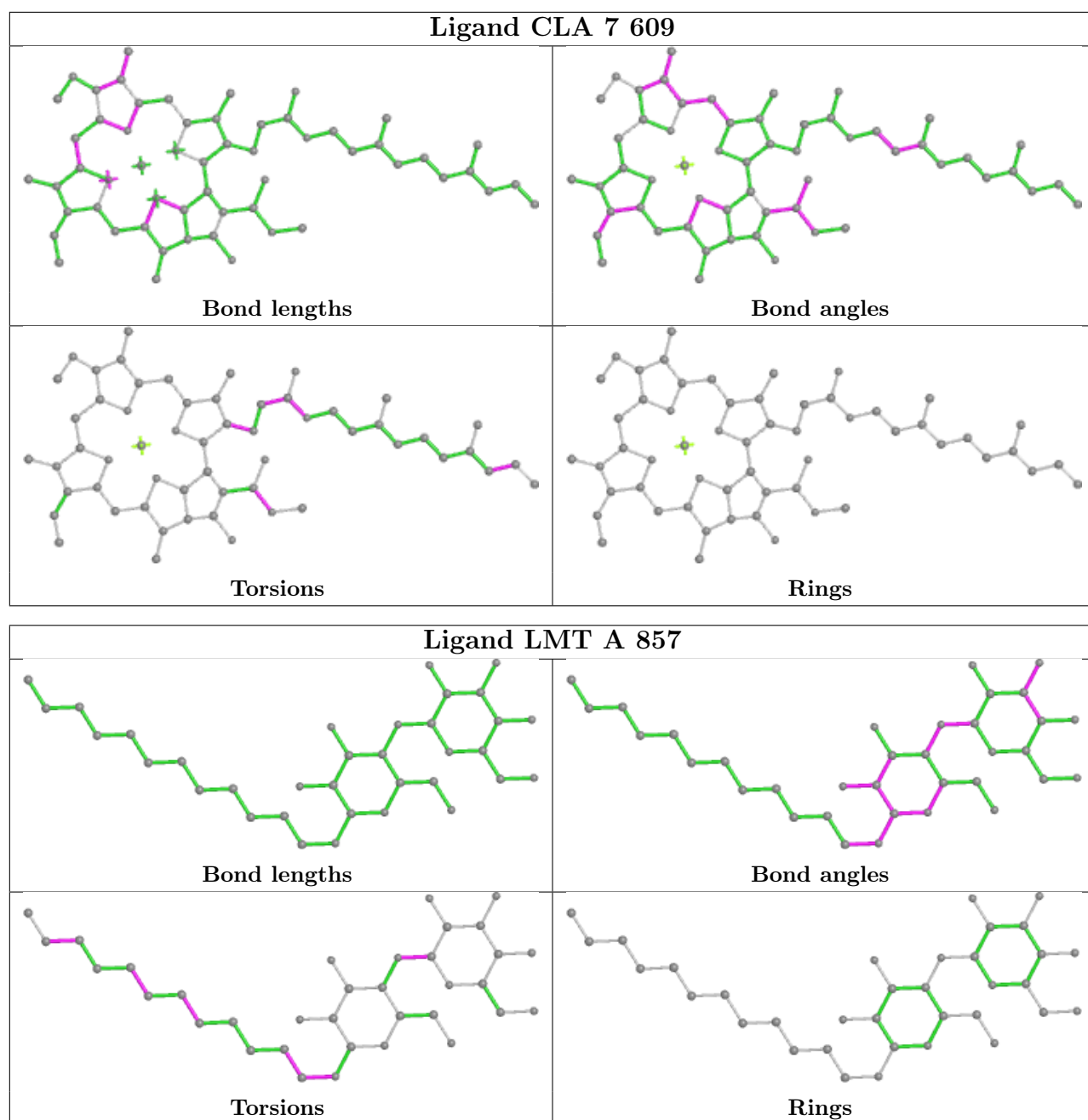
Bond angles



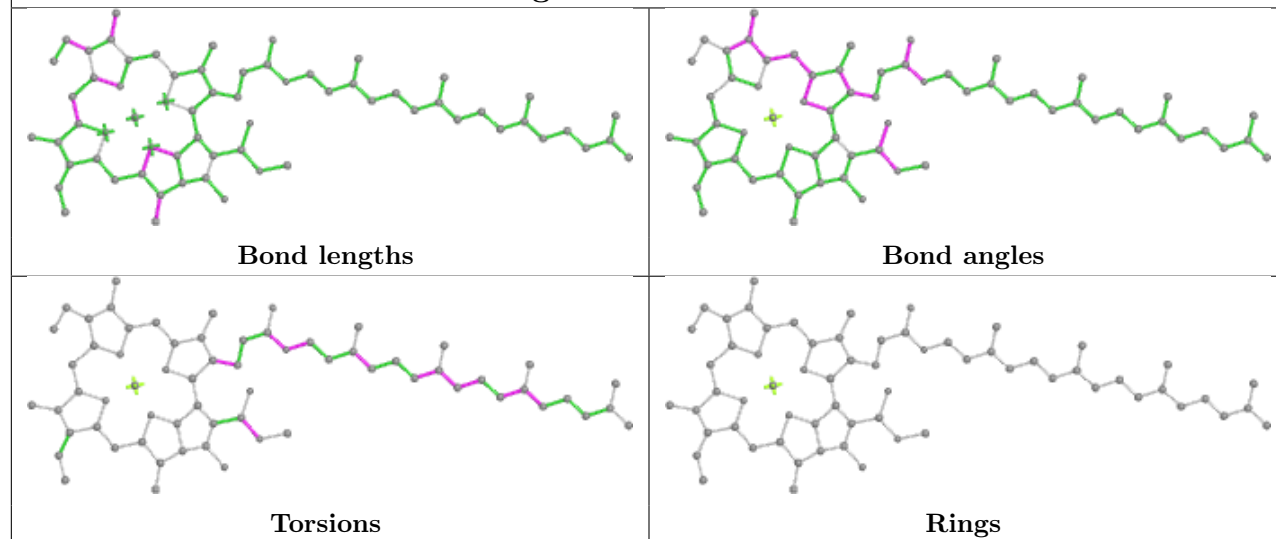
Torsions



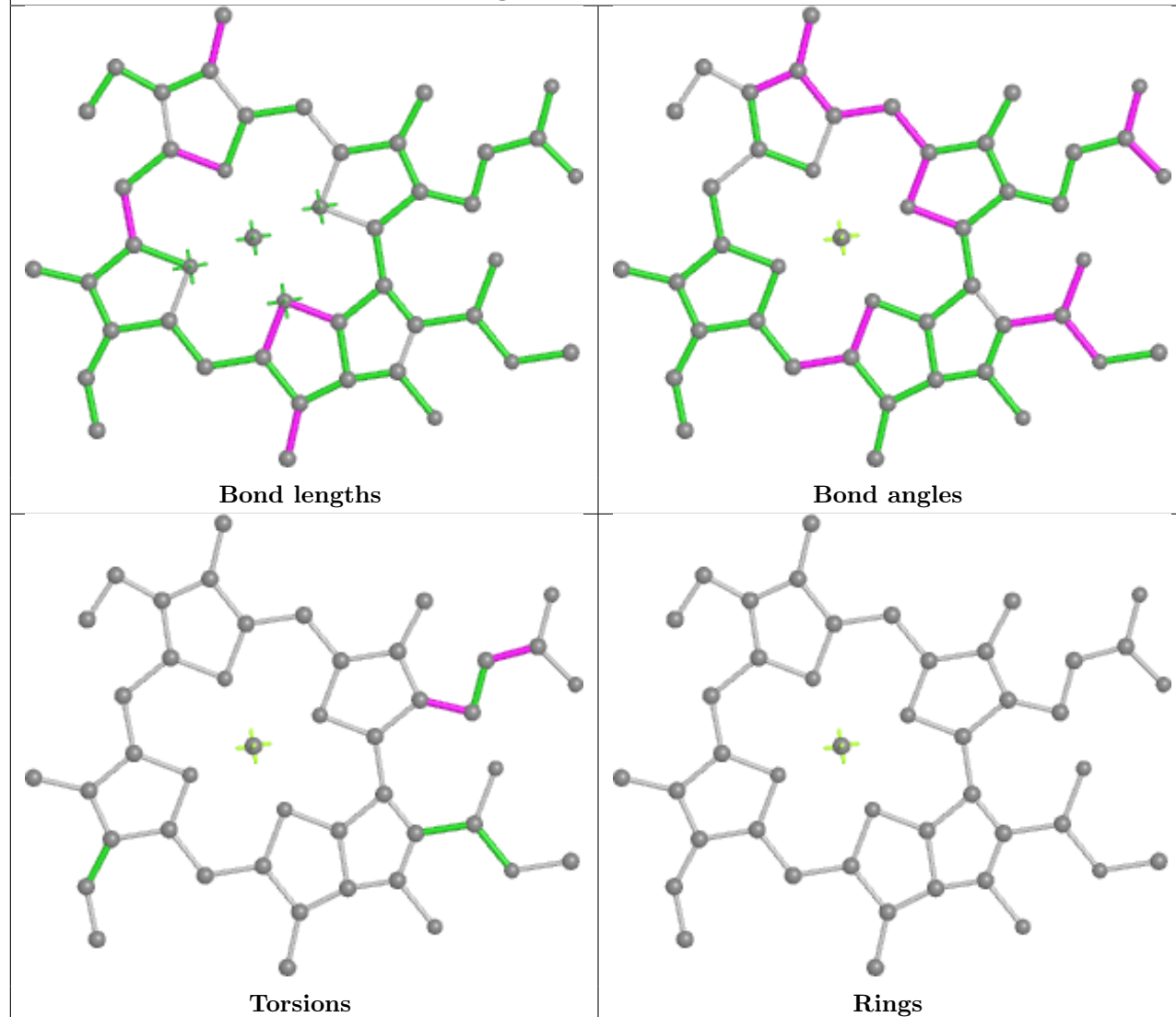
Rings

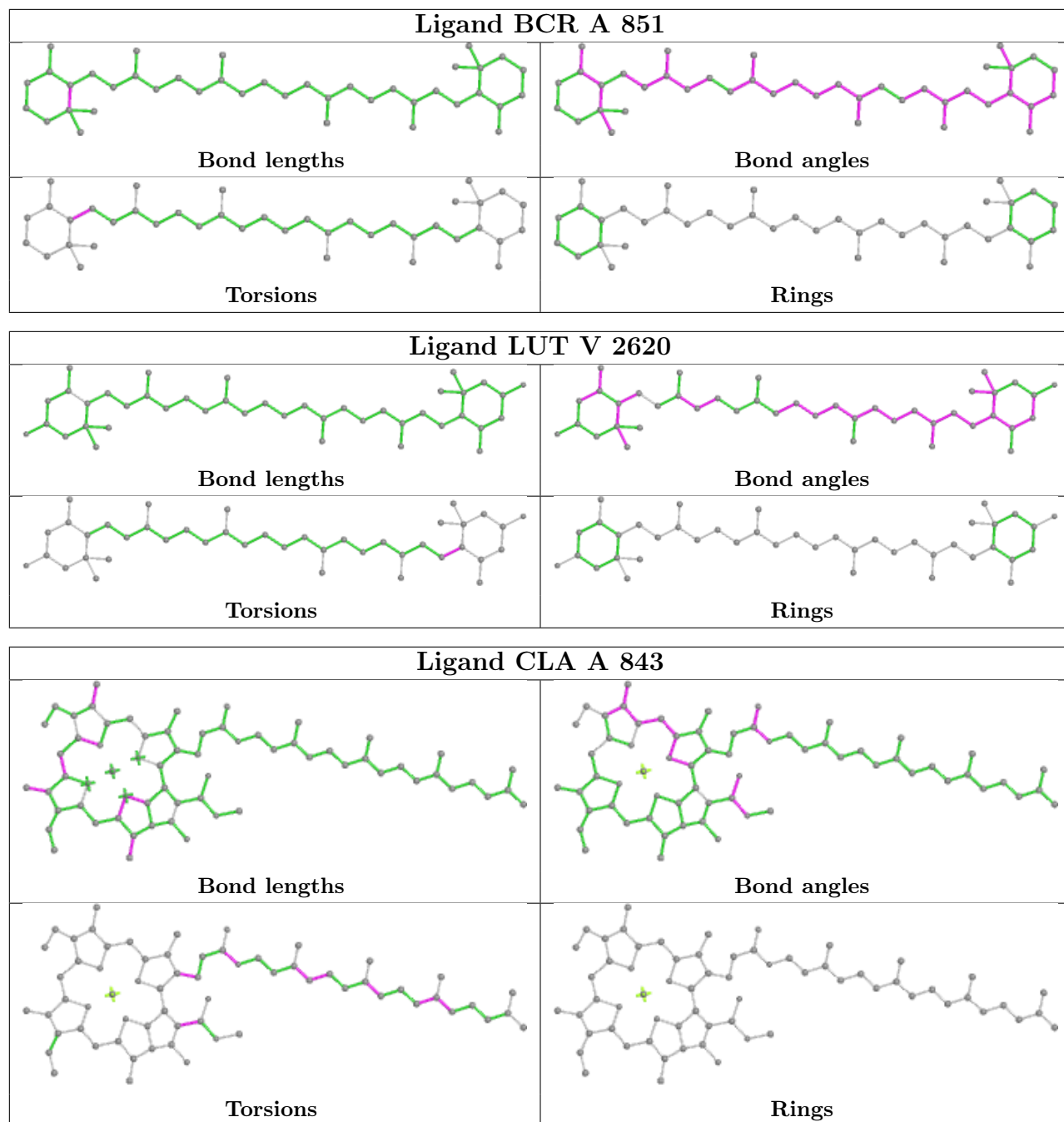


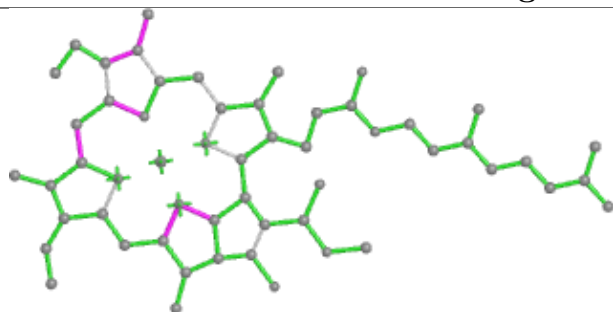
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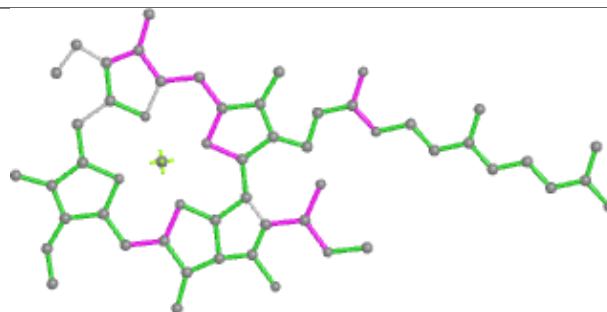
Ligand CLA 4 609



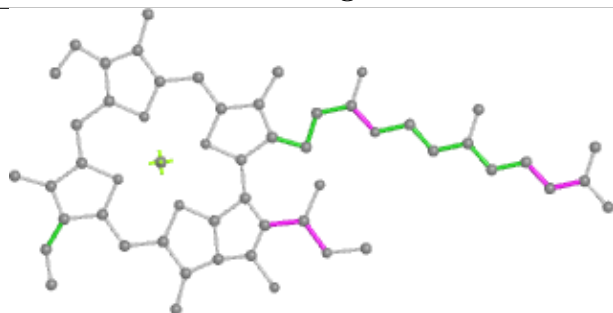


Ligand CLA 1 603

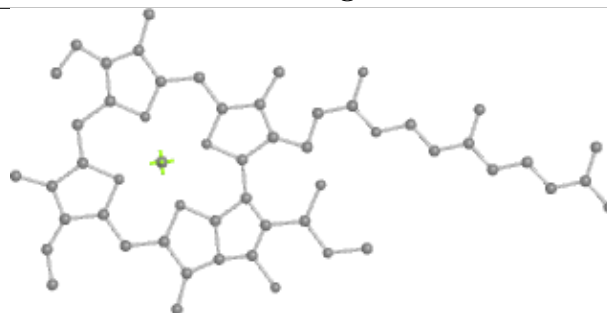
Bond lengths



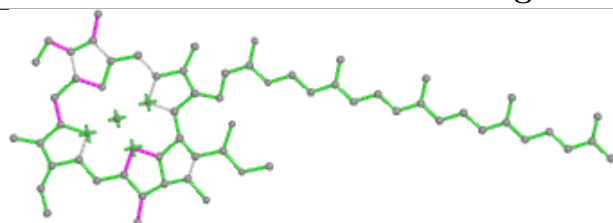
Bond angles



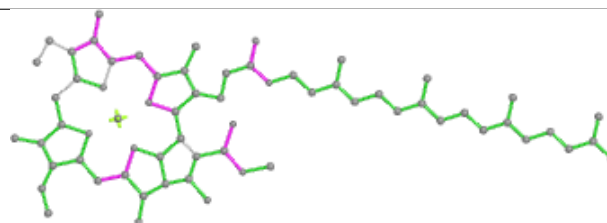
Torsions



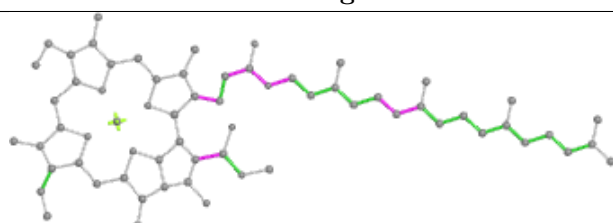
Rings

Ligand CLA B 839

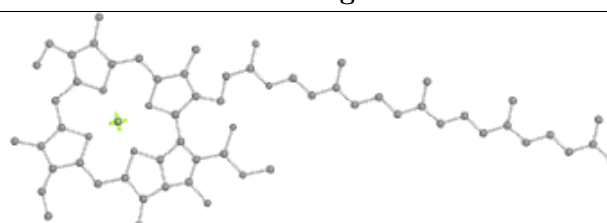
Bond lengths



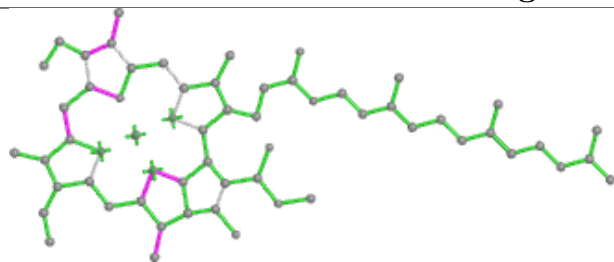
Bond angles



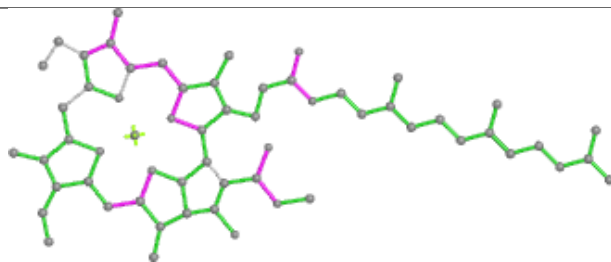
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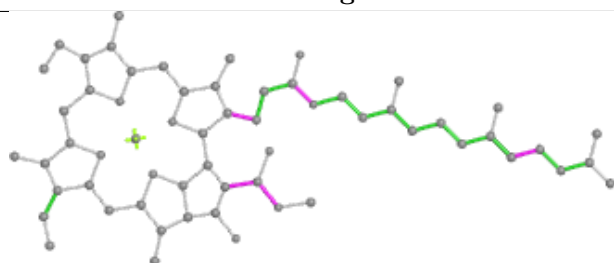
Rings

Ligand CLA 3 610

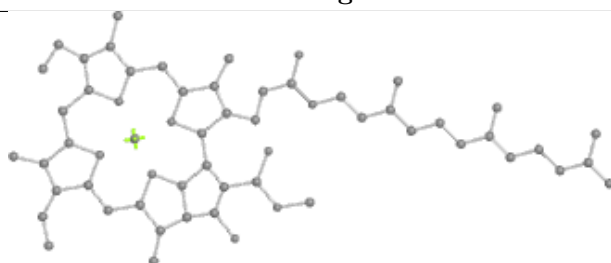
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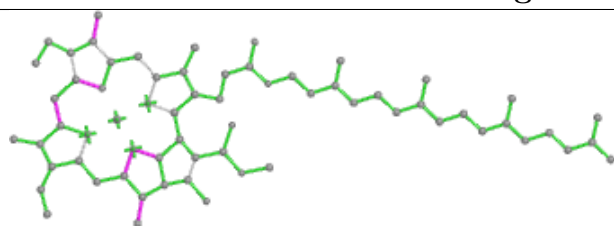
Bond angles



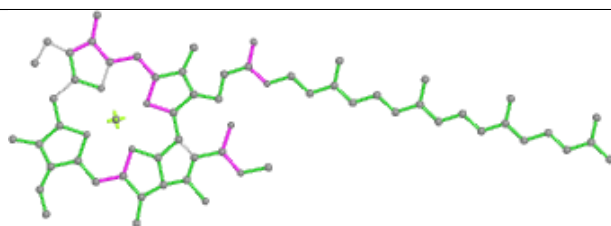
Torsions



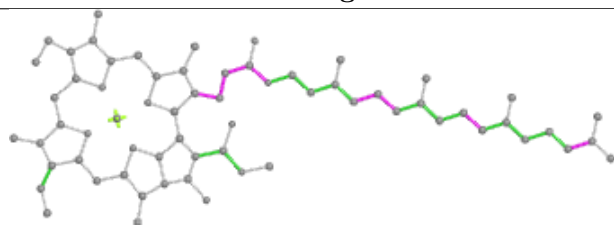
Rings

Ligand CLA B 825

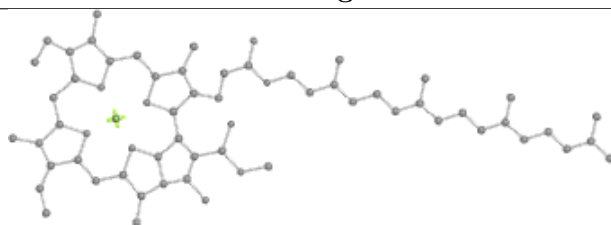
Bond lengths



Bond angles

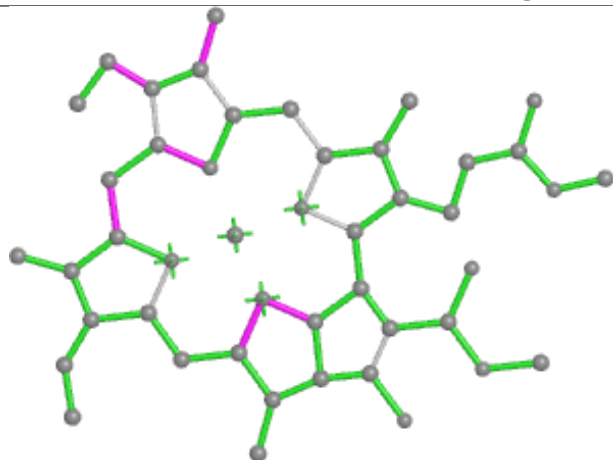


Torsions

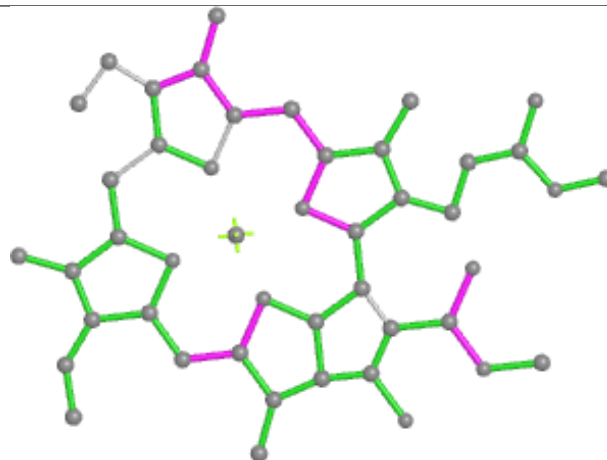


Rings

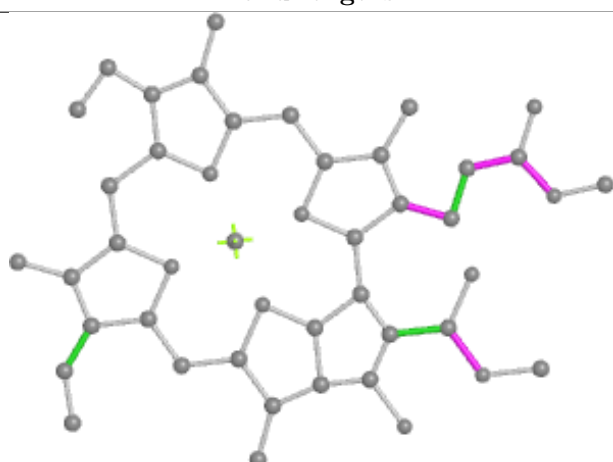
Ligand CLA 7 606



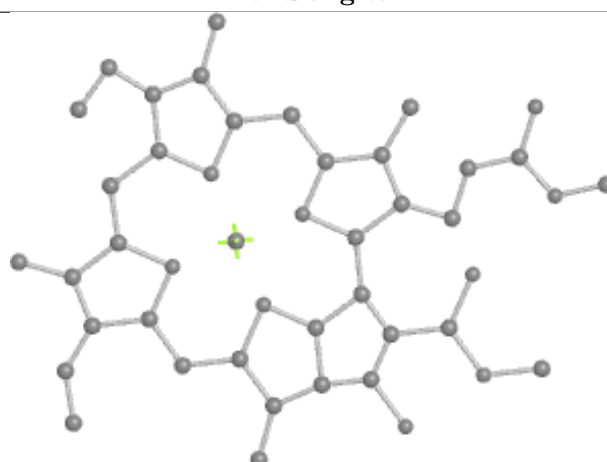
Bond lengths



Bond angles

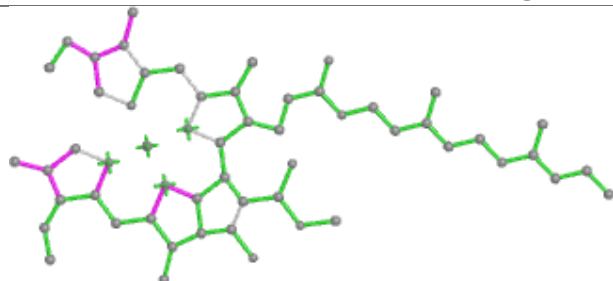


Torsions

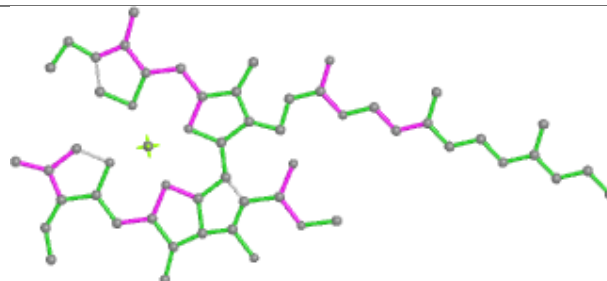


Rings

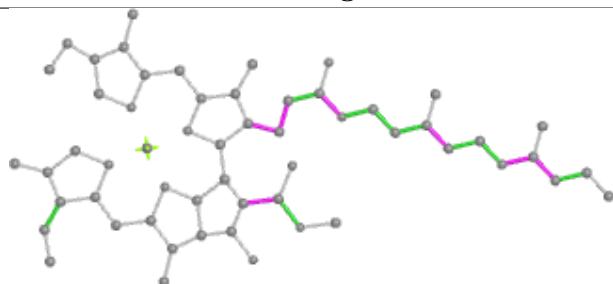
Ligand CLA 3 617



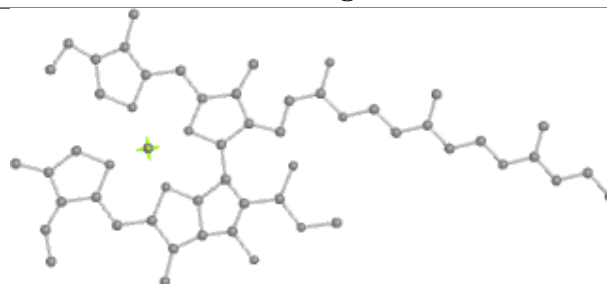
Bond lengths



Bond angles

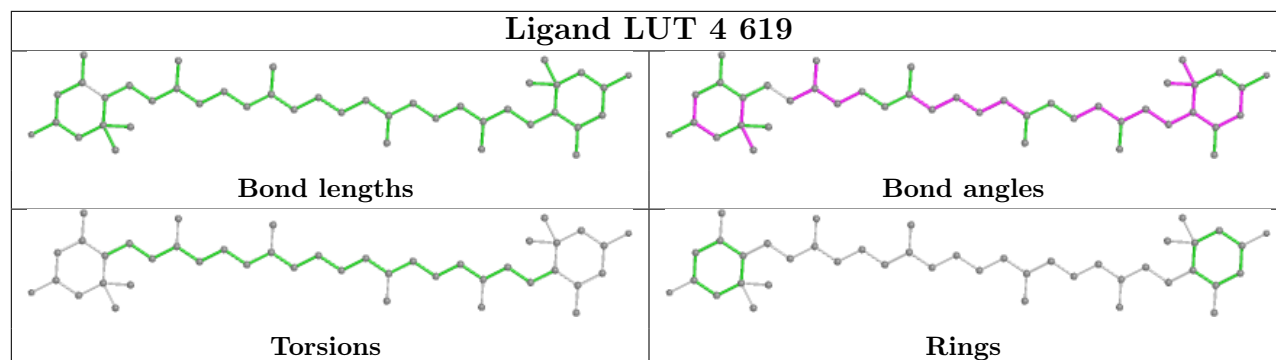


Torsions

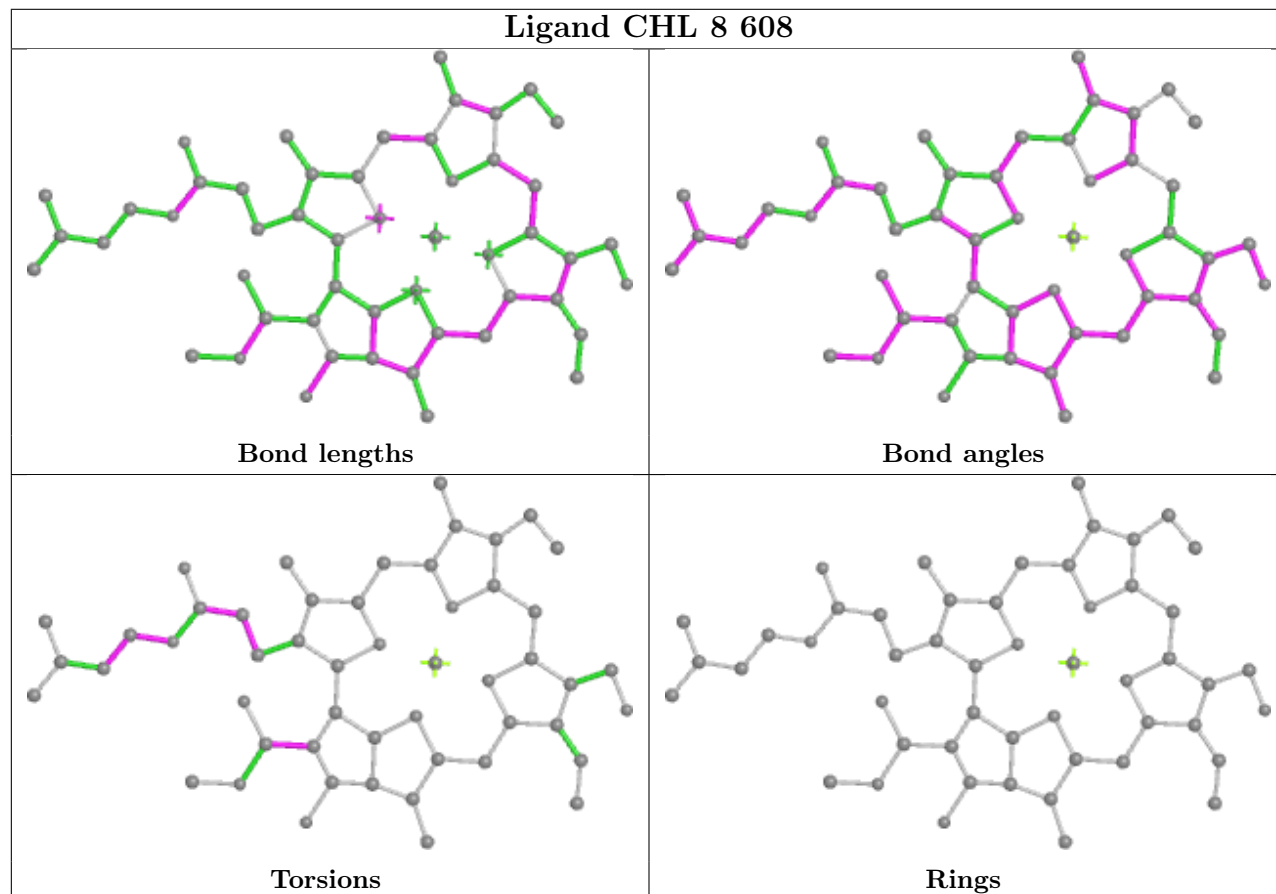


Rings

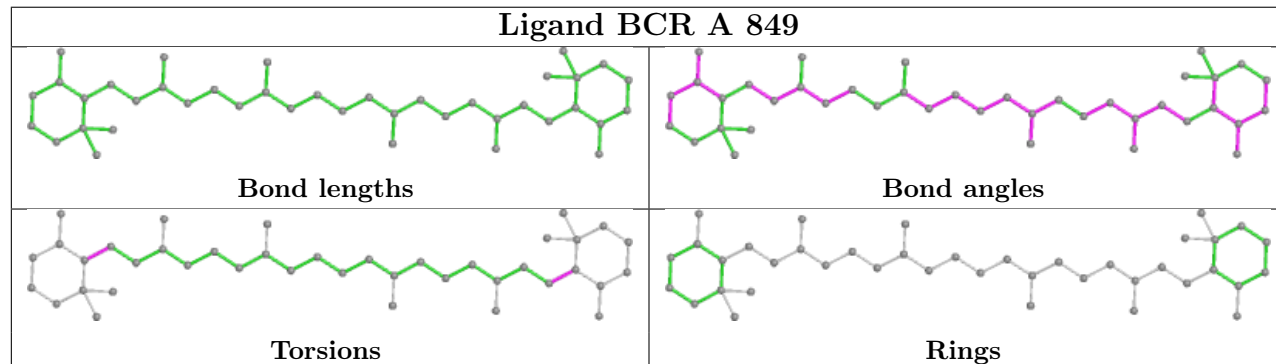
Ligand LUT 4 619

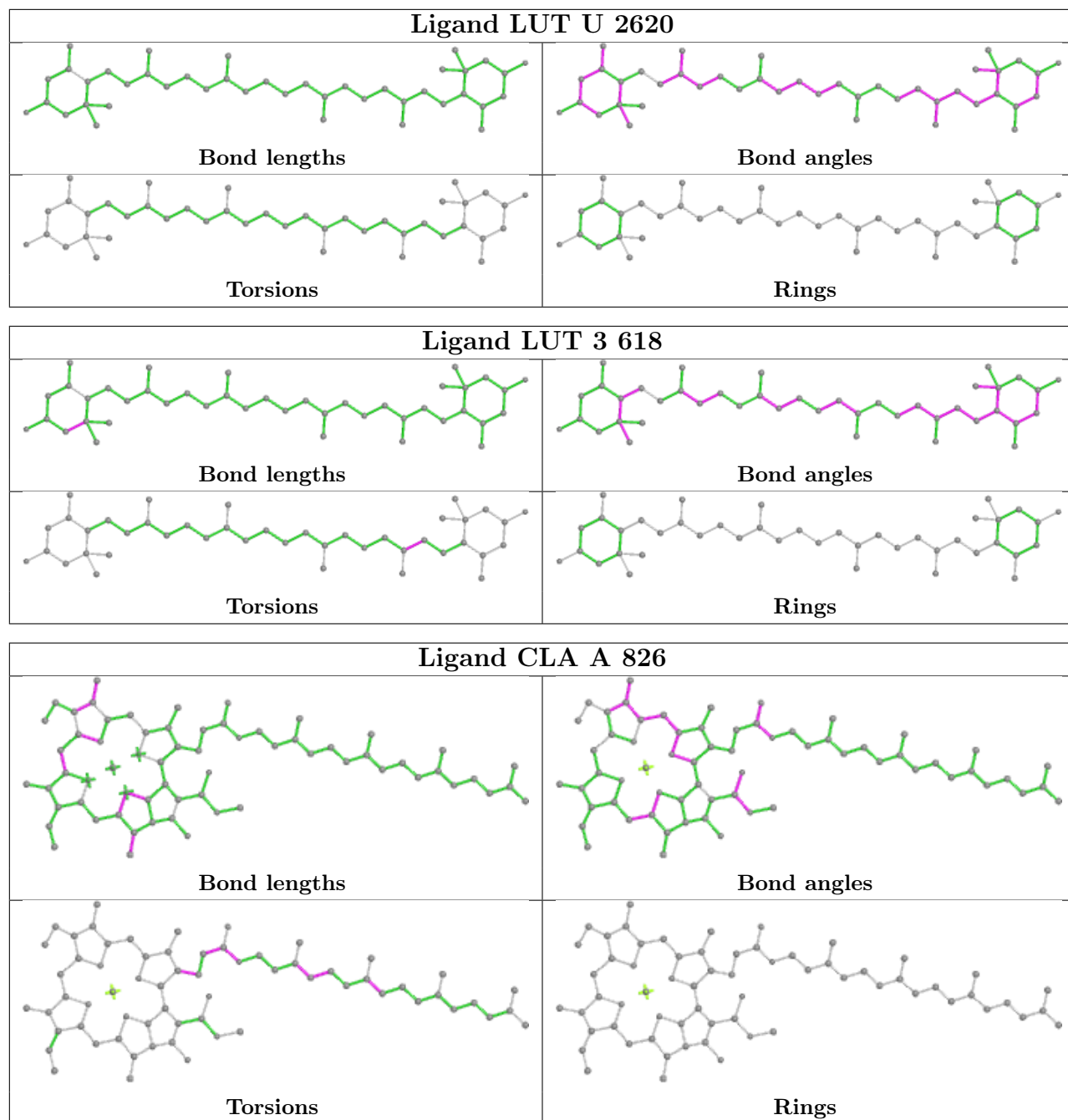


Ligand CHL 8 608

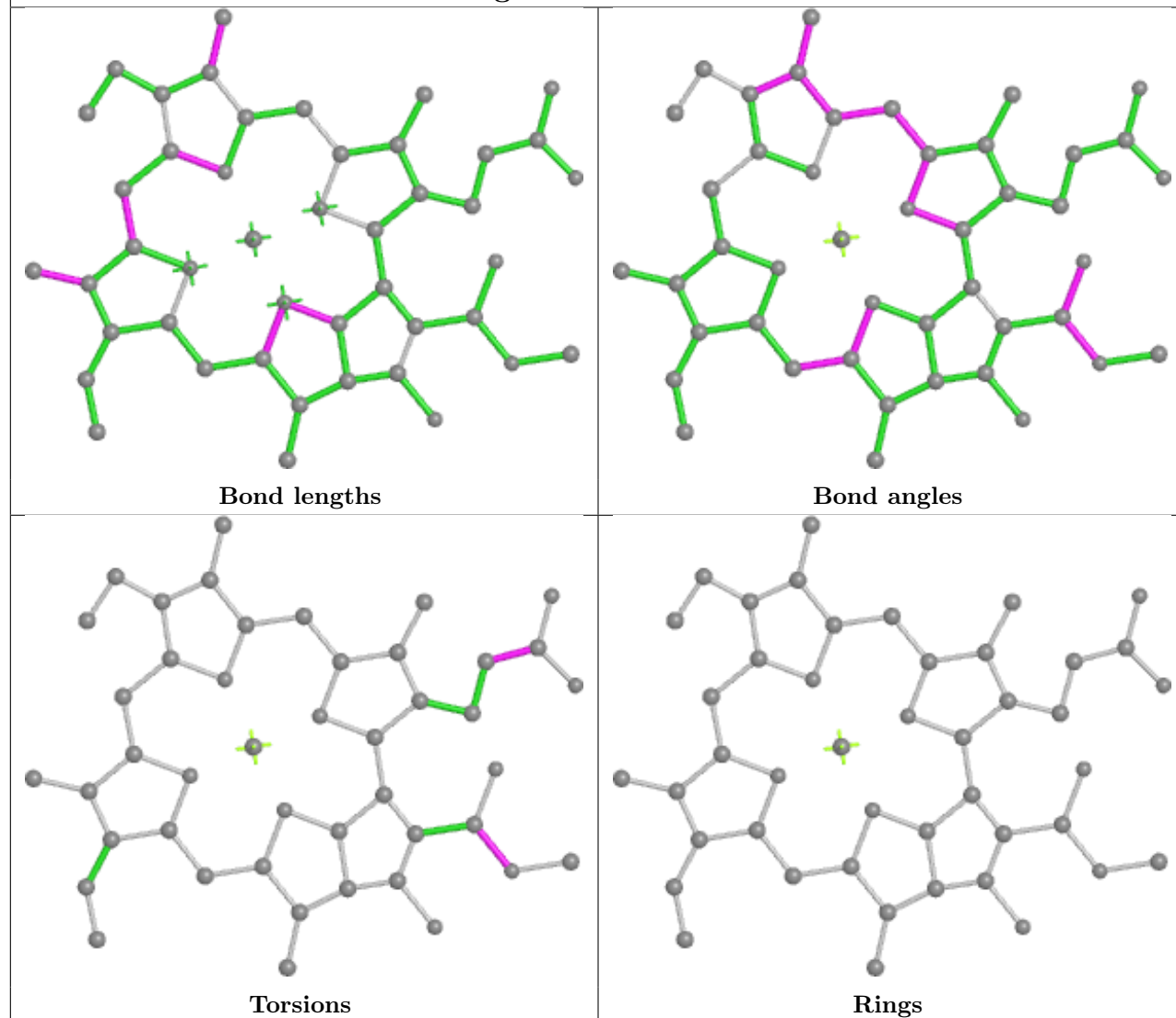


Ligand BCR A 849

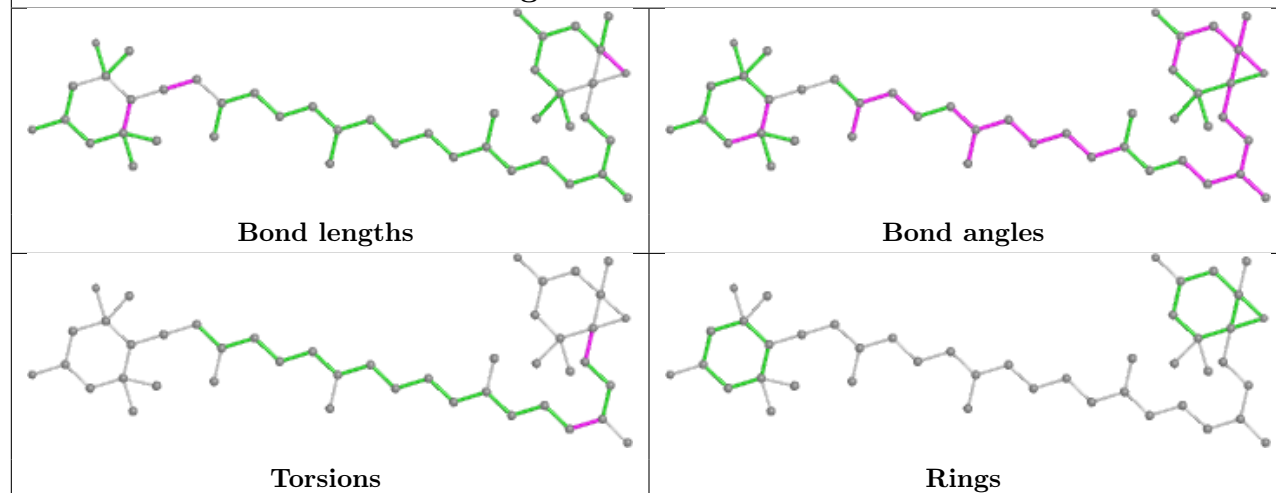


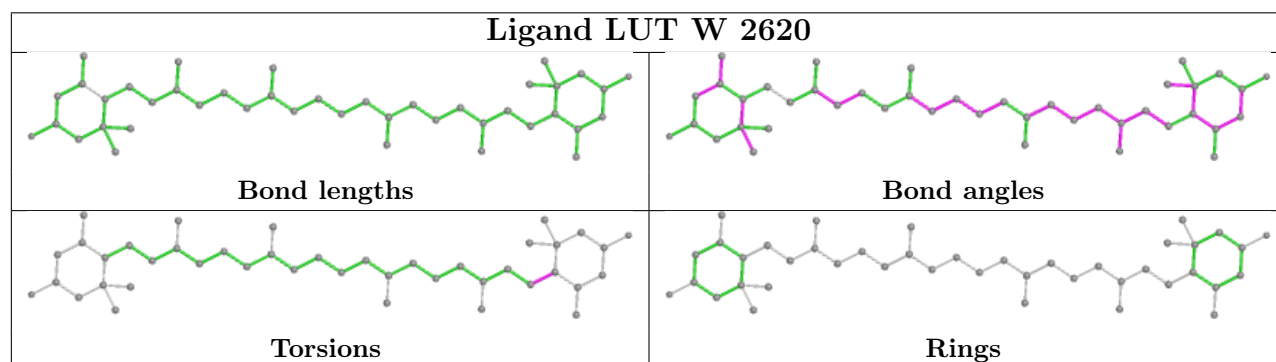
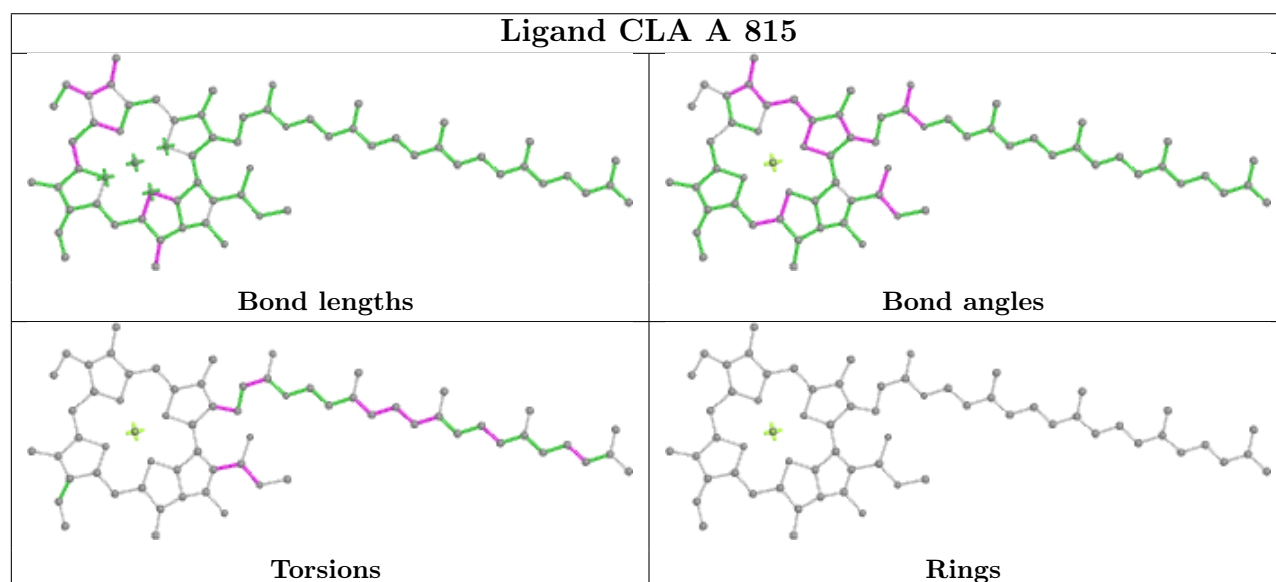
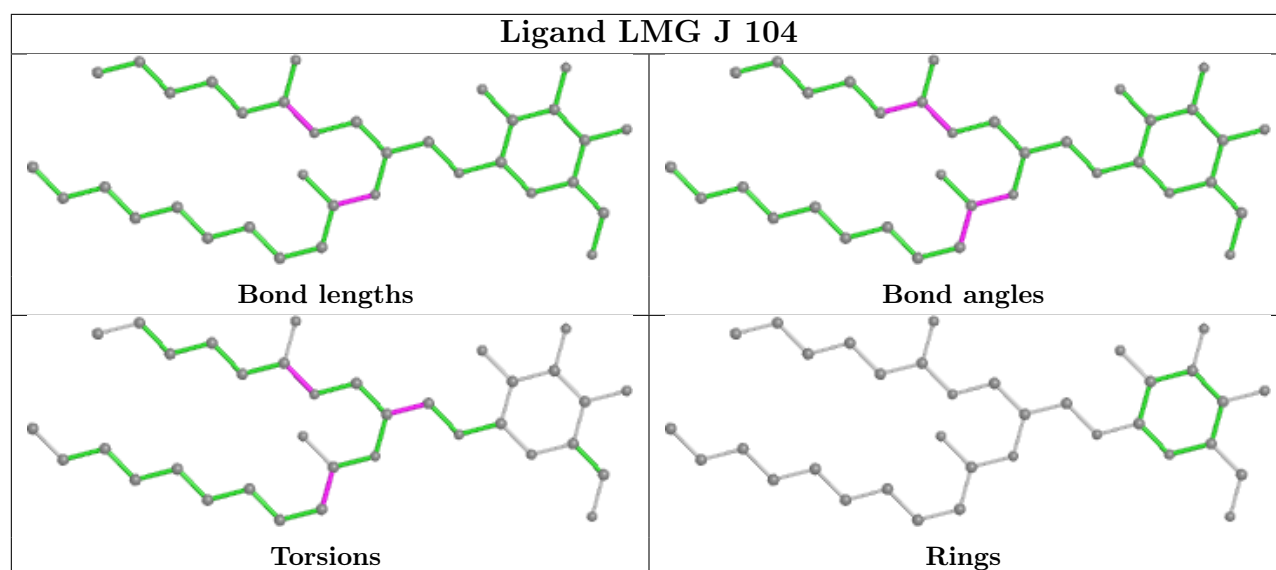


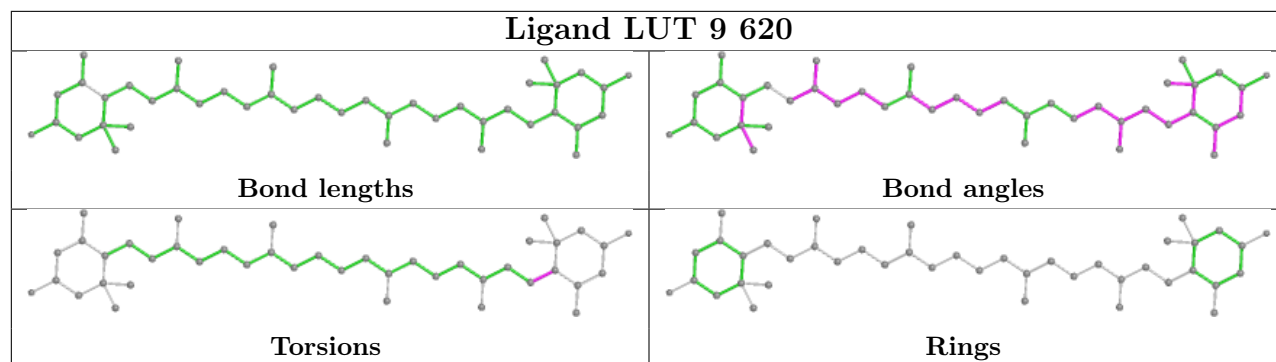
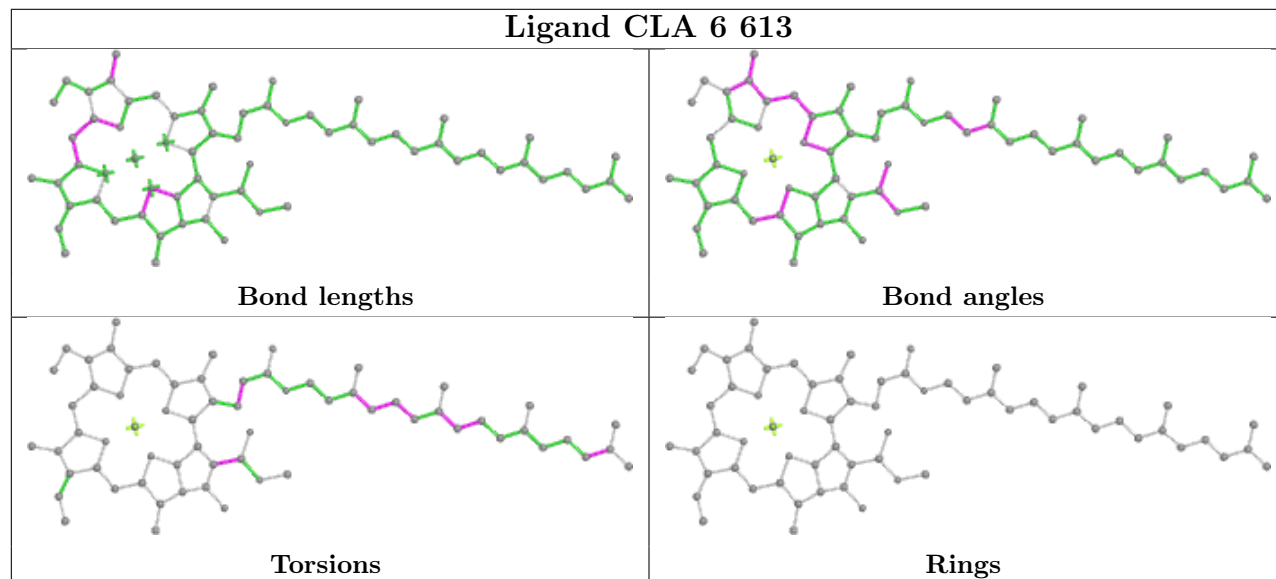
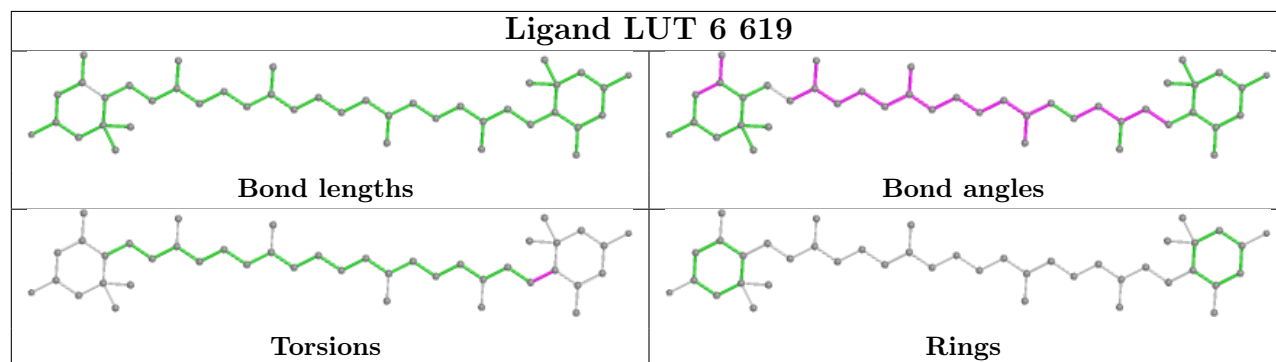
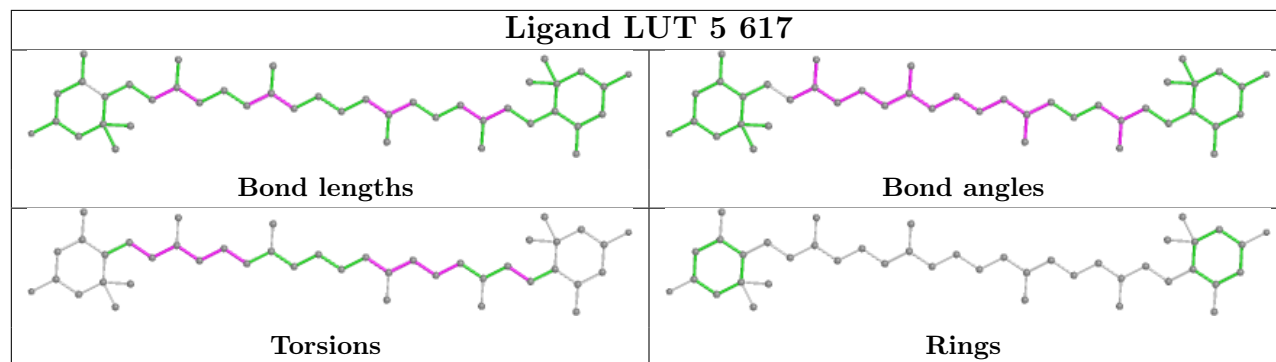
Ligand CLA 7 612

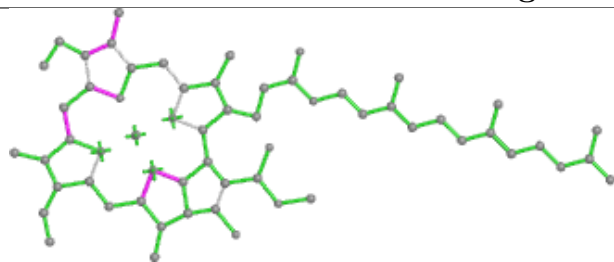


Ligand NEX U 2623

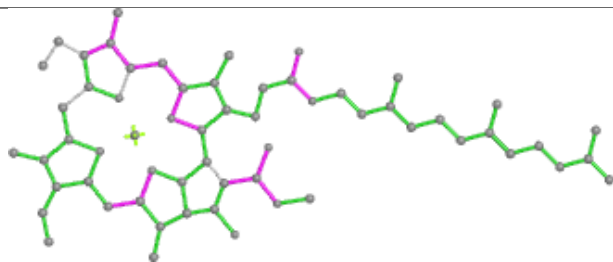




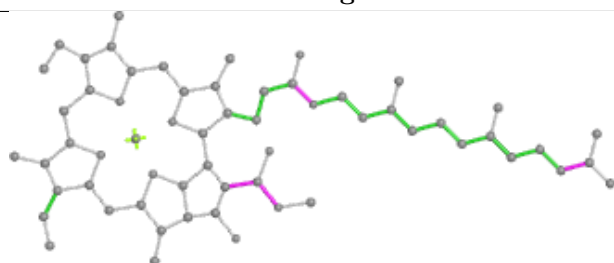
Ligand LUT 9 620**Ligand CLA 6 613****Ligand LUT 6 619****Ligand LUT 5 617**

Ligand CLA 8 602

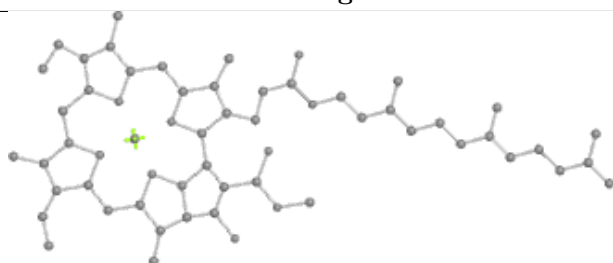
Bond lengths



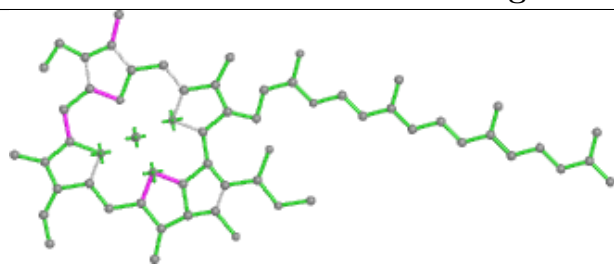
Bond angles



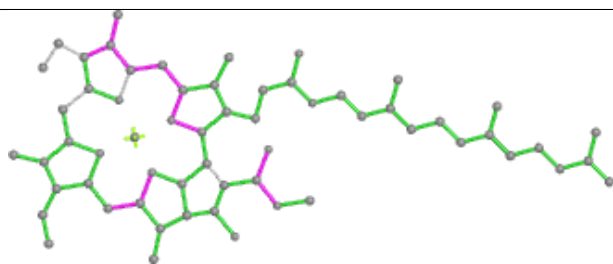
Torsions



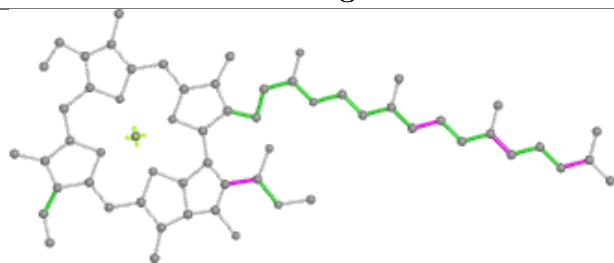
Rings

Ligand CLA W 602

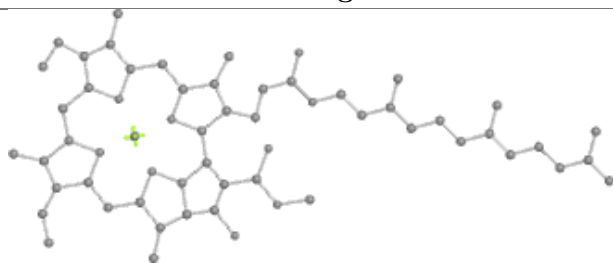
Bond lengths



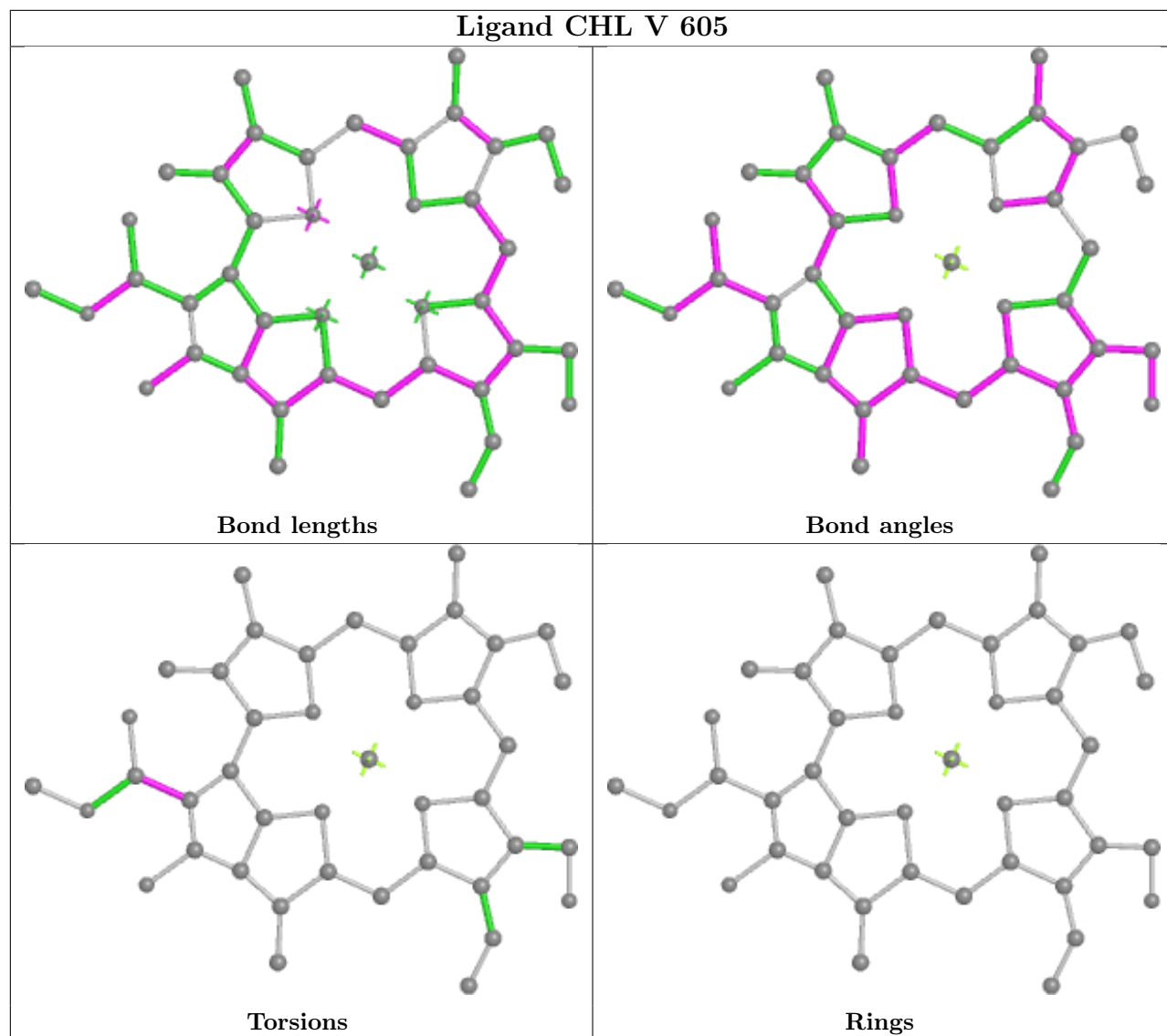
Bond angles



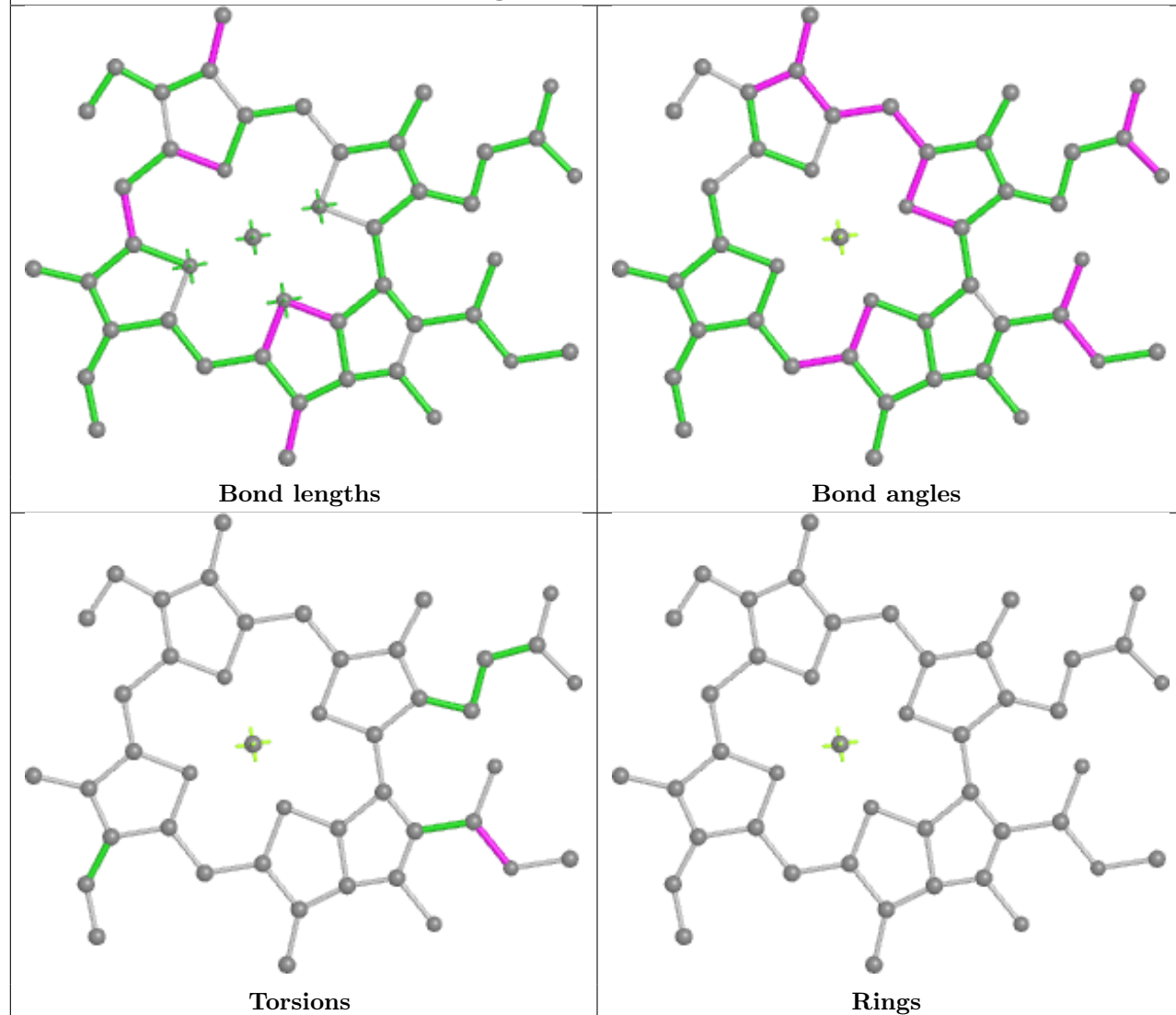
Torsions



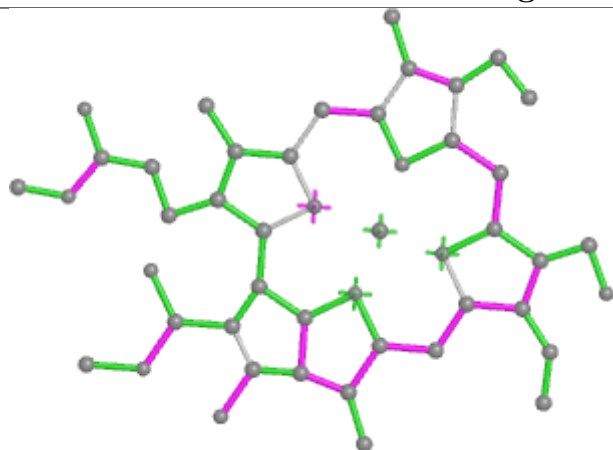
Rings



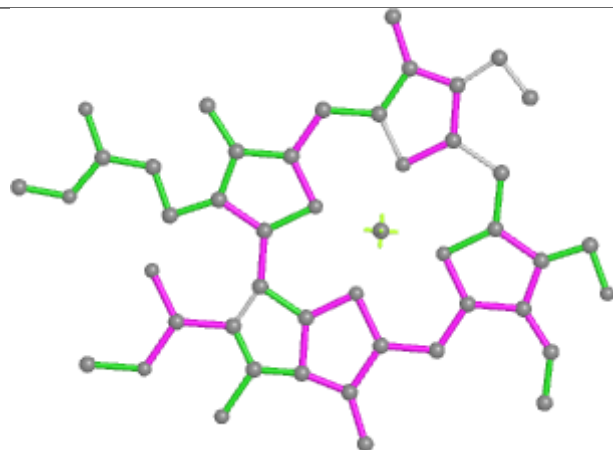
Ligand CLA F 303



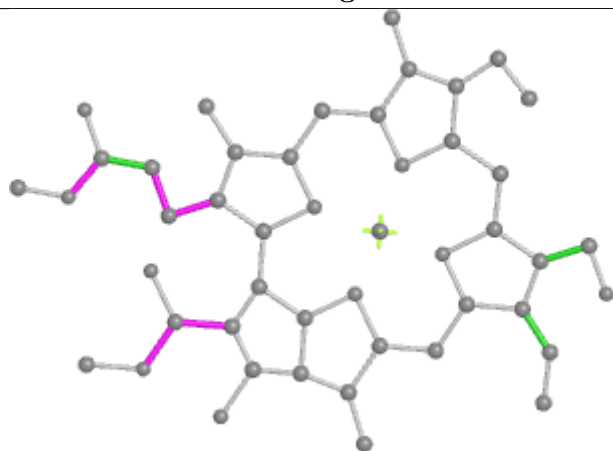
Ligand CHL 6 618



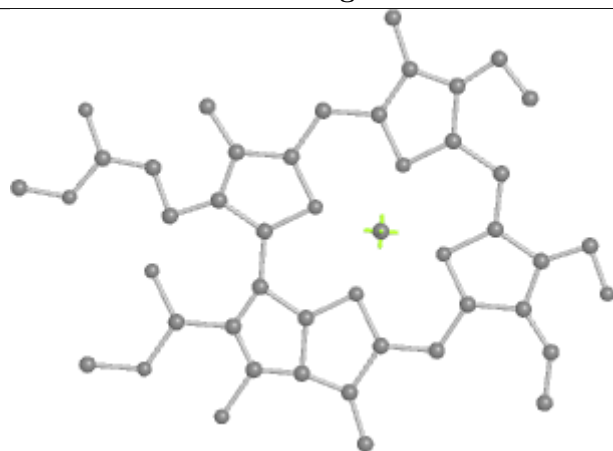
Bond lengths



Bond angles

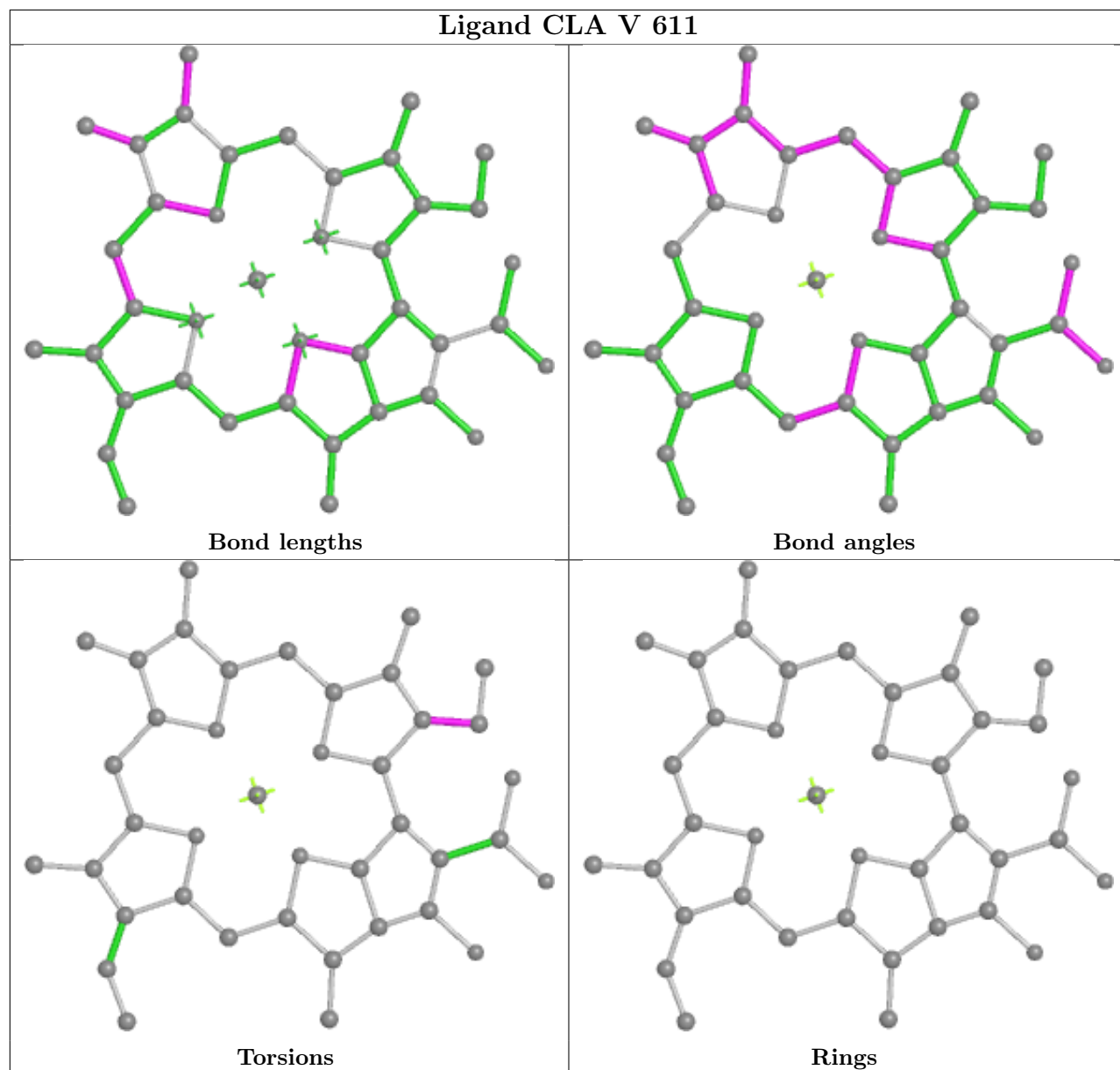


Torsions

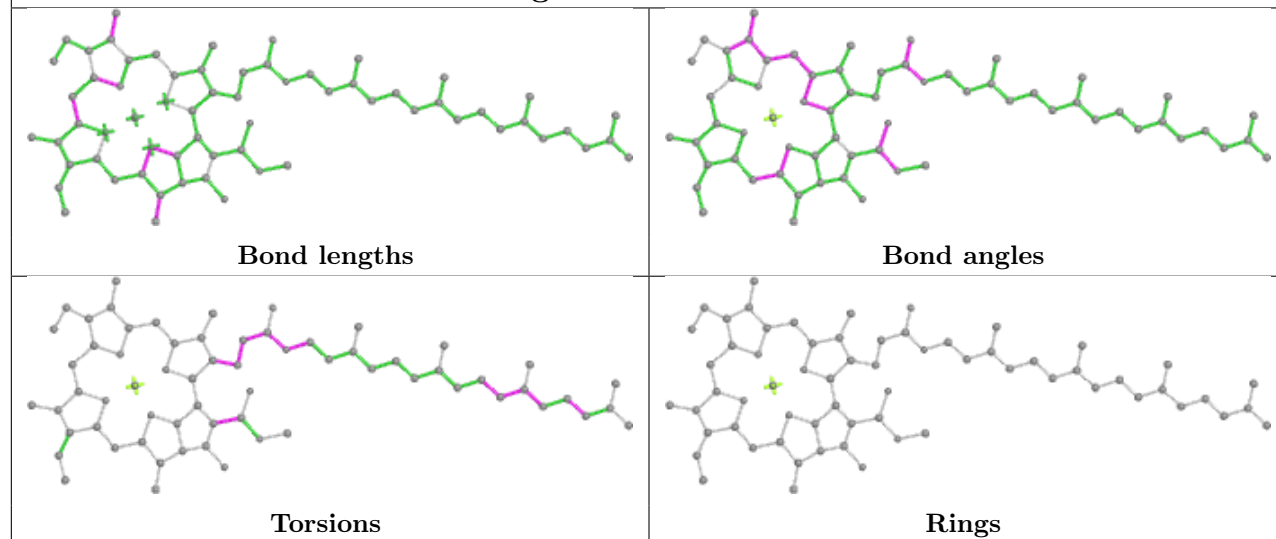


Rings

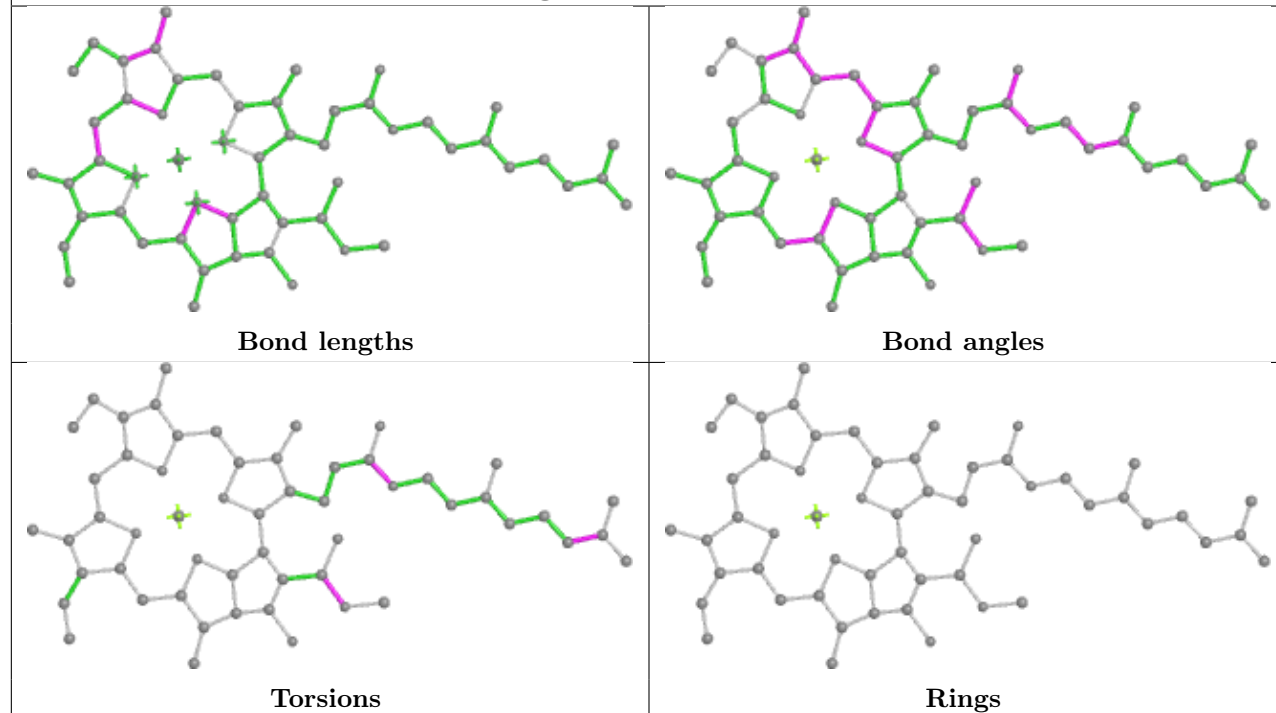
Ligand CLA V 611



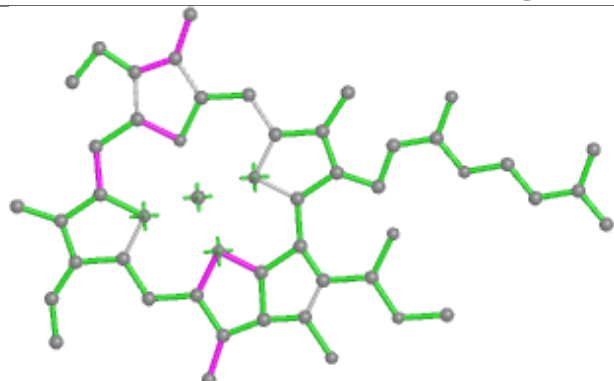
Ligand CLA A 806



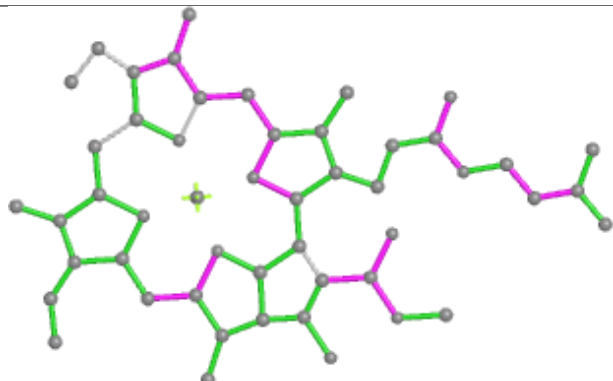
Ligand CLA 8 610



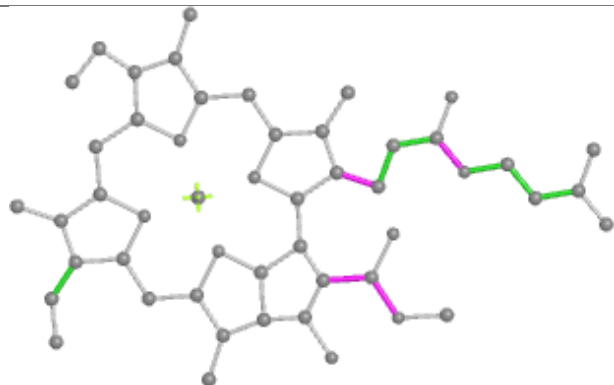
Ligand CLA 5 613



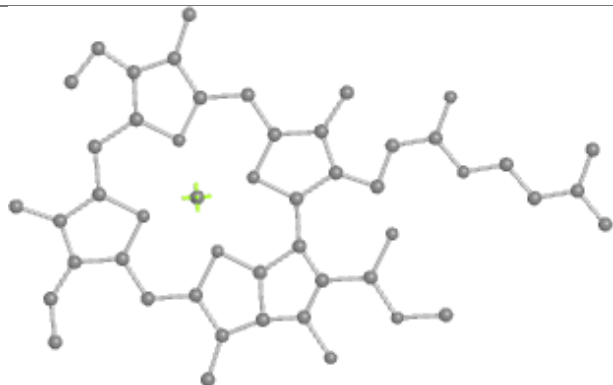
Bond lengths



Bond angles

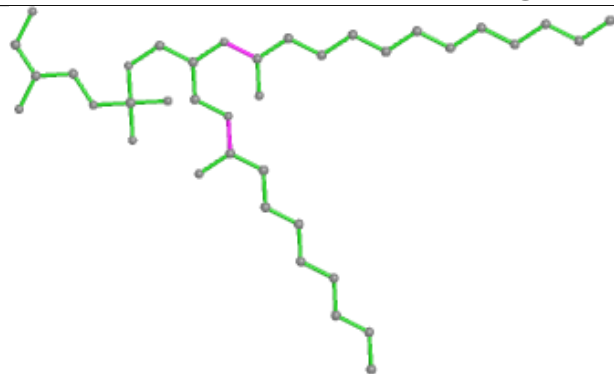


Torsions

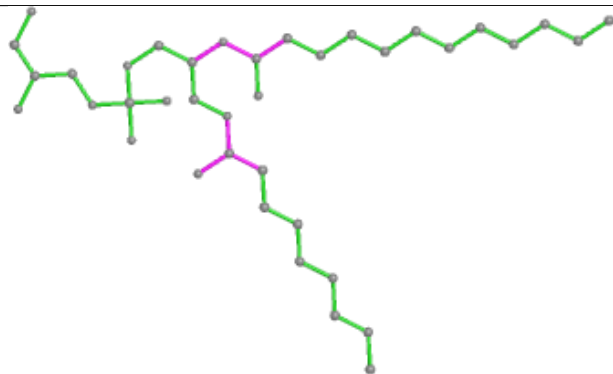


Rings

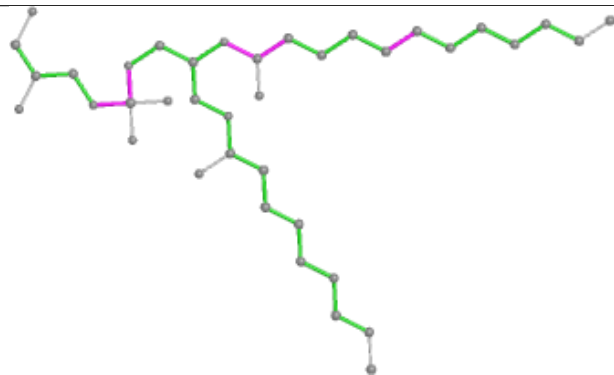
Ligand LHG 8 630



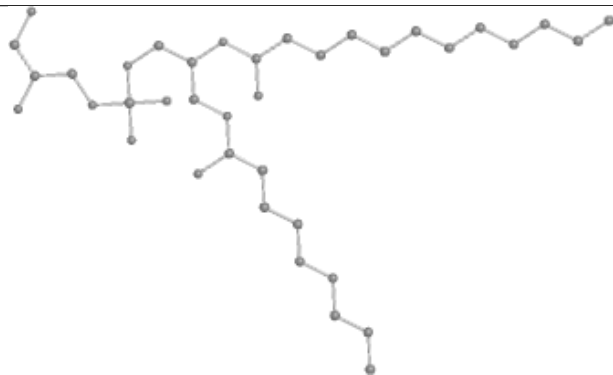
Bond lengths



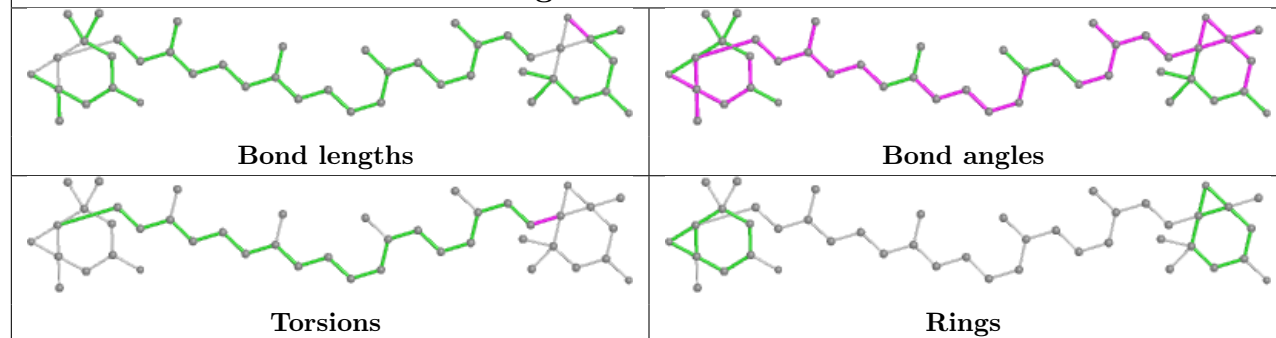
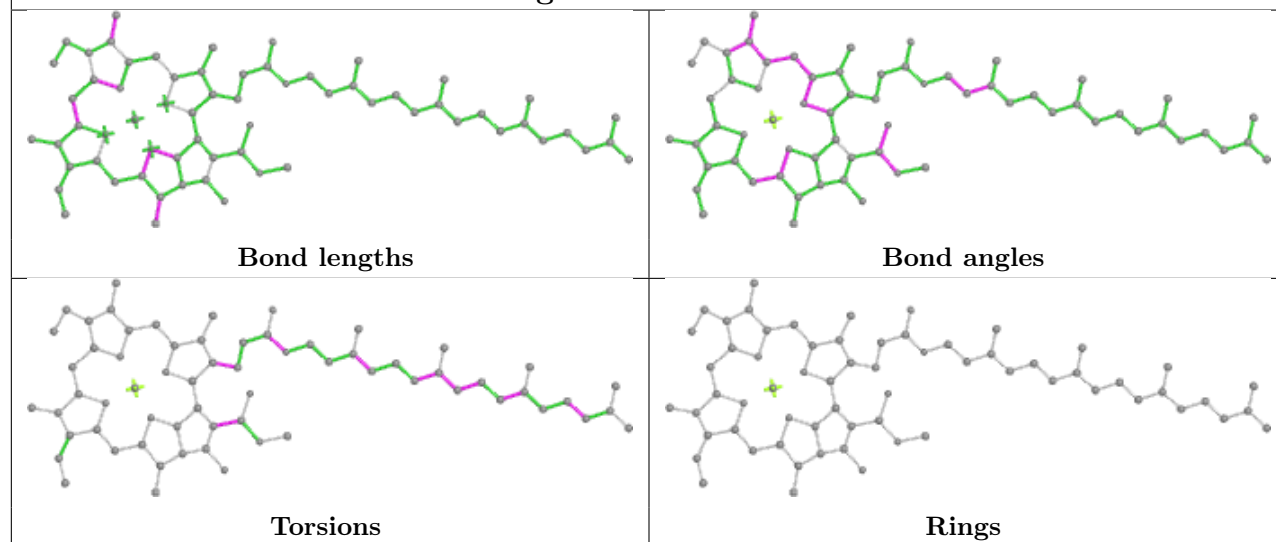
Bond angles



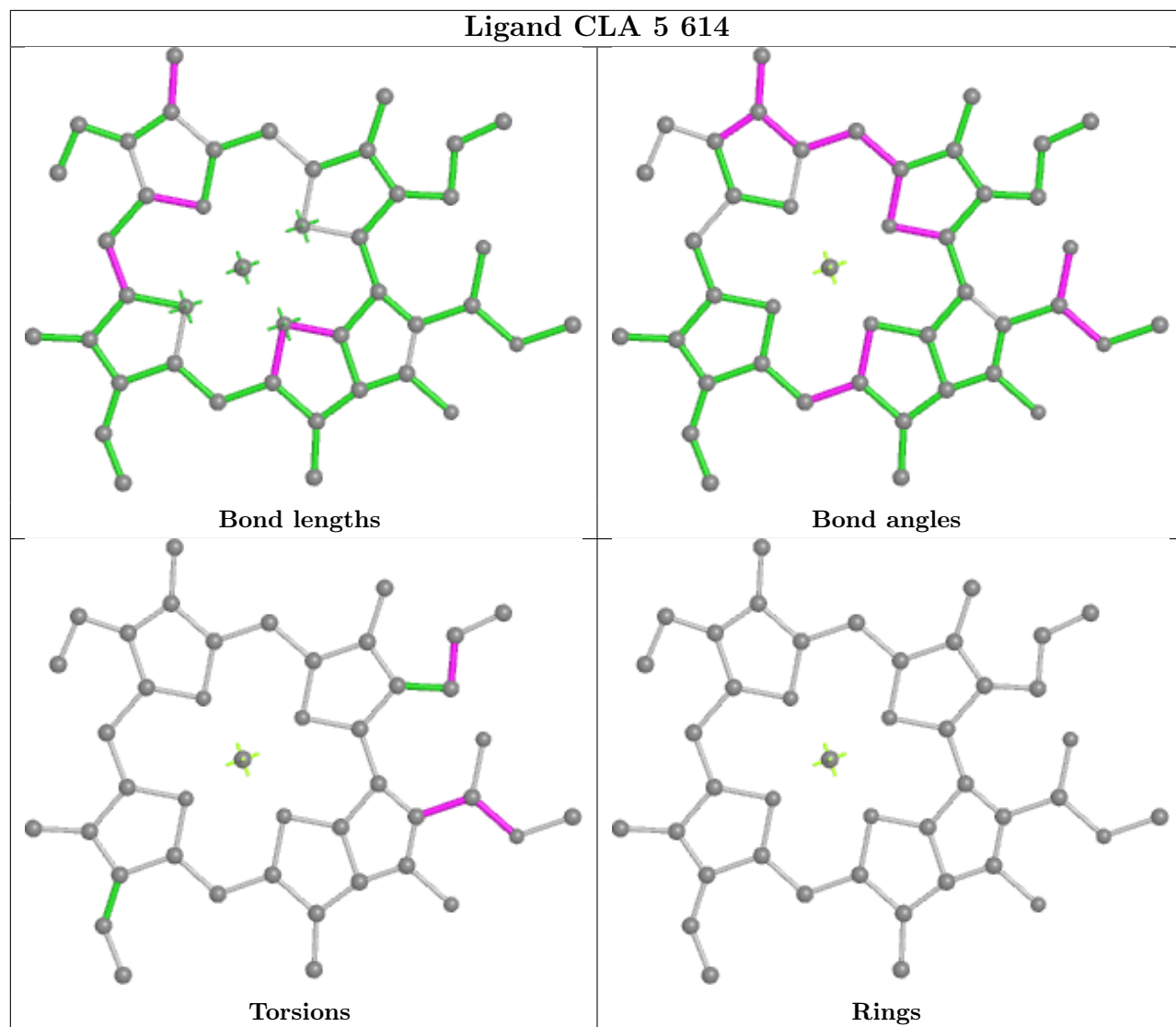
Torsions

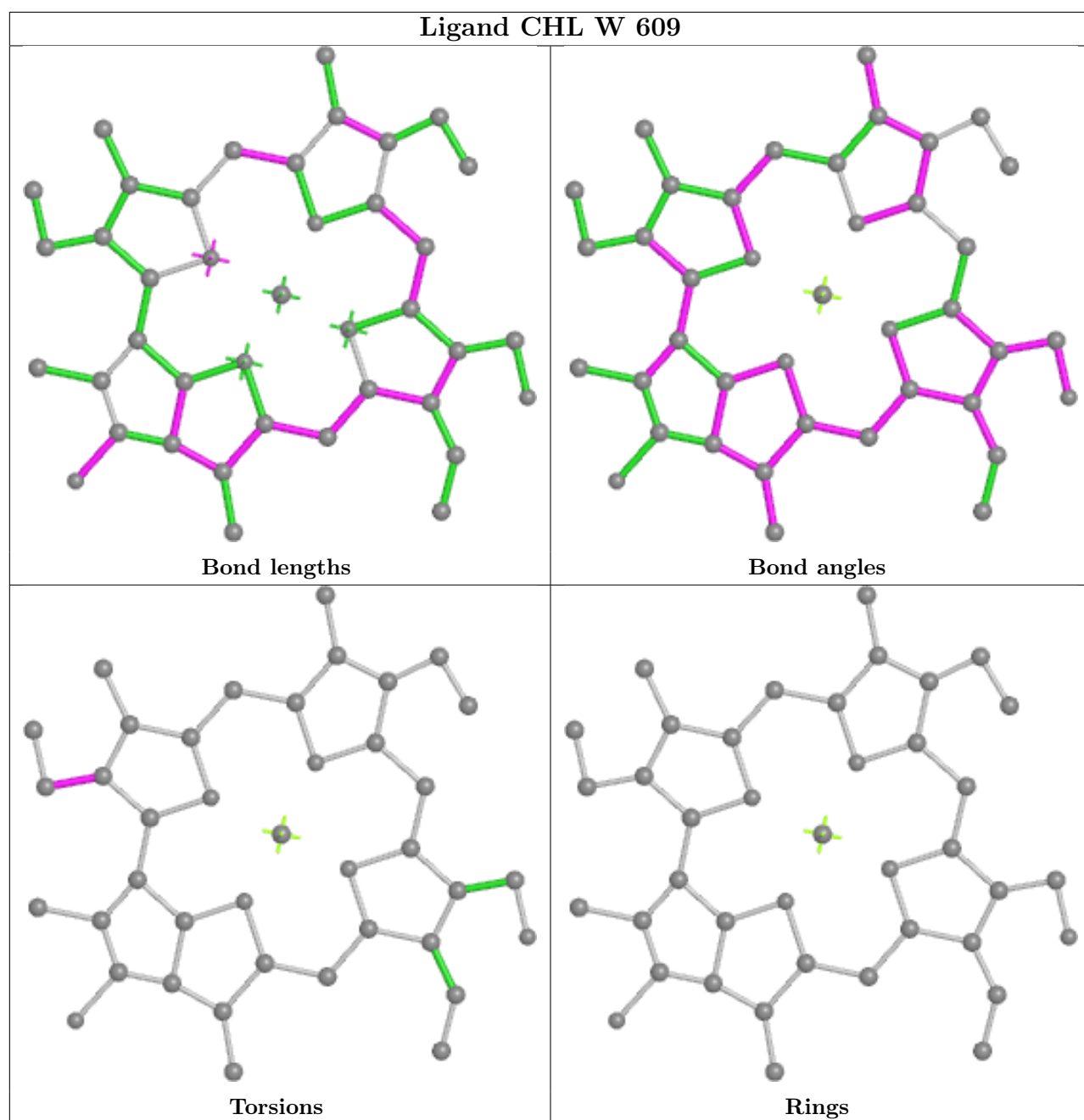


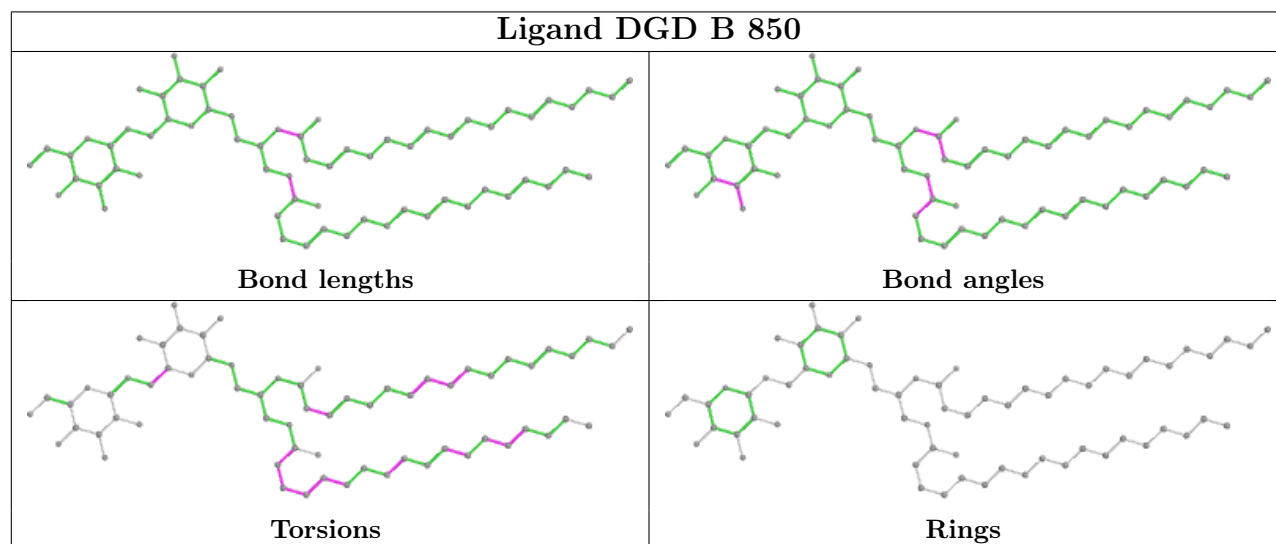
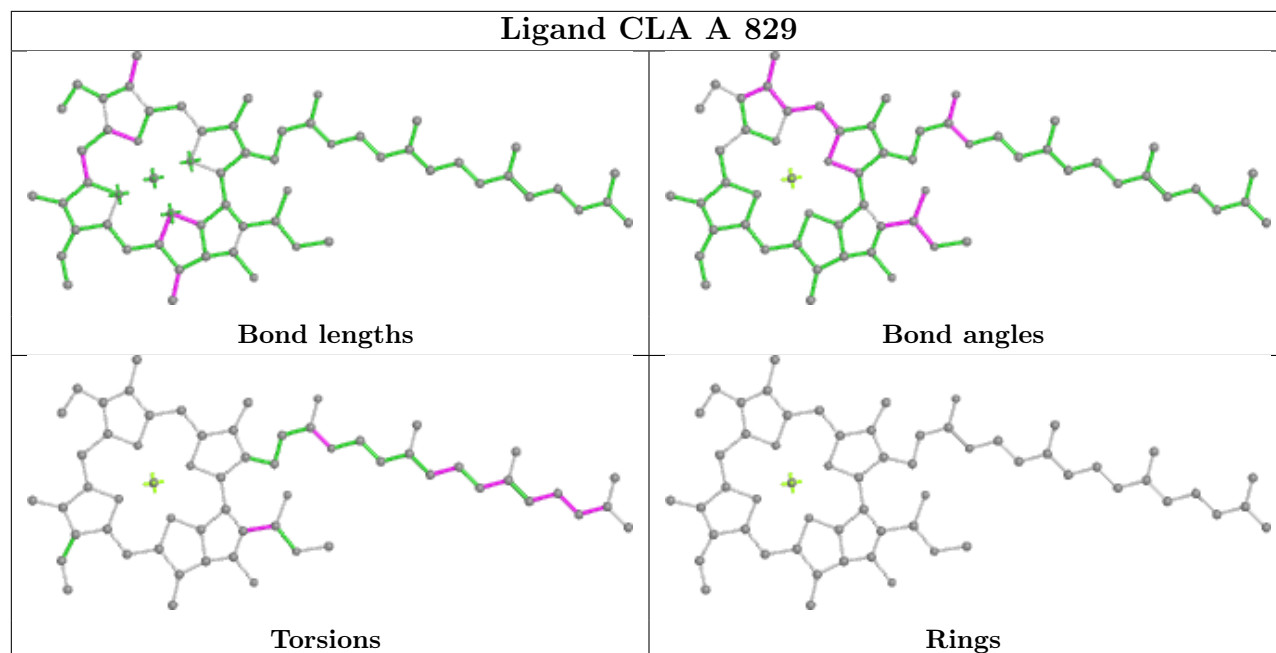
Rings

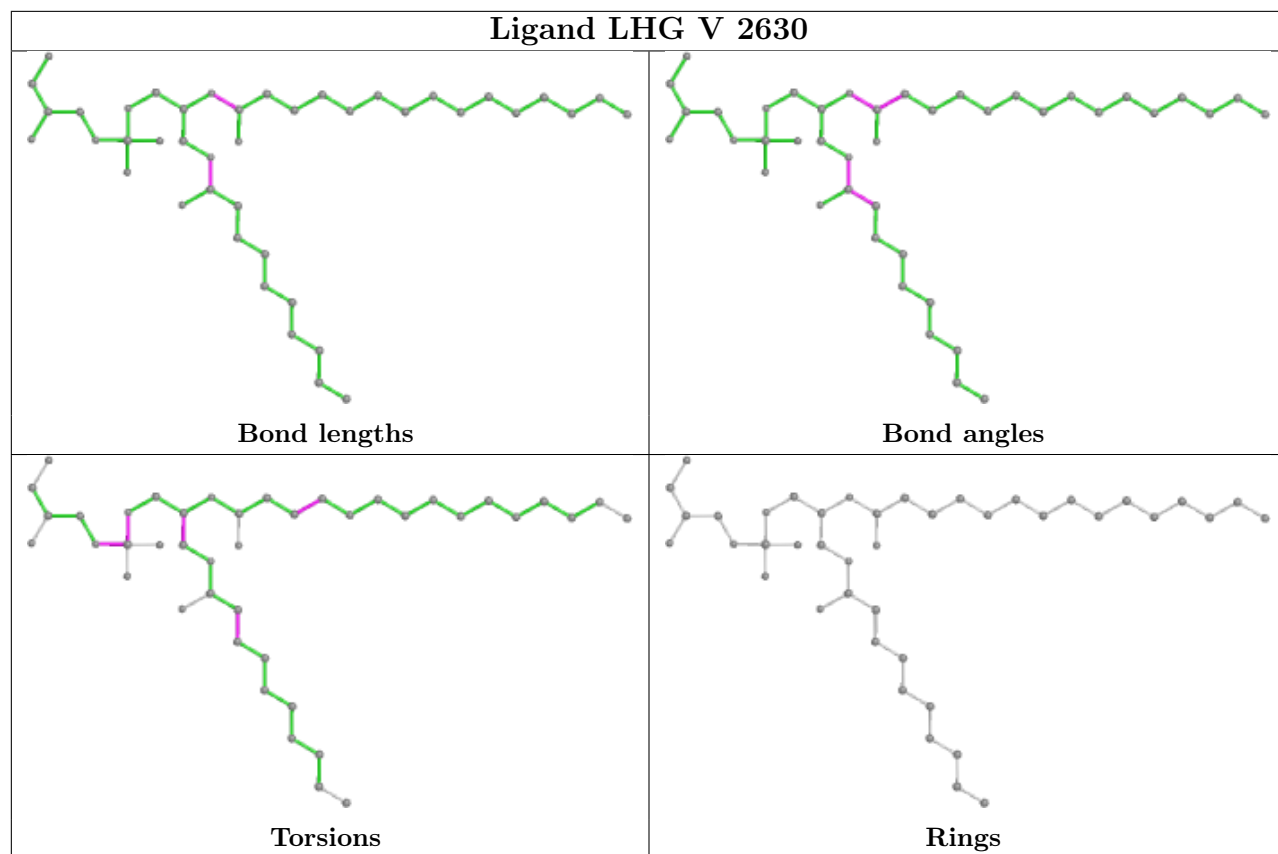
Ligand XAT 4 620**Ligand CLA 1 602**

Ligand CLA 5 614

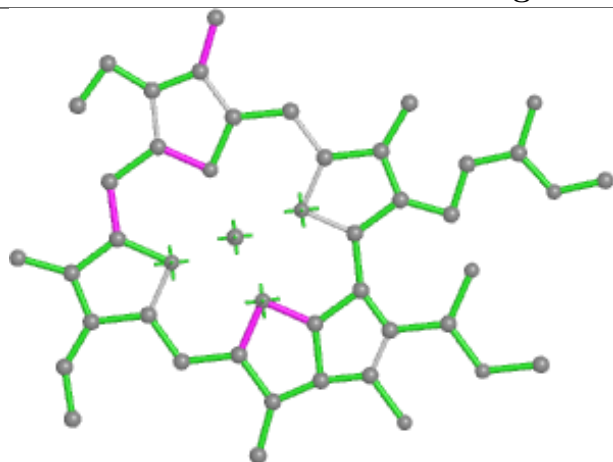




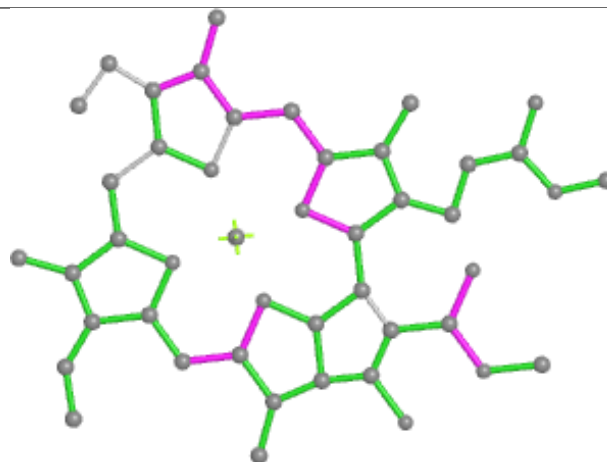




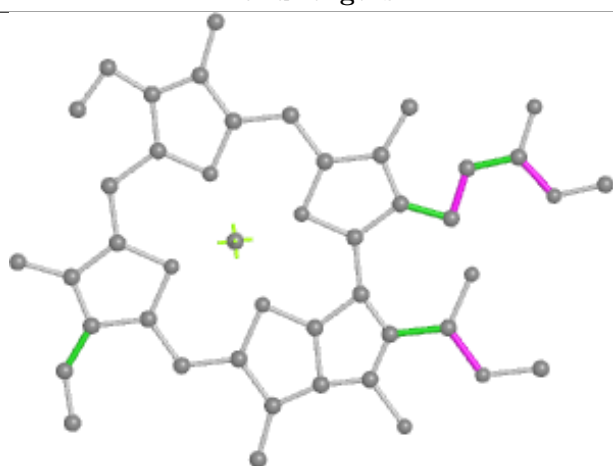
Ligand CLA G 204



Bond lengths



Bond angles

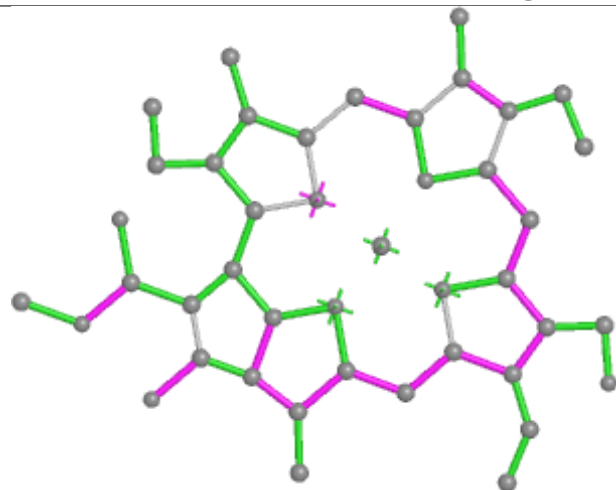


Torsions

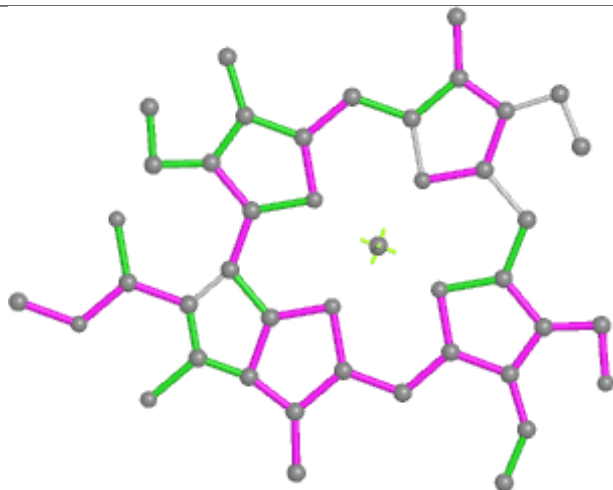


Rings

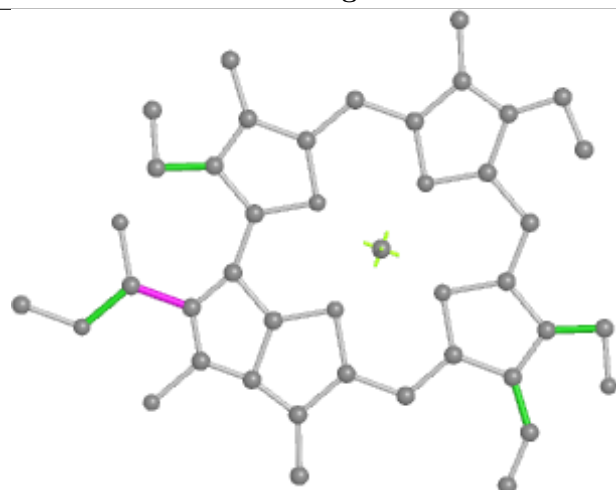
Ligand CHL 9 608



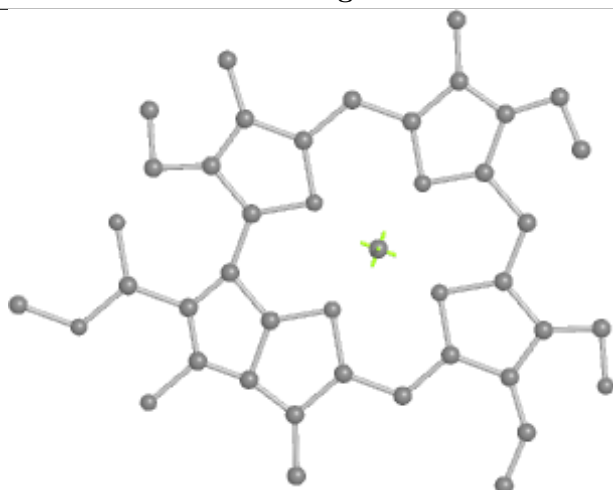
Bond lengths



Bond angles

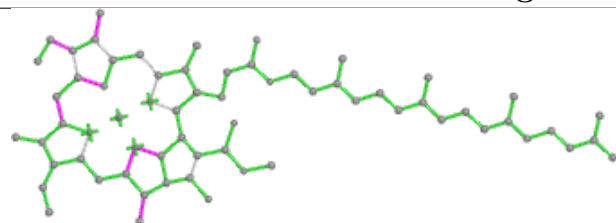


Torsions

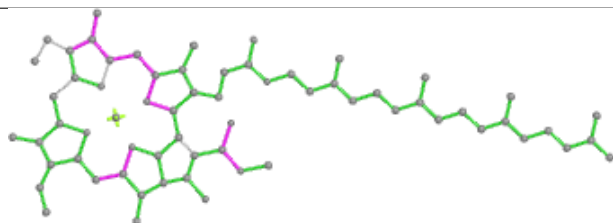


Rings

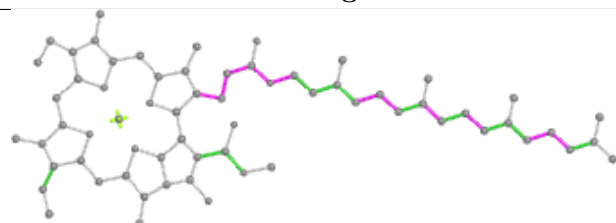
Ligand CLA B 828



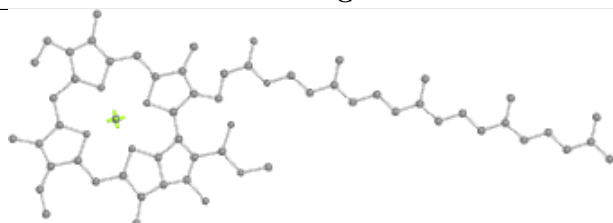
Bond lengths



Bond angles

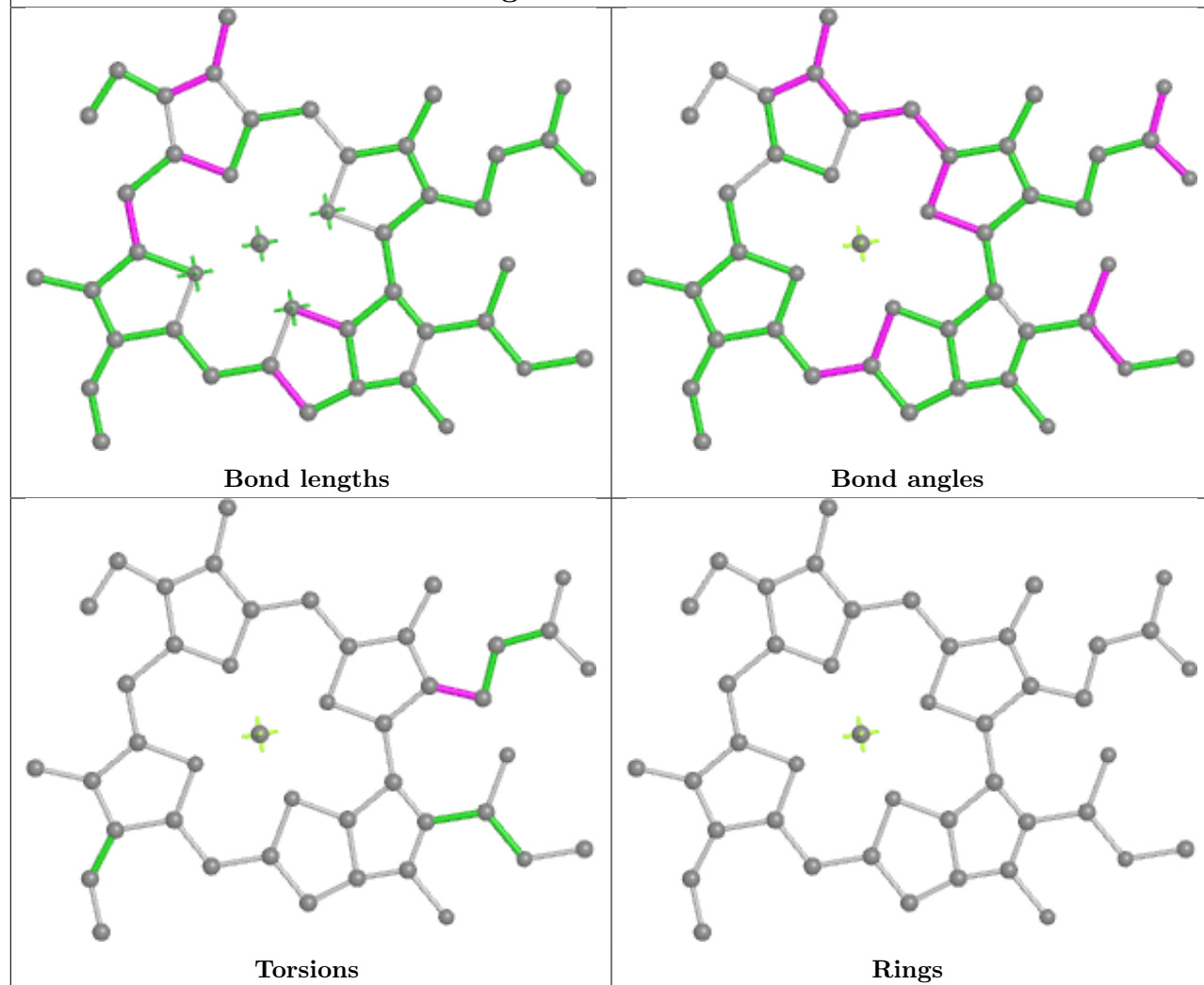


Torsions

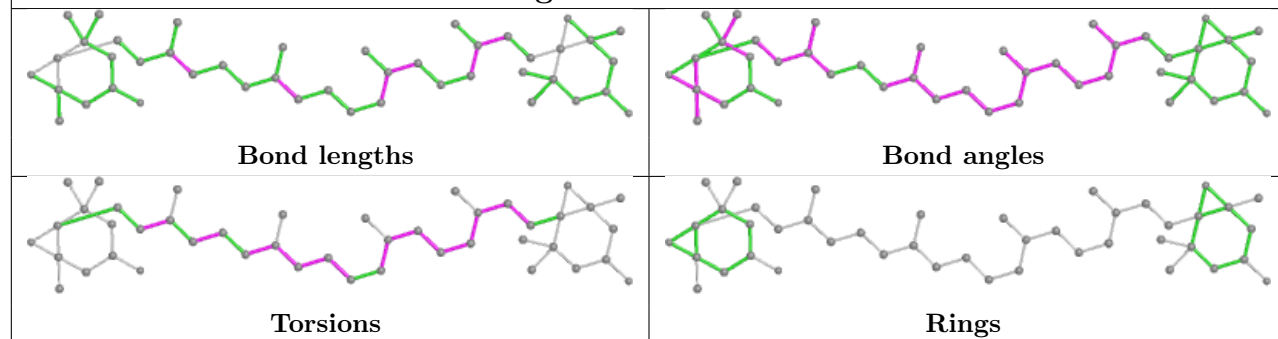


Rings

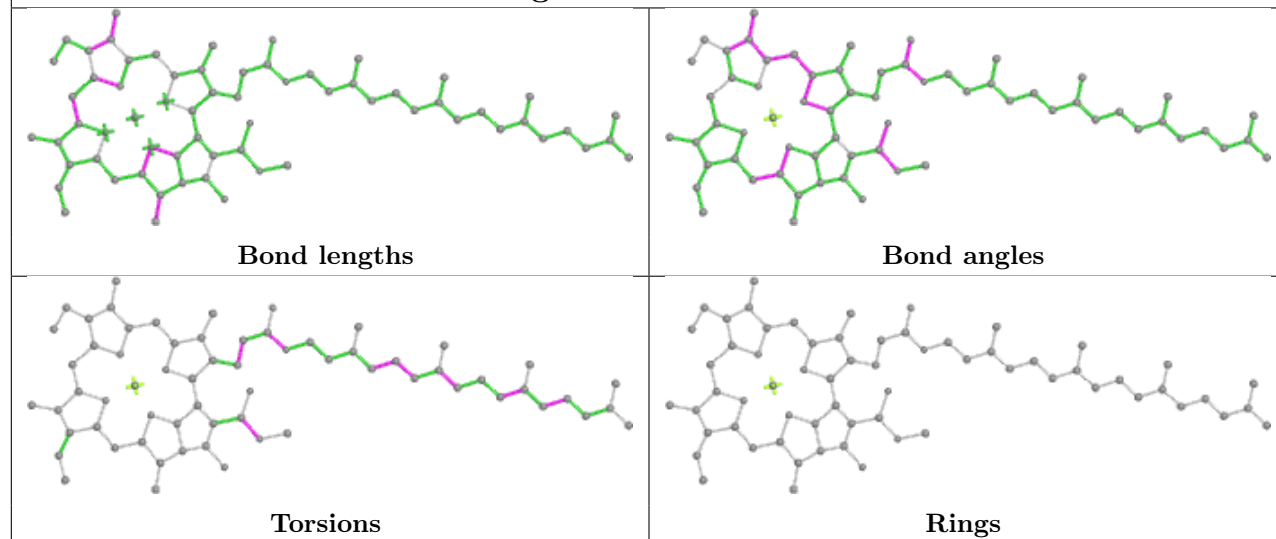
Ligand CLA B 812



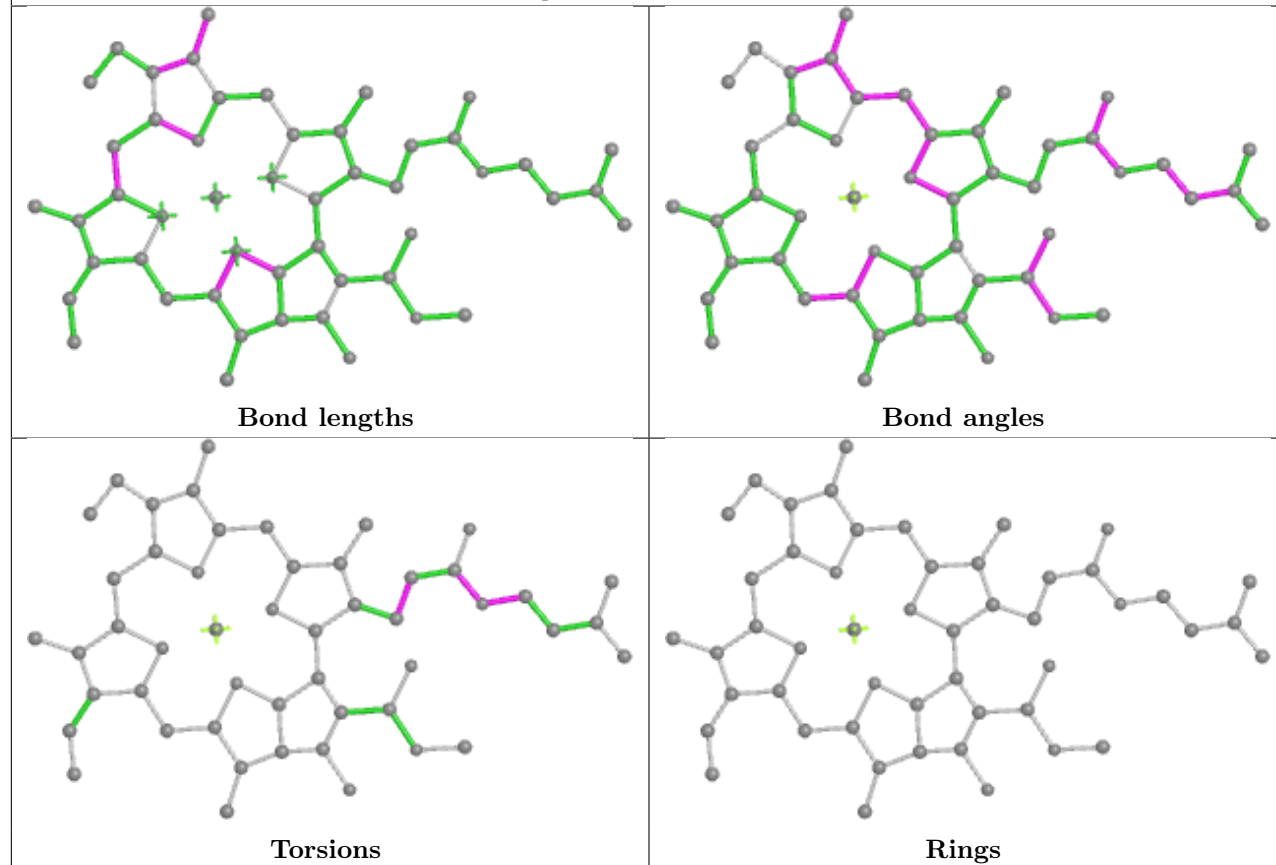
Ligand XAT 8 620



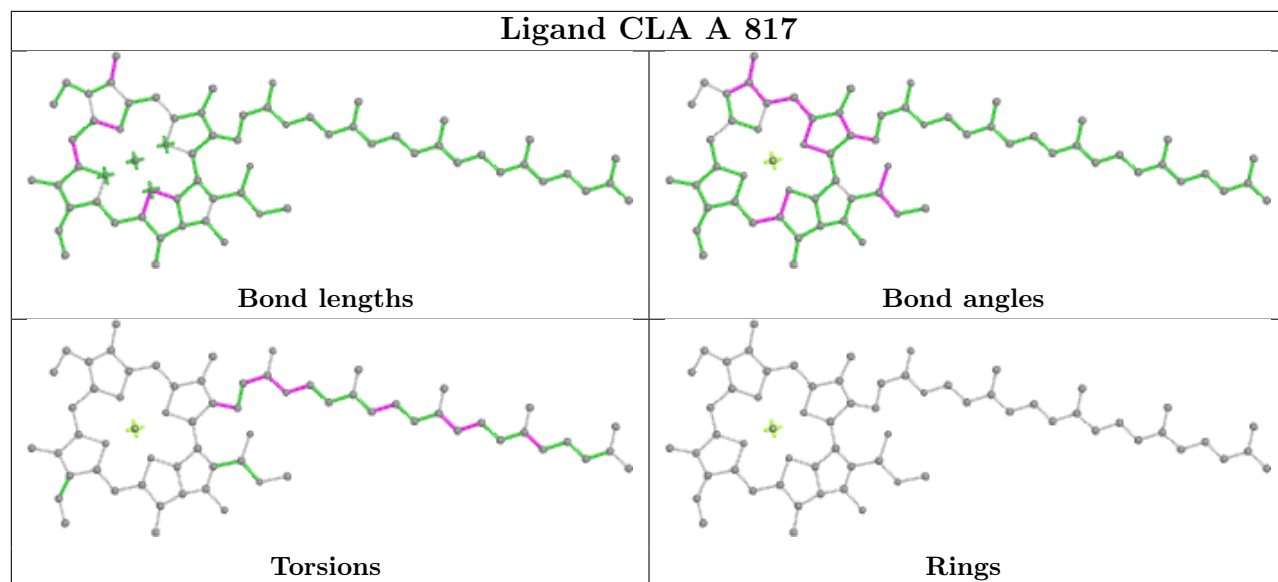
Ligand CLA A 822



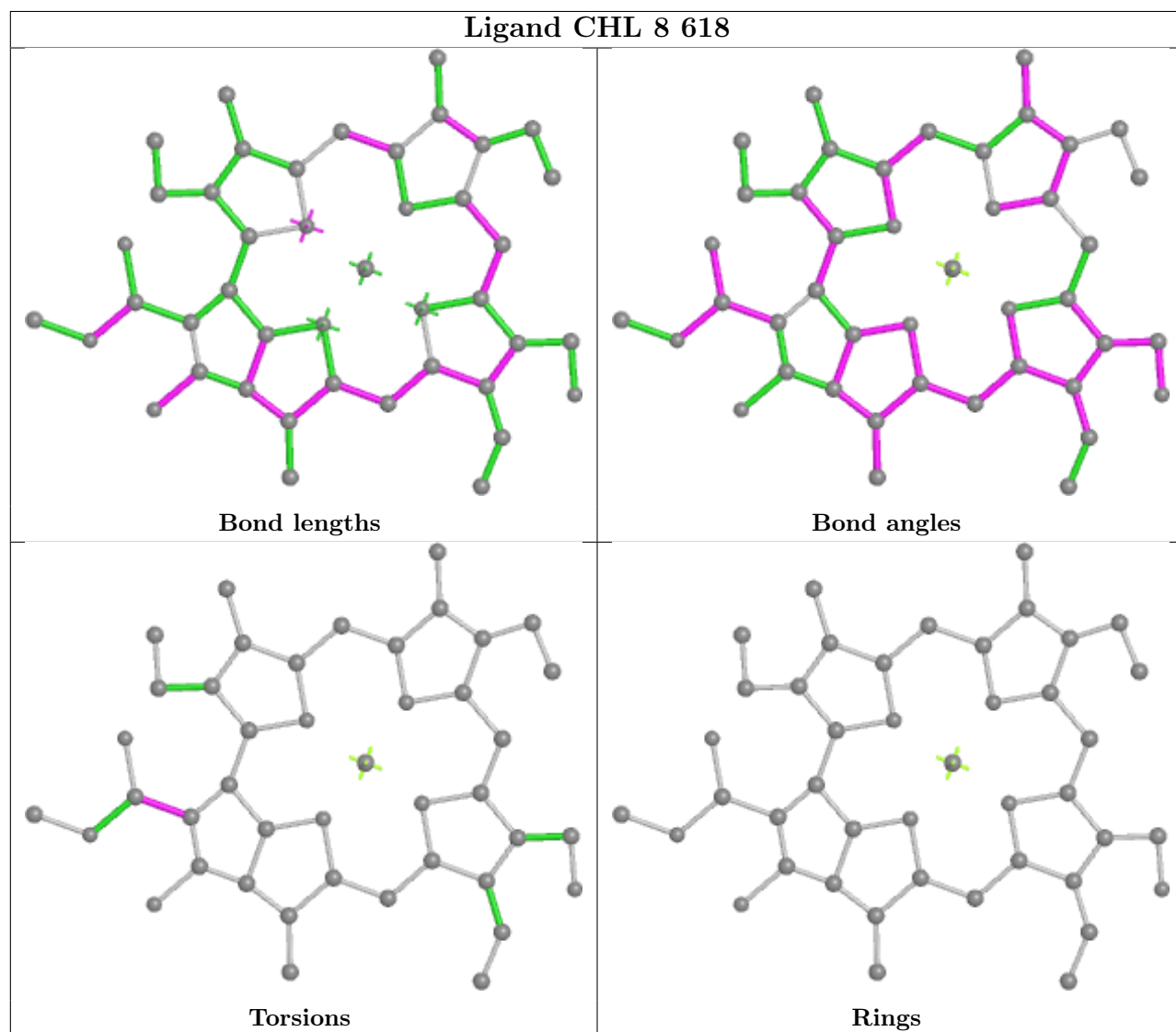
Ligand CLA 2 604

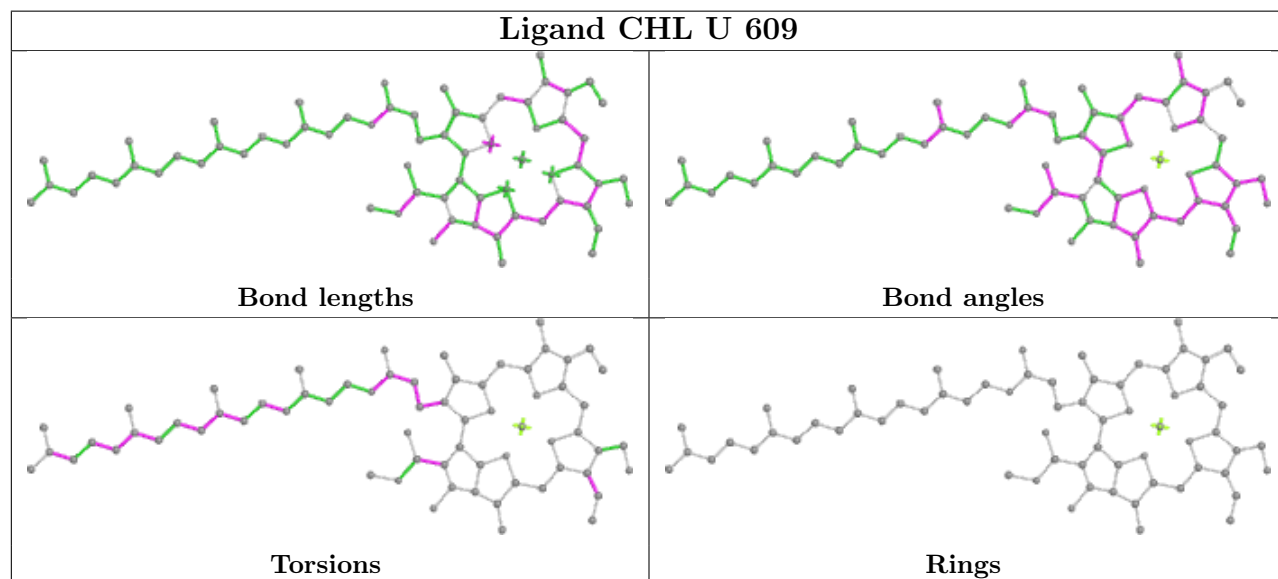
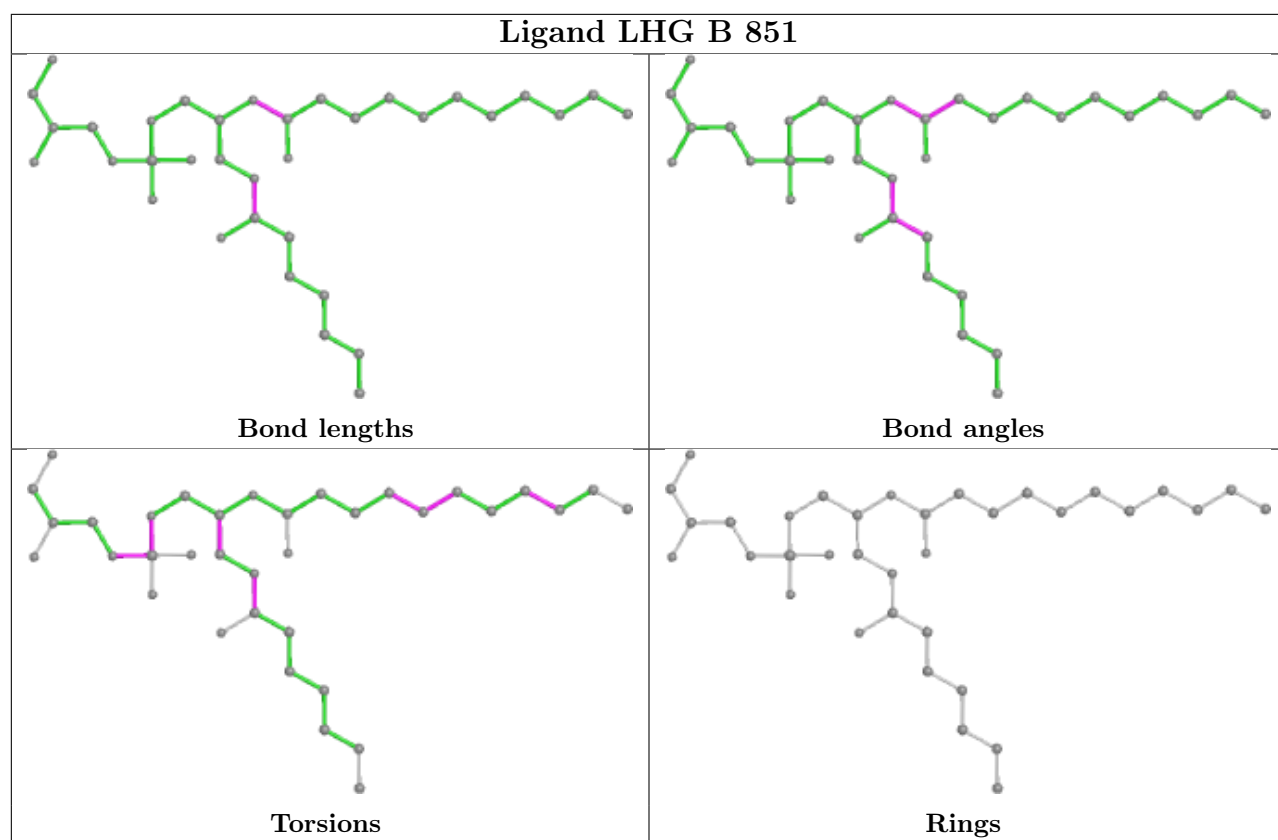


Ligand CLA A 817

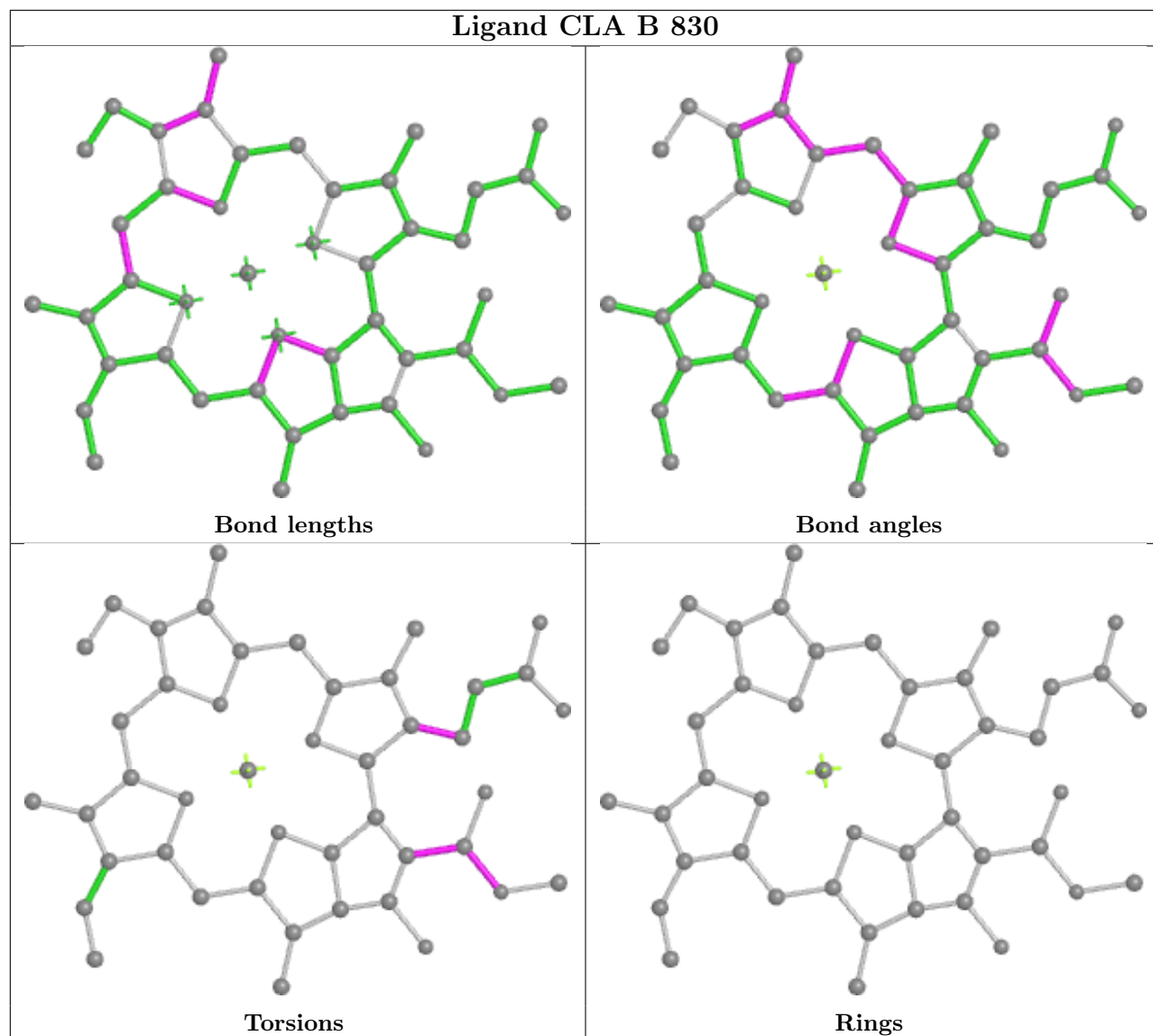


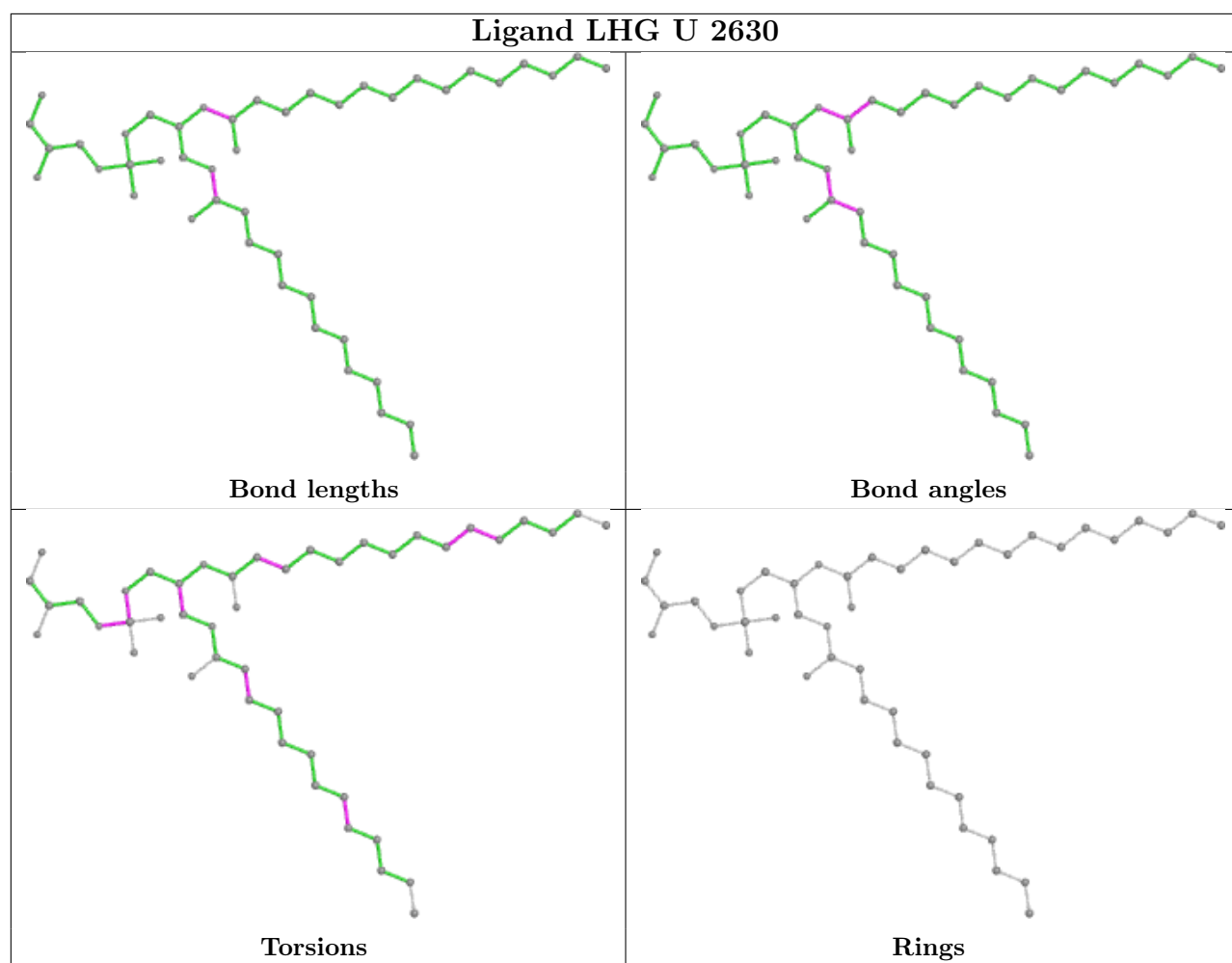
Ligand CHL 8 618



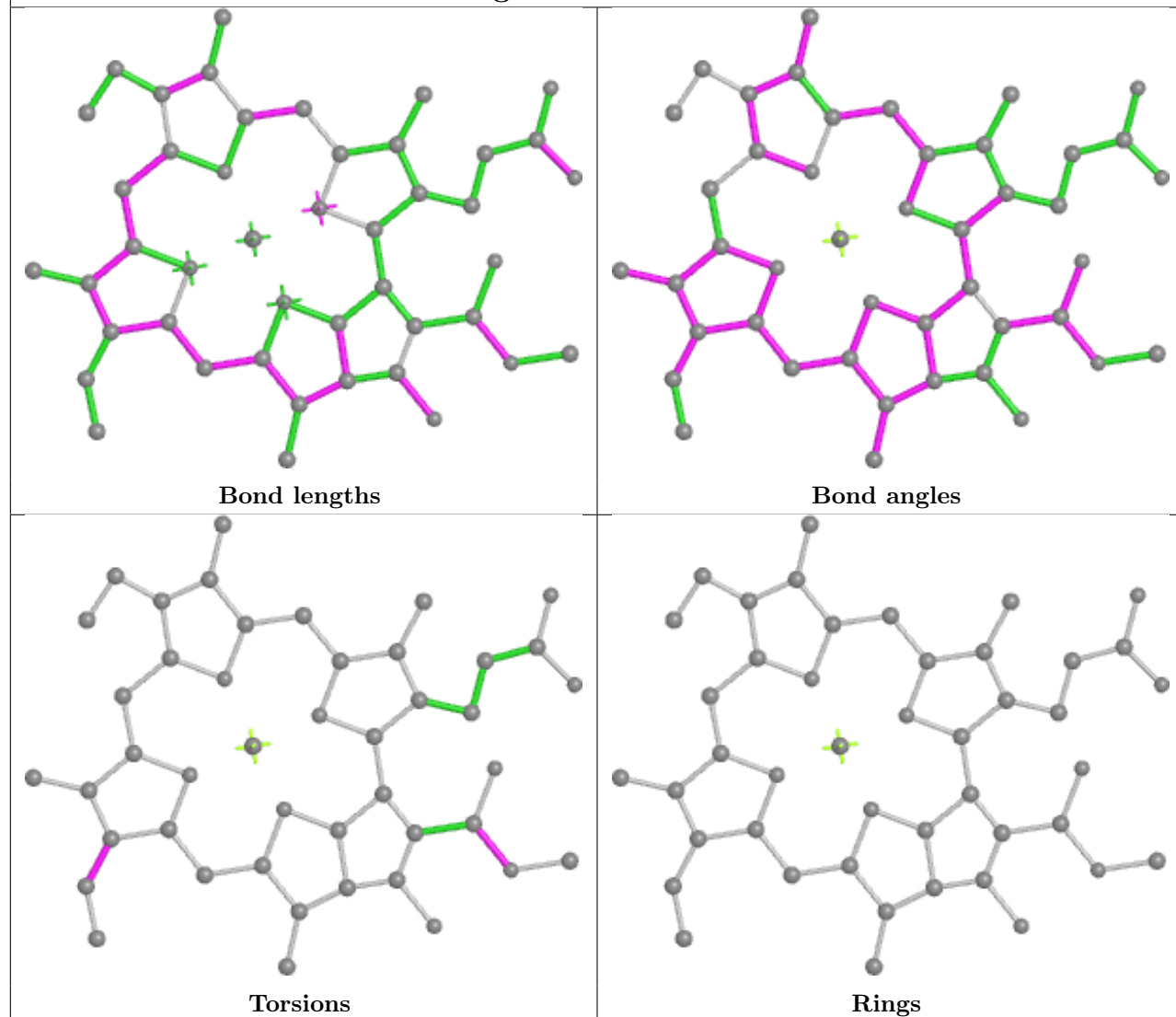


Ligand CLA B 830

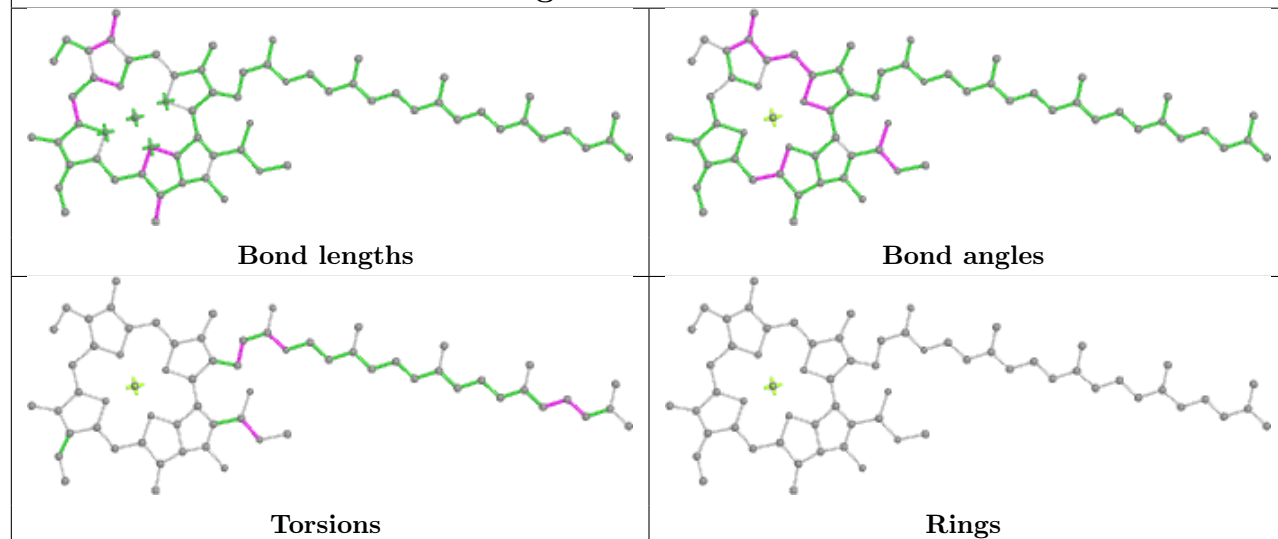




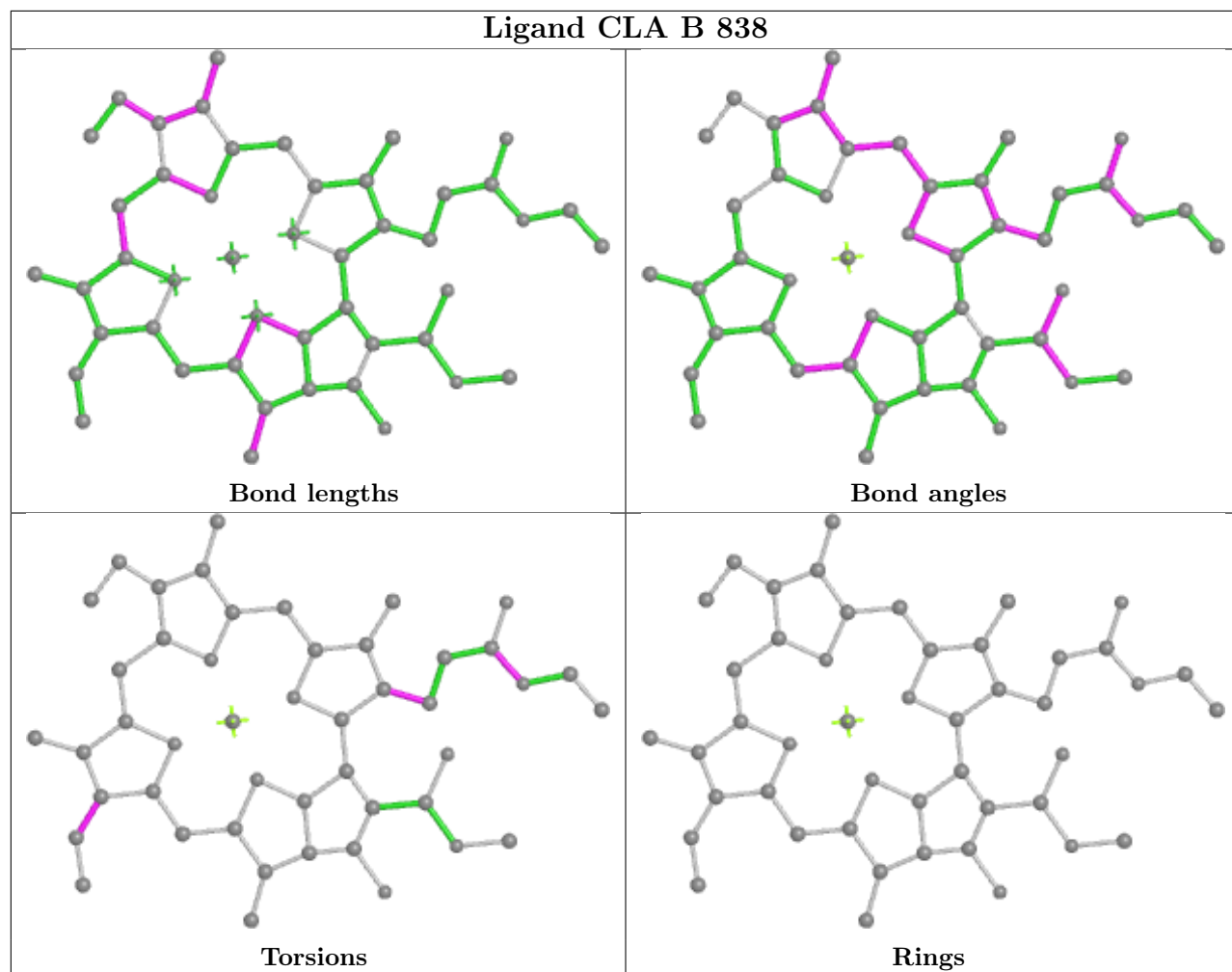
Ligand CLA 9 609



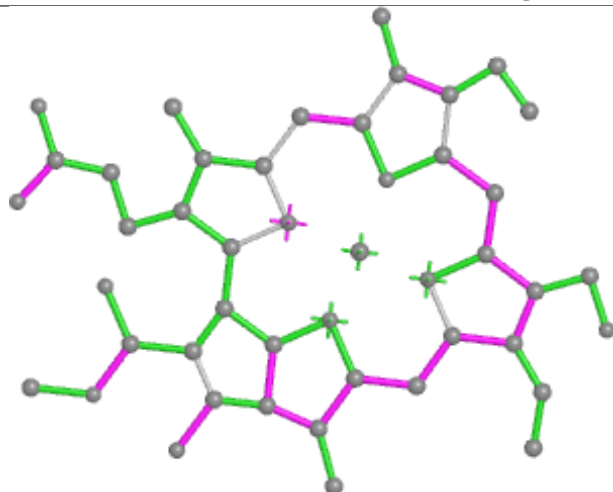
Ligand CLA 3 603



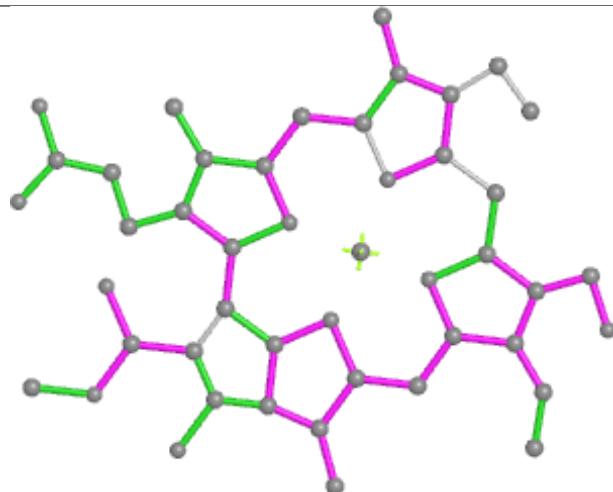
Ligand CLA B 838



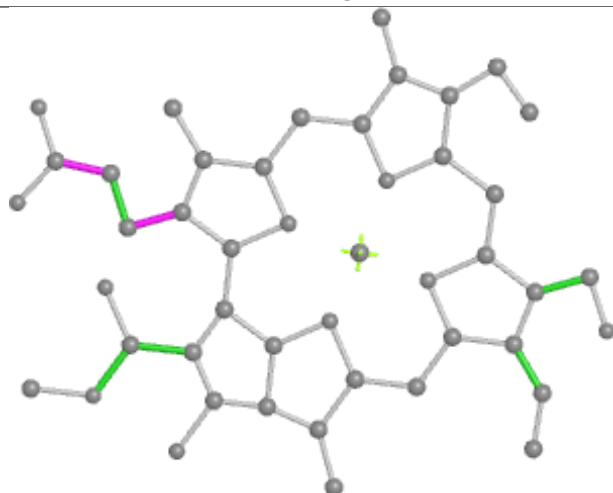
Ligand CHL 2 606



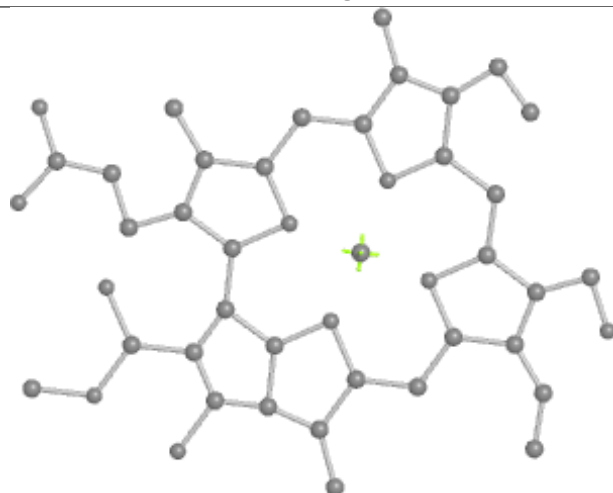
Bond lengths



Bond angles

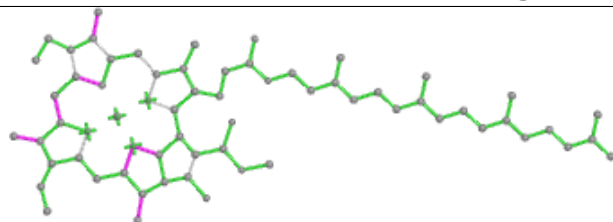


Torsions

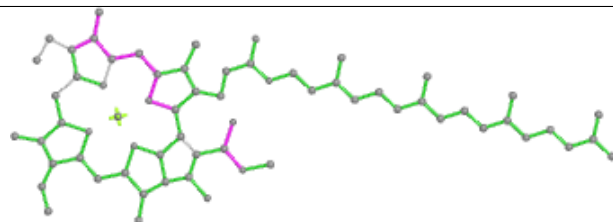


Rings

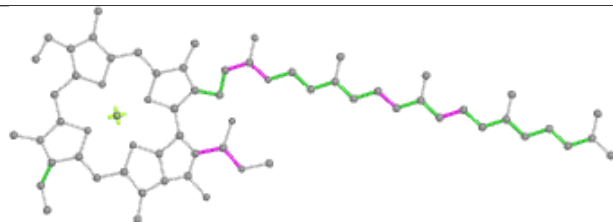
Ligand CLA B 802



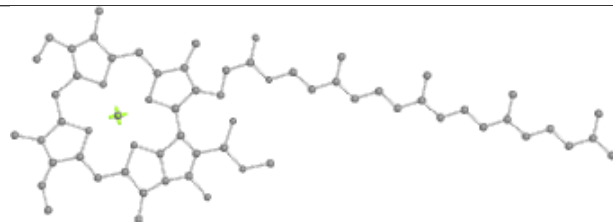
Bond lengths



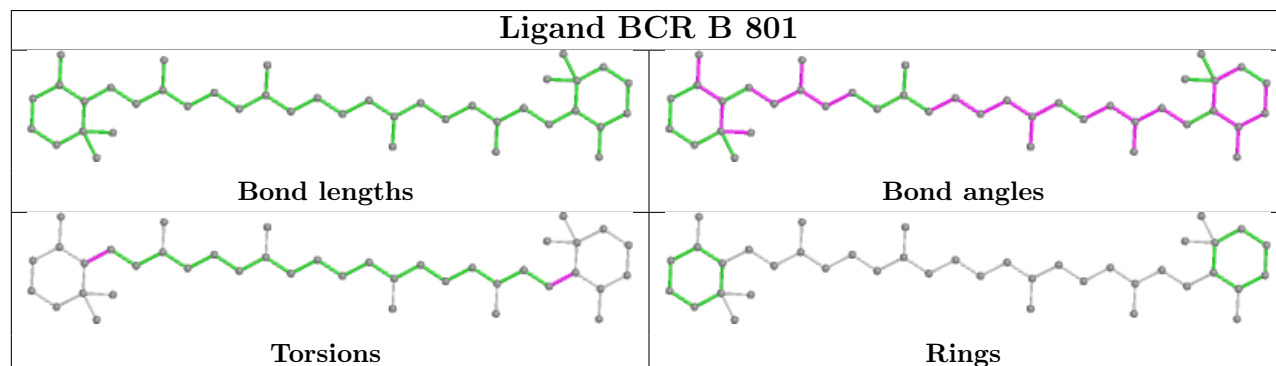
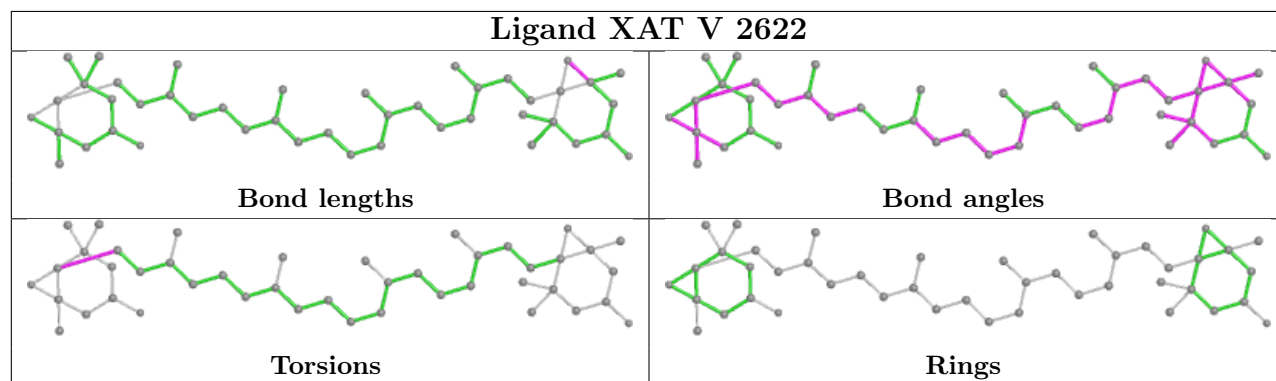
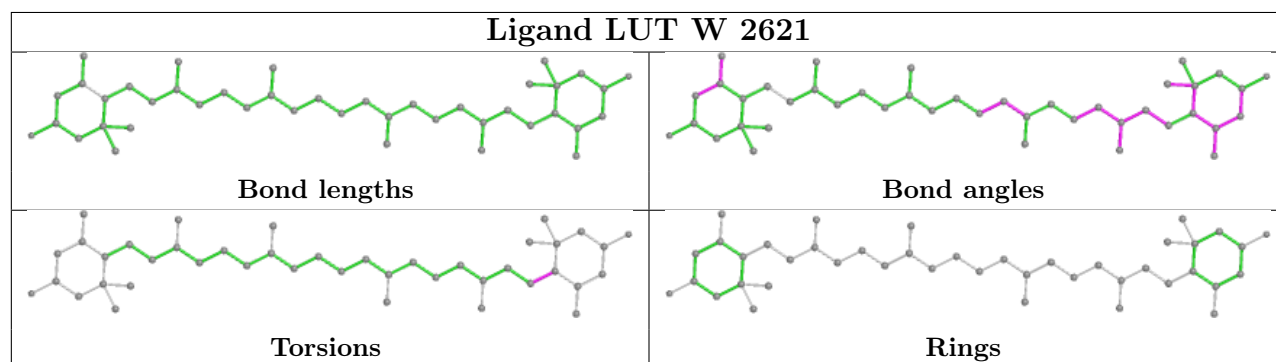
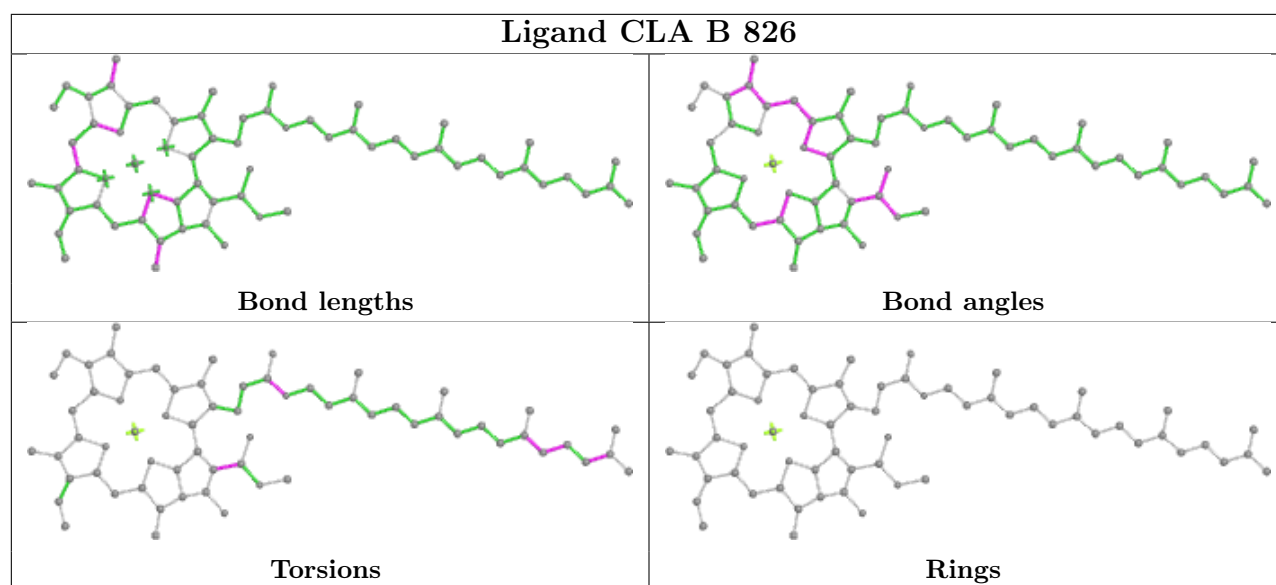
Bond angles



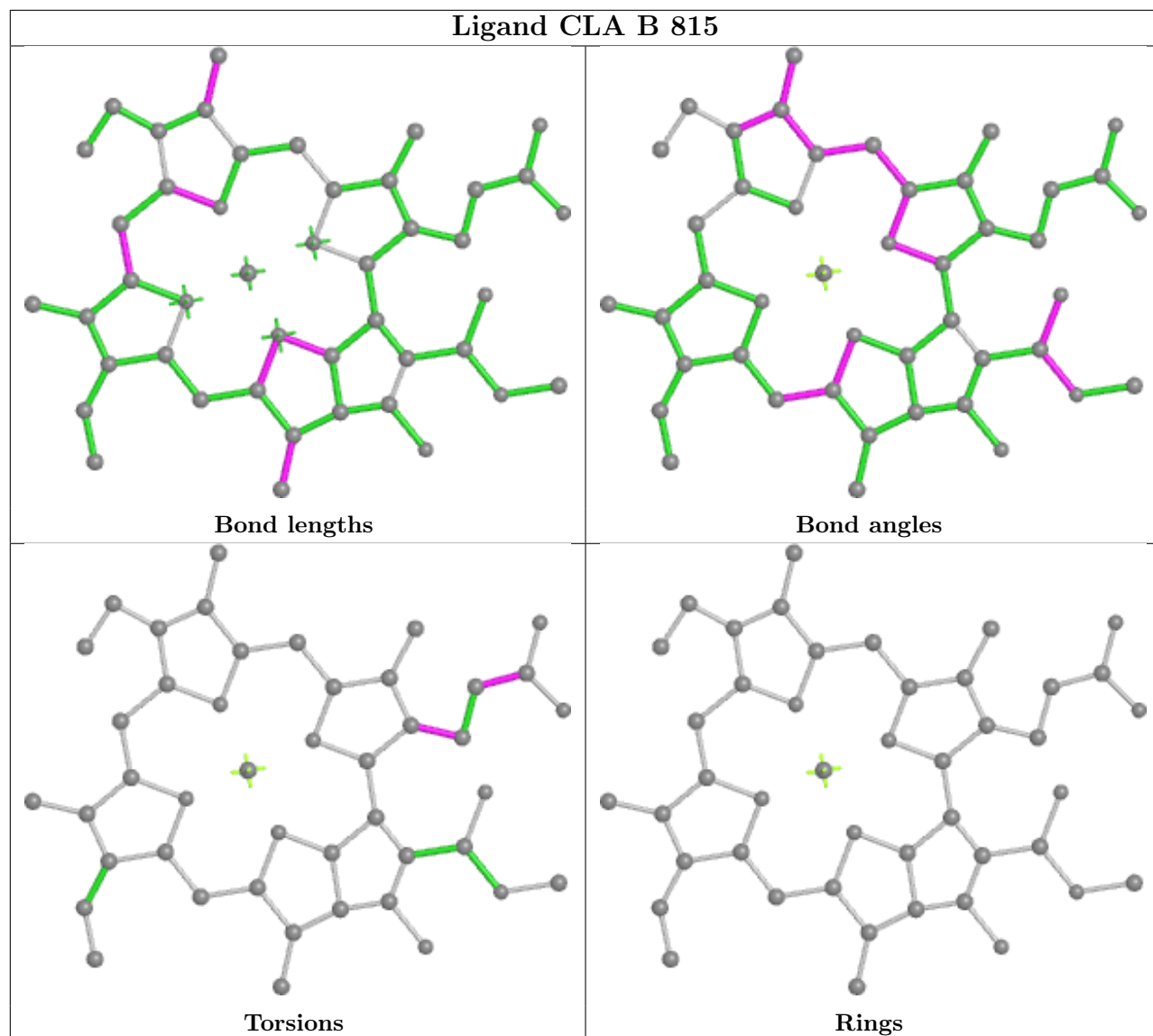
Torsions

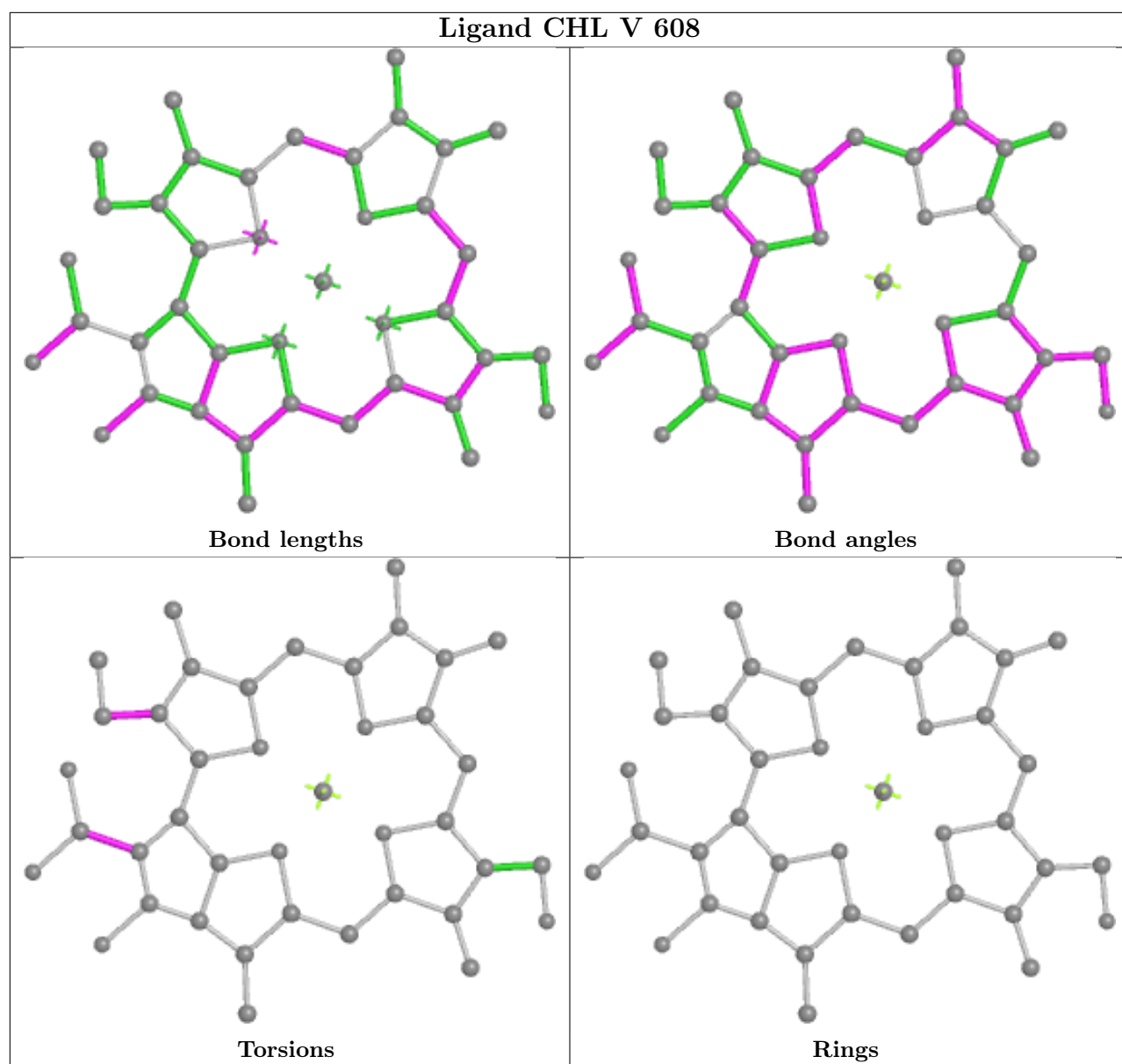


Rings

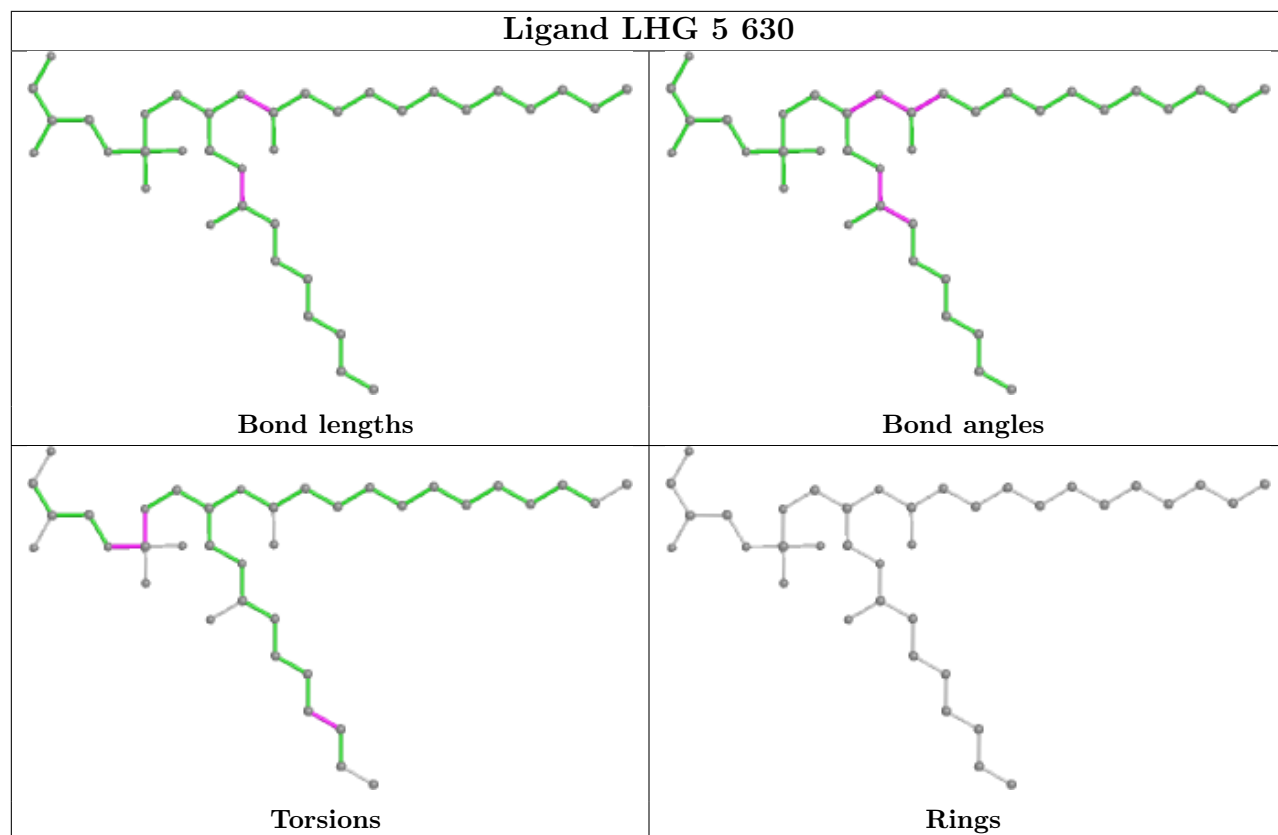


Ligand CLA B 815

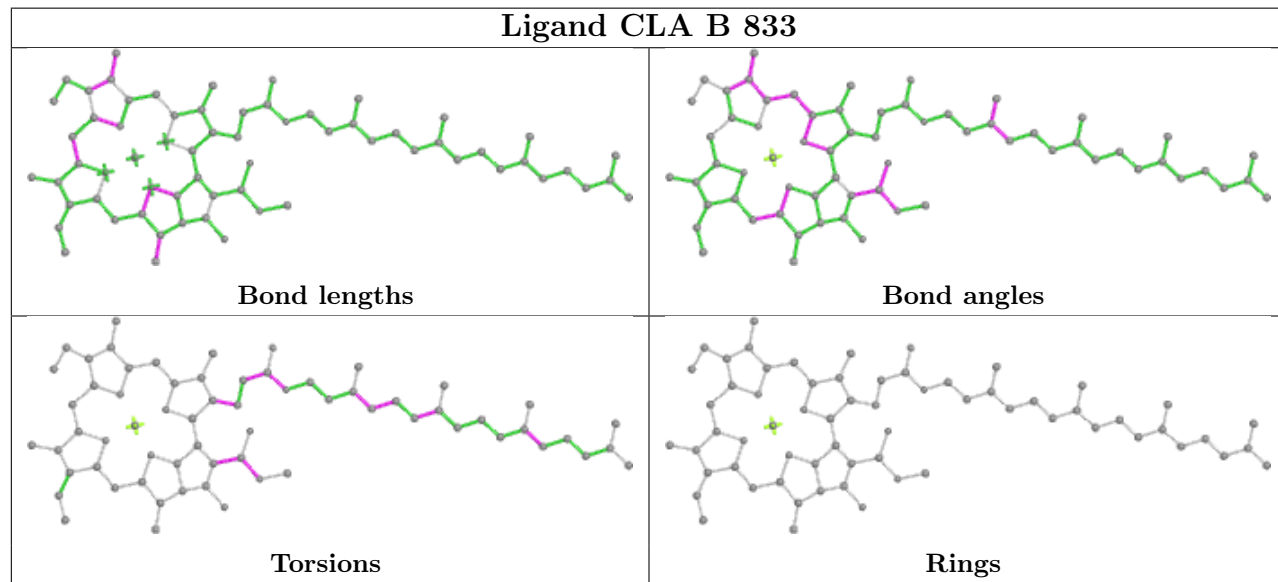




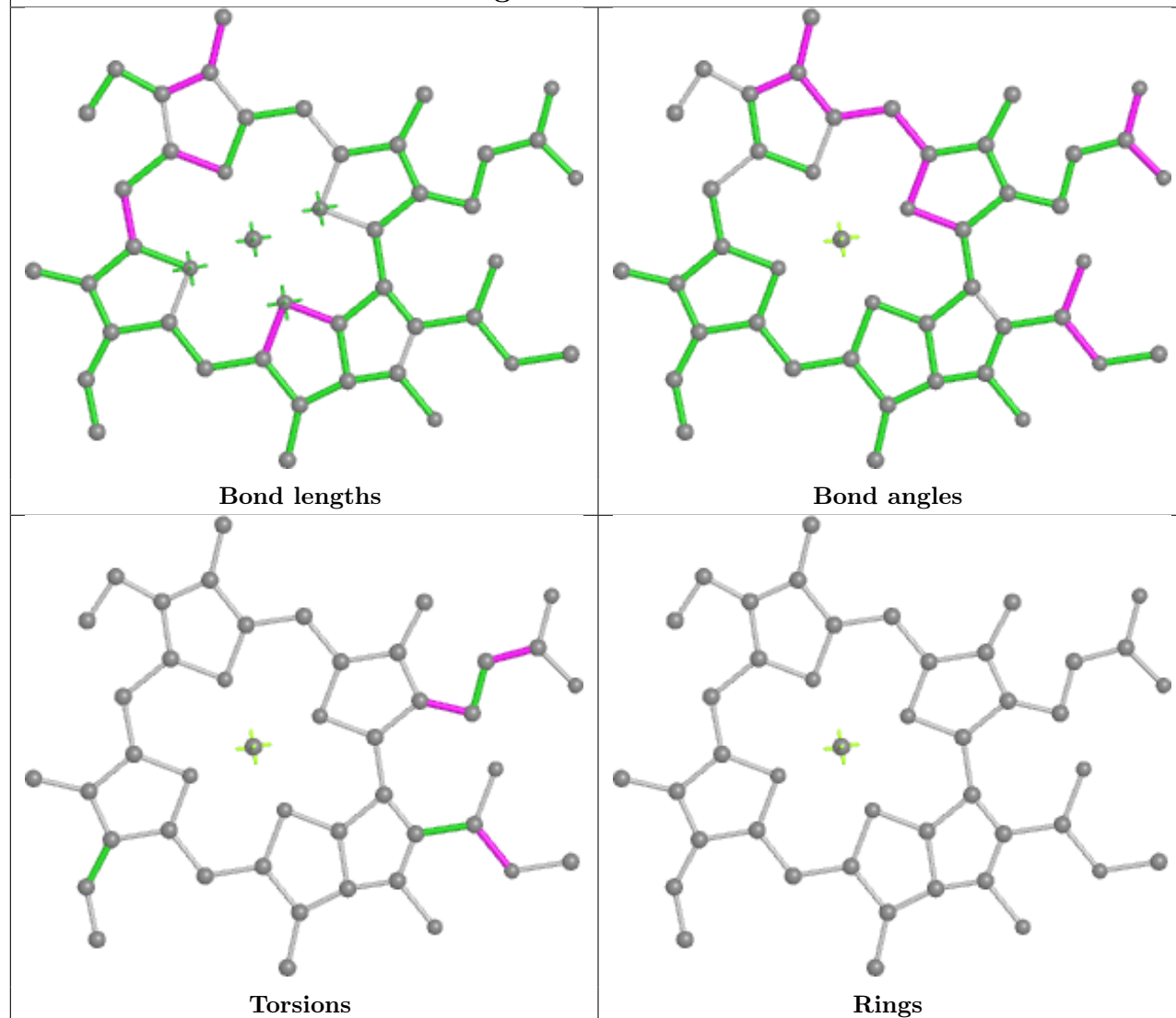
Ligand LHG 5 630



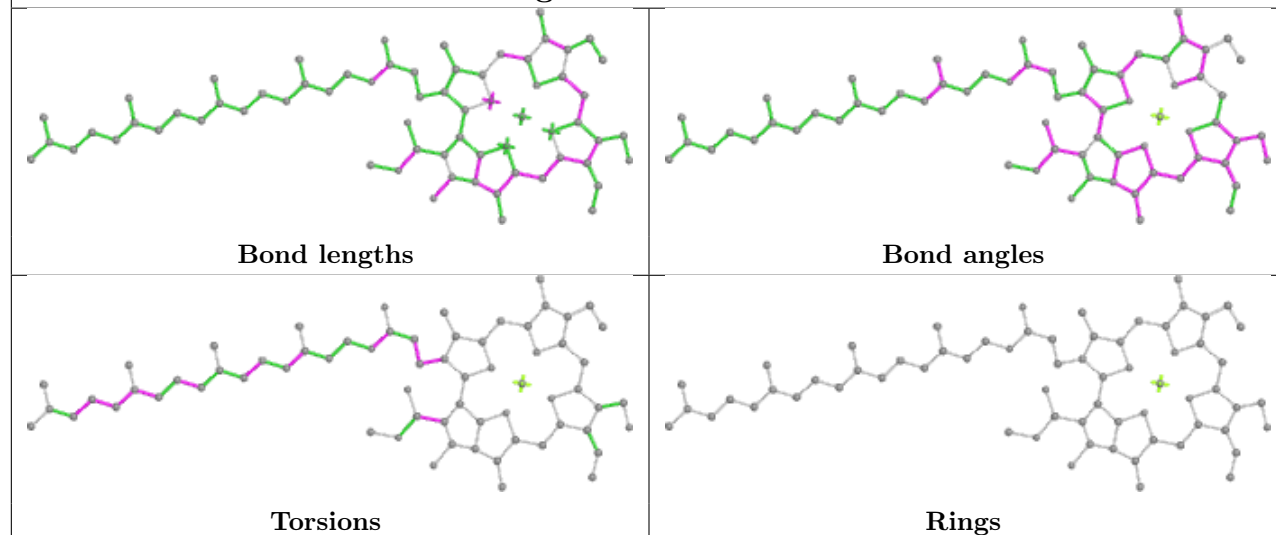
Ligand CLA B 833

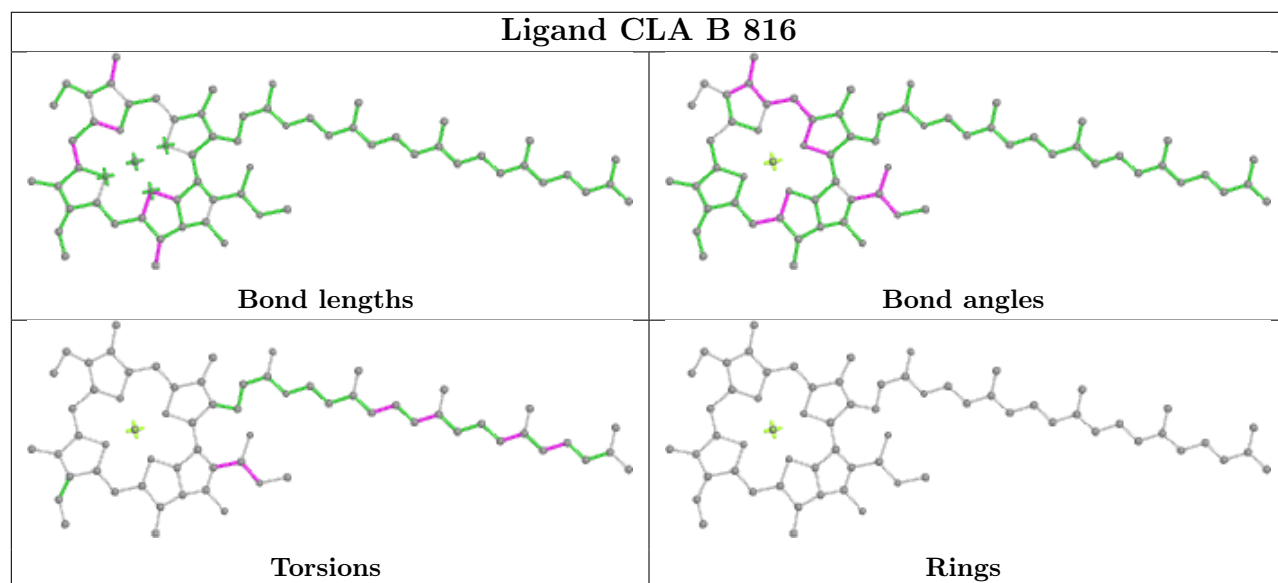
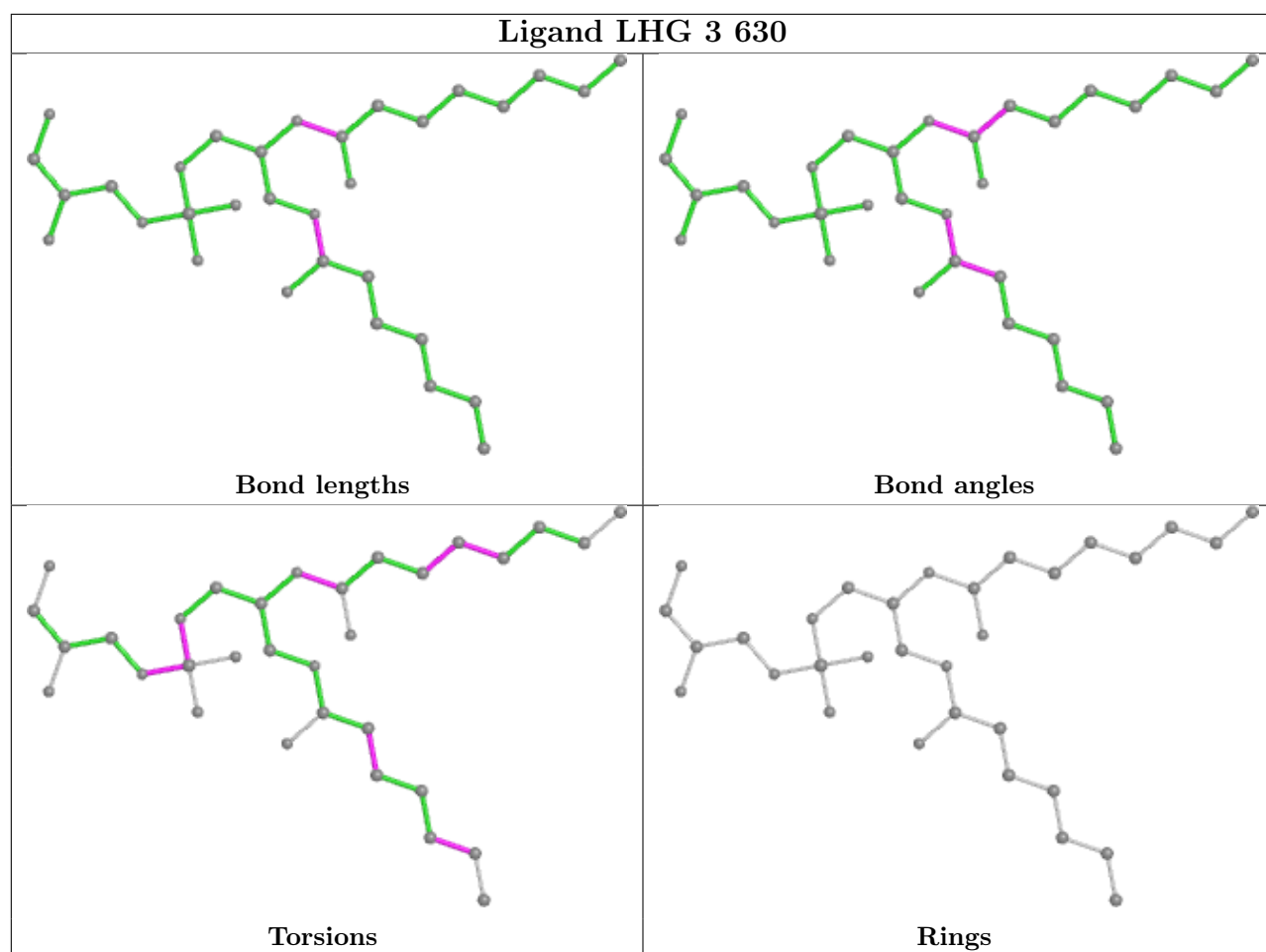


Ligand CLA 5 603

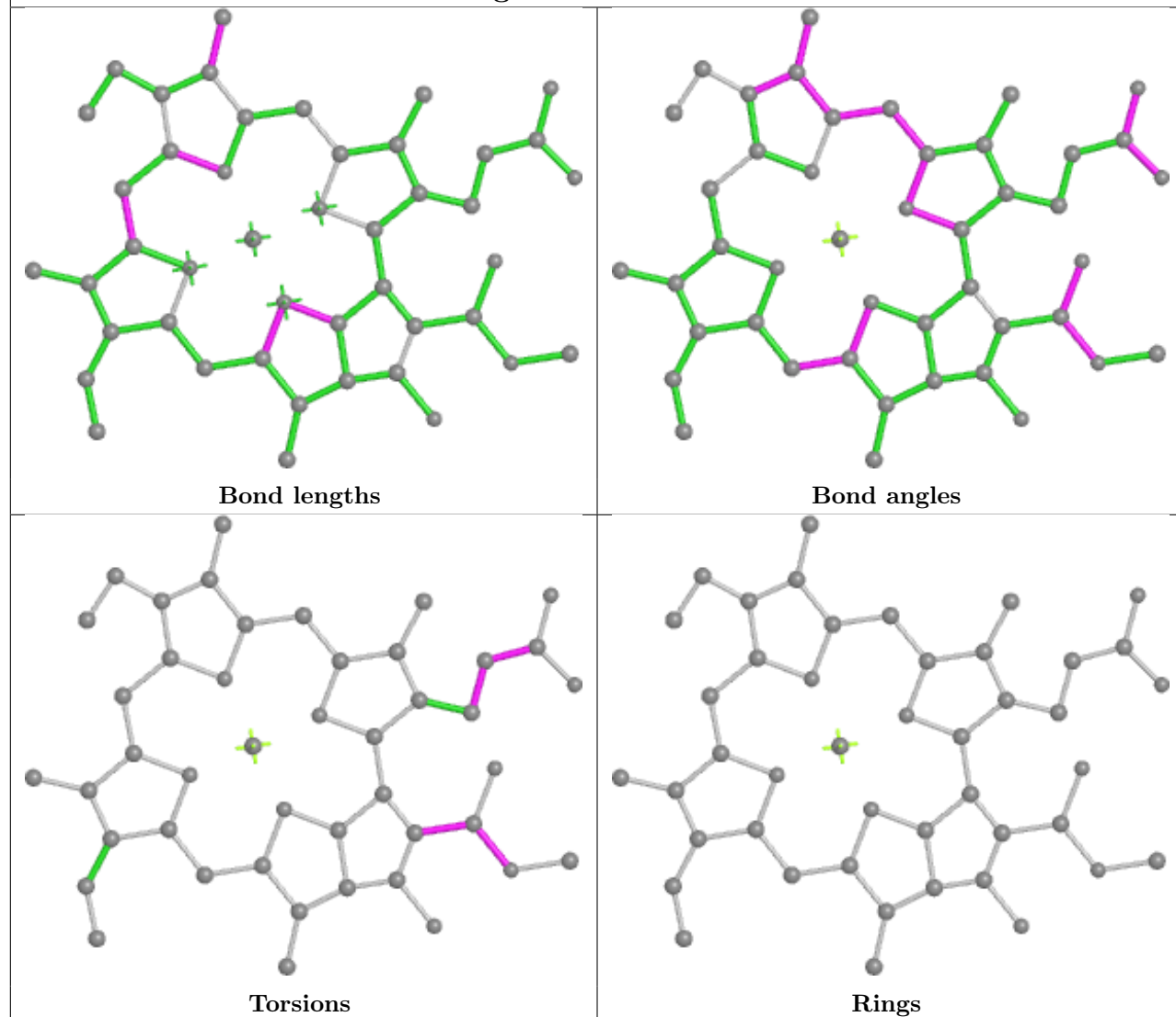


Ligand CHL 6 601

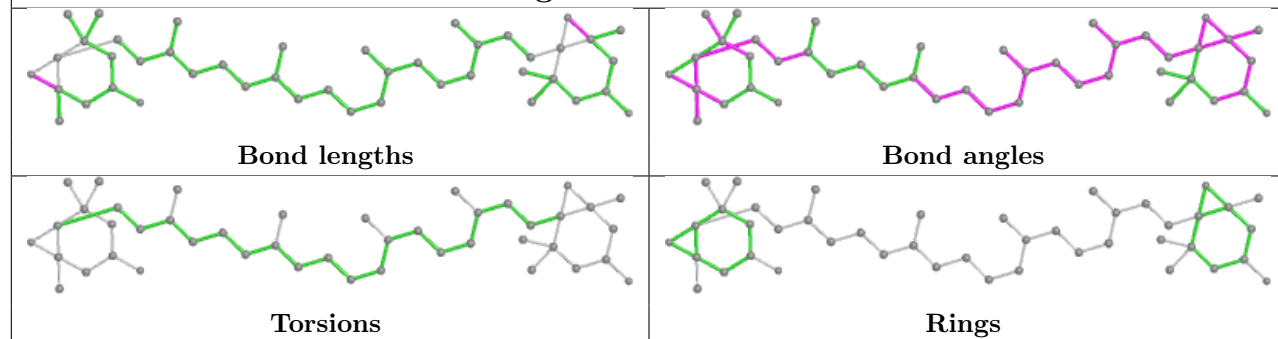




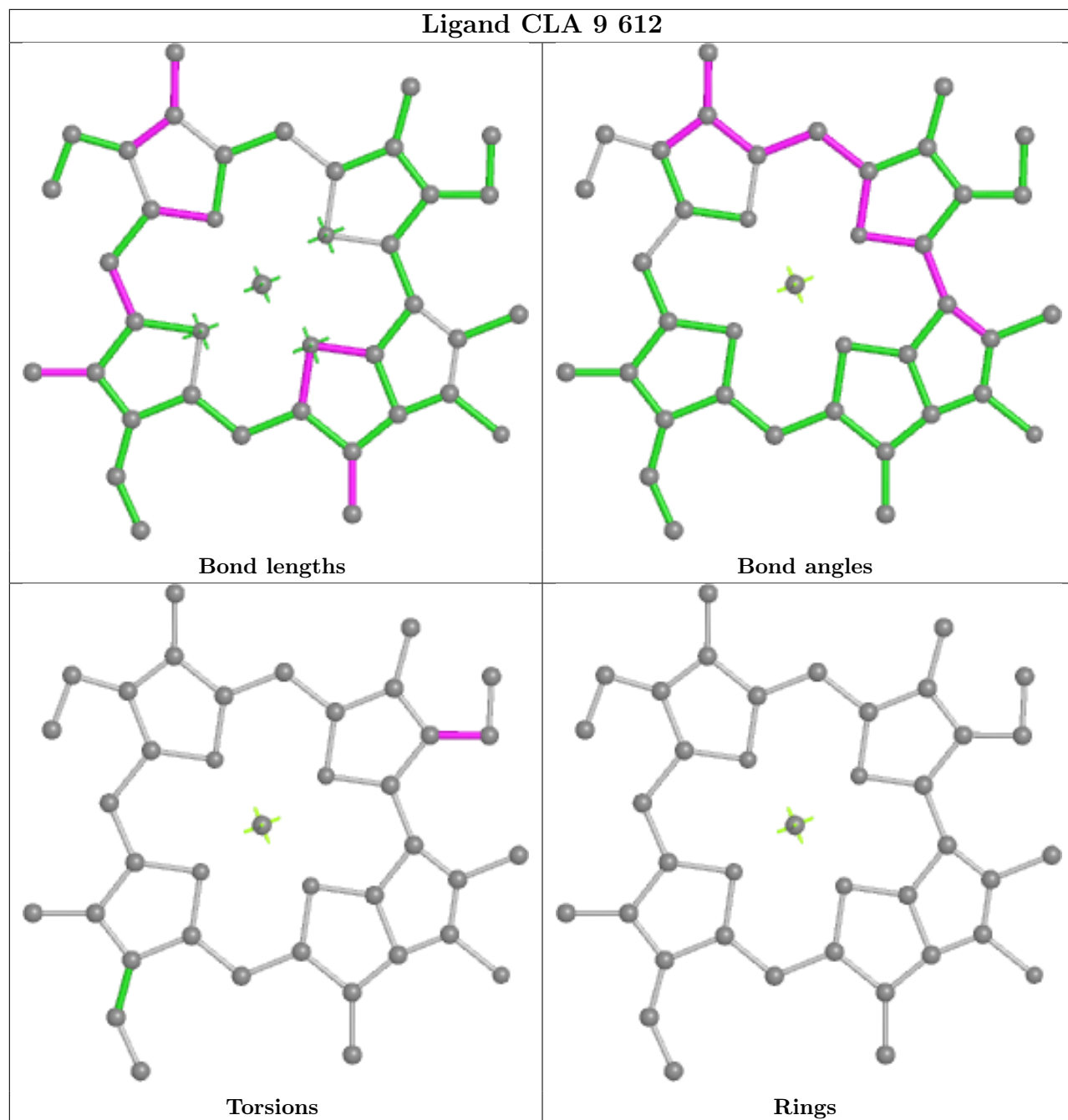
Ligand CLA 6 611

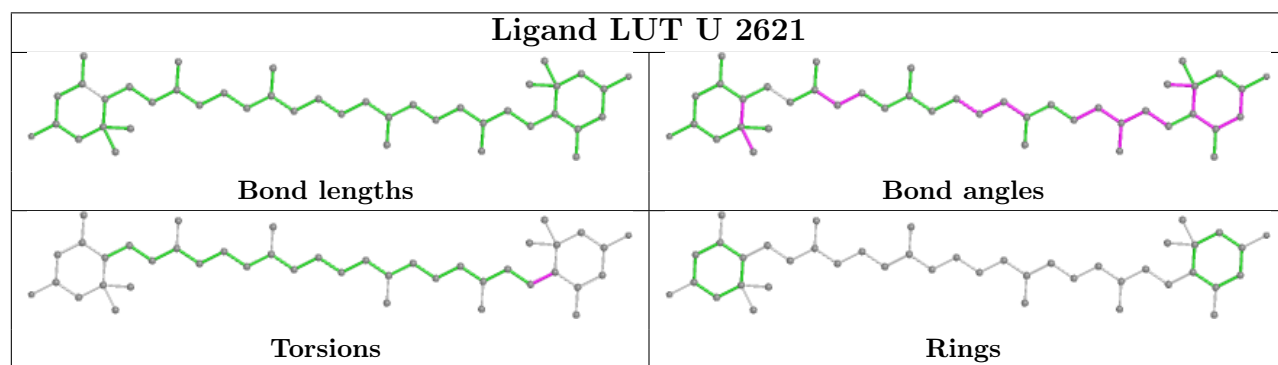
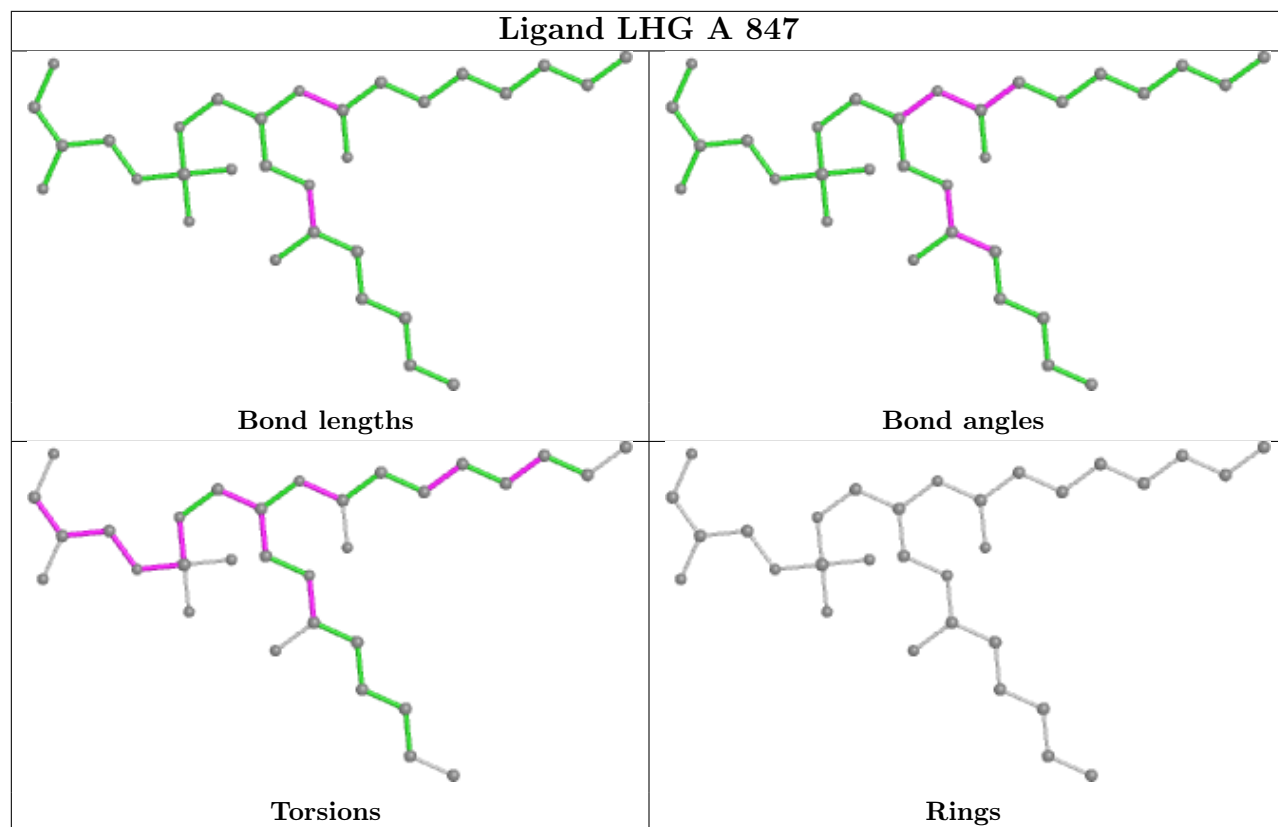


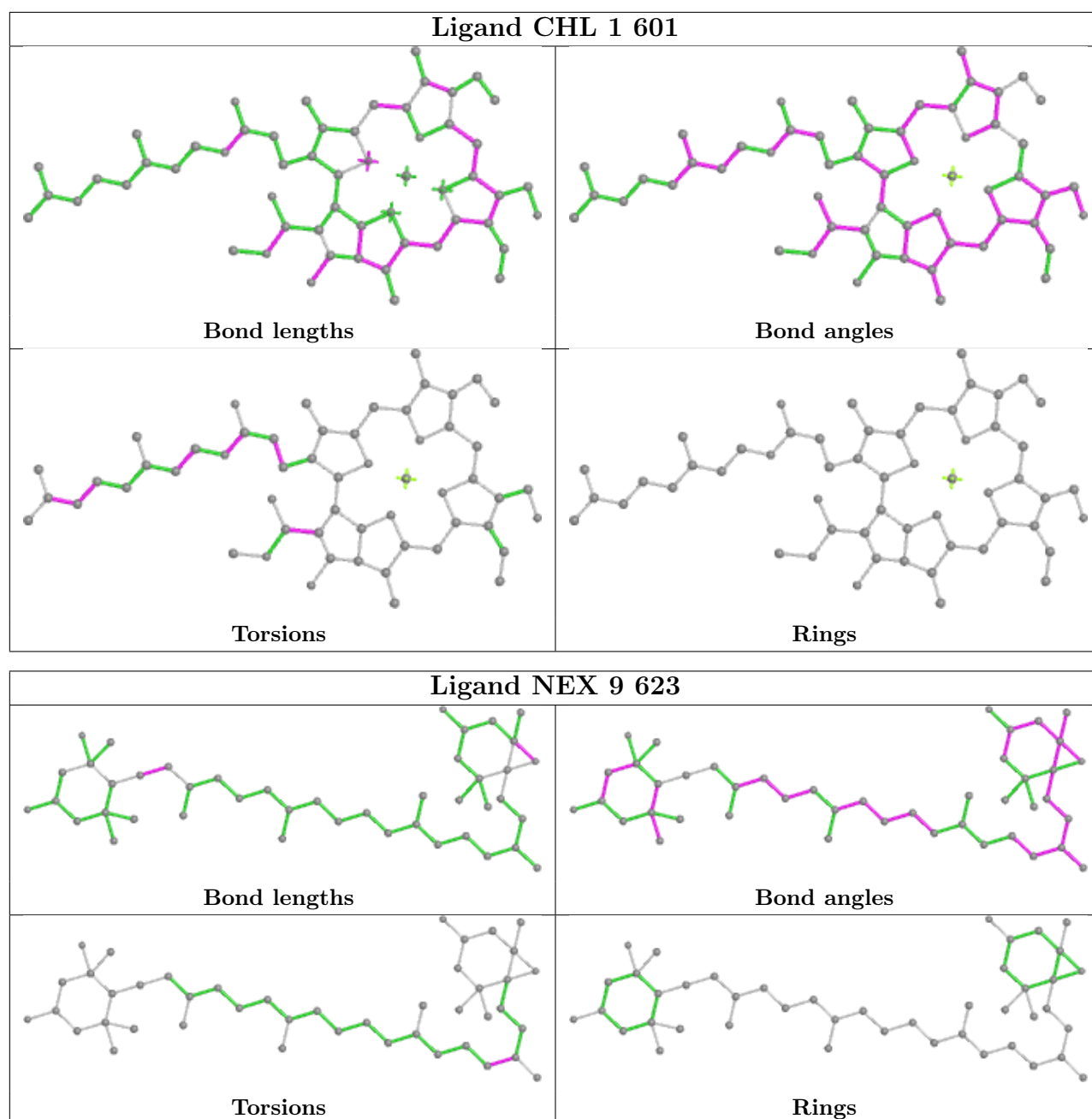
Ligand XAT 2 620

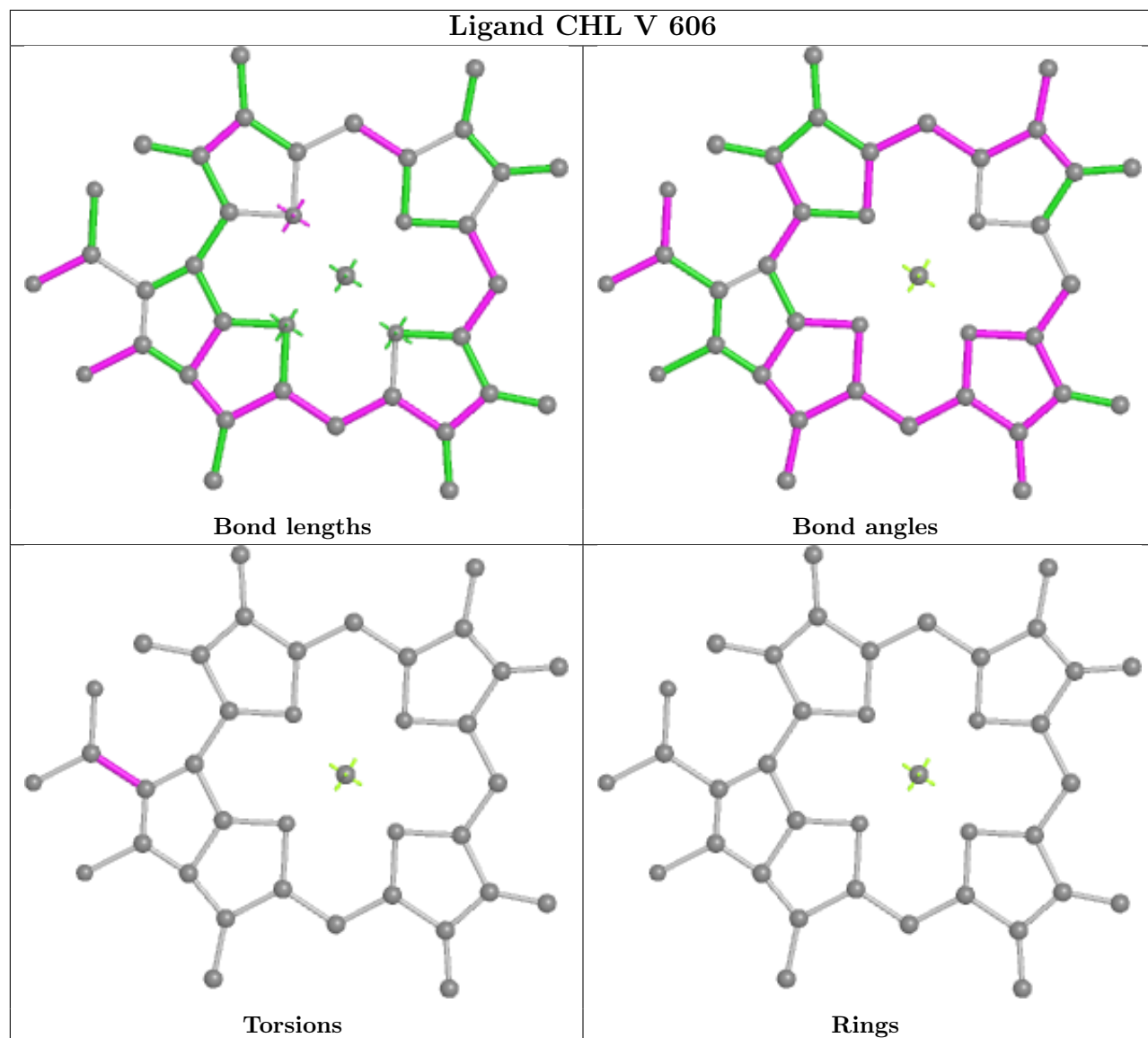


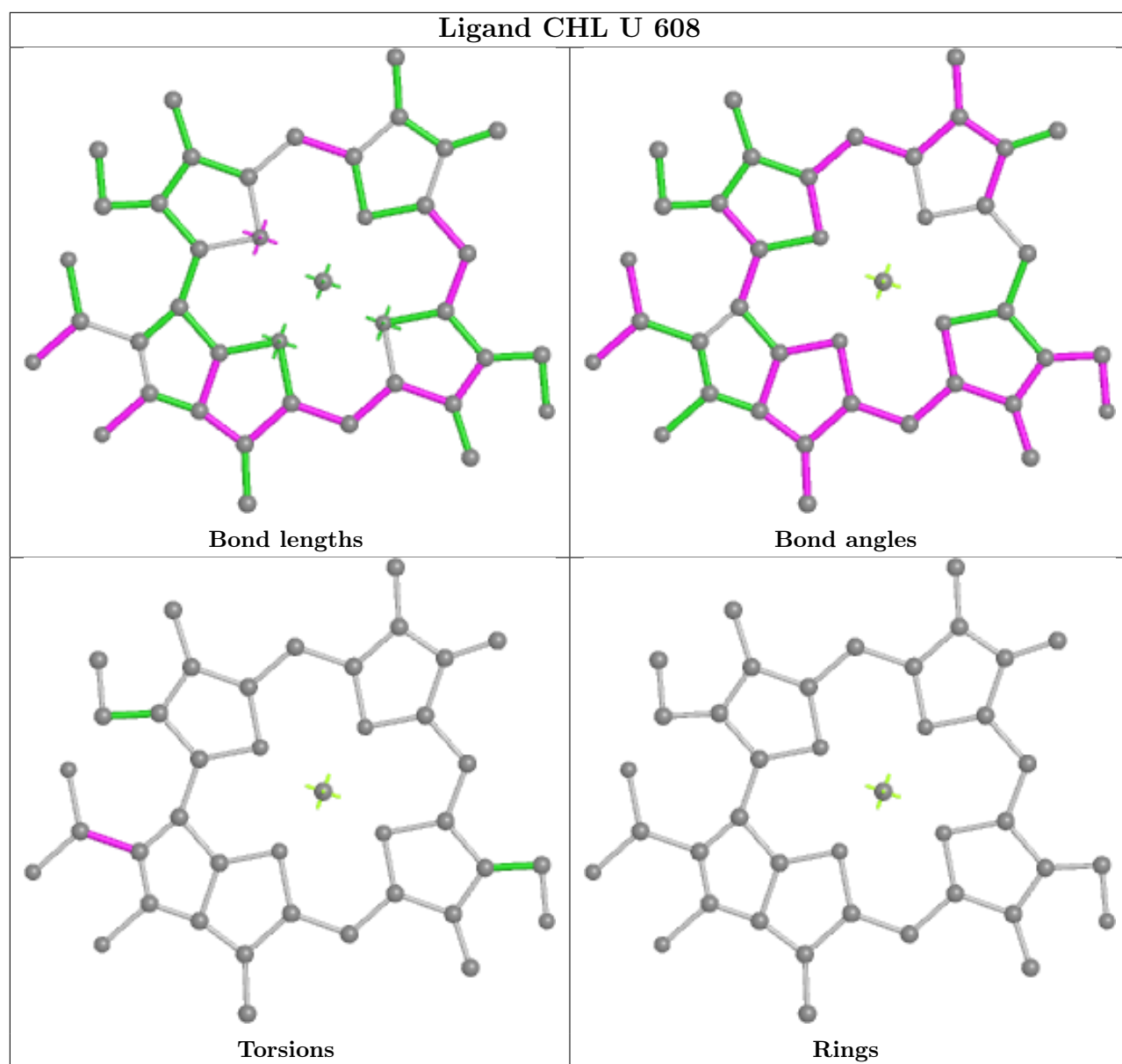
Ligand CLA 9 612



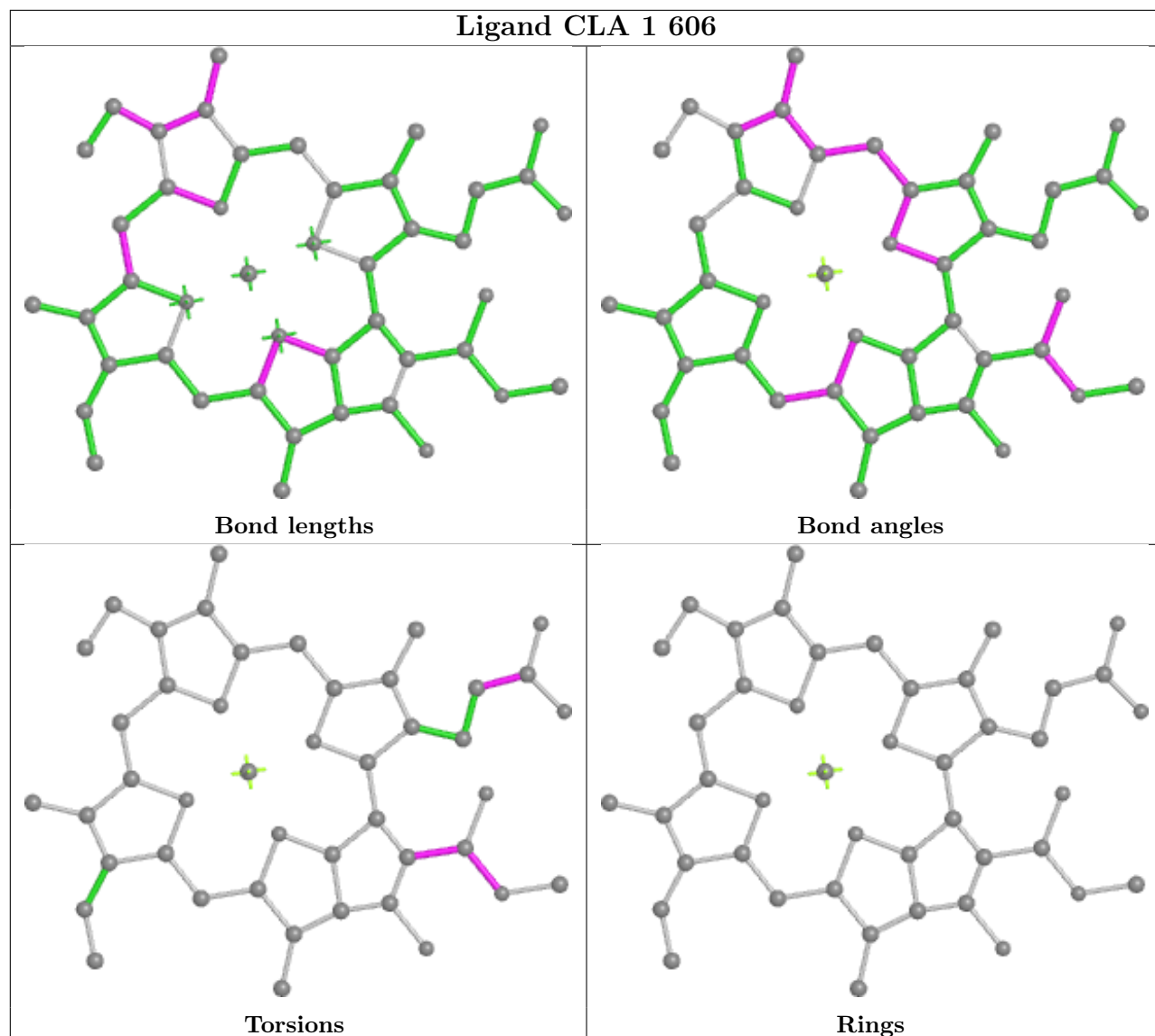




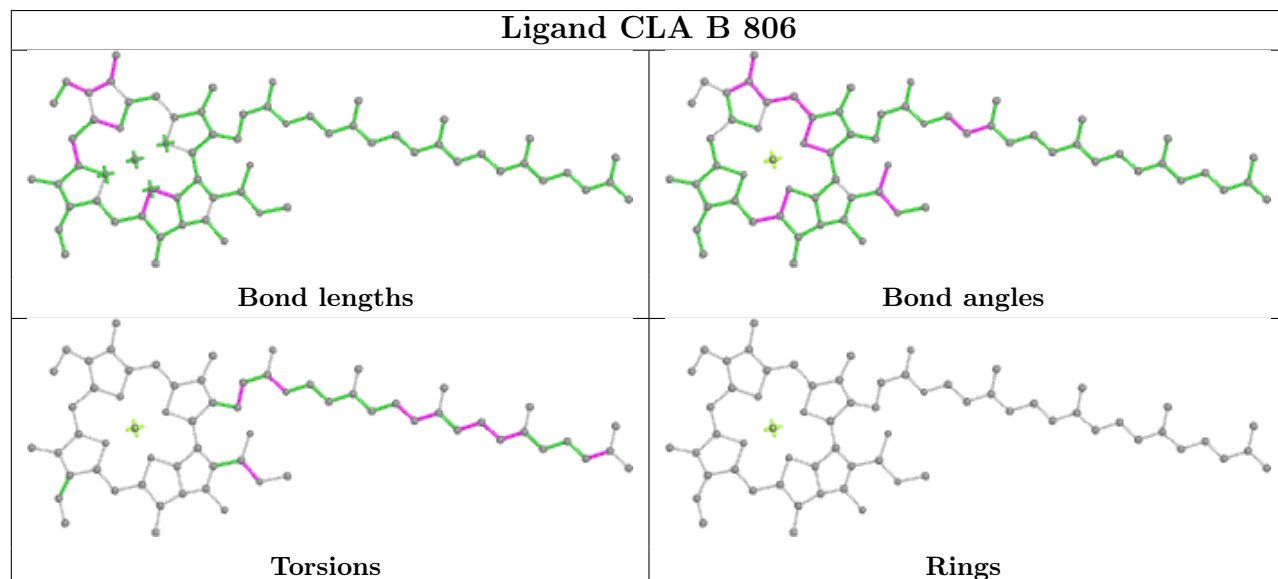




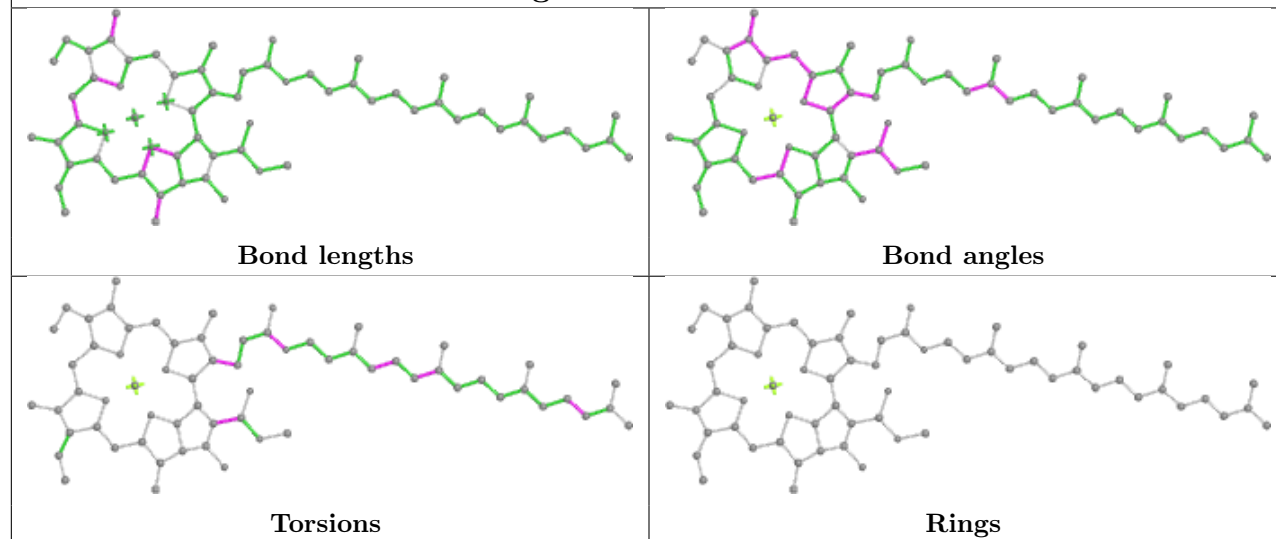
Ligand CLA 1 606



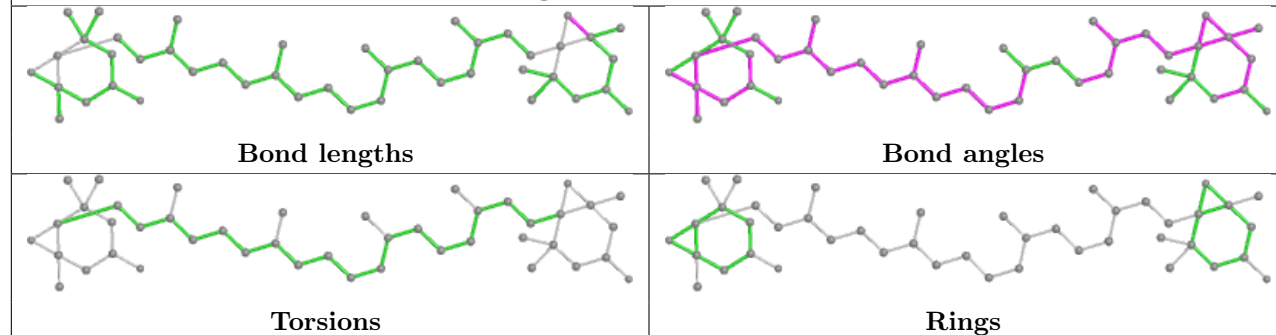
Ligand CLA B 806



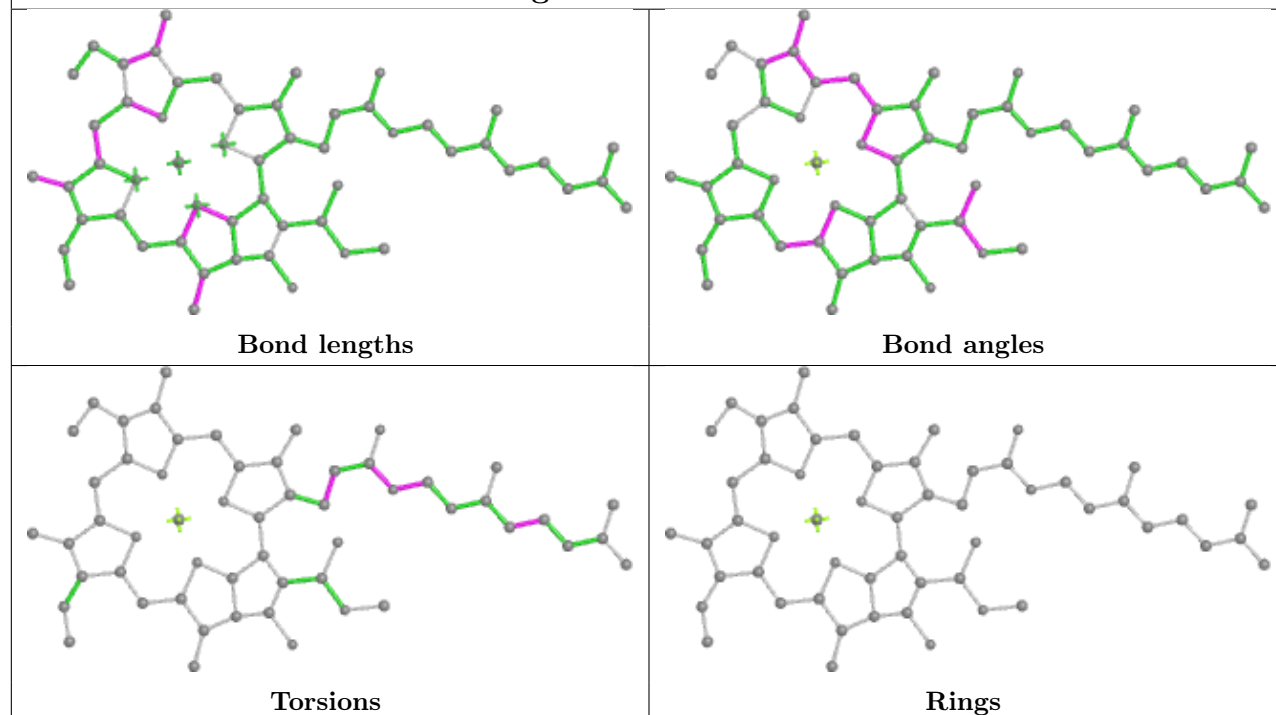
Ligand CLA B 805



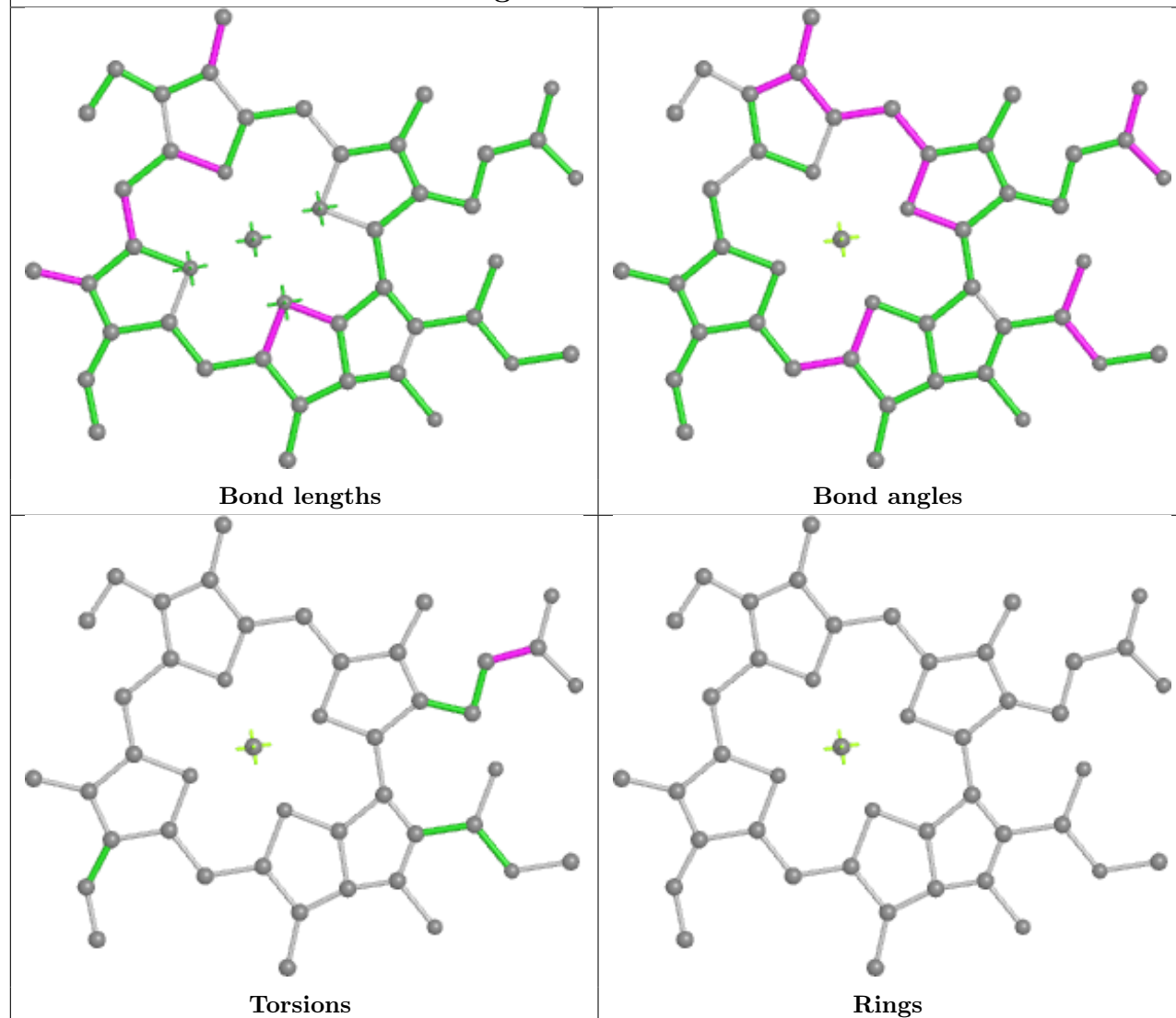
Ligand XAT 1 618



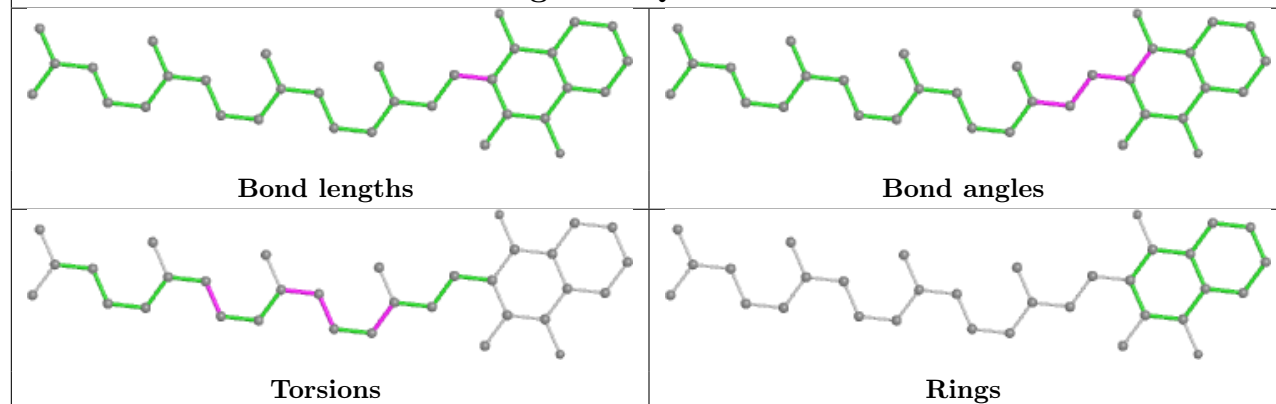
Ligand CLA A 832



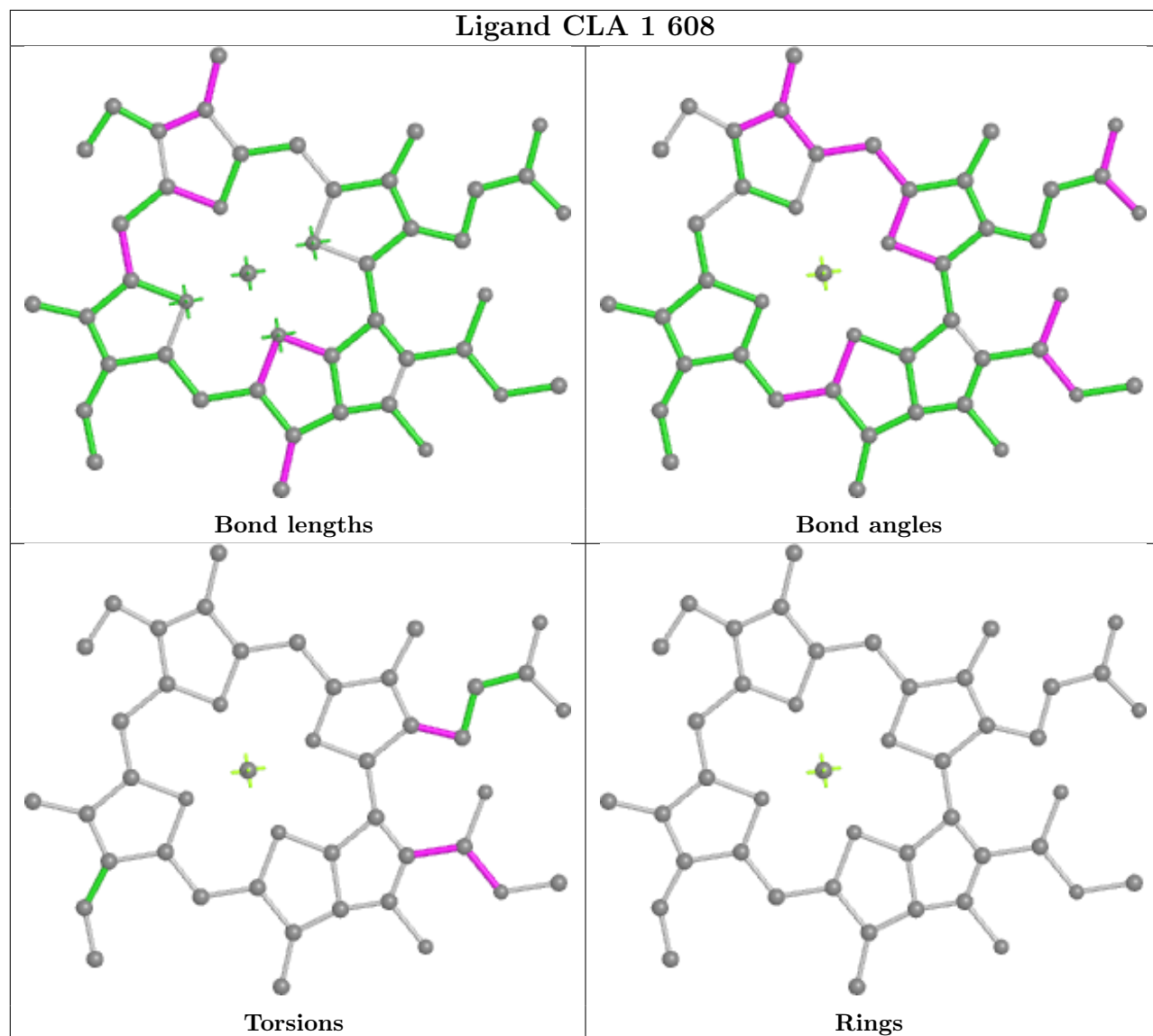
Ligand CLA 5 606



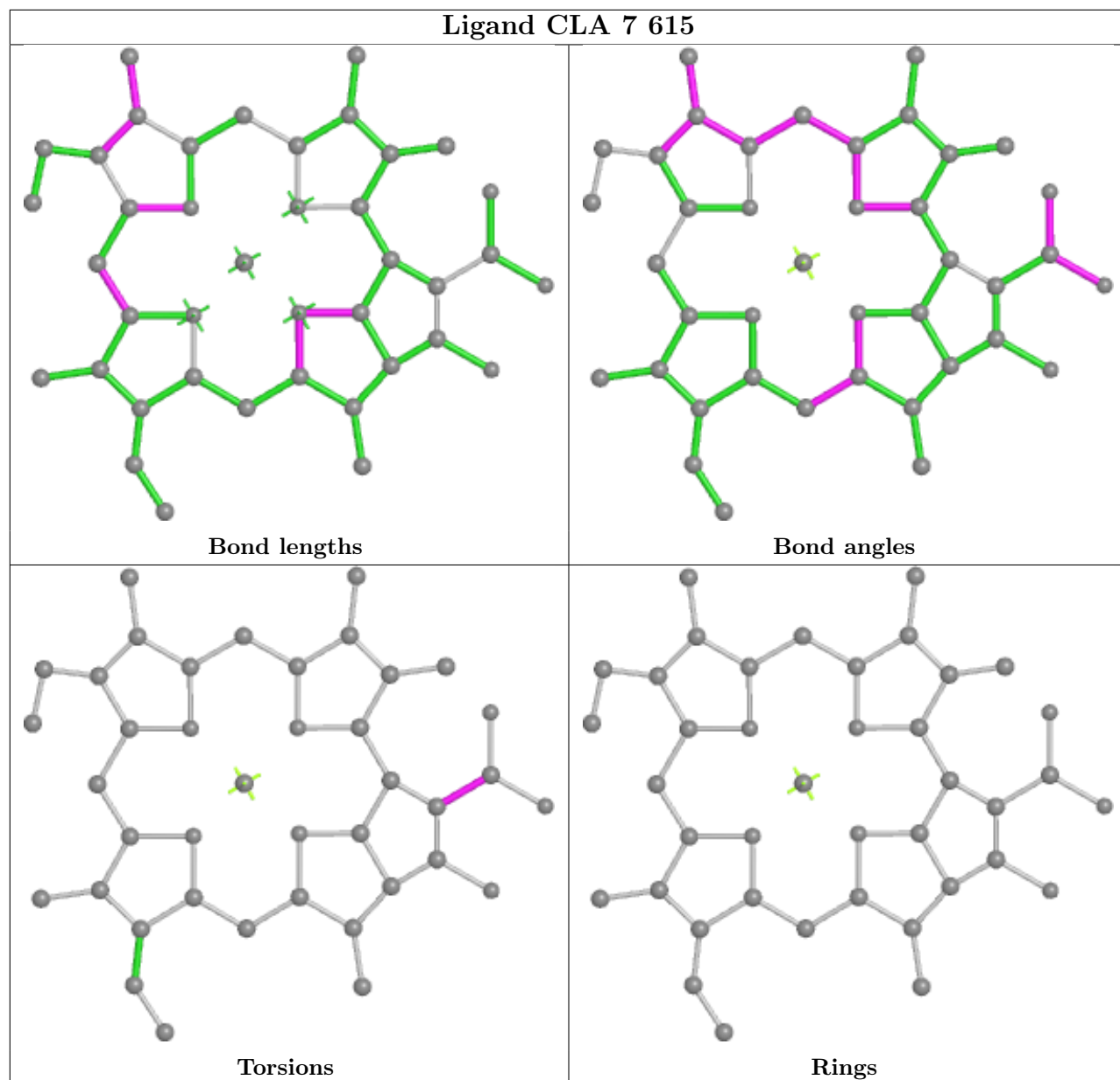
Ligand PQN B 842



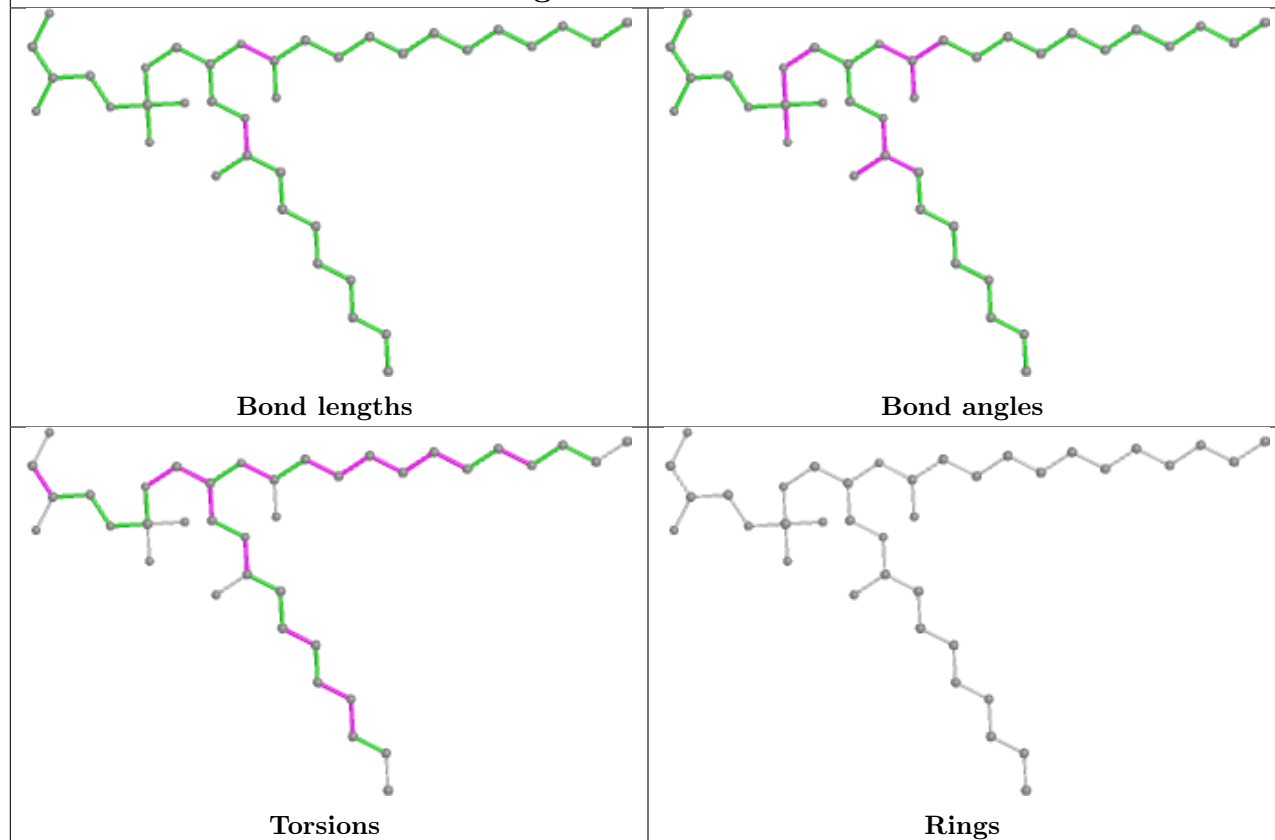
Ligand CLA 1 608



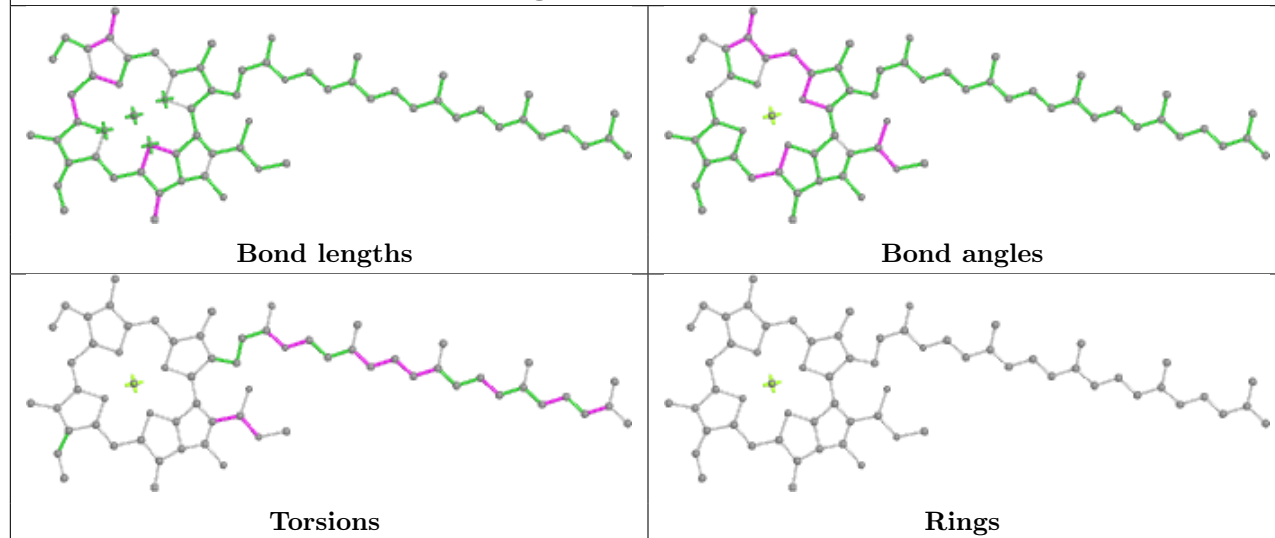
Ligand CLA 7 615

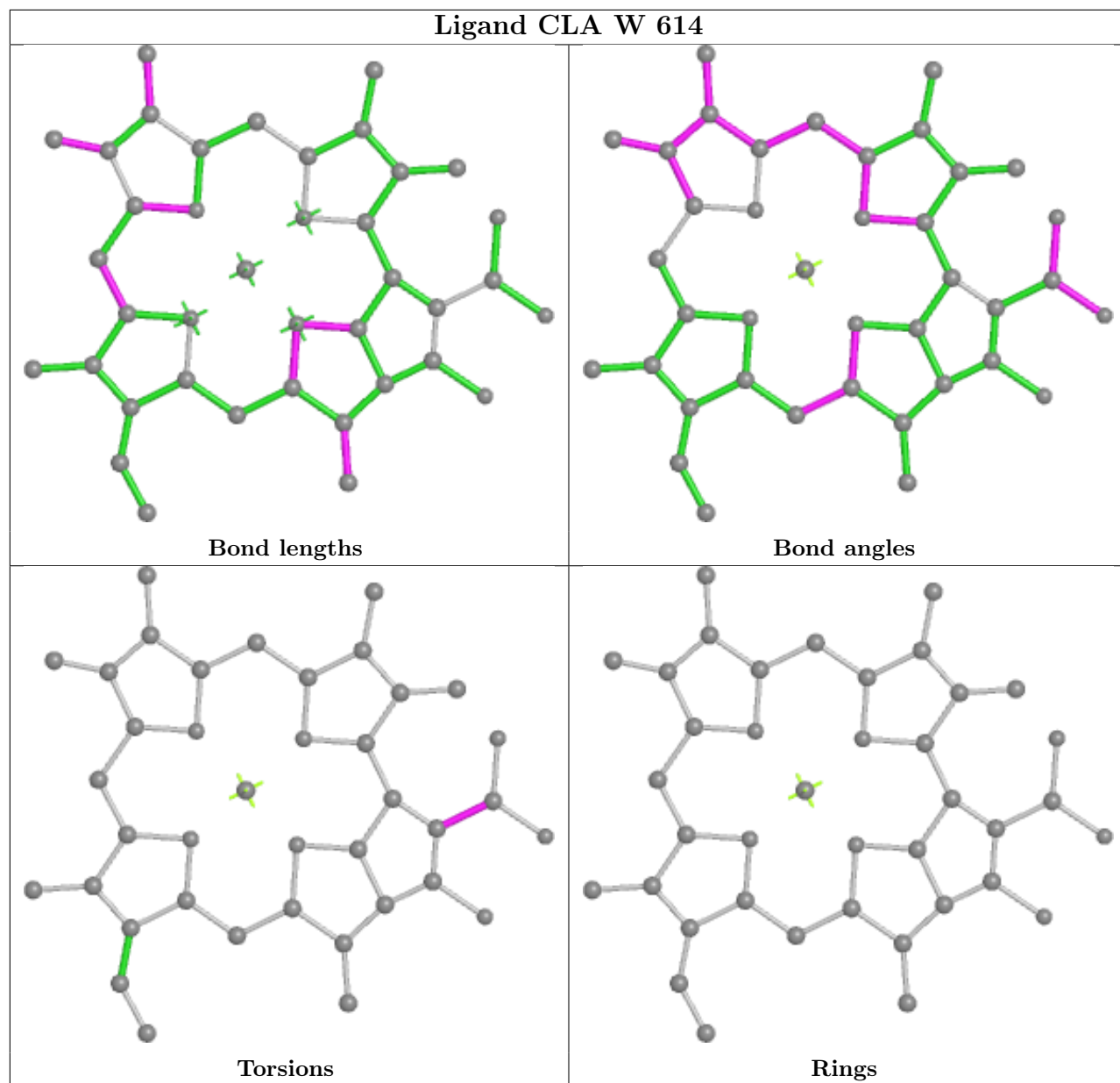


Ligand LHG 4 630

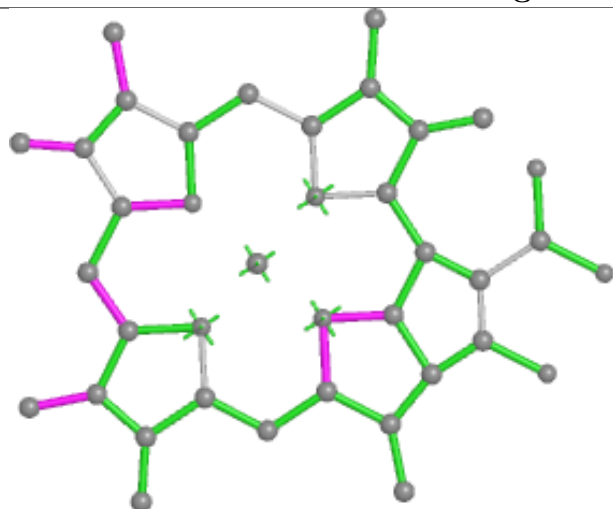


Ligand CLA A 837

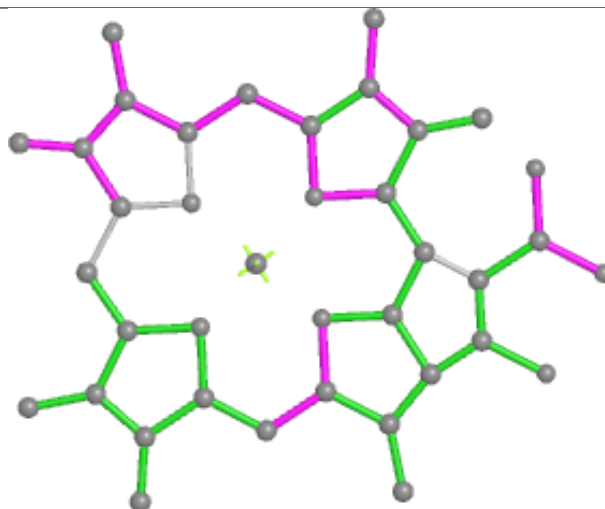




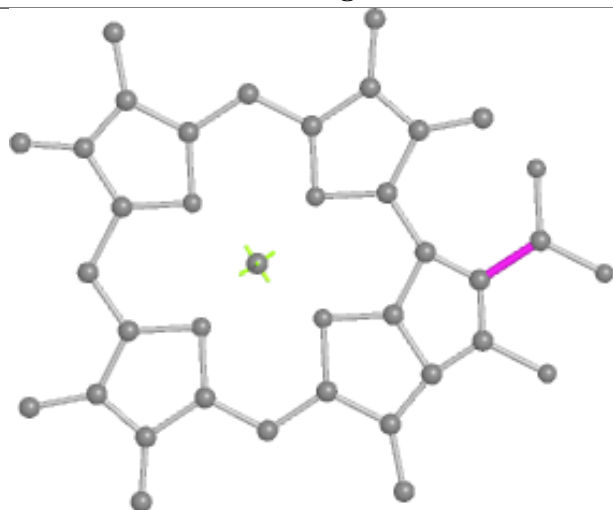
Ligand CLA V 612



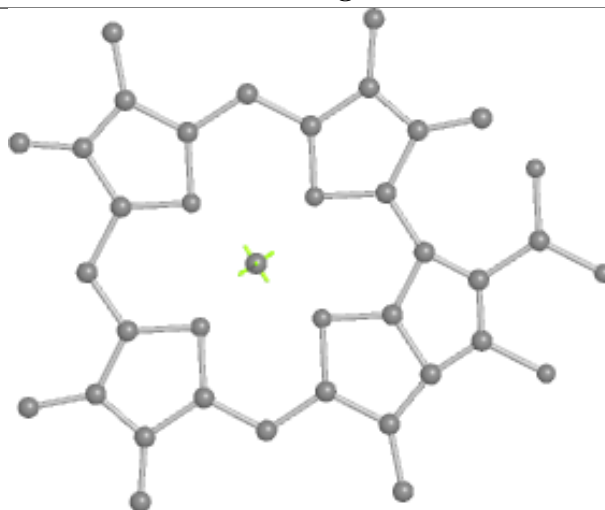
Bond lengths



Bond angles

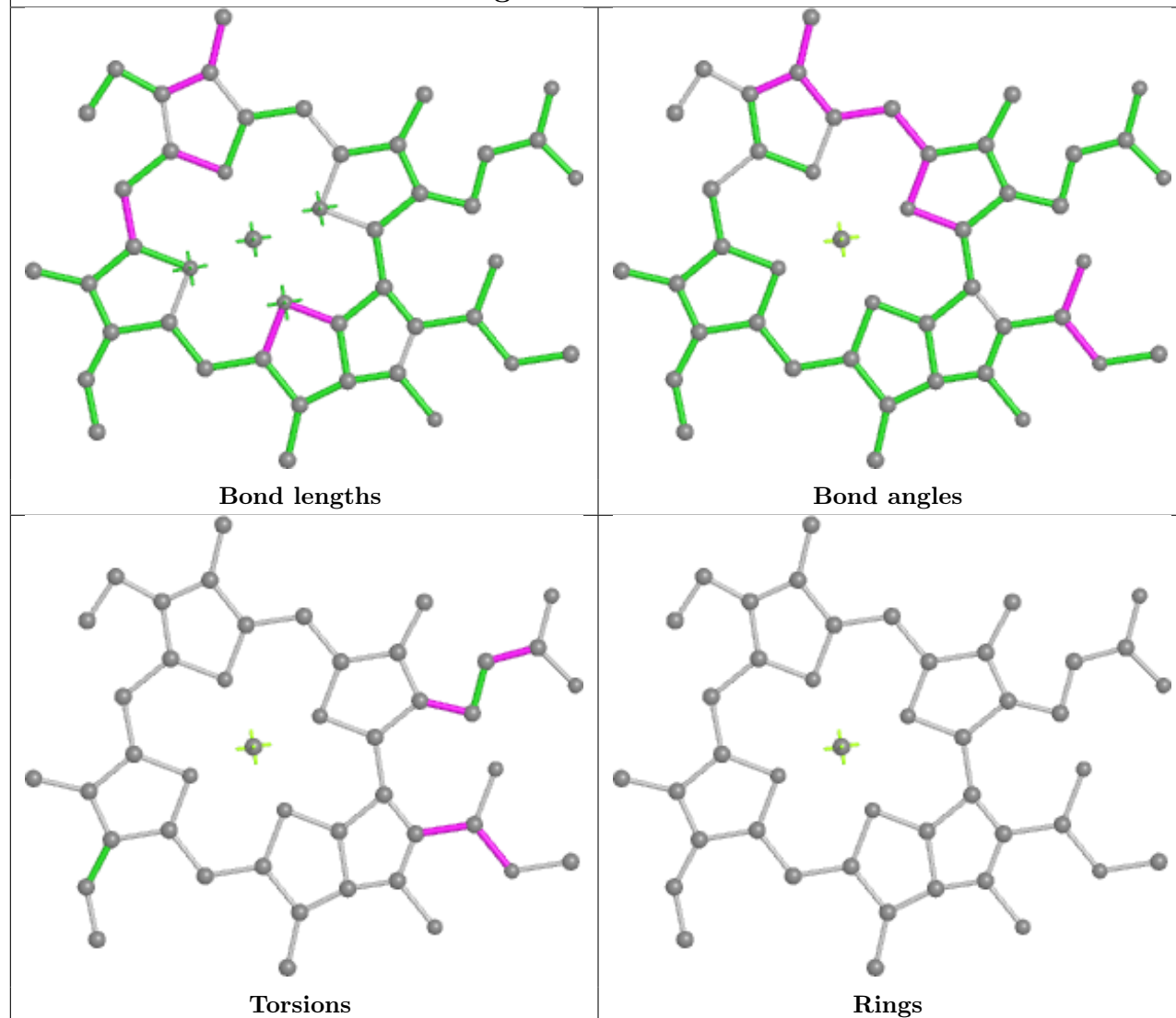


Torsions

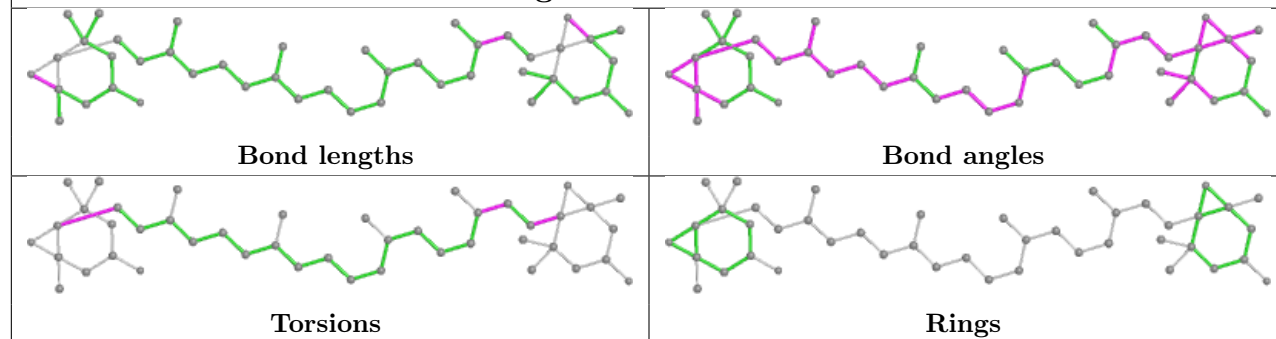


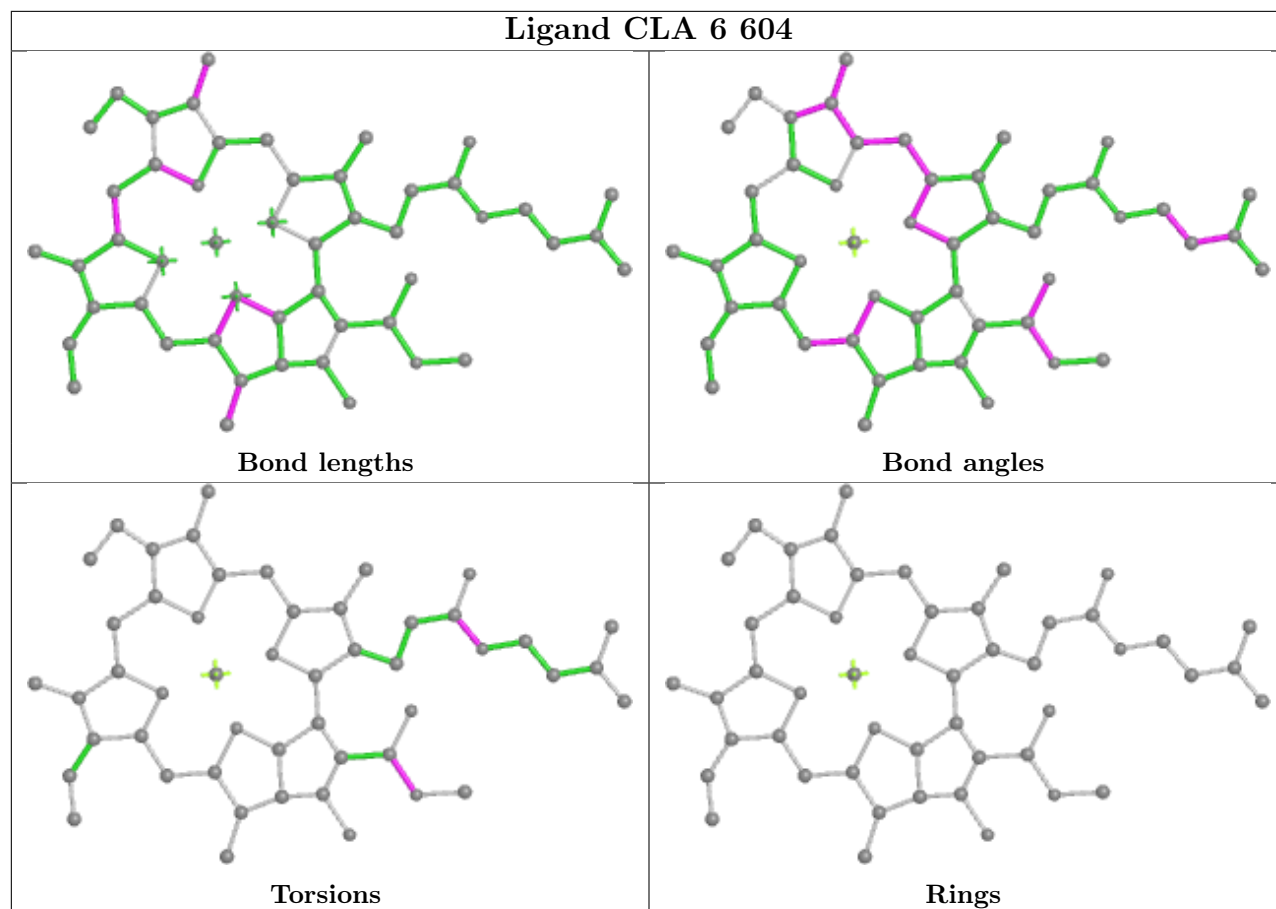
Rings

Ligand CLA 2 612

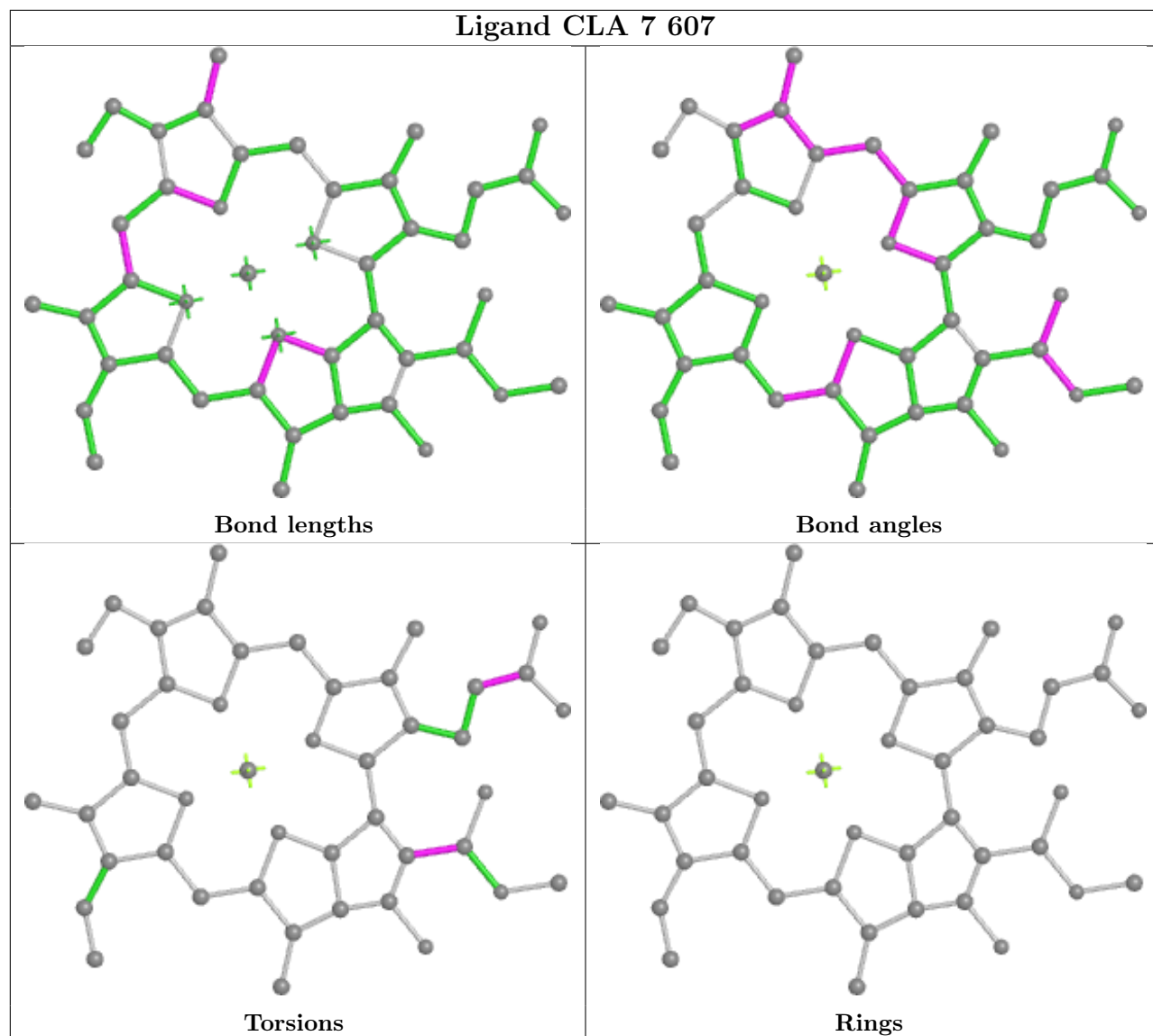


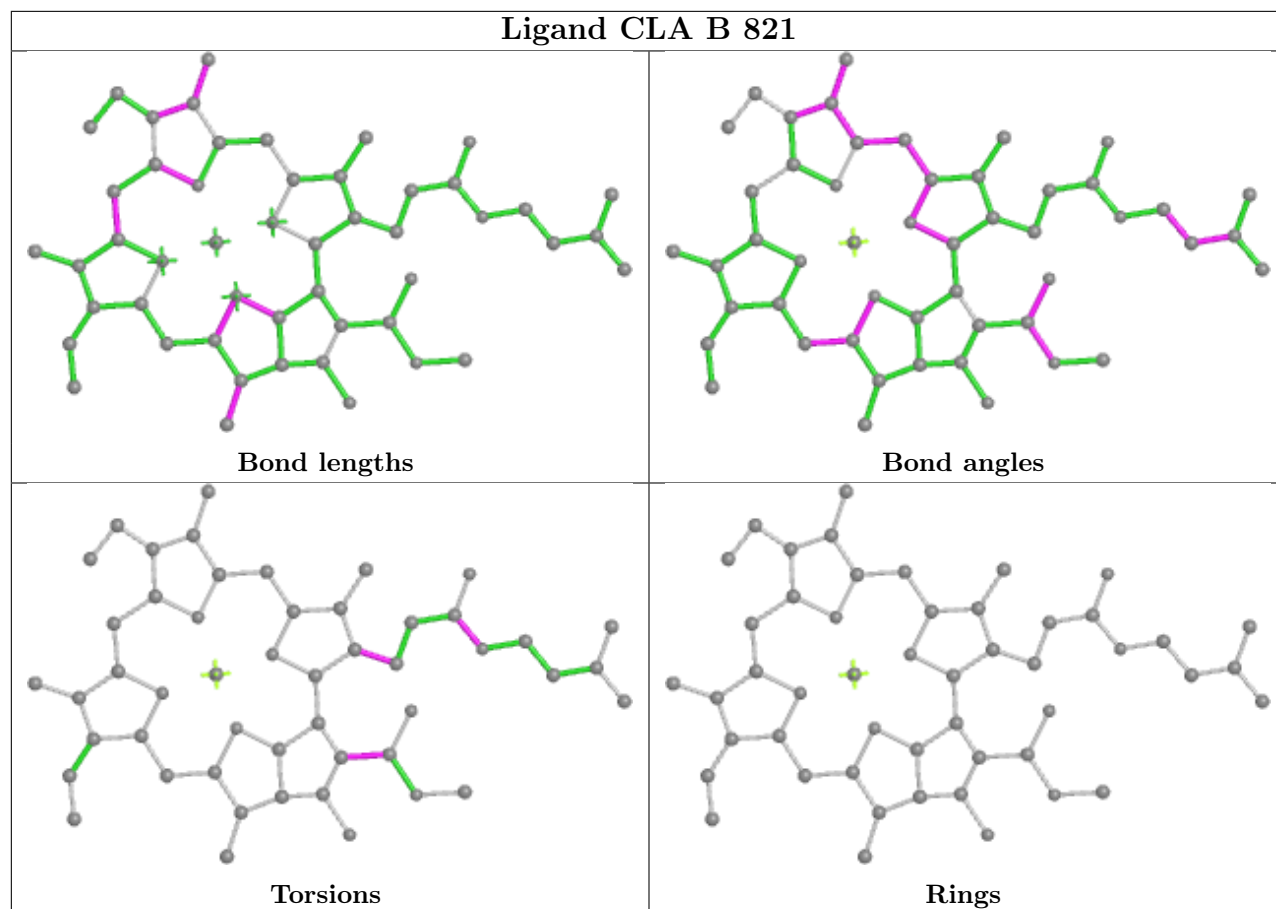
Ligand XAT 7 619

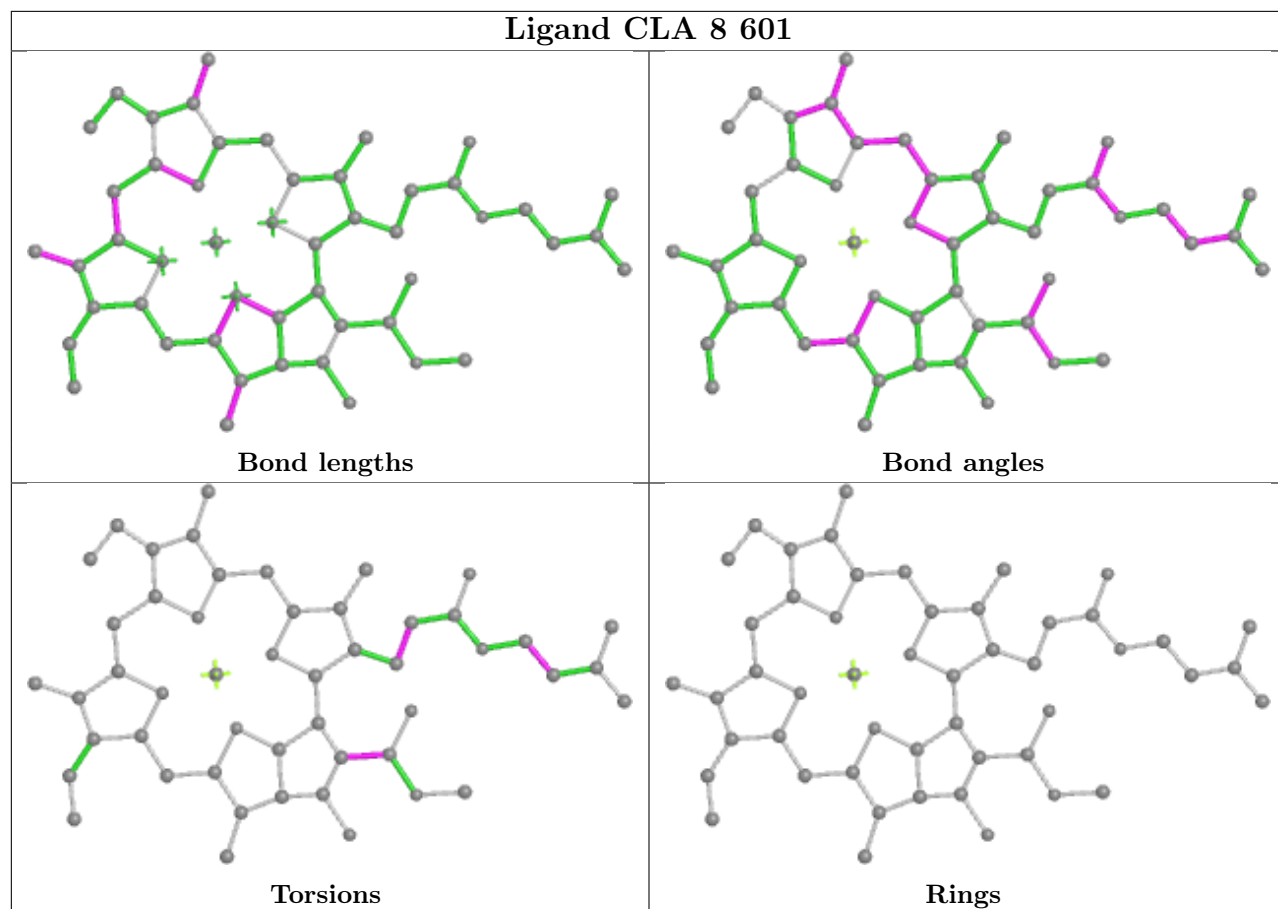




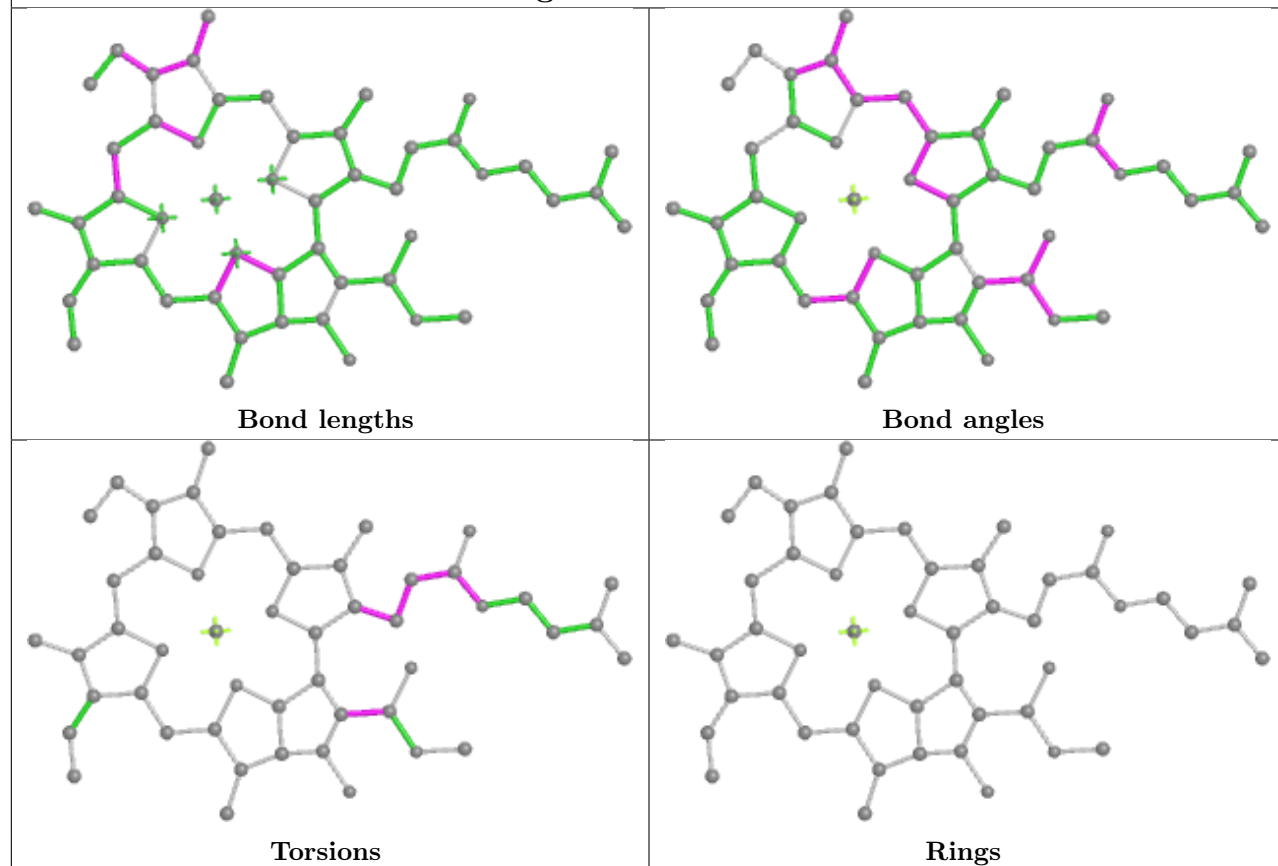
Ligand CLA 7 607



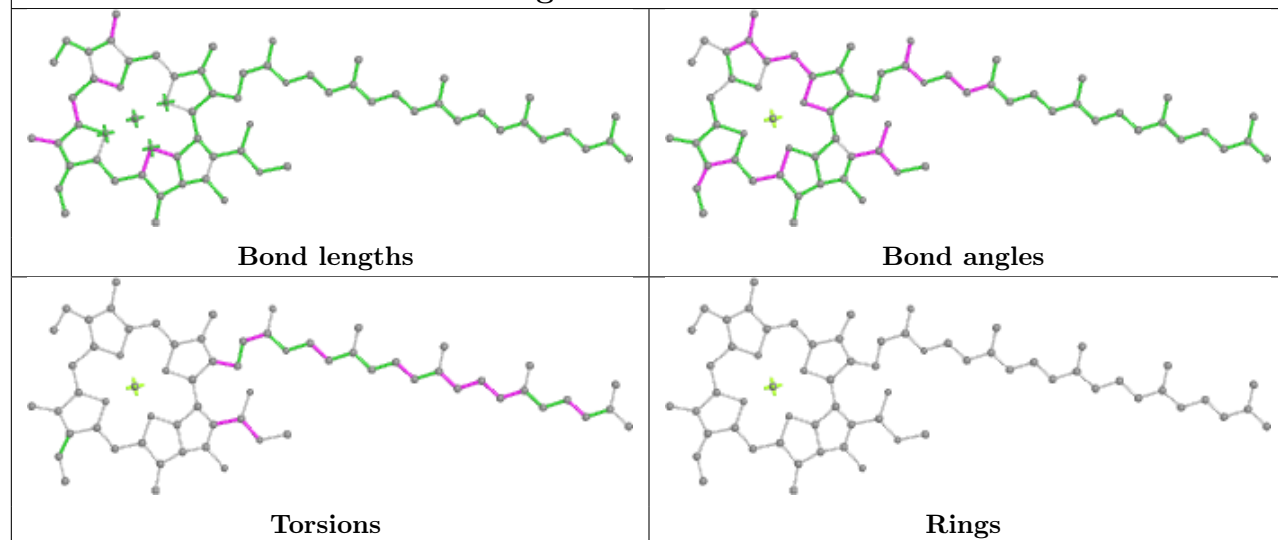




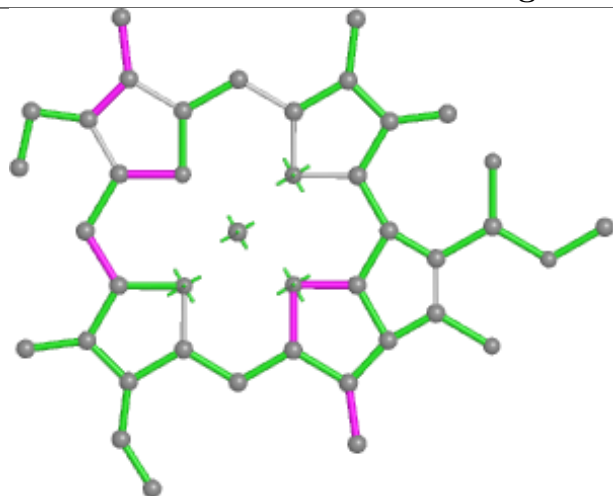
Ligand CLA 3 607



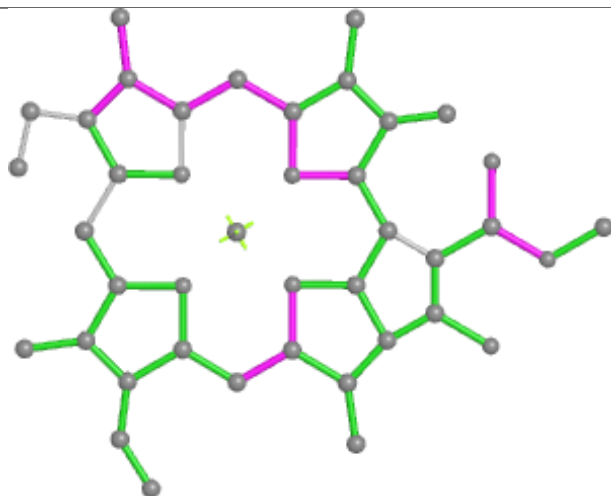
Ligand CLA 1 611



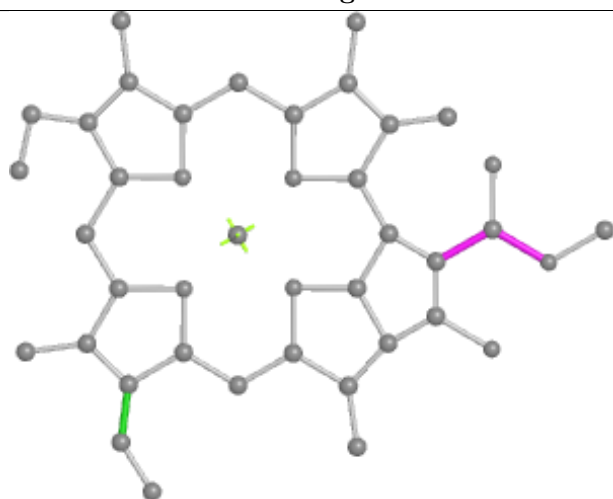
Ligand CLA 5 604



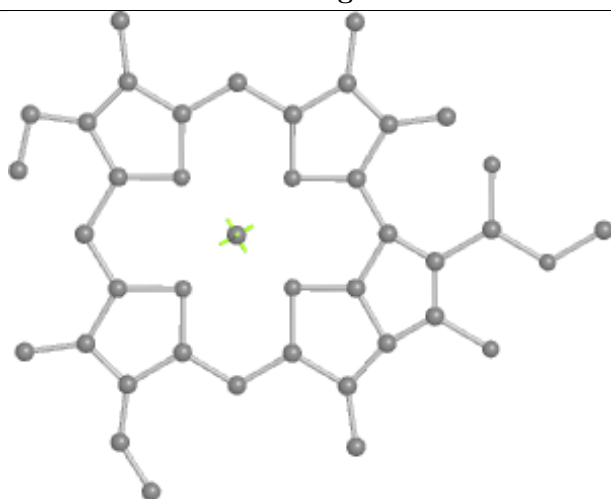
Bond lengths



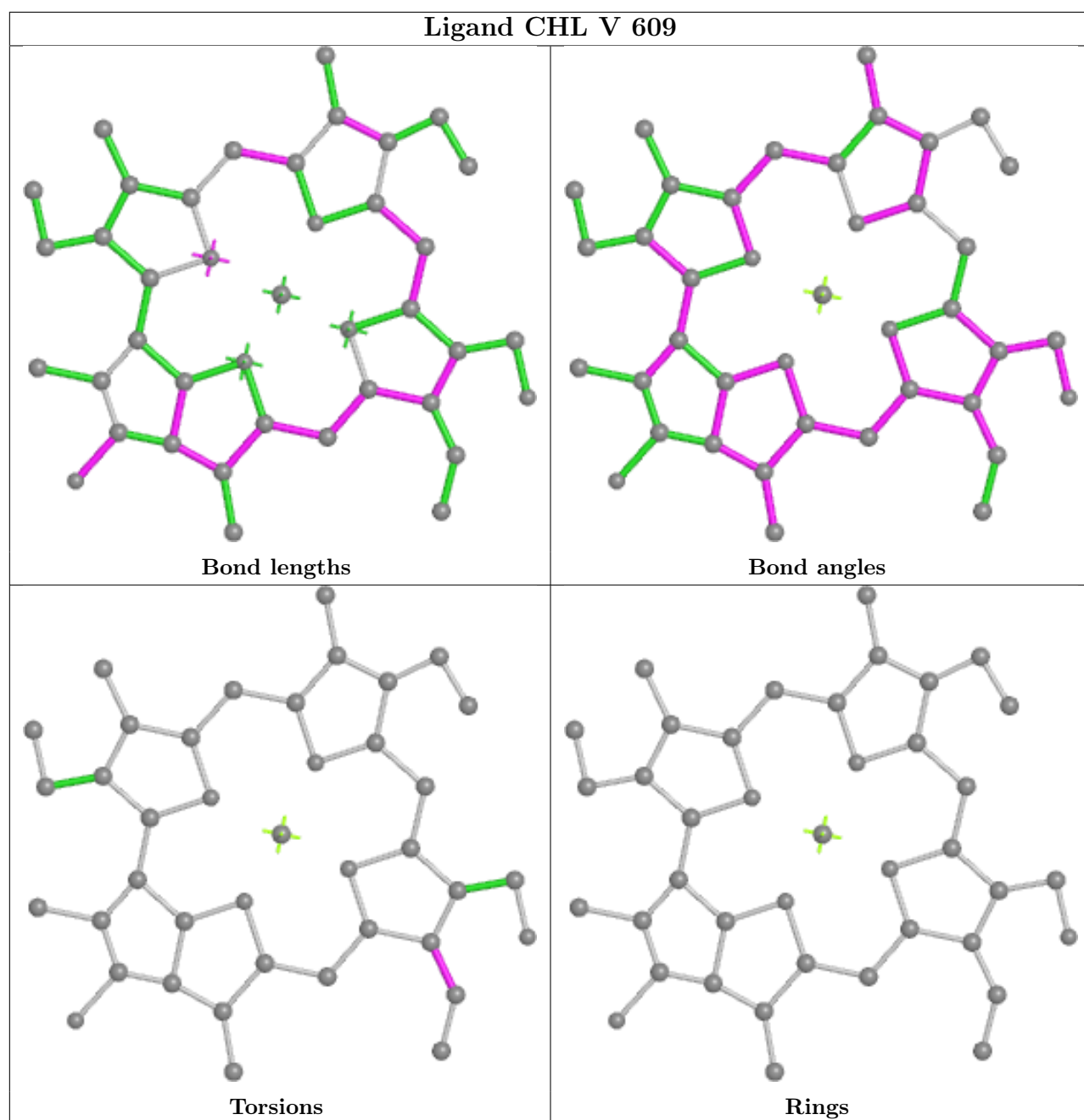
Bond angles

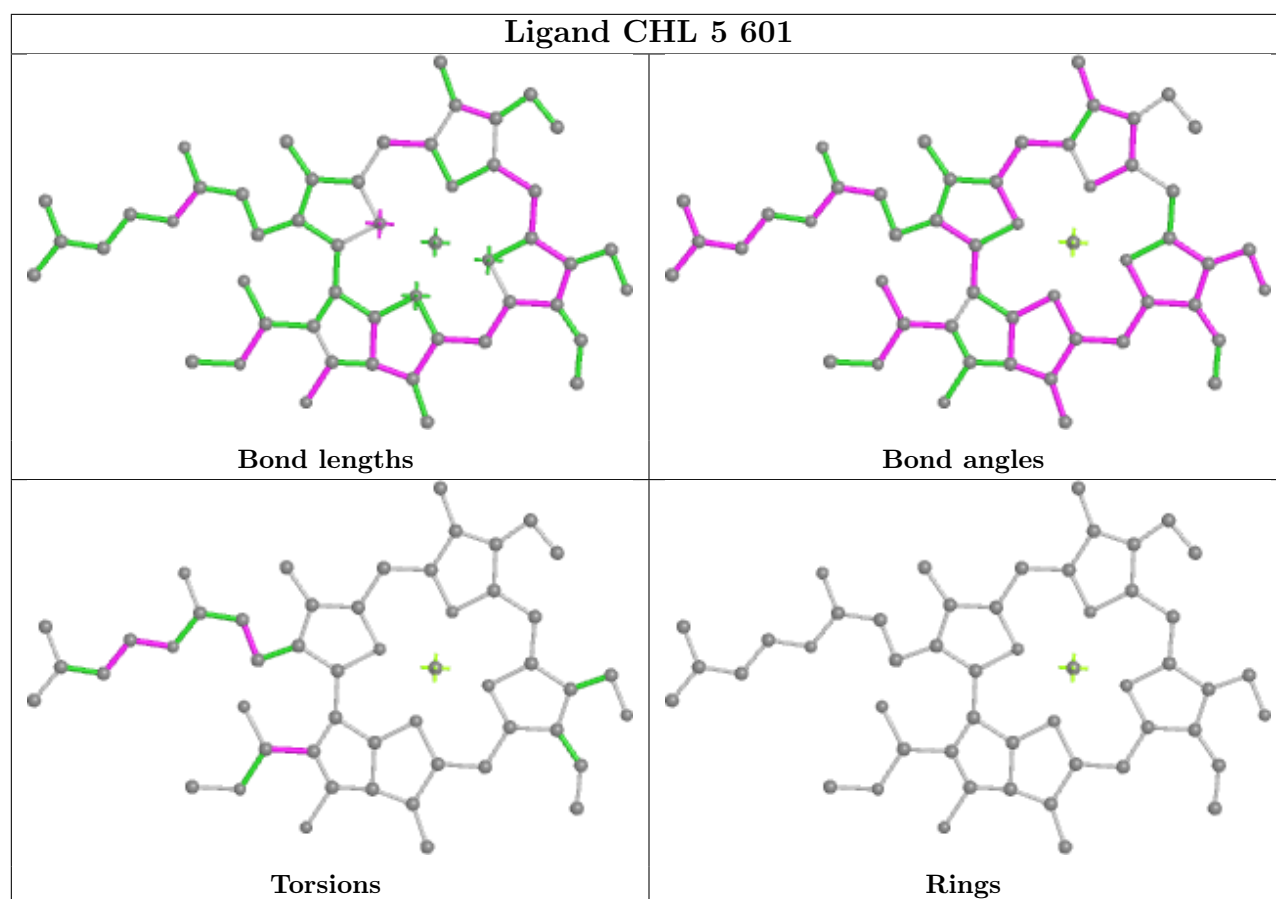


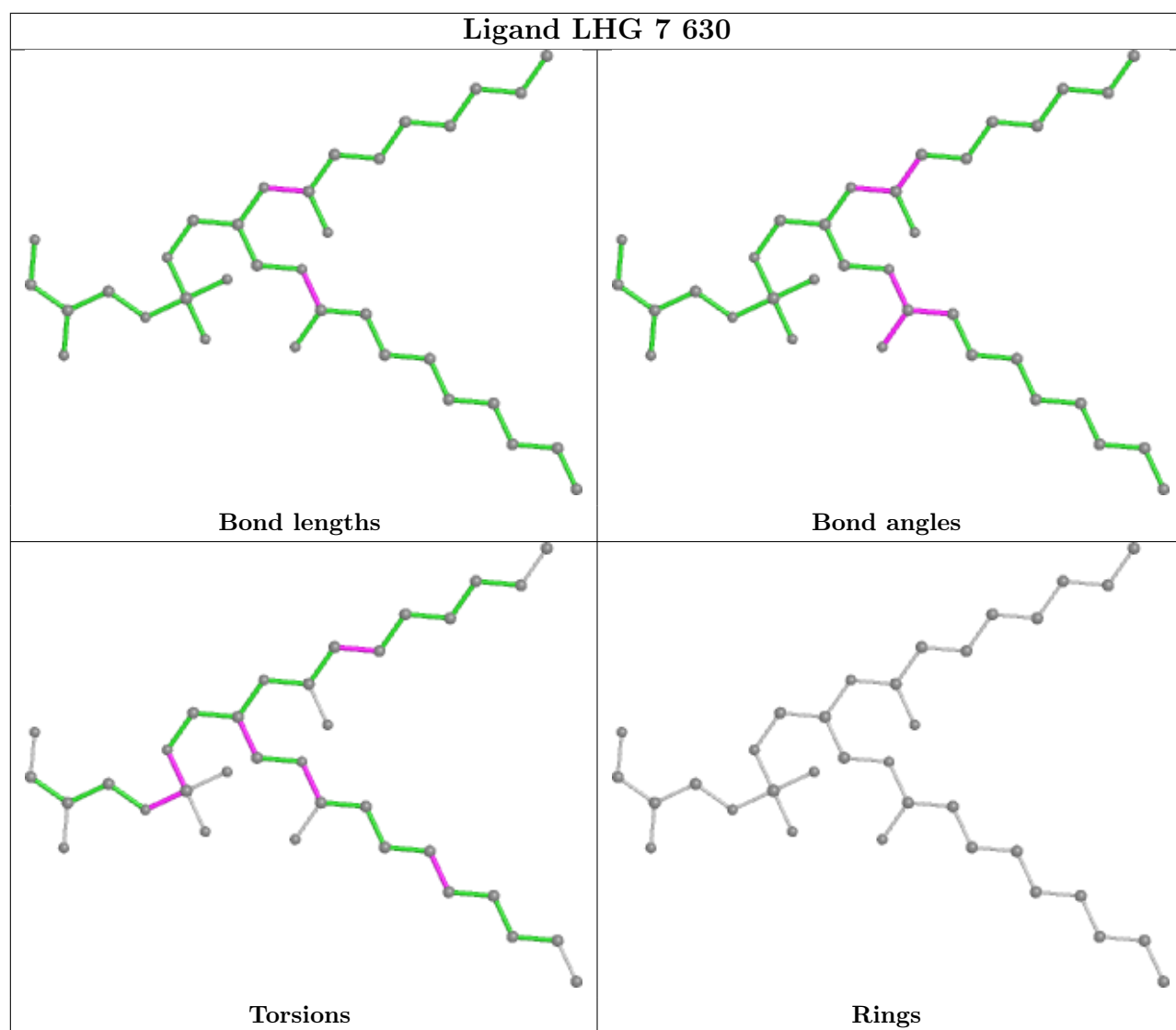
Torsions

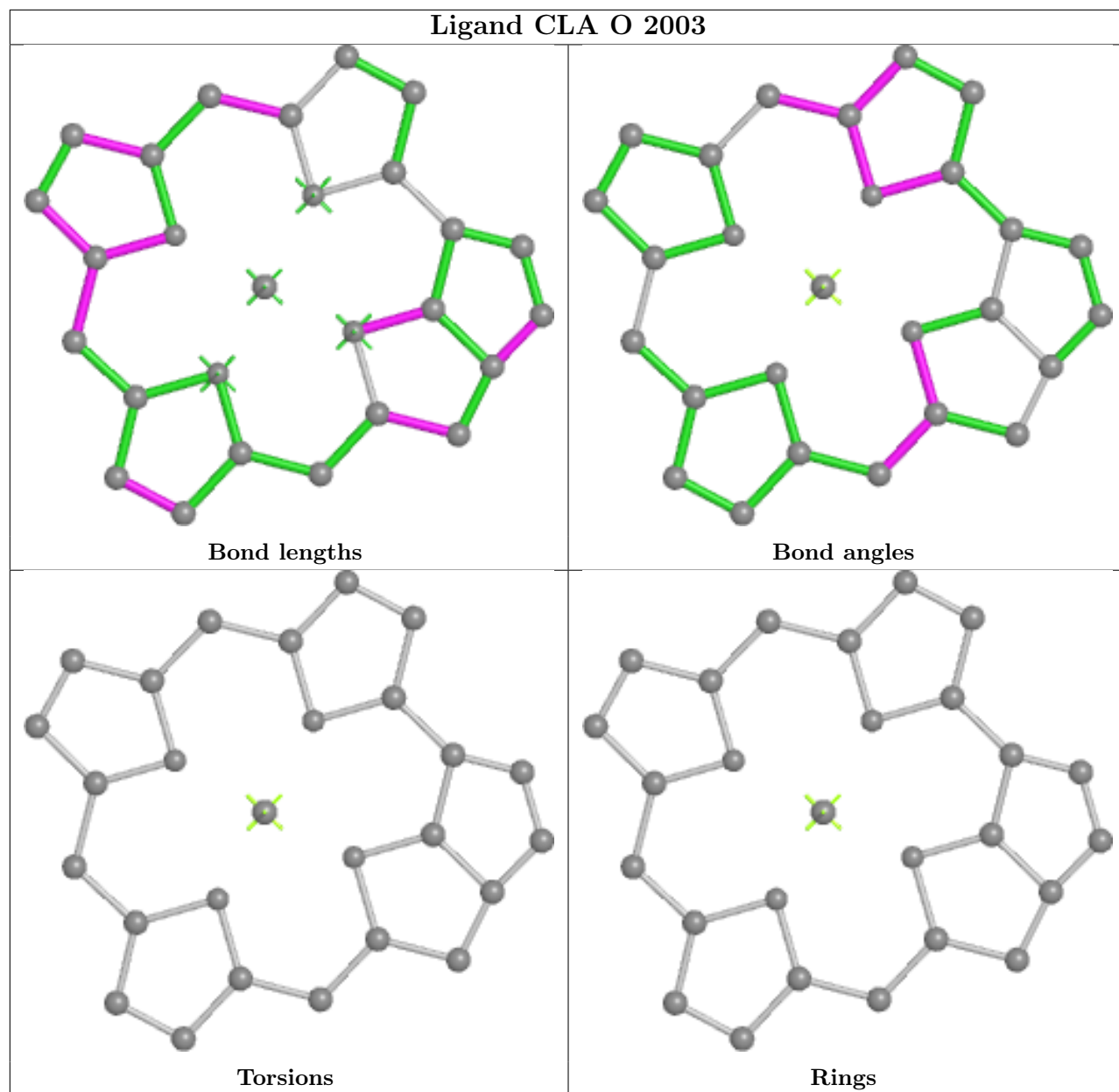


Rings

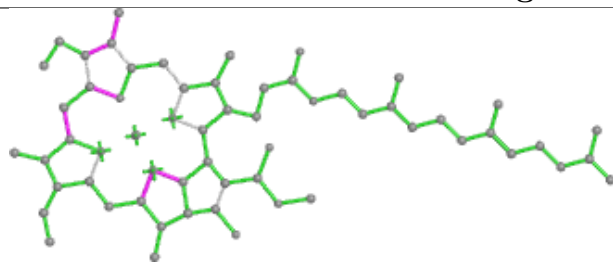




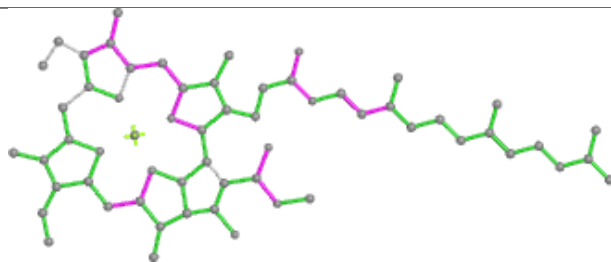




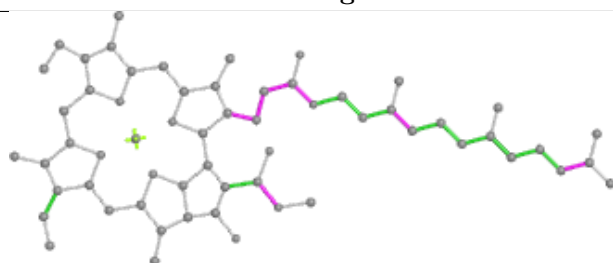
Ligand CLA L 304



Bond lengths



Bond angles

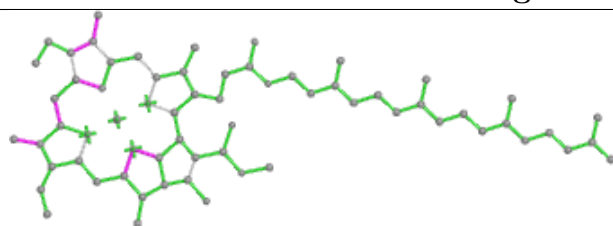


Torsions

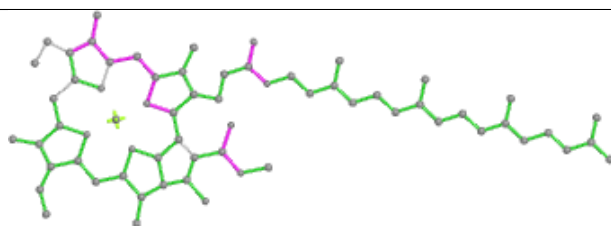


Rings

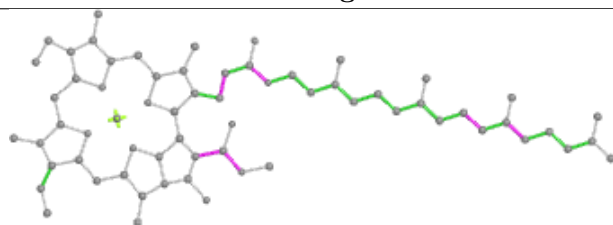
Ligand CLA U 612



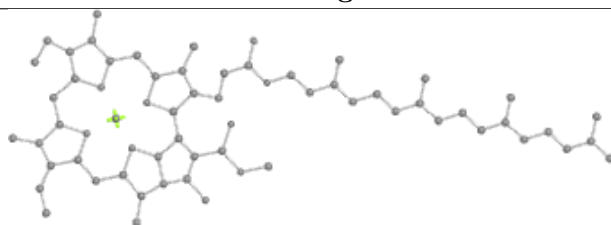
Bond lengths



Bond angles

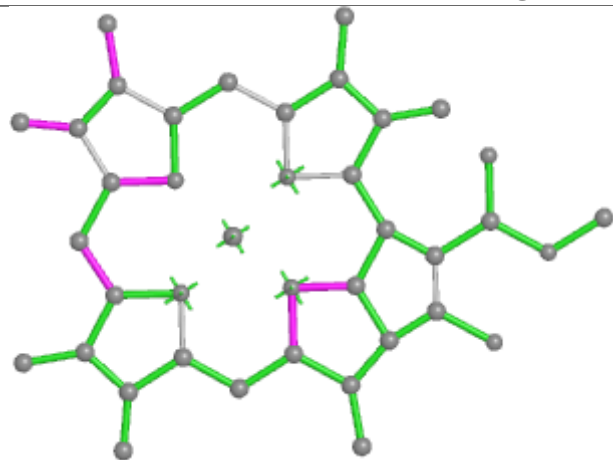


Torsions

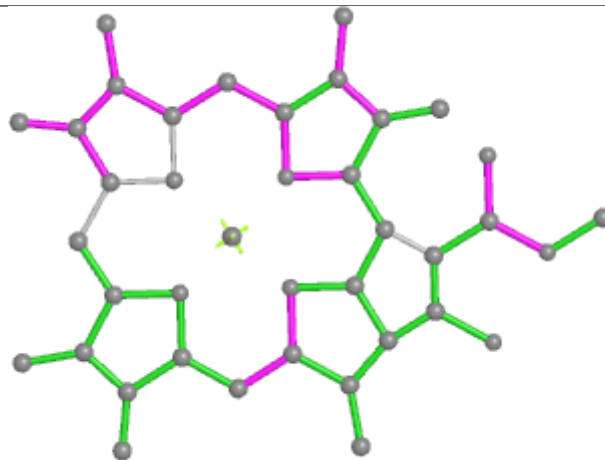


Rings

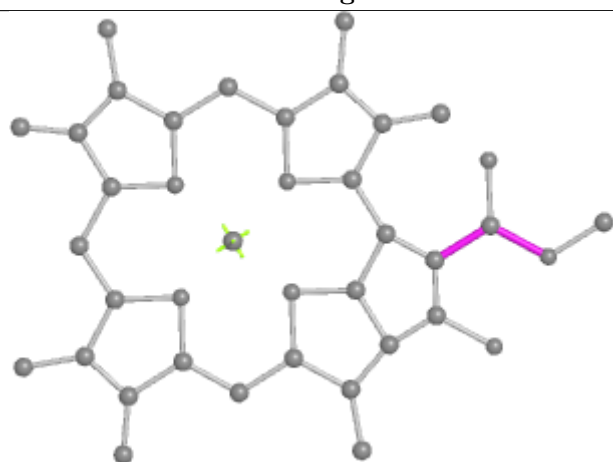
Ligand CLA V 610



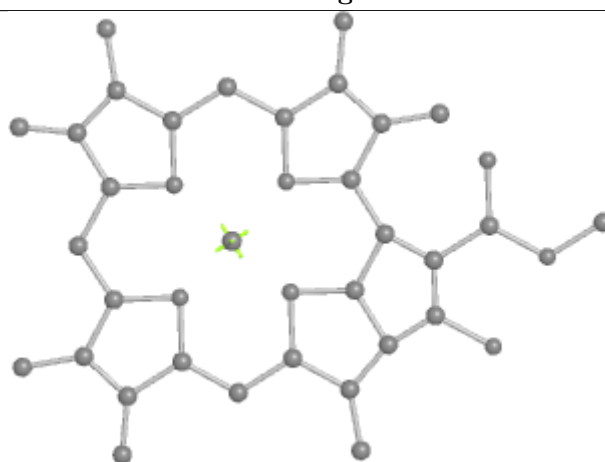
Bond lengths



Bond angles

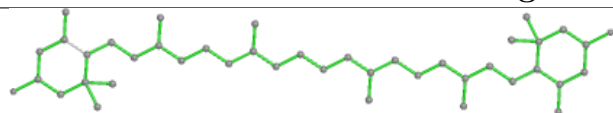


Torsions

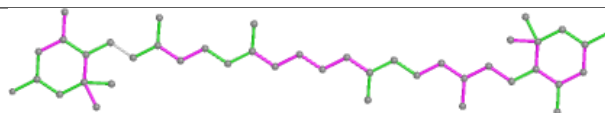


Rings

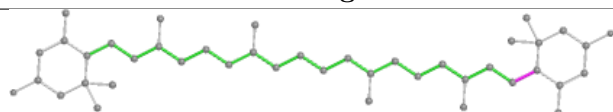
Ligand LUT 9 621



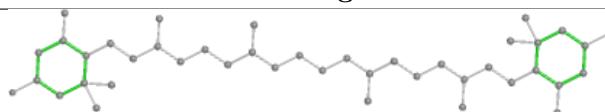
Bond lengths



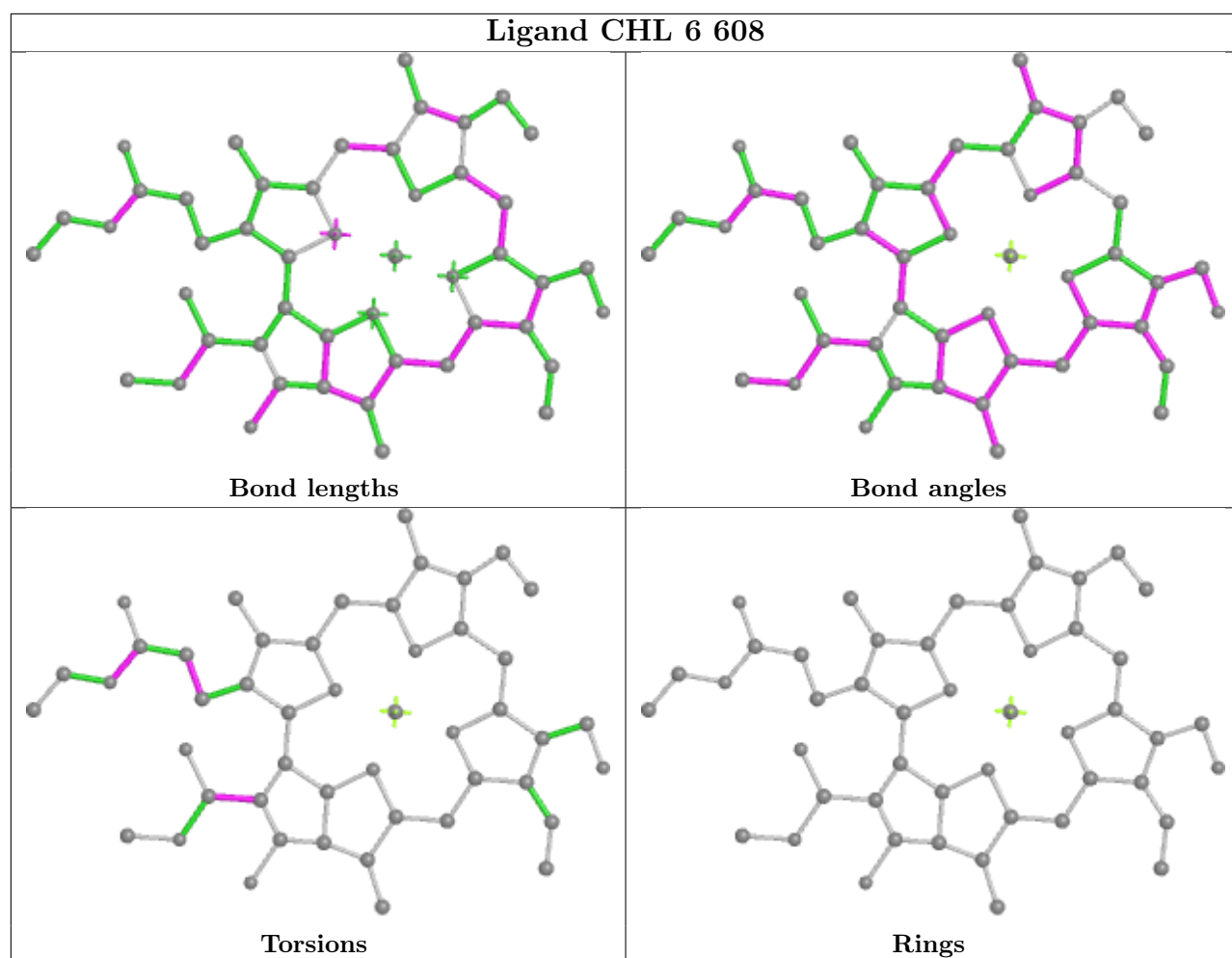
Bond angles



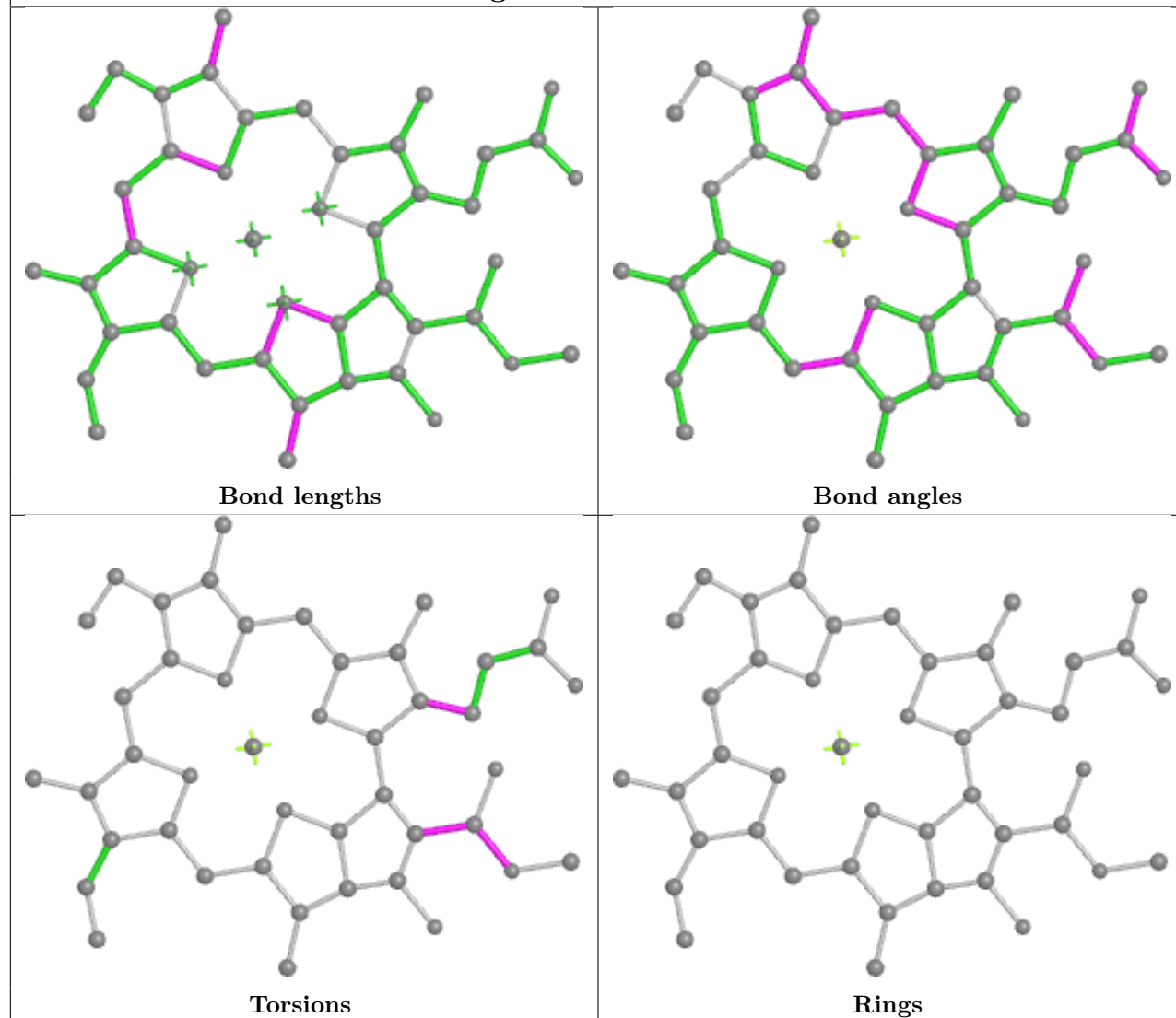
Torsions



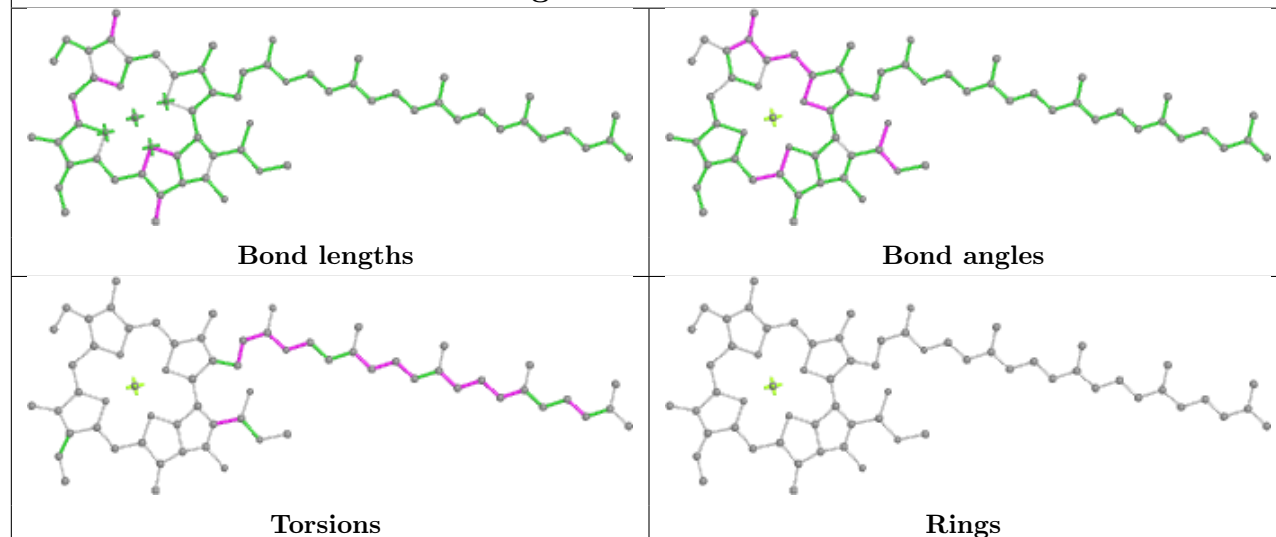
Rings



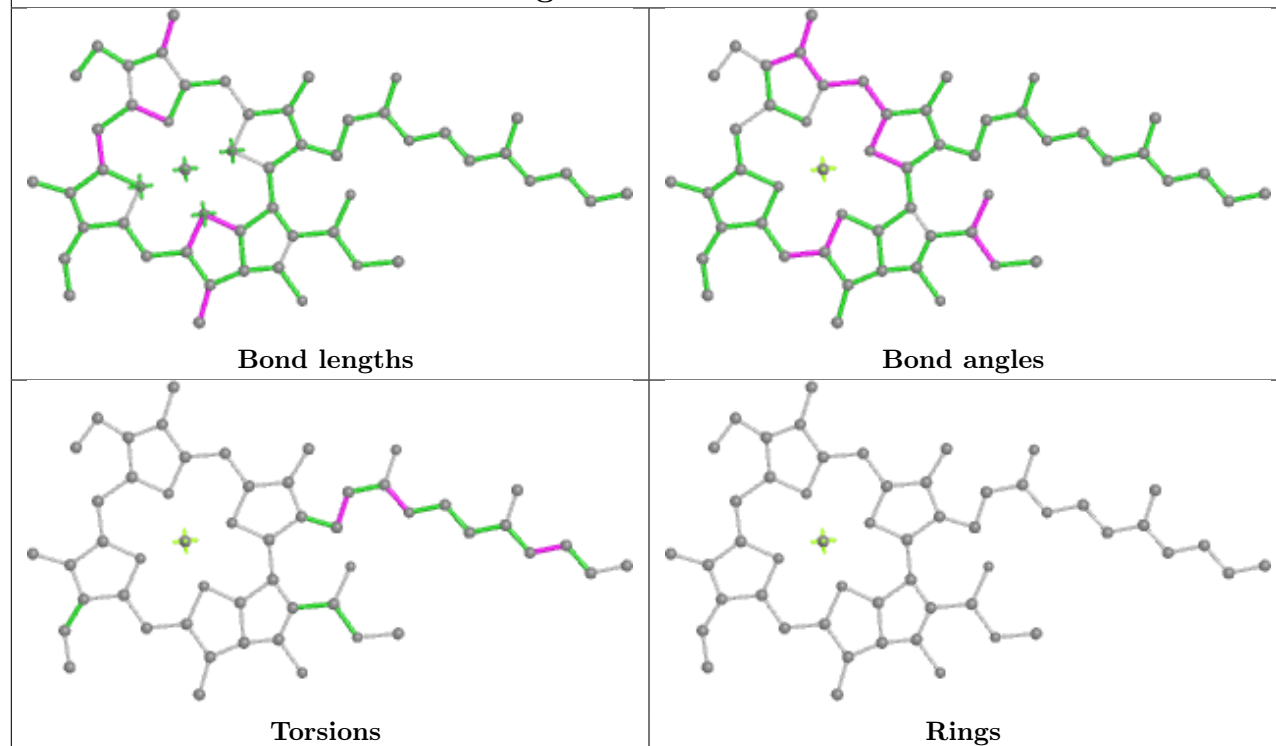
Ligand CLA V 614



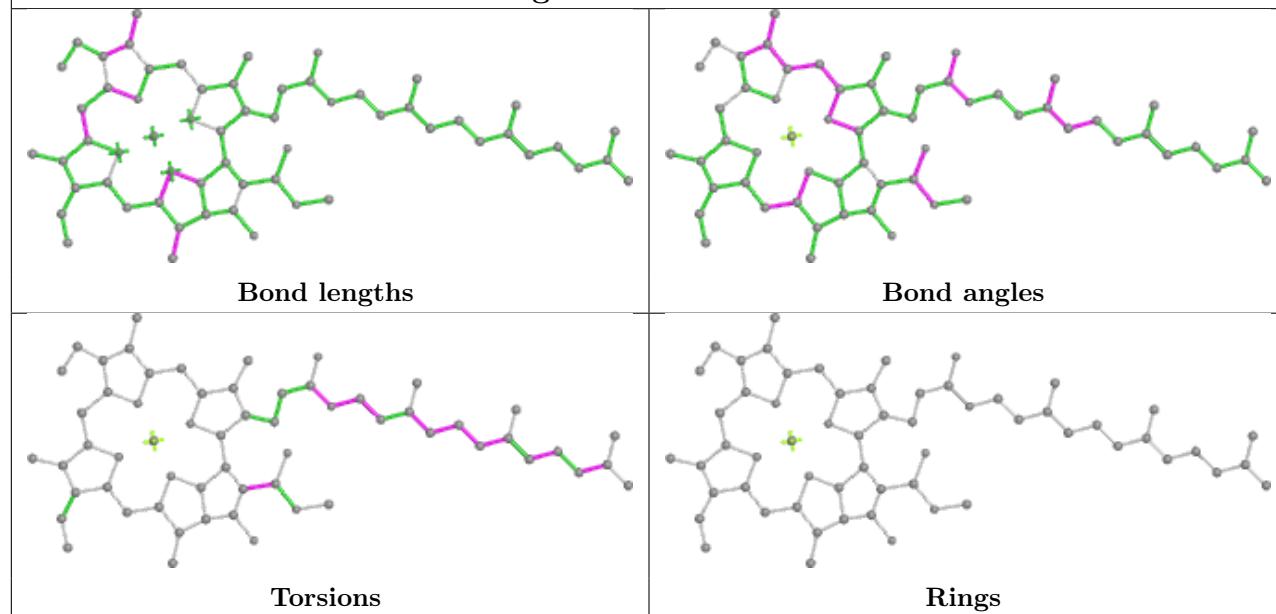
Ligand CLA A 807

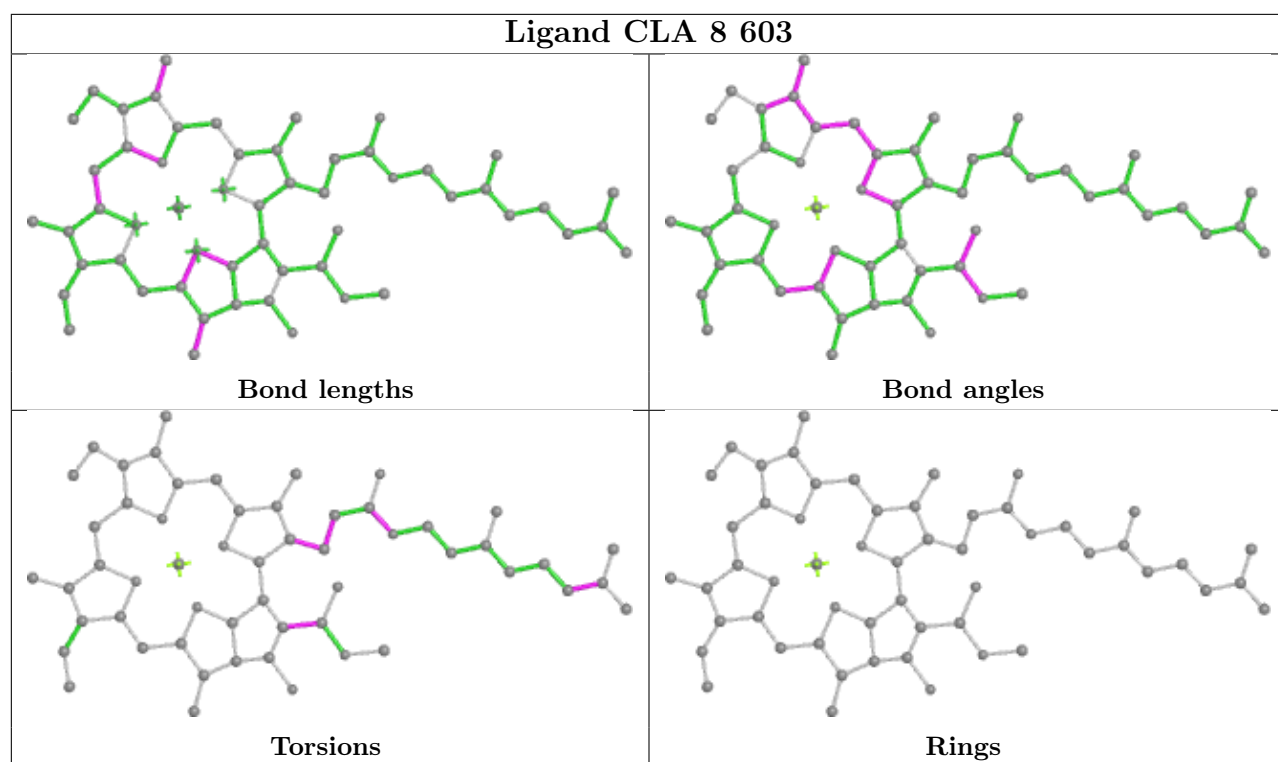


Ligand CLA 3 615

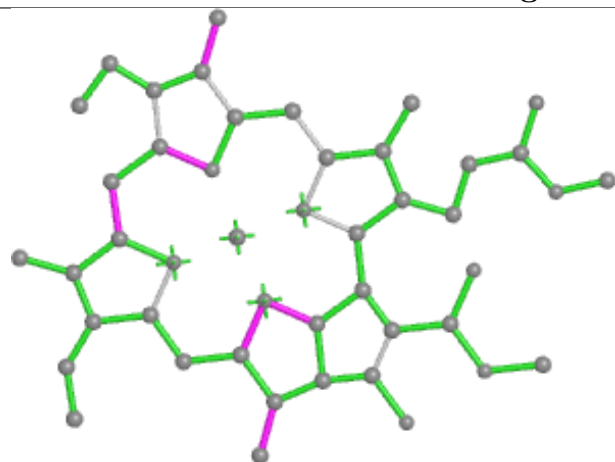


Ligand CLA B 819

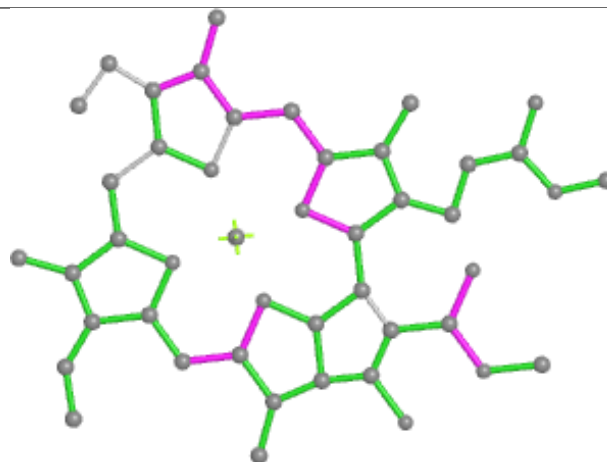




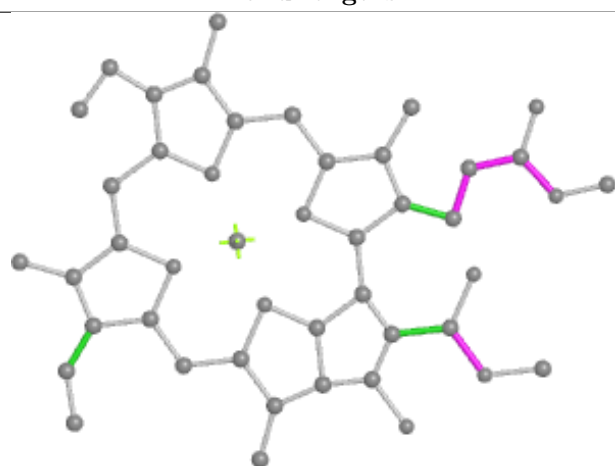
Ligand CLA 6 603



Bond lengths



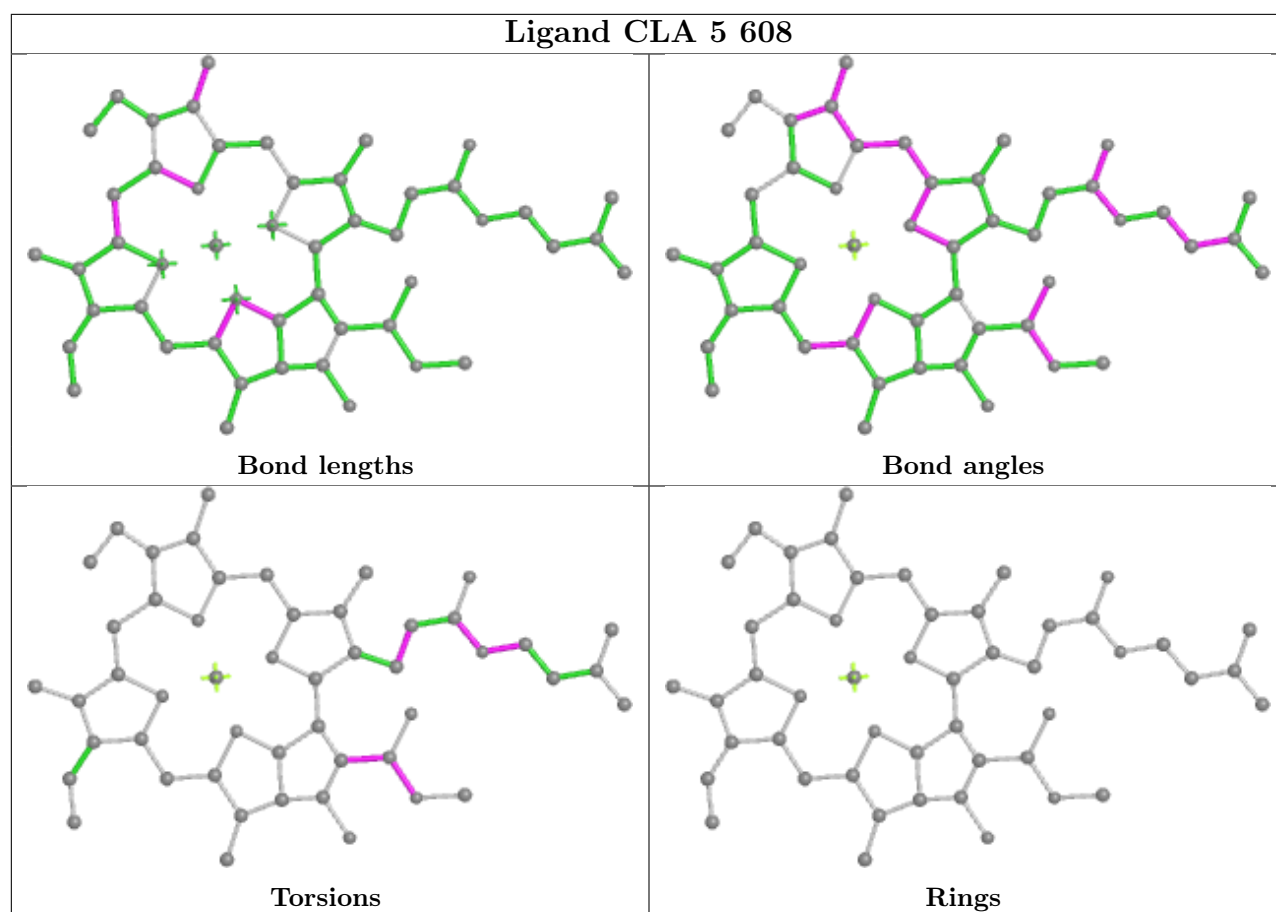
Bond angles



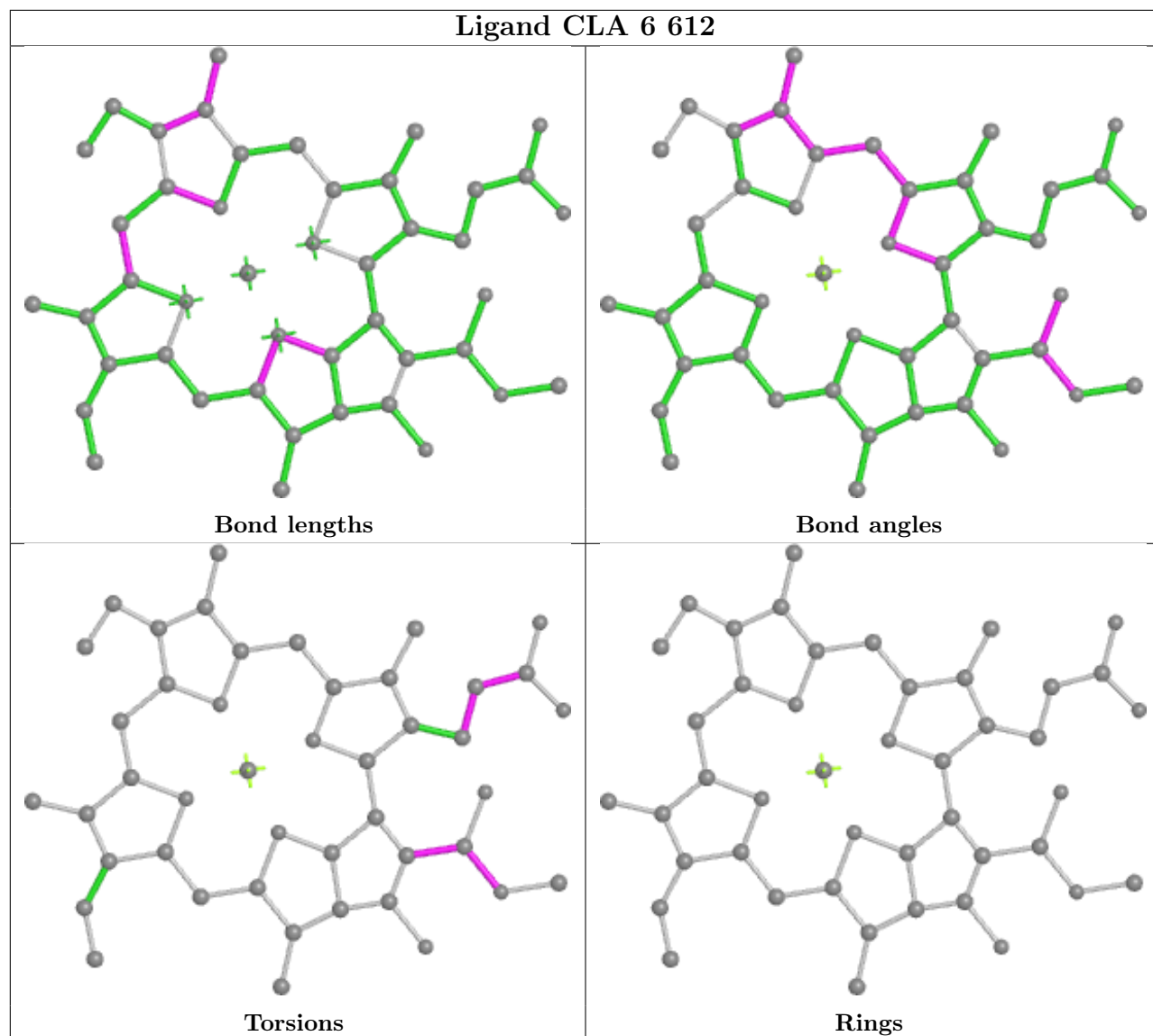
Torsions



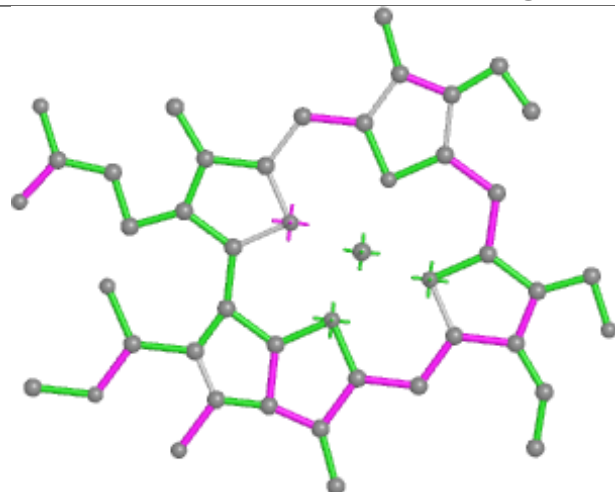
Rings



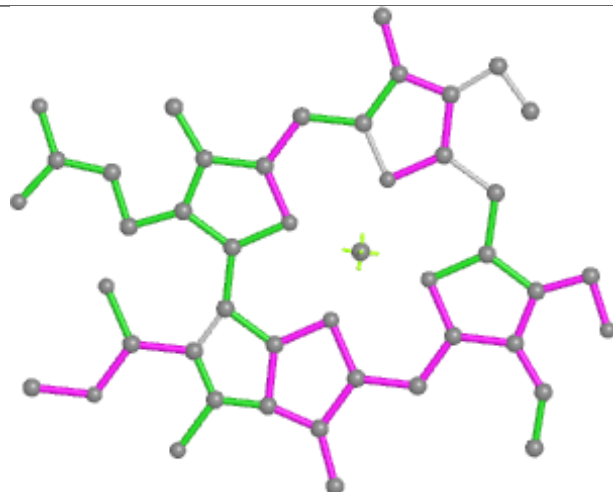
Ligand CLA 6 612



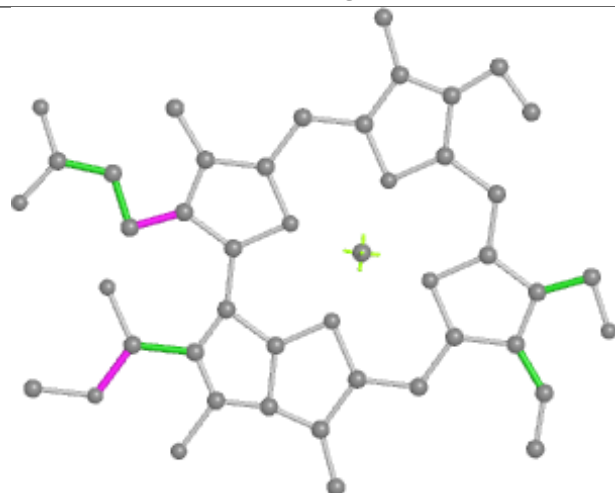
Ligand CHL 4 608



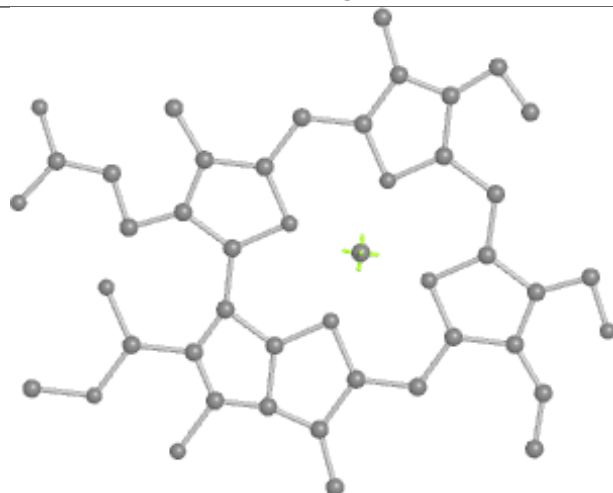
Bond lengths



Bond angles

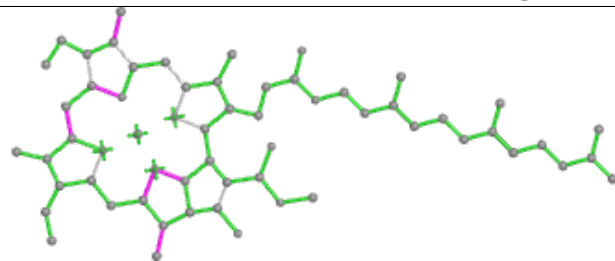


Torsions

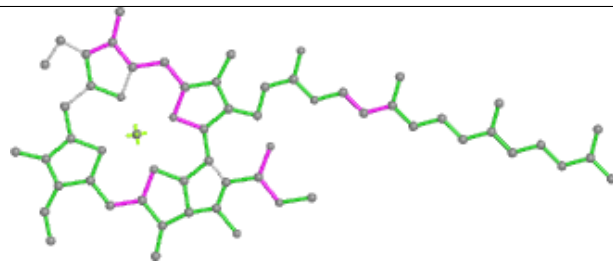


Rings

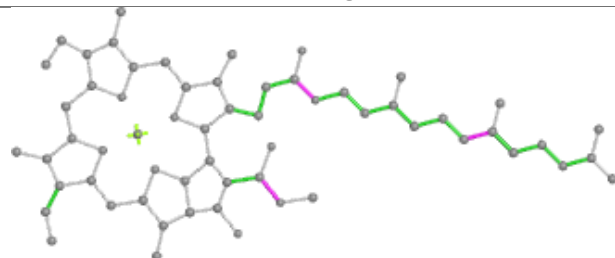
Ligand CLA A 839



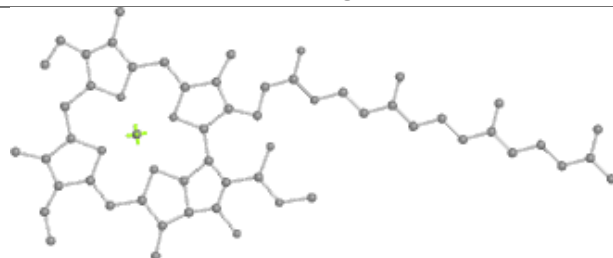
Bond lengths



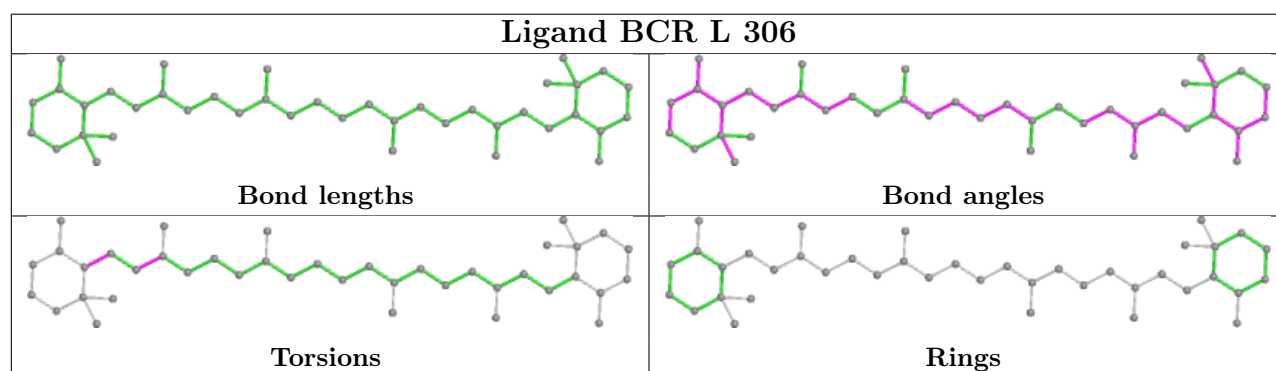
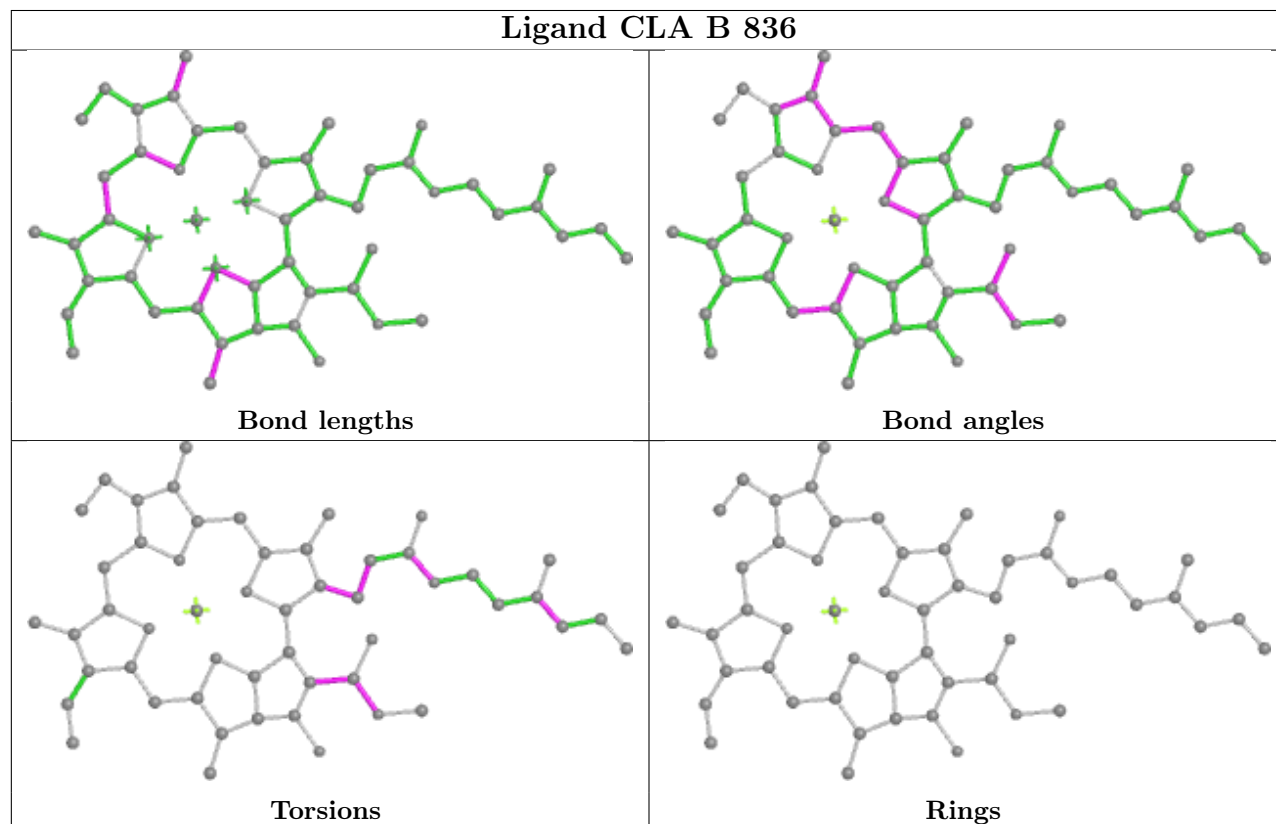
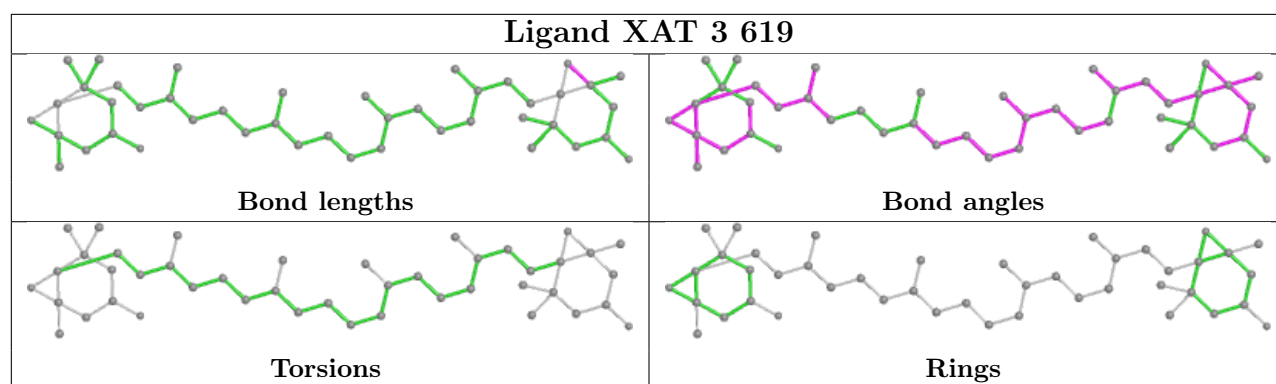
Bond angles



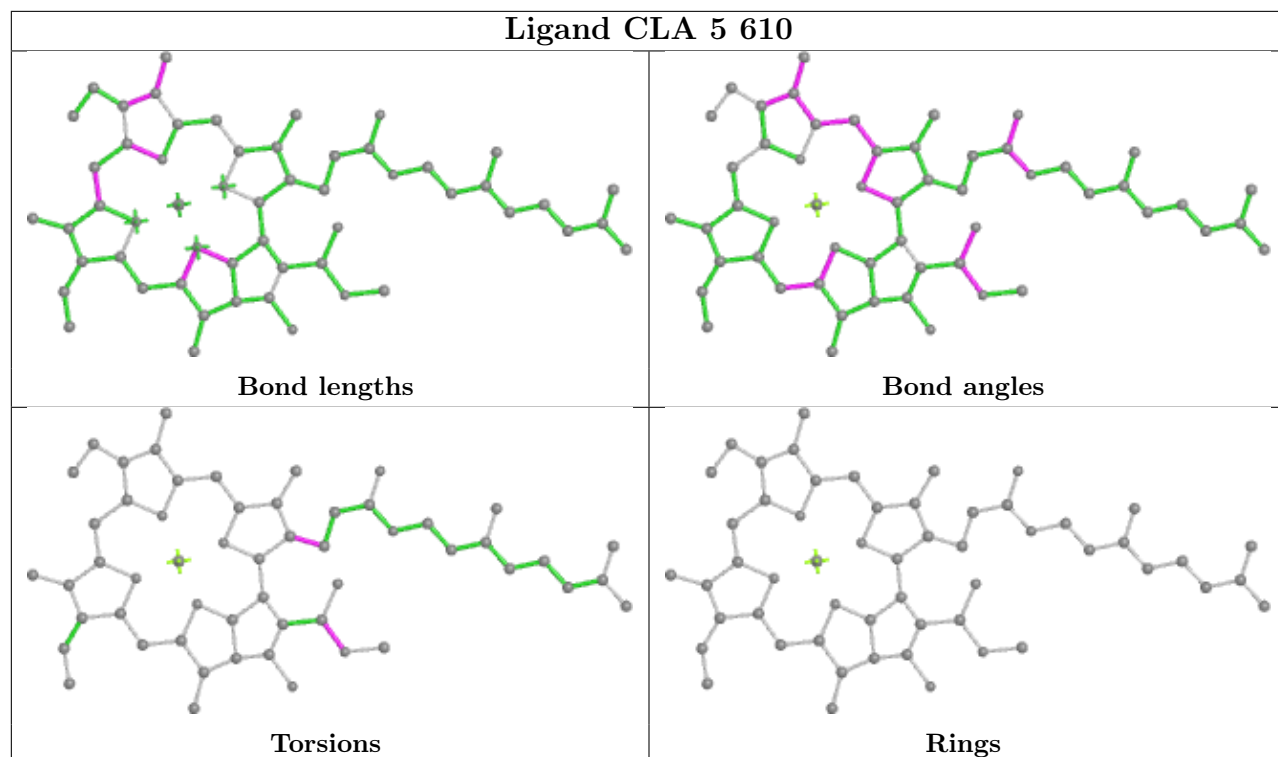
Torsions



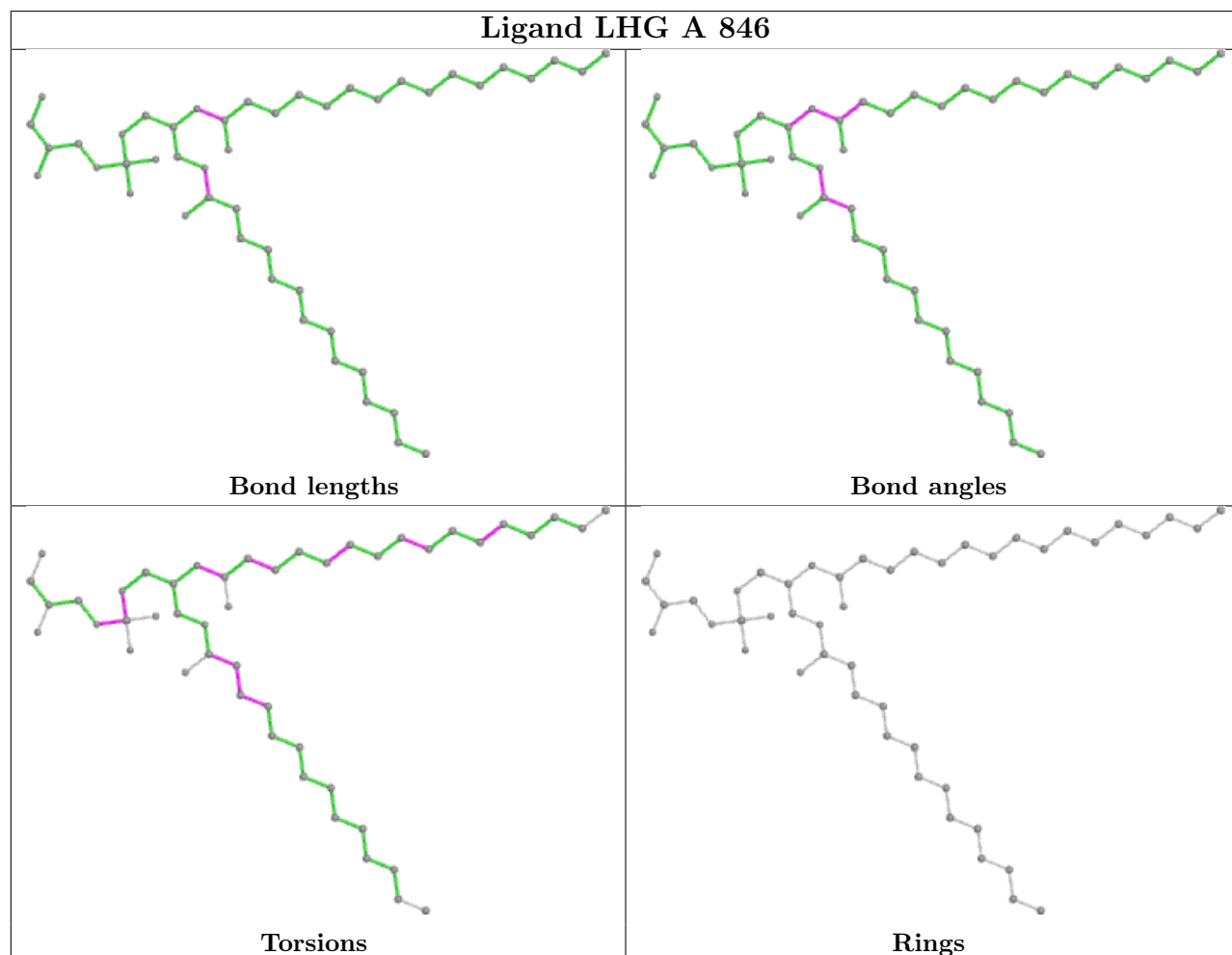
Rings

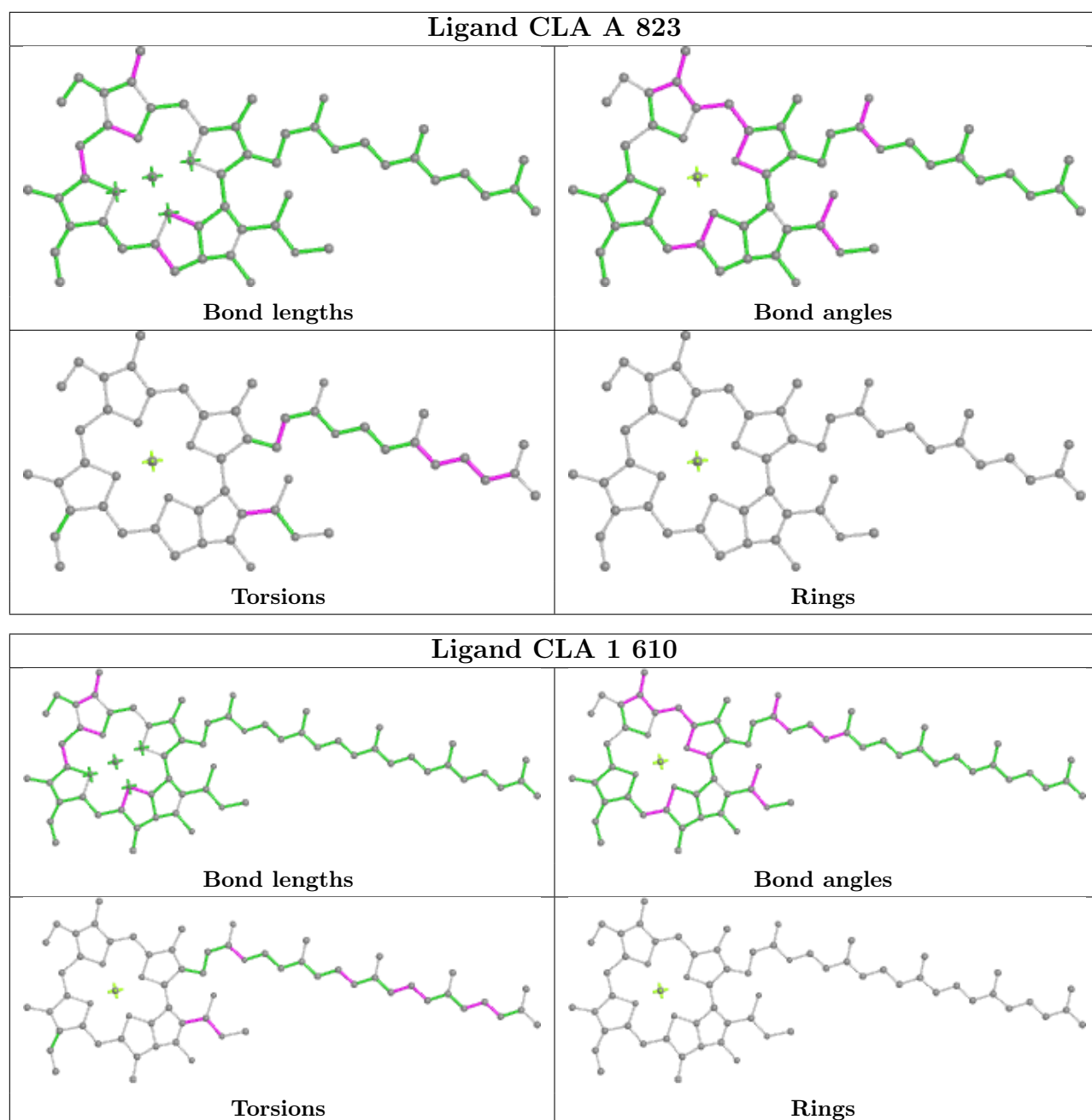


Ligand CLA 5 610

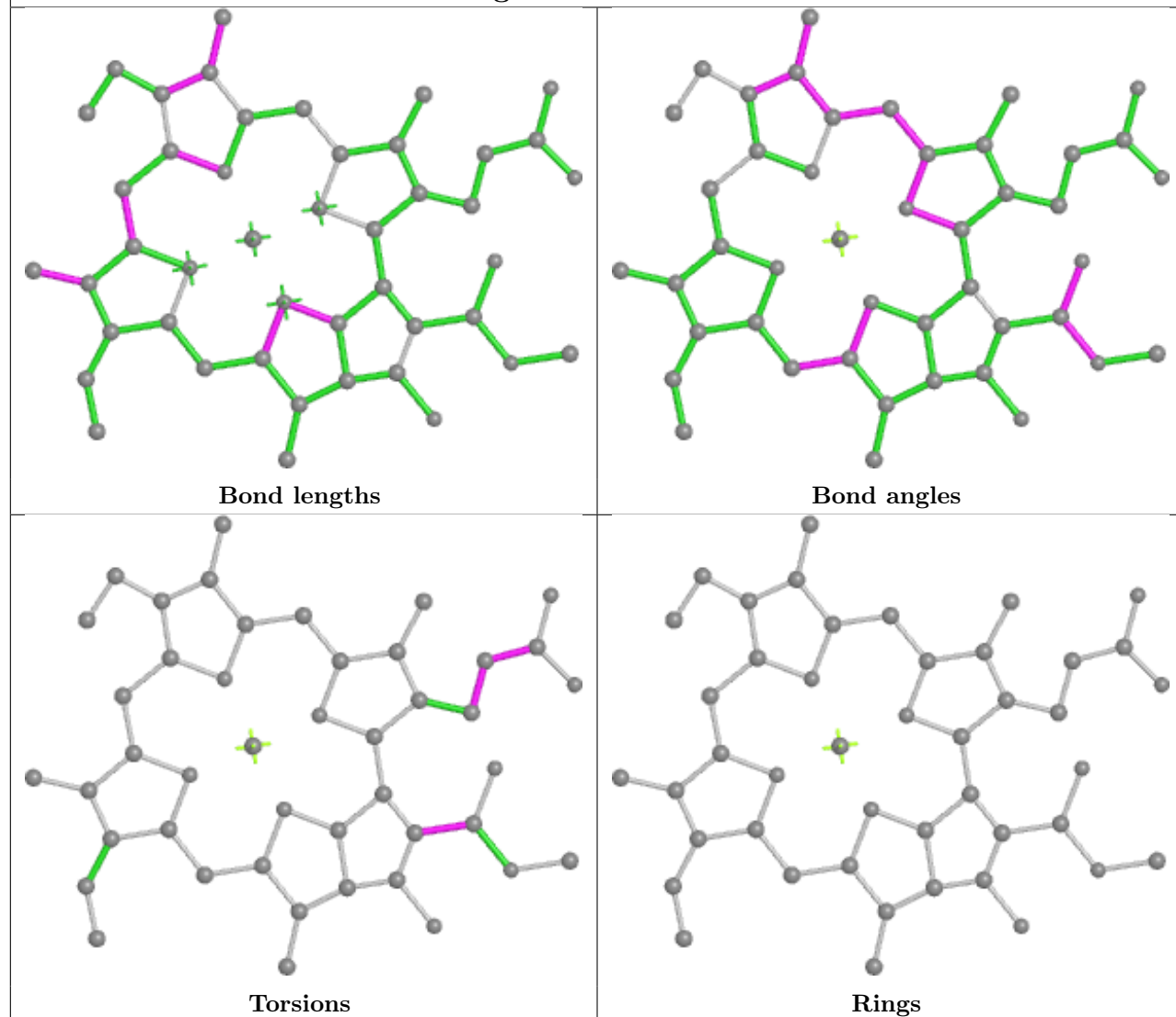


Ligand LHG A 846

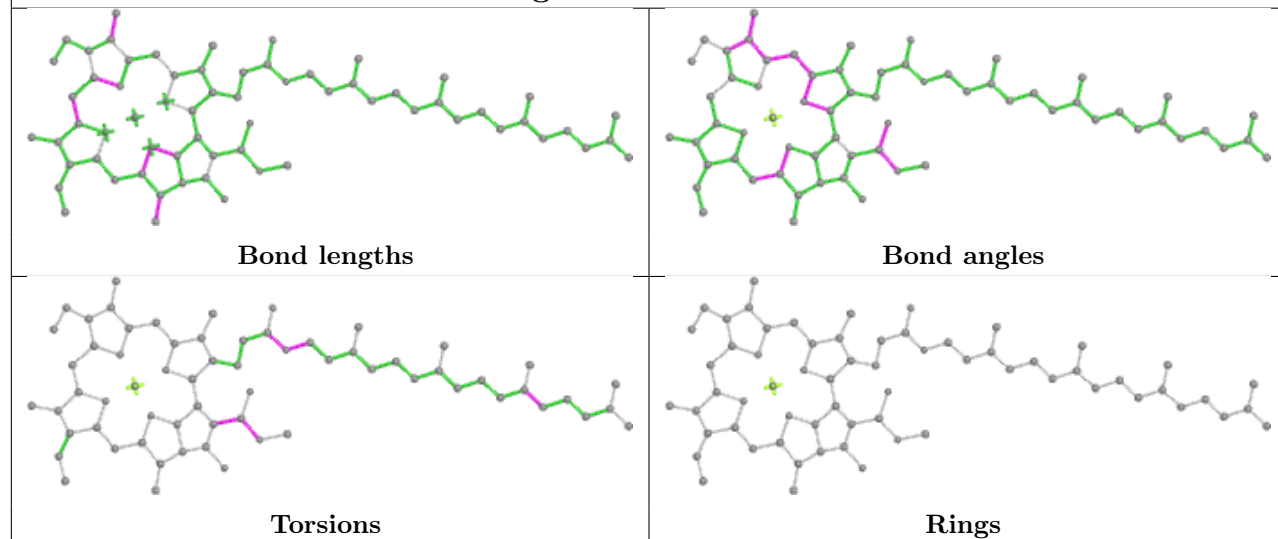


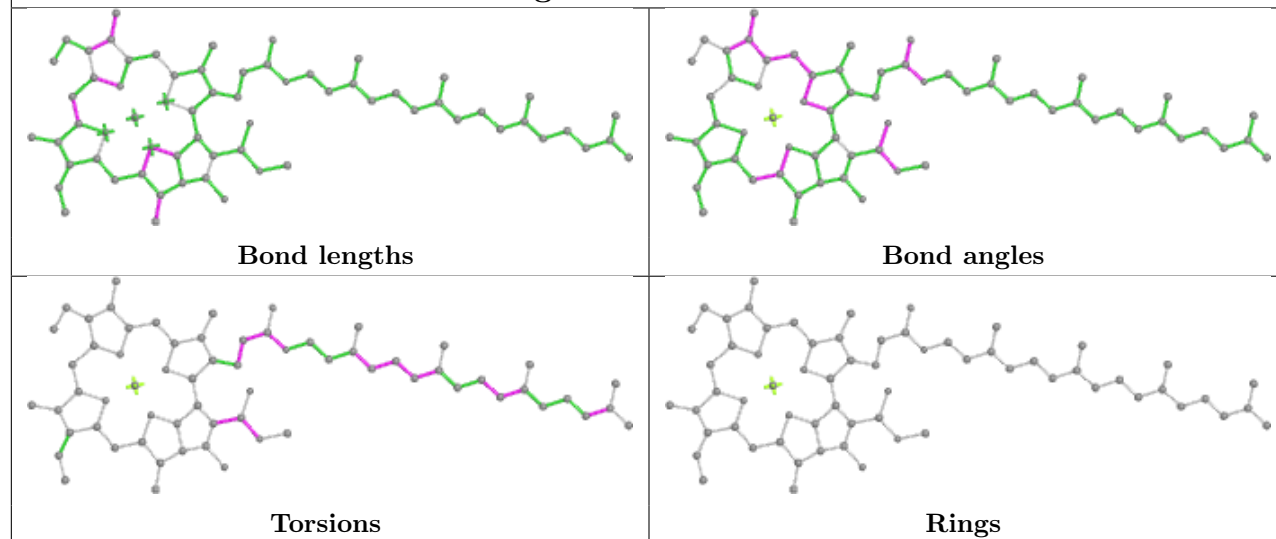
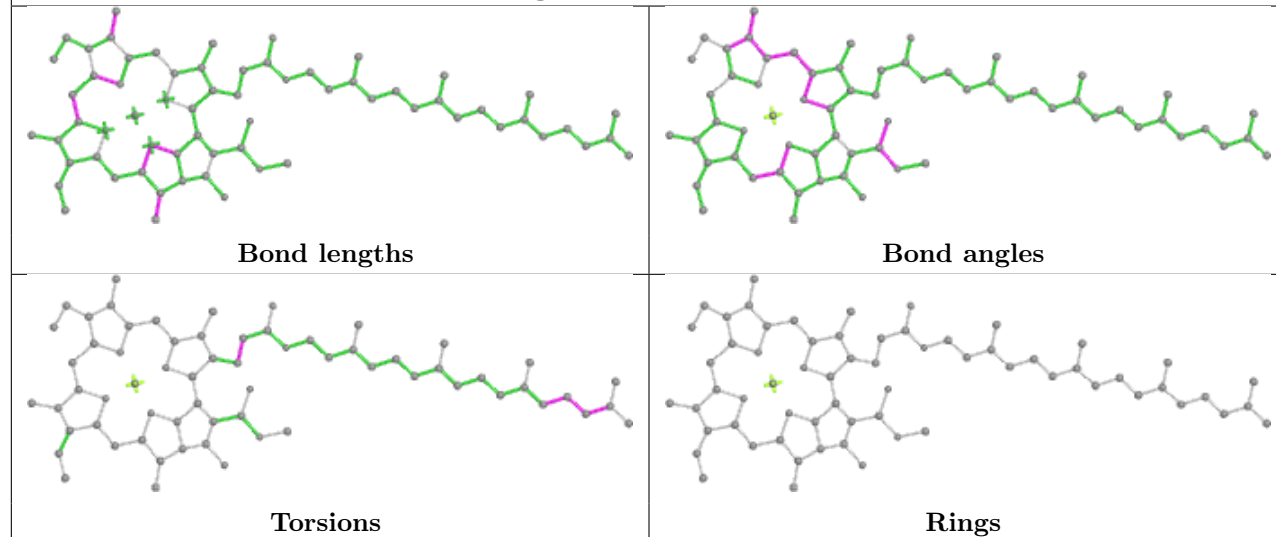


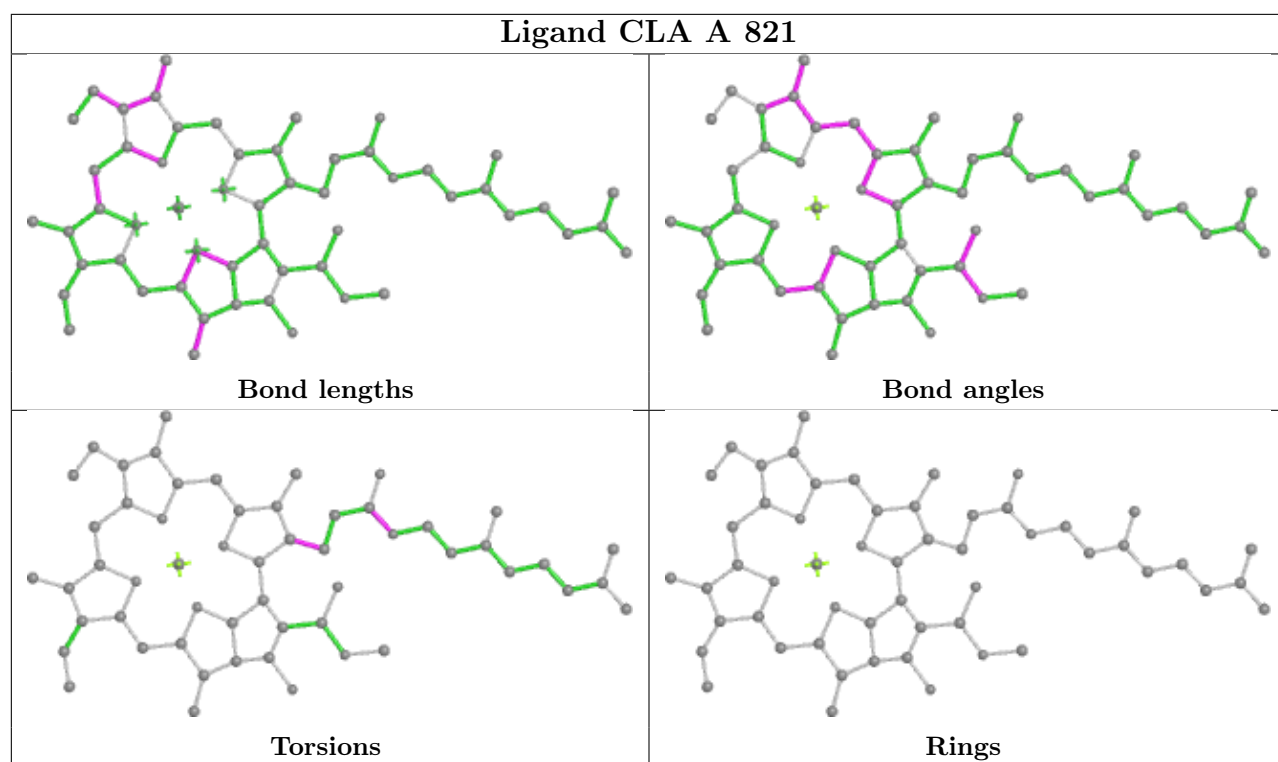
Ligand CLA 4 612



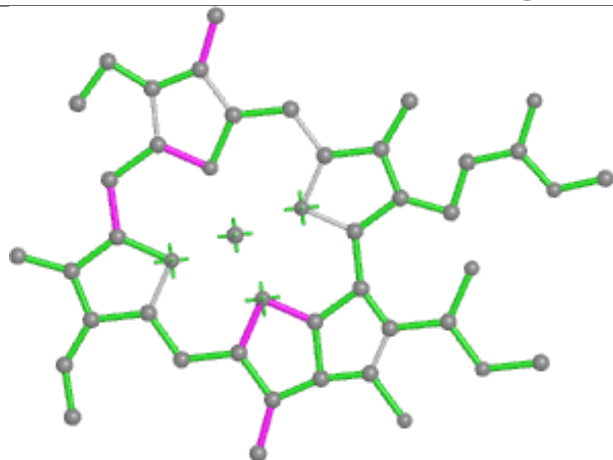
Ligand CLA B 829



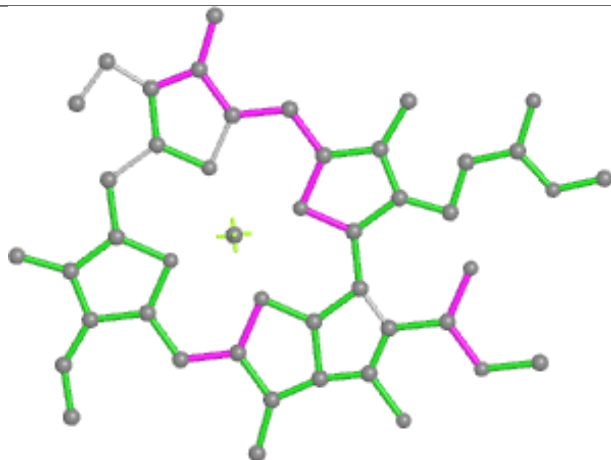
Ligand CLA L 302**Ligand CLA A 818**



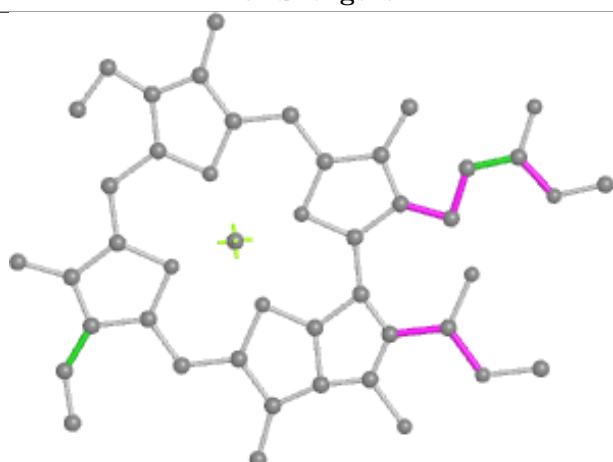
Ligand CLA 3 606



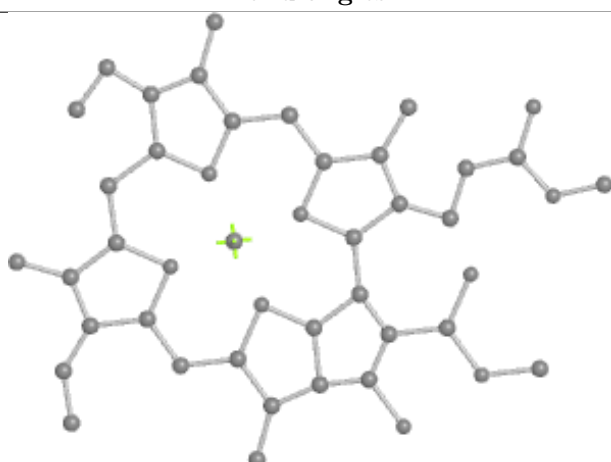
Bond lengths



Bond angles

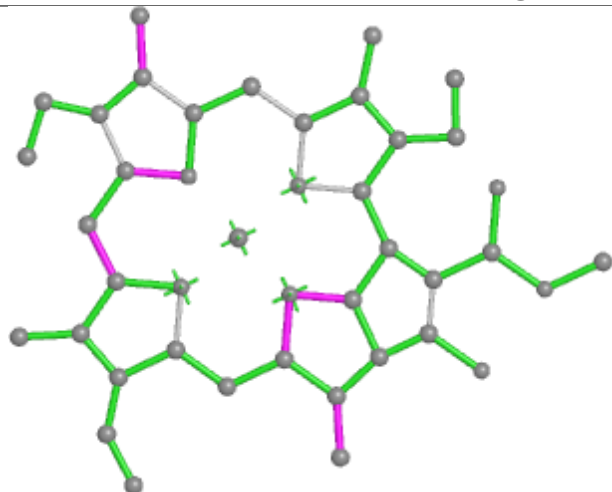


Torsions

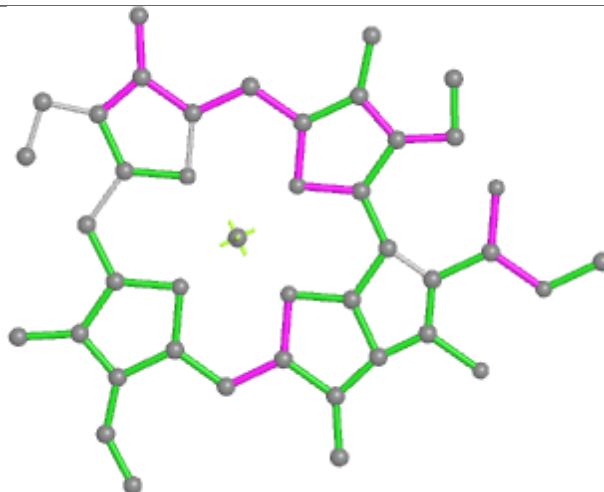


Rings

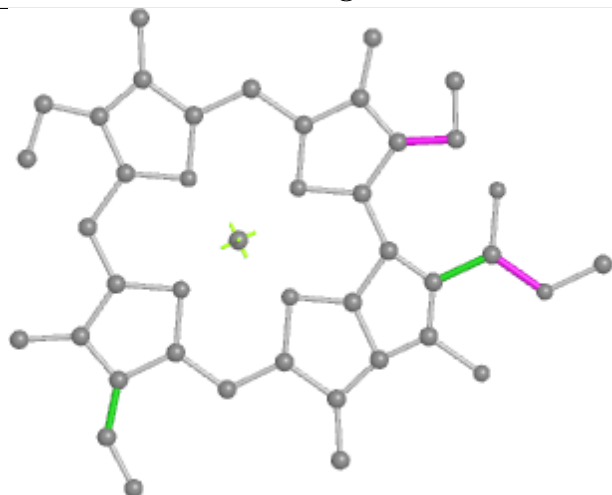
Ligand CLA K 201



Bond lengths



Bond angles

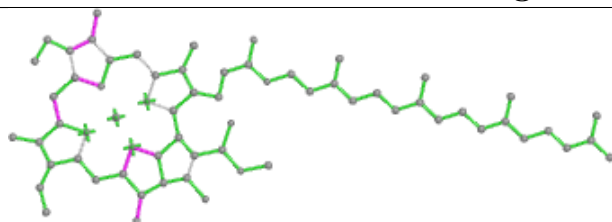


Torsions

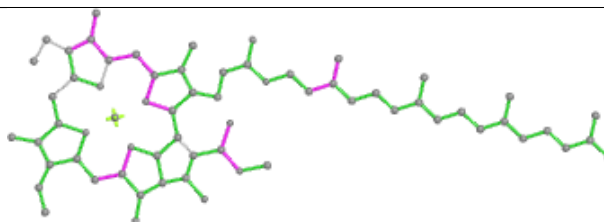


Rings

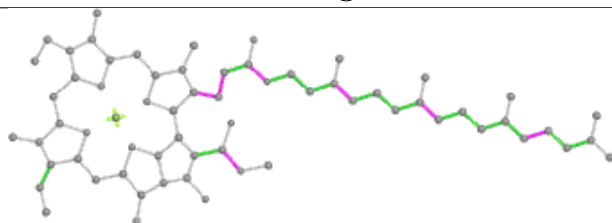
Ligand CLA B 809



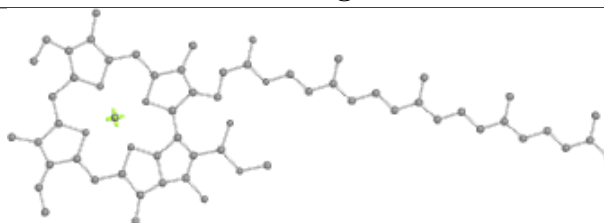
Bond lengths



Bond angles

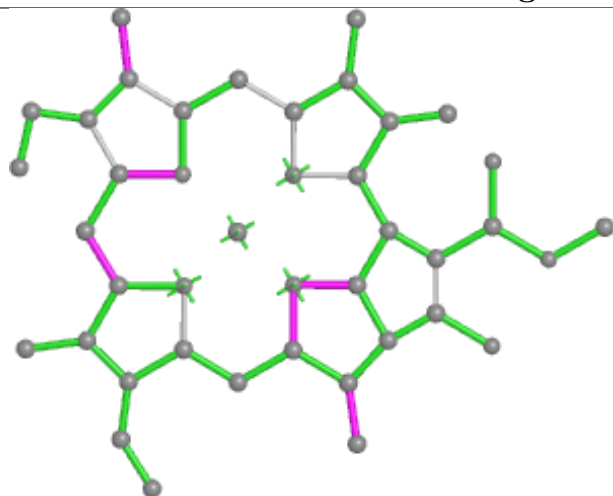


Torsions

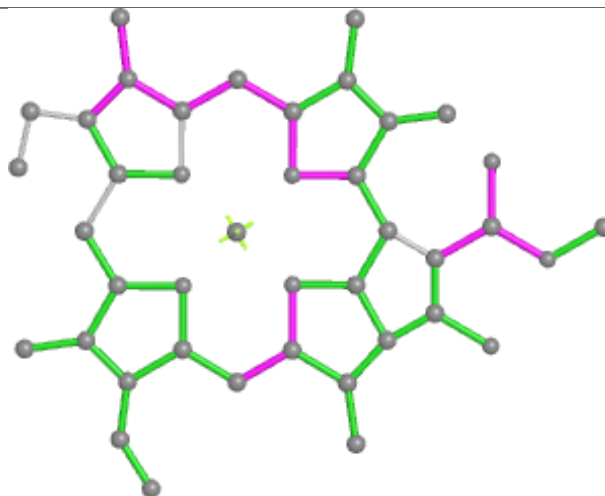


Rings

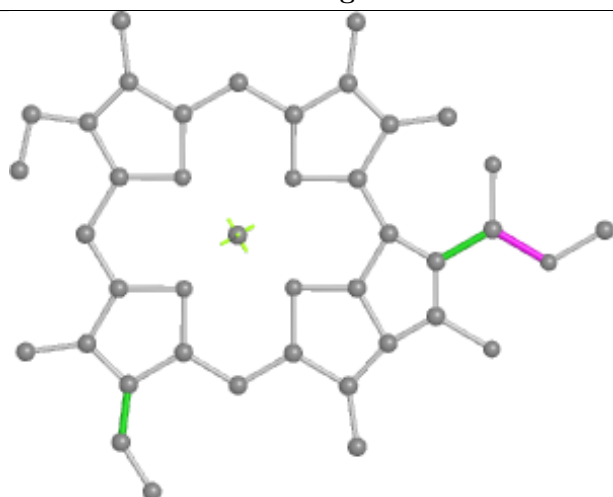
Ligand CLA 7 611



Bond lengths



Bond angles

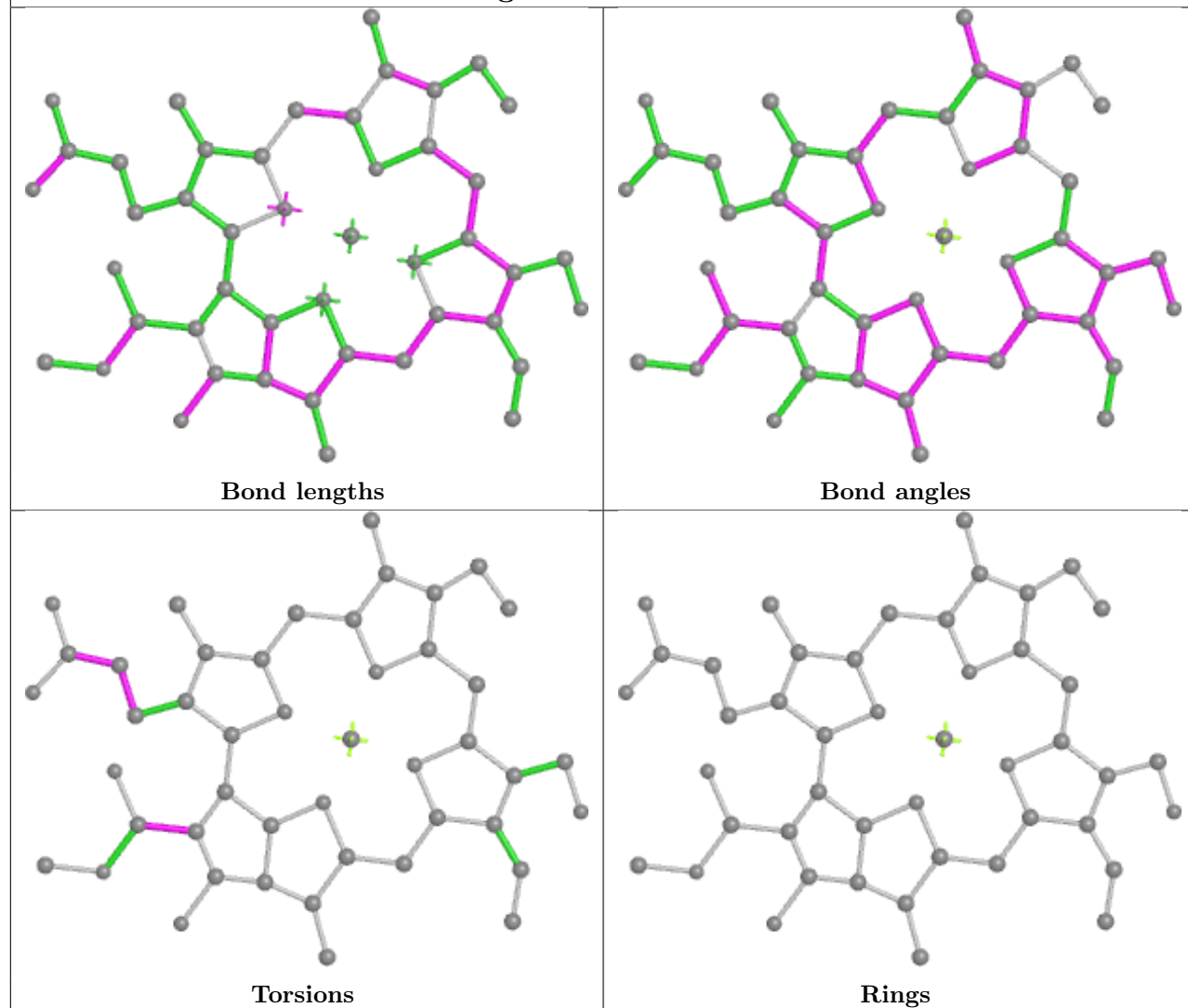


Torsions

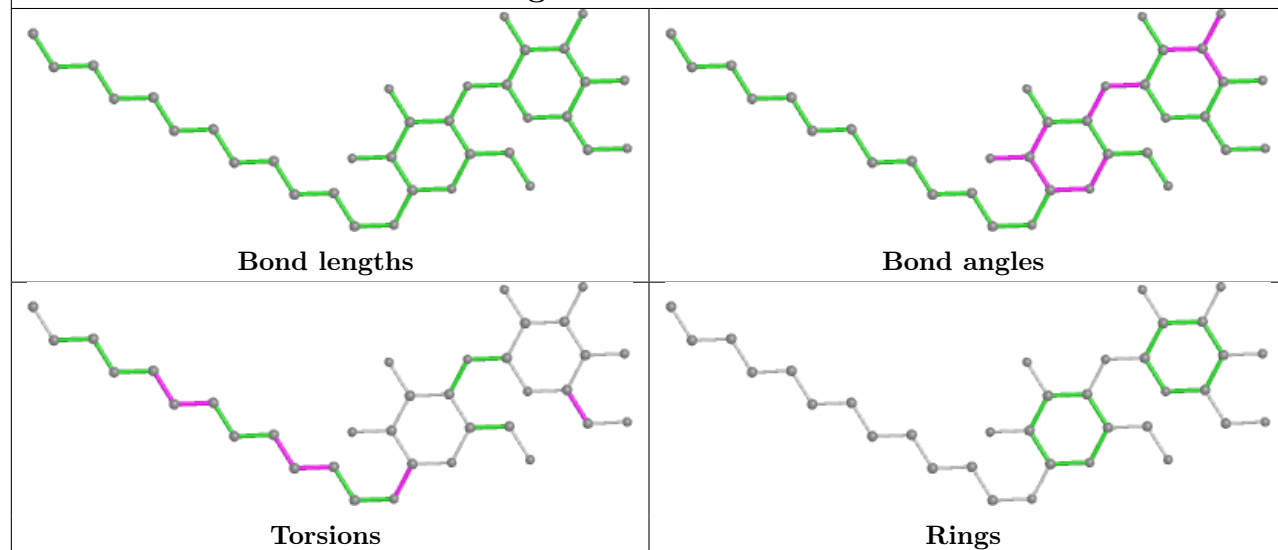


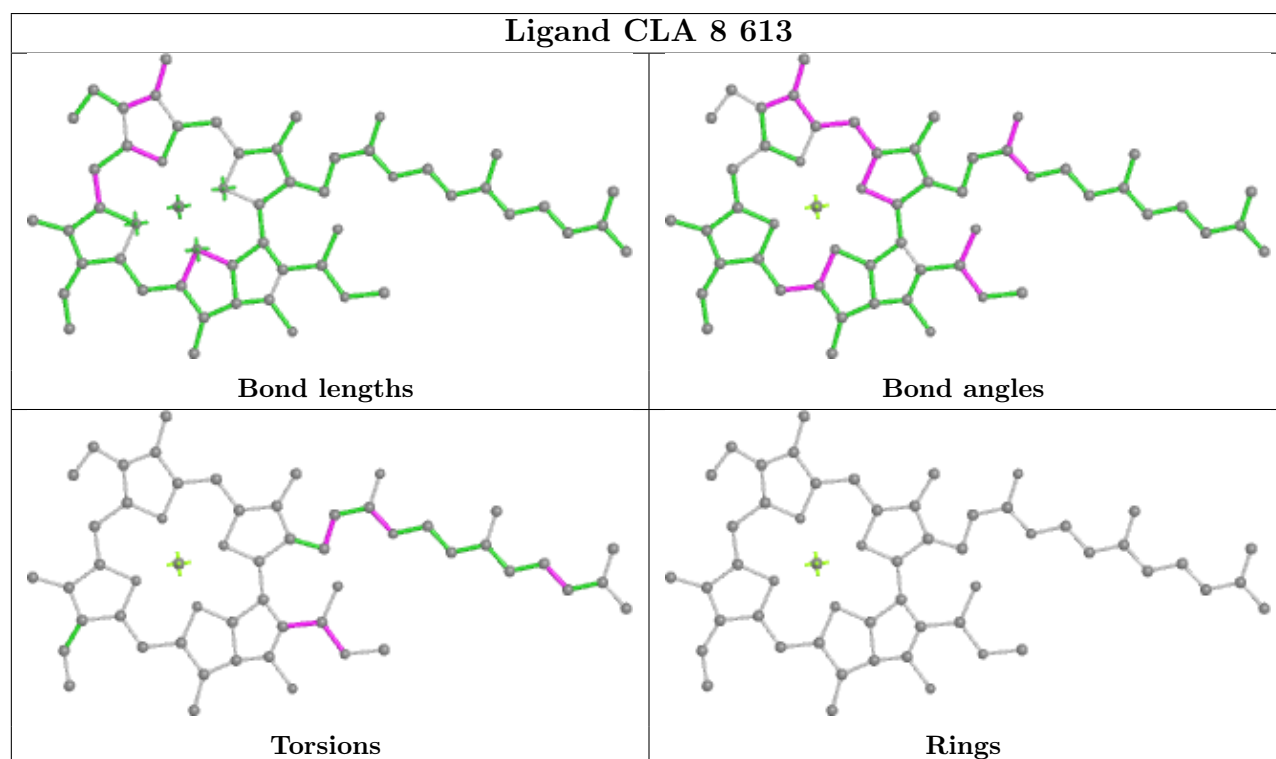
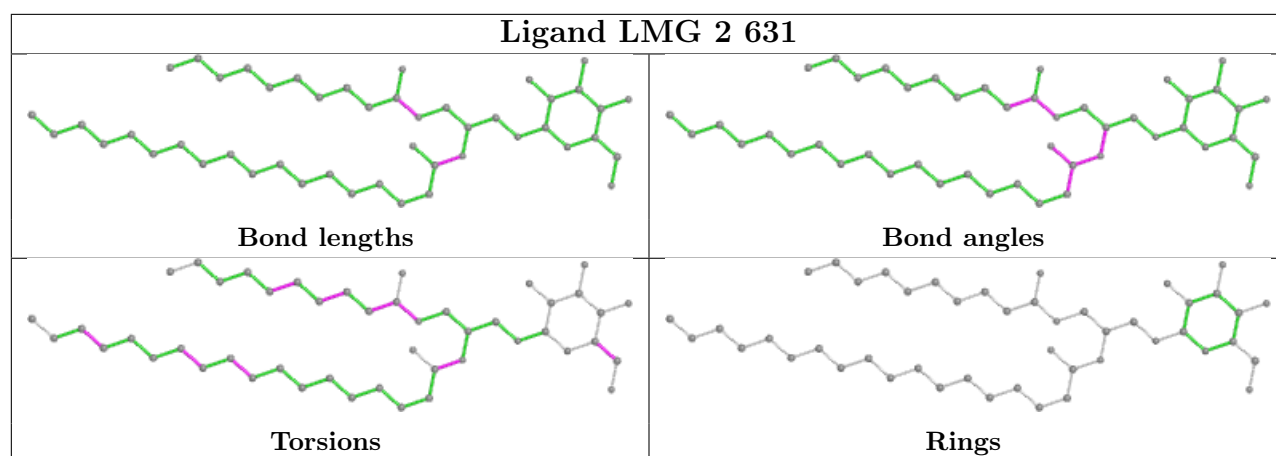
Rings

Ligand CHL 8 607

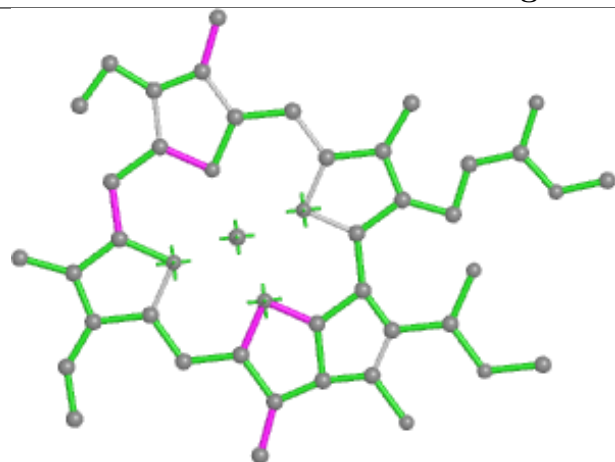


Ligand LMT G 206

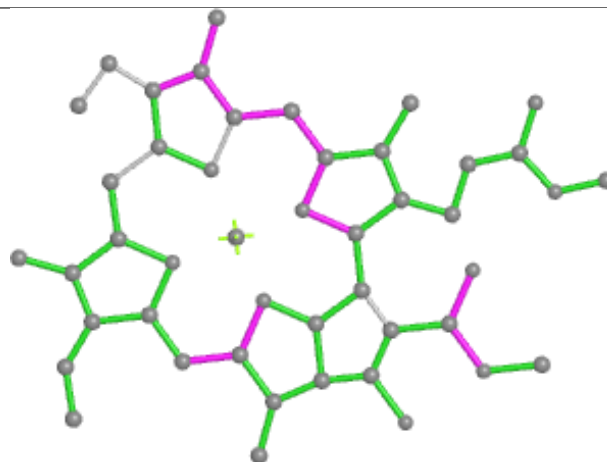




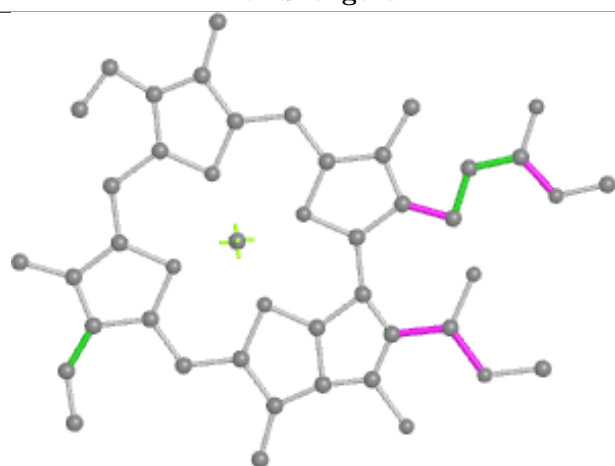
Ligand CLA 4 614



Bond lengths



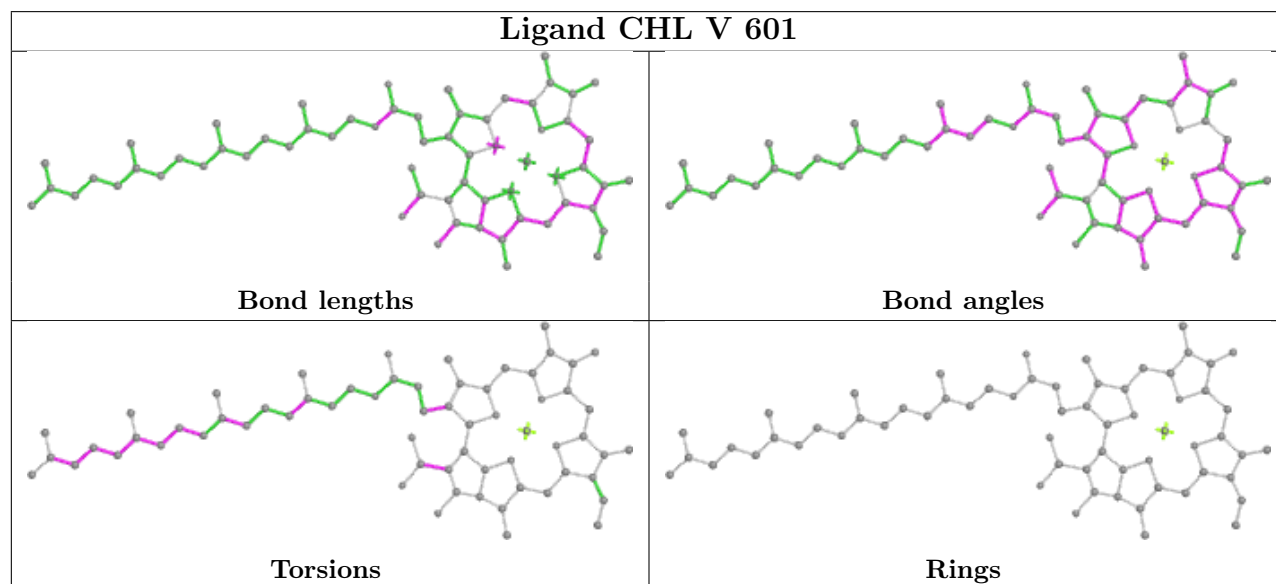
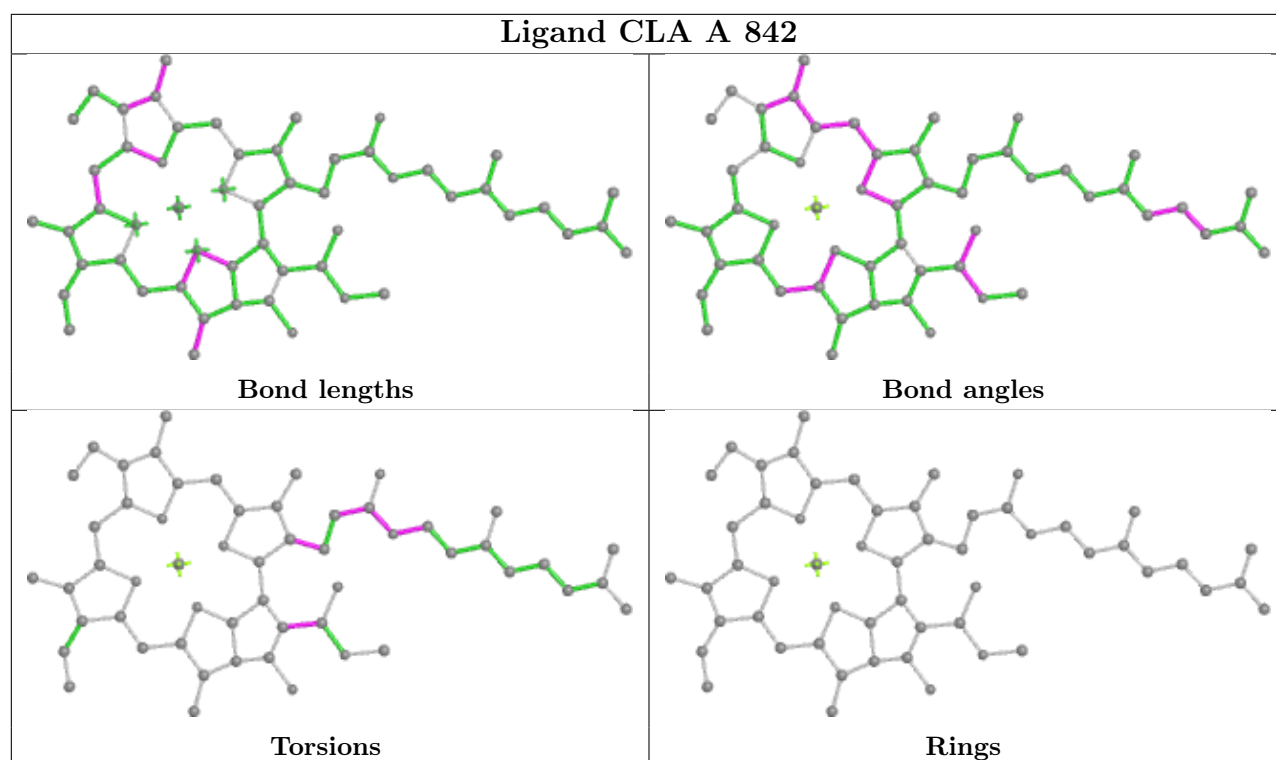
Bond angles

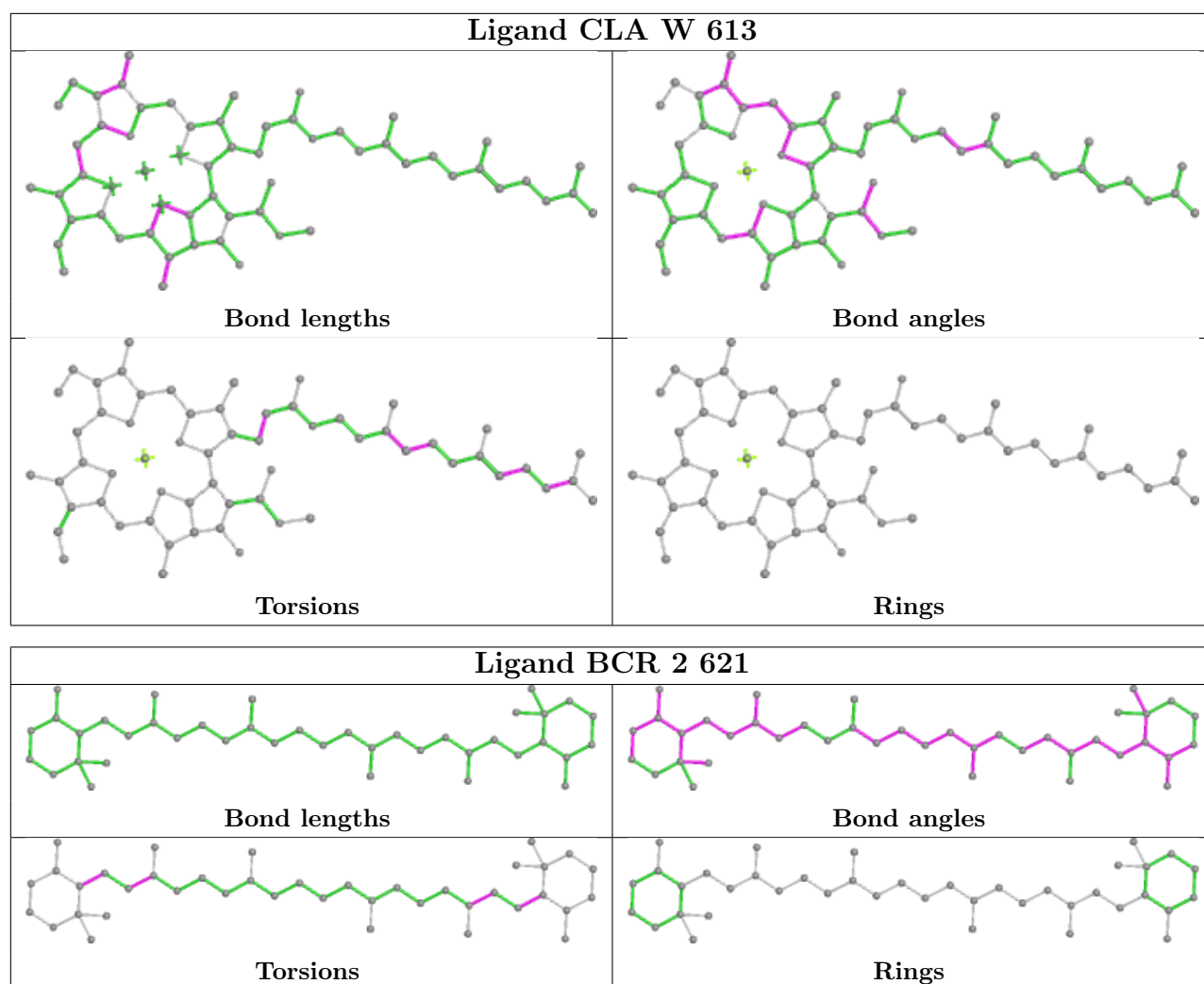


Torsions

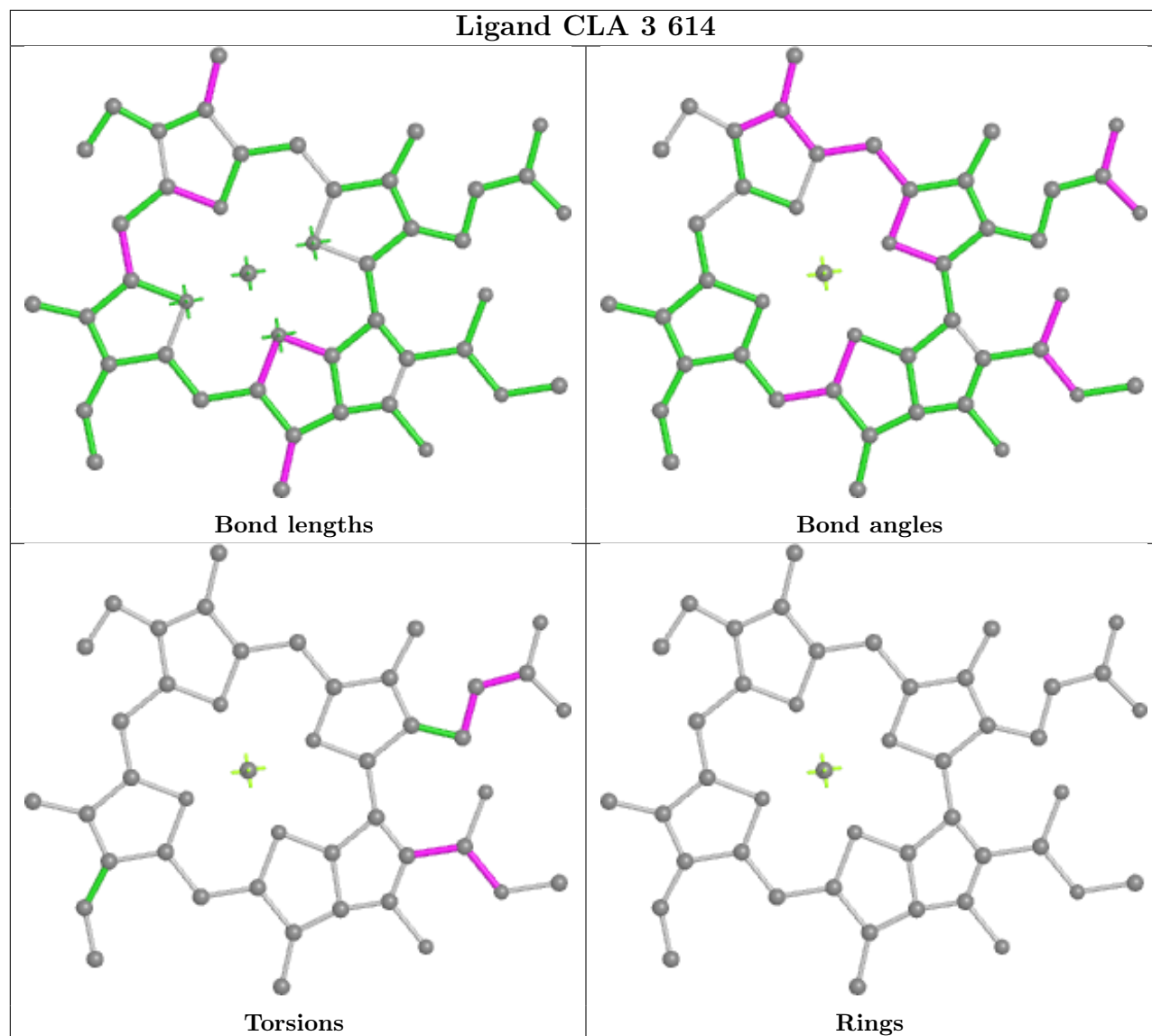


Rings

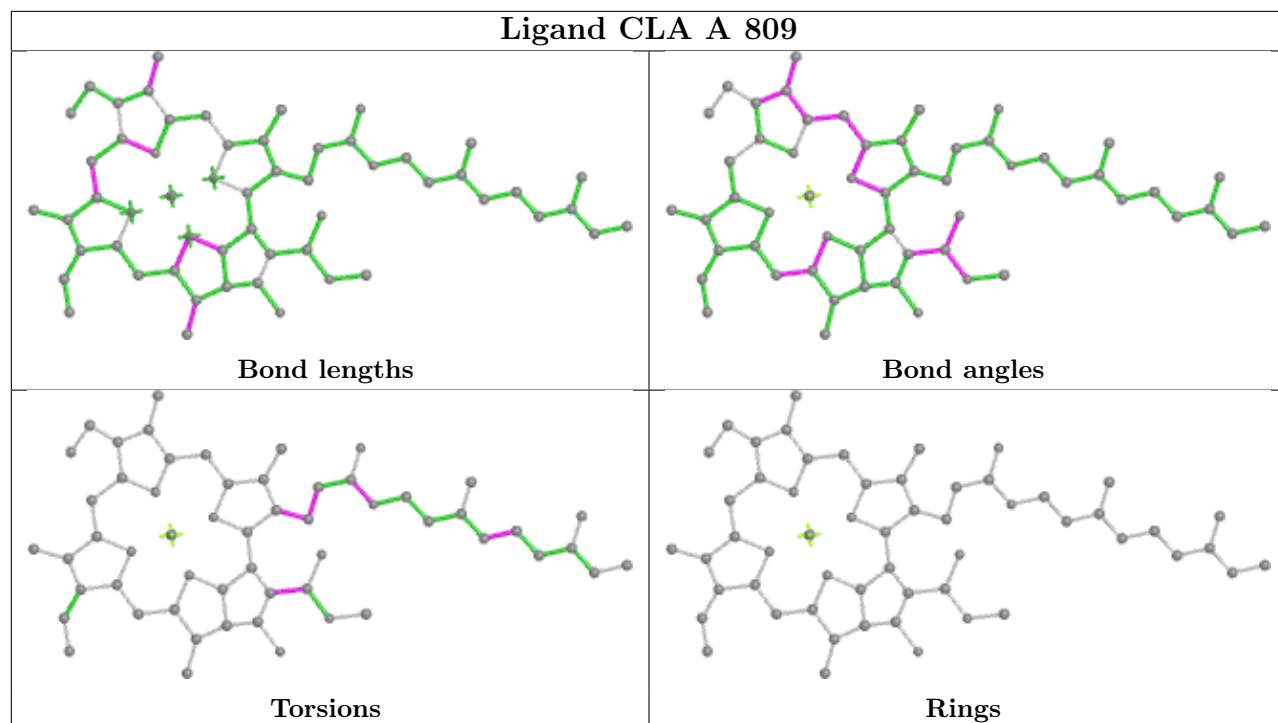




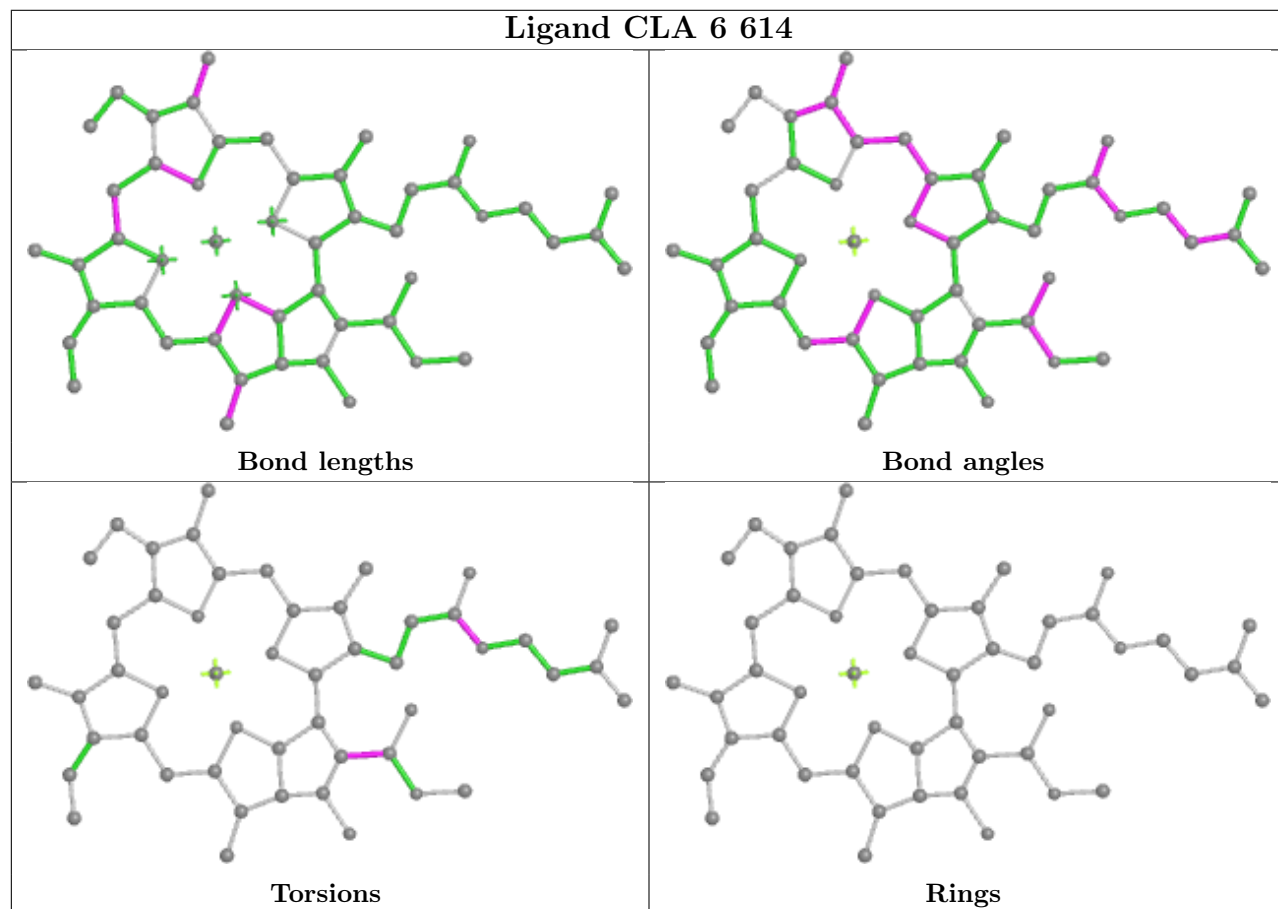
Ligand CLA 3 614



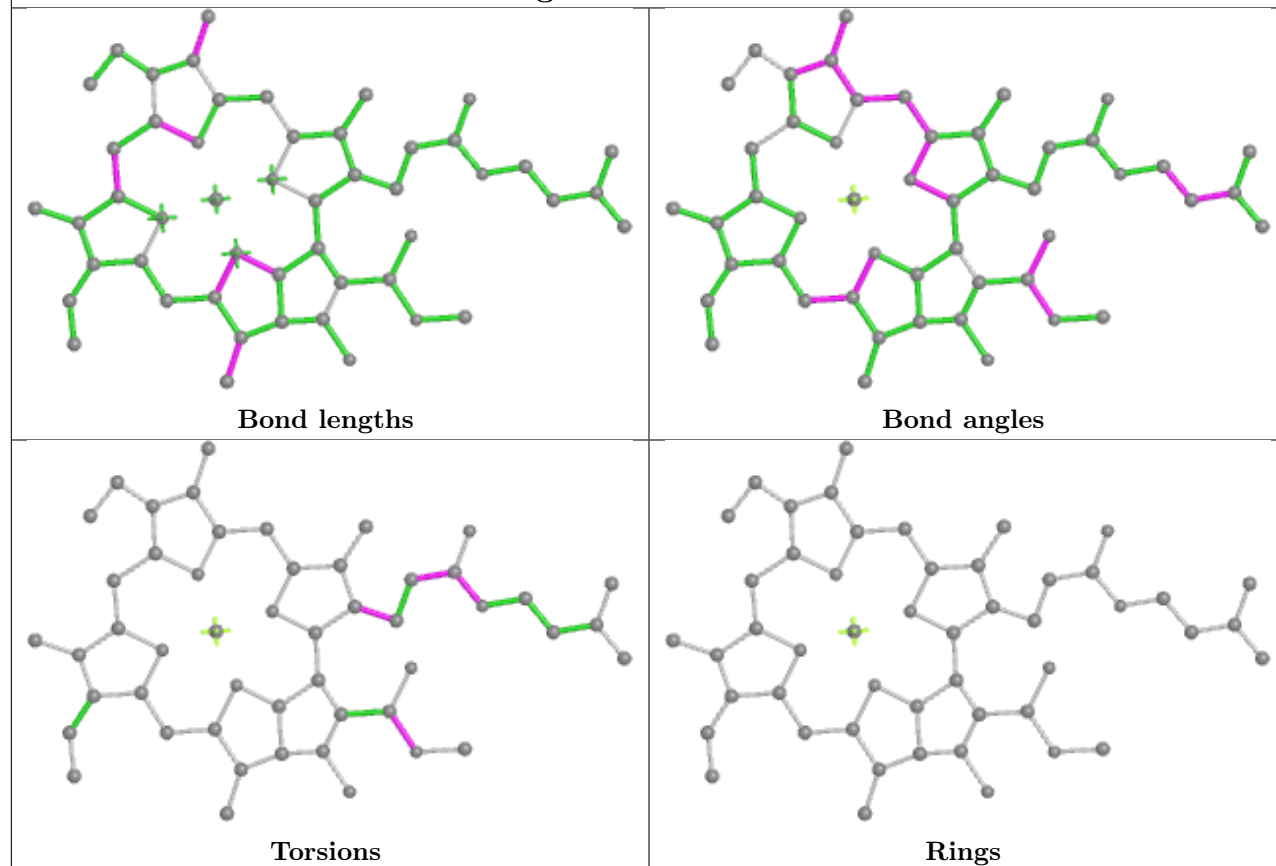
Ligand CLA A 809



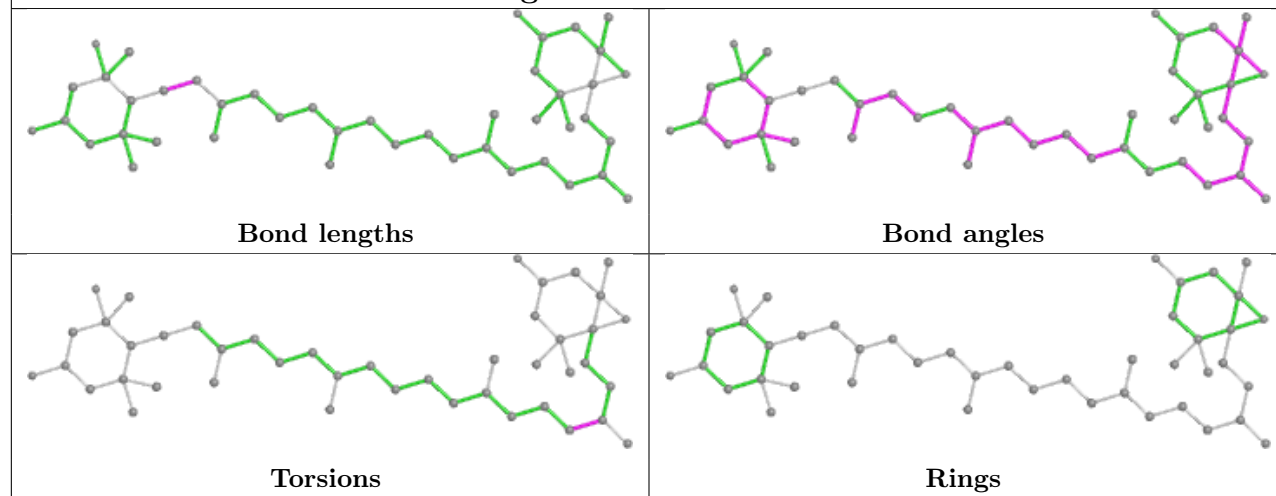
Ligand CLA 6 614

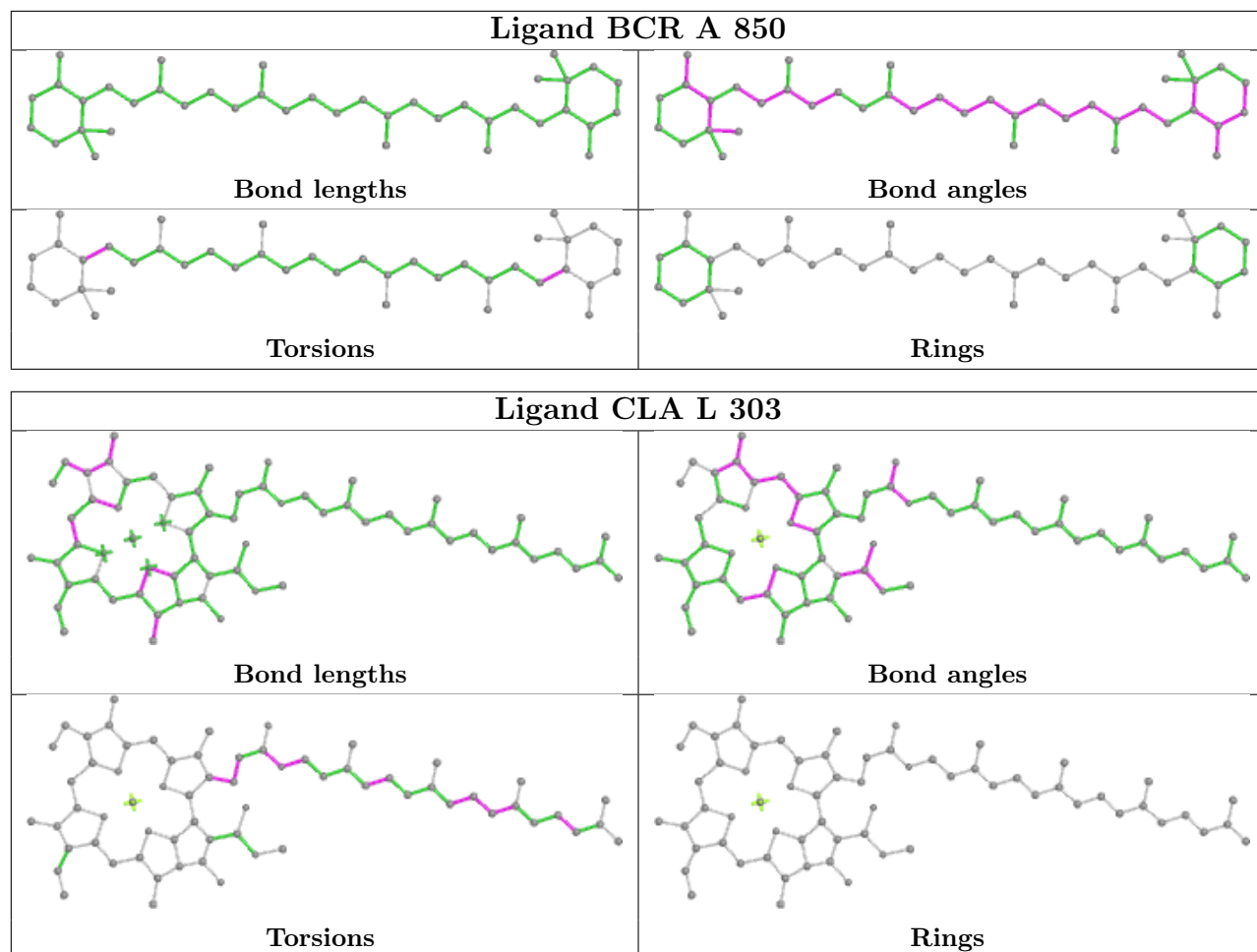


Ligand CLA 1 613

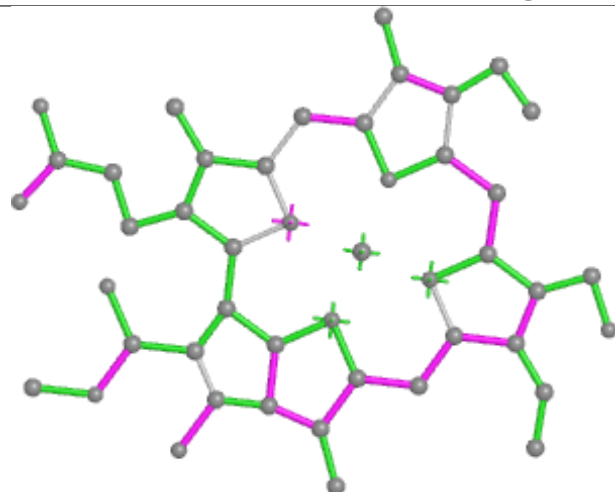


Ligand NEX V 2623

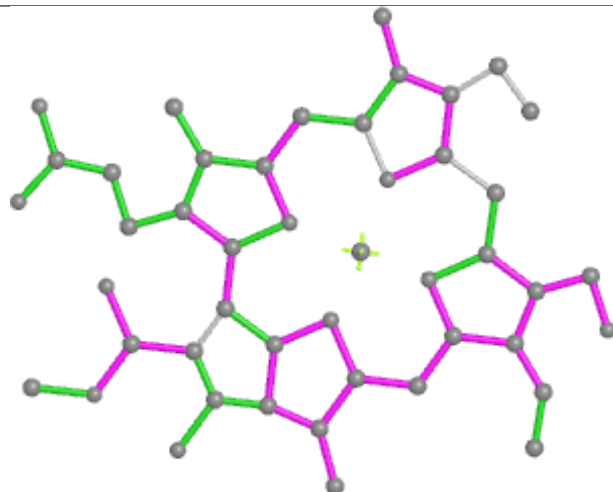




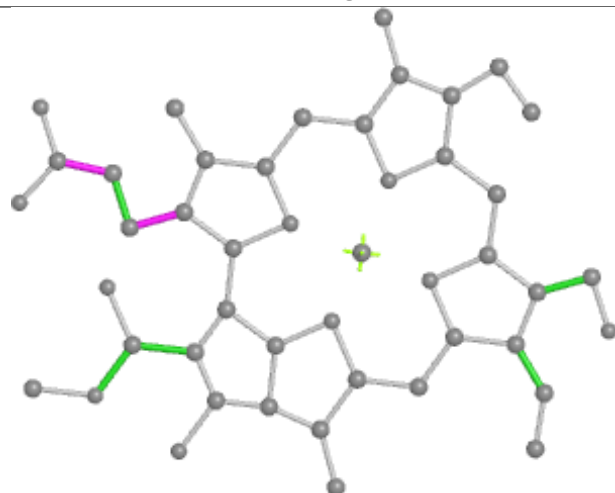
Ligand CHL 6 606



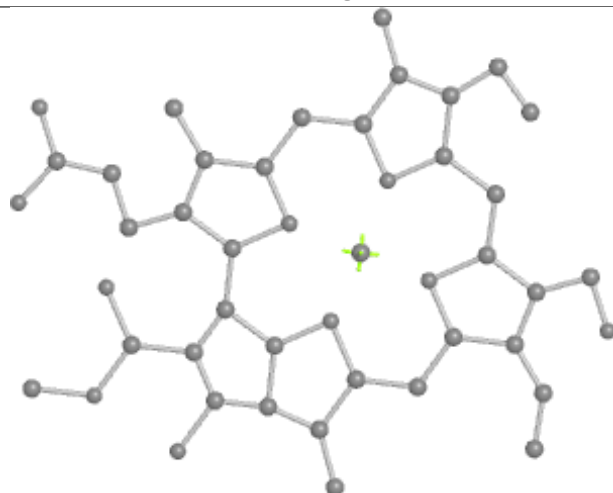
Bond lengths



Bond angles

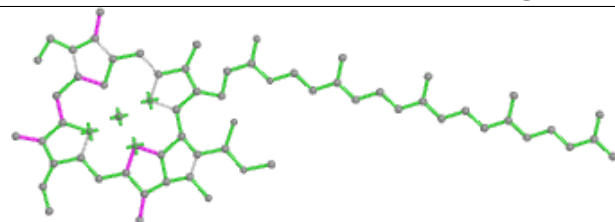


Torsions

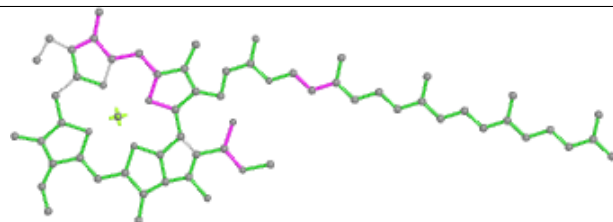


Rings

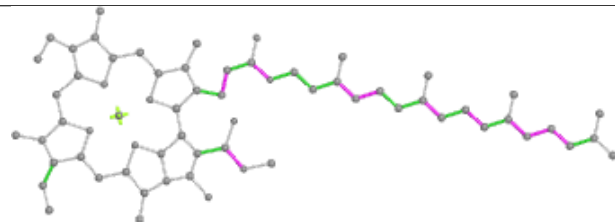
Ligand CLA F 301



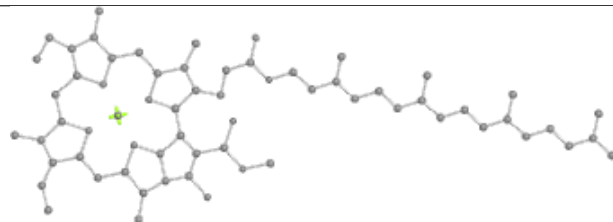
Bond lengths



Bond angles

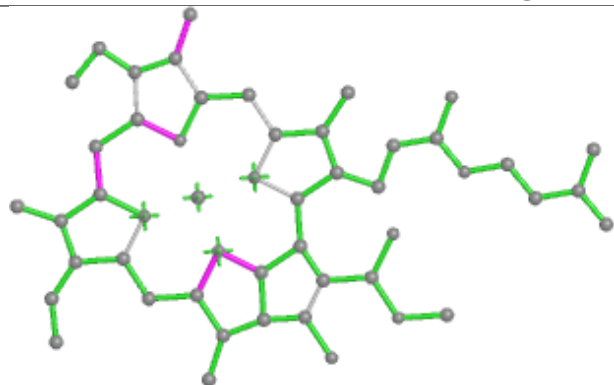


Torsions

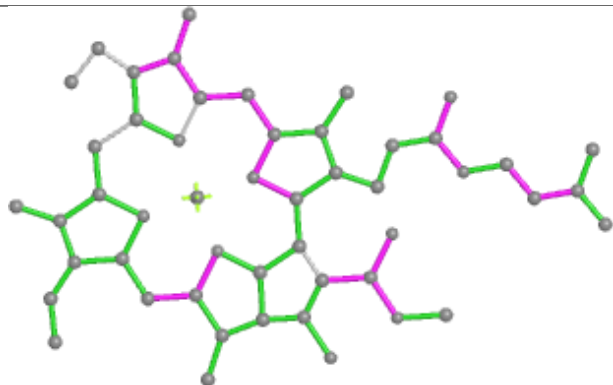


Rings

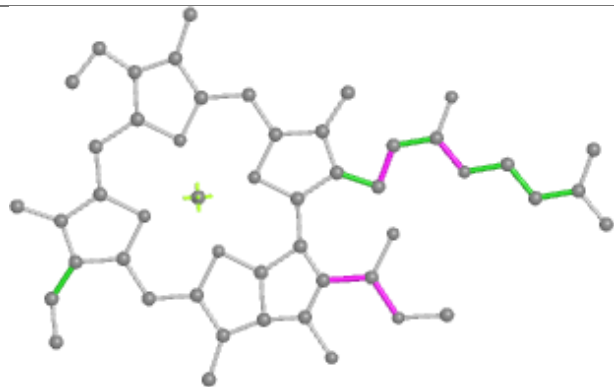
Ligand CLA 4 601



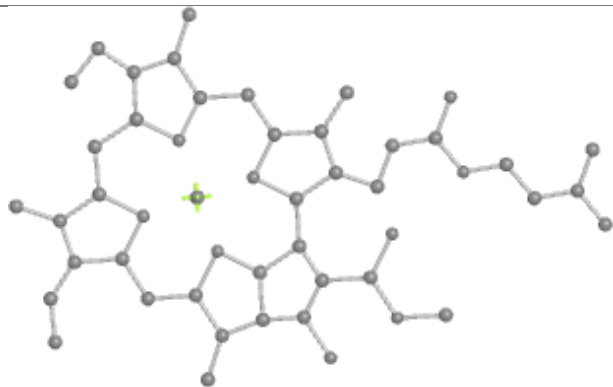
Bond lengths



Bond angles

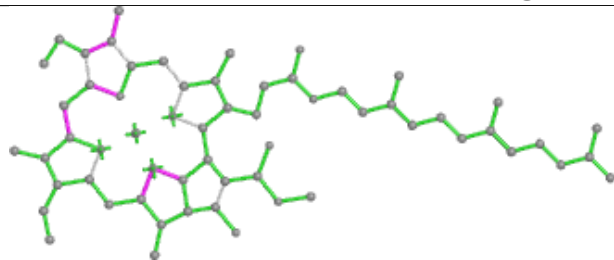


Torsions

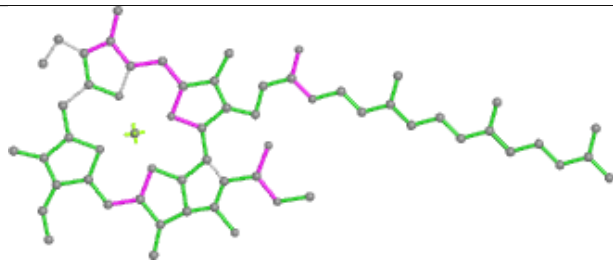


Rings

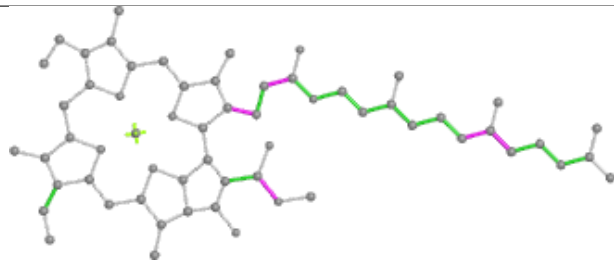
Ligand CLA 6 610



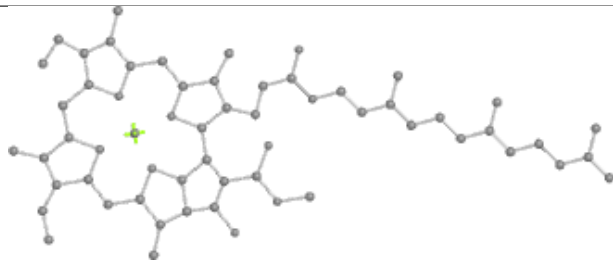
Bond lengths



Bond angles

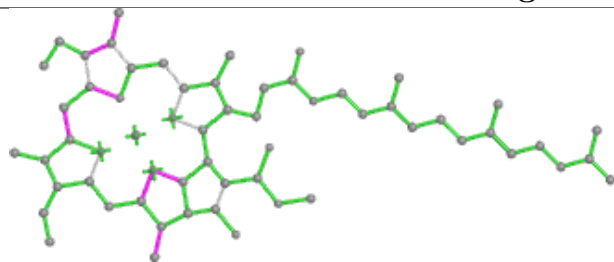


Torsions

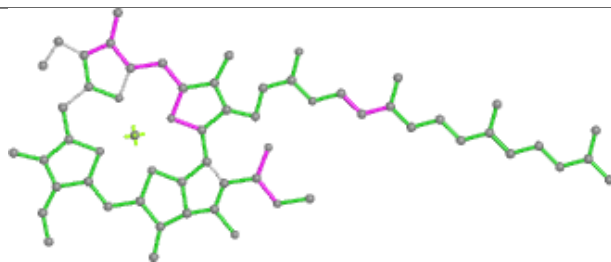


Rings

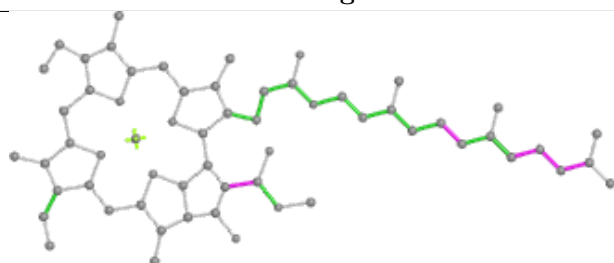
Ligand CLA 2 610



Bond lengths



Bond angles

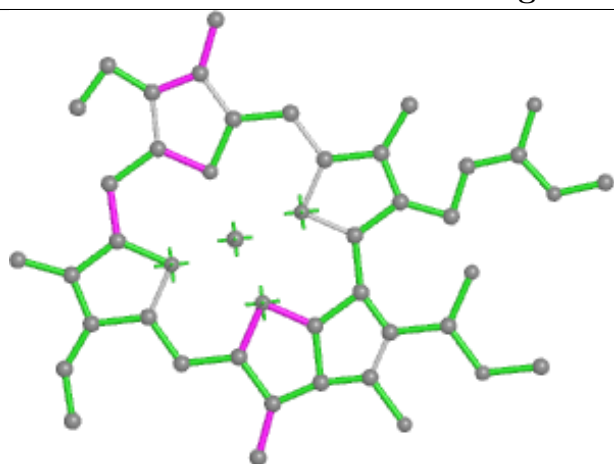


Torsions

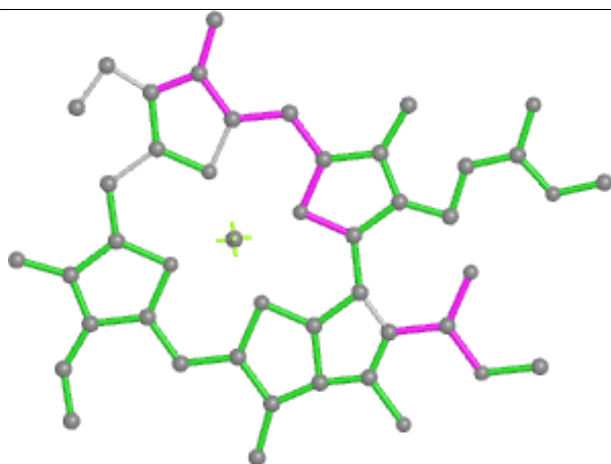


Rings

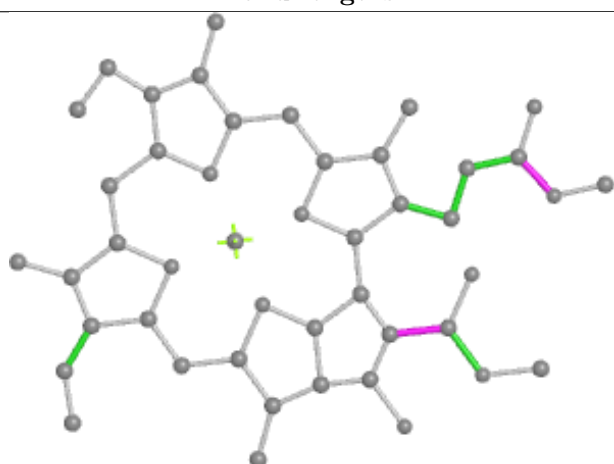
Ligand CLA 5 611



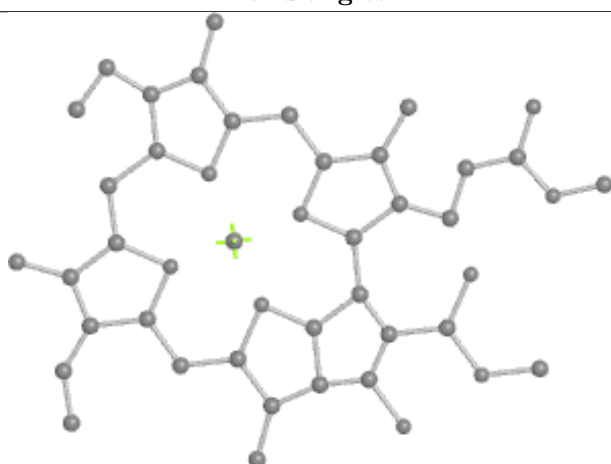
Bond lengths



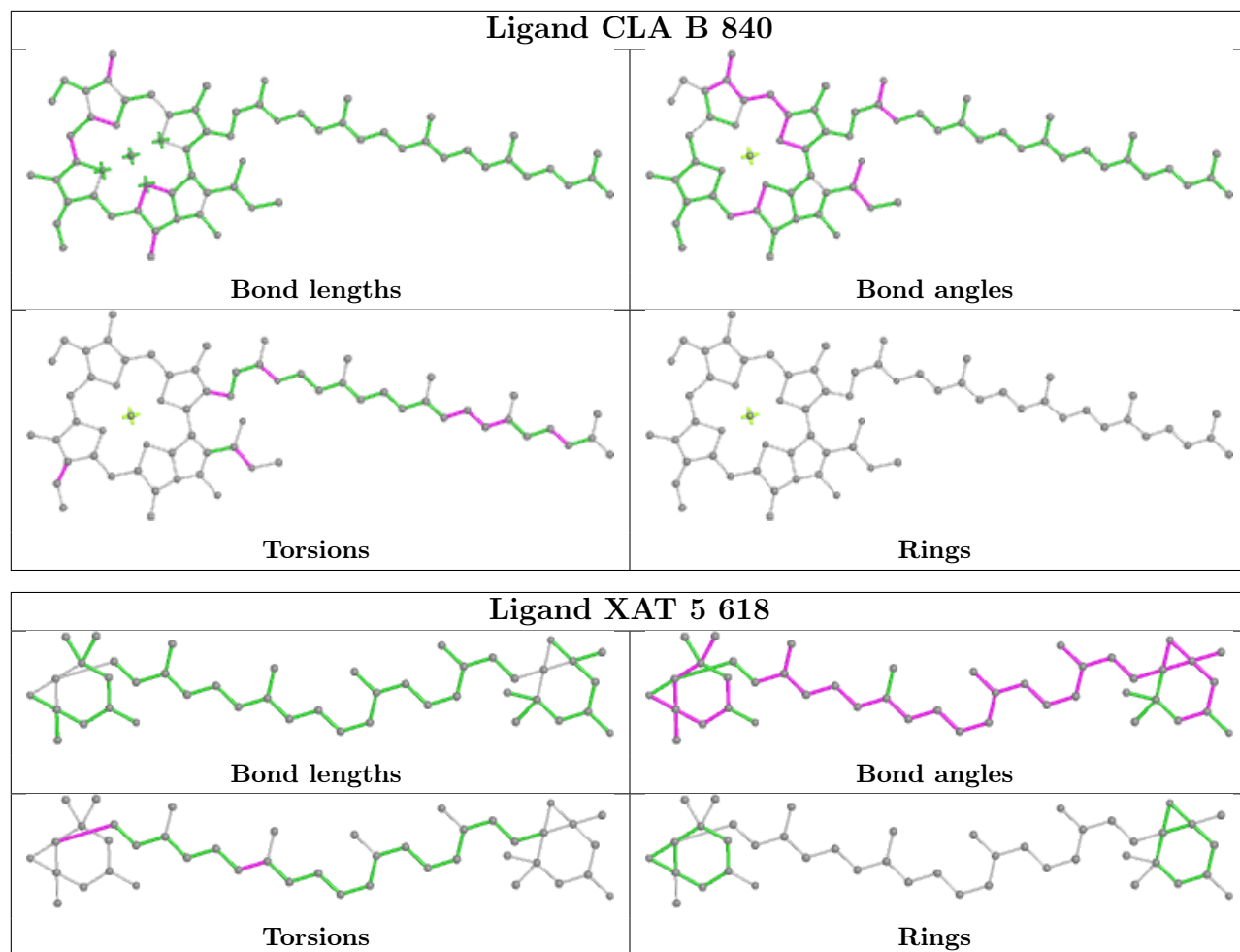
Bond angles



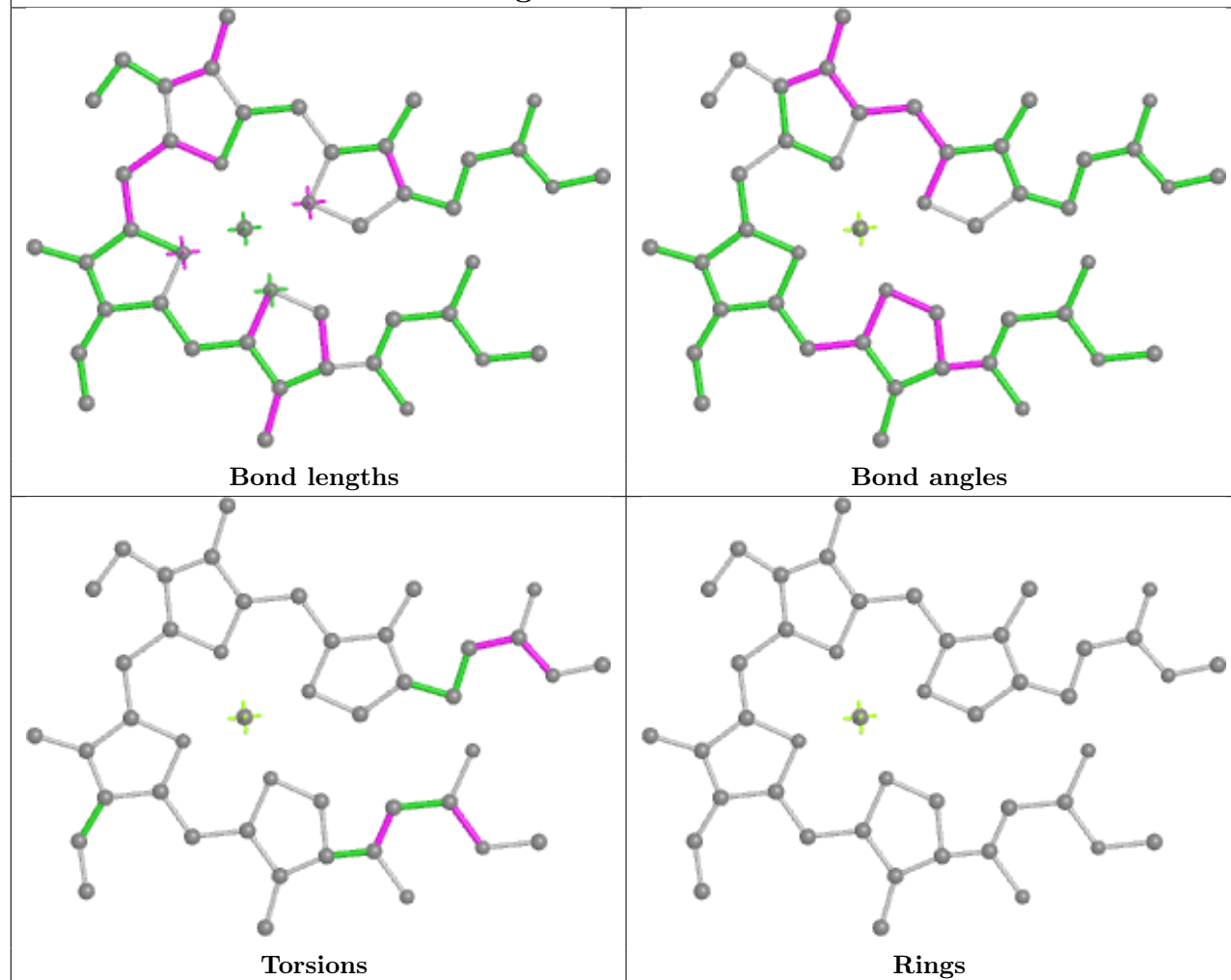
Torsions



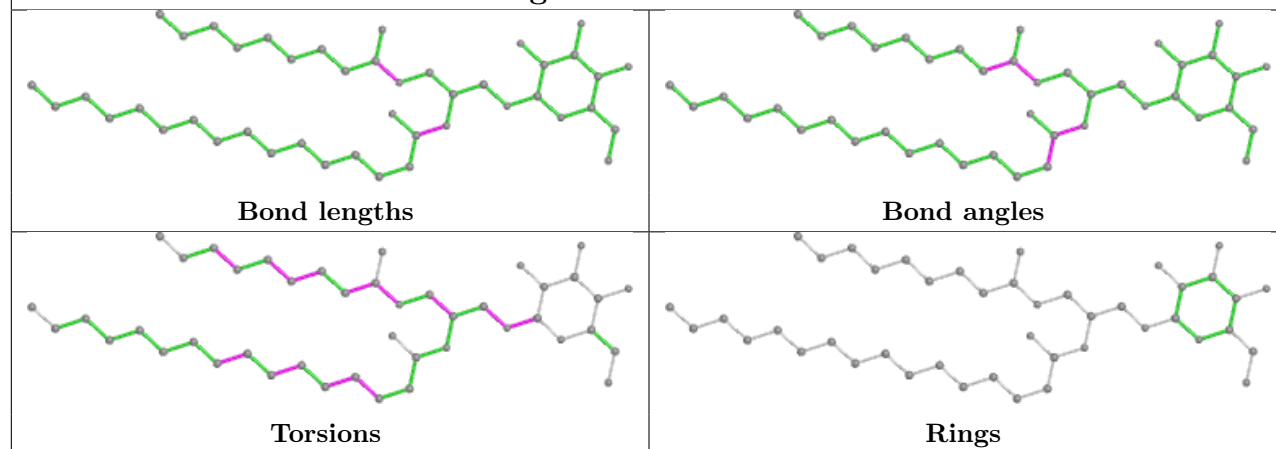
Rings



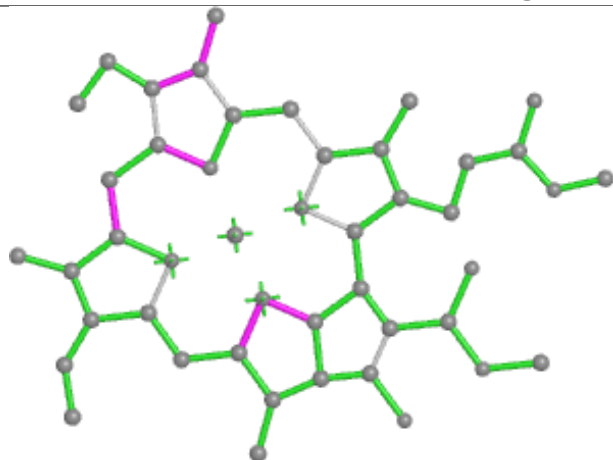
Ligand CLA F 304



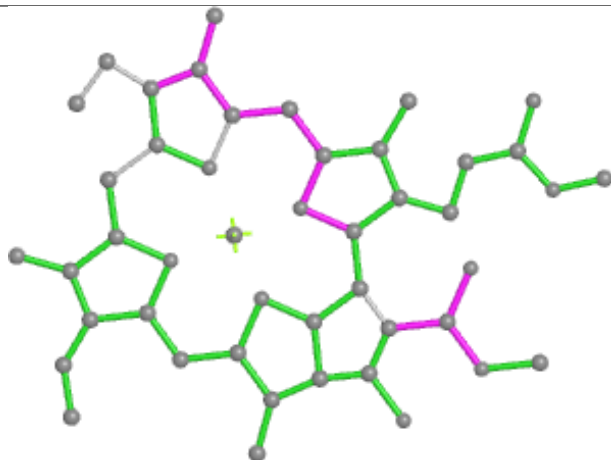
Ligand LMG L 307



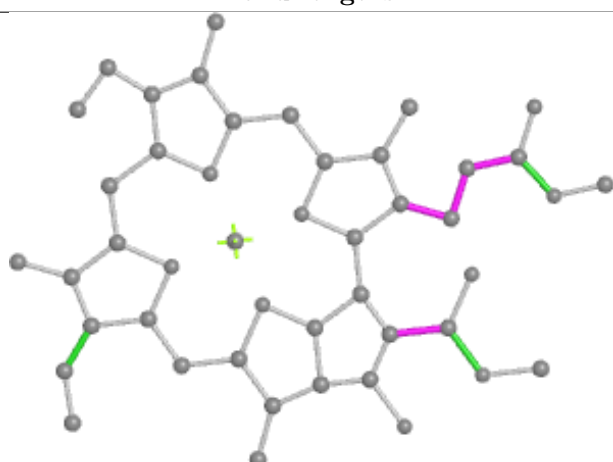
Ligand CLA 2 609



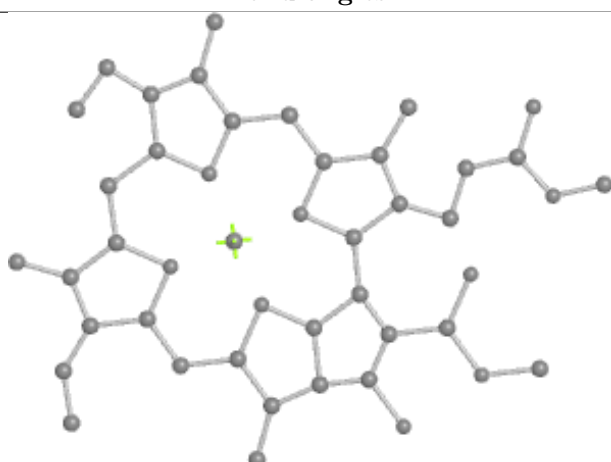
Bond lengths



Bond angles

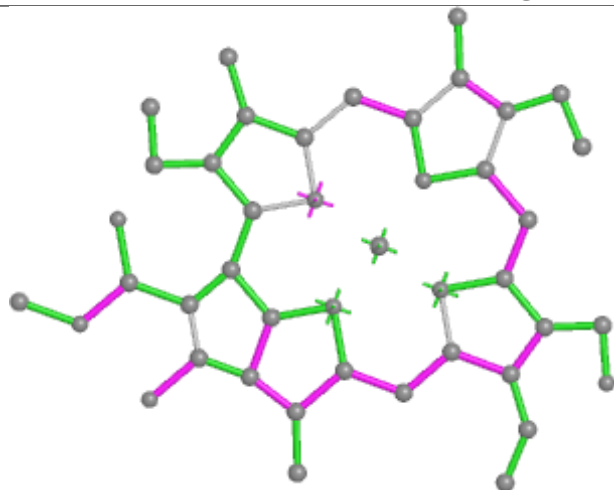


Torsions

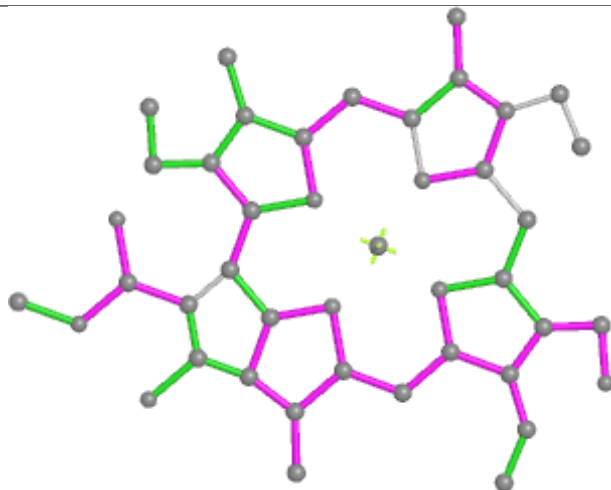


Rings

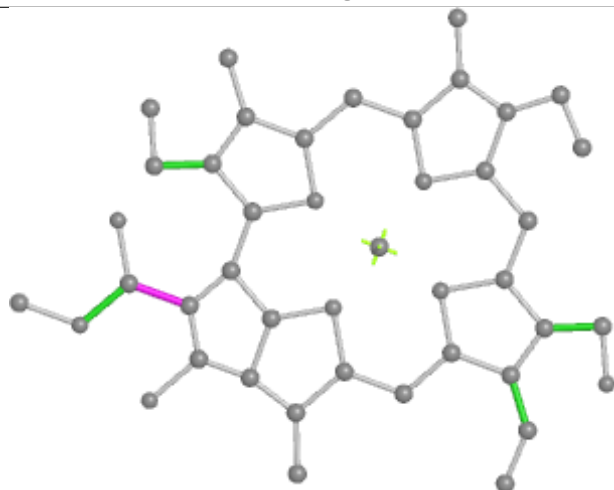
Ligand CHL 4 618



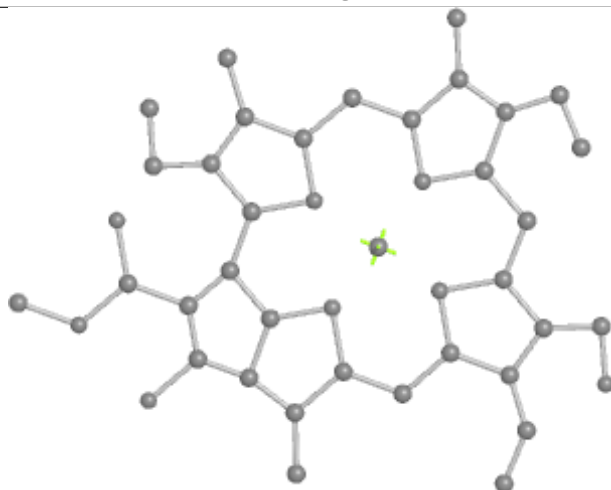
Bond lengths



Bond angles

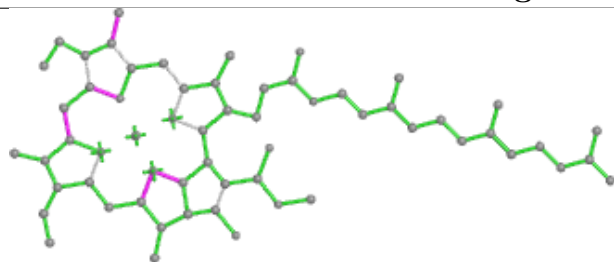


Torsions

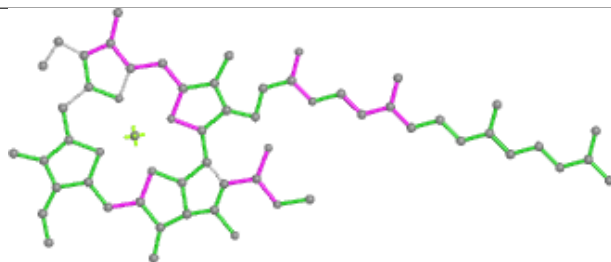


Rings

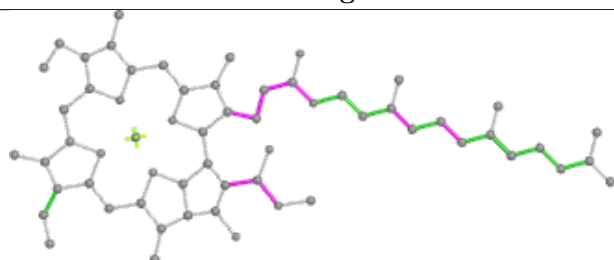
Ligand CLA B 822



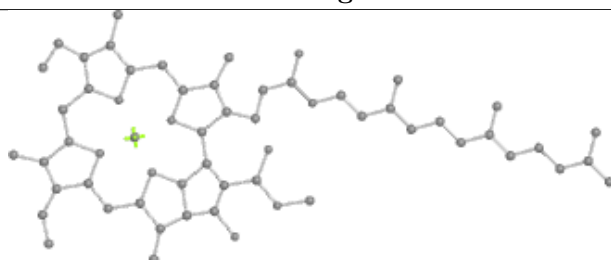
Bond lengths



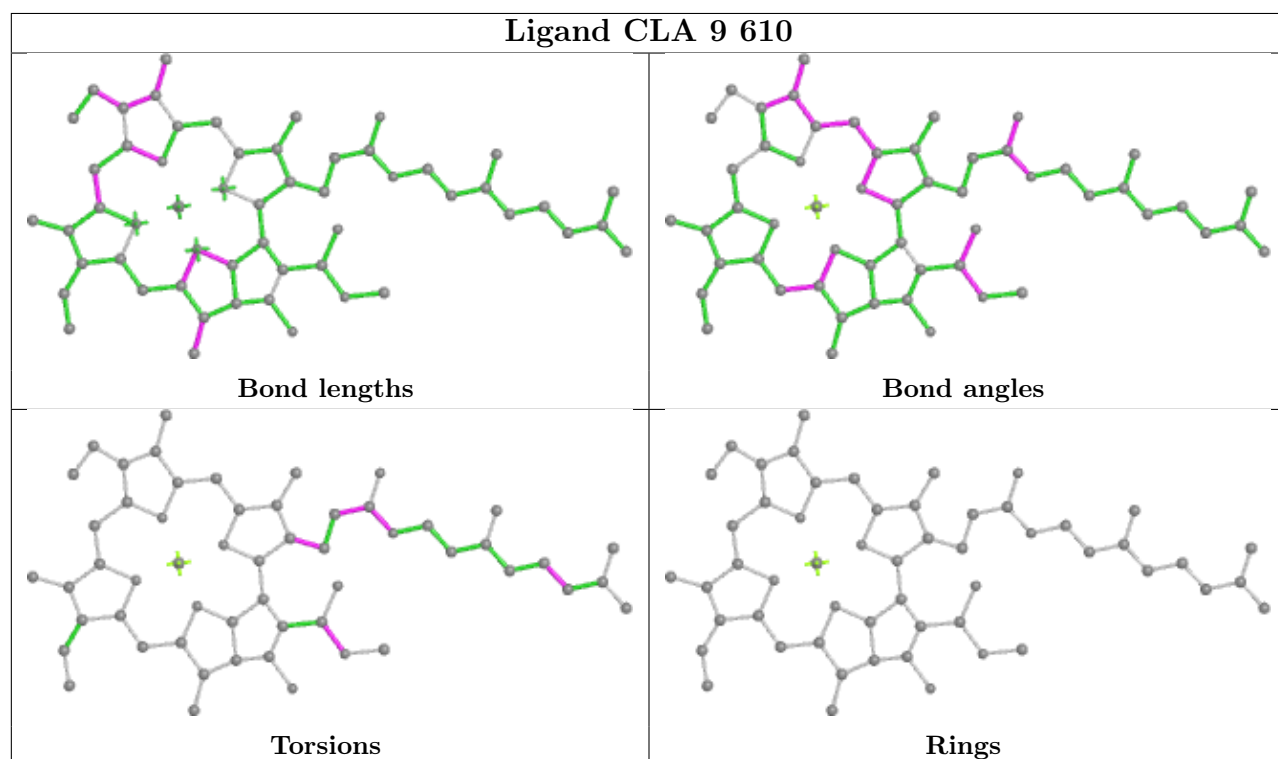
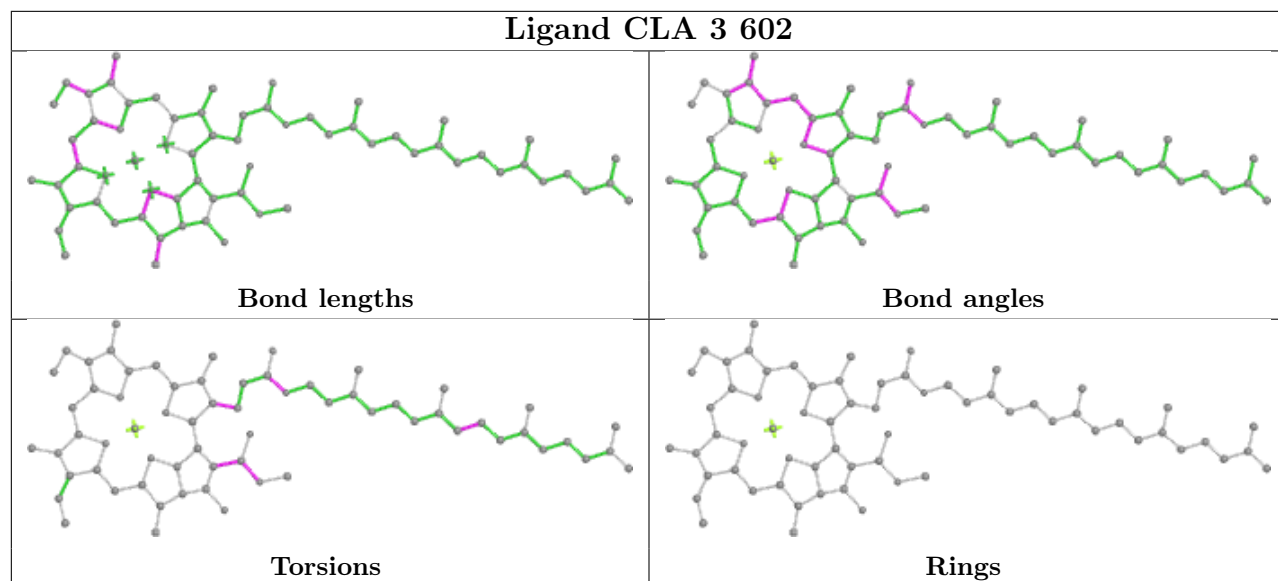
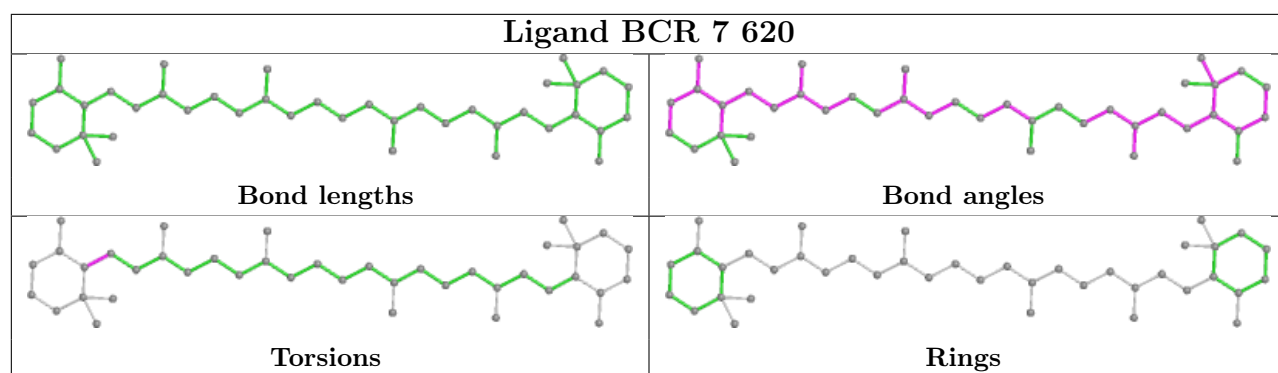
Bond angles

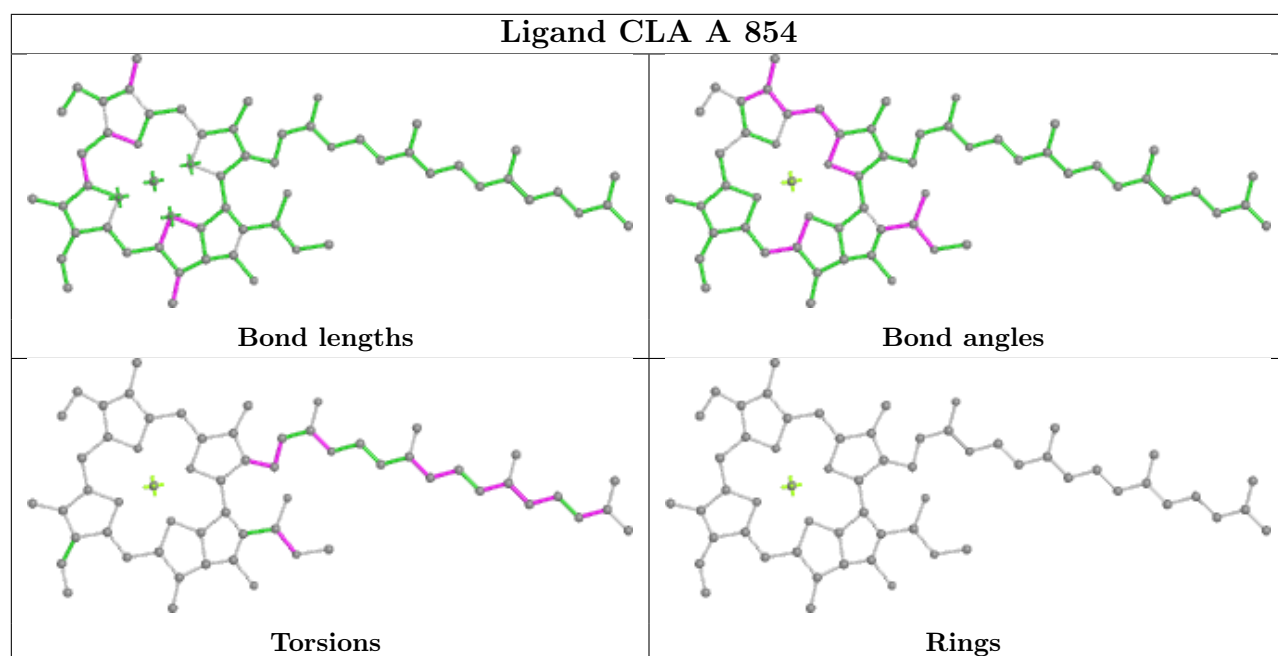


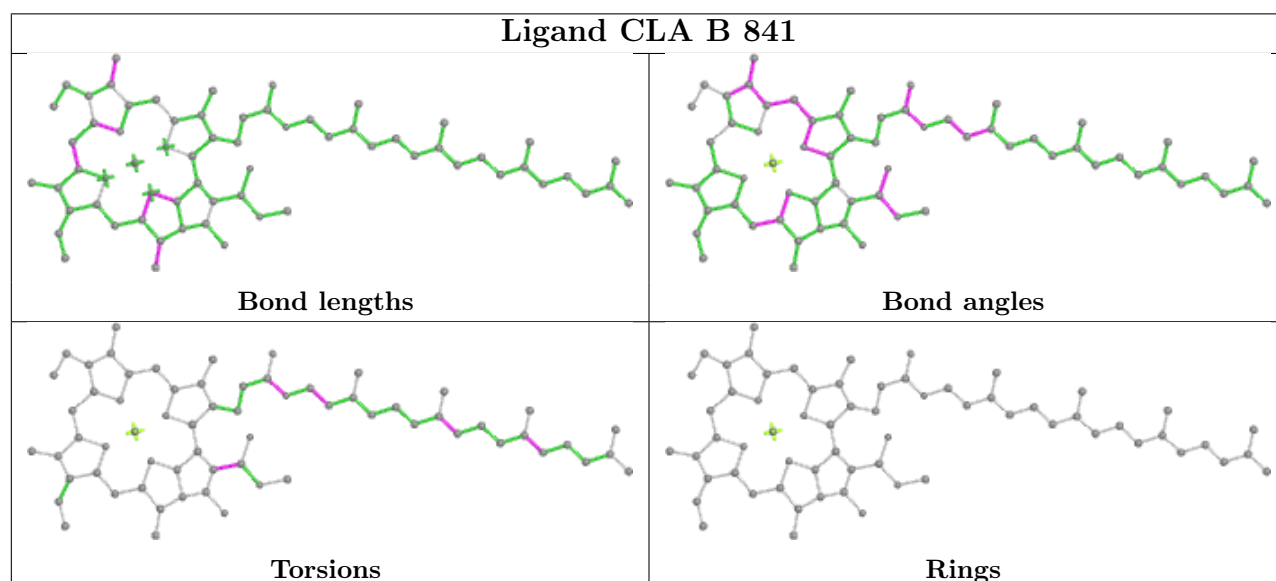
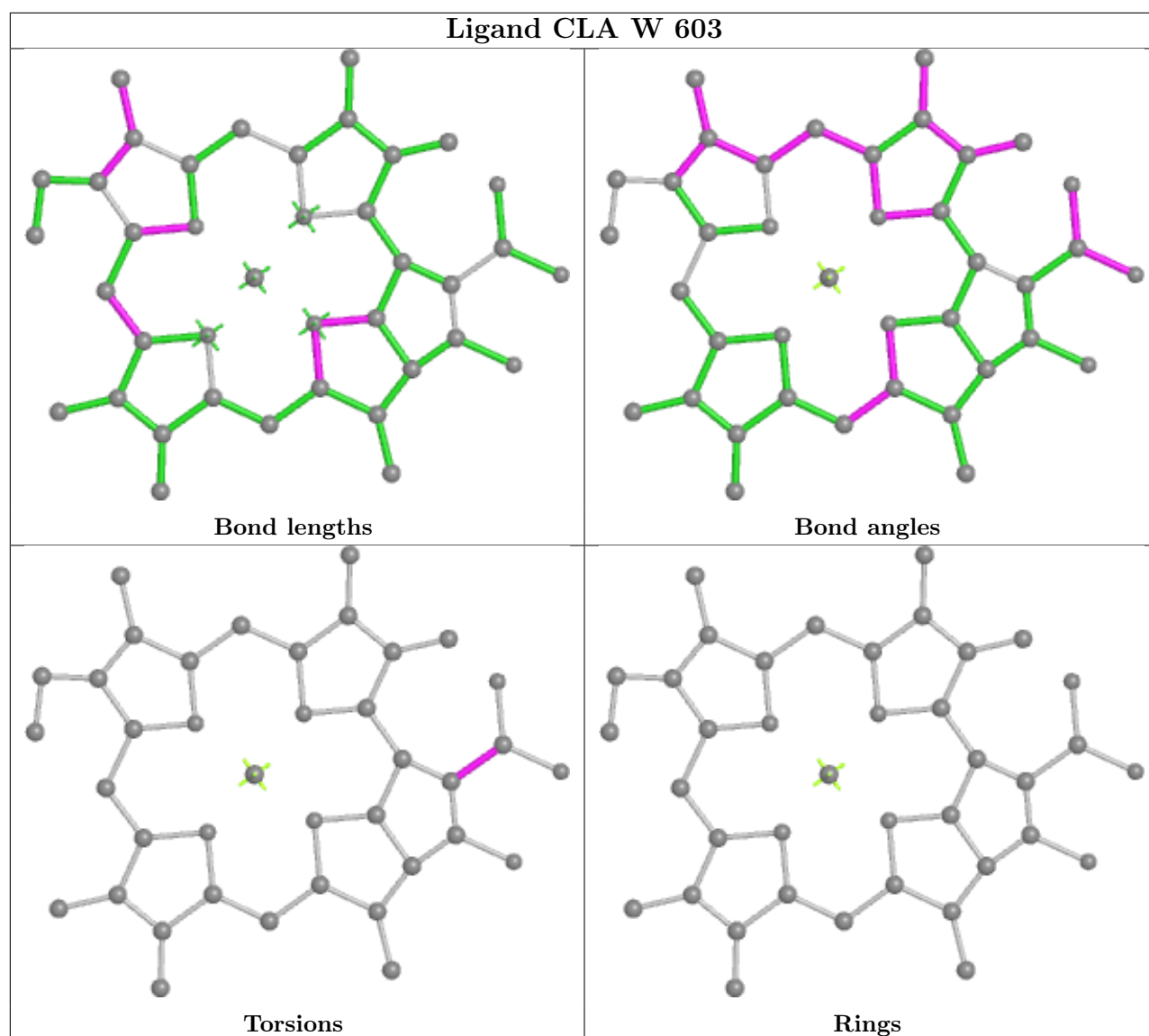
Torsions

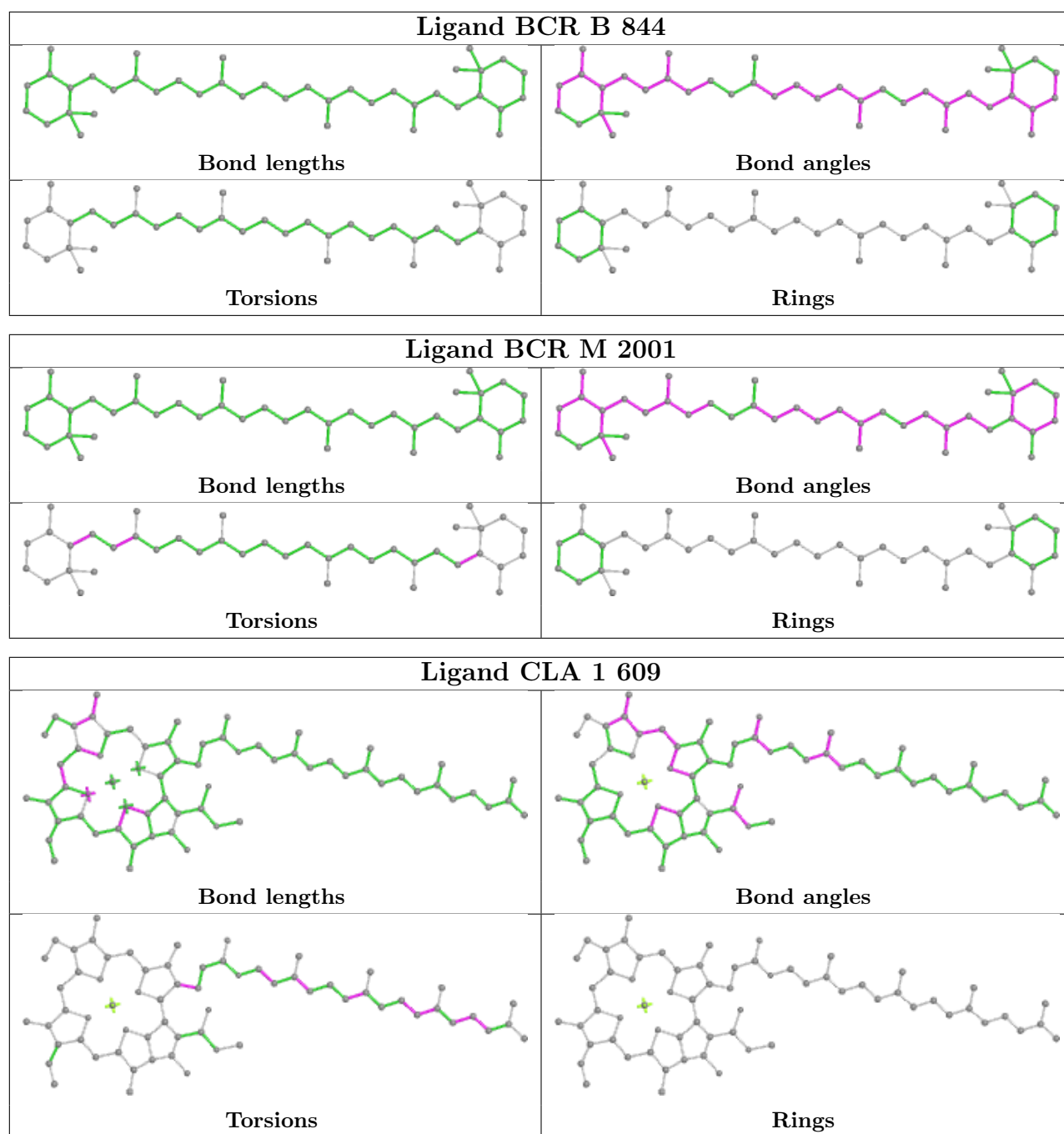


Rings

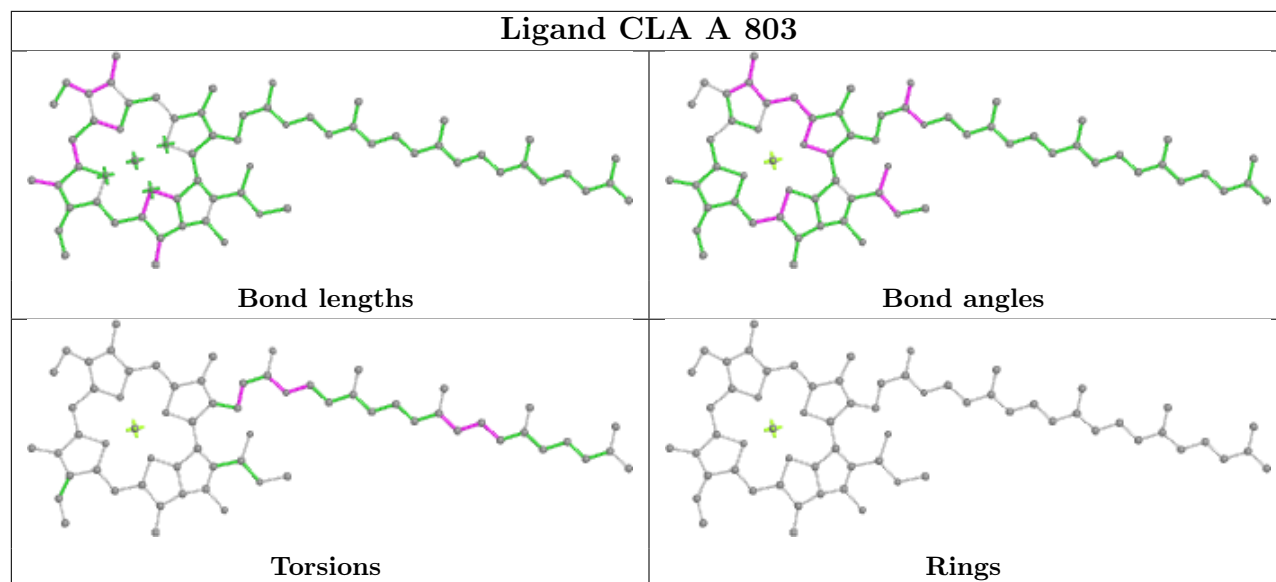




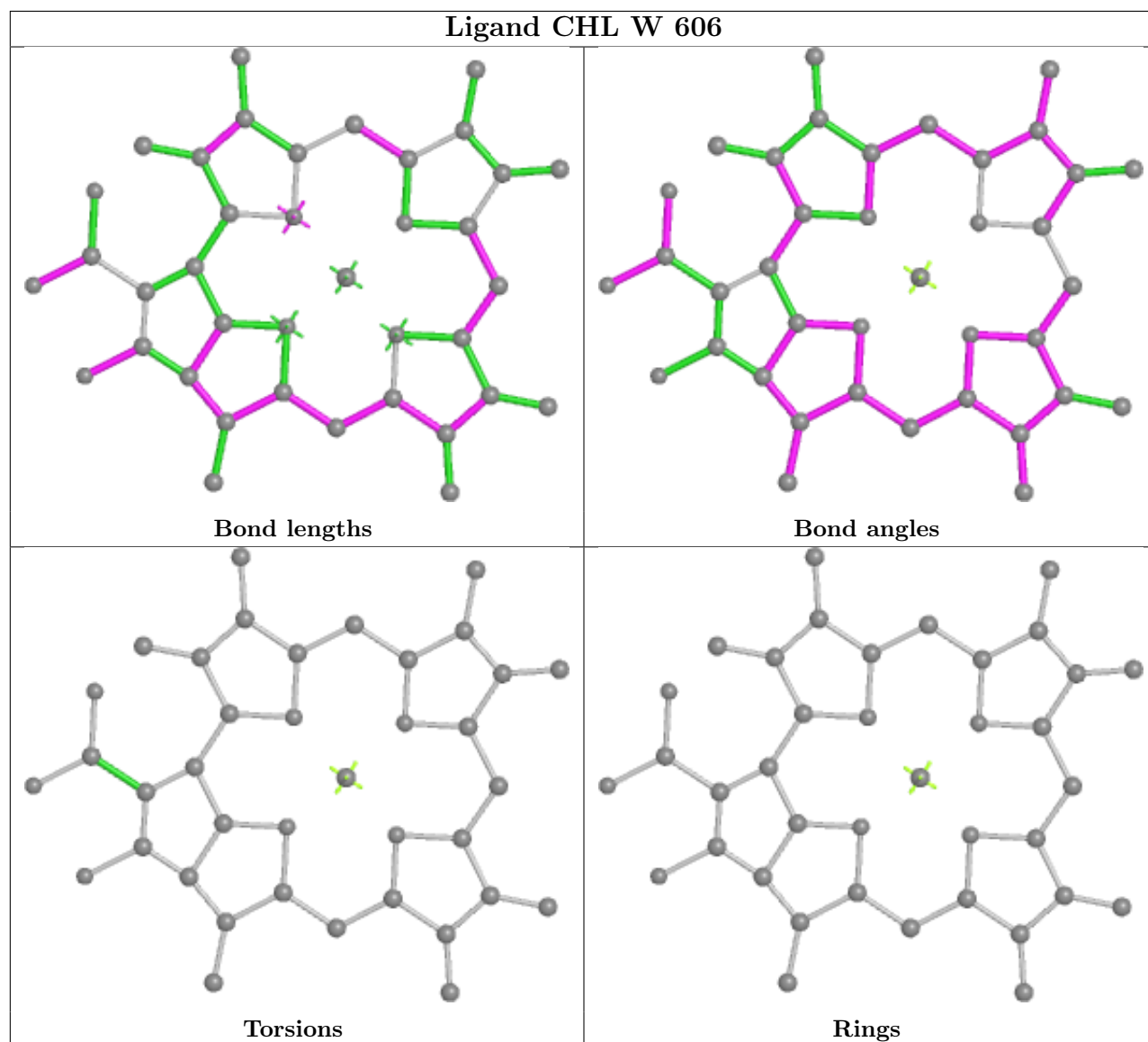




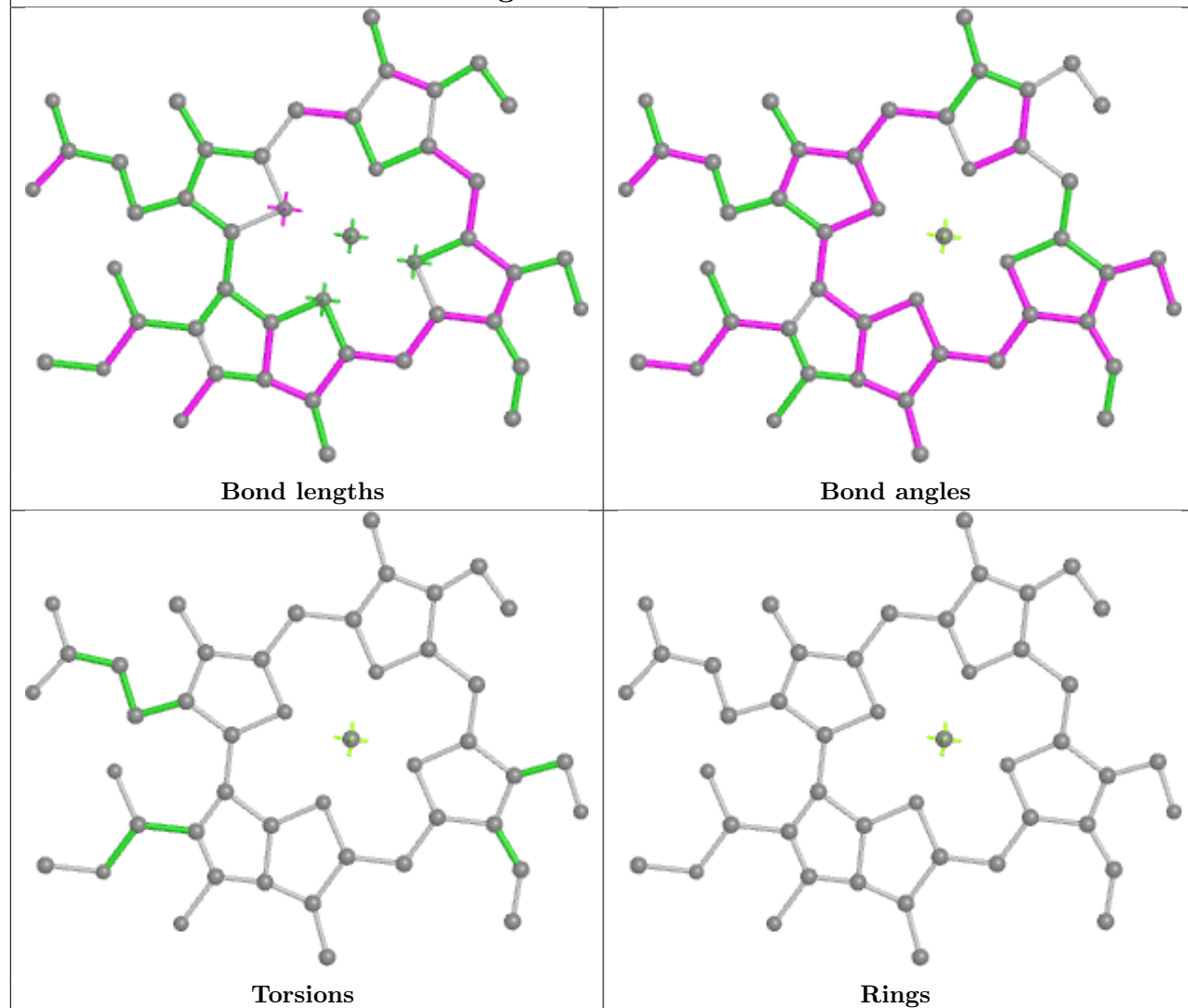
Ligand CLA A 803



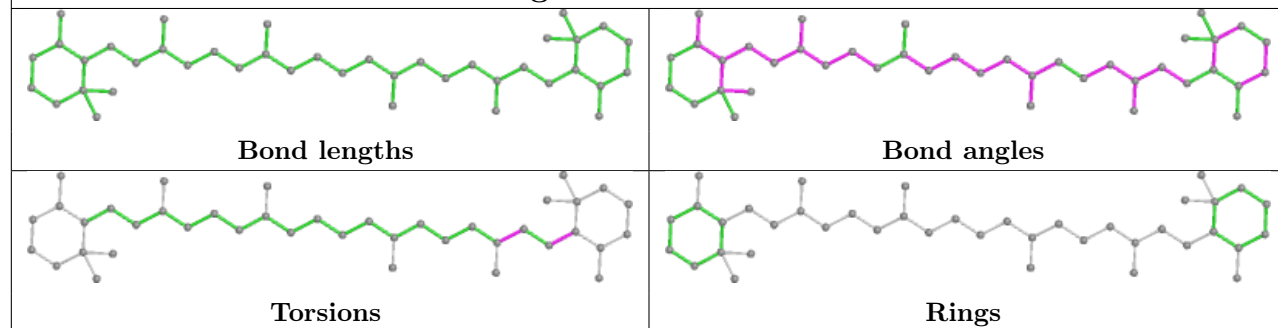
Ligand CHL W 606

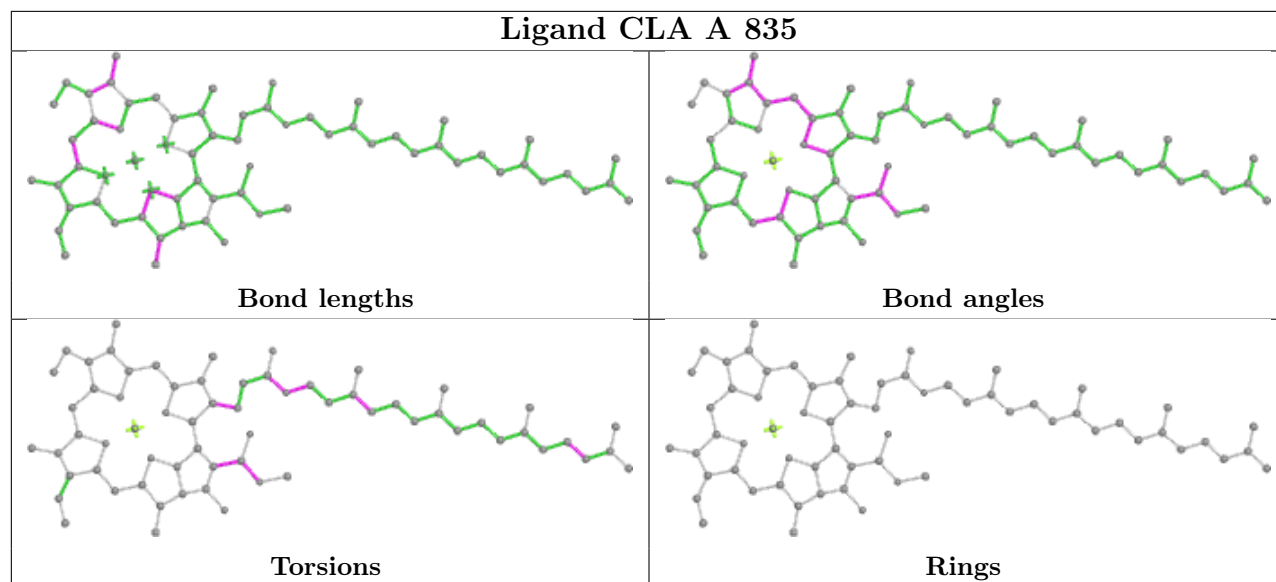
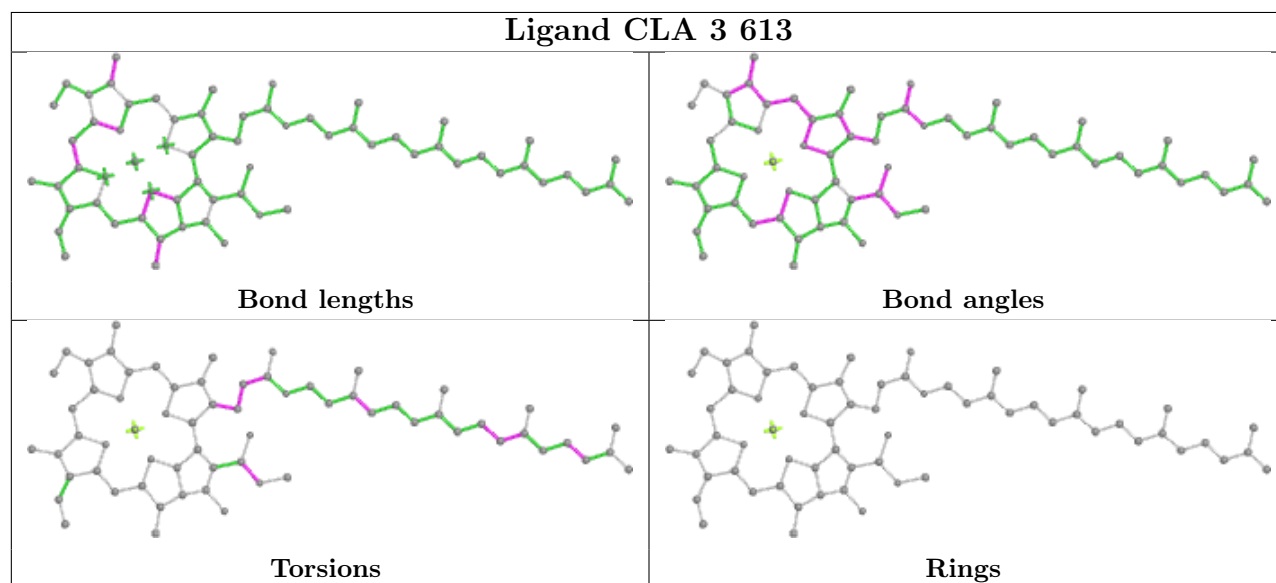


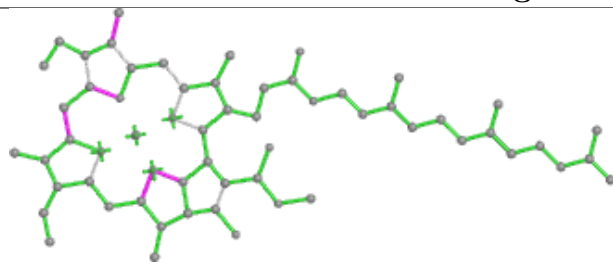
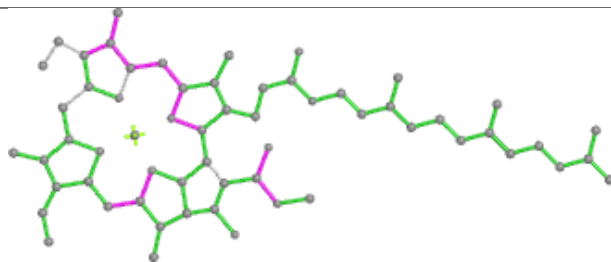
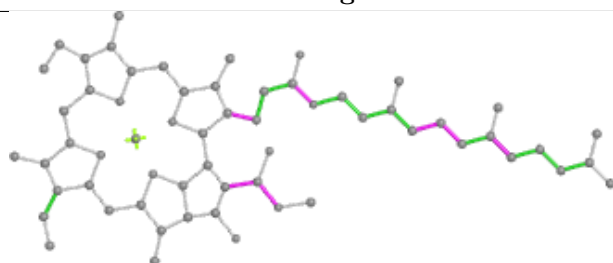
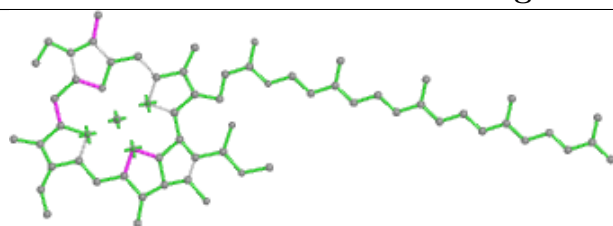
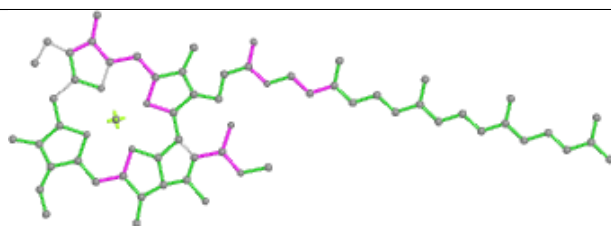
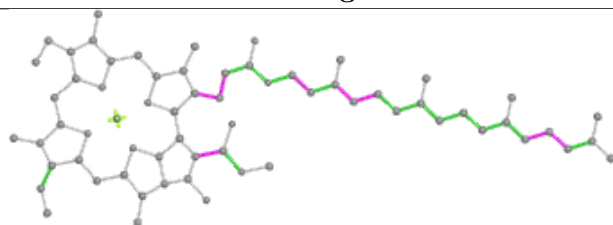
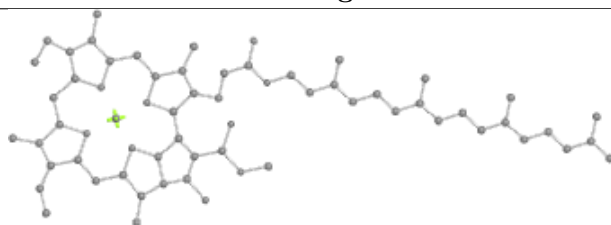
Ligand CHL 2 608

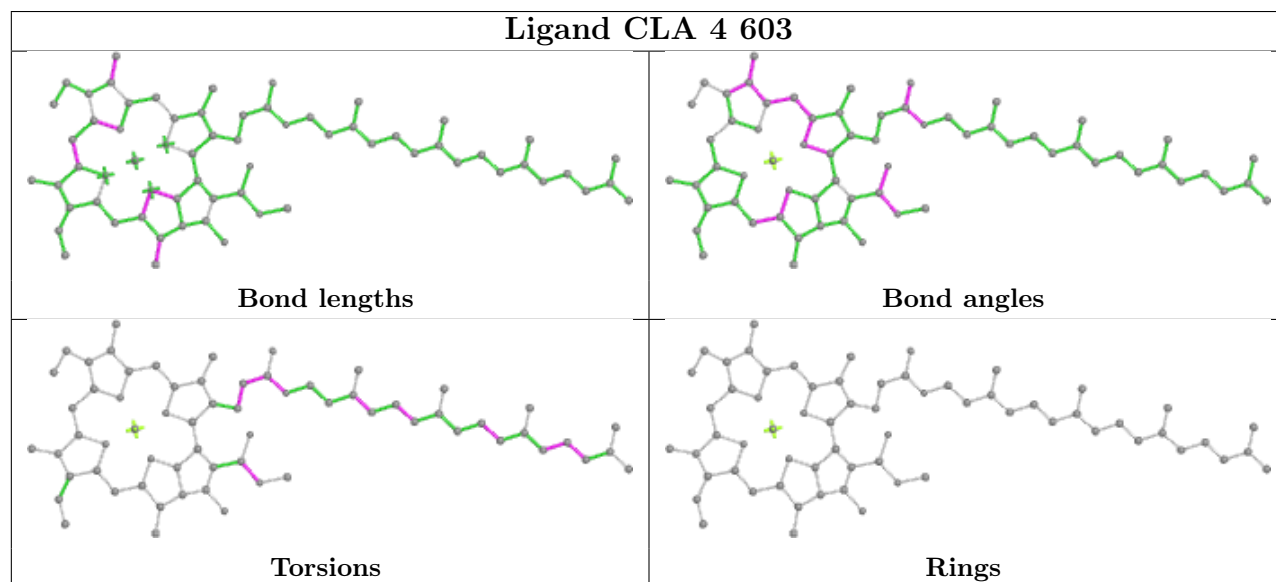
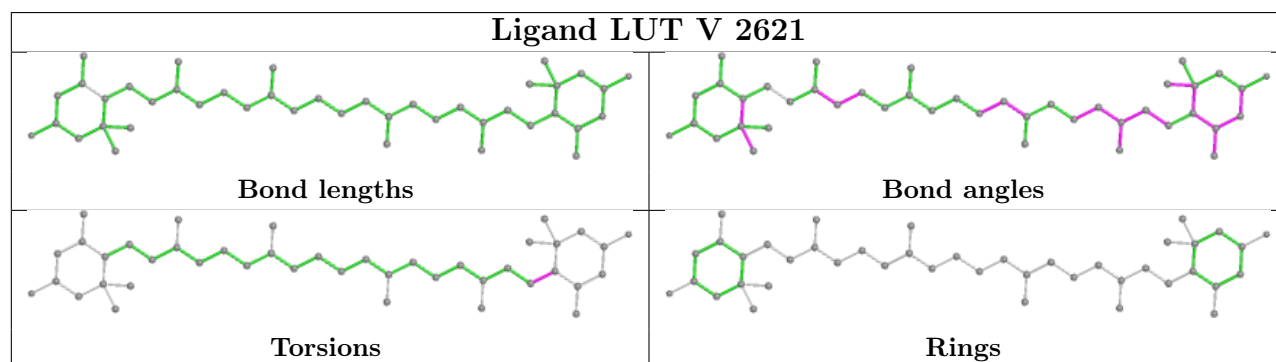
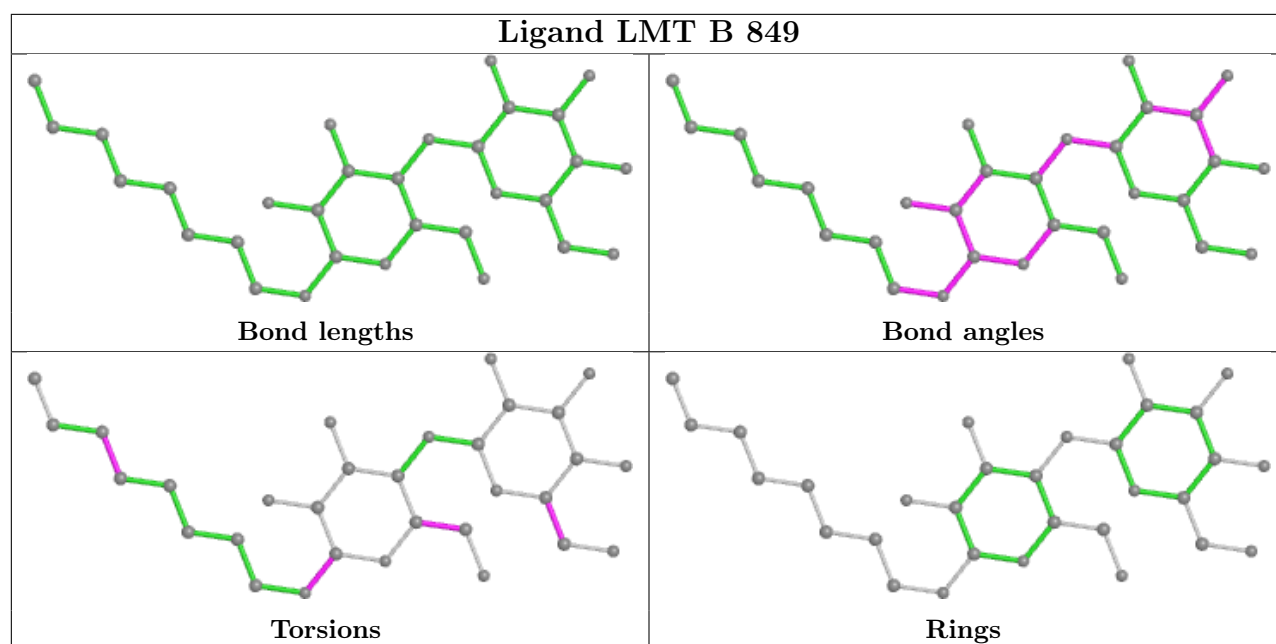


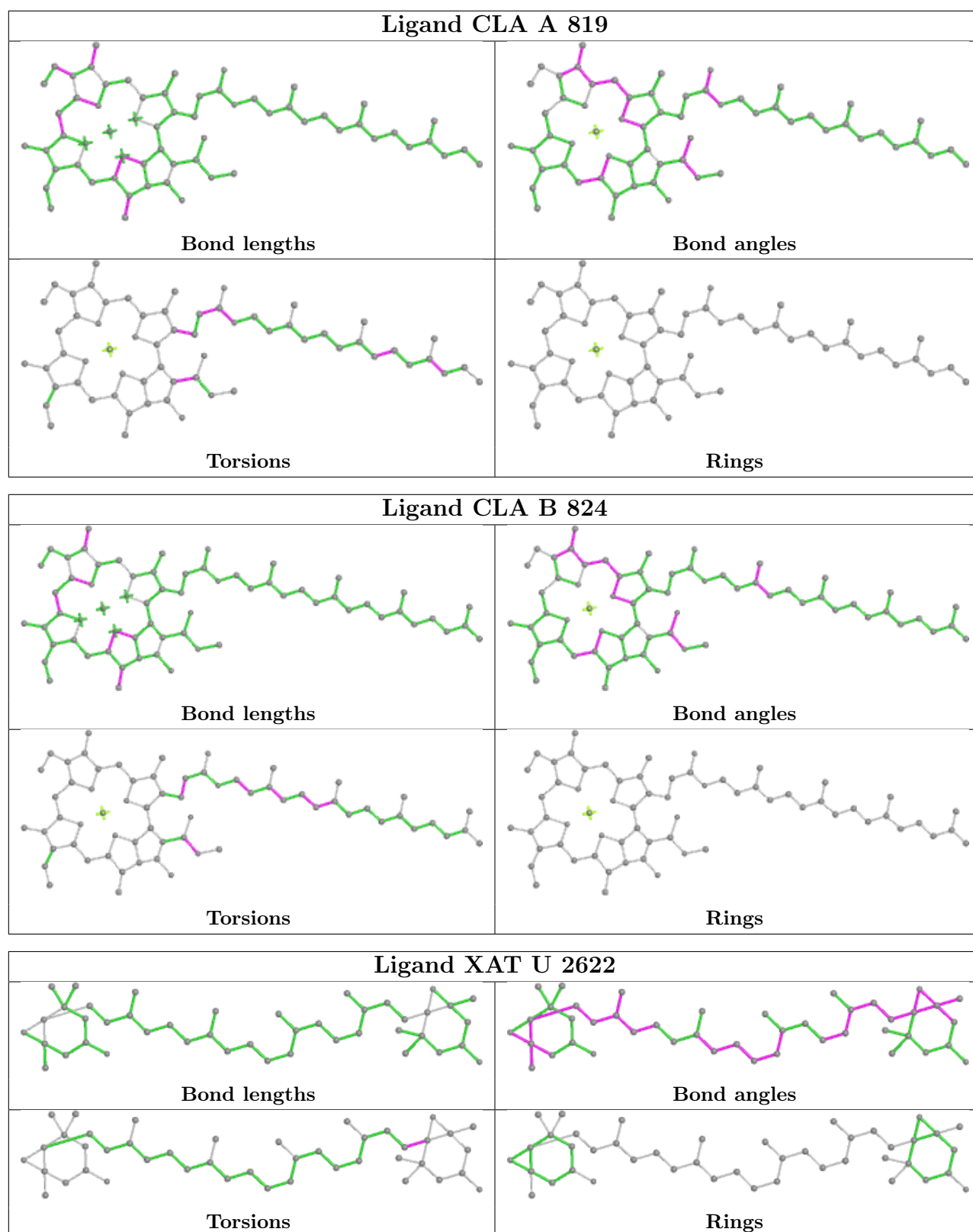
Ligand BCR B 848

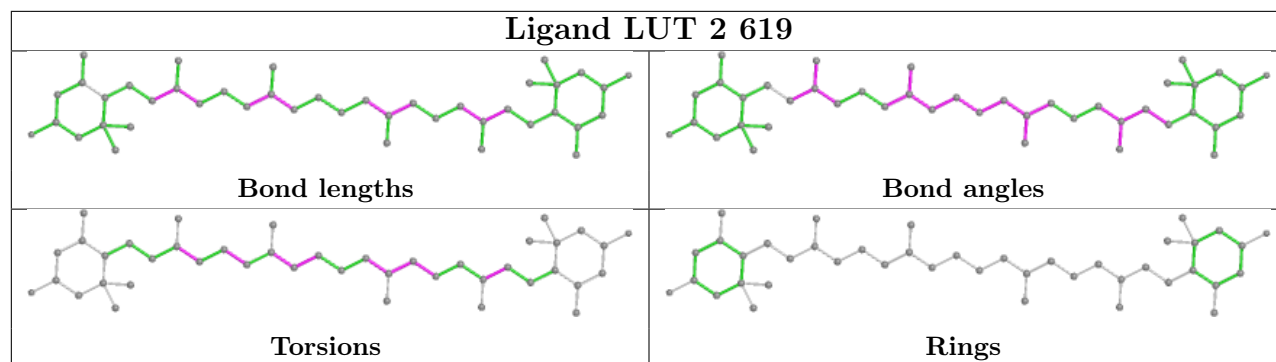
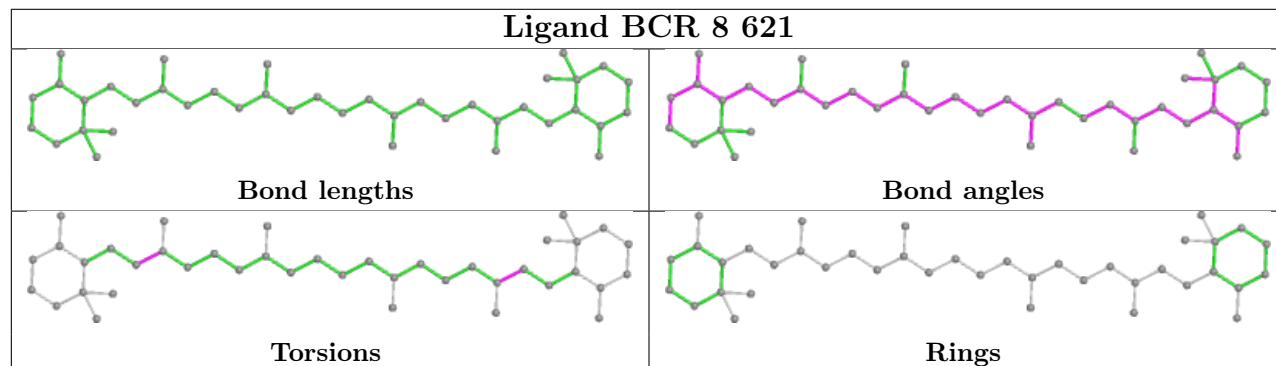
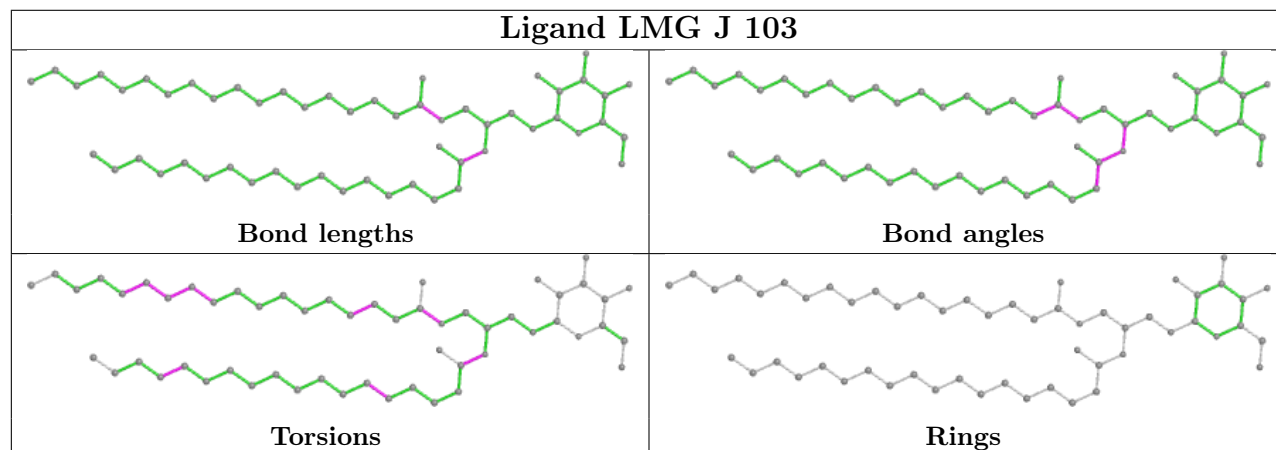
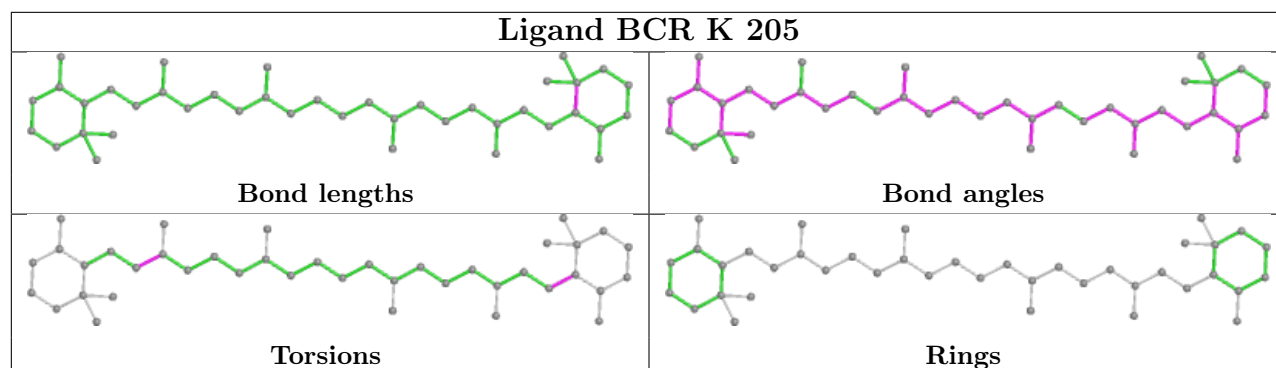


Ligand CLA A 835**Ligand CLA 3 613**

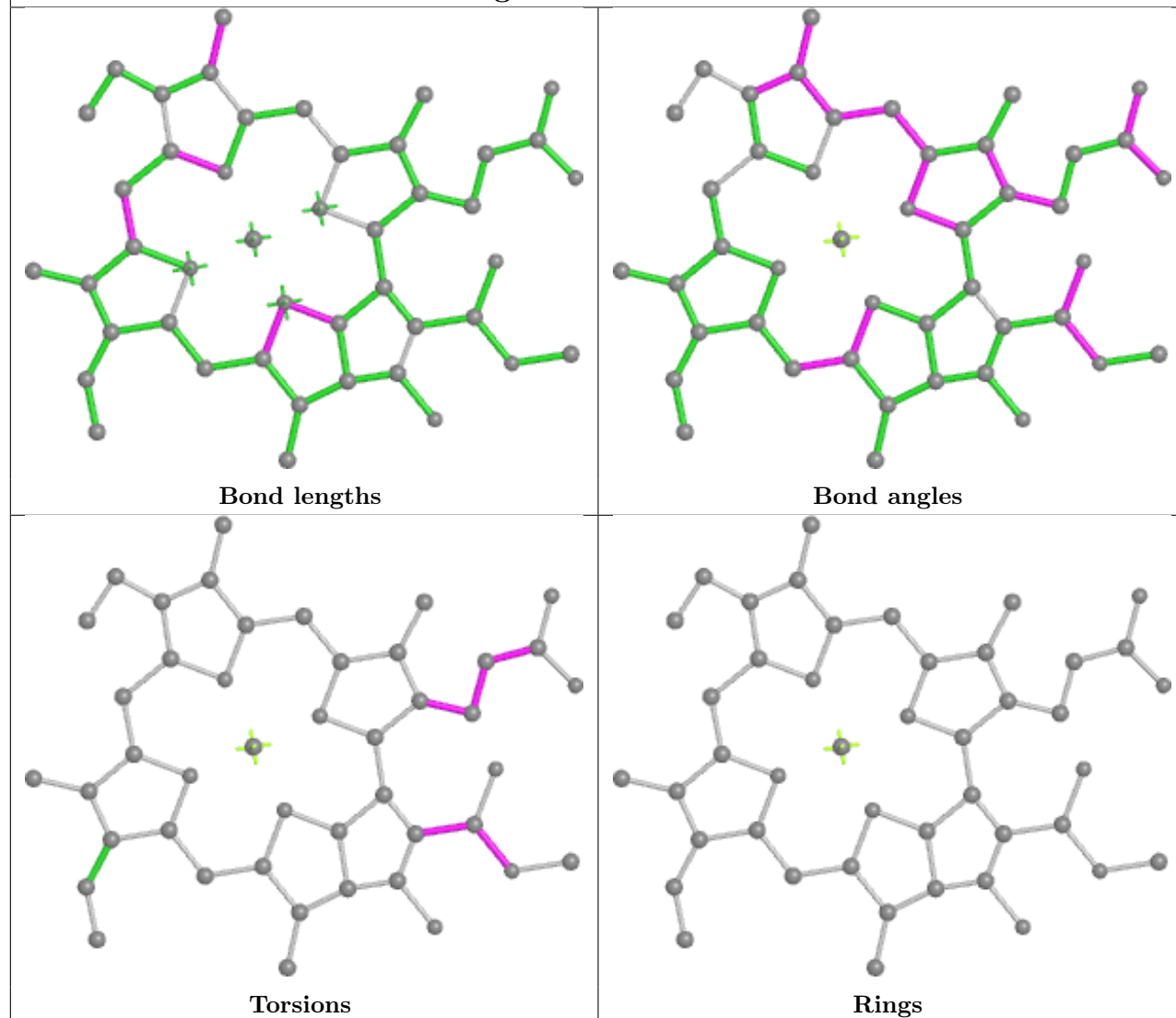
Ligand CLA V 603**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA B 804****Bond lengths****Bond angles****Torsions****Rings**



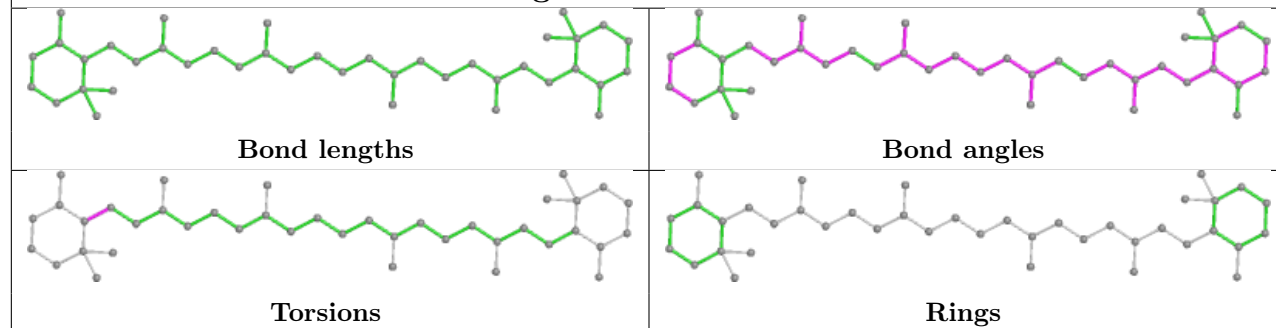


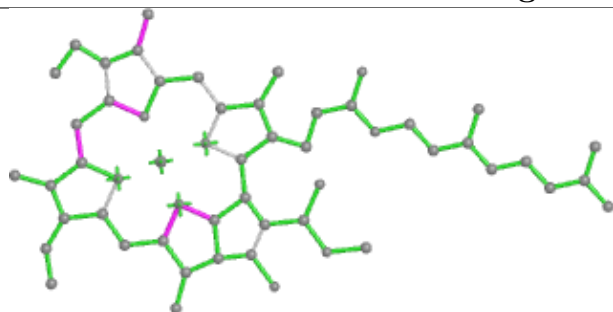
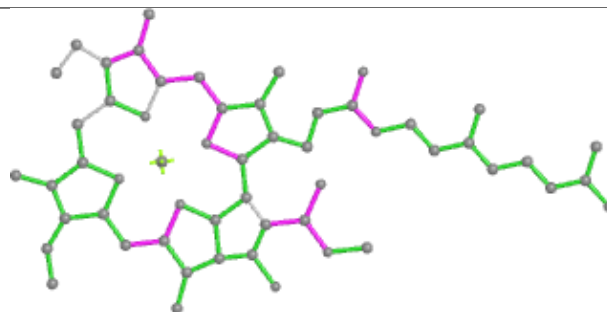
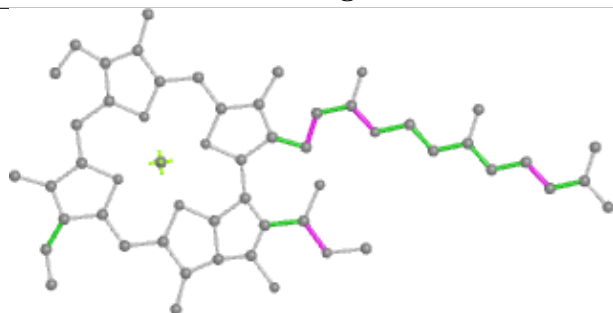
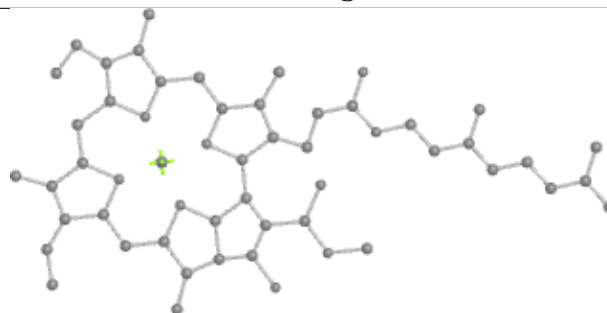
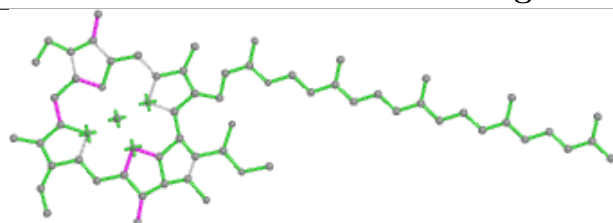
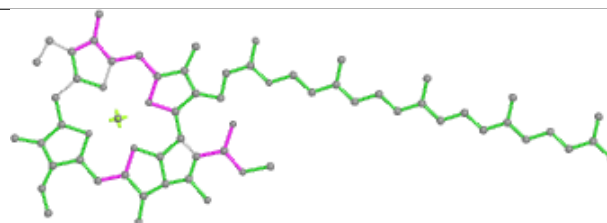
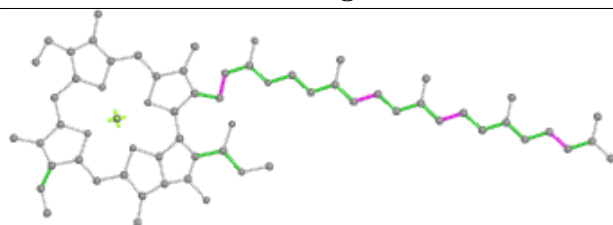
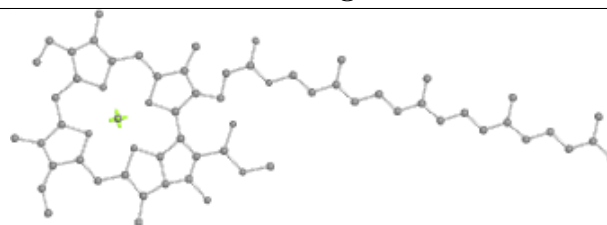
Ligand LUT 2 619**Ligand BCR 8 621****Ligand LMG J 103****Ligand BCR K 205**

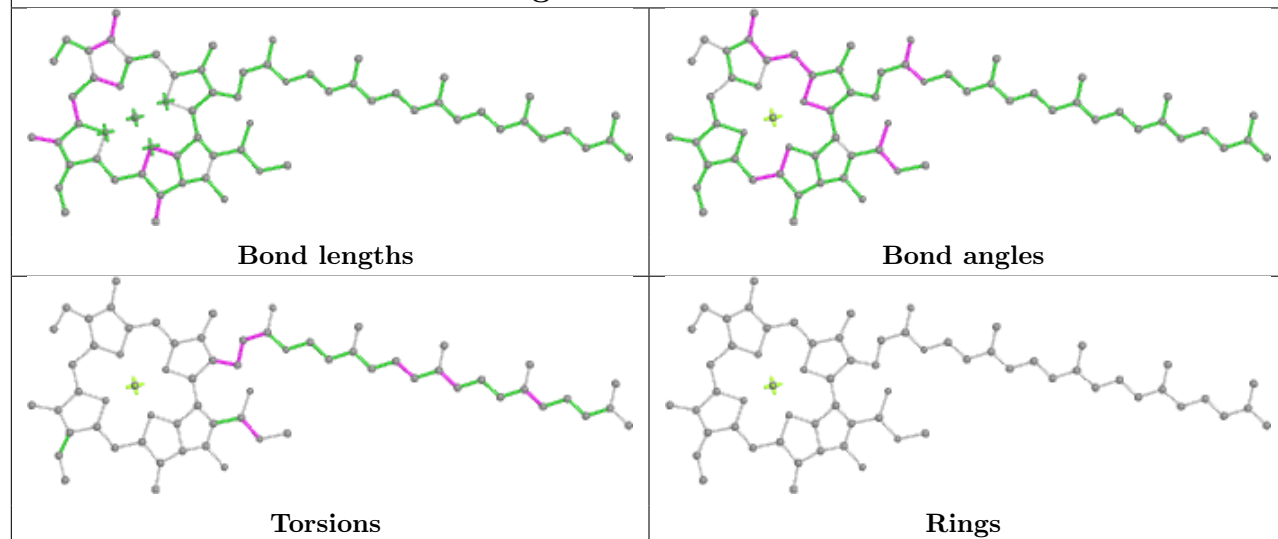
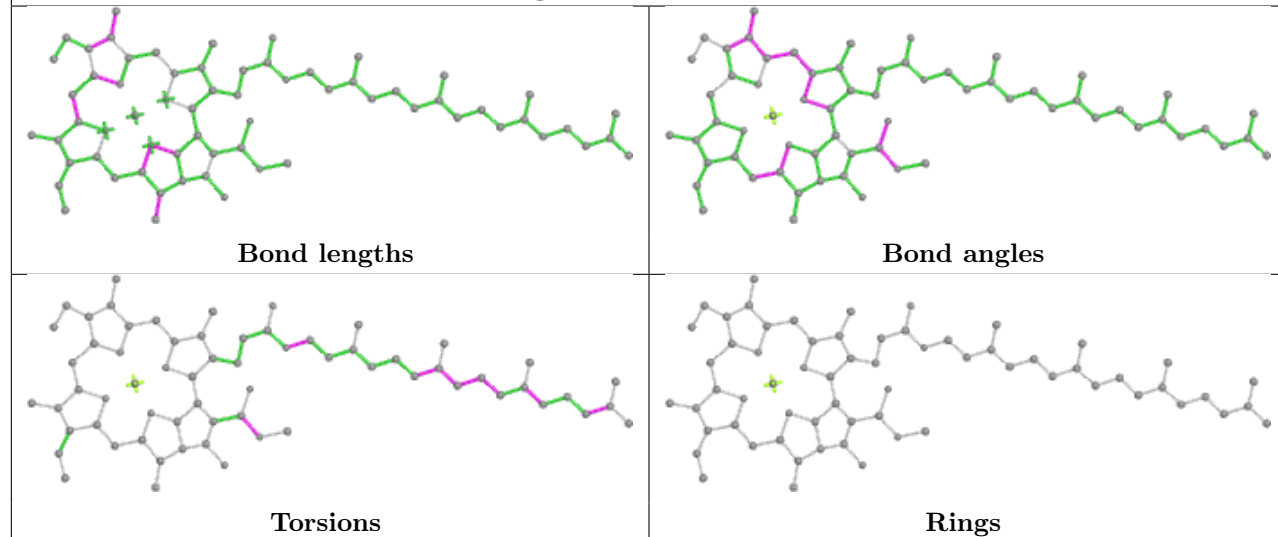
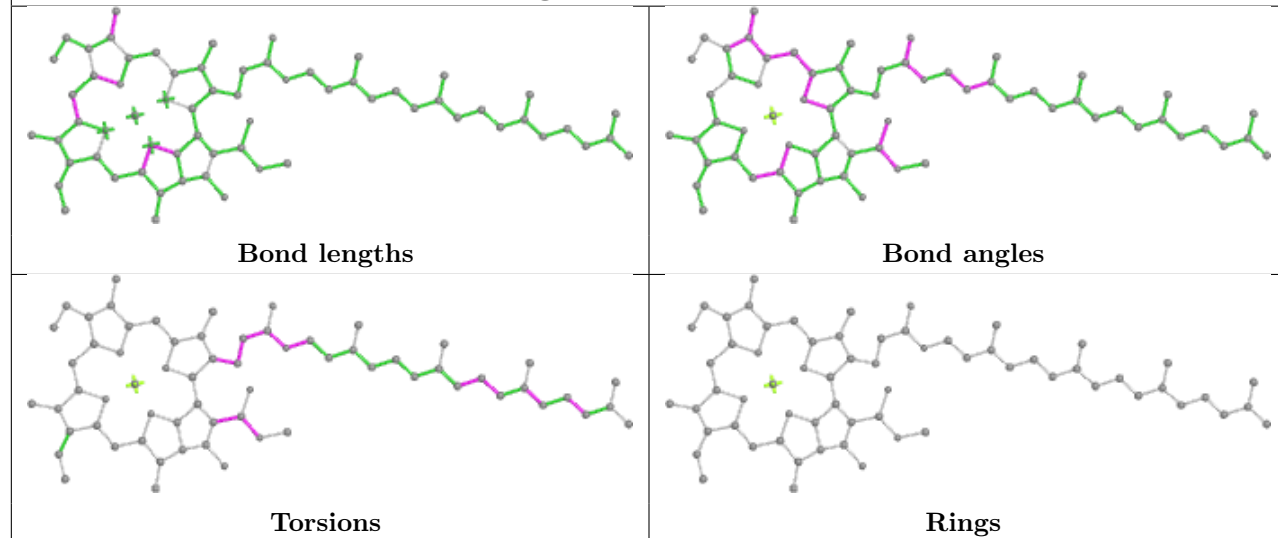
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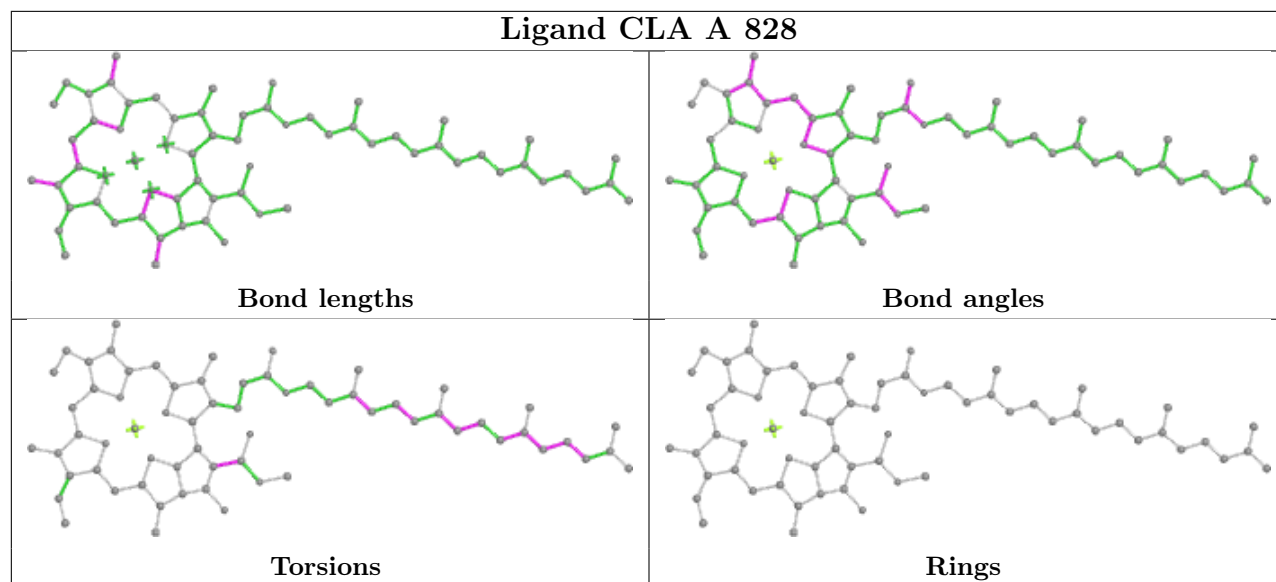
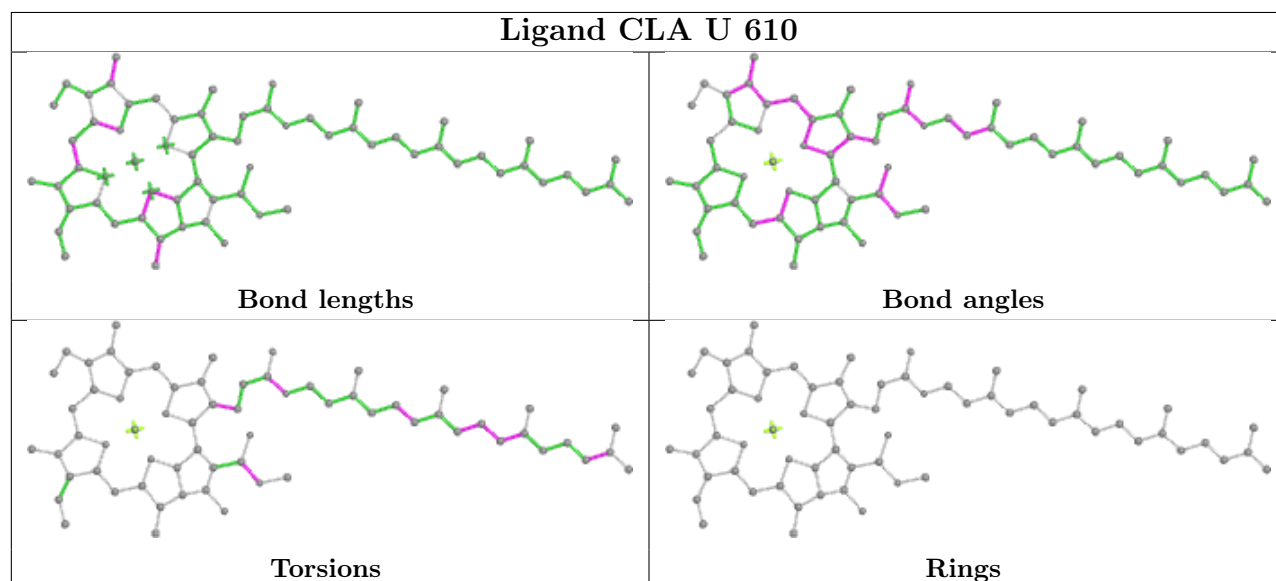


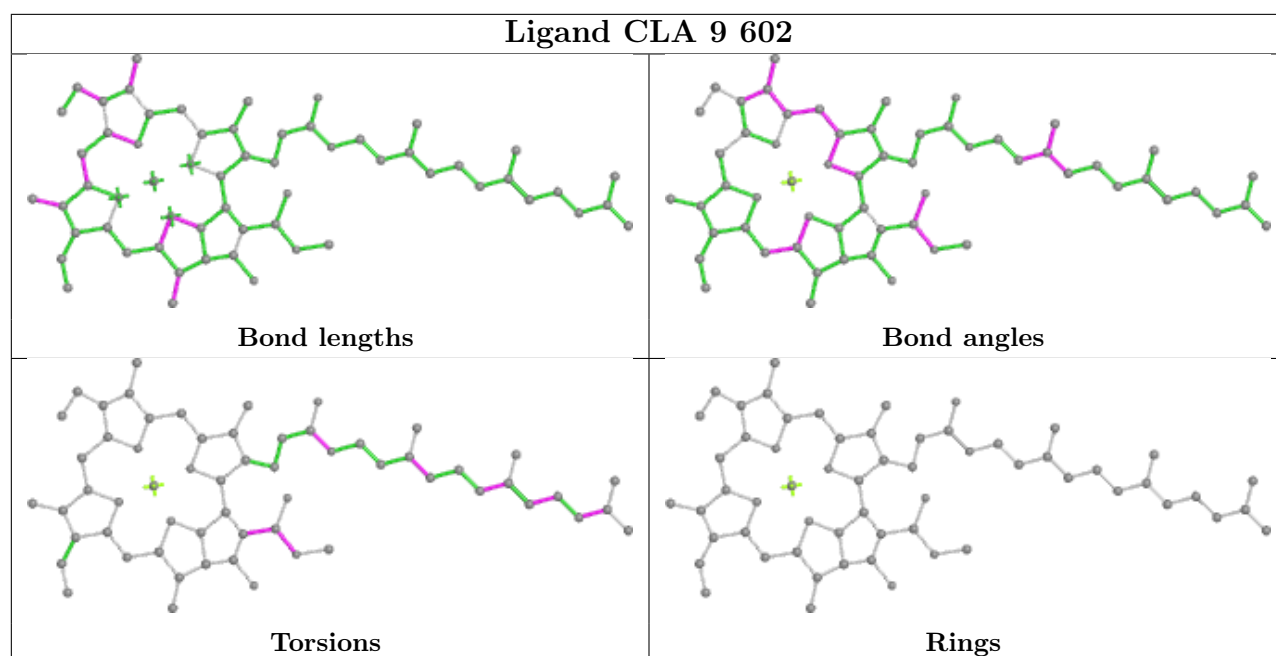
Ligand BCR L 305



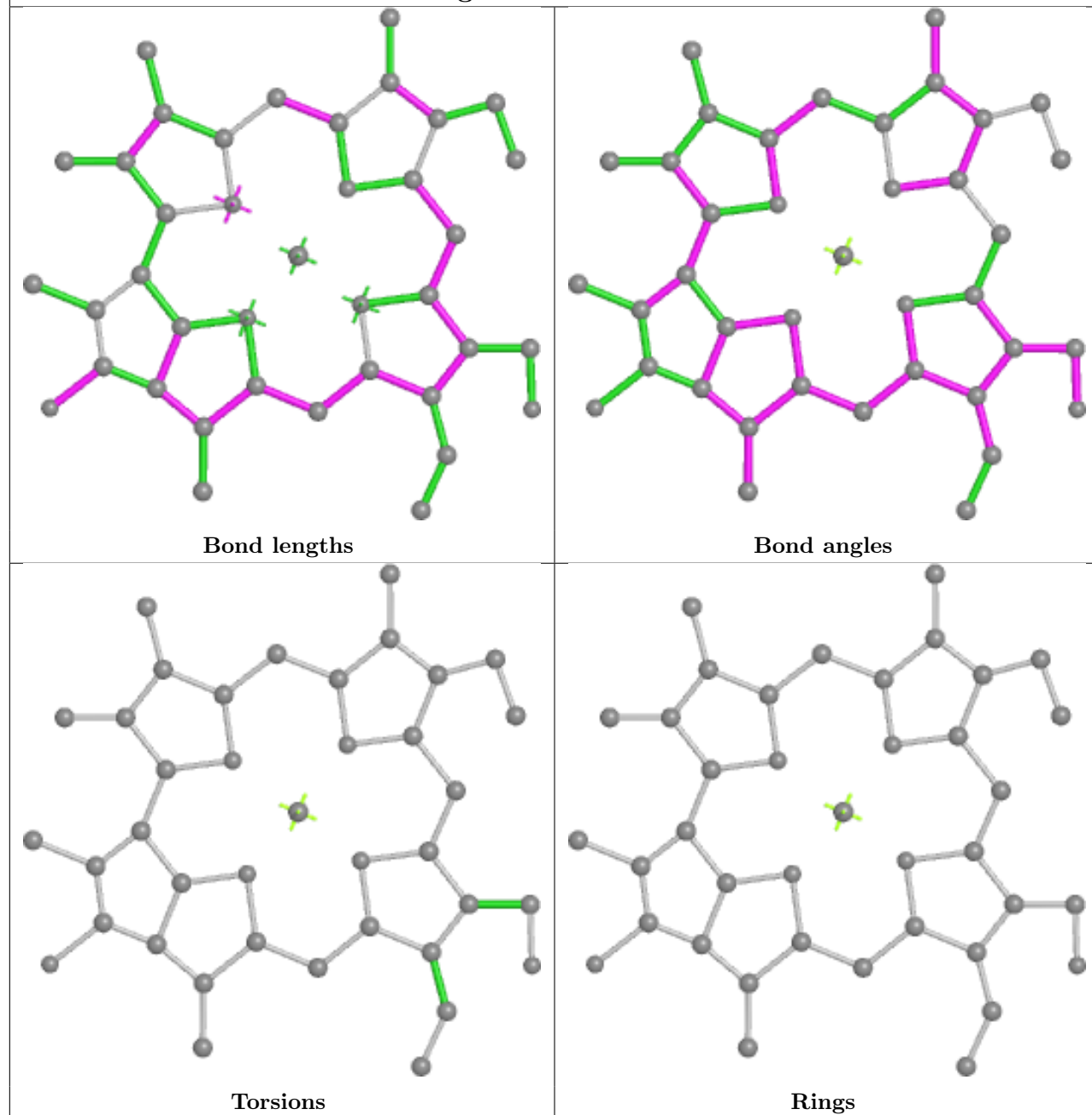
Ligand CLA 4 613**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA B 807****Bond lengths****Bond angles****Torsions****Rings**

Ligand CLA B 808**Ligand CLA U 603****Ligand CLA 4 602**

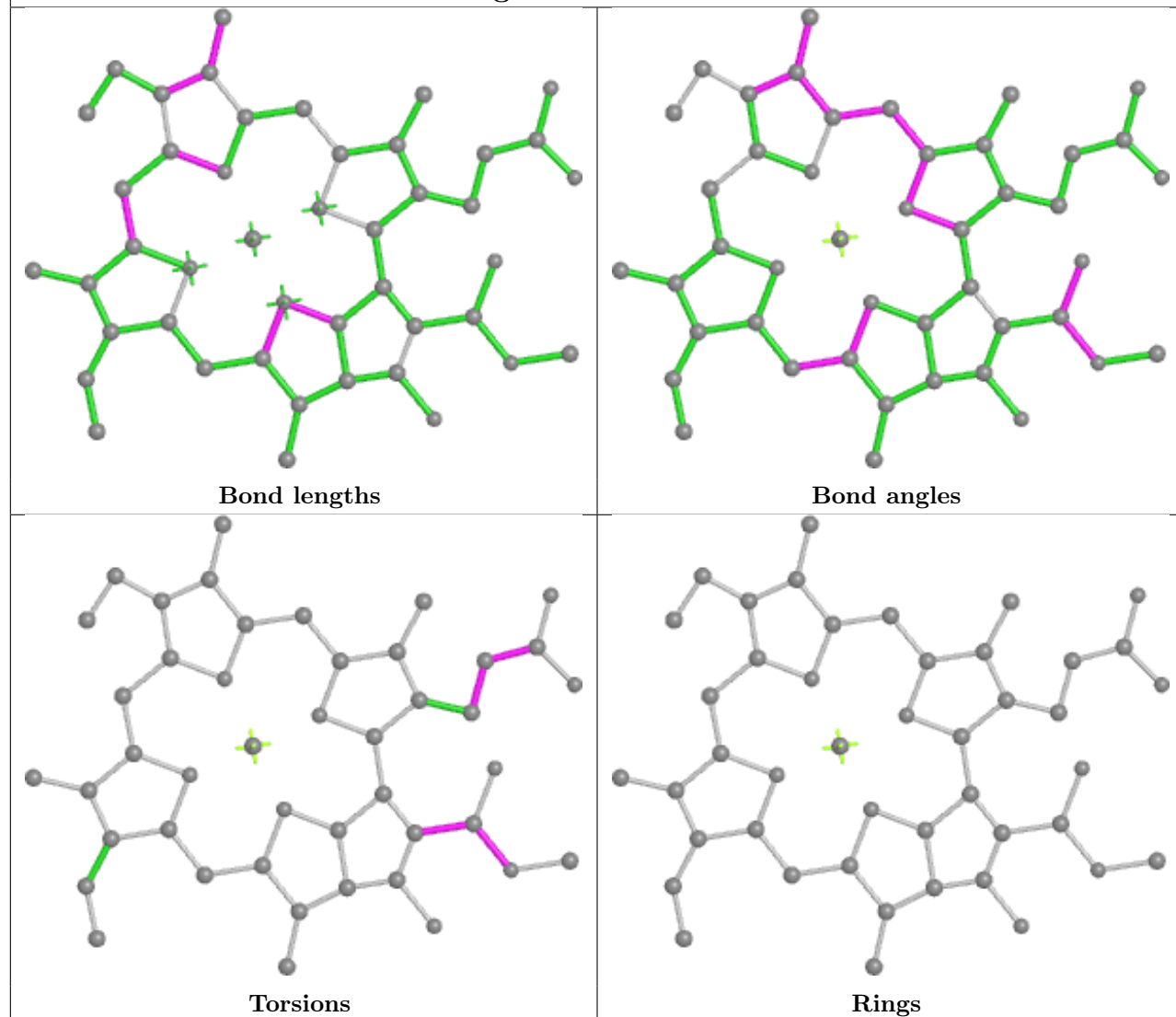
Ligand CLA A 828**Ligand CLA U 610**



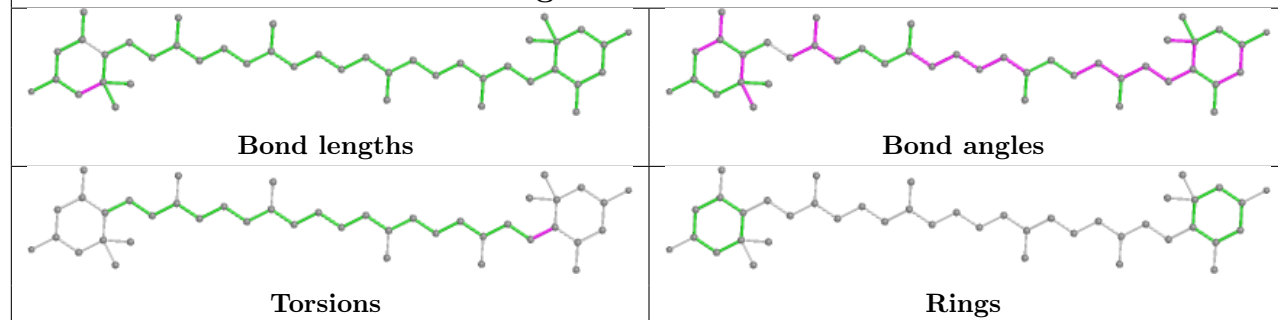
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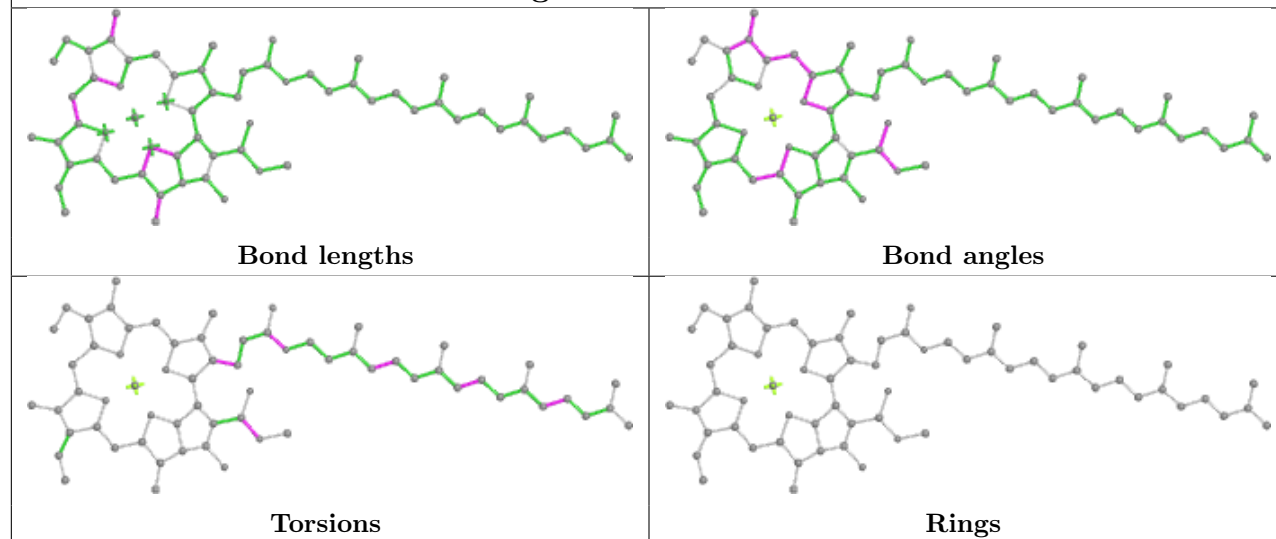
Ligand CLA 1 616



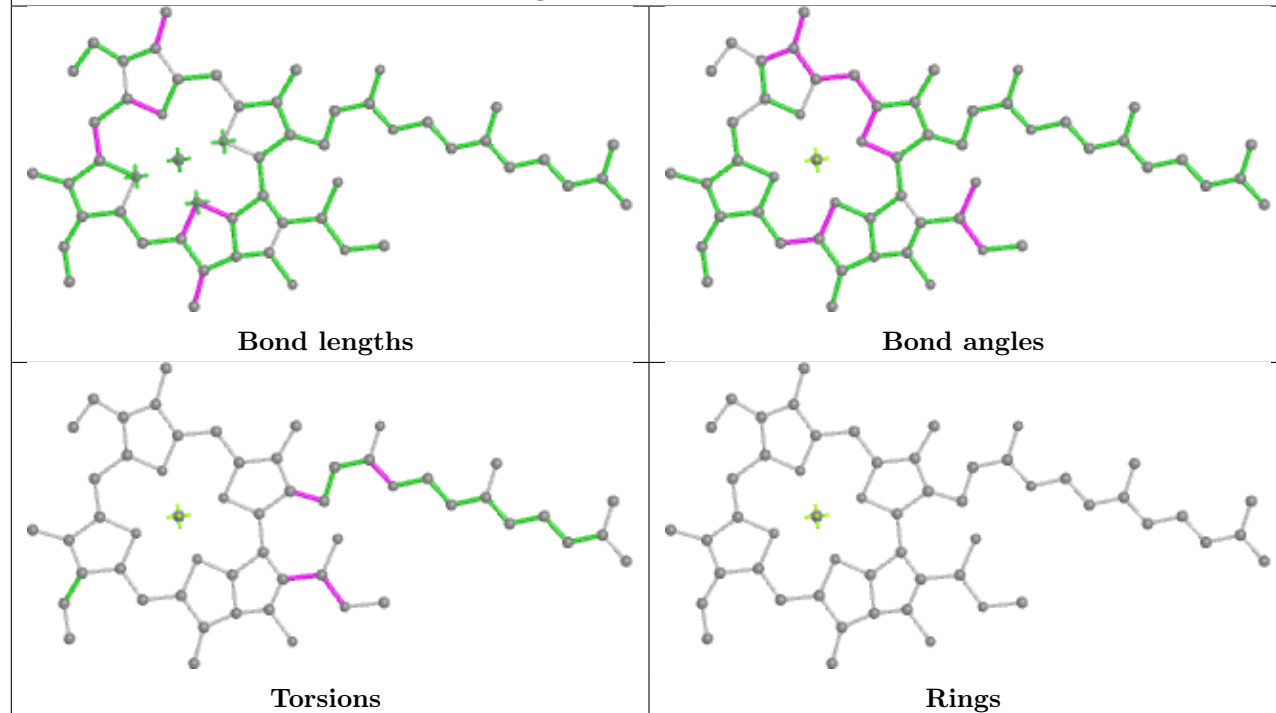
Ligand LUT 8 619



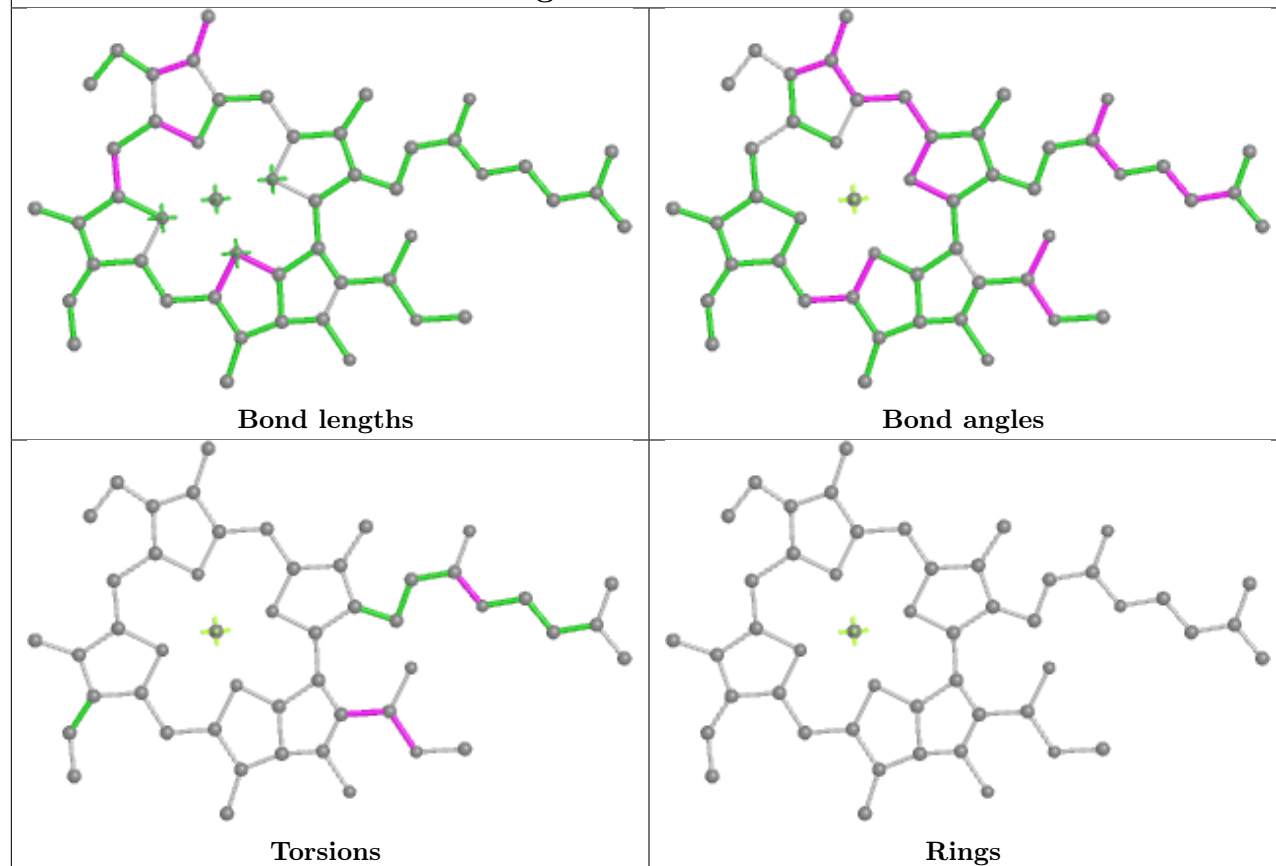
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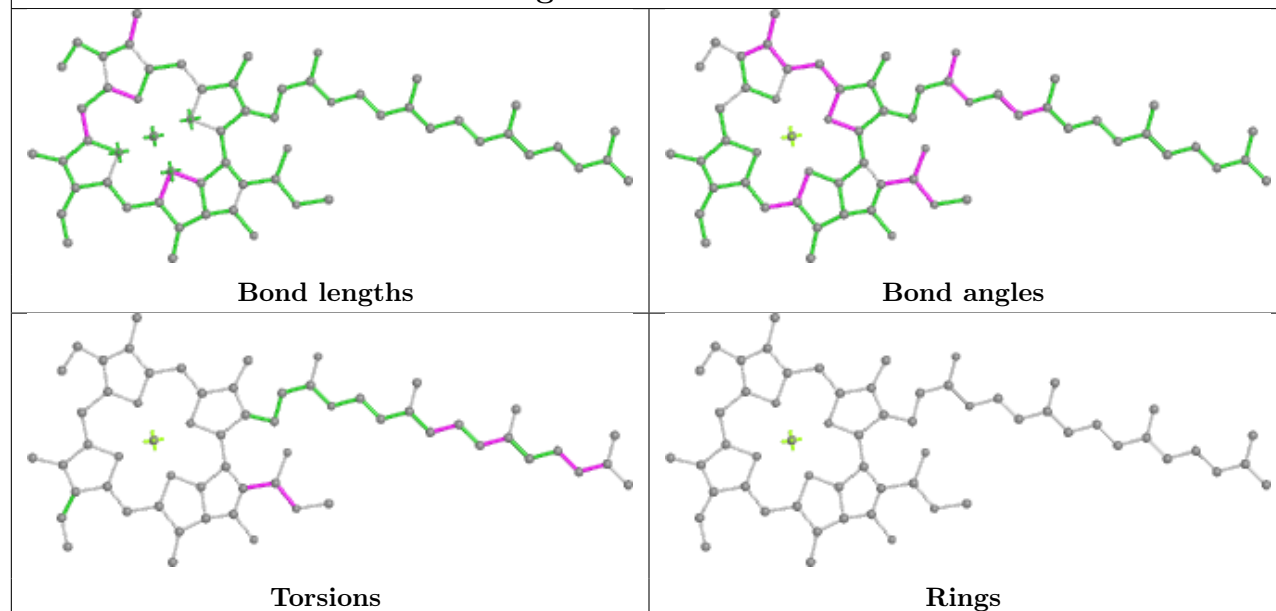
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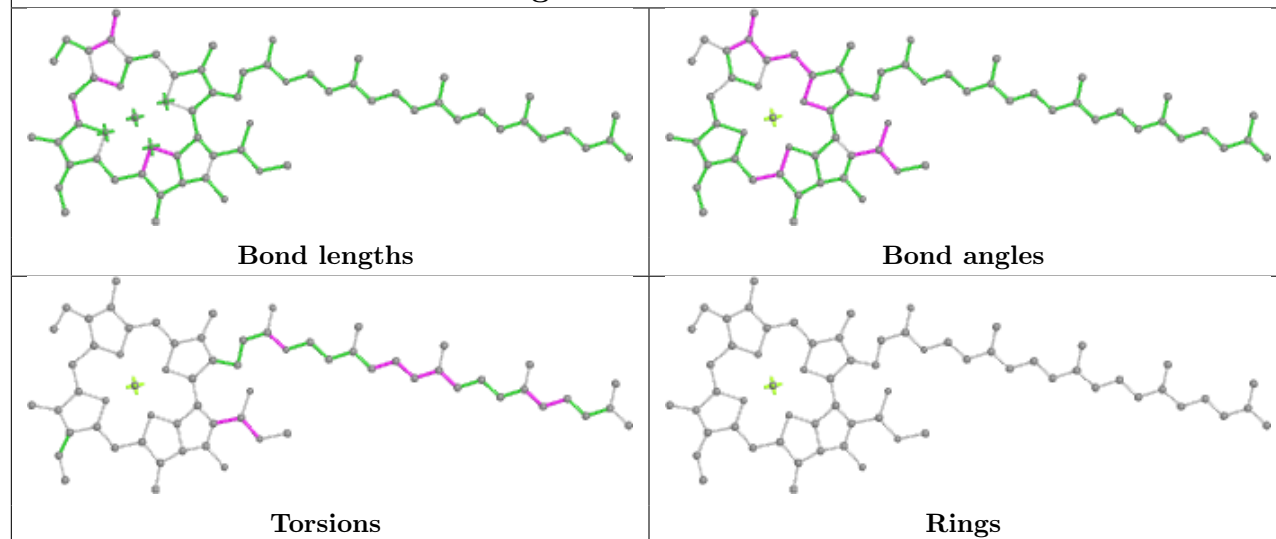
Ligand CLA 8 604



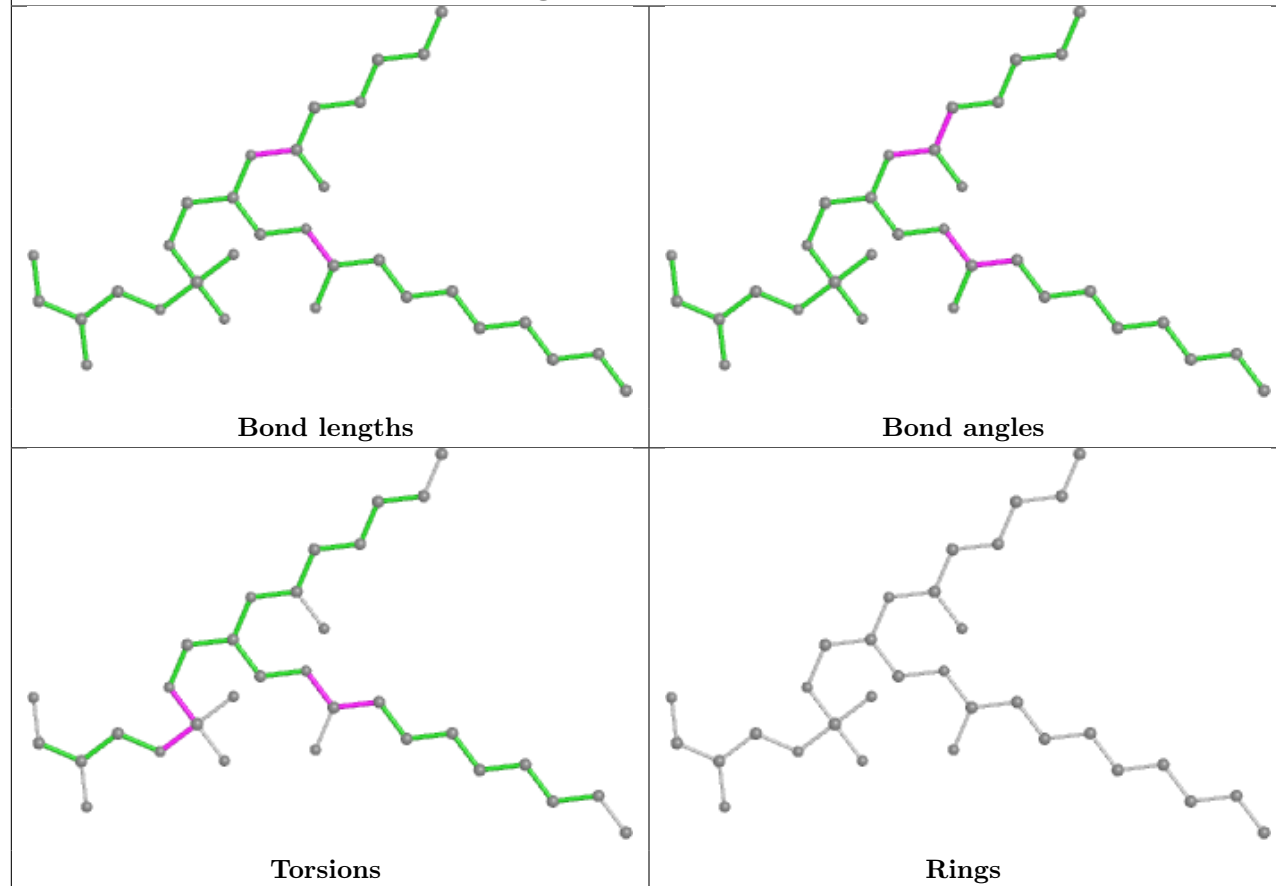
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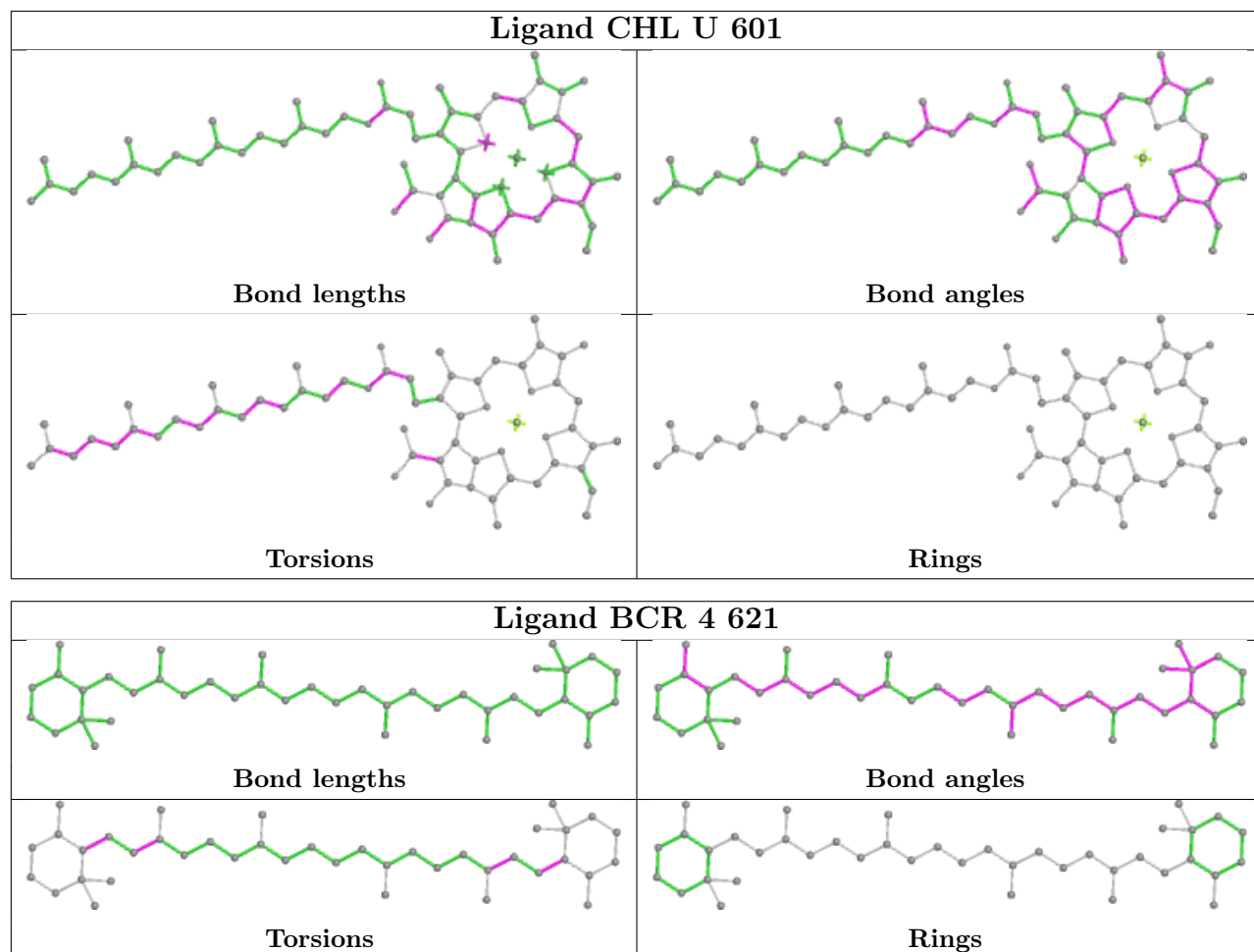


Ligand CLA A 827

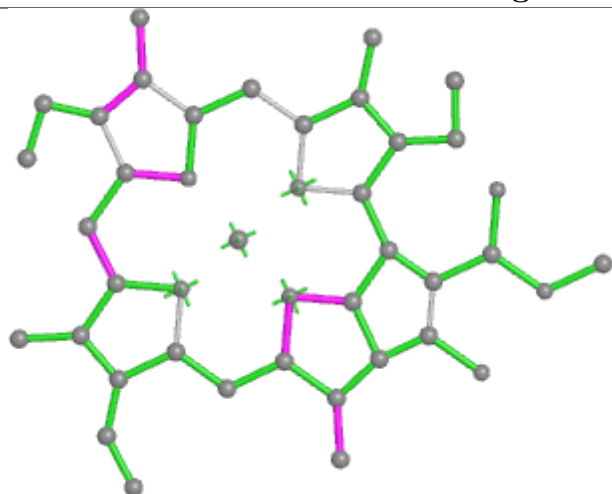


Ligand LHG 6 630

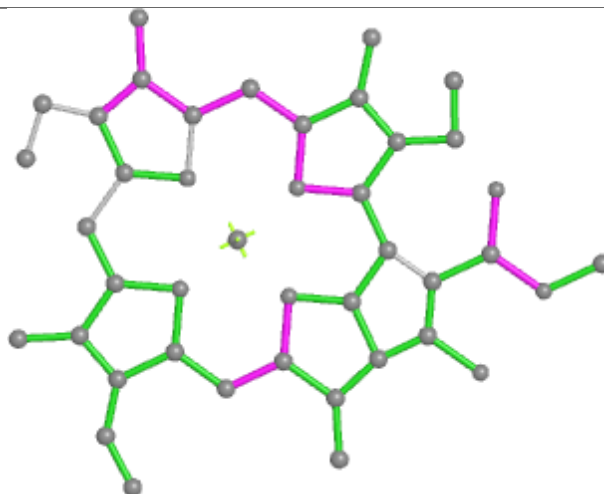




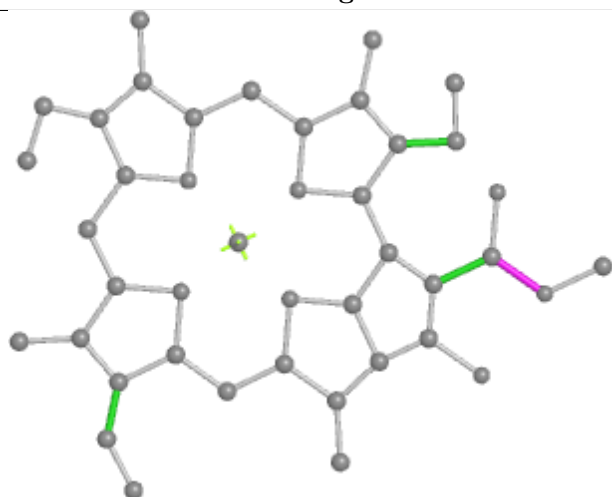
Ligand CLA K 206



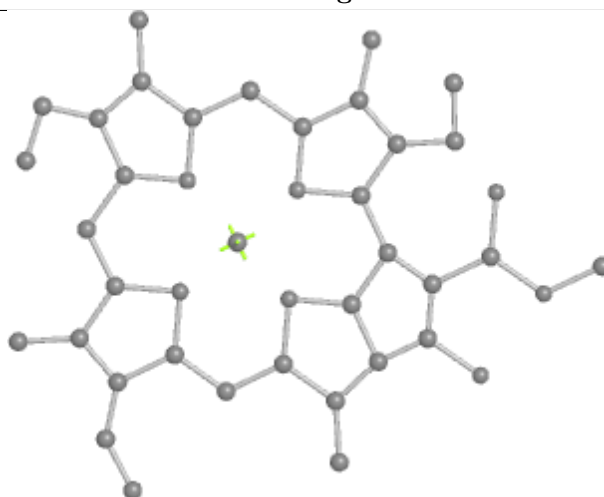
Bond lengths



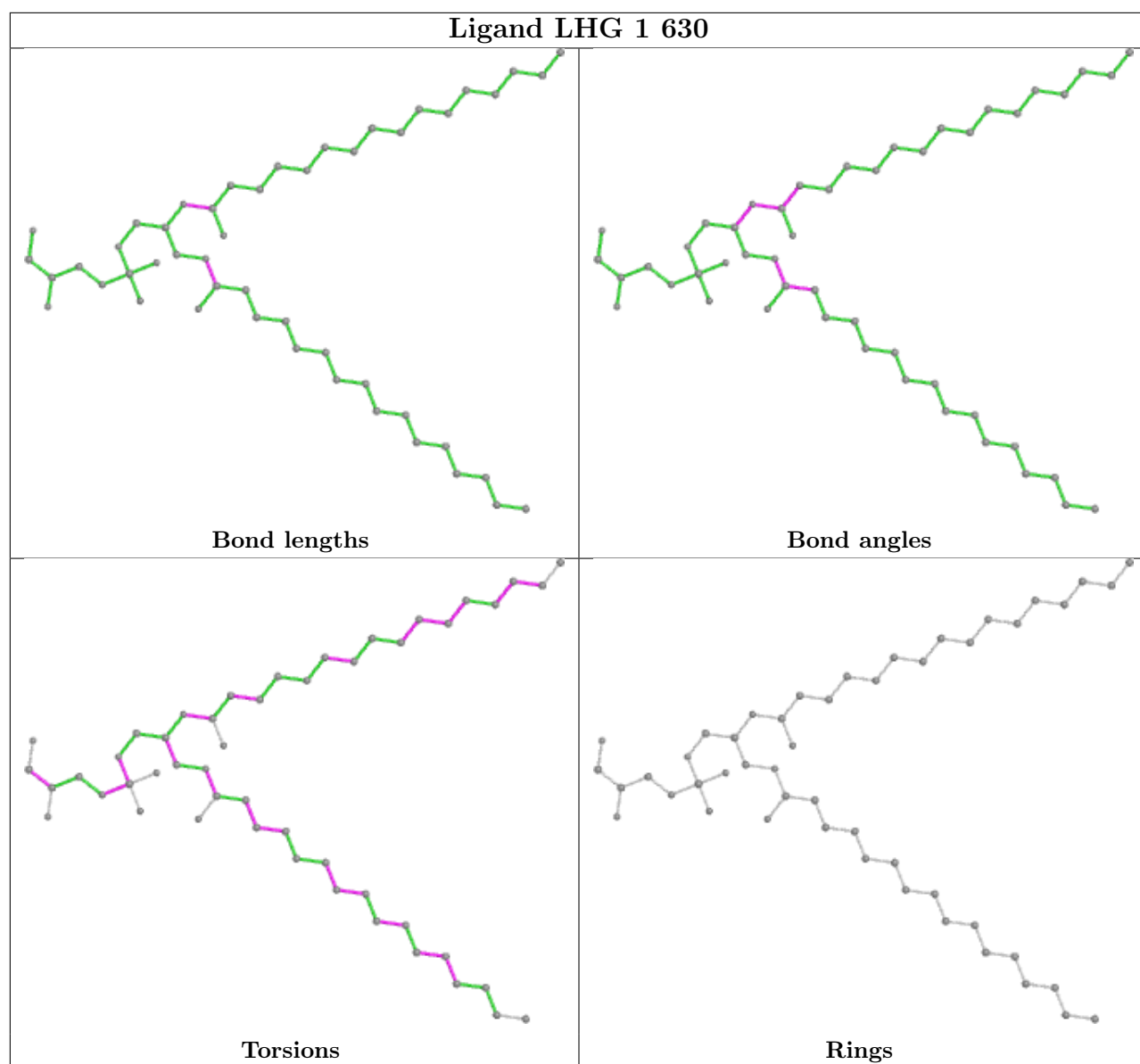
Bond angles

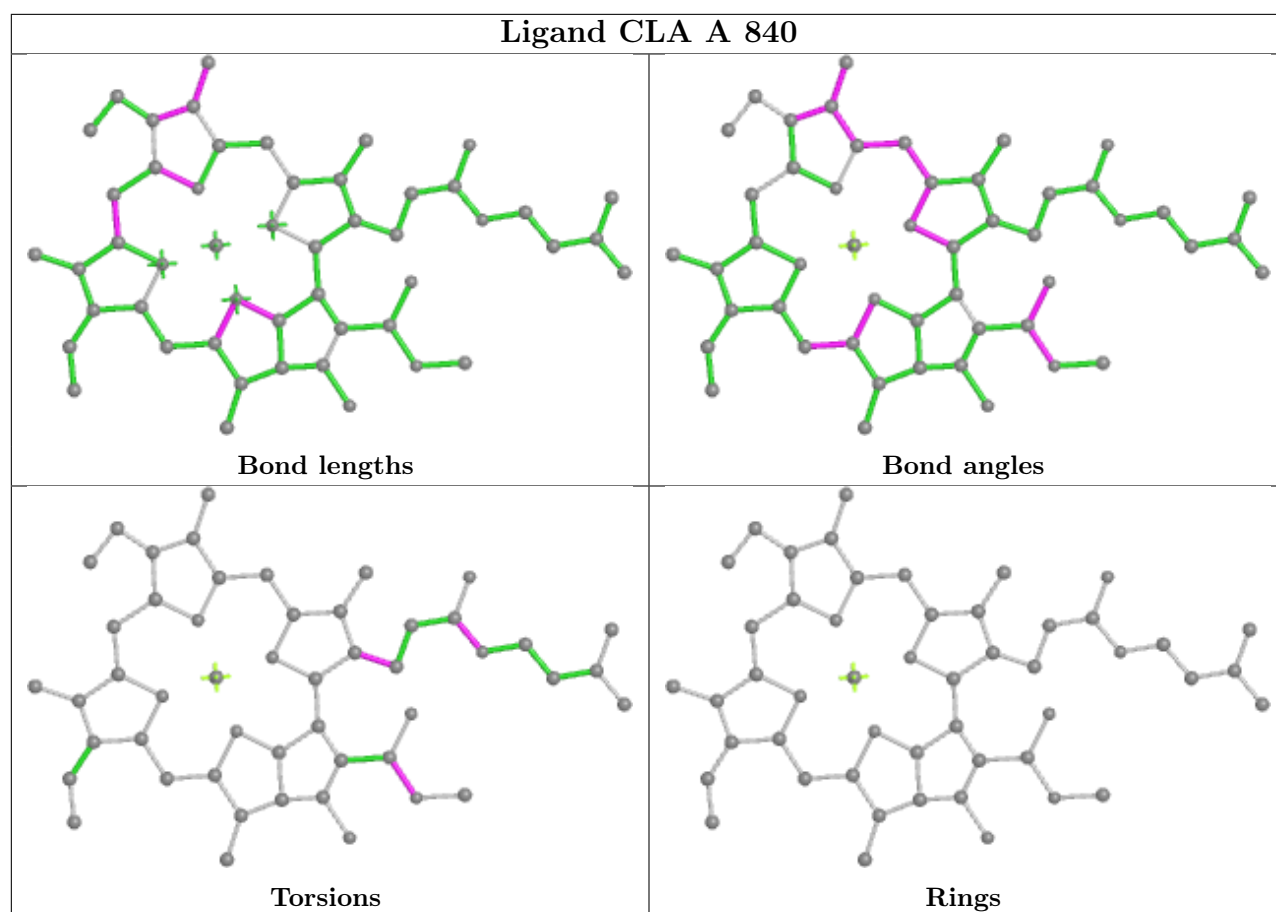


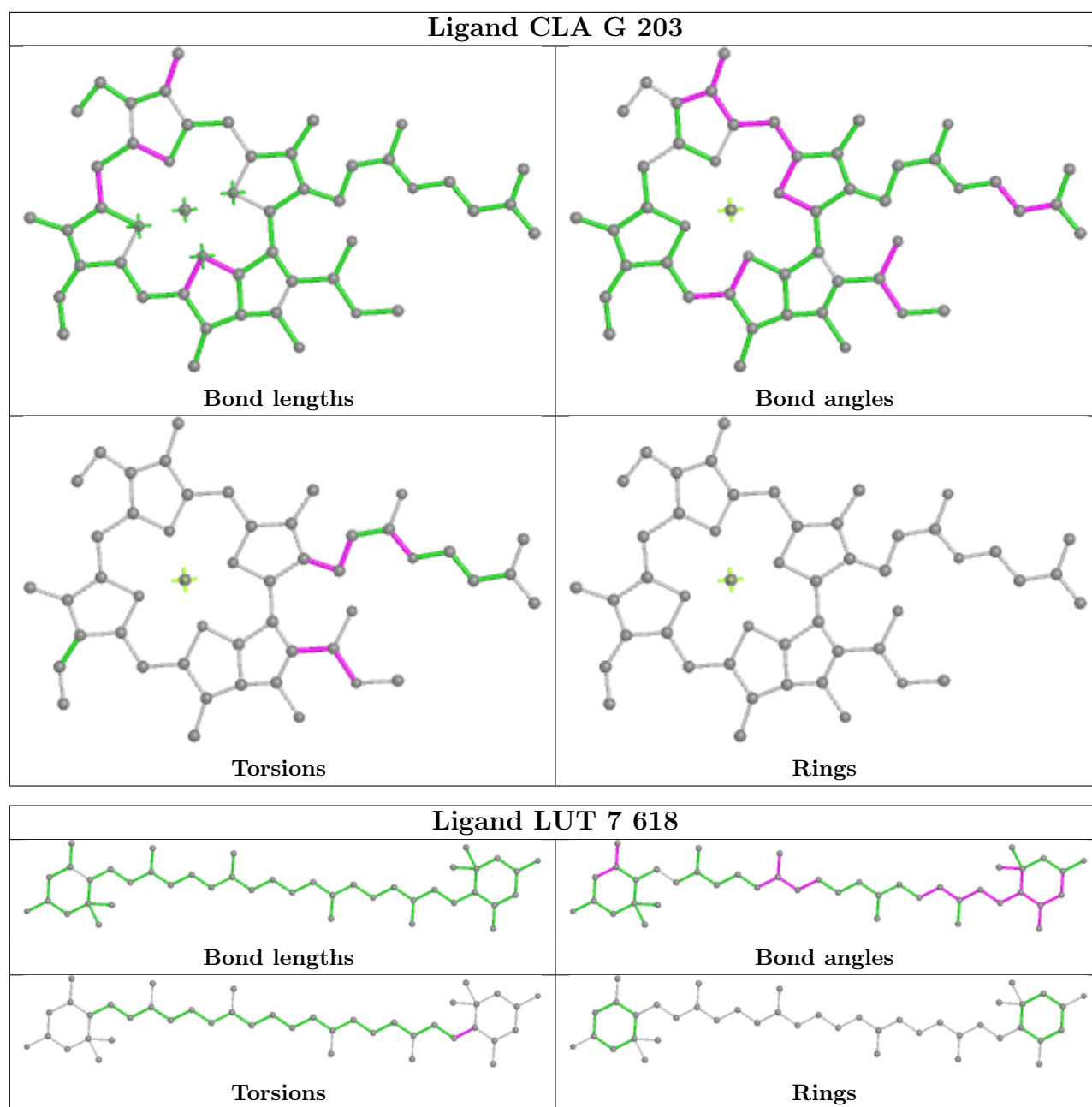
Torsions

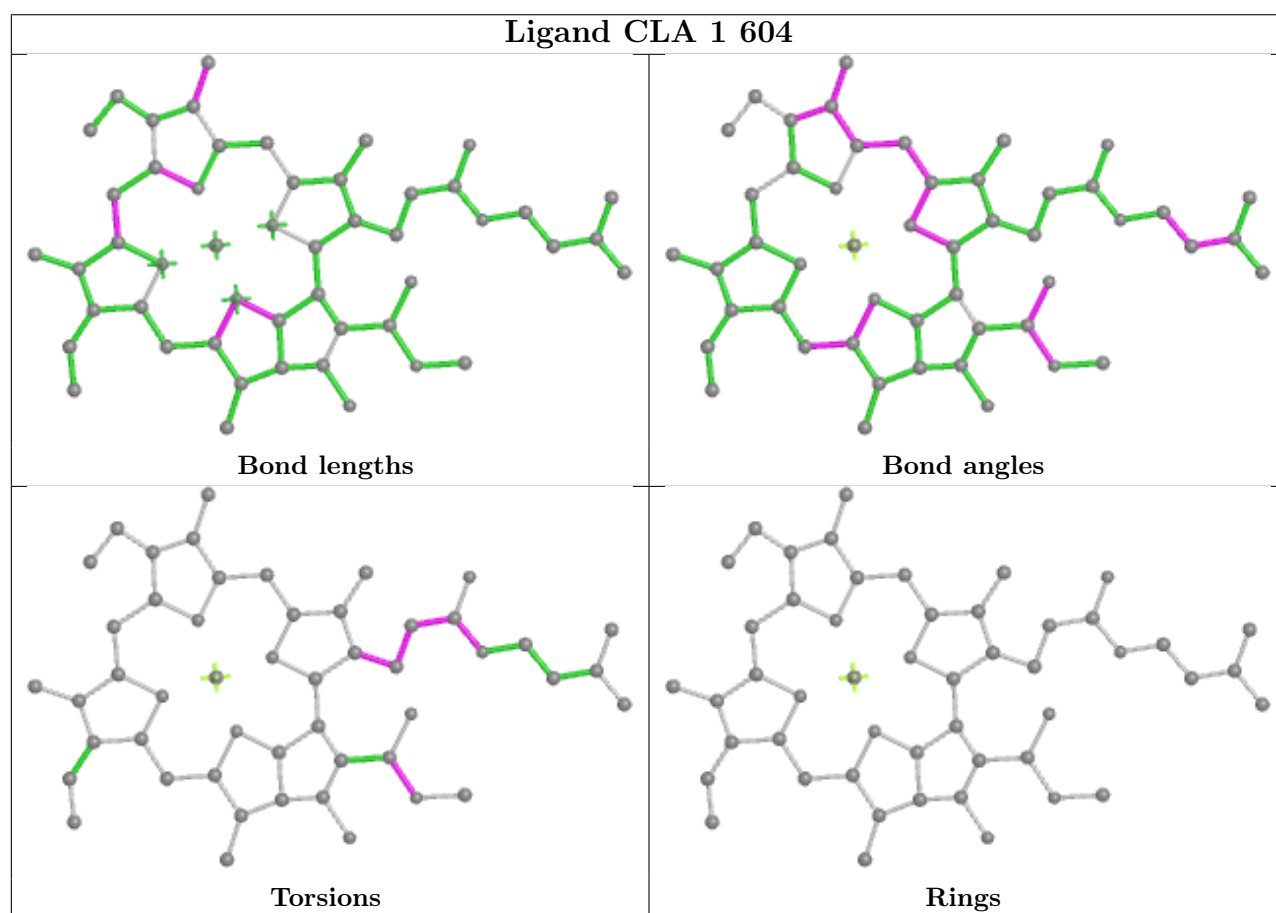
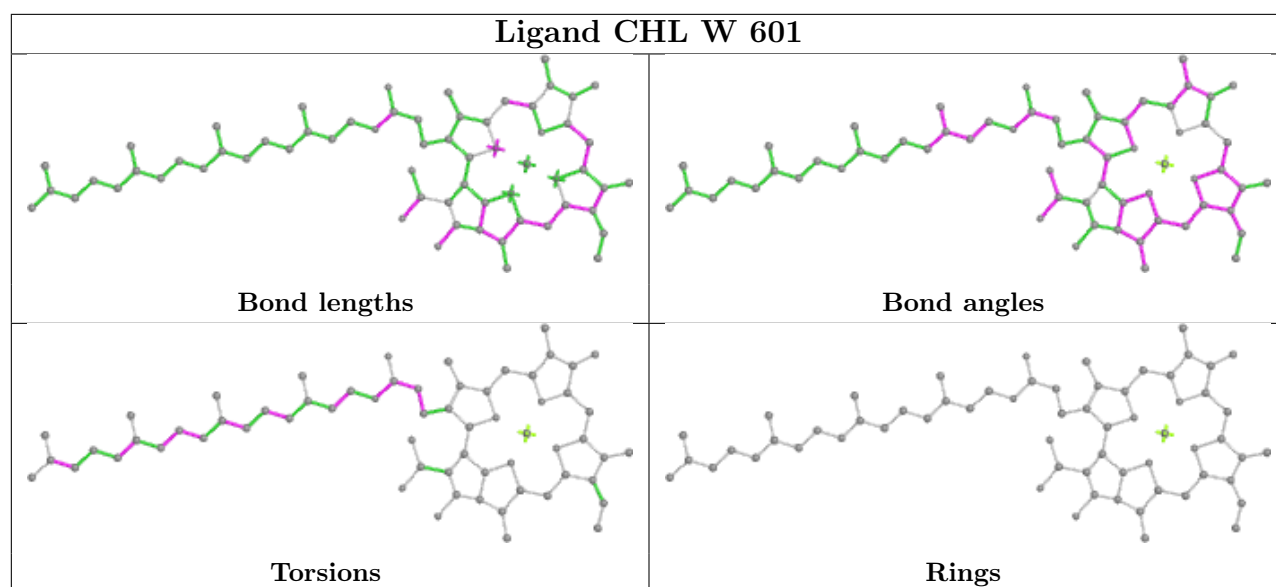


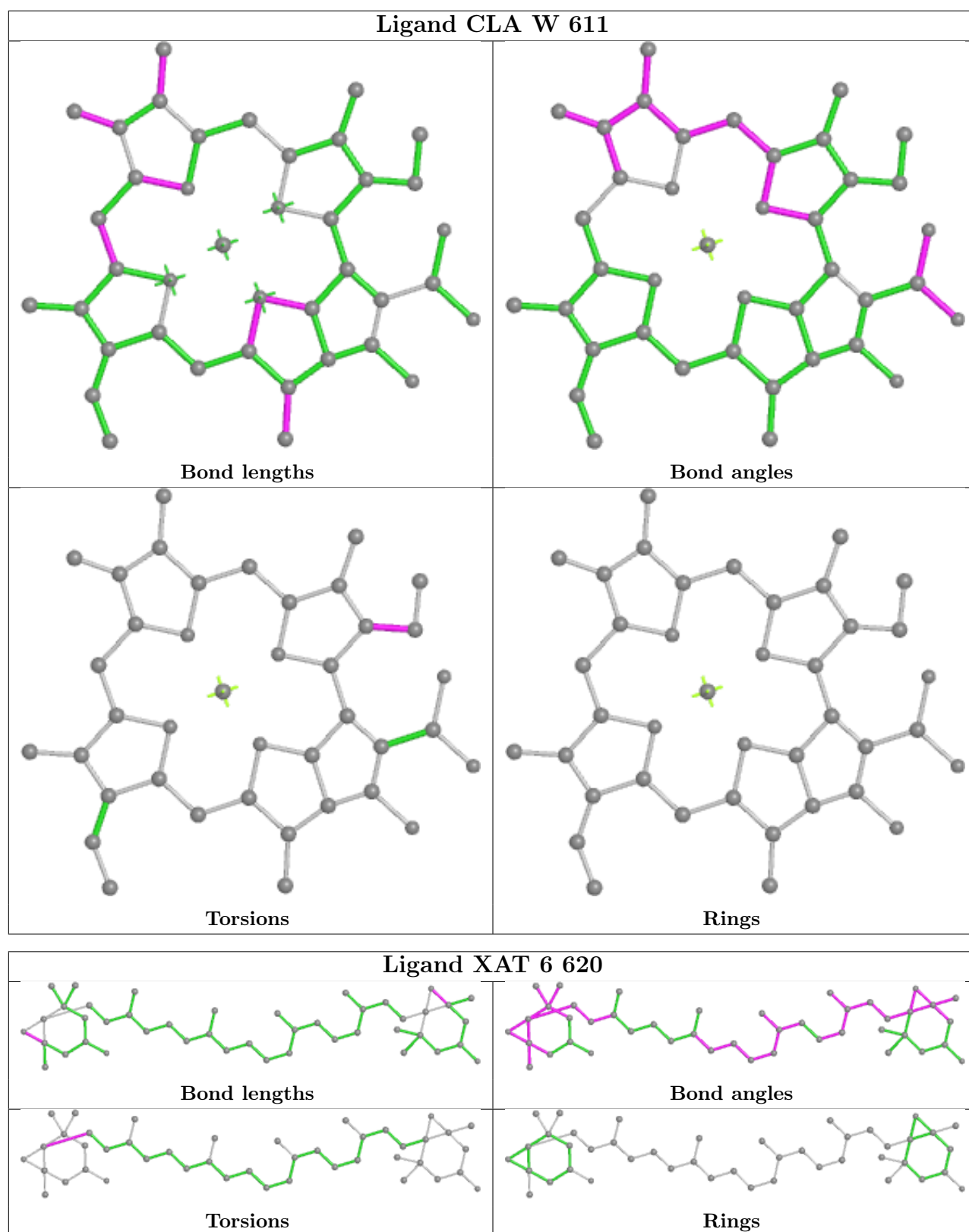
Rings



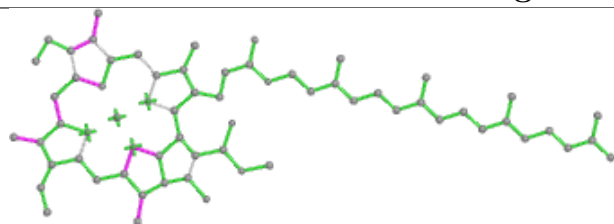




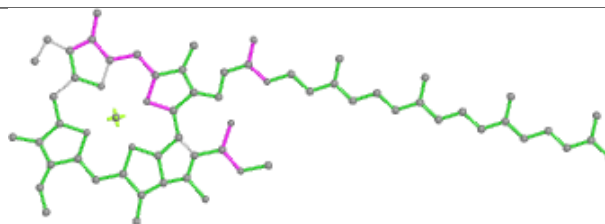




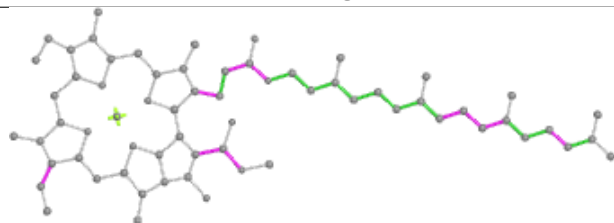
Ligand CLA B 803



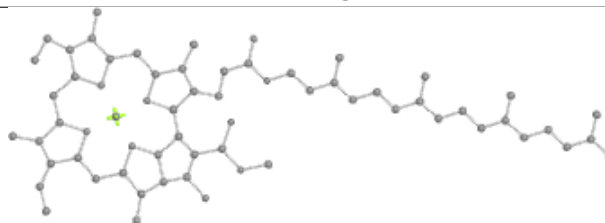
Bond lengths



Bond angles

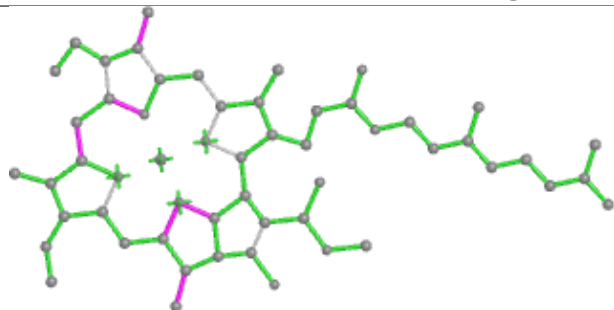


Torsions

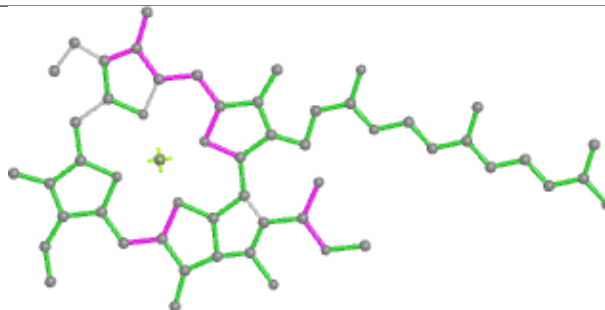


Rings

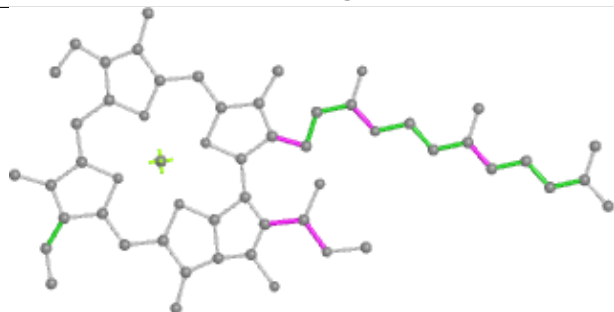
Ligand CLA O 2002



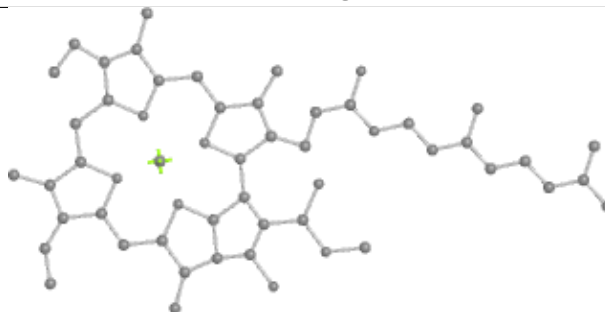
Bond lengths



Bond angles

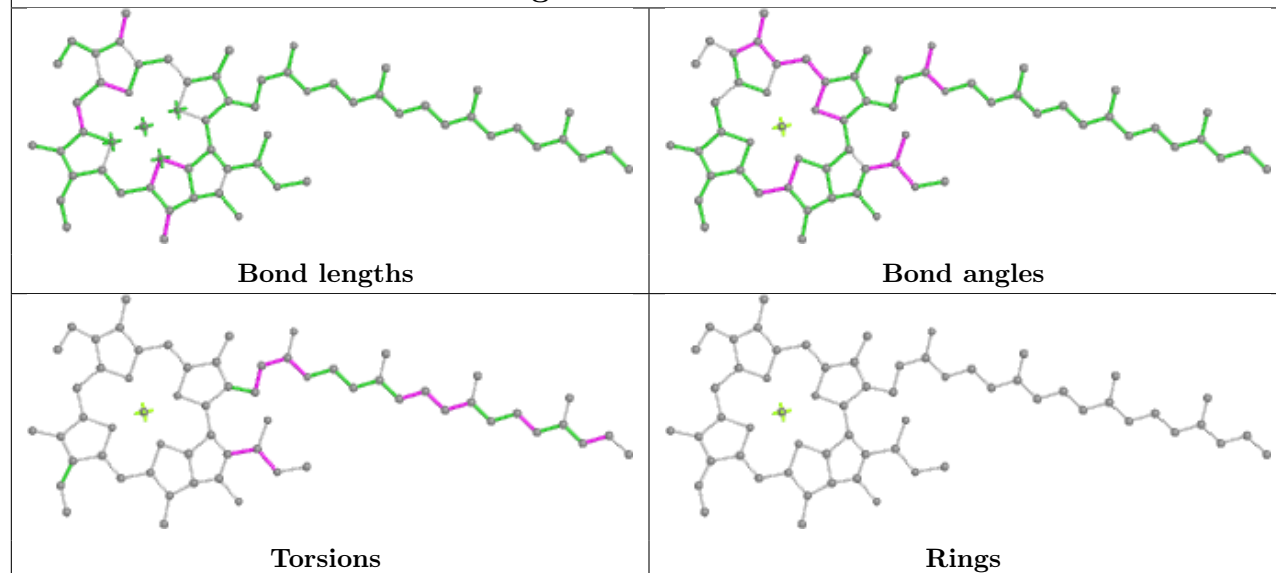


Torsions

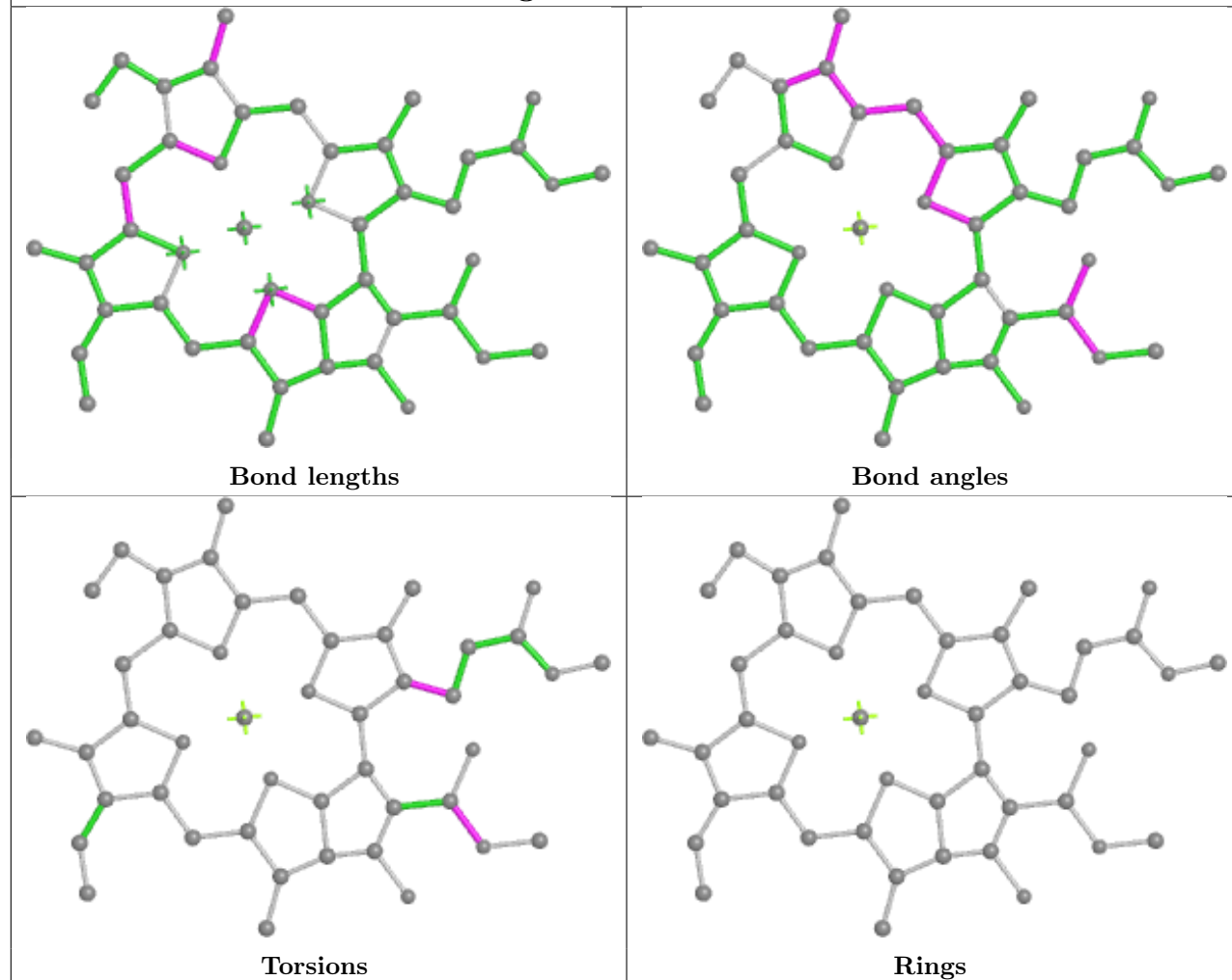


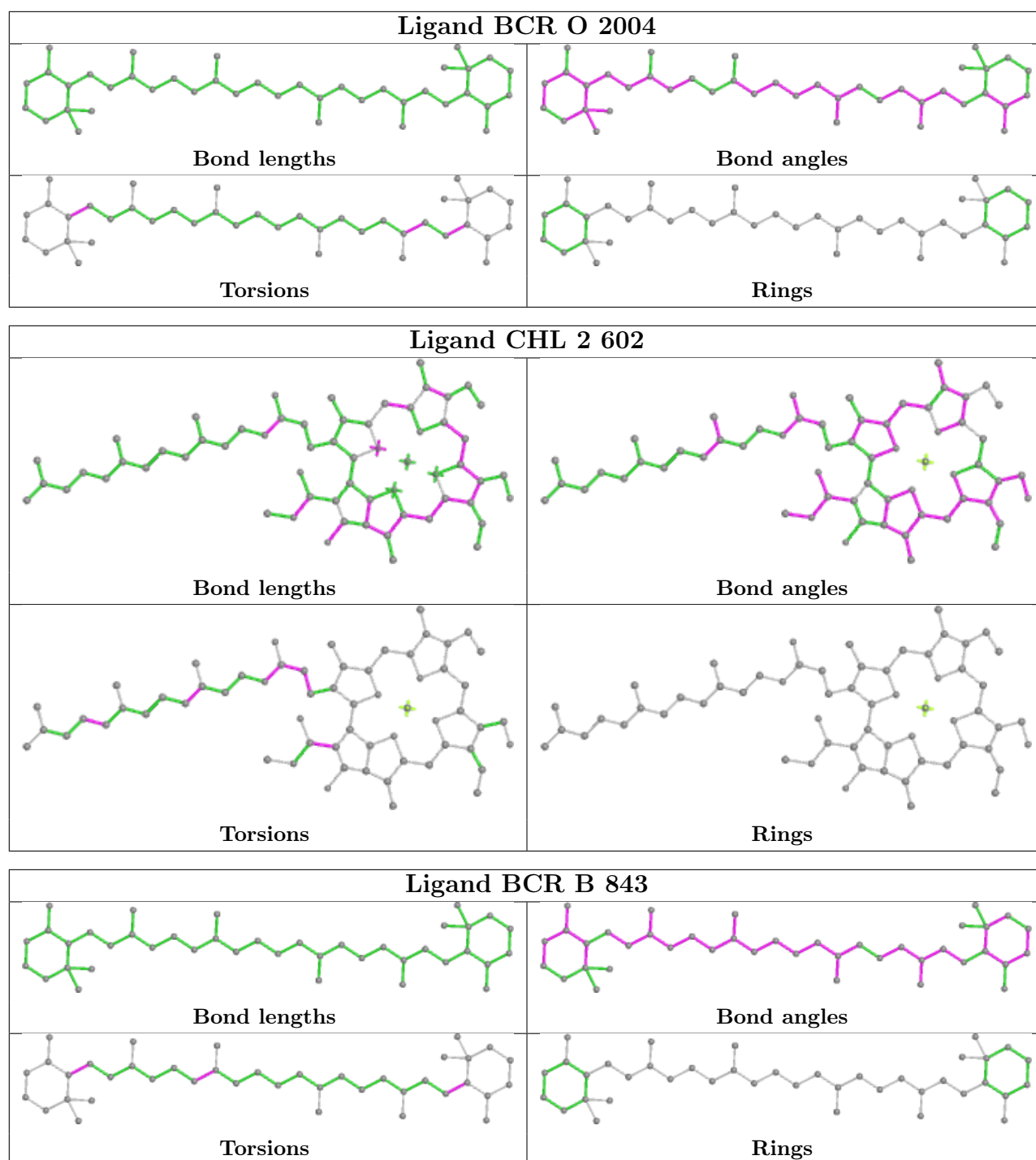
Rings

Ligand CLA A 824

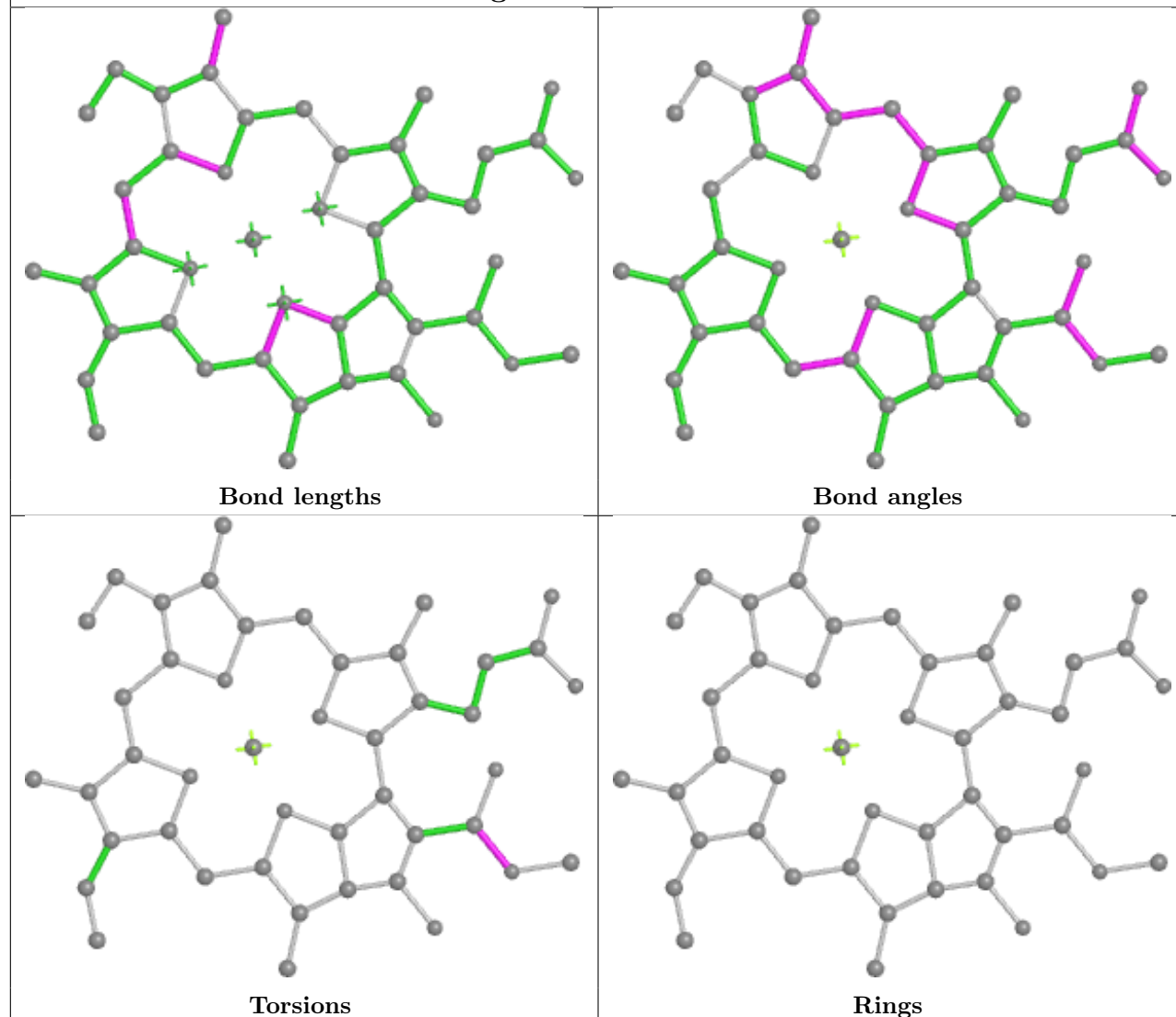


Ligand CLA 5 616

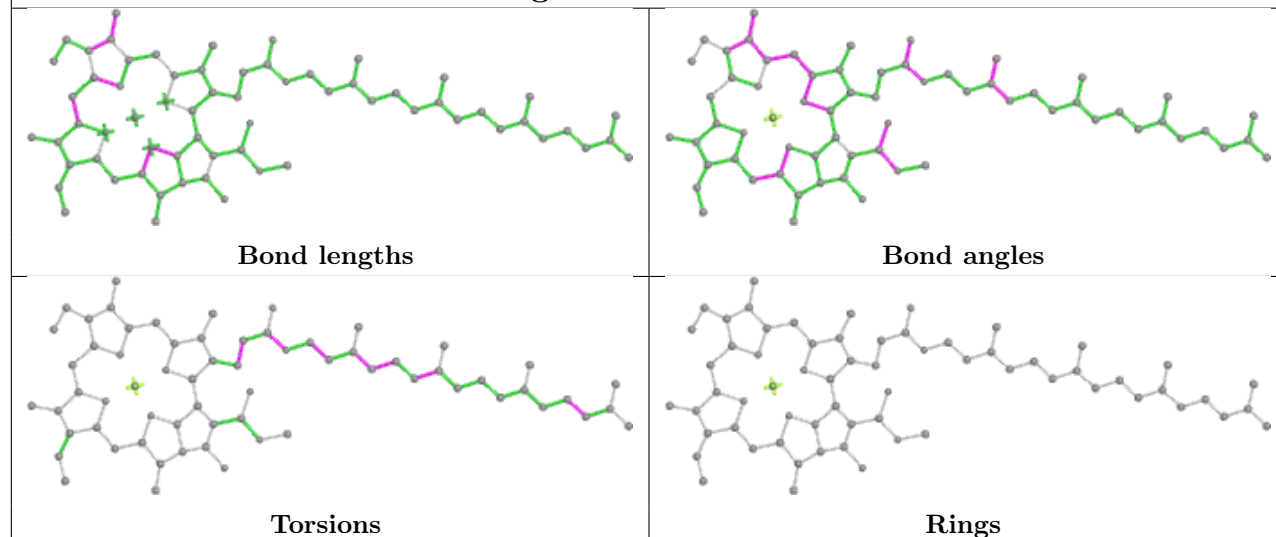




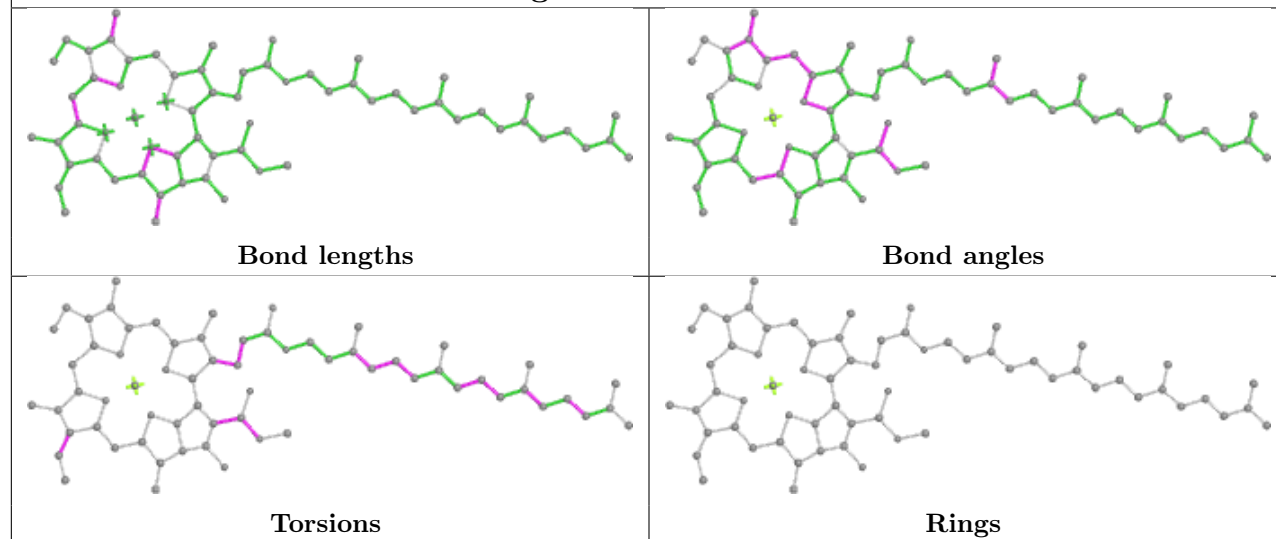
Ligand CLA B 835



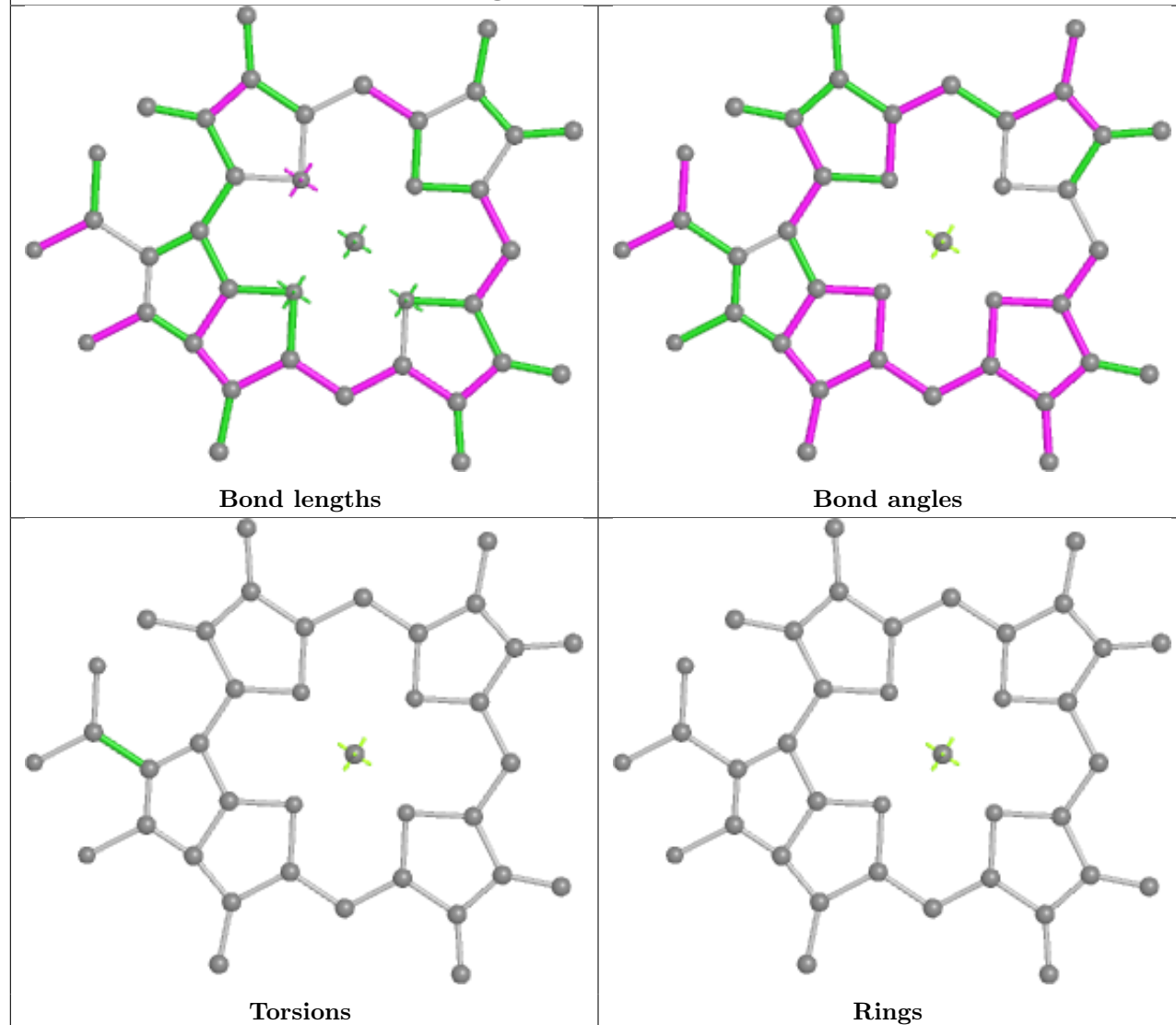
Ligand CLA U 602



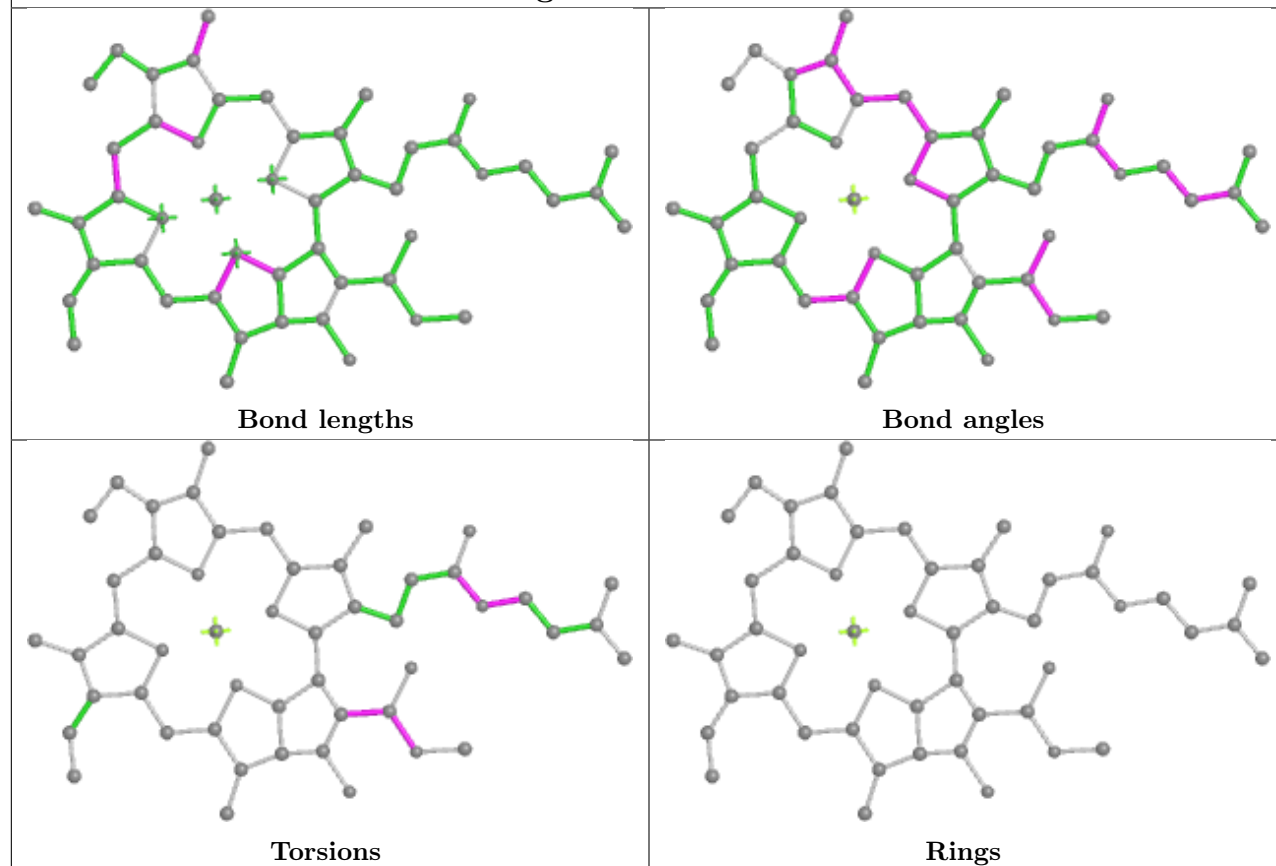
Ligand CLA K 204



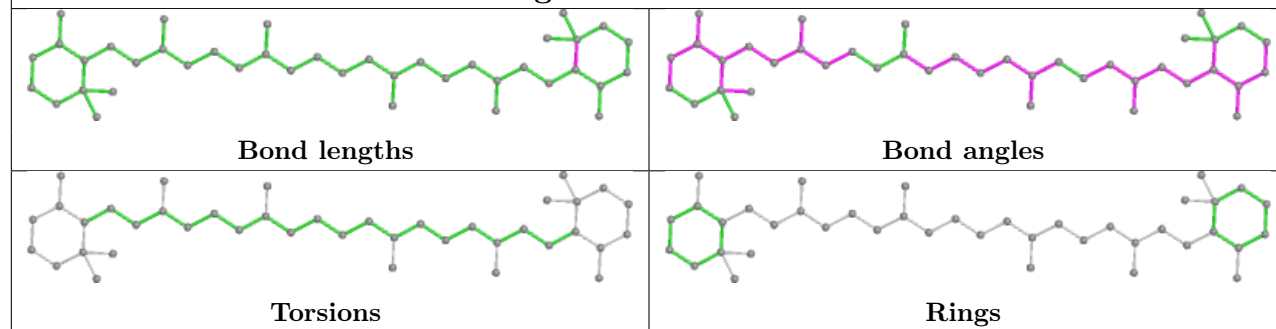
Ligand CHL U 605



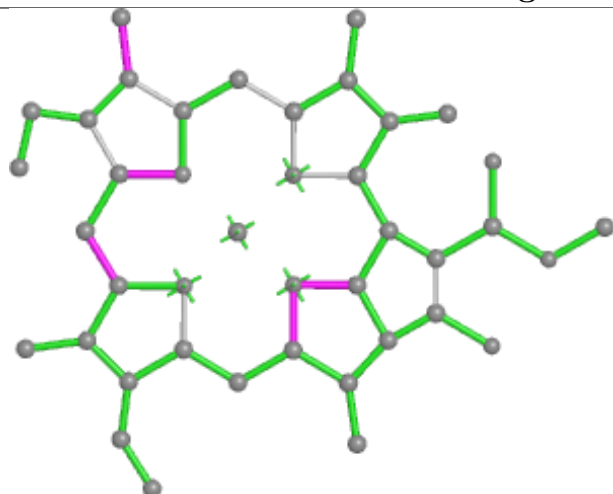
Ligand CLA 7 604



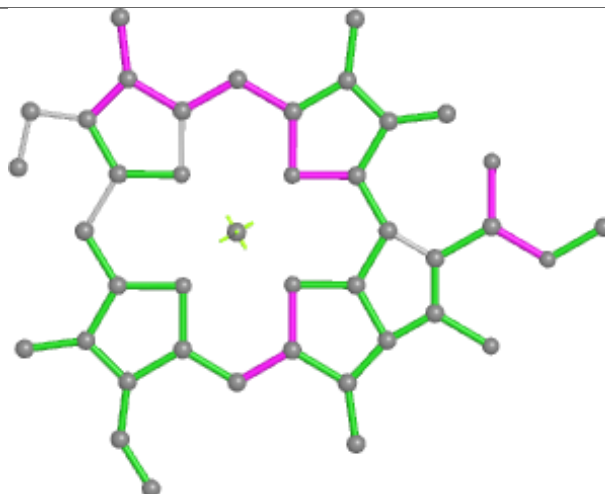
Ligand BCR 3 621



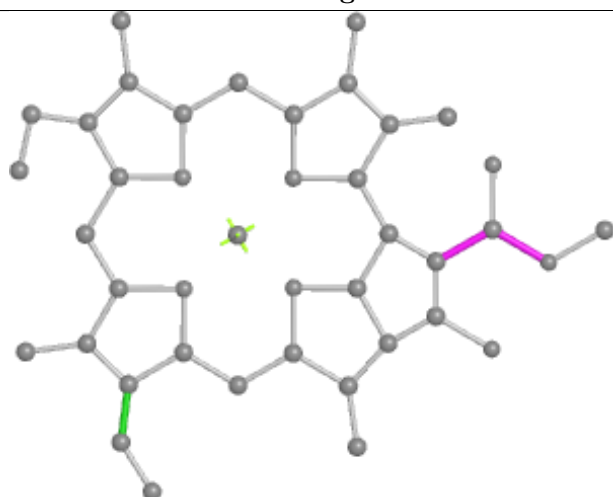
Ligand CLA 7 614



Bond lengths



Bond angles

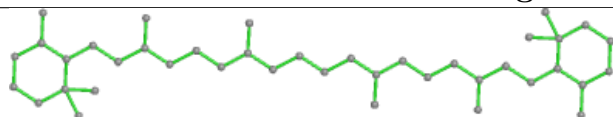


Torsions

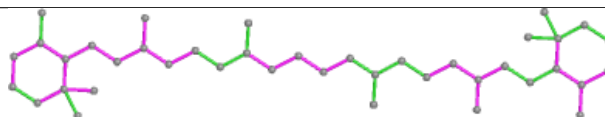


Rings

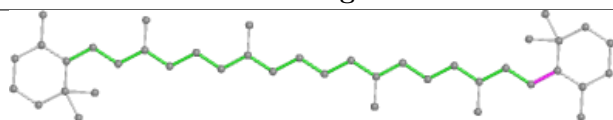
Ligand BCR J 102



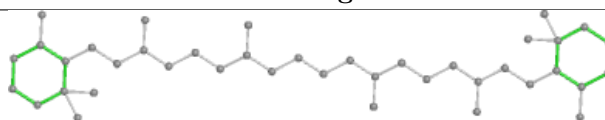
Bond lengths



Bond angles

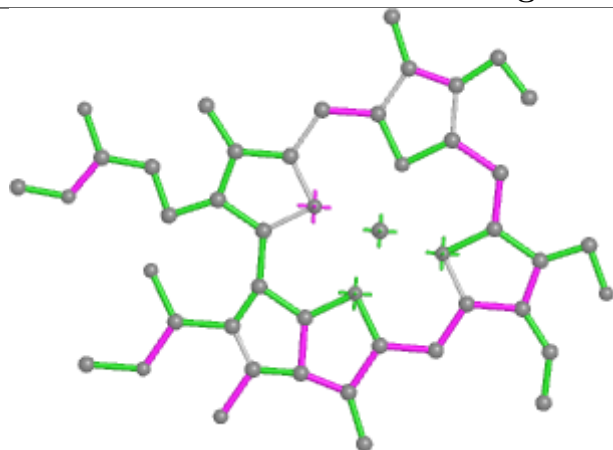


Torsions

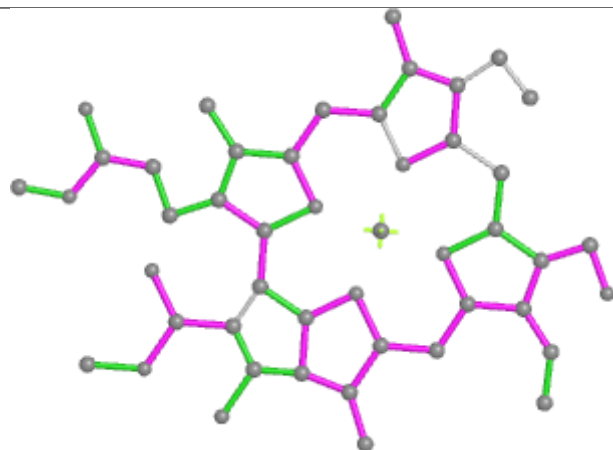


Rings

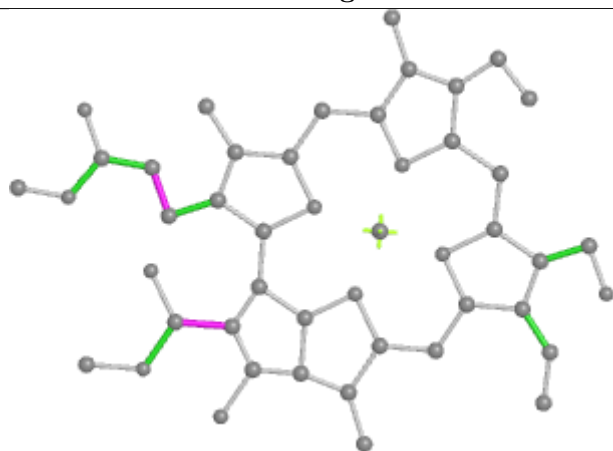
Ligand CHL 2 607



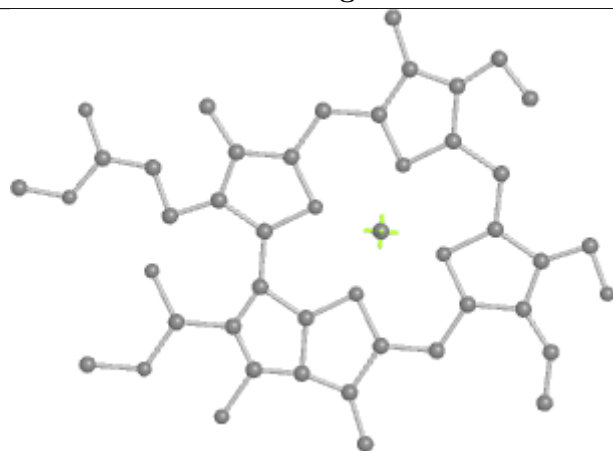
Bond lengths



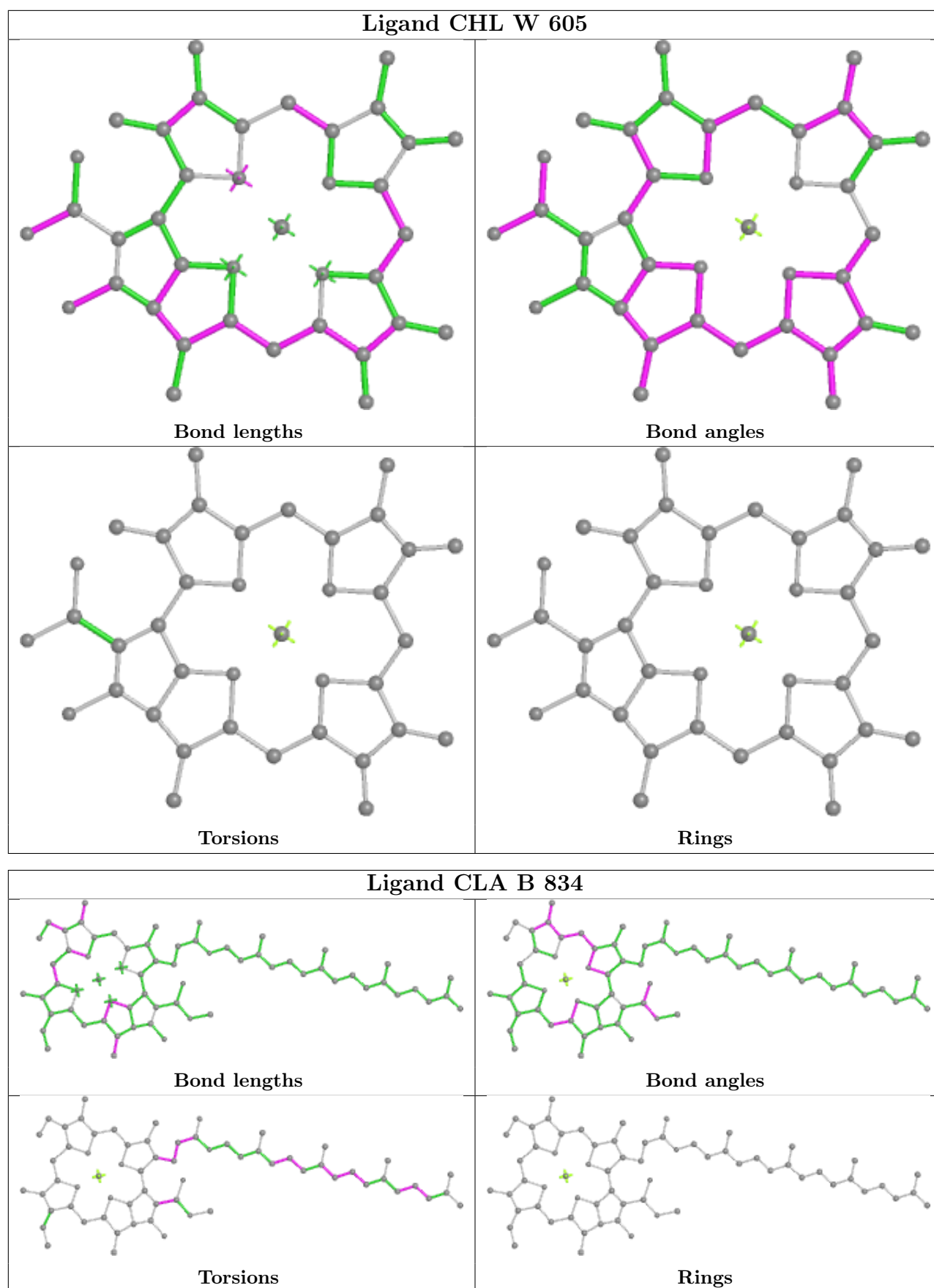
Bond angles

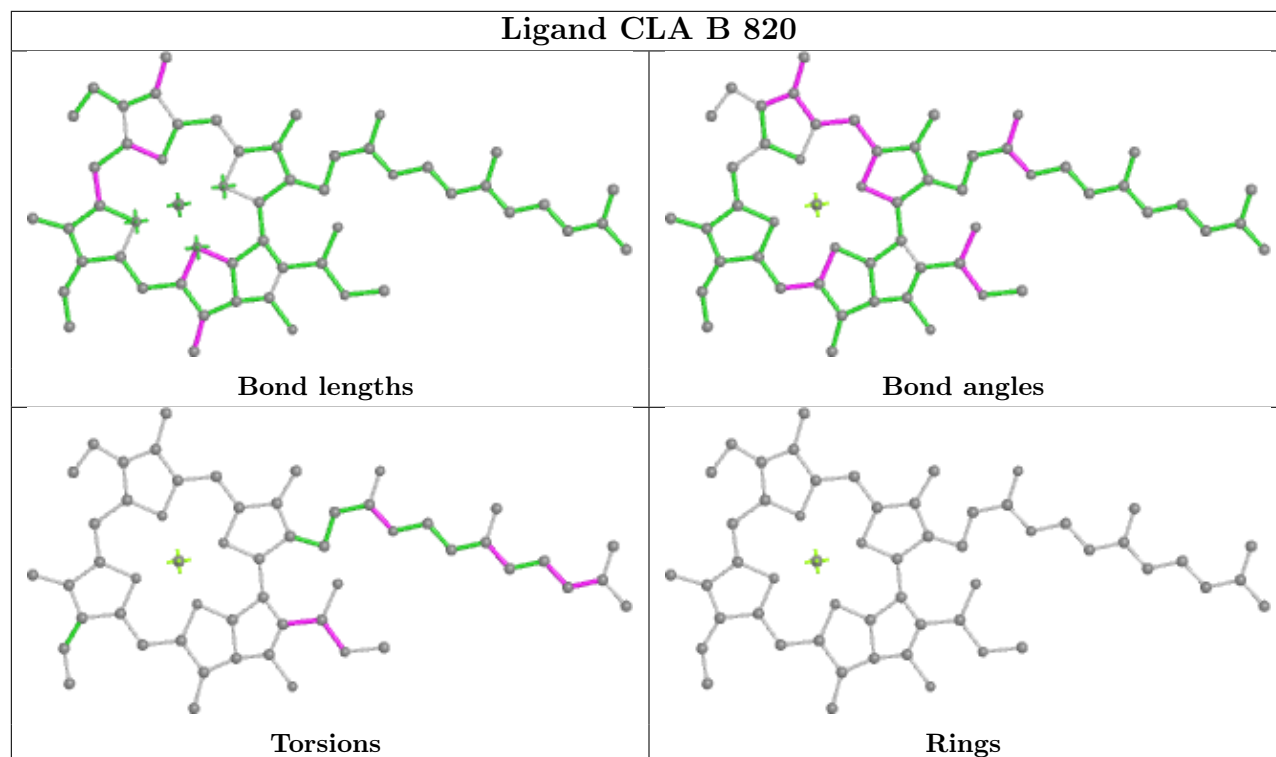
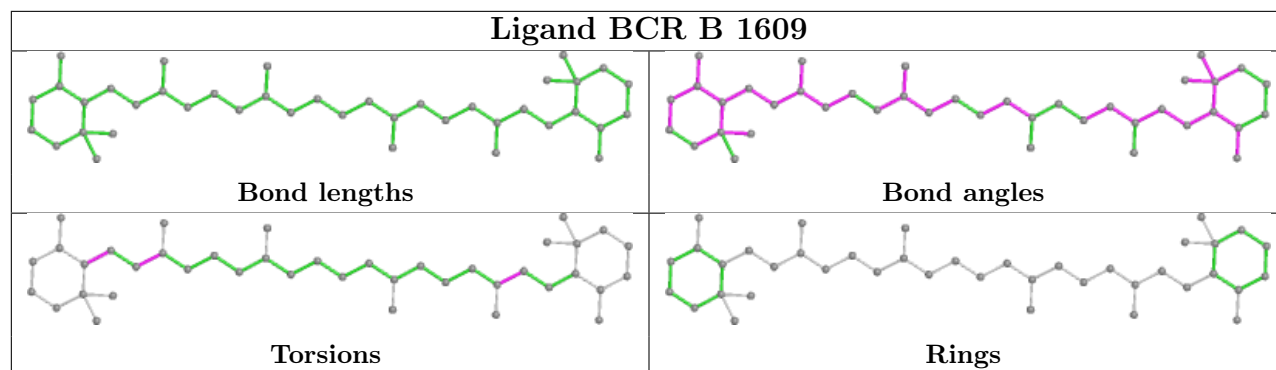


Torsions

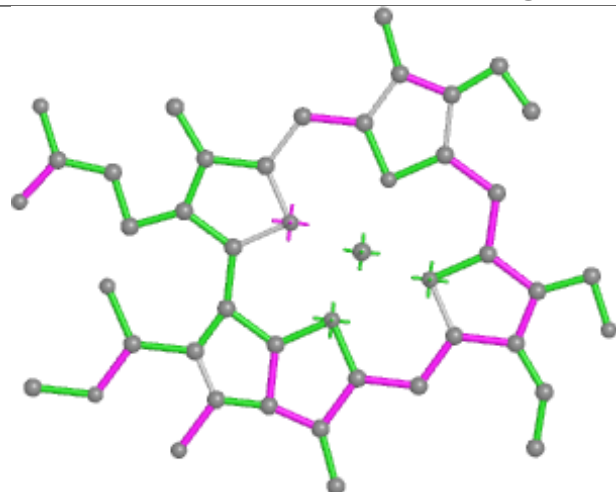


Rings

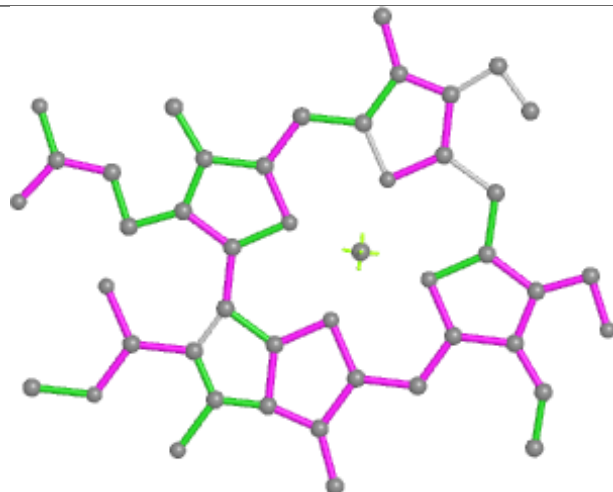




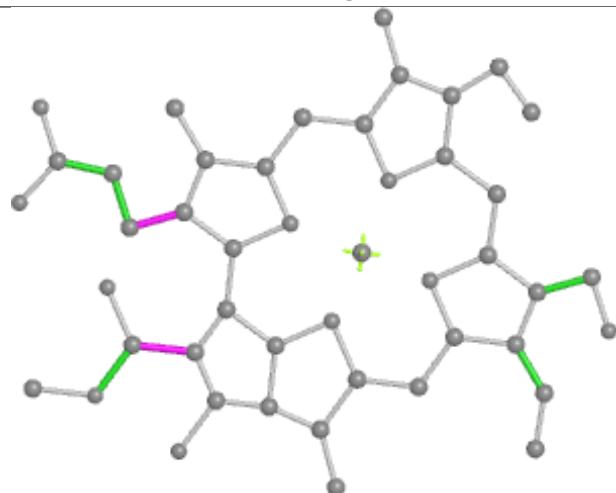
Ligand CHL 8 606



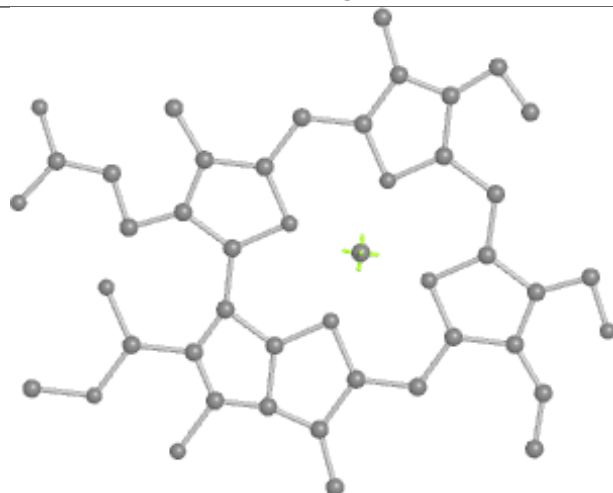
Bond lengths



Bond angles

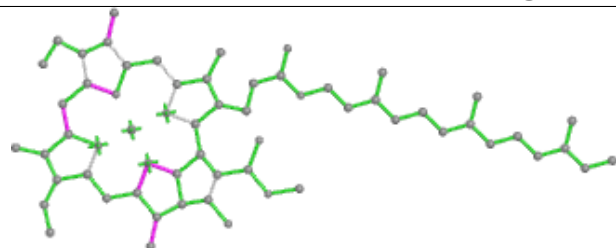


Torsions

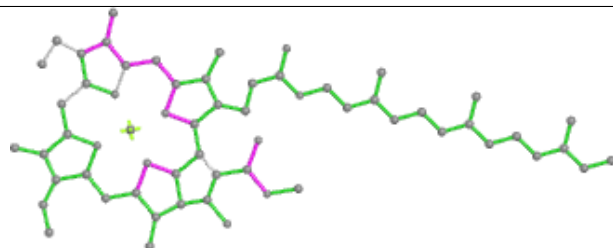


Rings

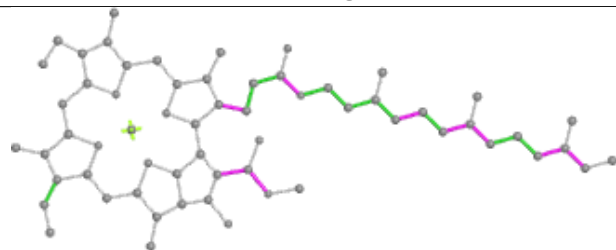
Ligand CLA 4 610



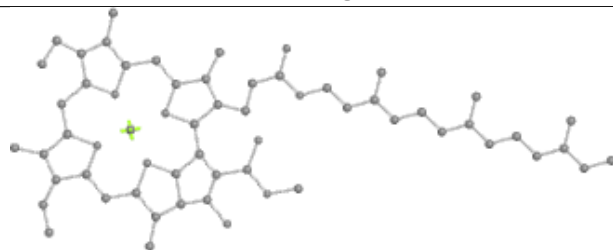
Bond lengths



Bond angles

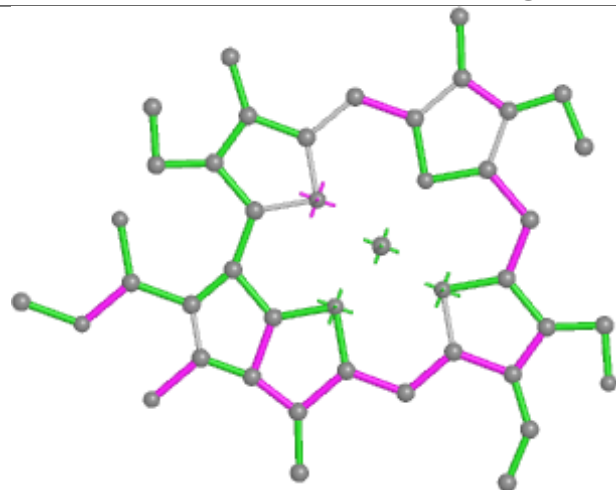


Torsions

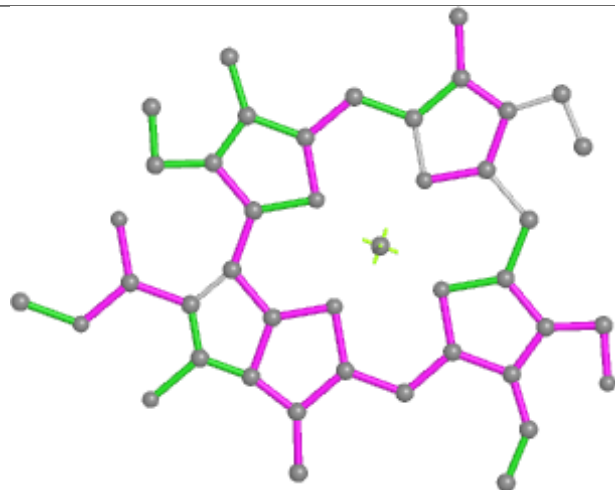


Rings

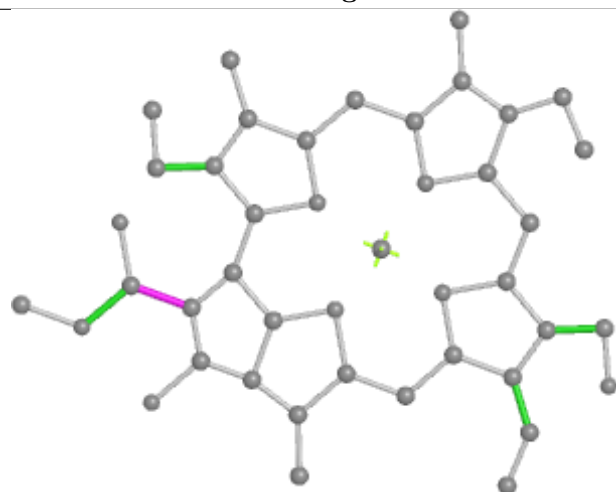
Ligand CHL 2 618



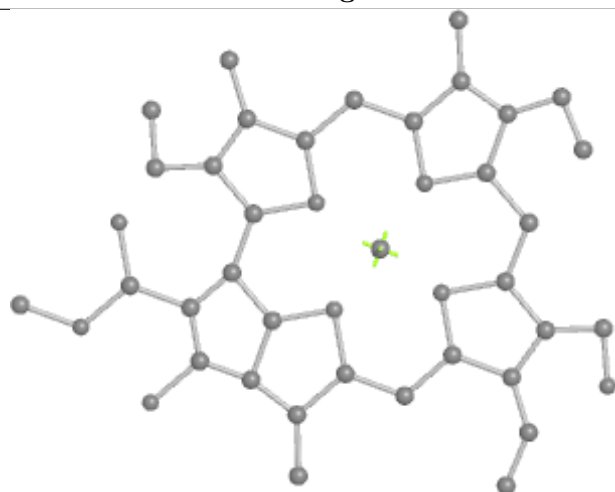
Bond lengths



Bond angles

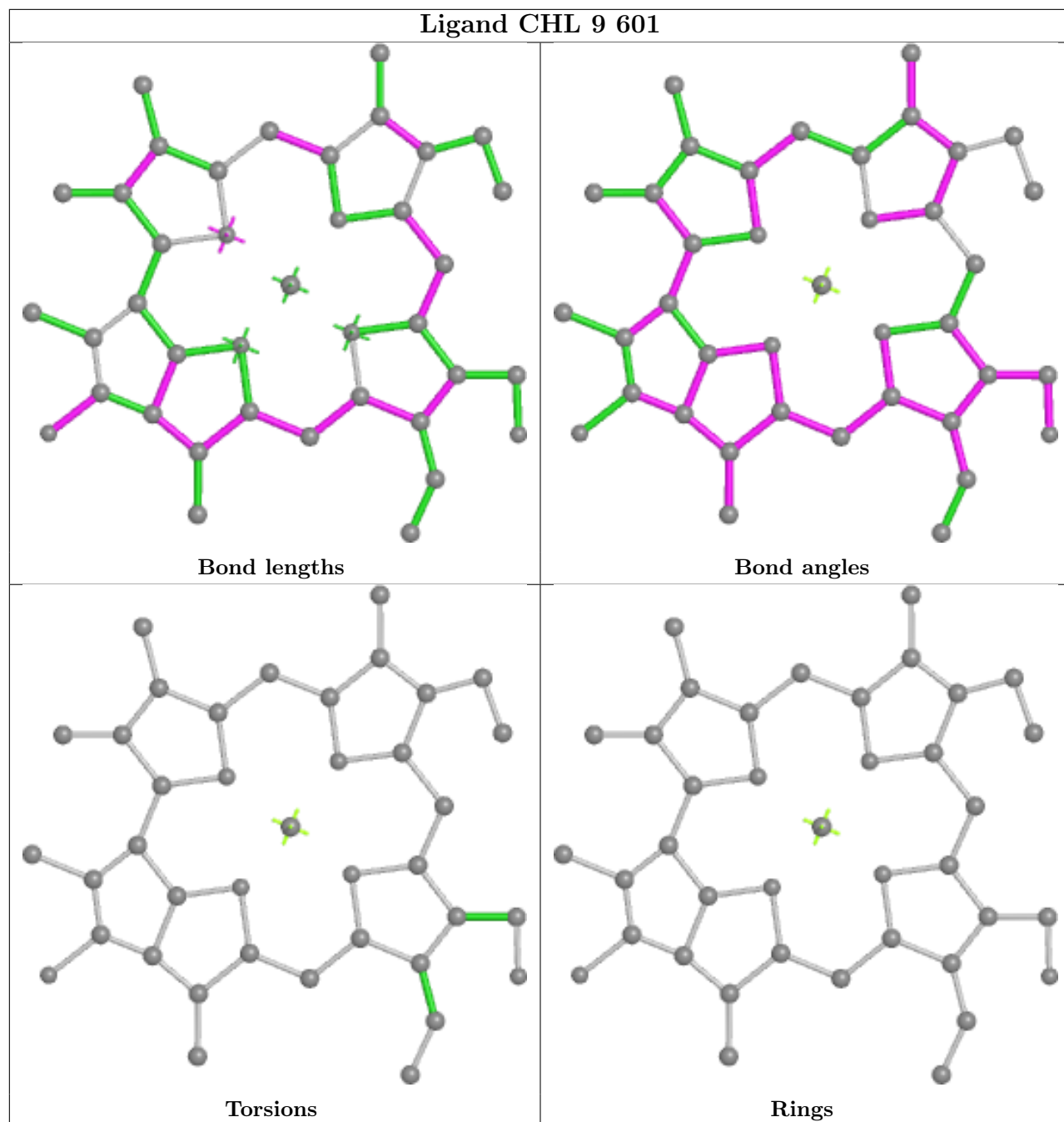


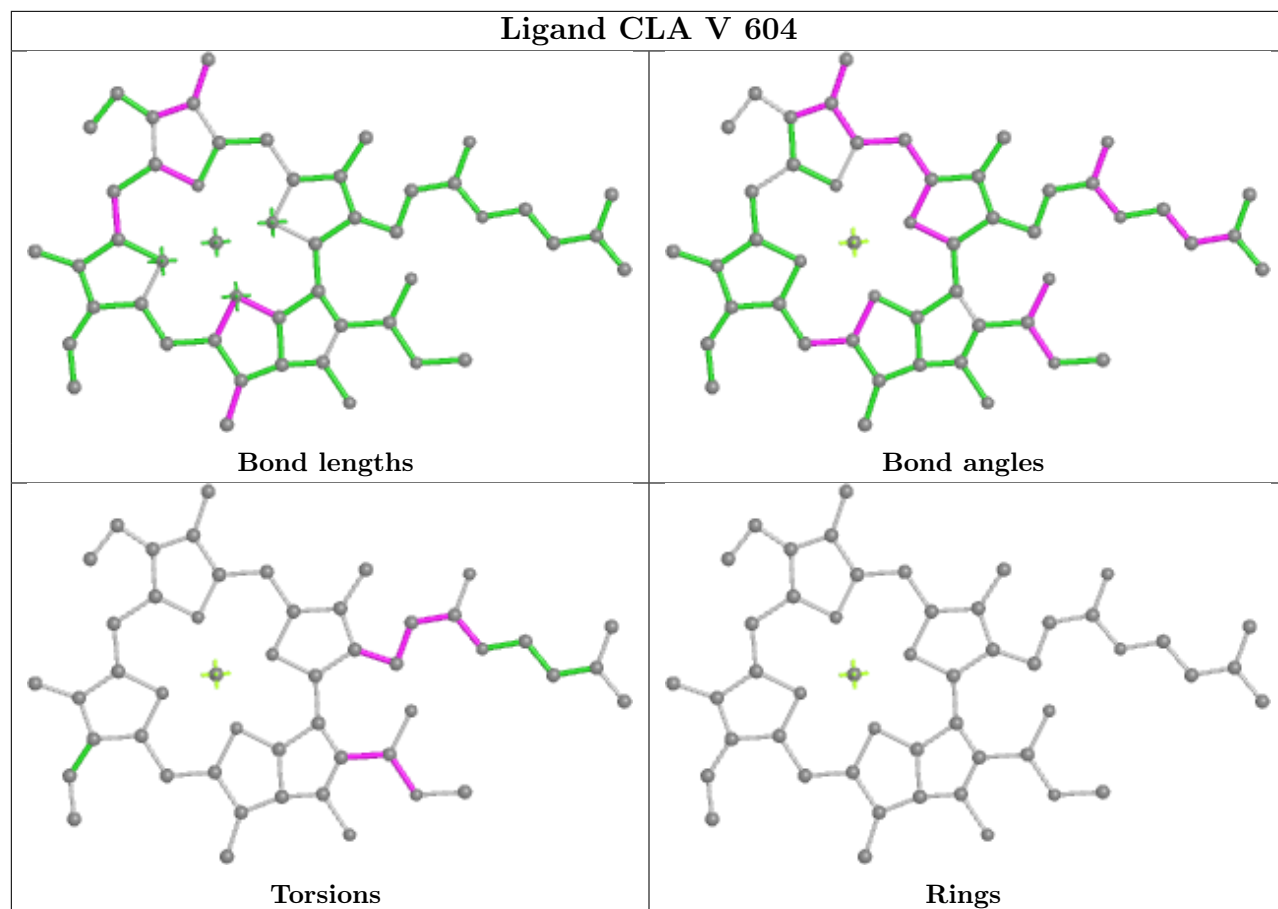
Torsions



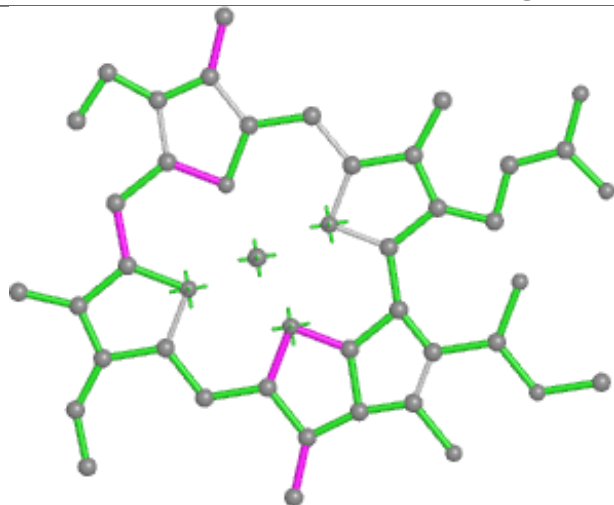
Rings

Ligand CHL 9 601

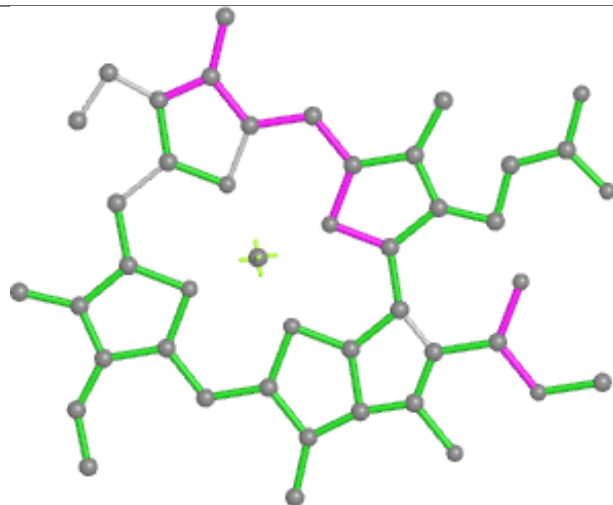




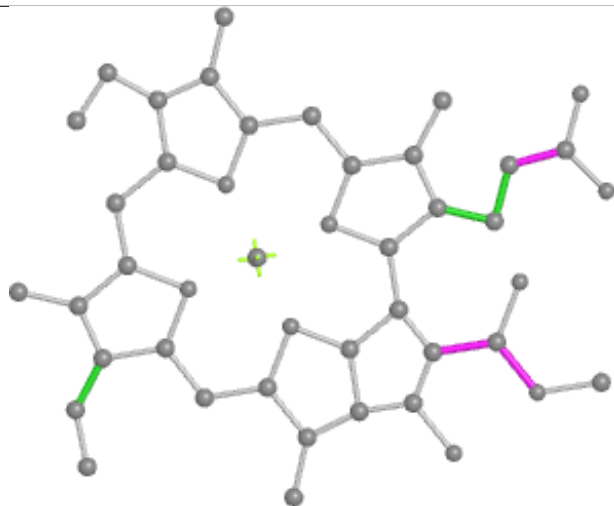
Ligand CLA 4 611



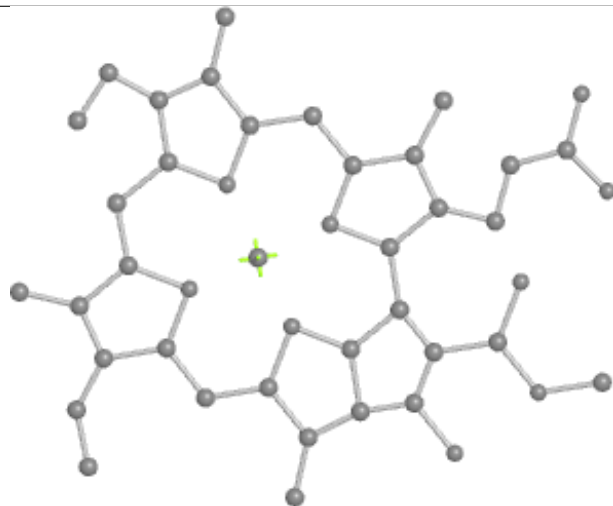
Bond lengths



Bond angles

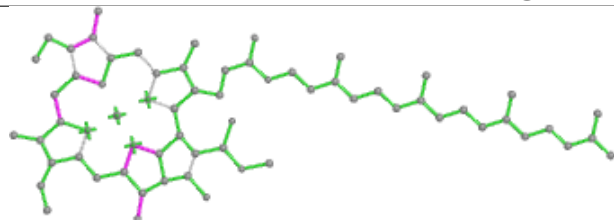


Torsions

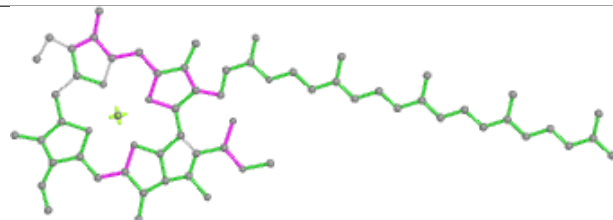


Rings

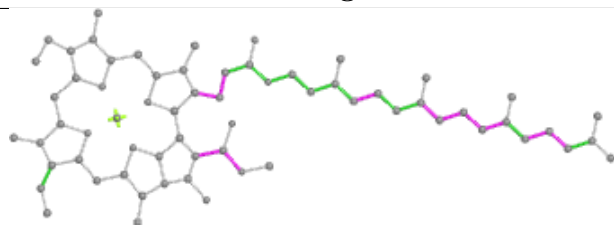
Ligand CLA 9 611



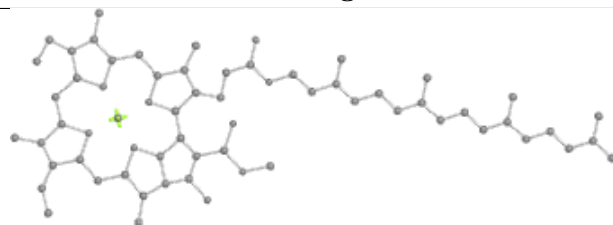
Bond lengths



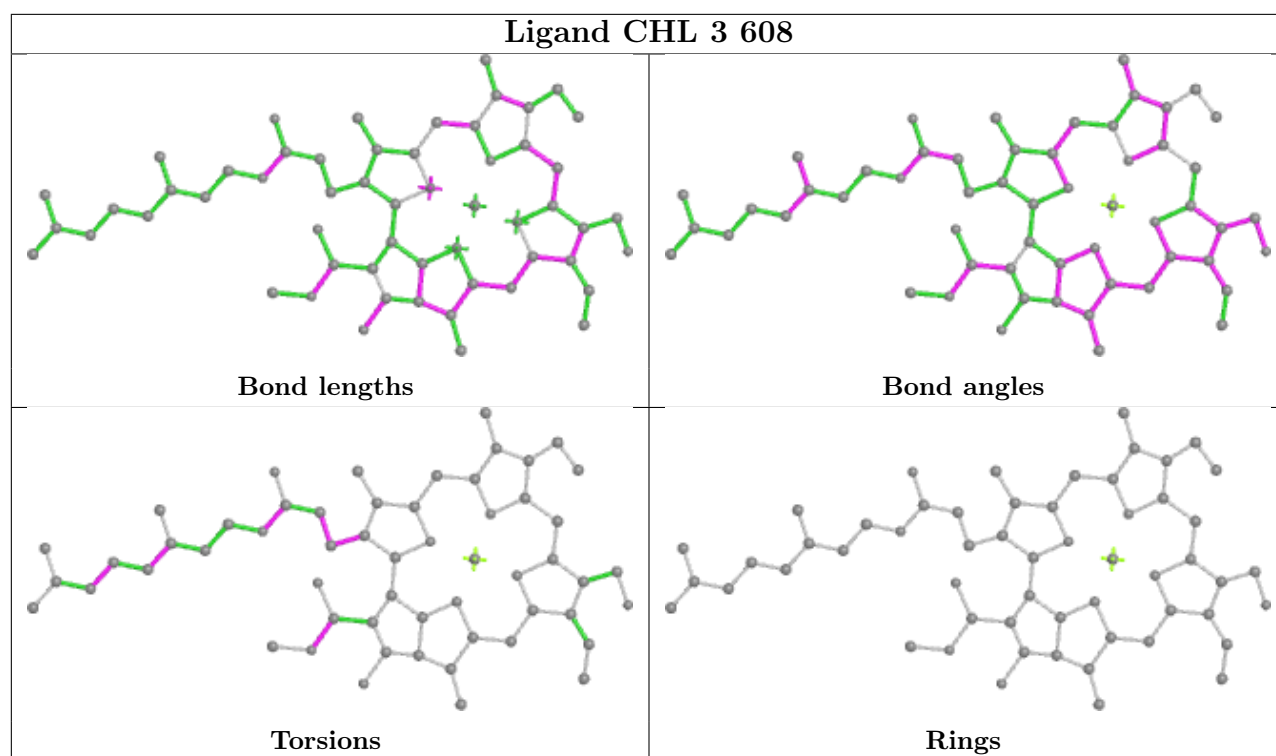
Bond angles

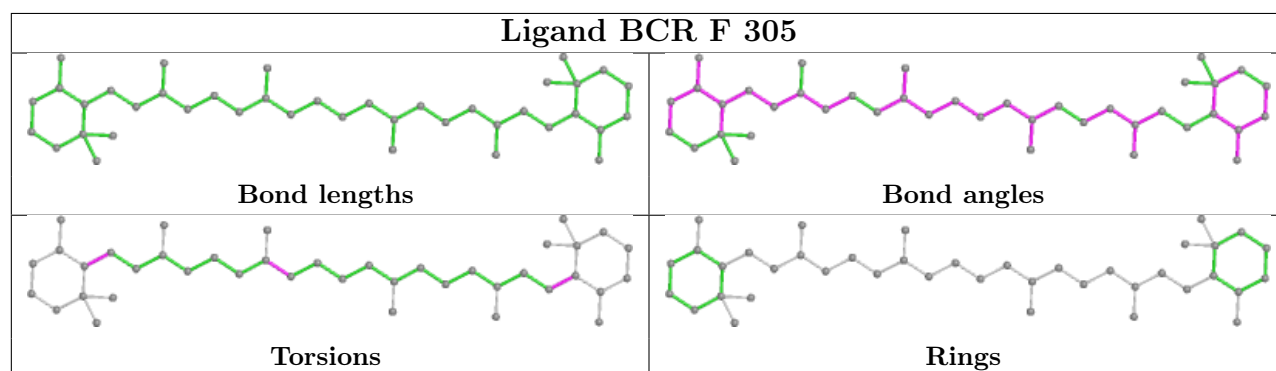
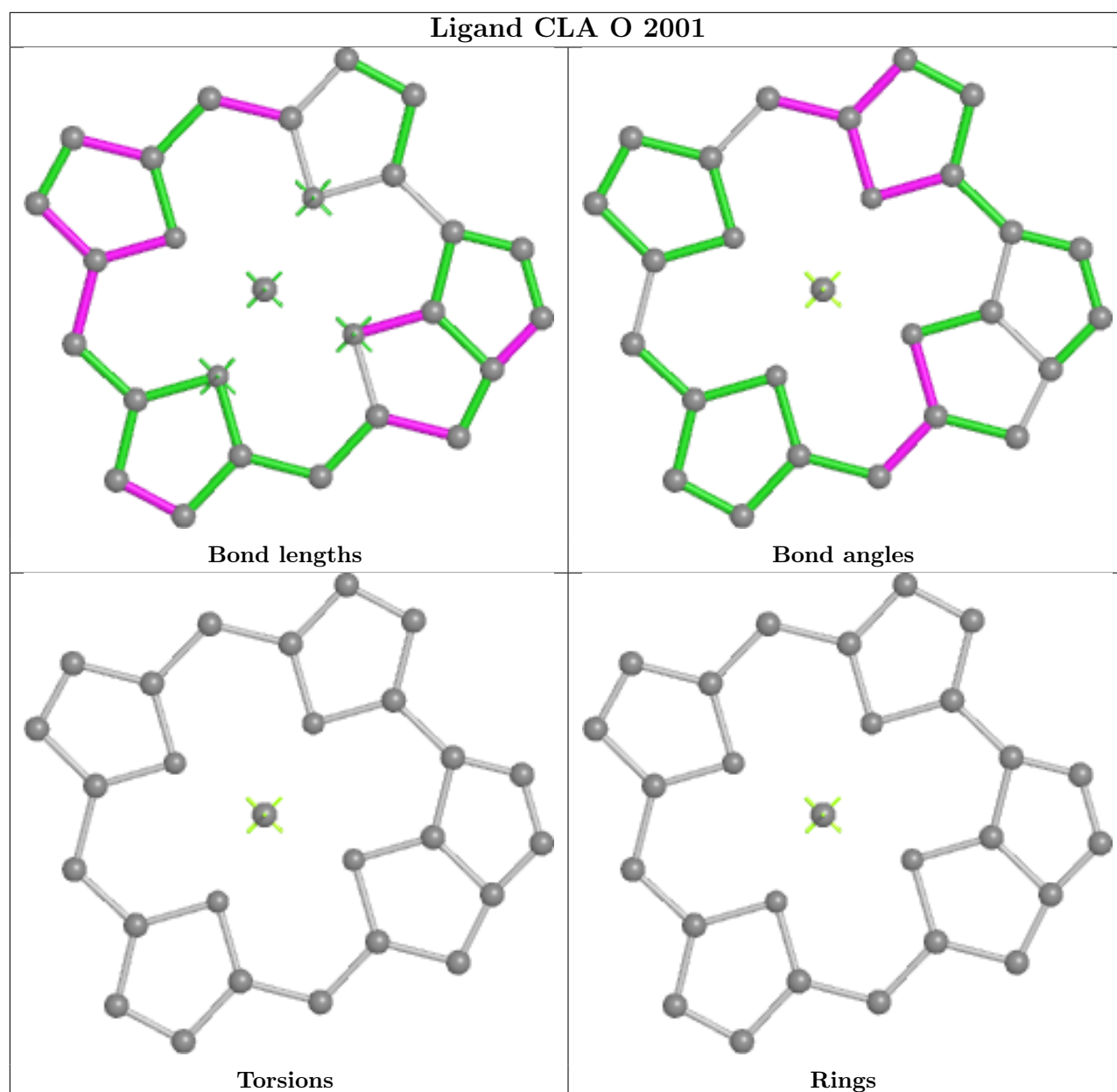


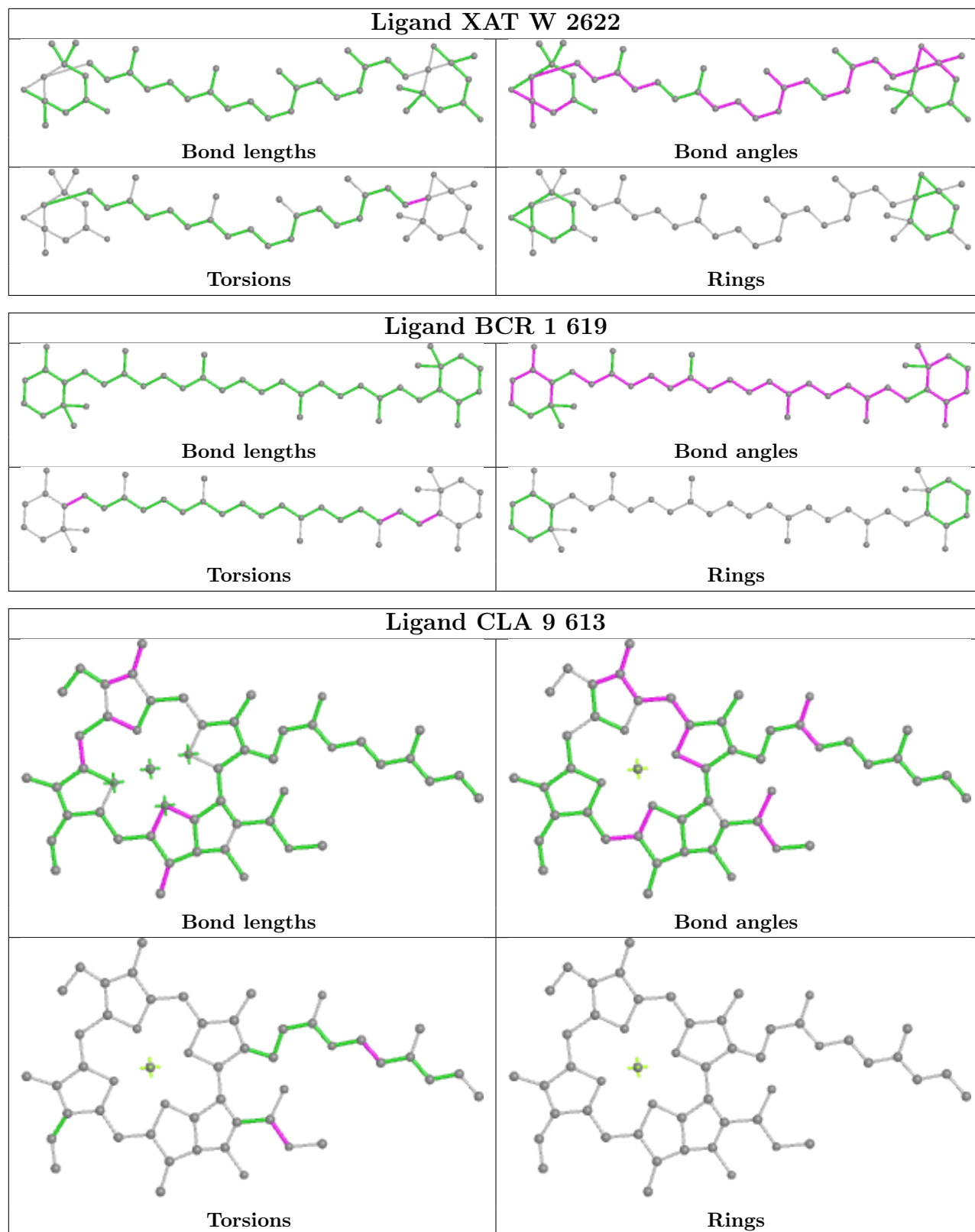
Torsions



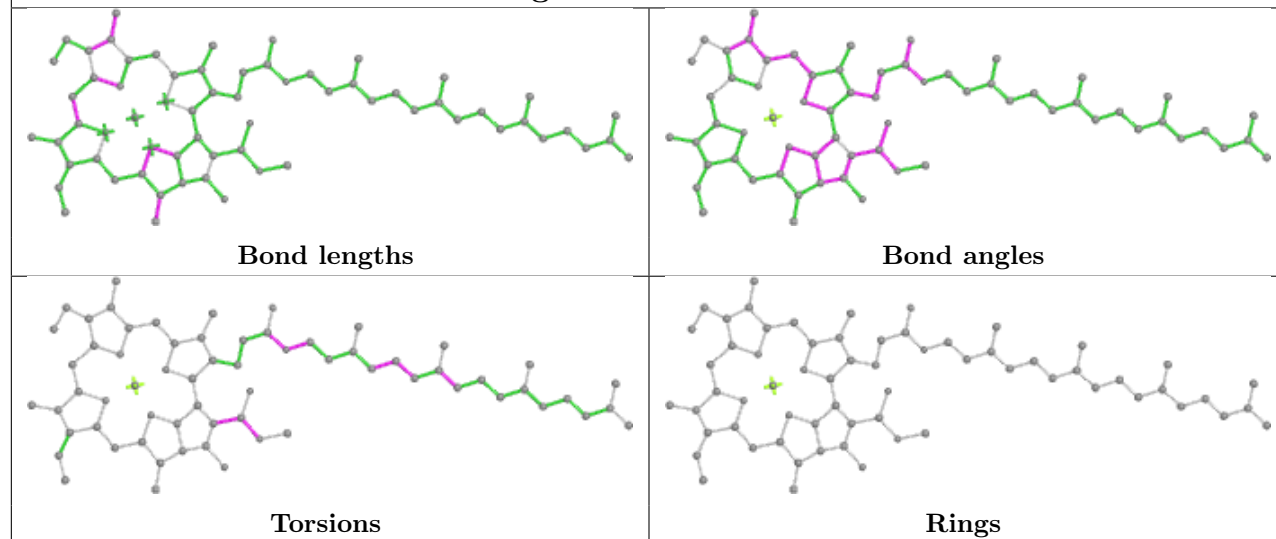
Rings



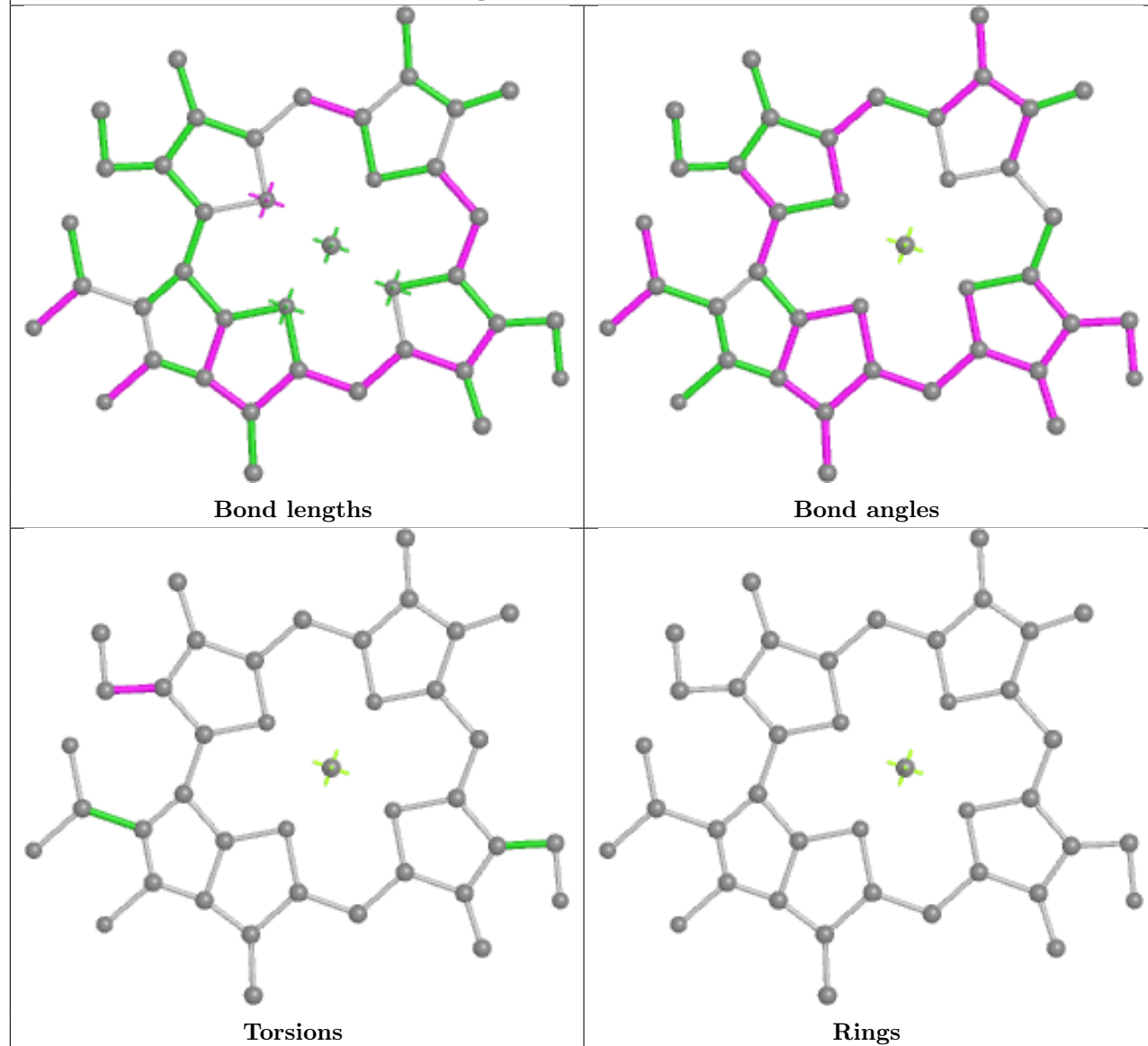




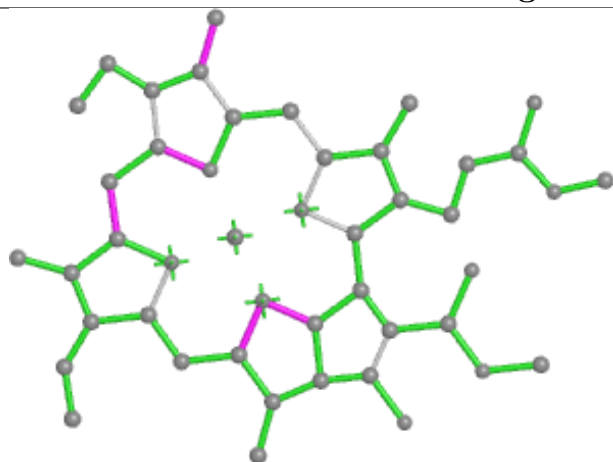
Ligand CLA A 801



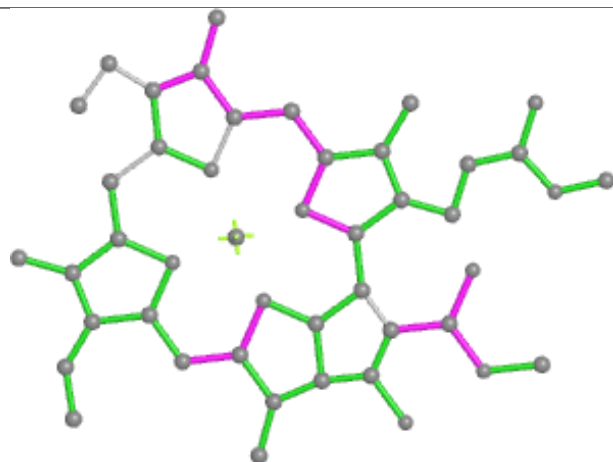
Ligand CHL W 608



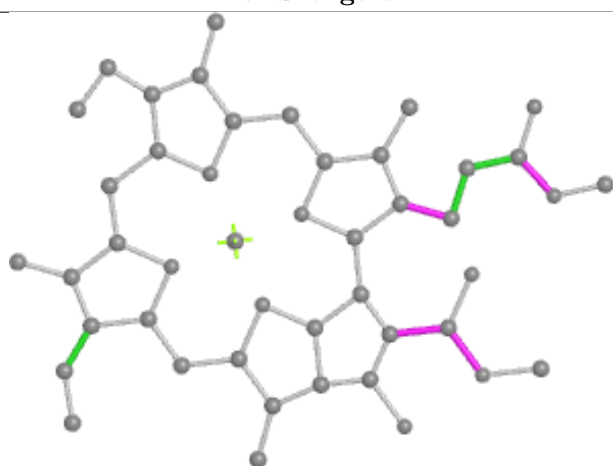
Ligand CLA 7 617



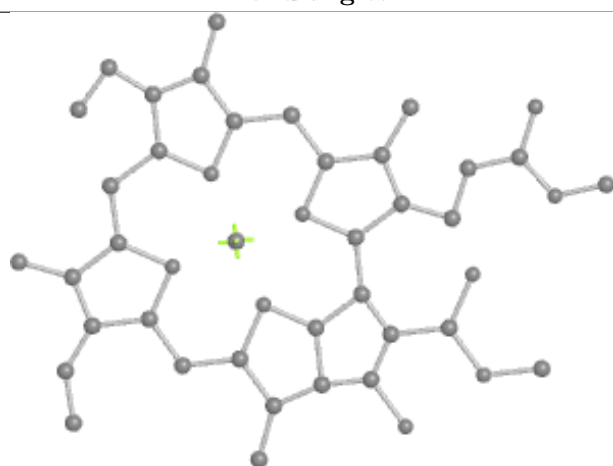
Bond lengths



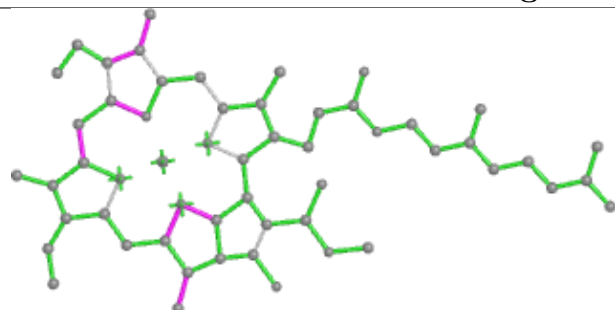
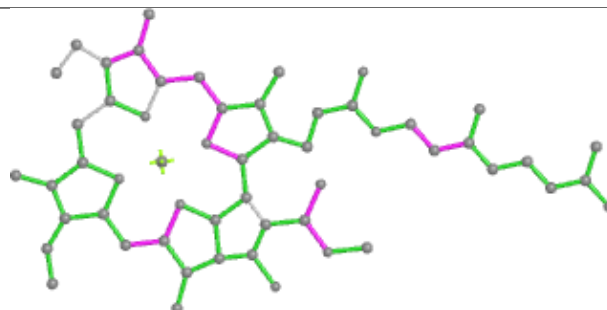
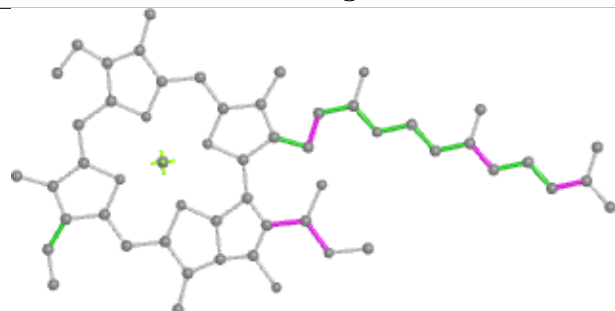
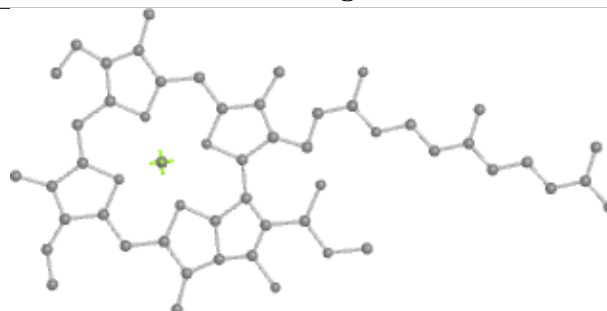
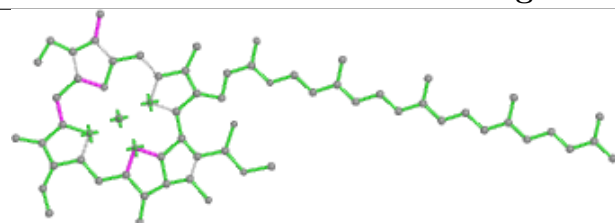
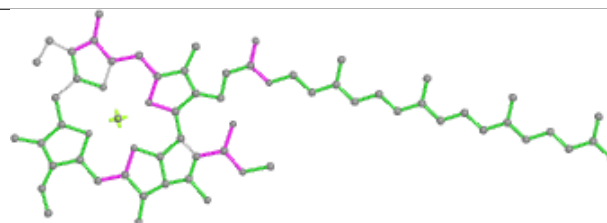
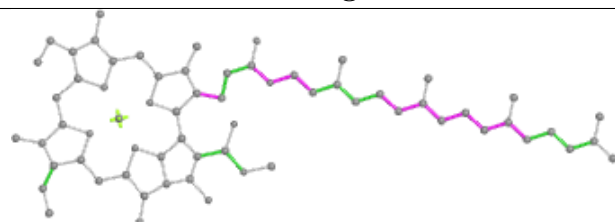
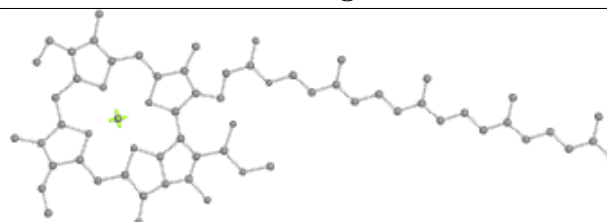
Bond angles

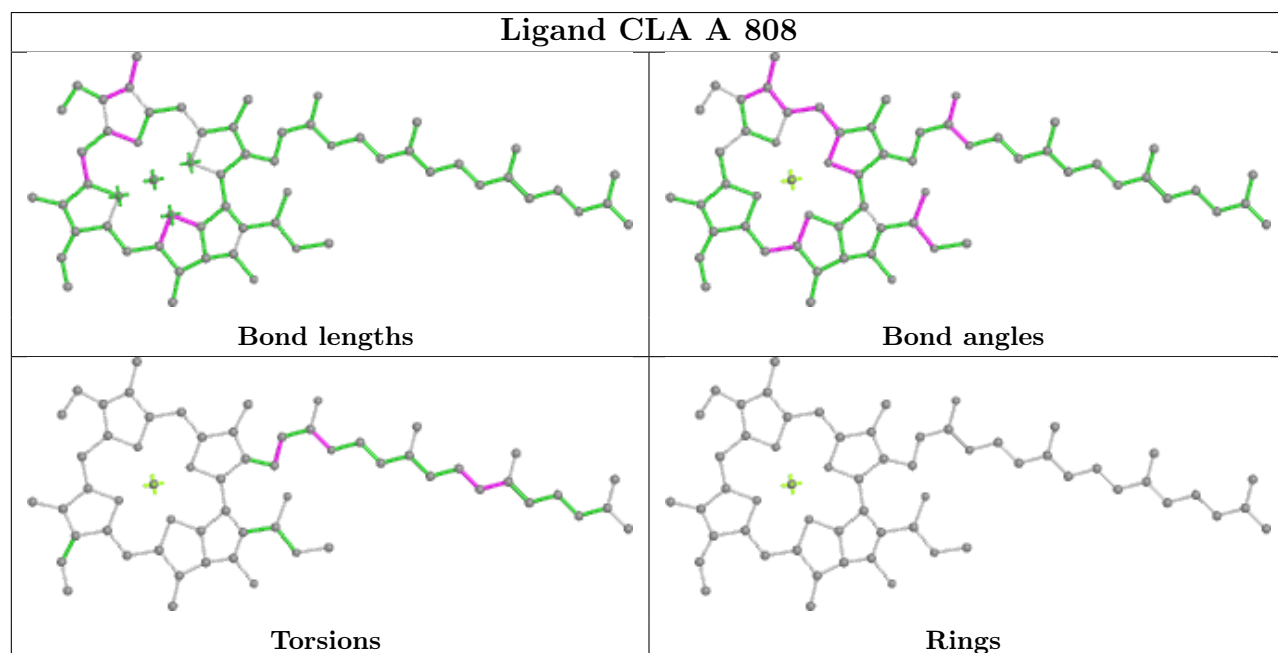
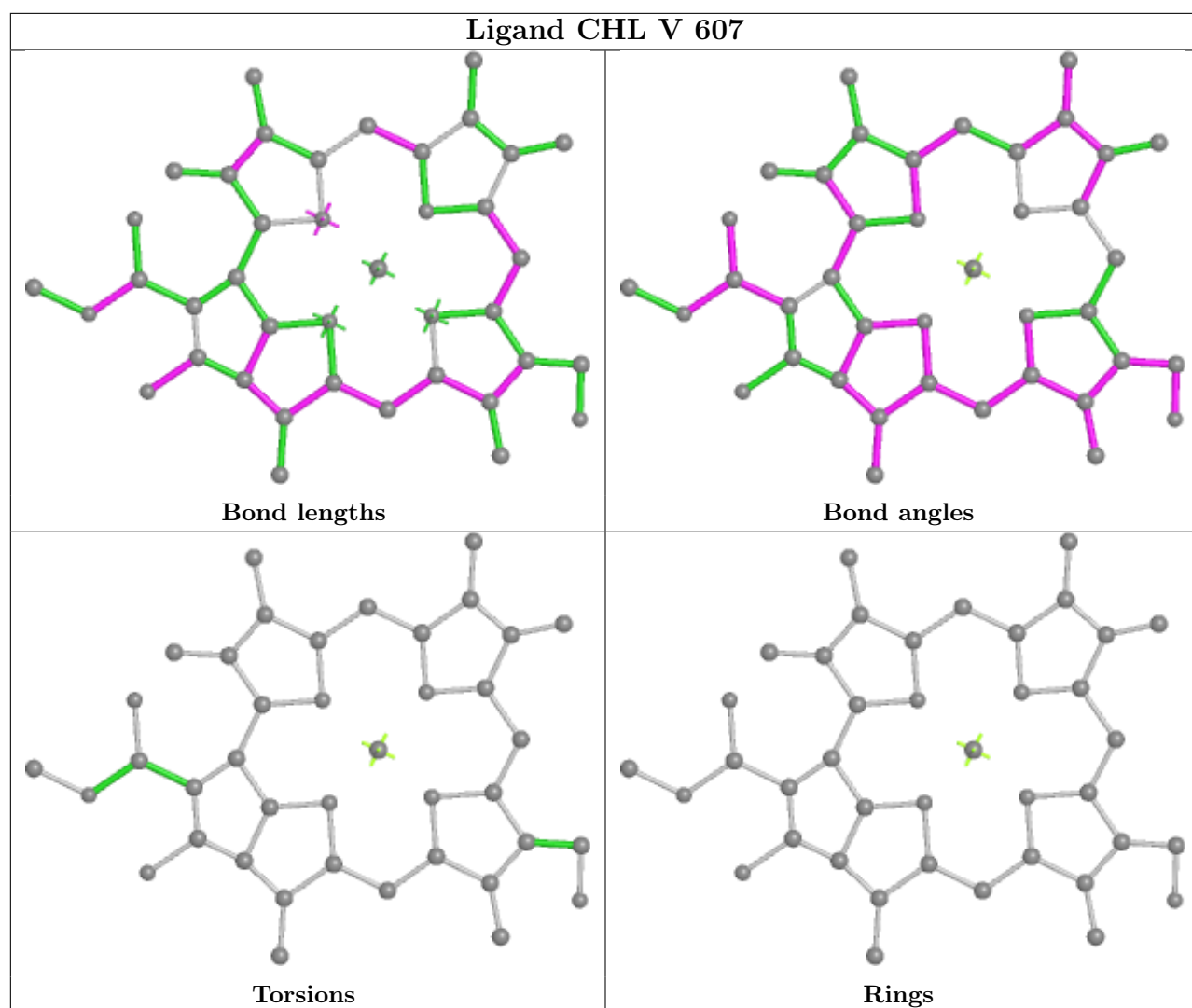


Torsions

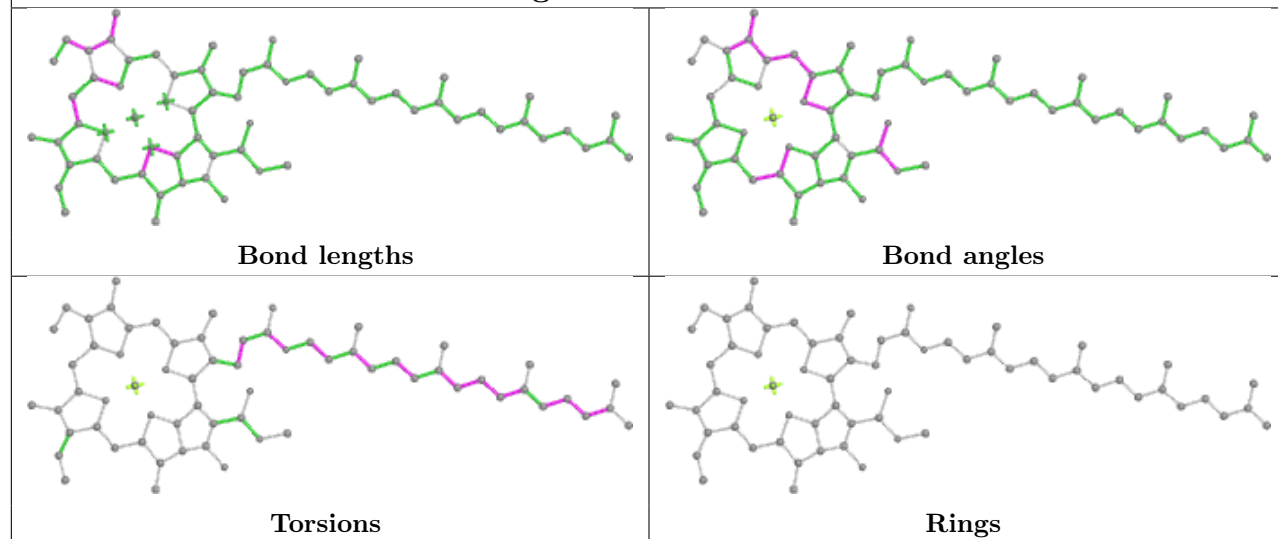


Rings

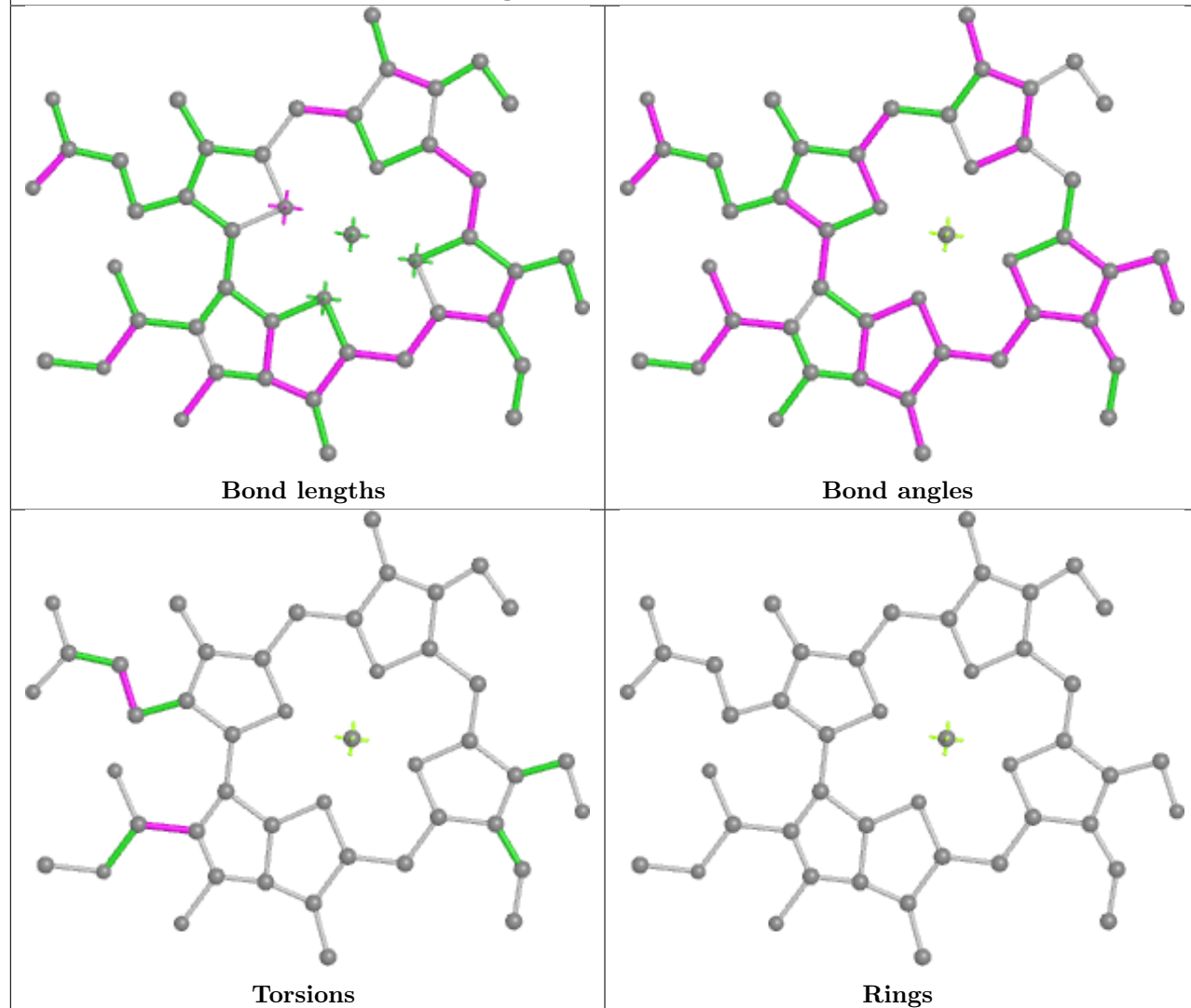
Ligand CLA 7 613**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA A 805****Bond lengths****Bond angles****Torsions****Rings**

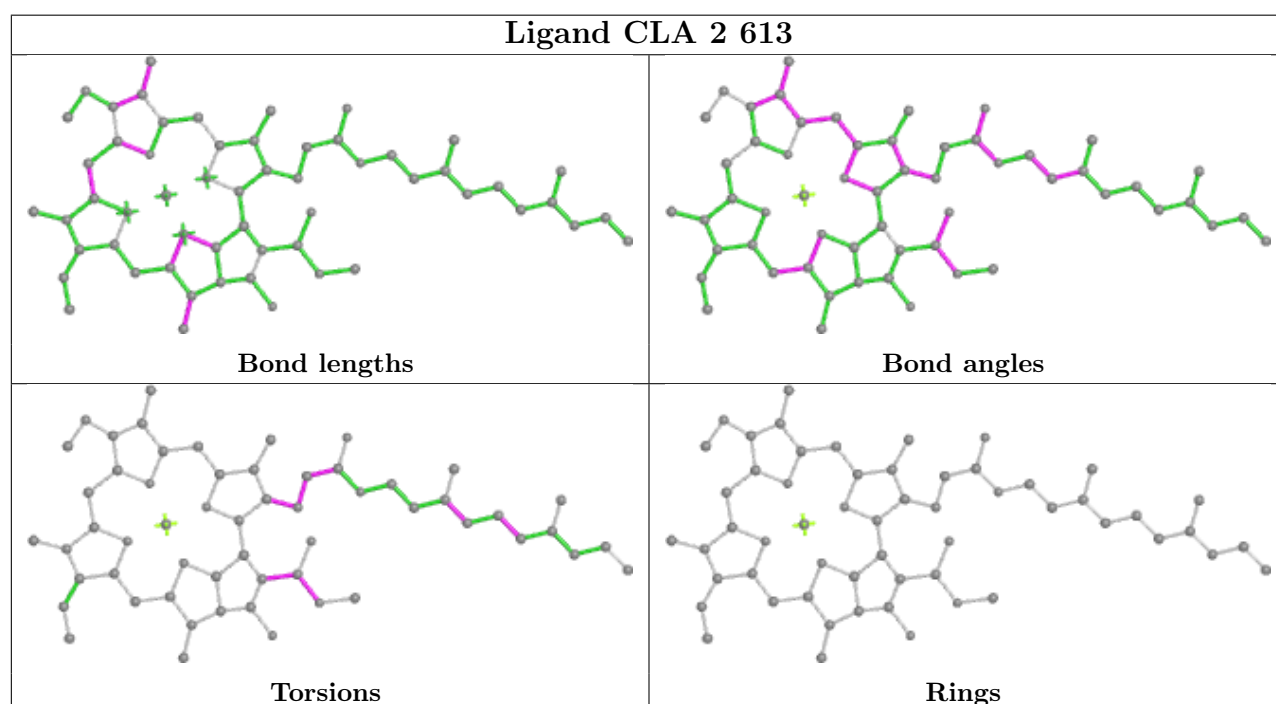
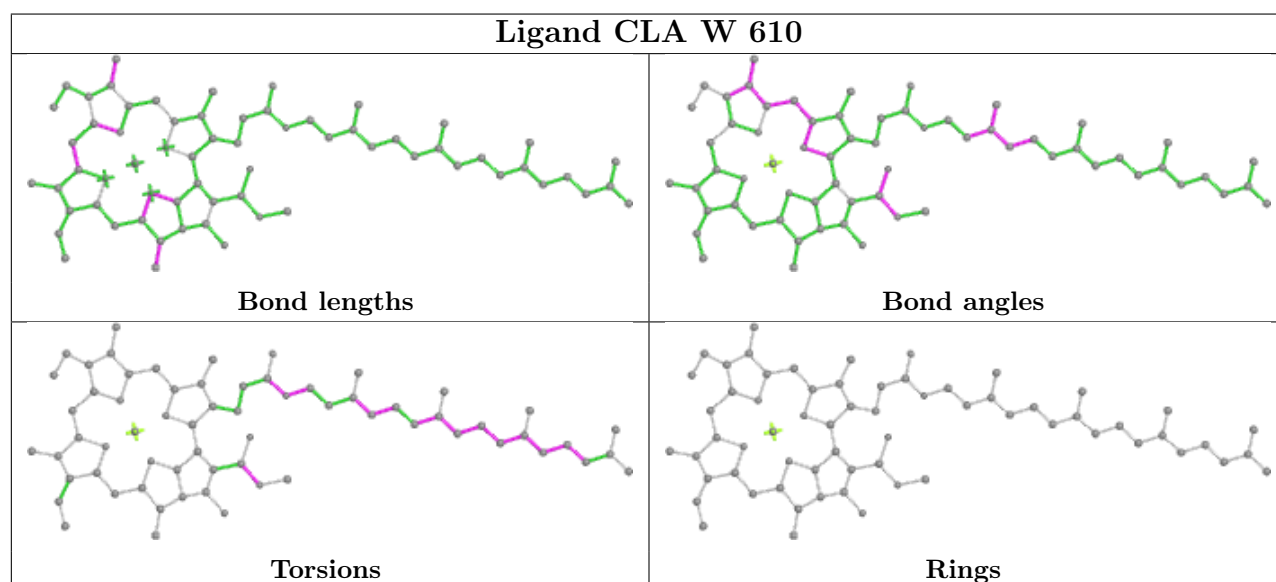
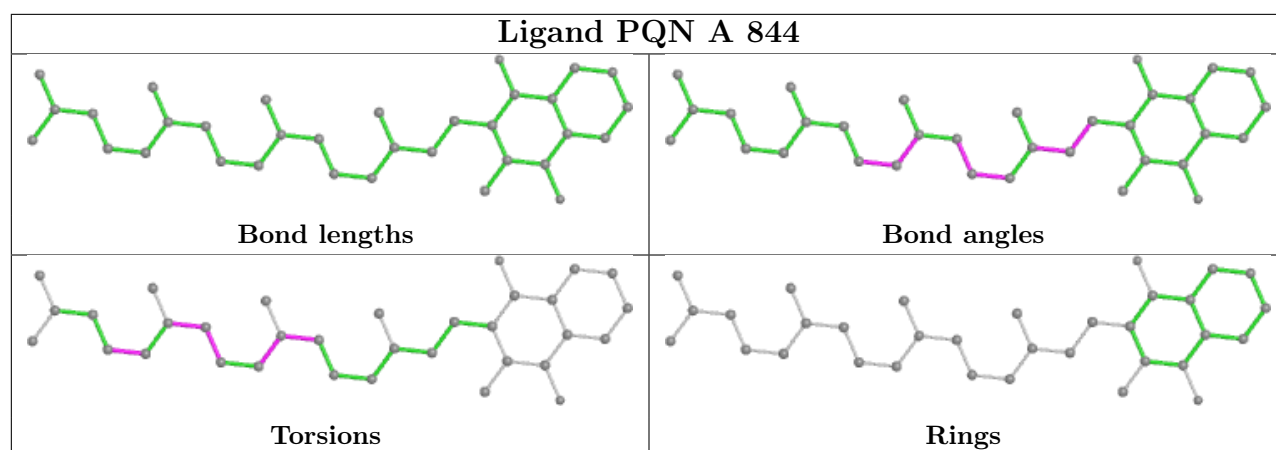


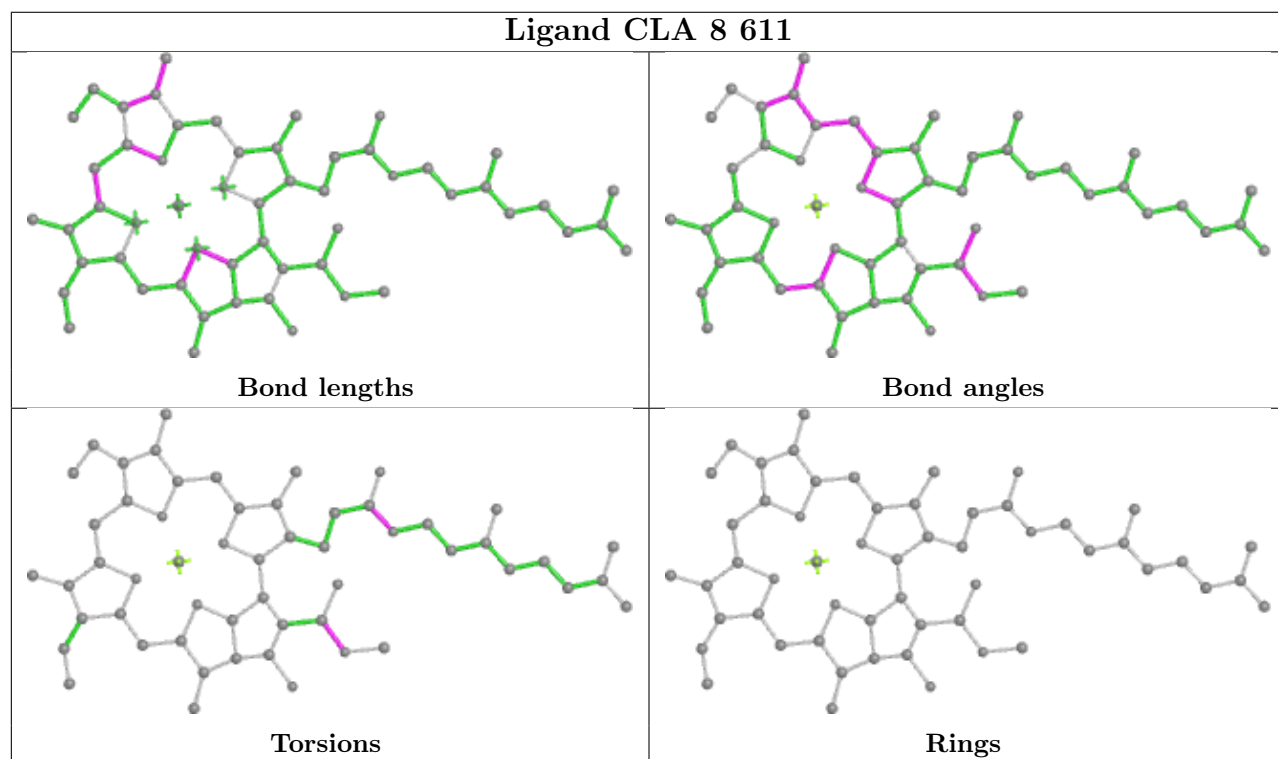
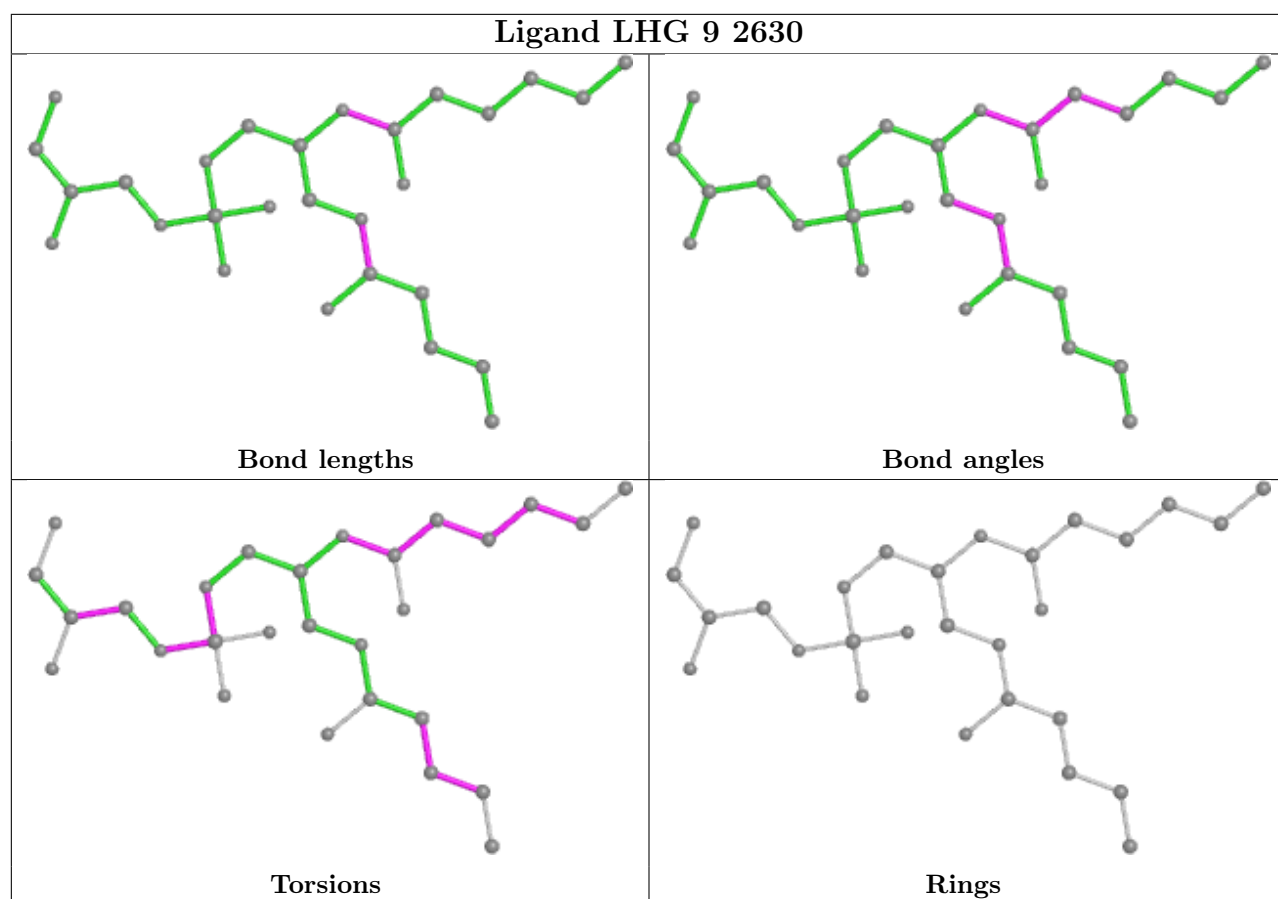
Ligand CLA B 817



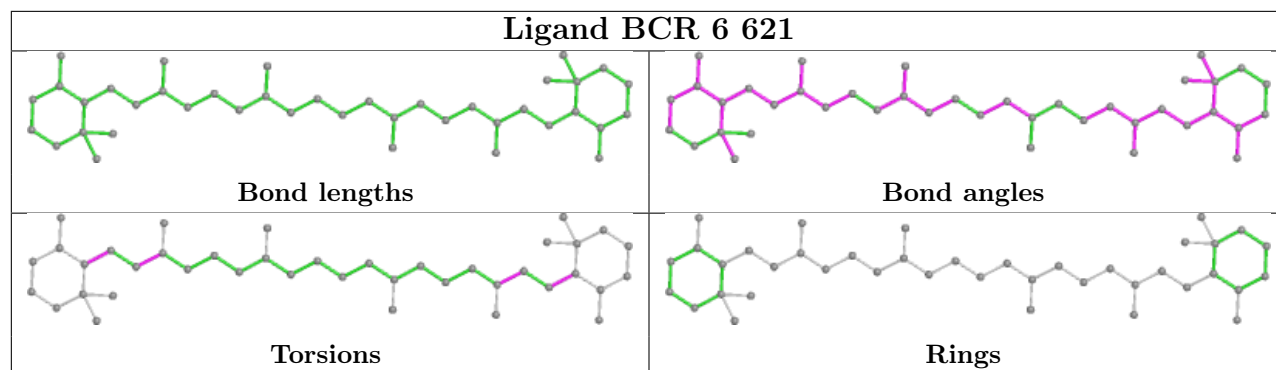
Ligand CHL 2 601



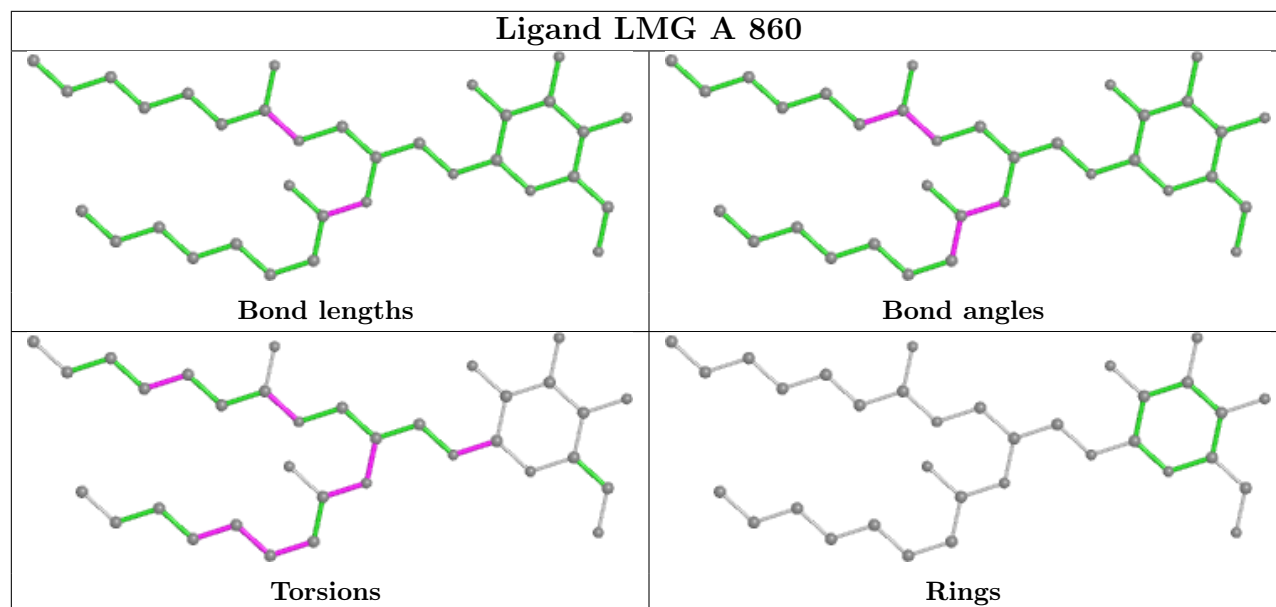




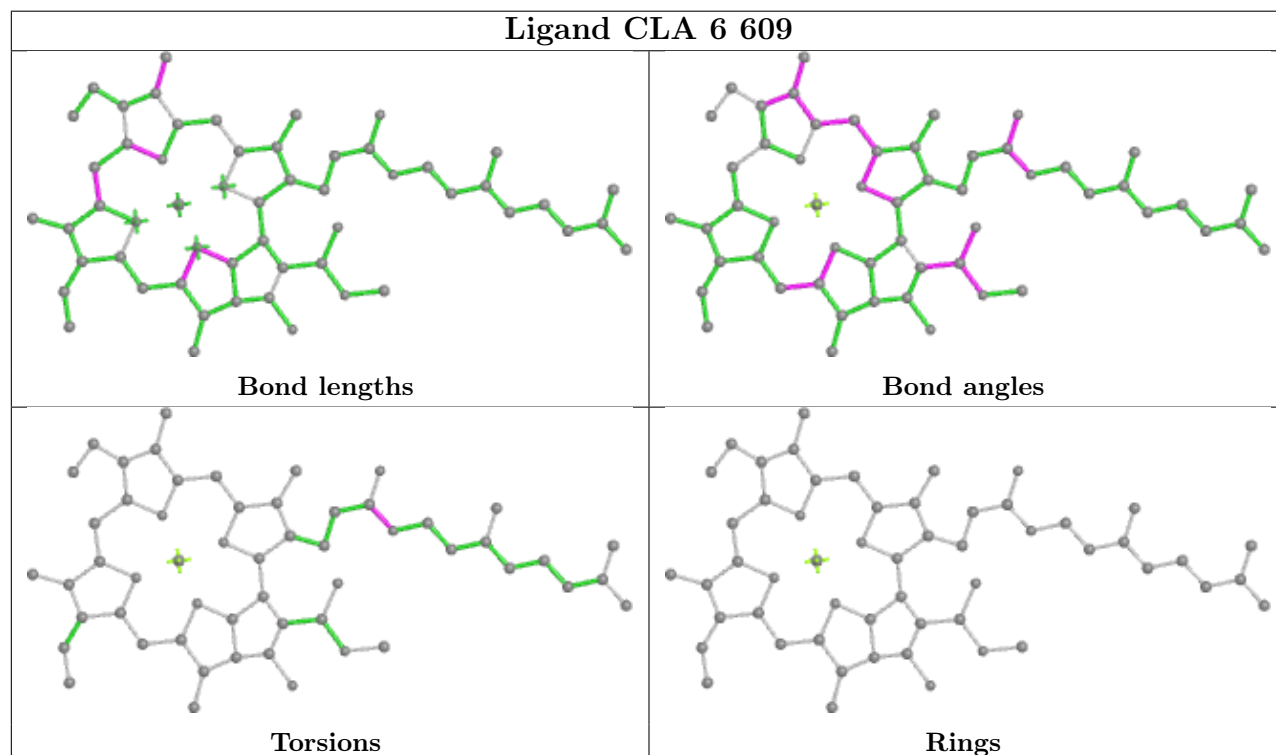
Ligand BCR 6 621



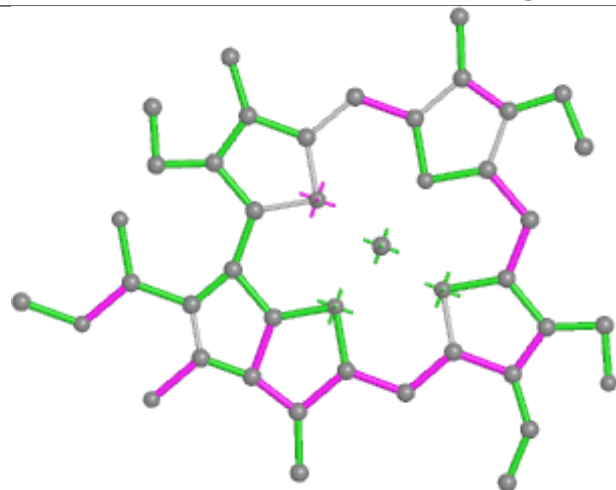
Ligand LMG A 860



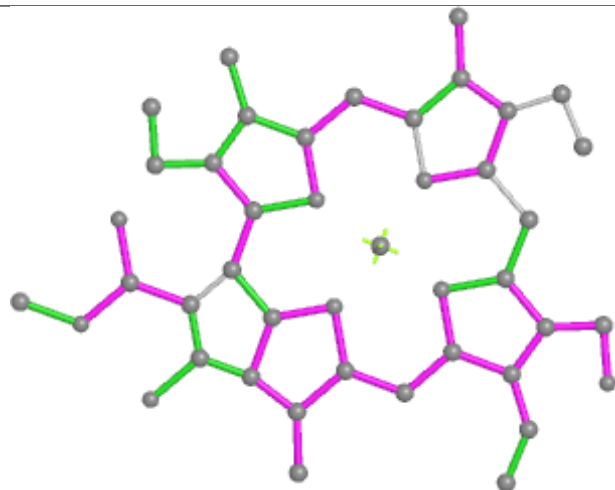
Ligand CLA 6 609



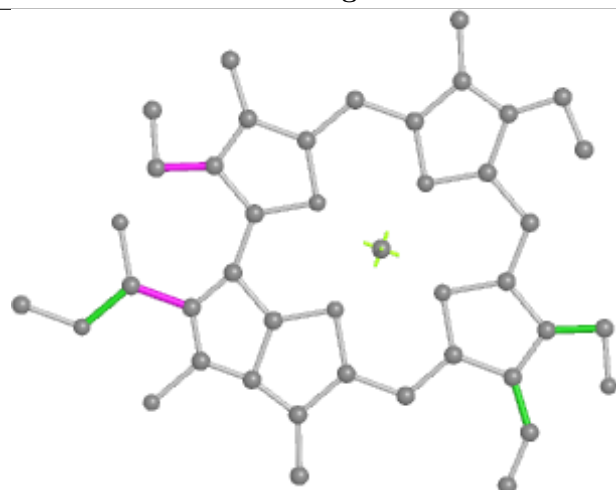
Ligand CHL 9 607



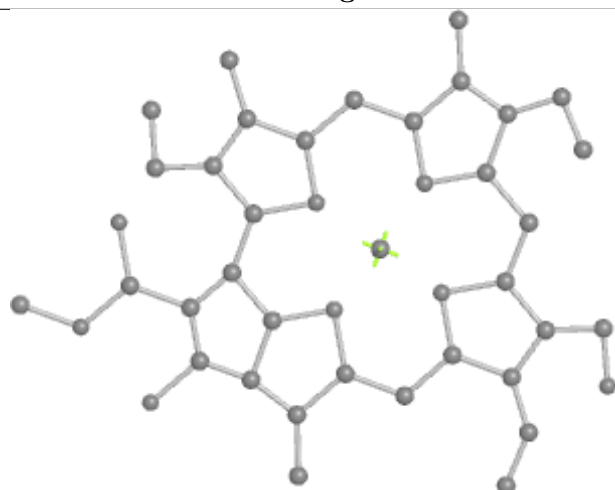
Bond lengths



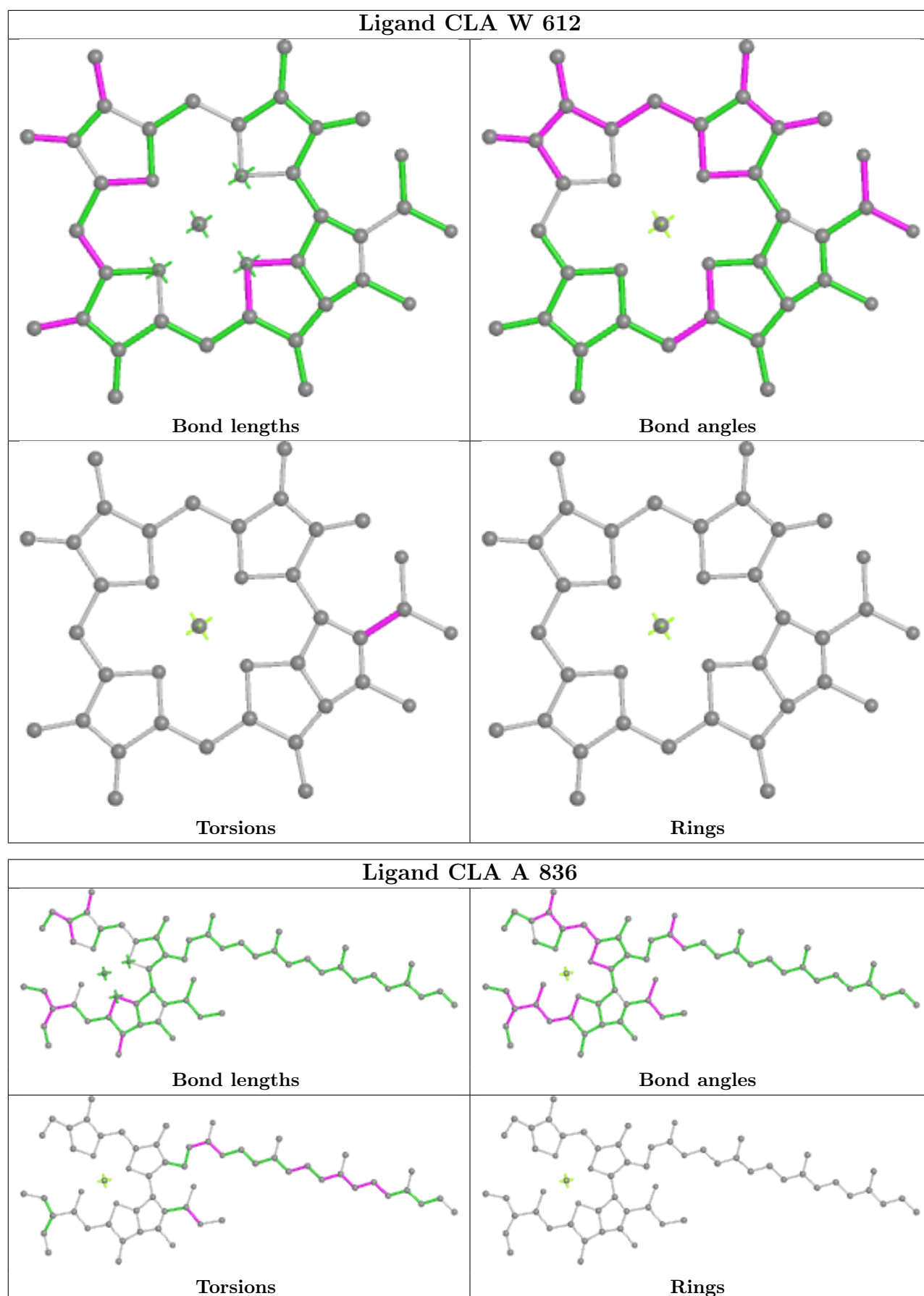
Bond angles

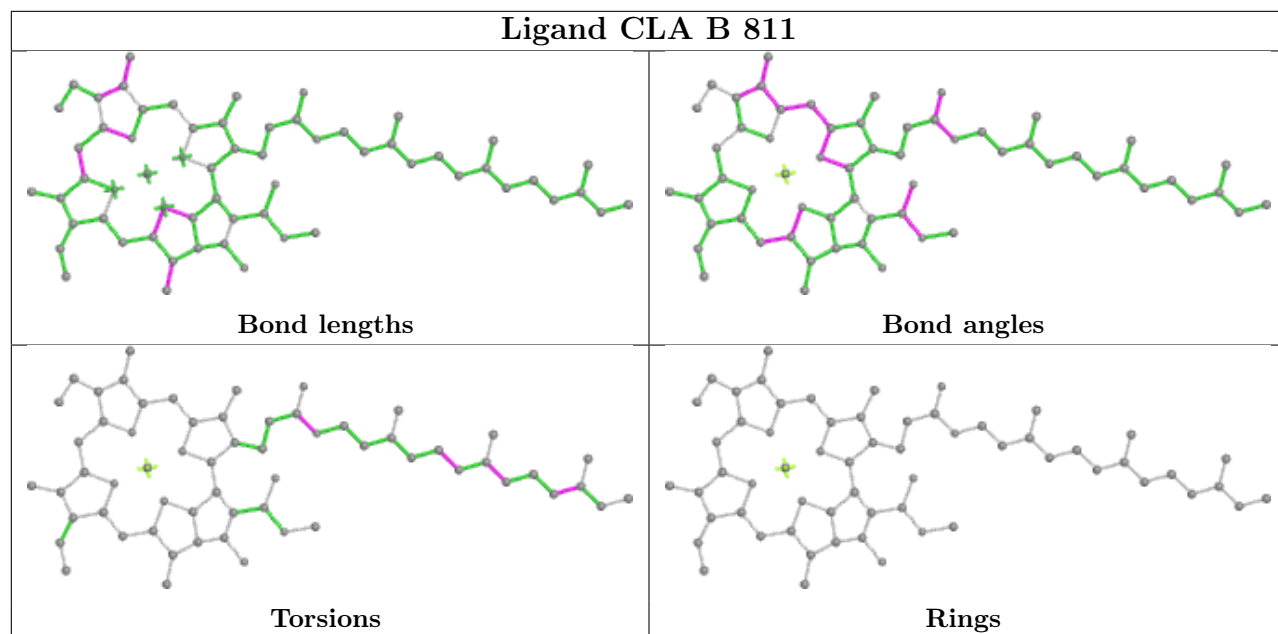
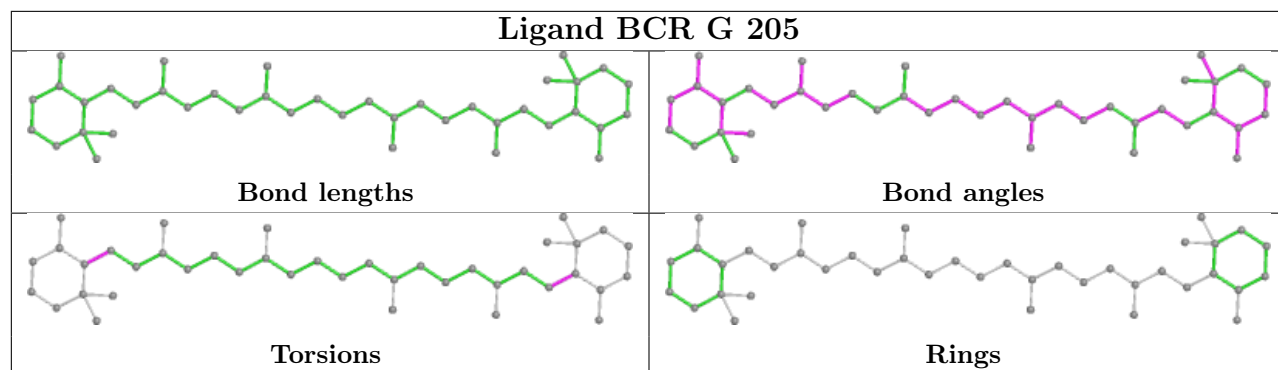


Torsions

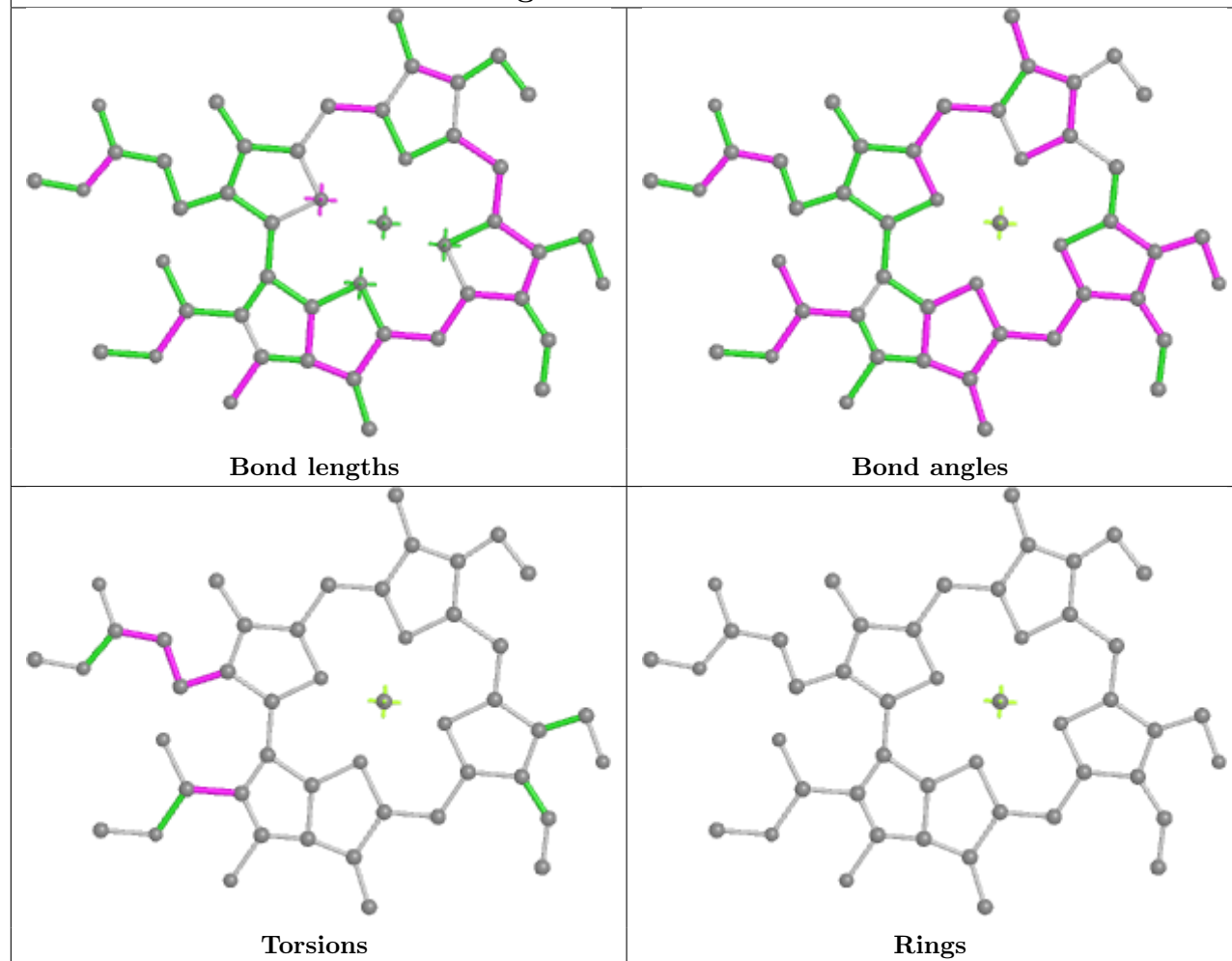


Rings

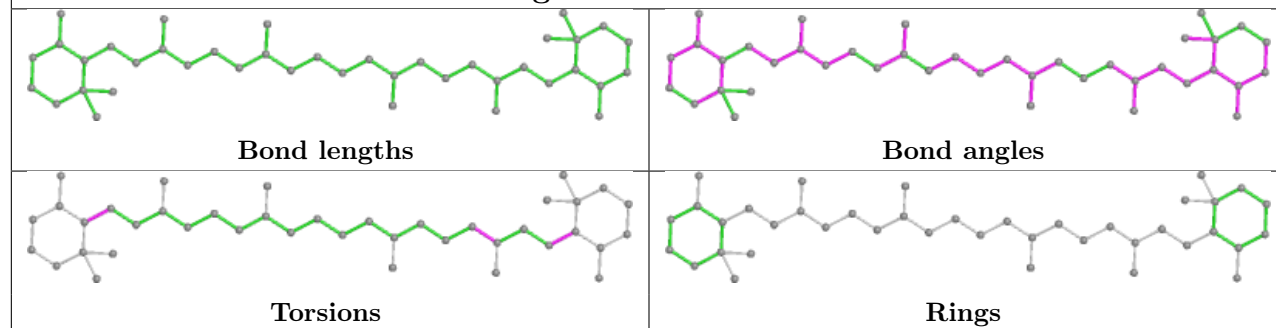




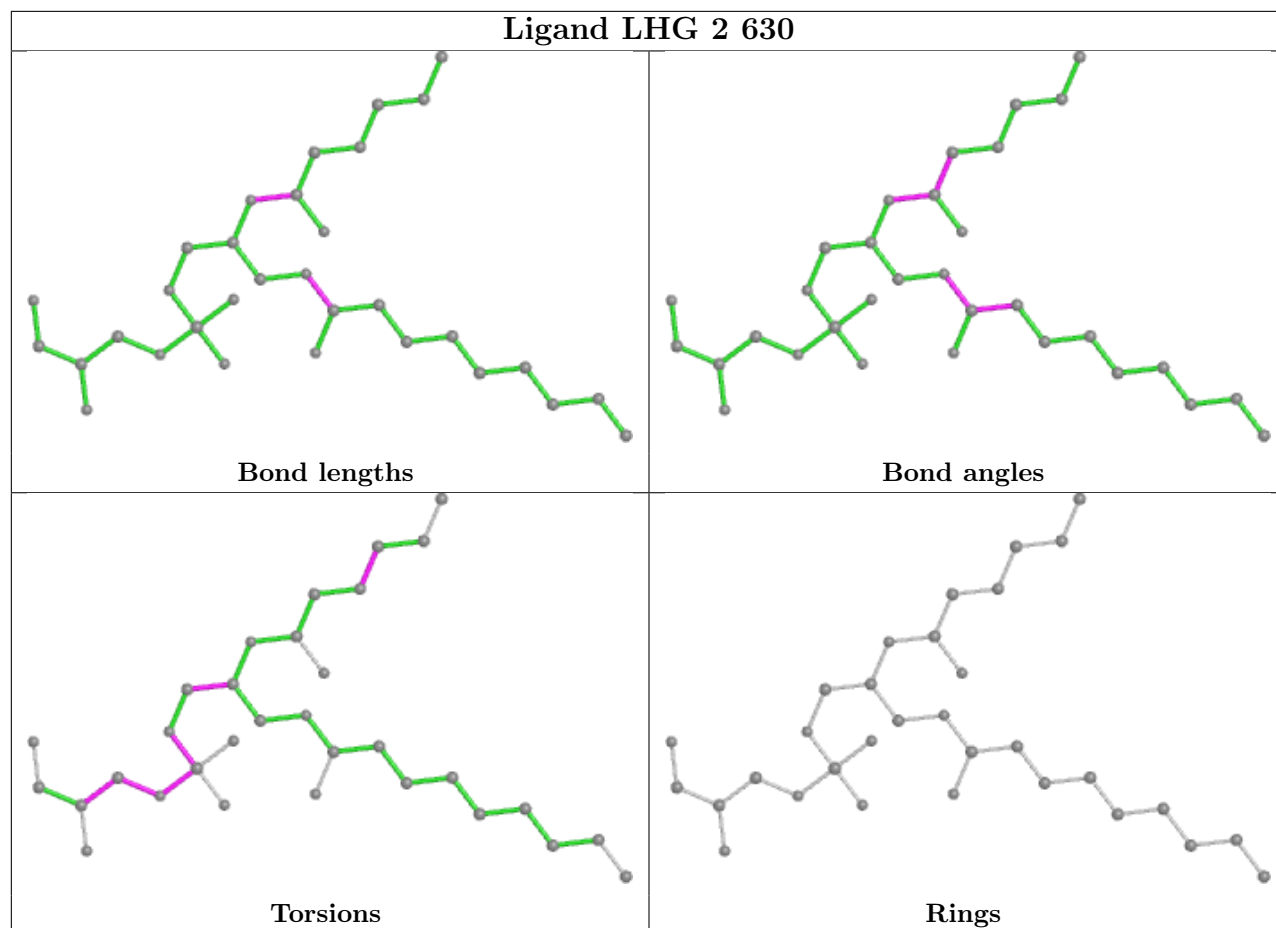
Ligand CHL 1 607



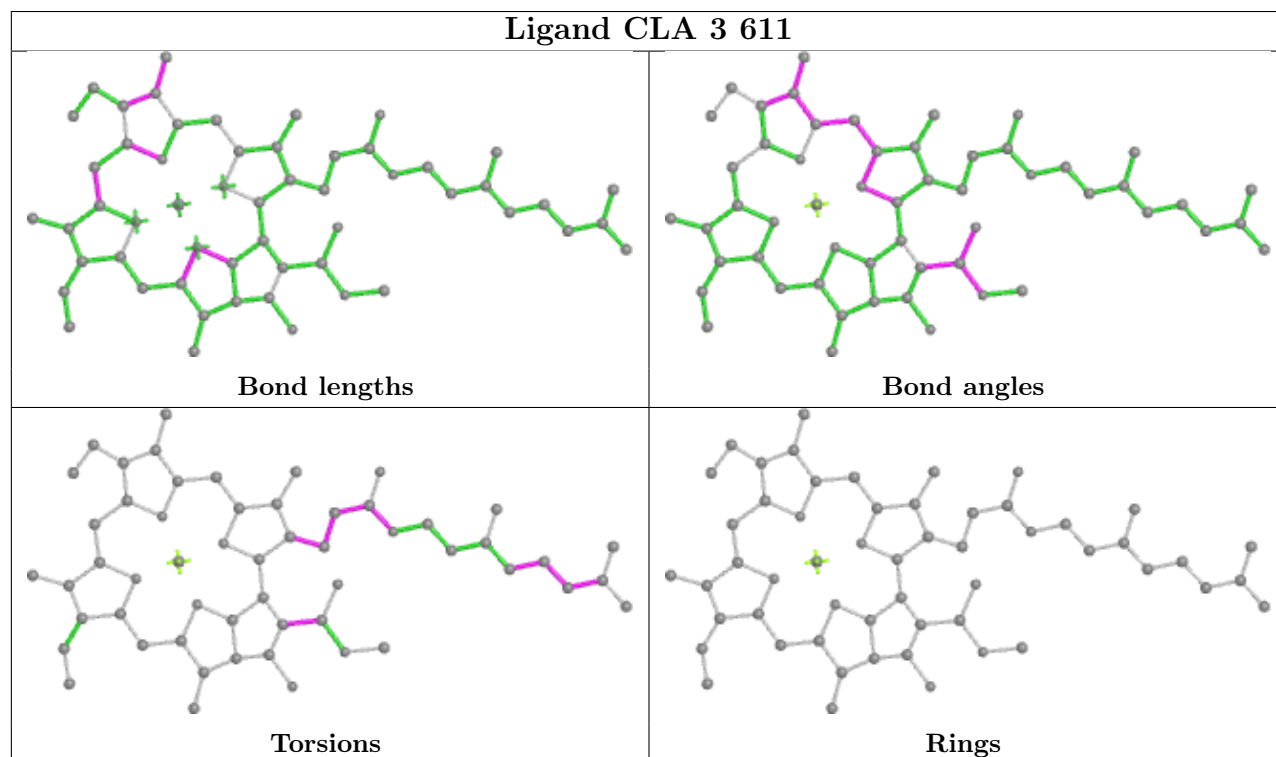
Ligand BCR L 301

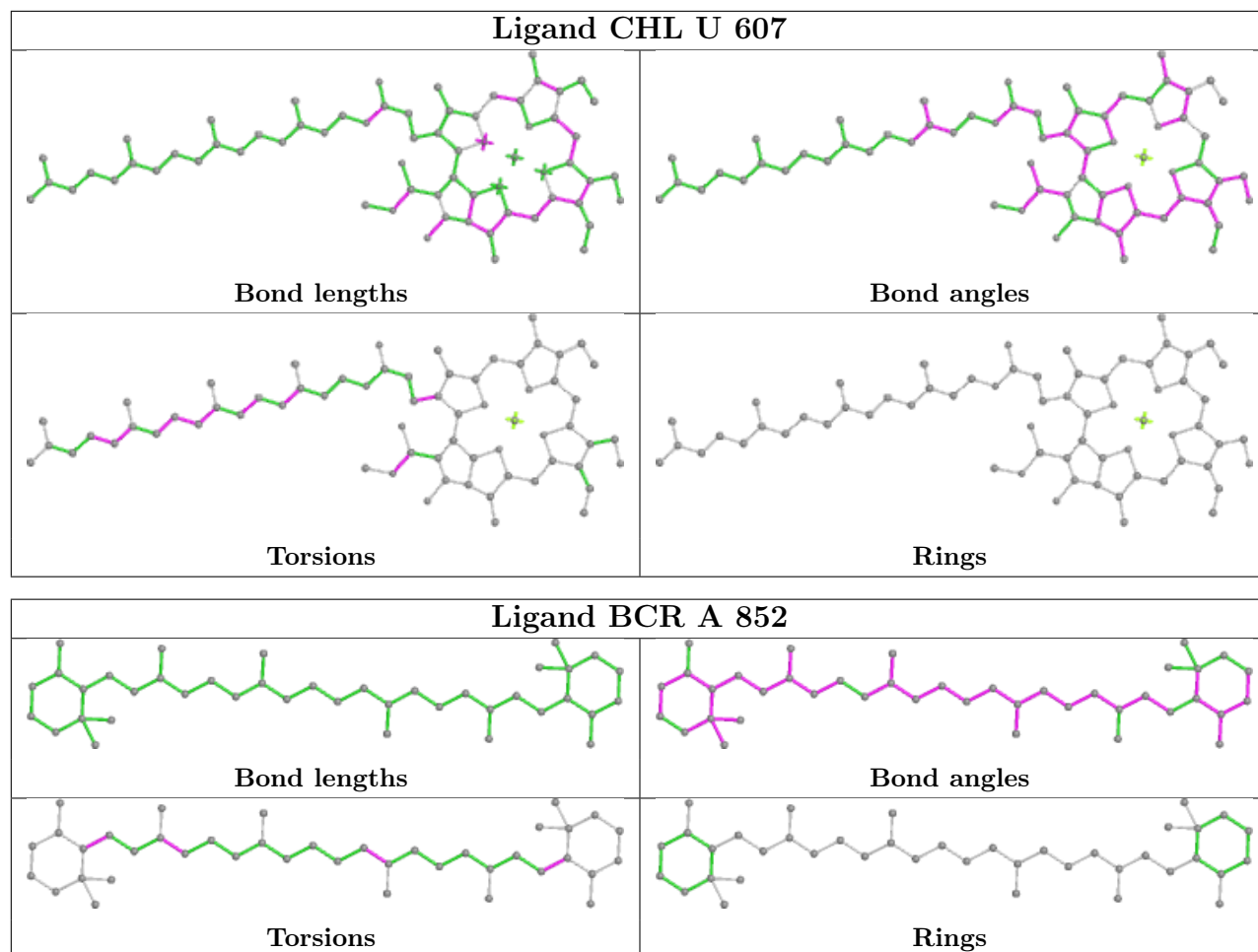


Ligand LHG 2 630

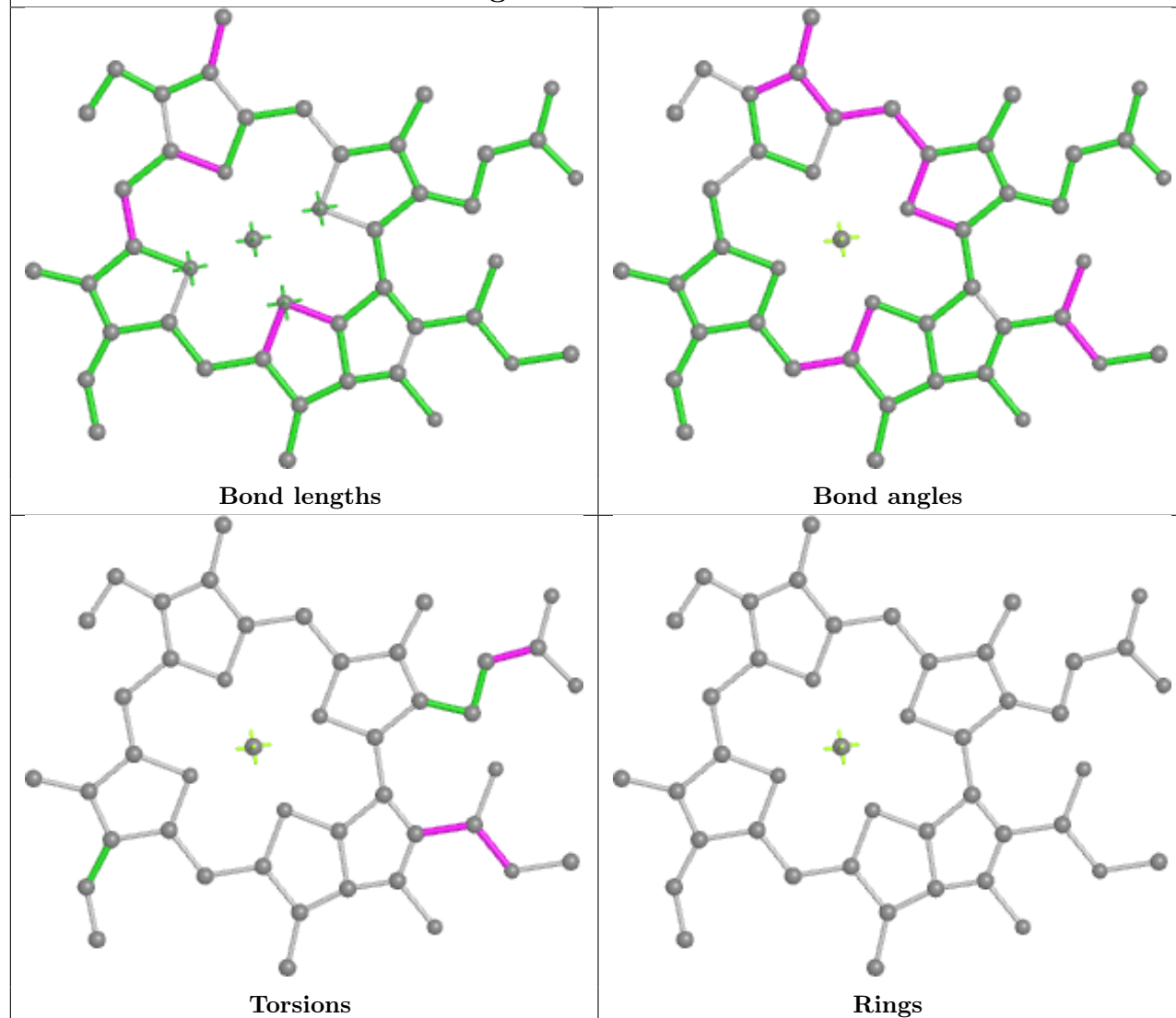


Ligand CLA 3 611

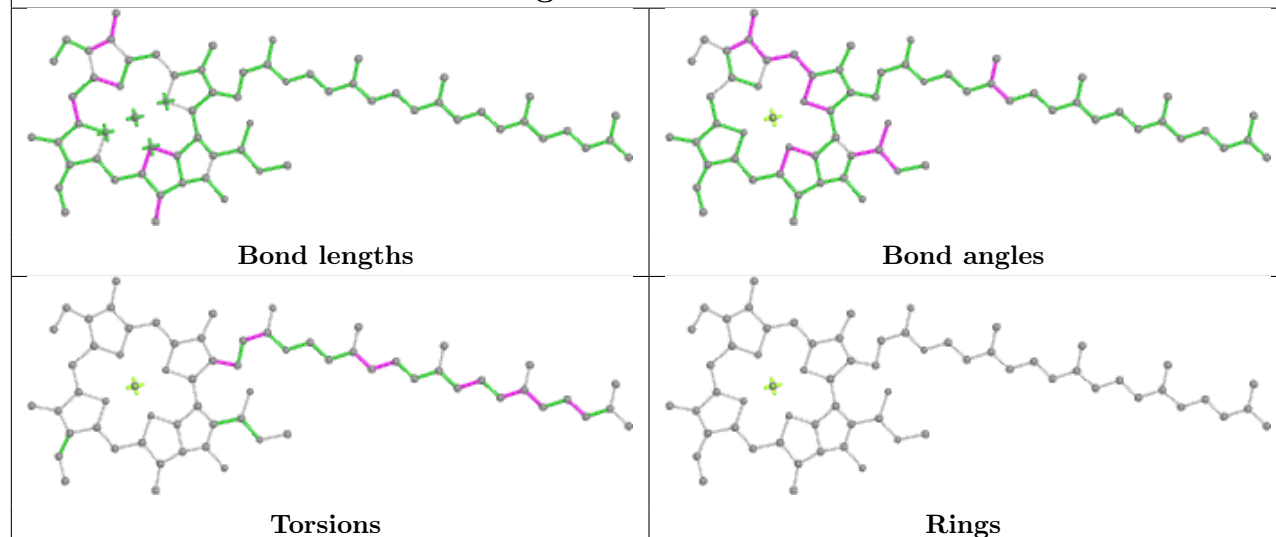


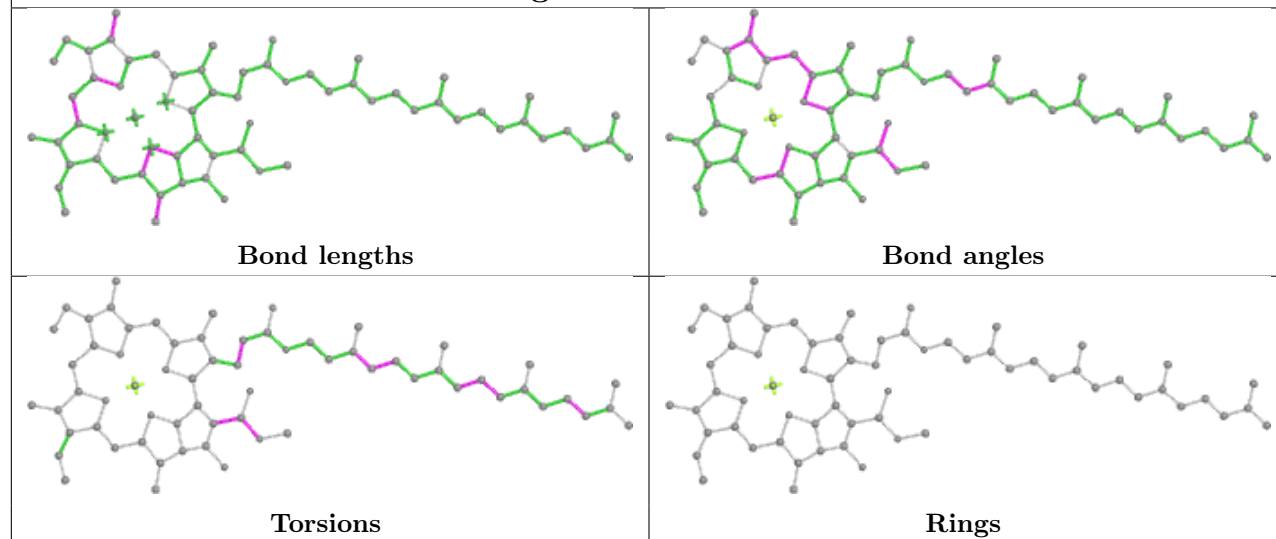
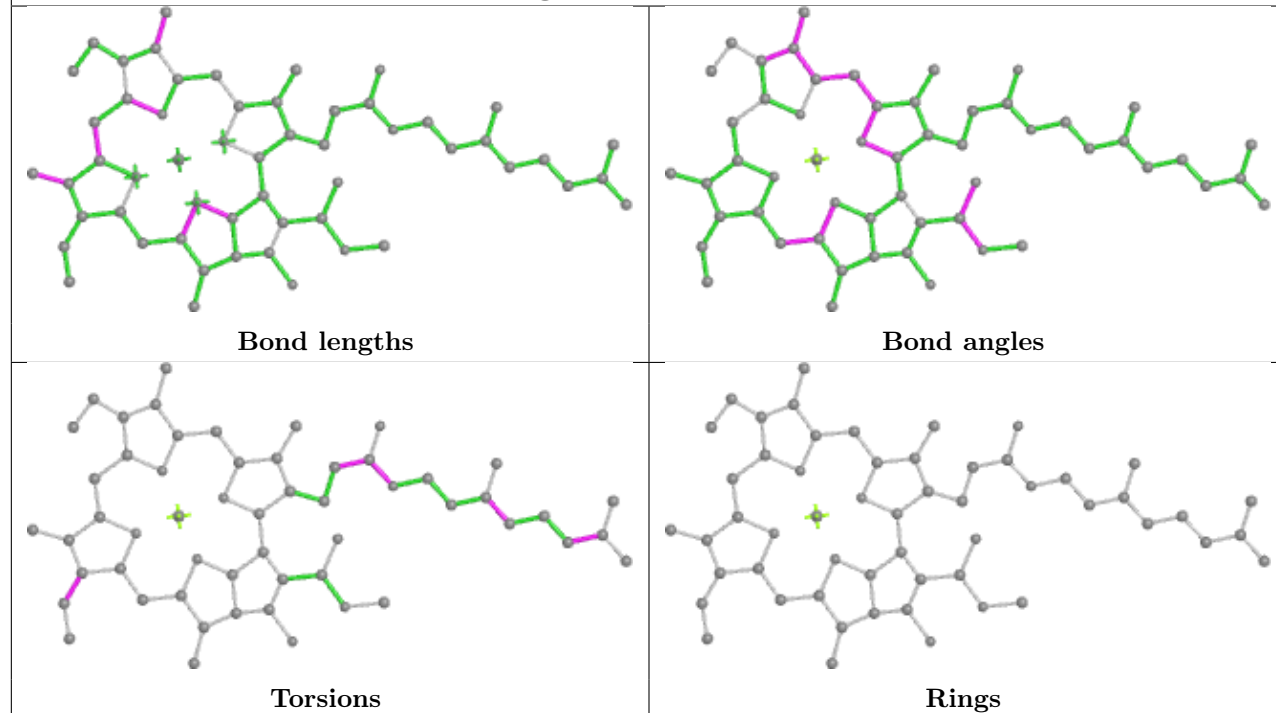


Ligand CLA U 611

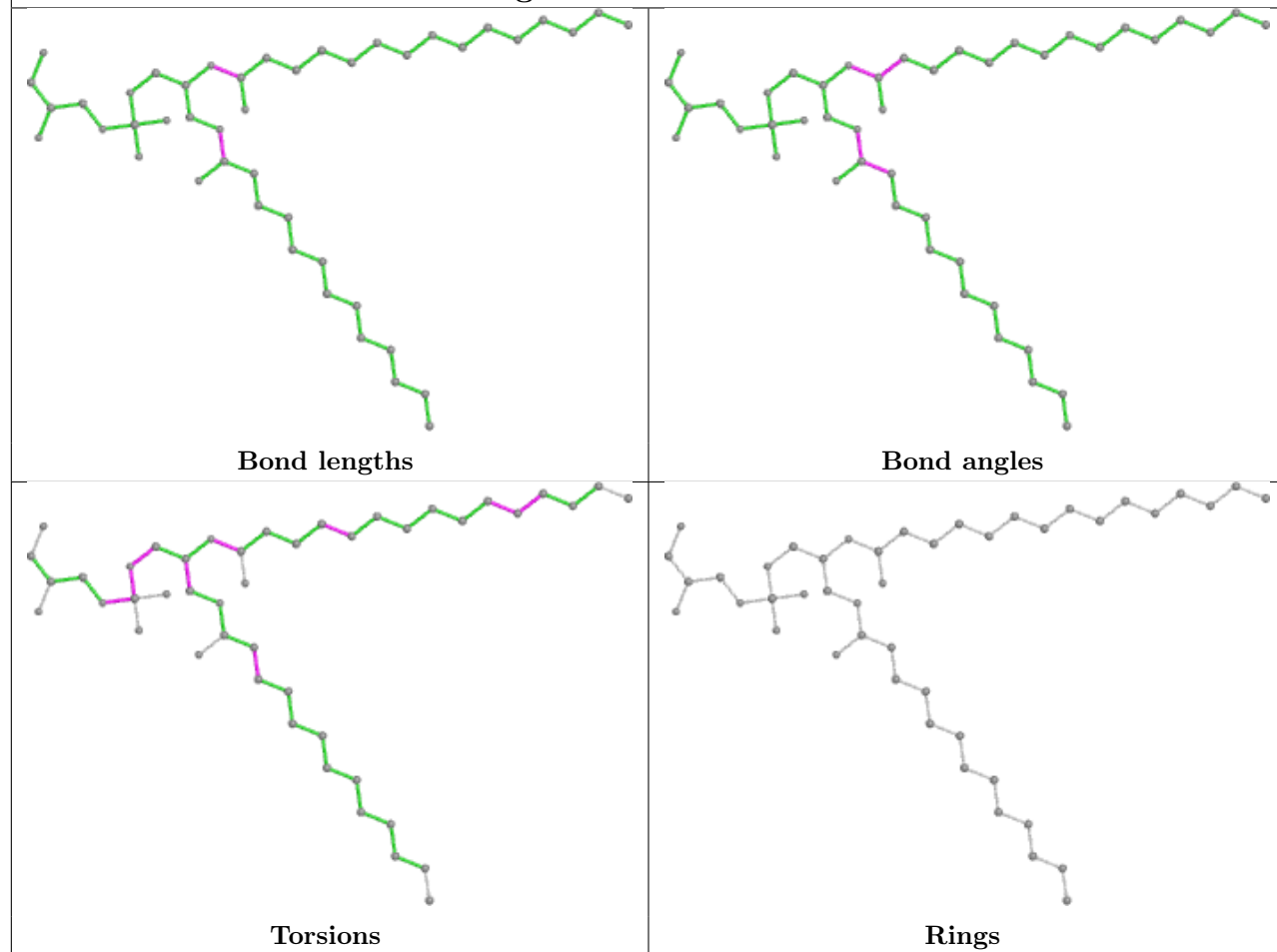


Ligand CLA 3 609

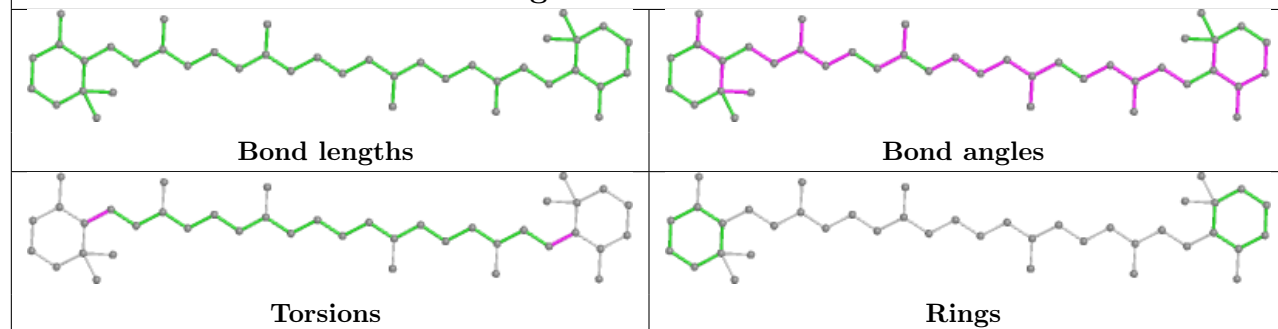


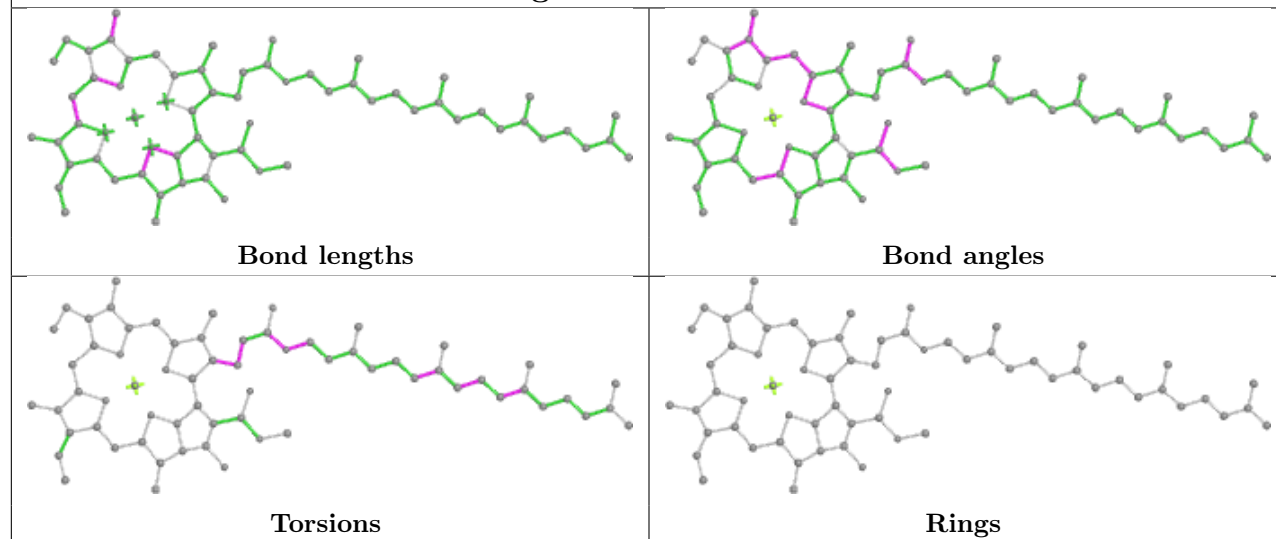
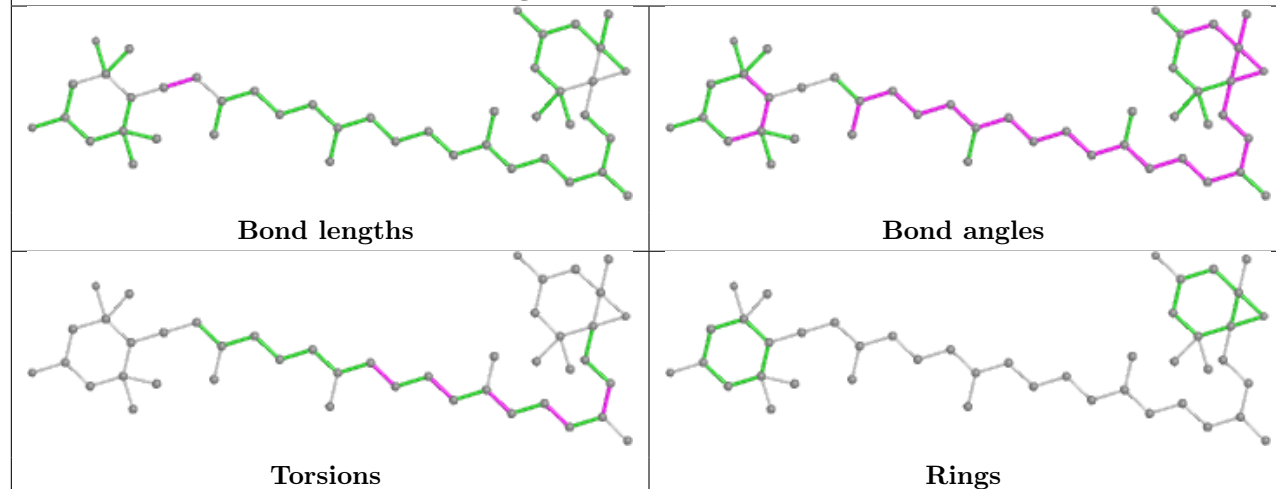
Ligand CLA U 613**Ligand CLA 8 609**

Ligand LHG W 2630

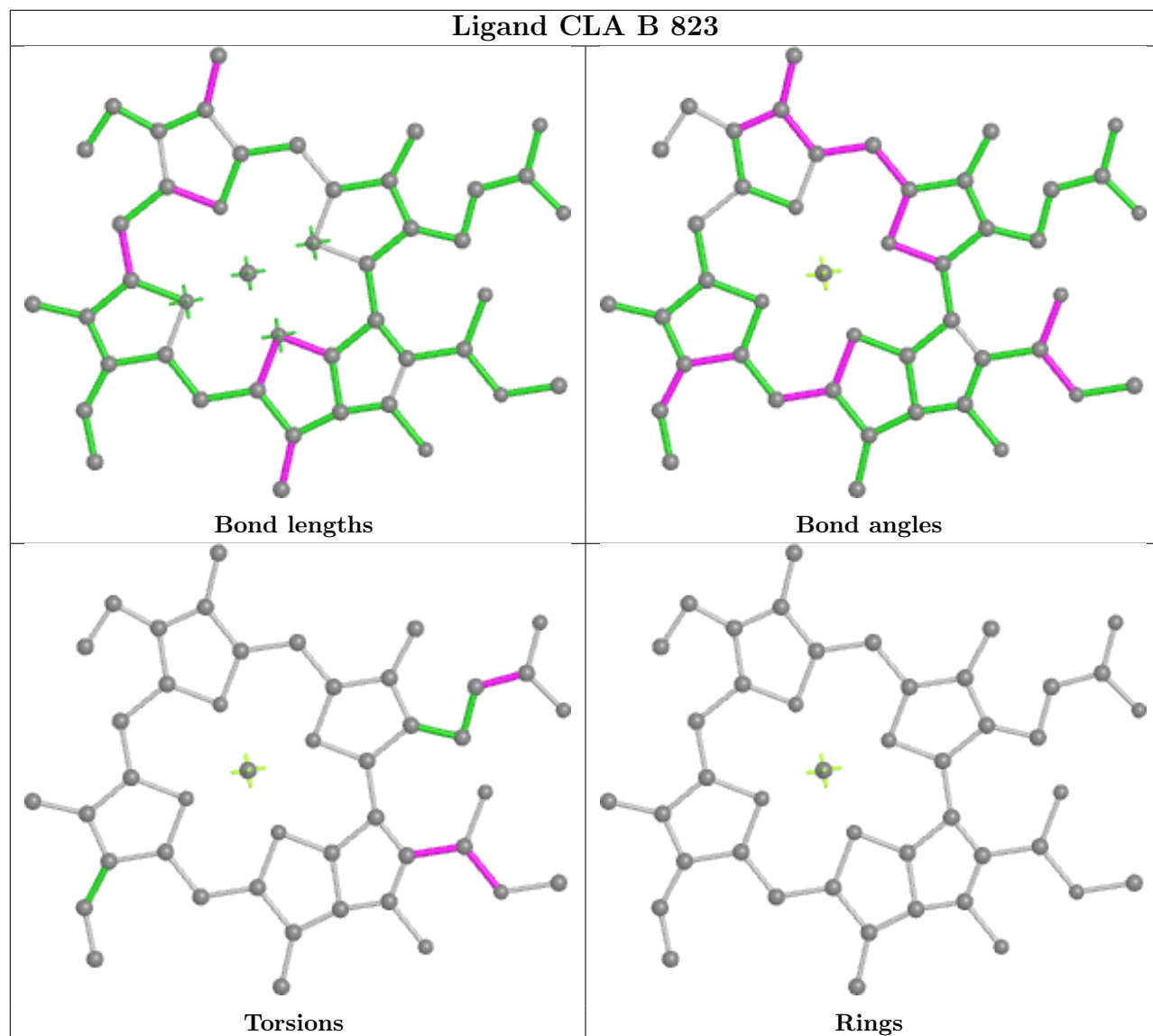


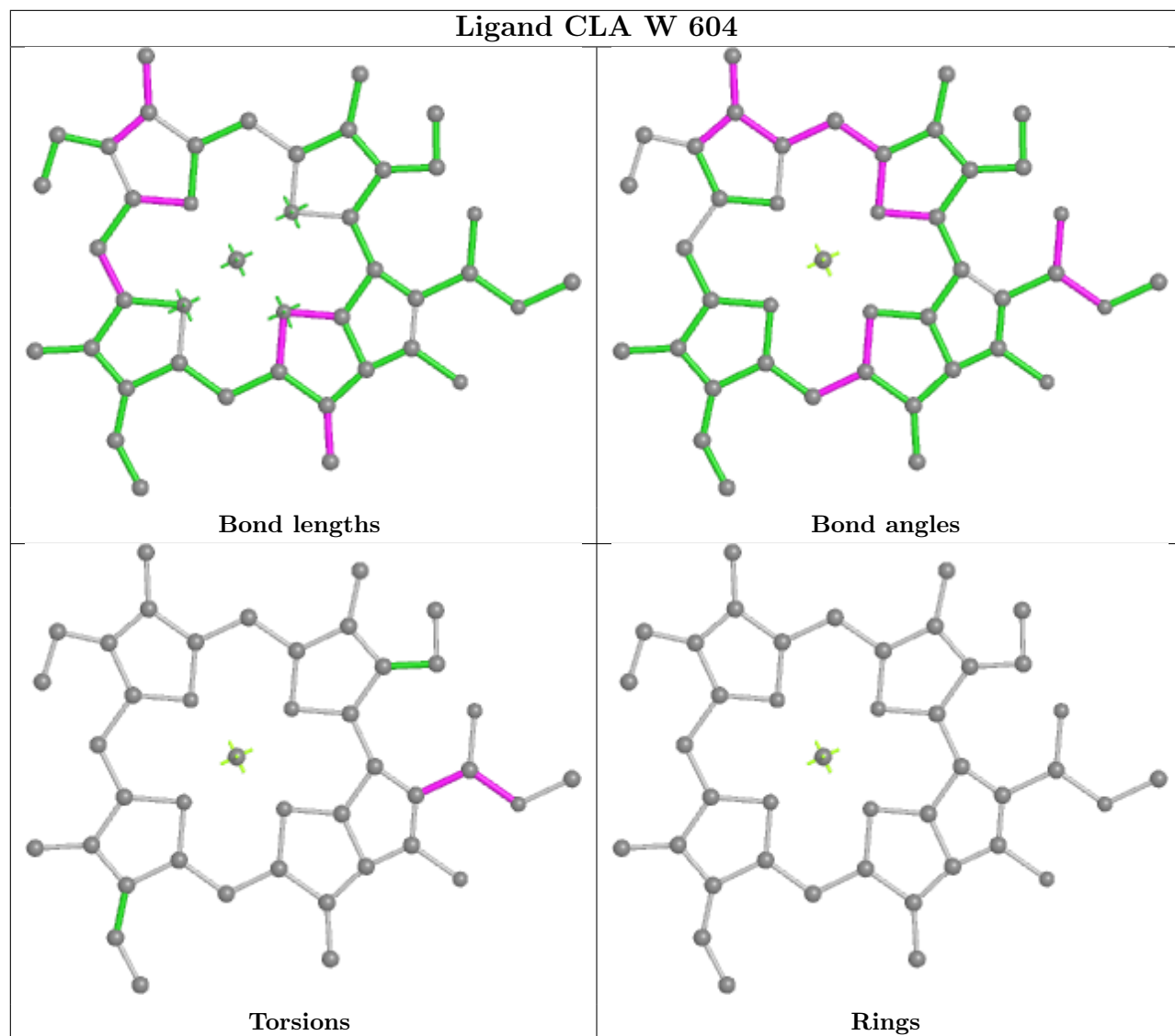
Ligand BCR A 848

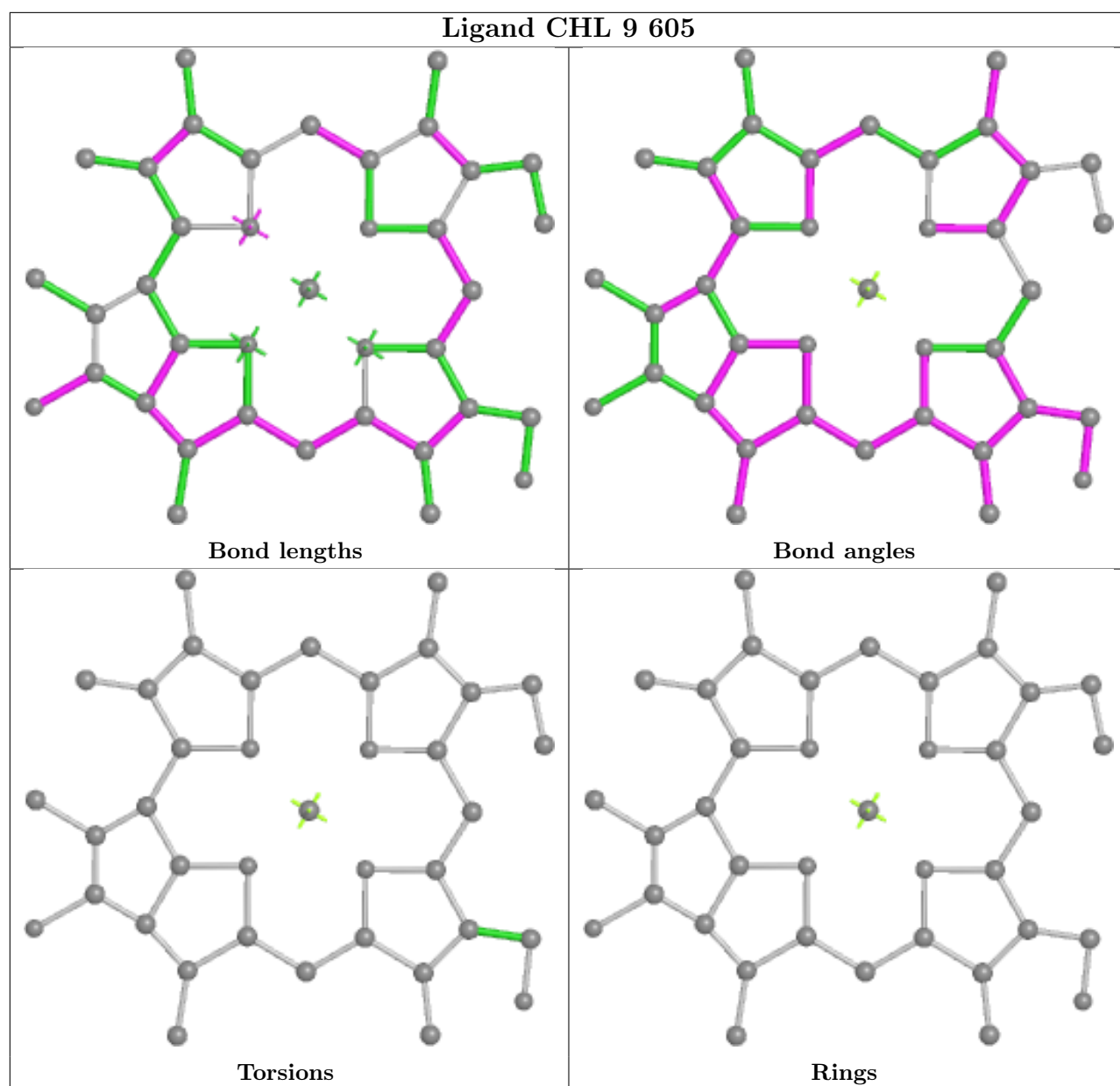


Ligand CLA A 831**Ligand NEX W 2623**

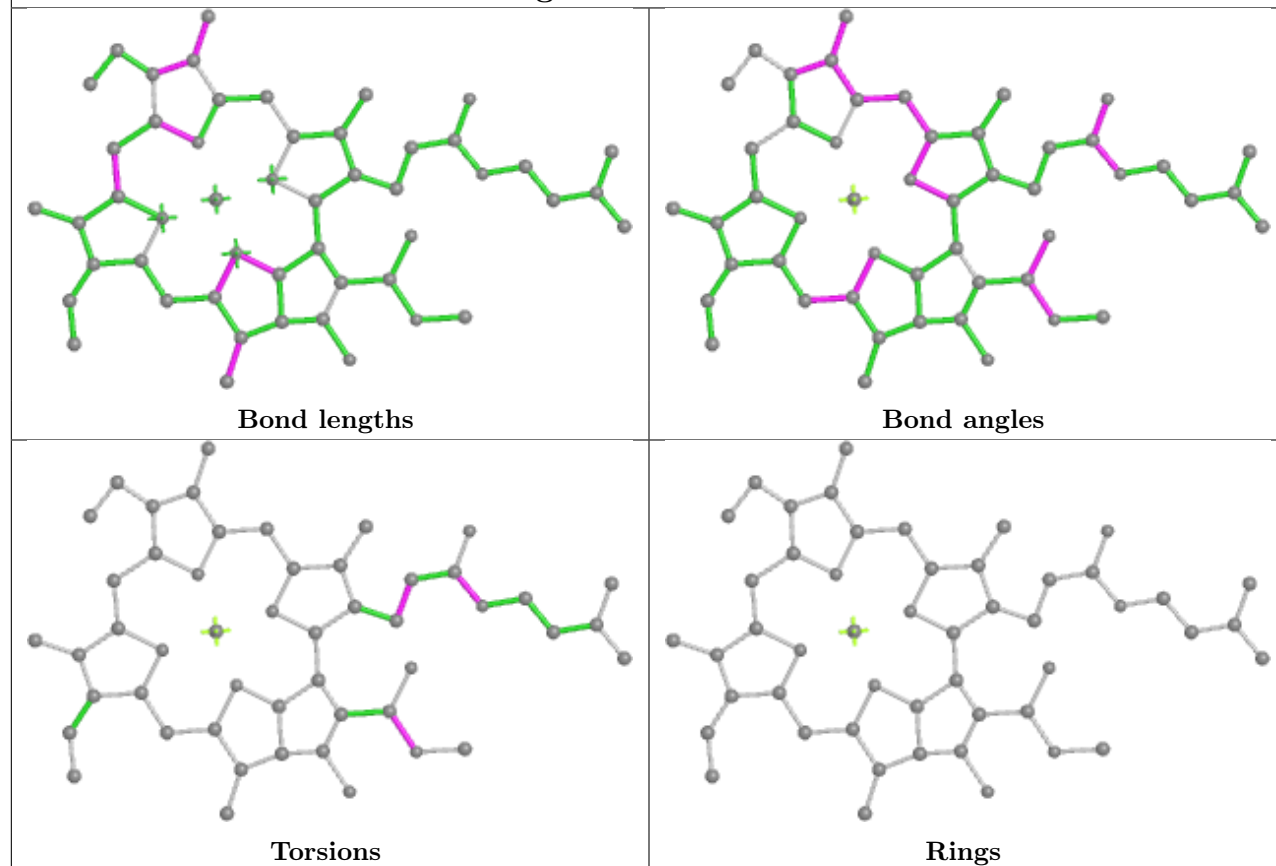
Ligand CLA B 823



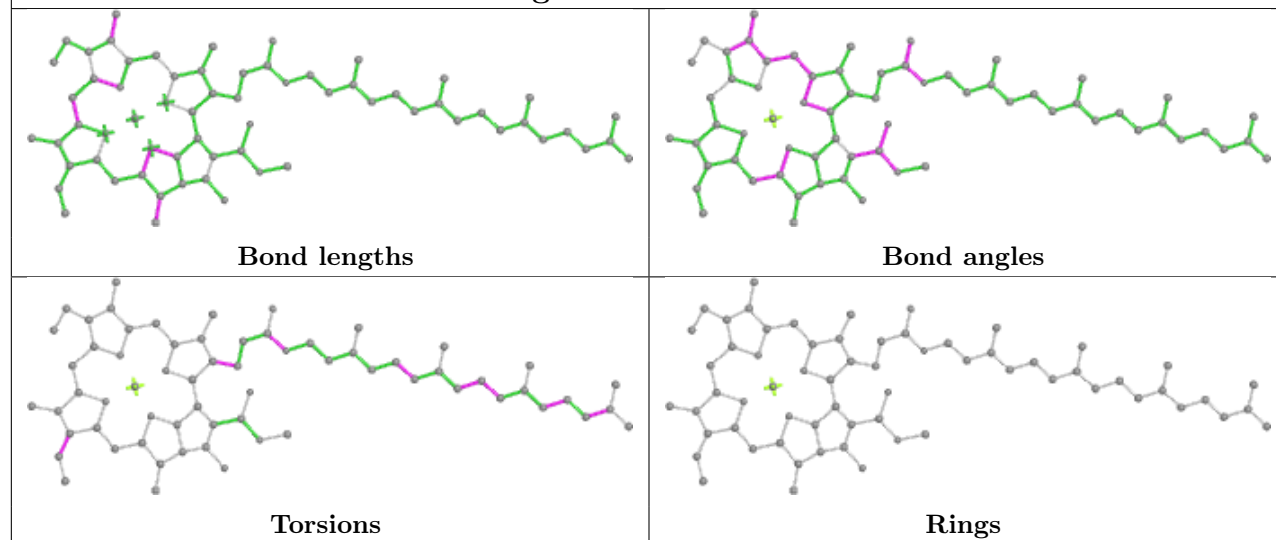




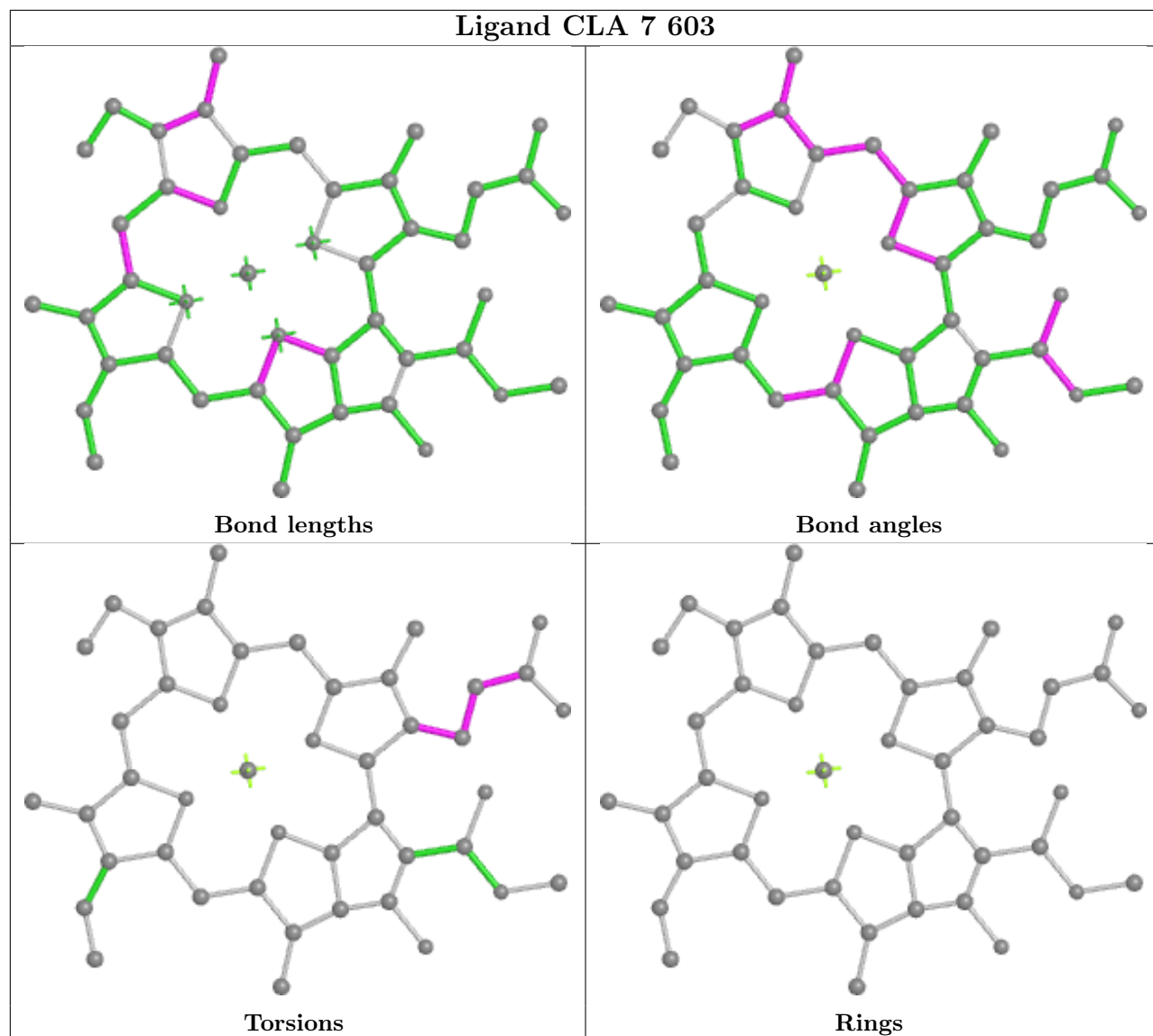
Ligand CLA J 101



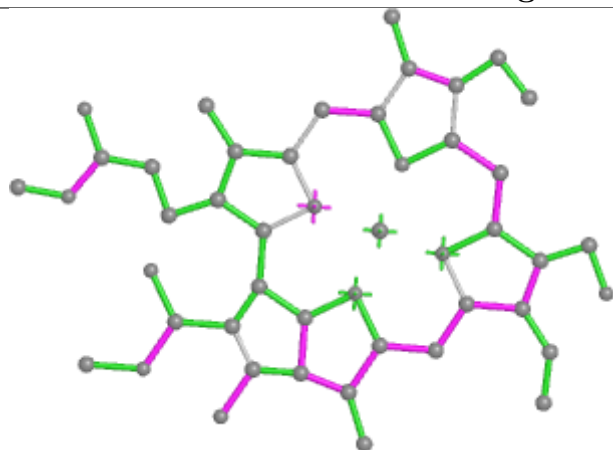
Ligand CLA B 813



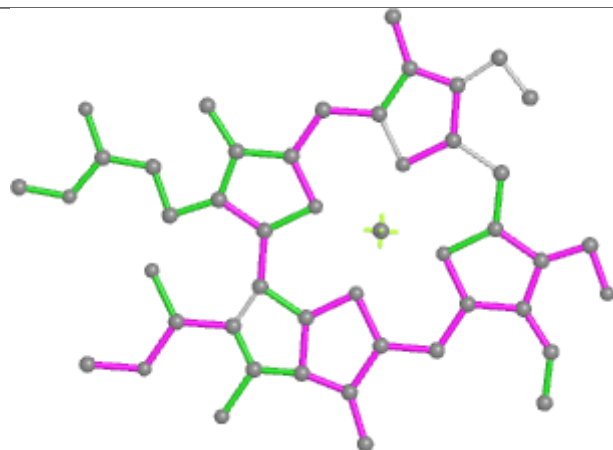
Ligand CLA 7 603



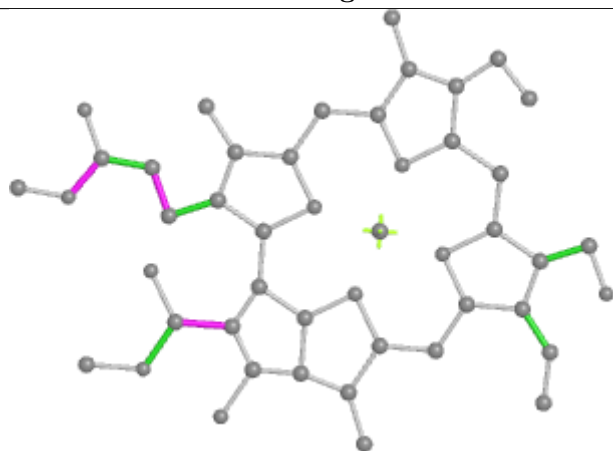
Ligand CHL 4 607



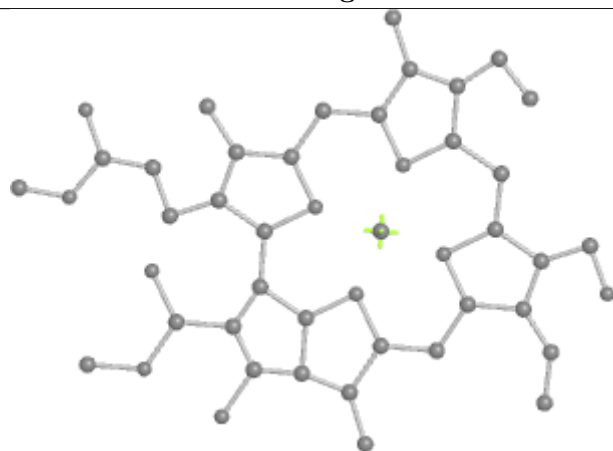
Bond lengths



Bond angles

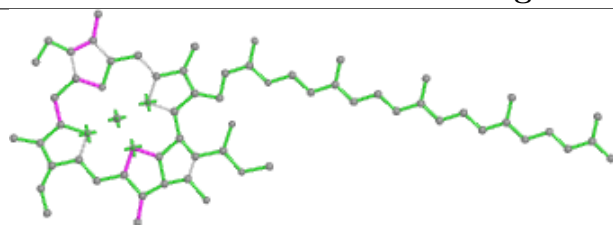


Torsions

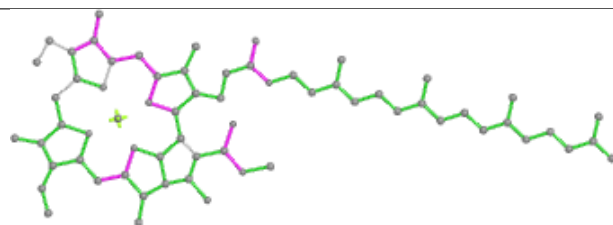


Rings

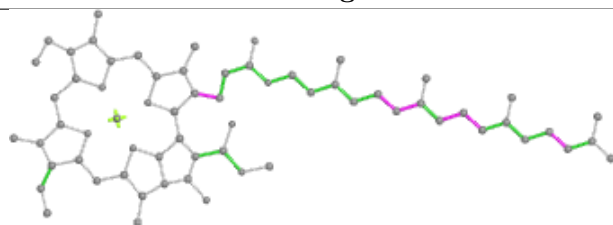
Ligand CLA B 837



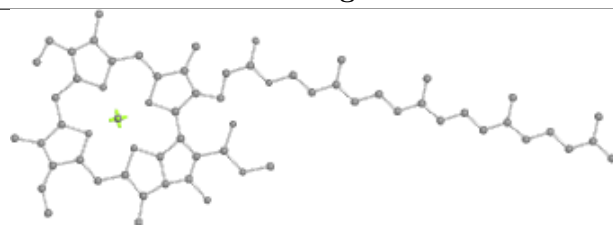
Bond lengths



Bond angles

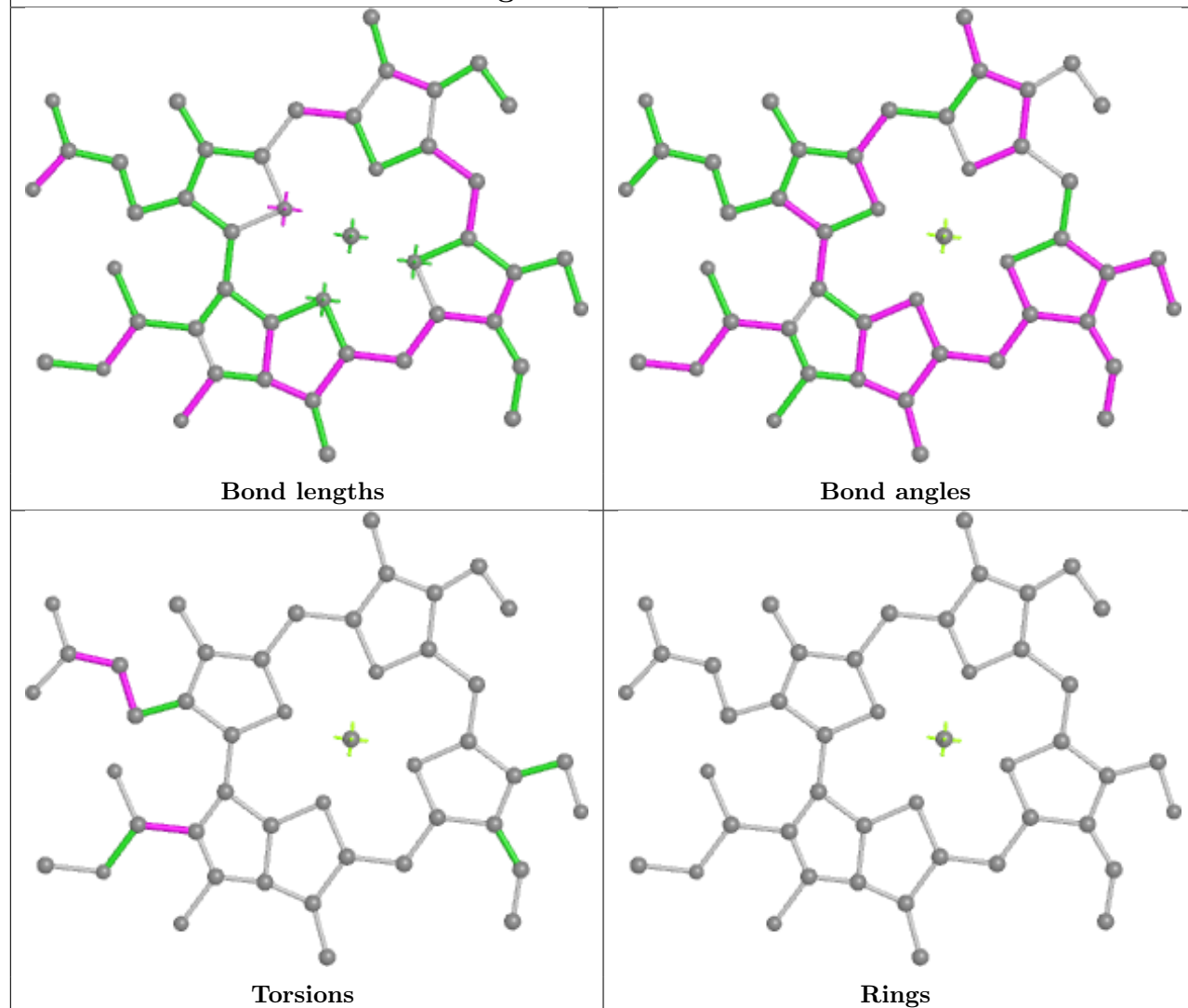


Torsions

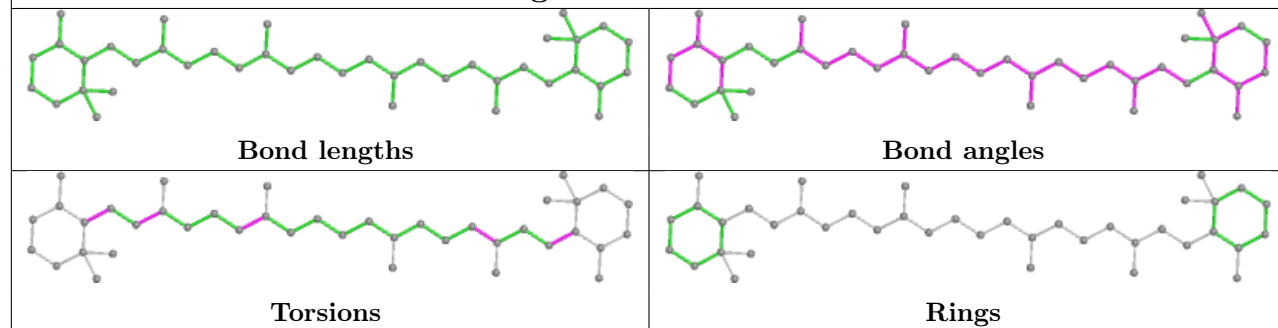


Rings

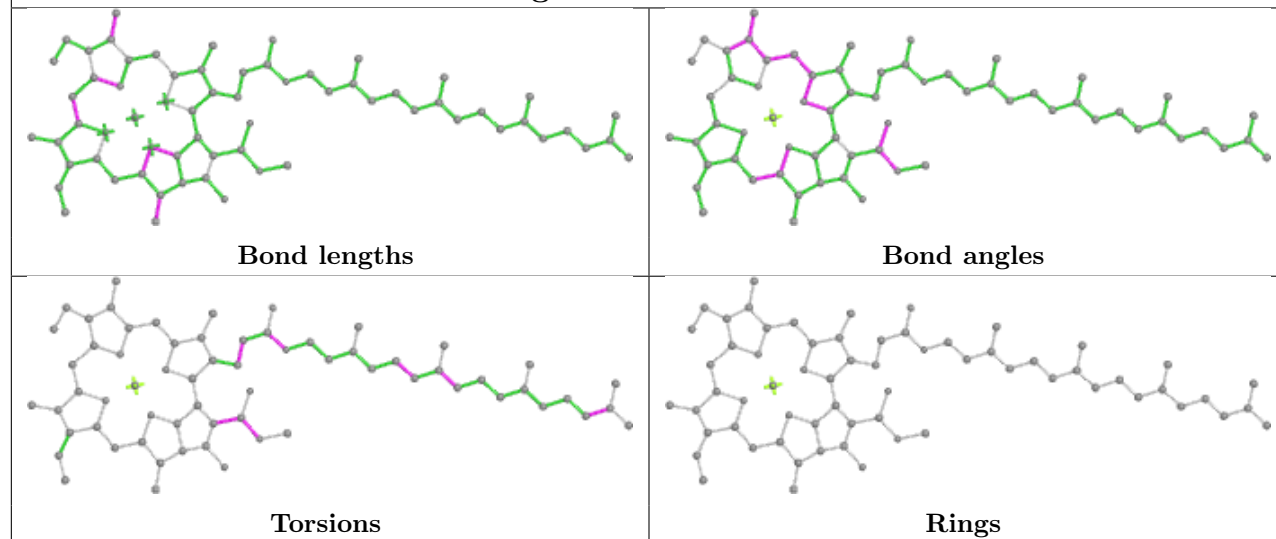
Ligand CHL 7 608



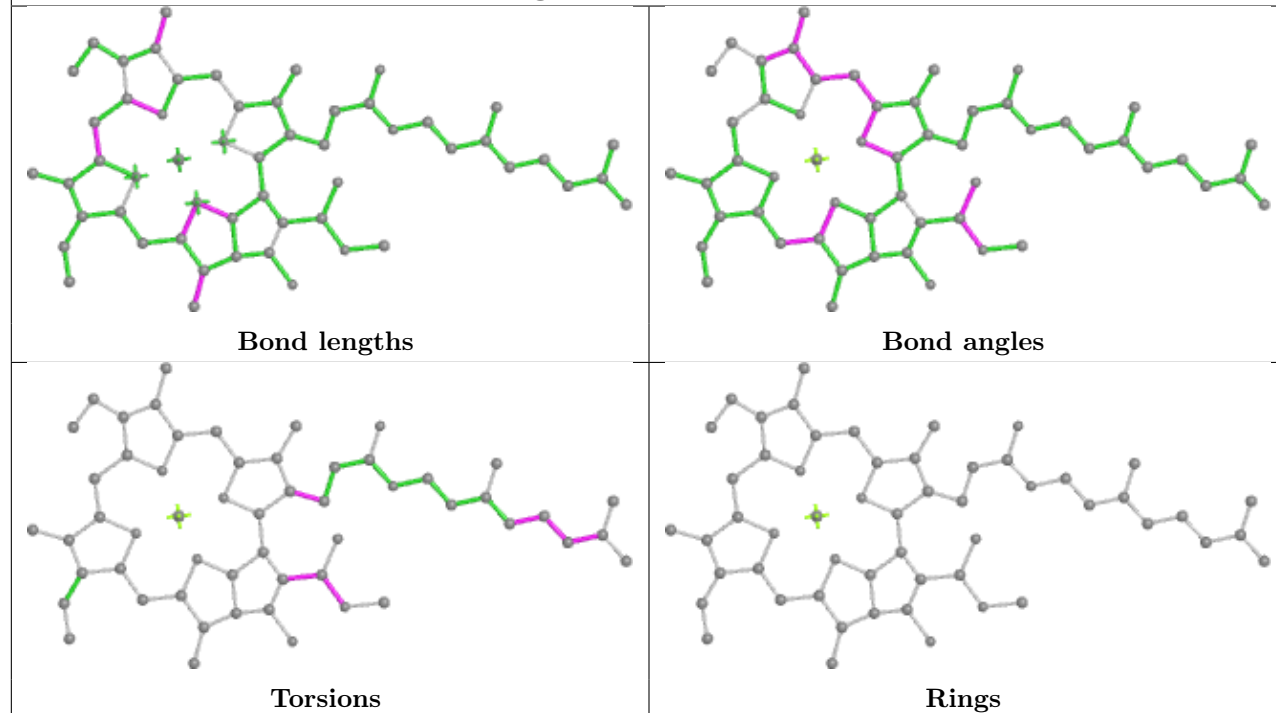
Ligand BCR B 845



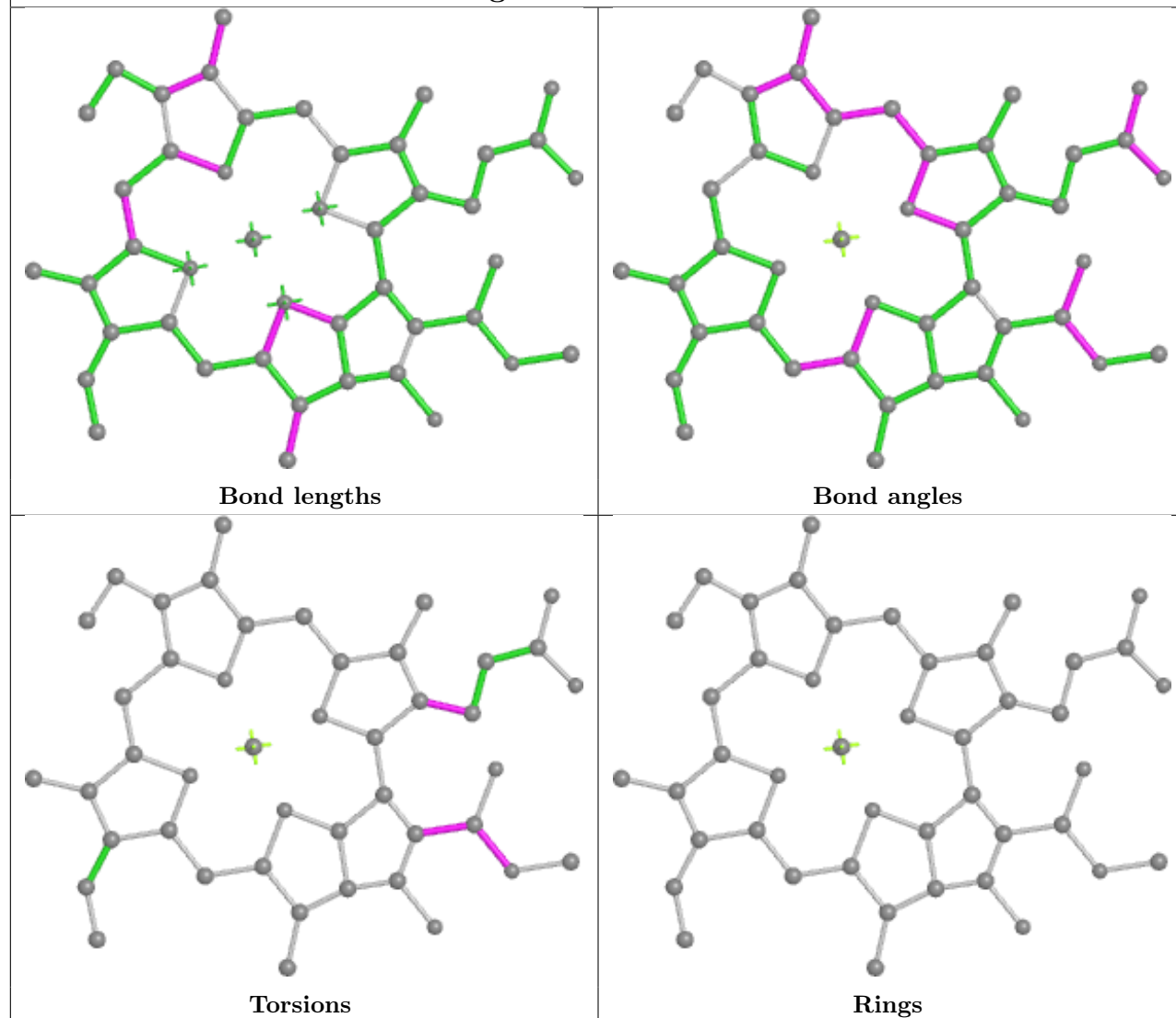
Ligand CLA A 845



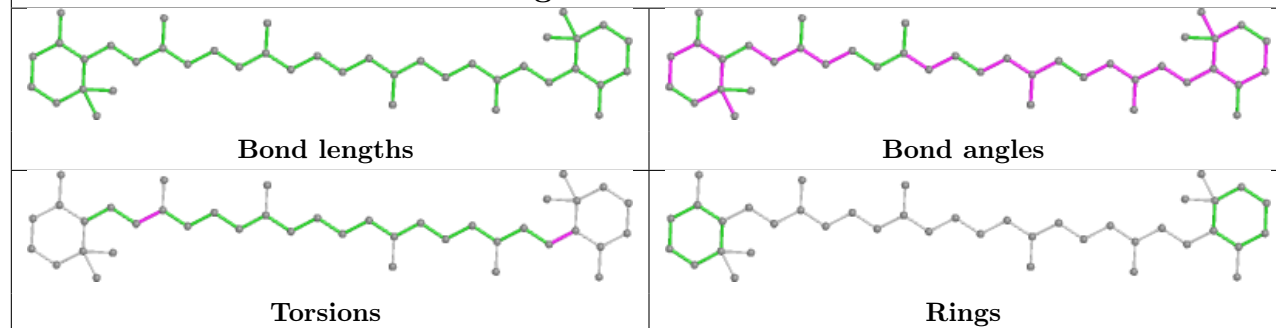
Ligand CLA A 838



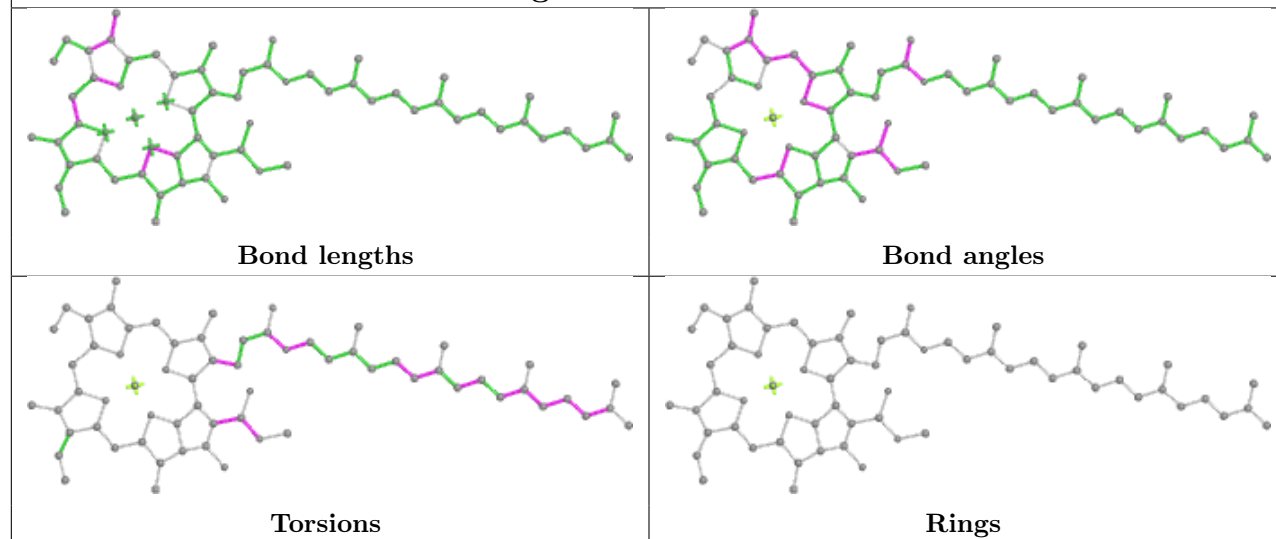
Ligand CLA G 201



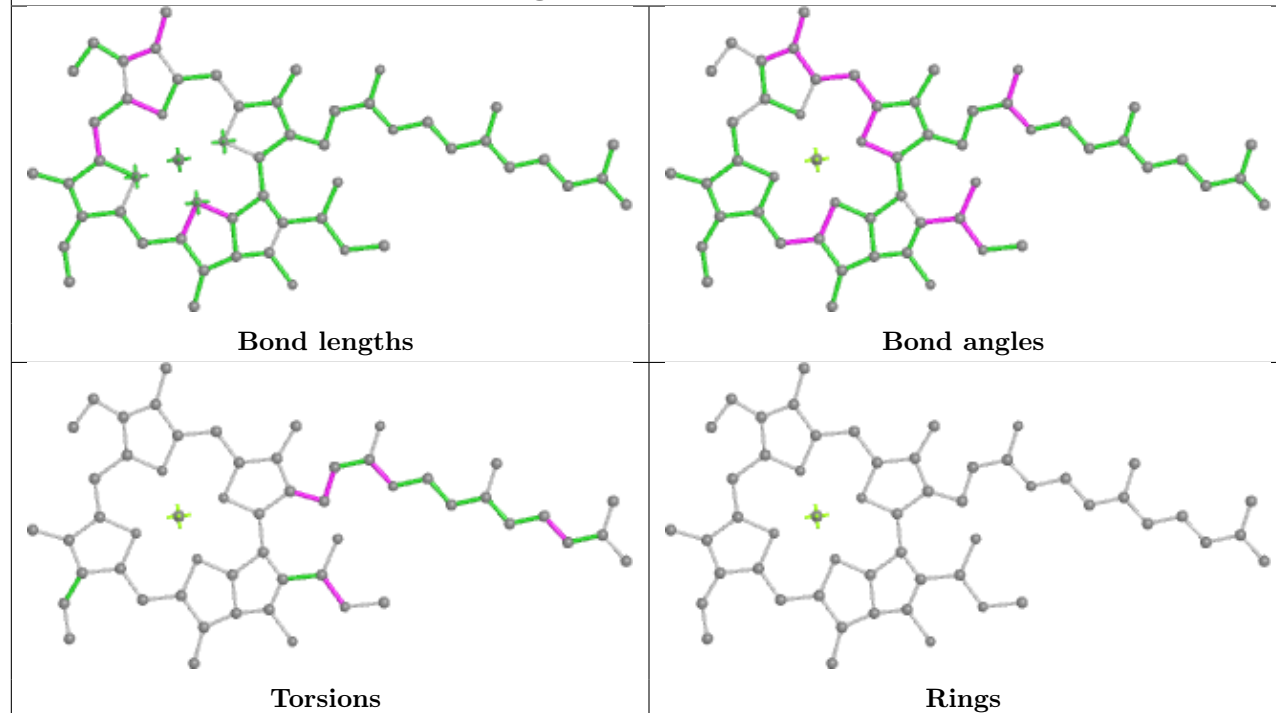
Ligand BCR 3 620



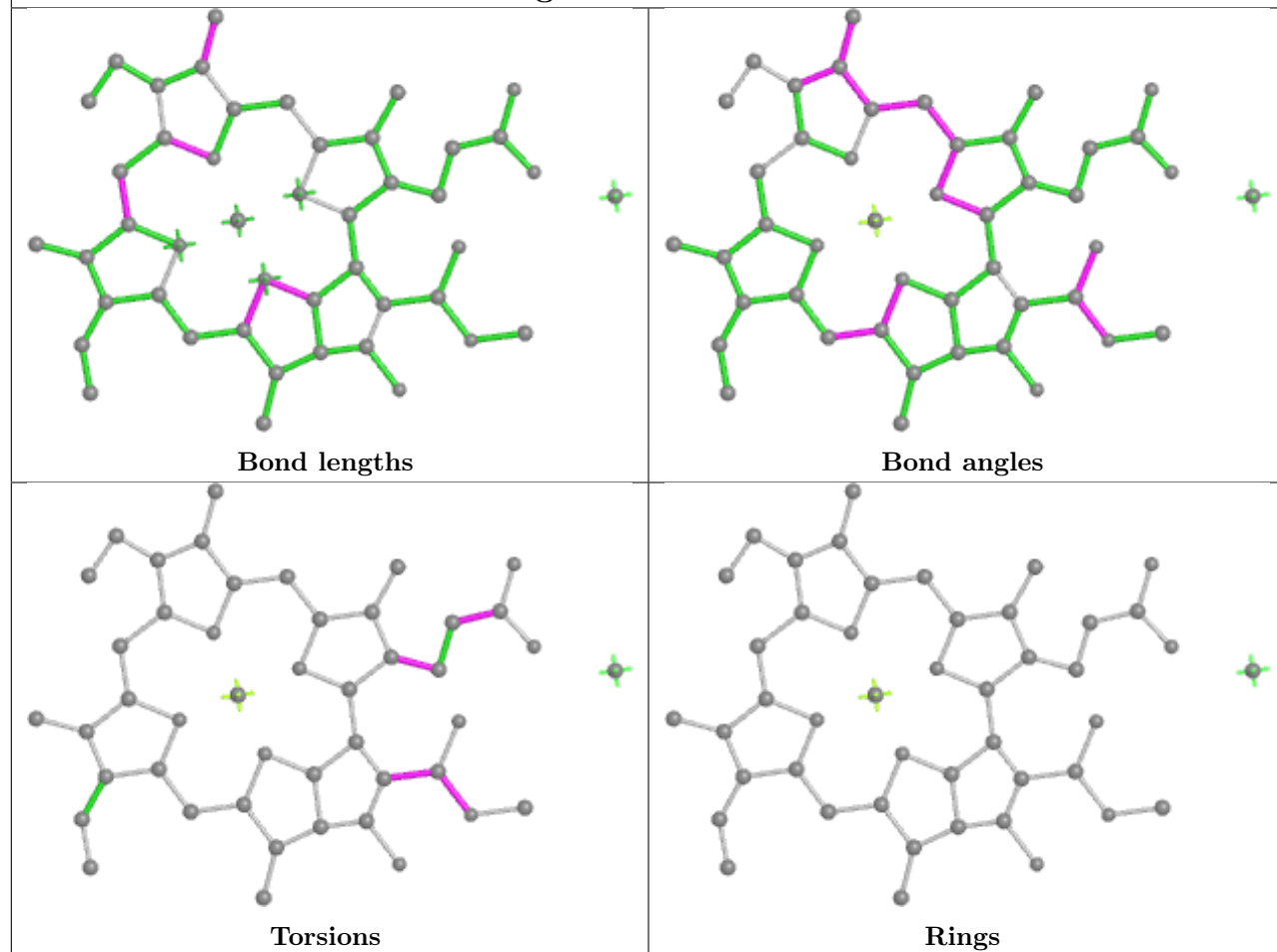
Ligand CLA A 804



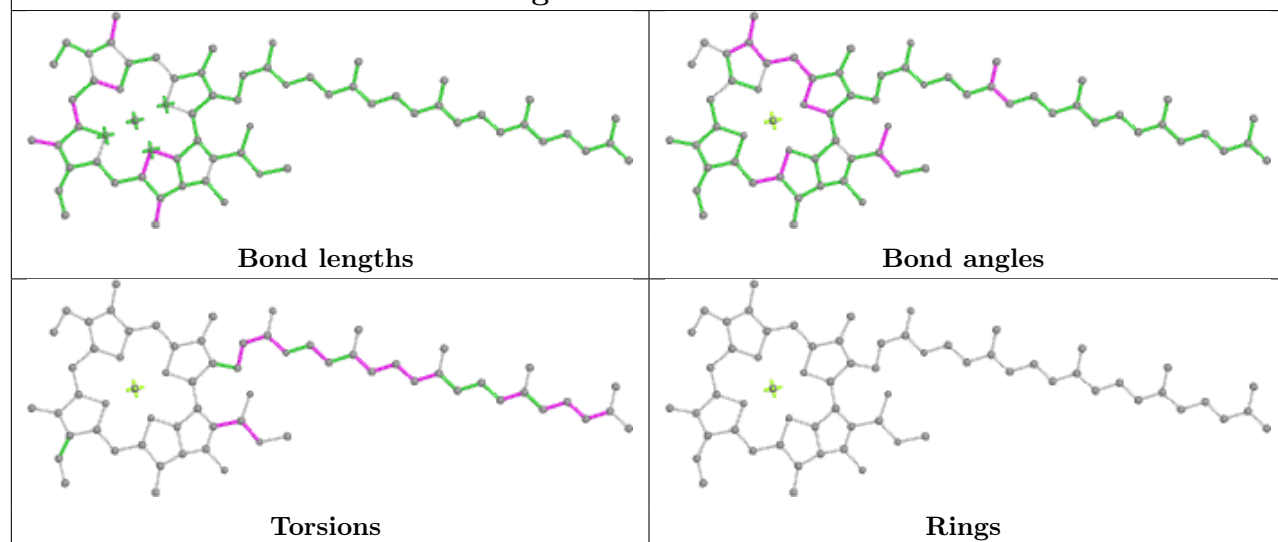
Ligand CLA K 203



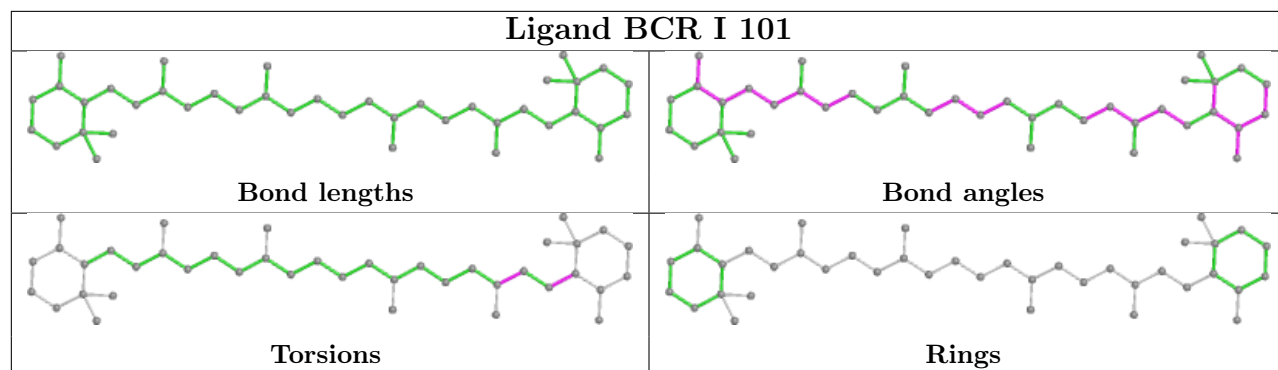
Ligand CLA 2 611



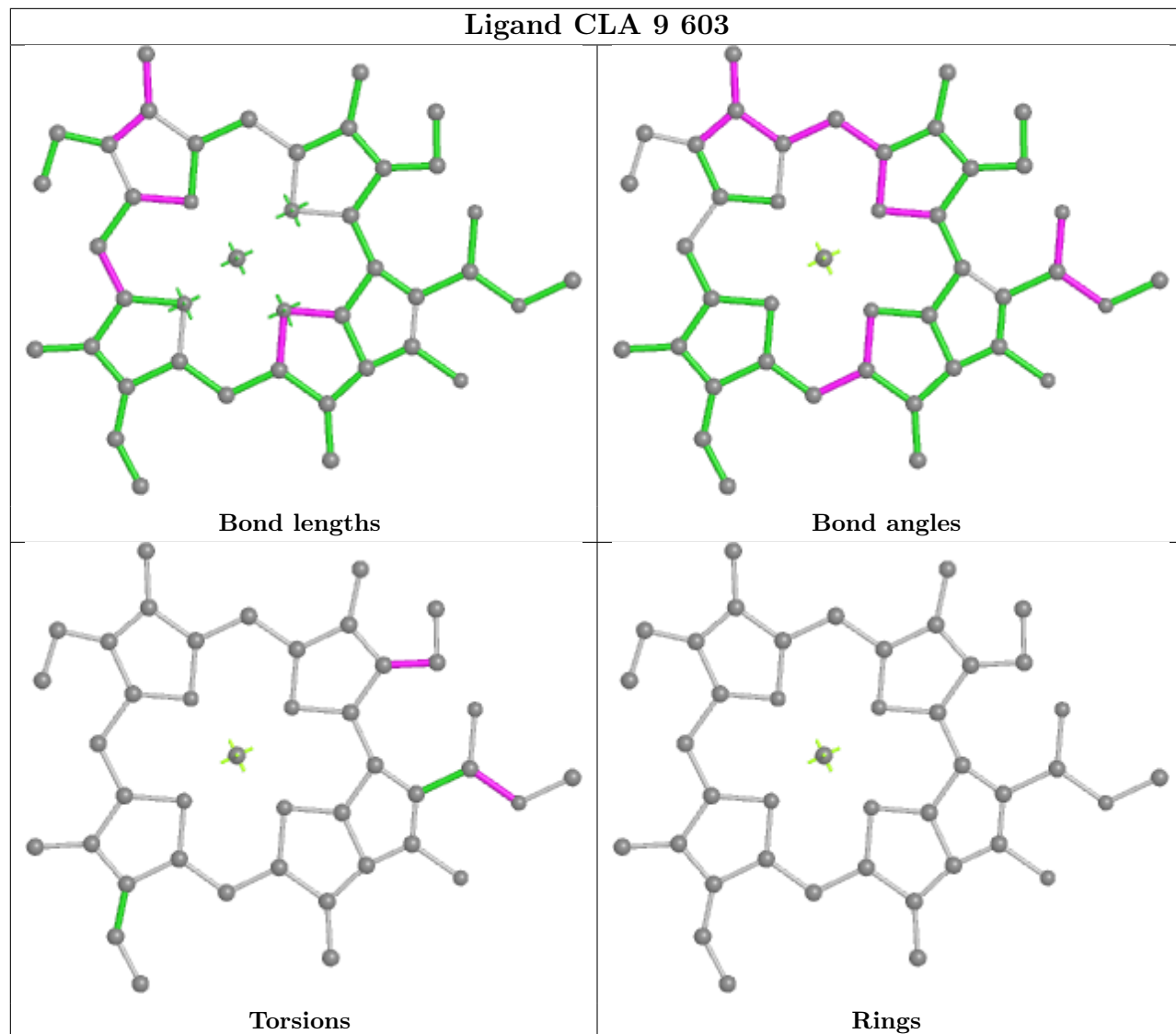
Ligand CLA A 814

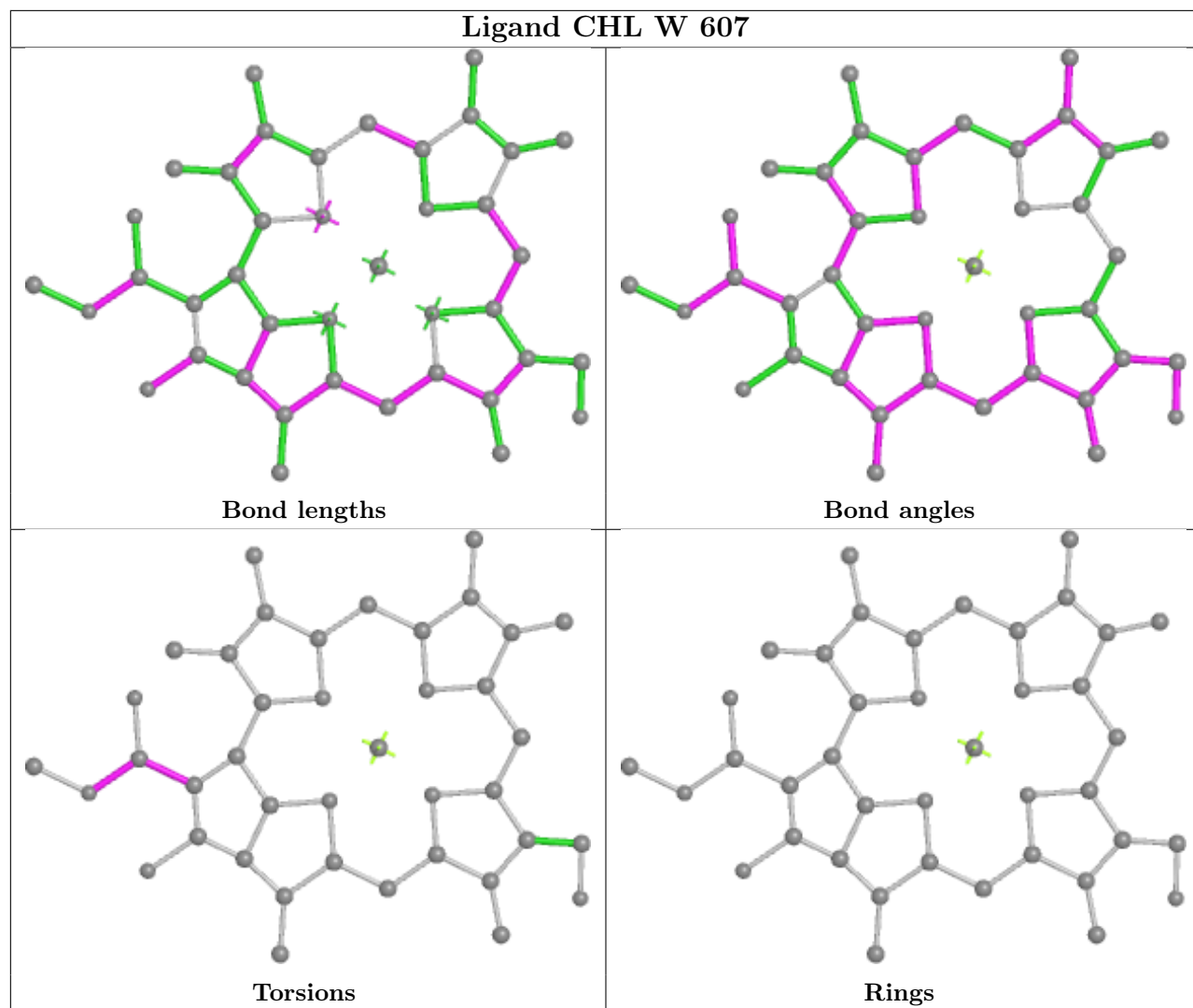


Ligand BCR I 101

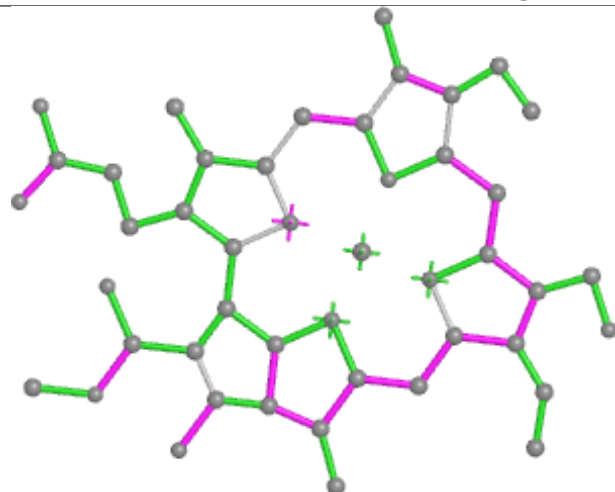


Ligand CLA 9 603

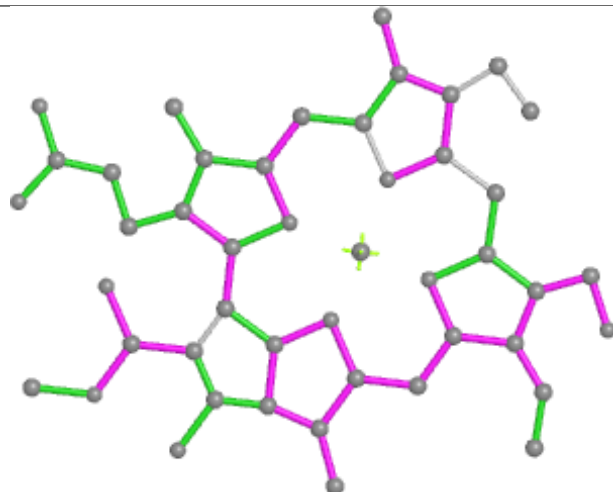




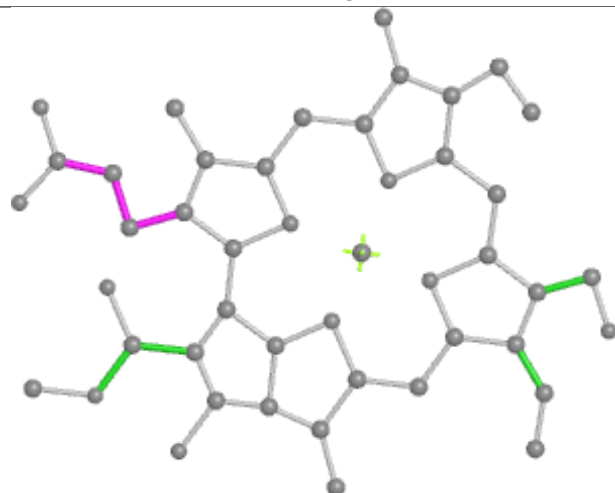
Ligand CHL U 606



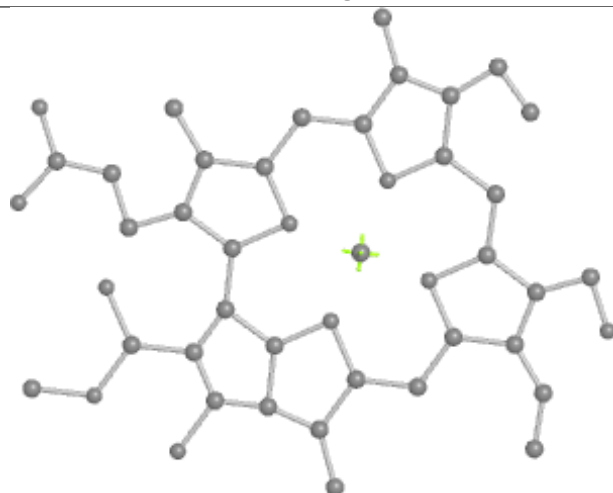
Bond lengths



Bond angles

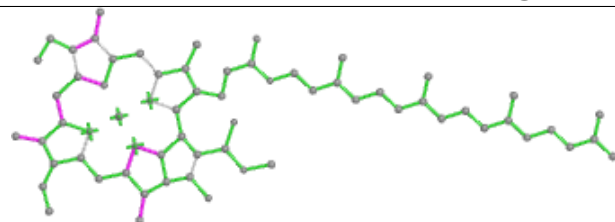


Torsions

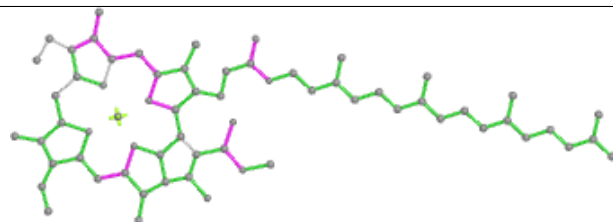


Rings

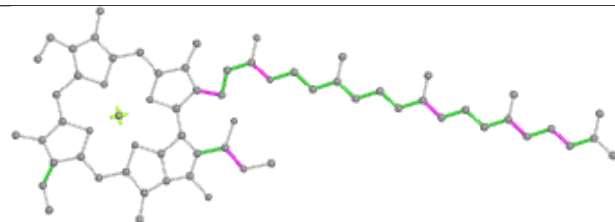
Ligand CLA A 812



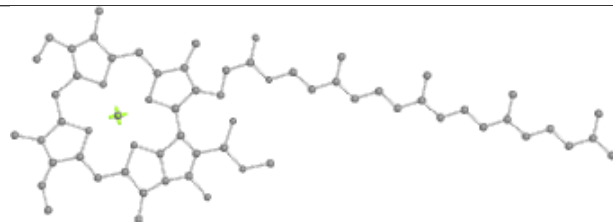
Bond lengths



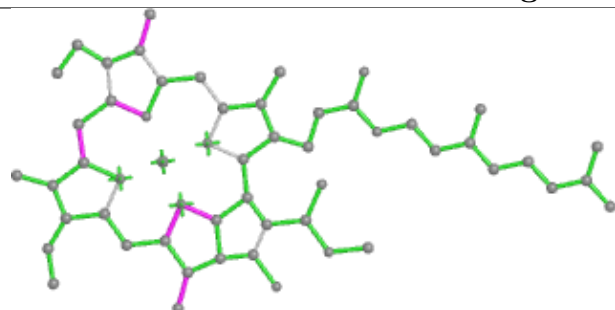
Bond angles



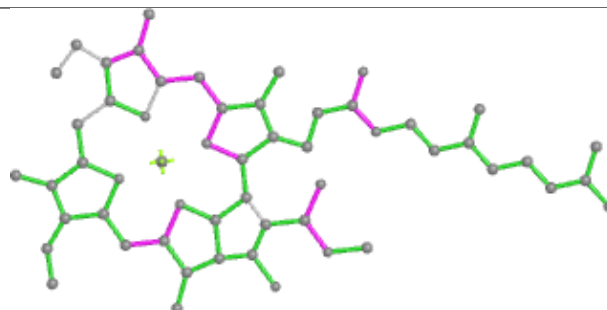
Torsions



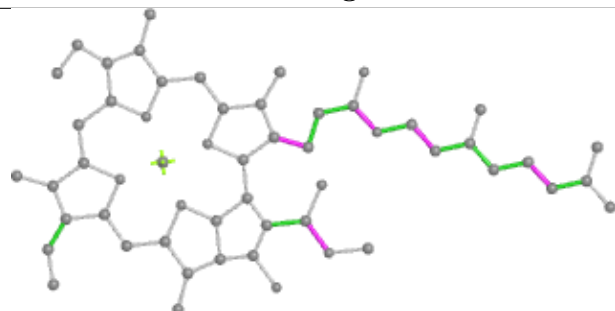
Rings

Ligand CLA 4 604

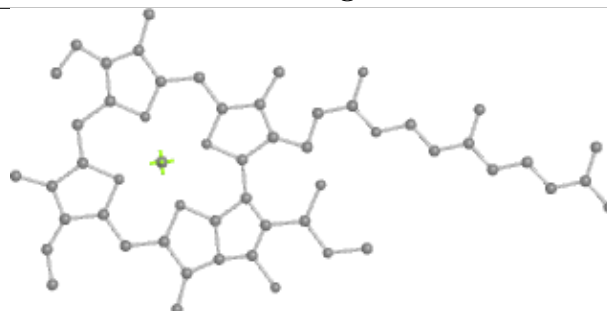
Bond lengths



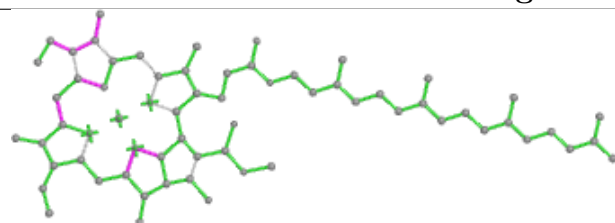
Bond angles



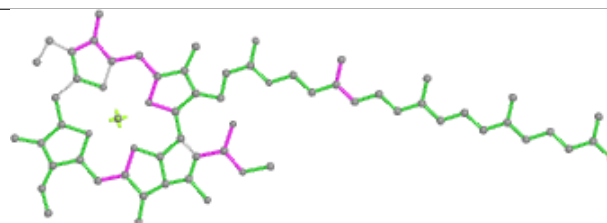
Torsions



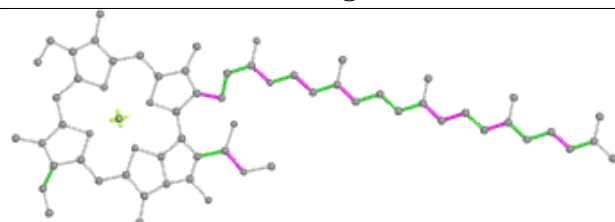
Rings

Ligand CLA A 810

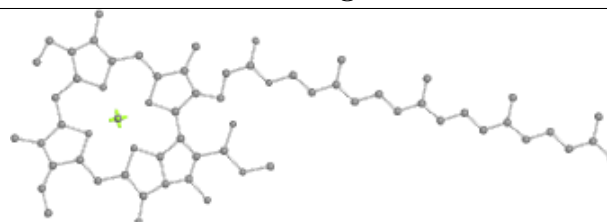
Bond lengths



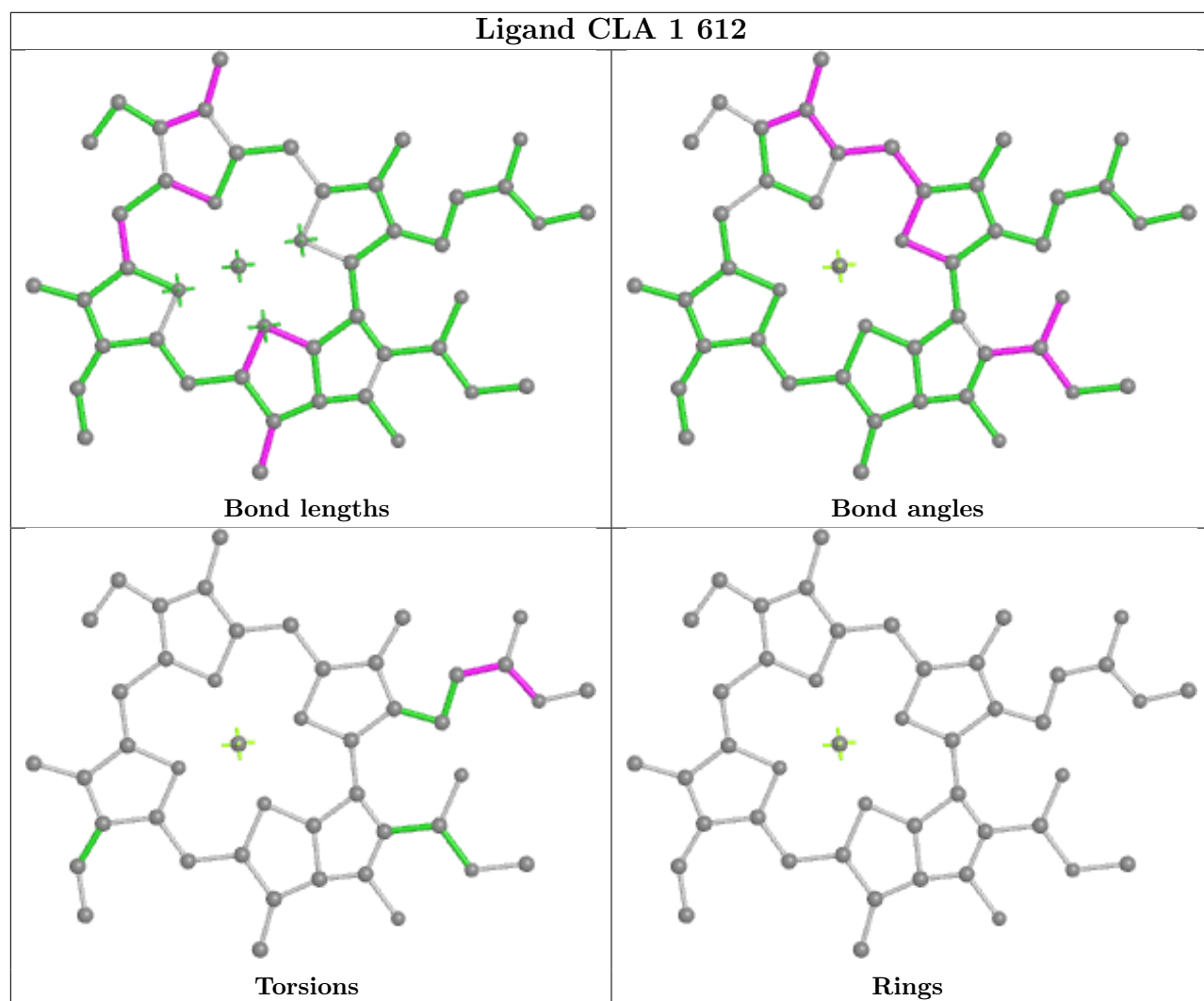
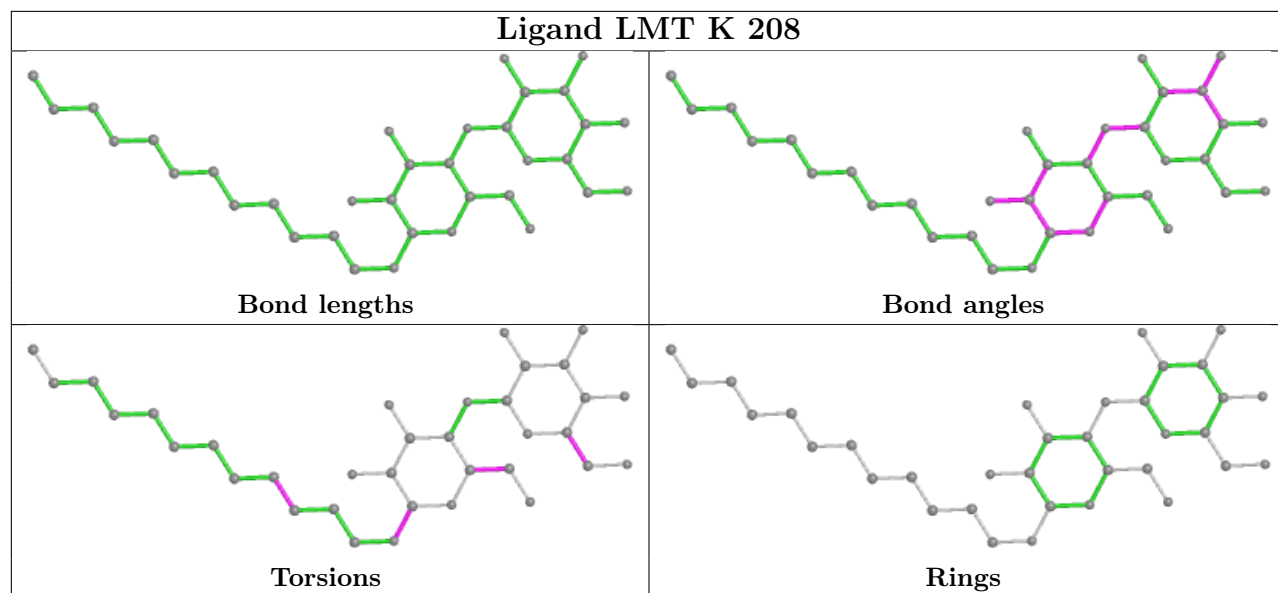
Bond angles



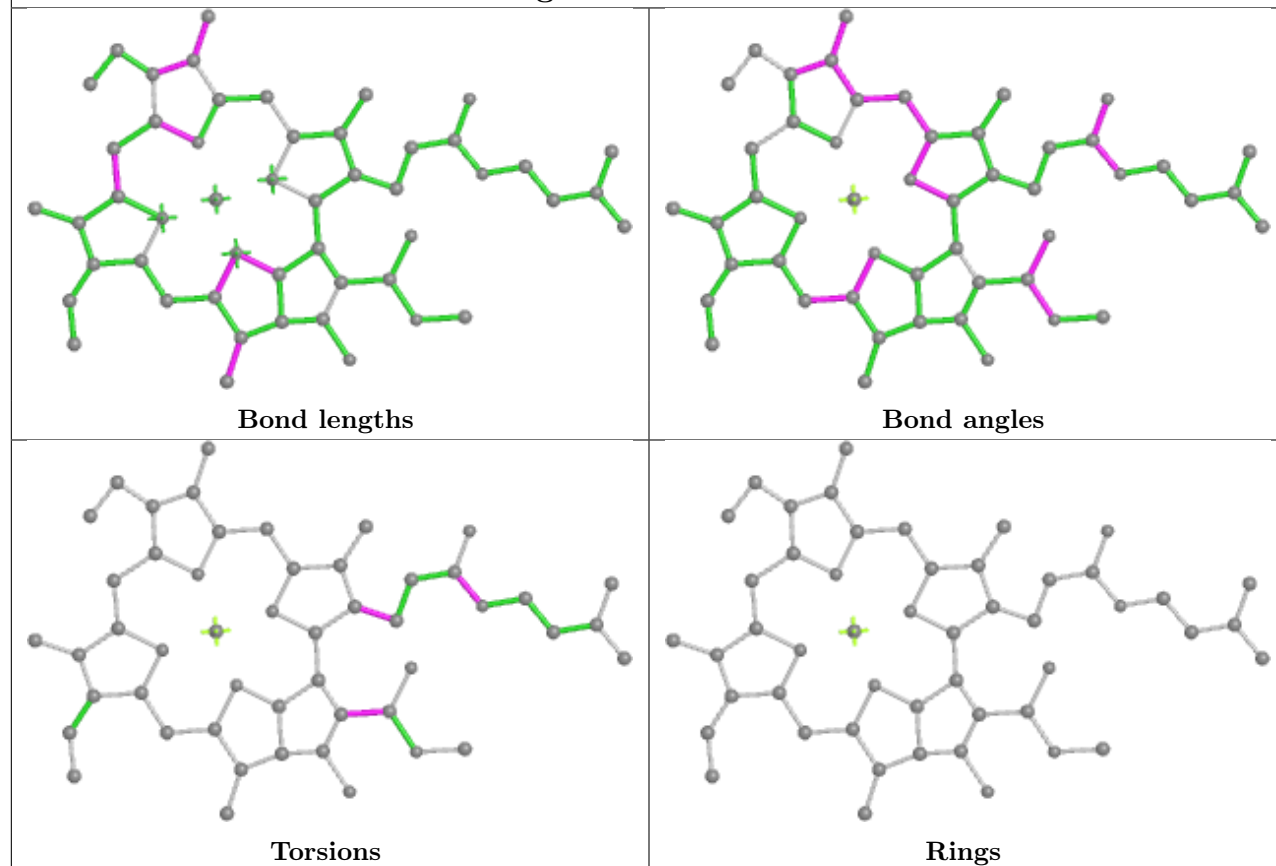
Torsions



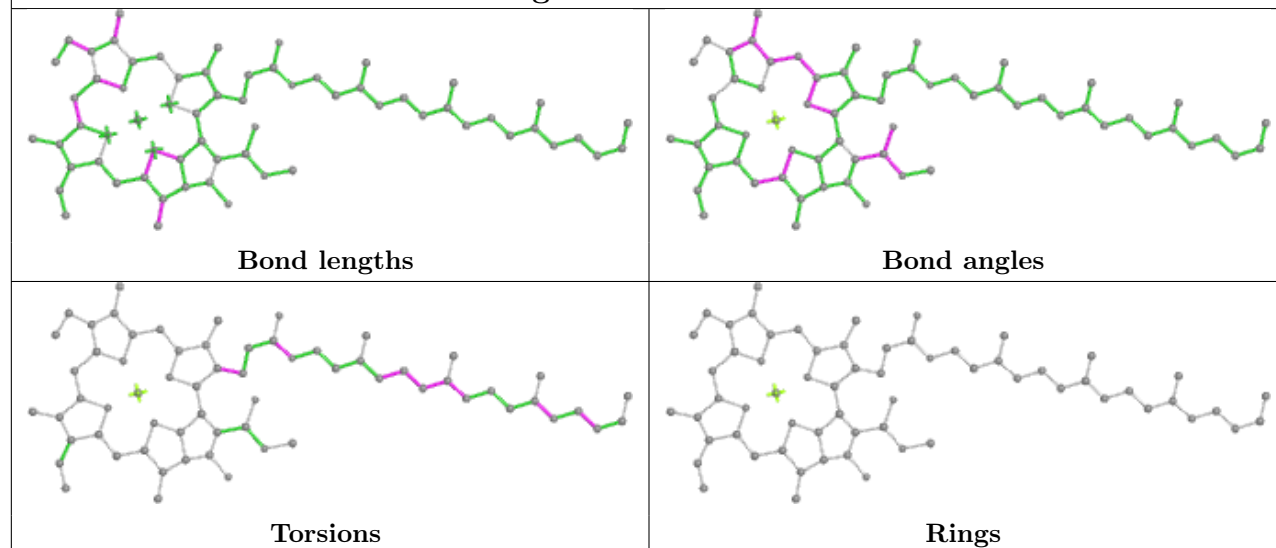
Rings

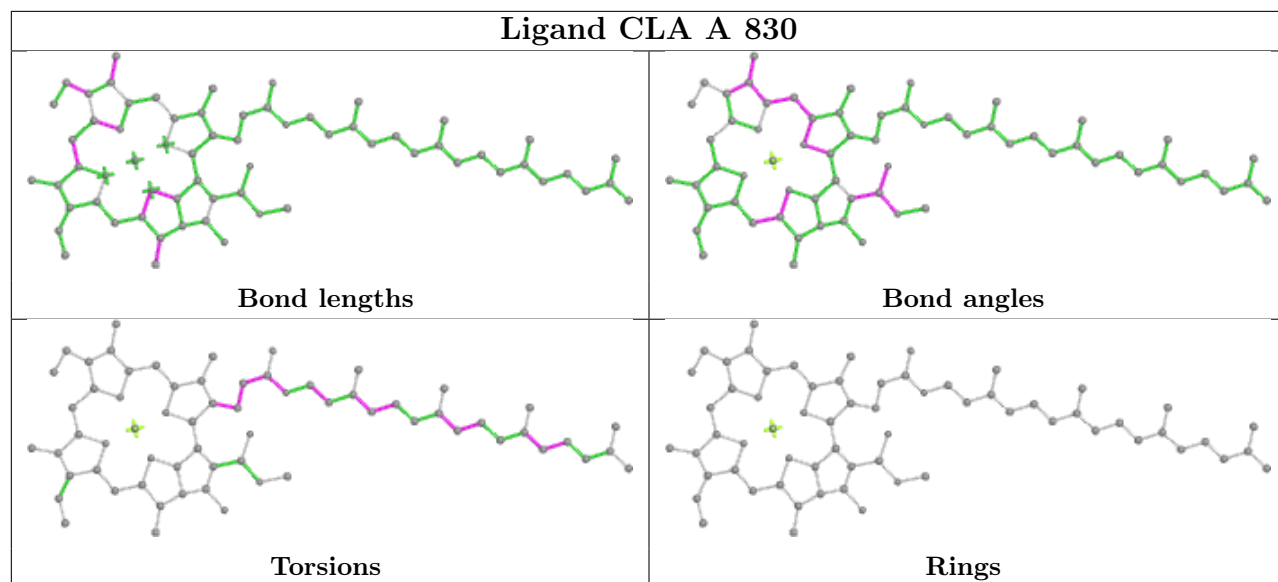


Ligand CLA 2 614

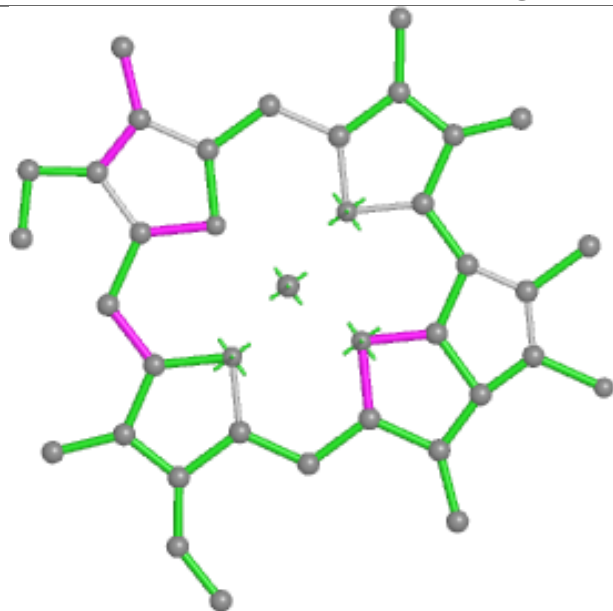


Ligand CLA B 818

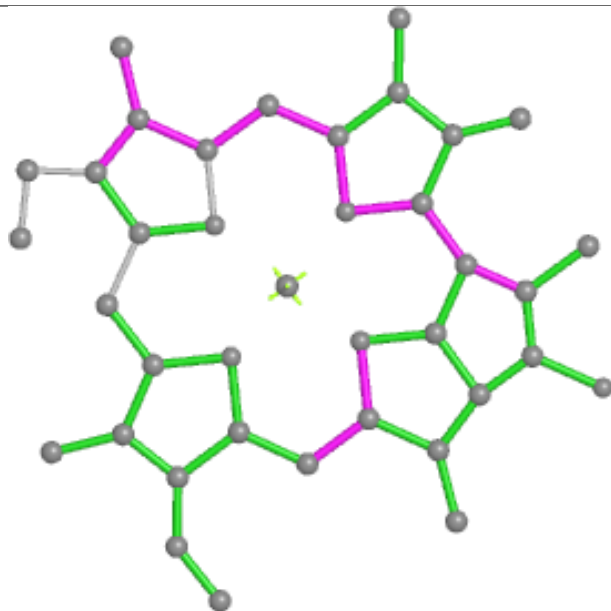




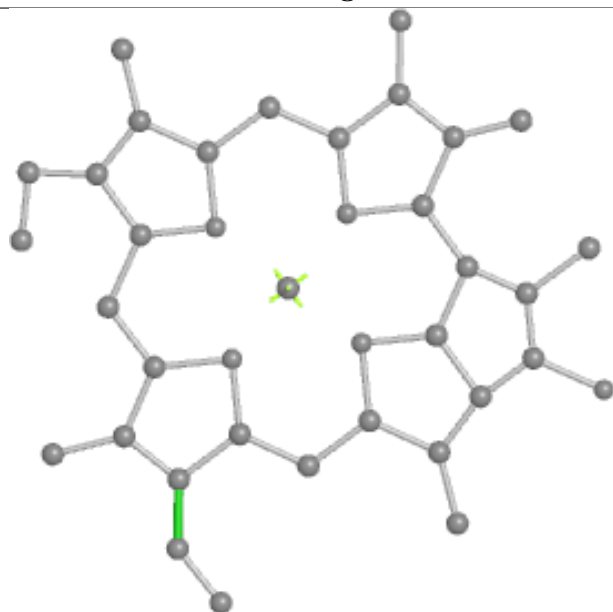
Ligand CLA H 201



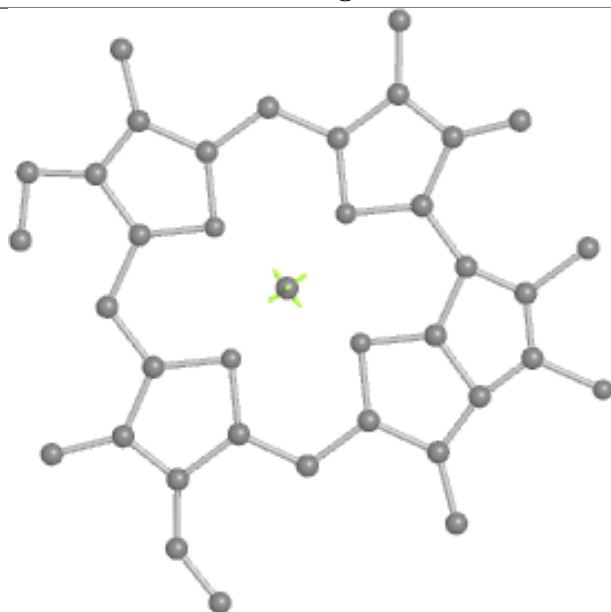
Bond lengths



Bond angles

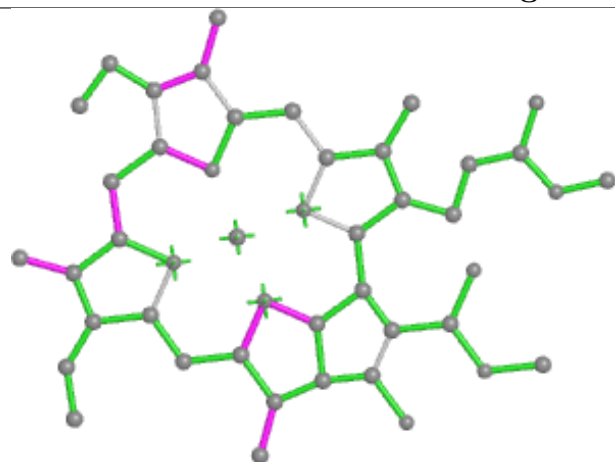


Torsions

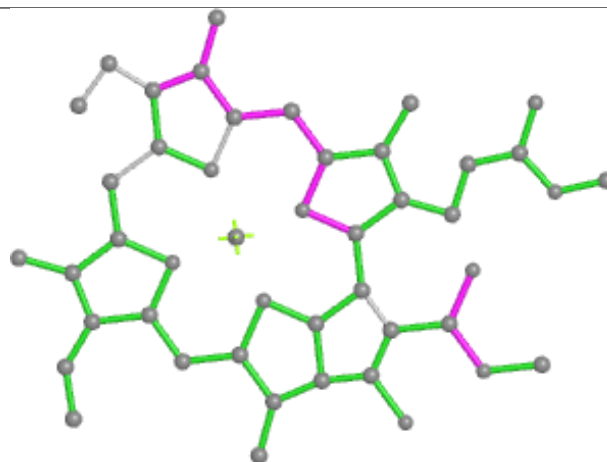


Rings

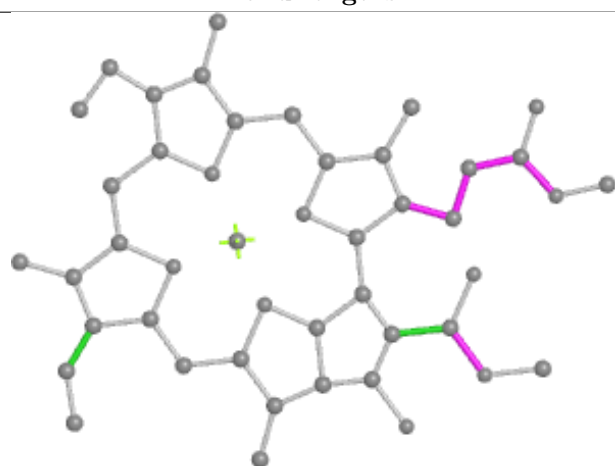
Ligand CLA 5 612



Bond lengths



Bond angles

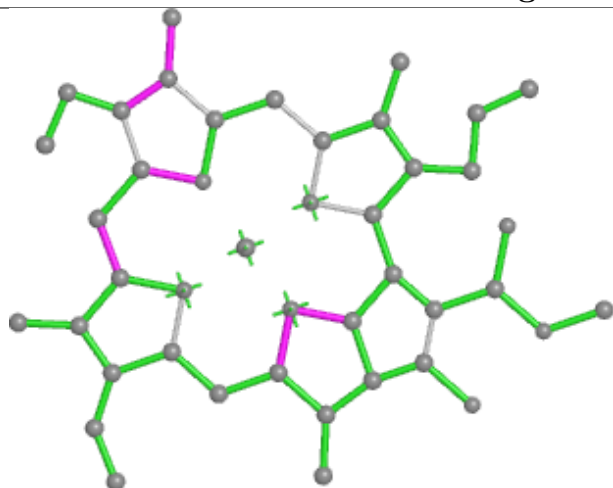


Torsions

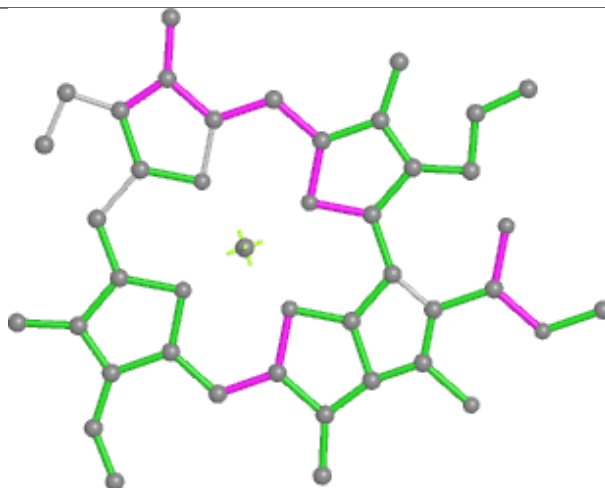


Rings

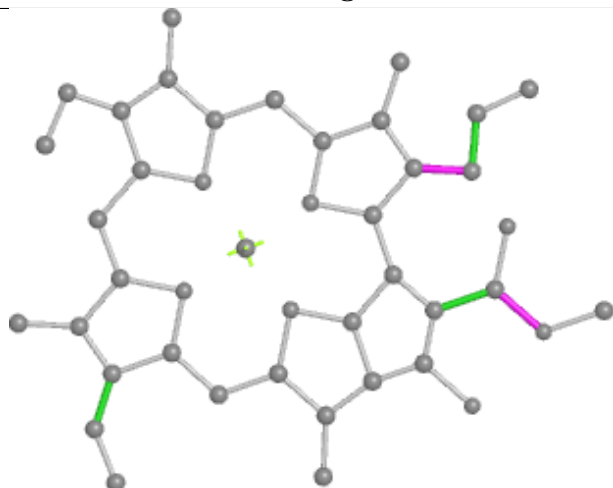
Ligand CLA 9 604



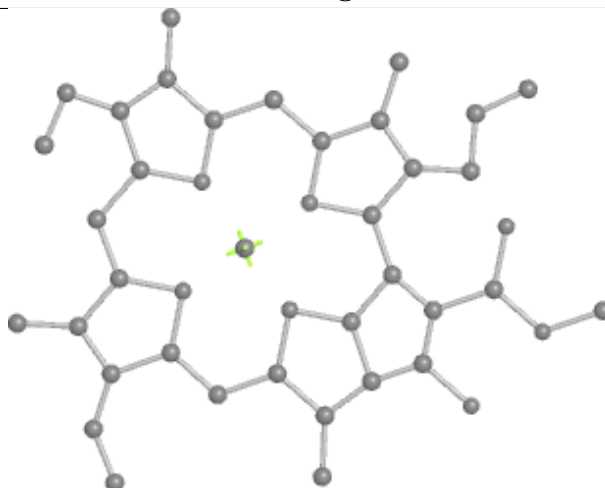
Bond lengths



Bond angles

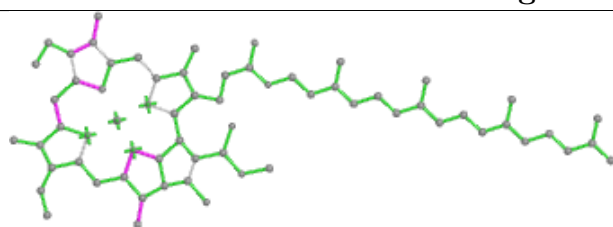


Torsions

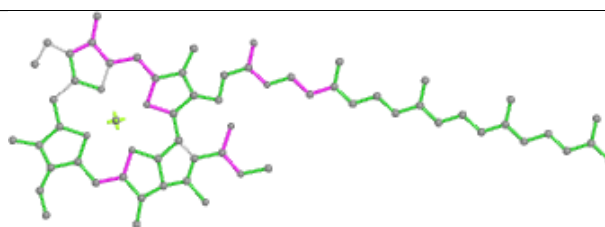


Rings

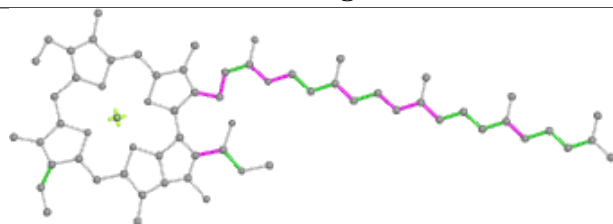
Ligand CLA 3 612



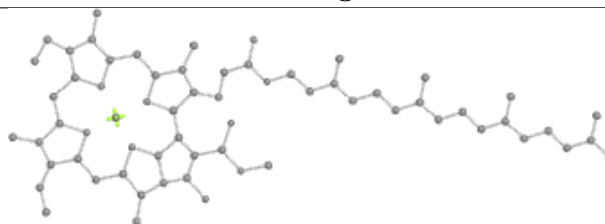
Bond lengths



Bond angles

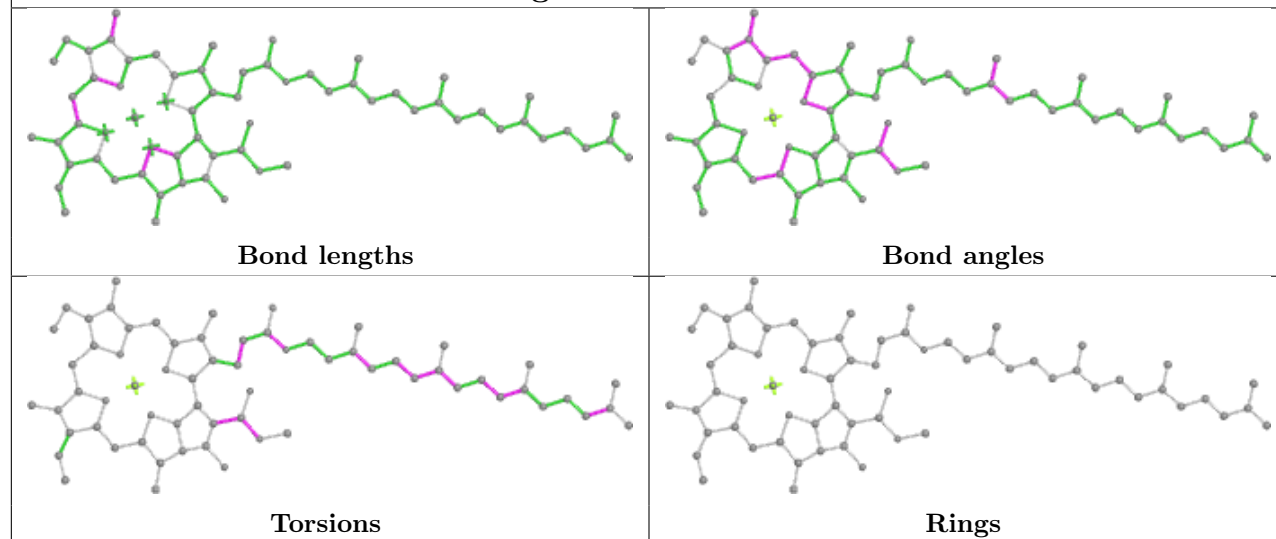


Torsions

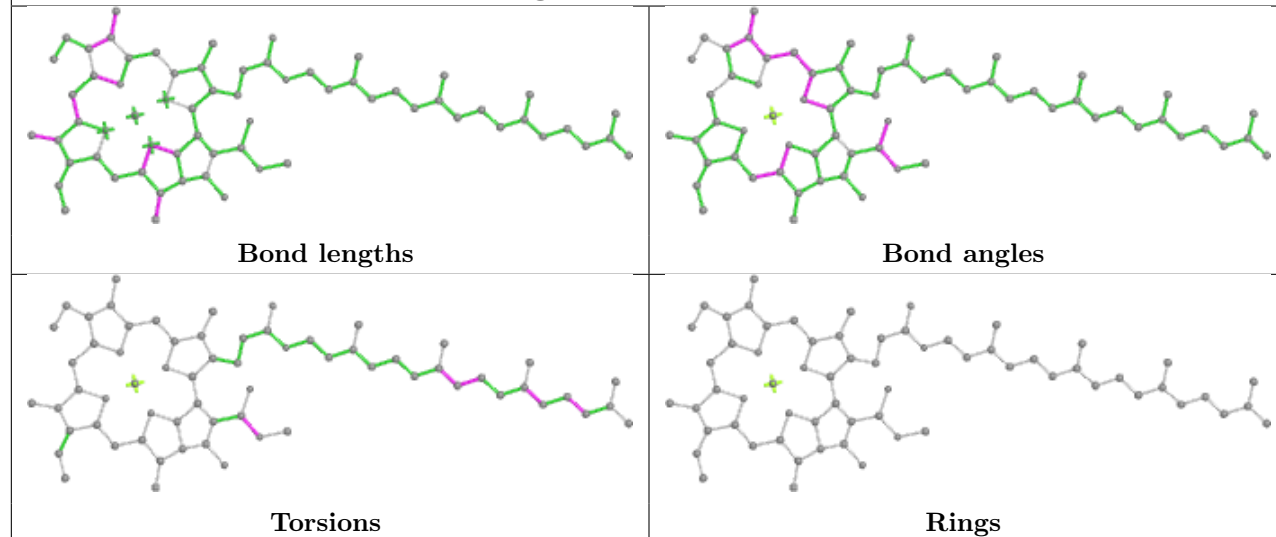


Rings

Ligand CLA A 825



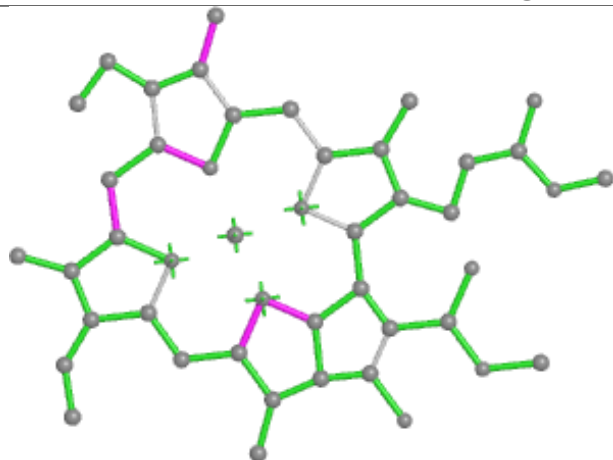
Ligand CLA A 802



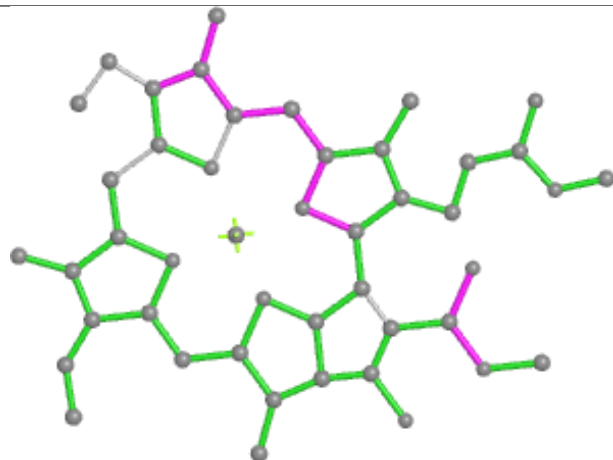
Ligand LUT 9 624



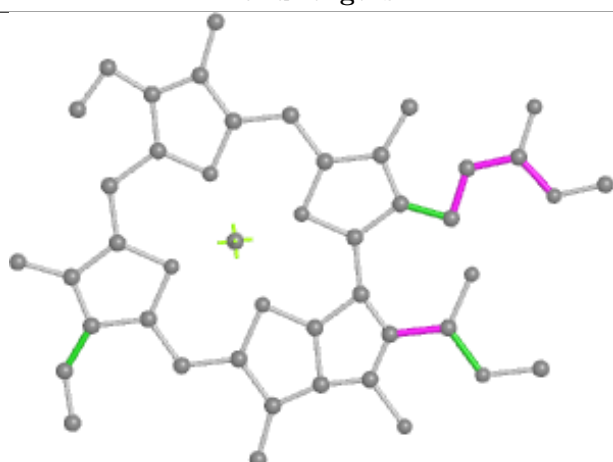
Ligand CLA 8 612



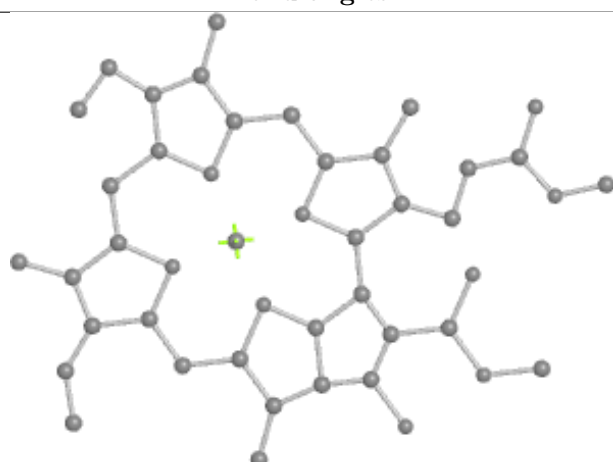
Bond lengths



Bond angles

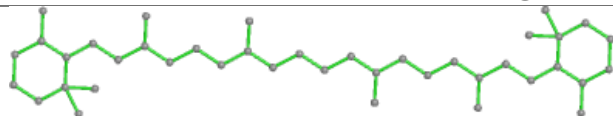


Torsions

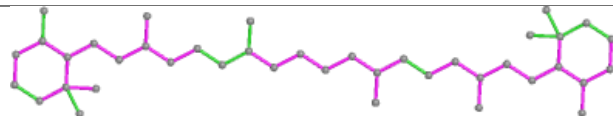


Rings

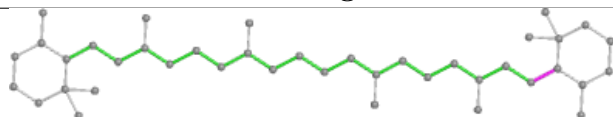
Ligand BCR 7 621



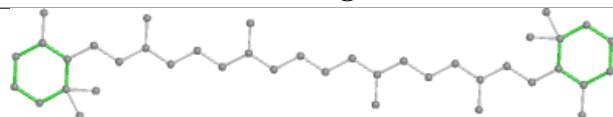
Bond lengths



Bond angles

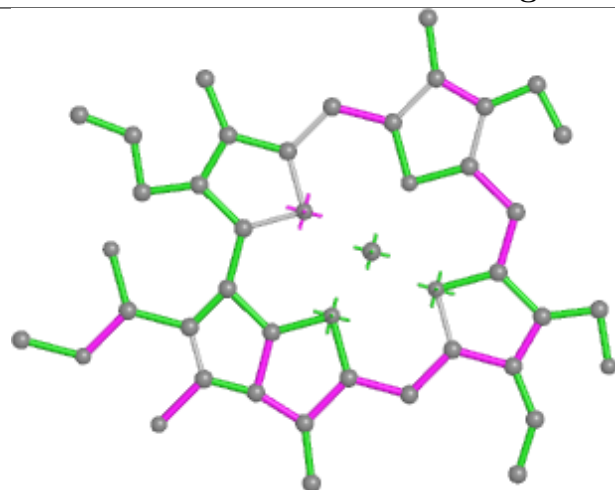


Torsions

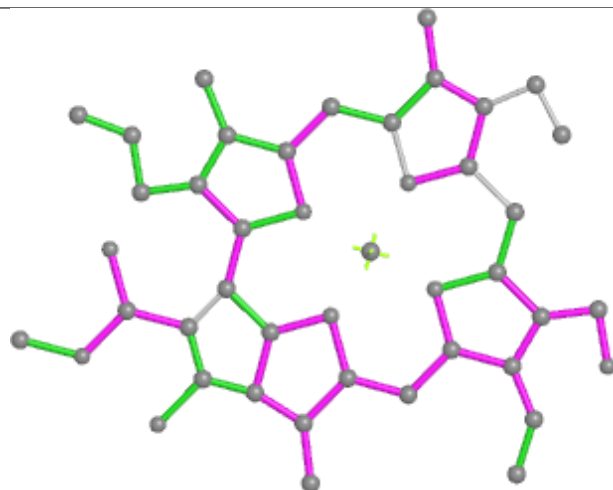


Rings

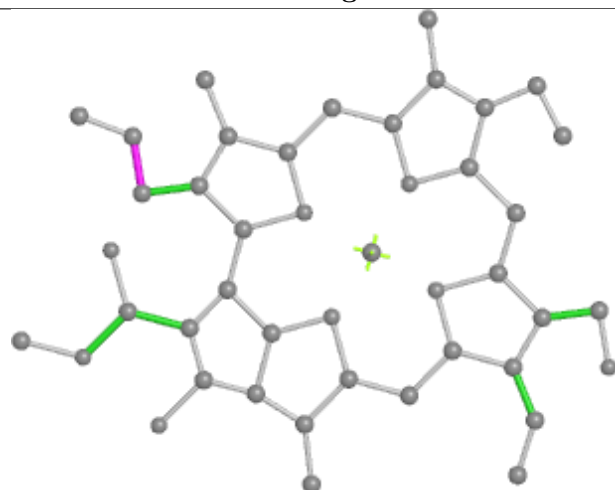
Ligand CHL 9 606



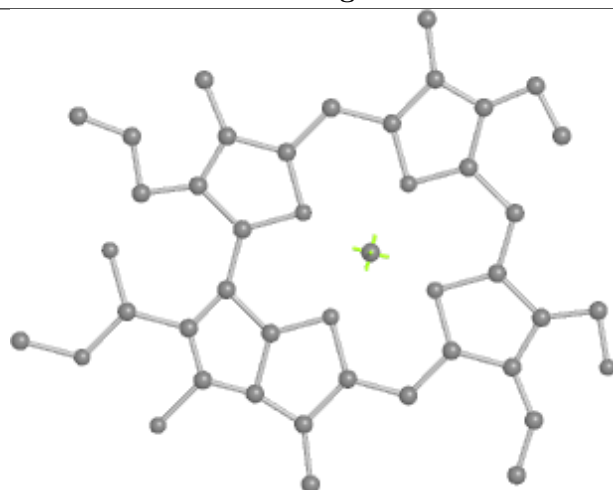
Bond lengths



Bond angles

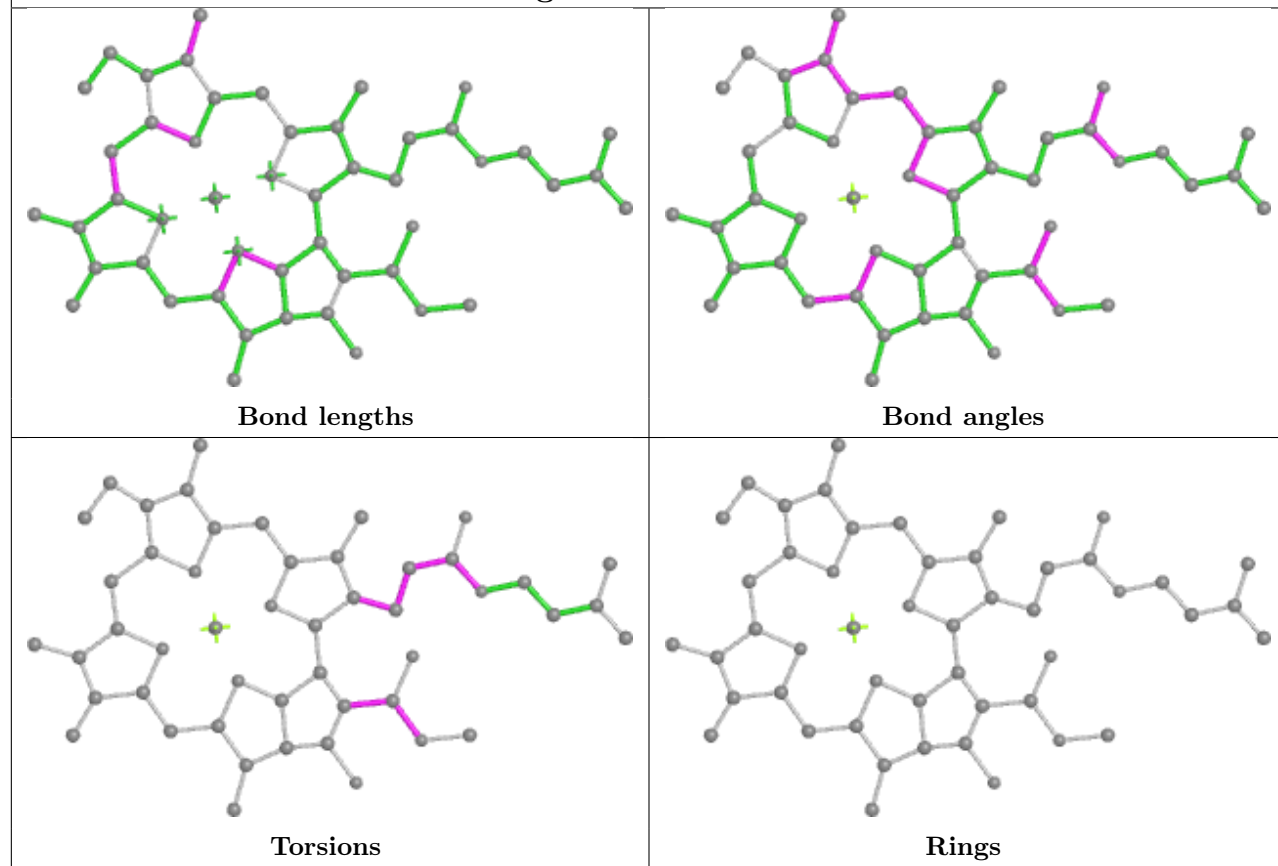


Torsions

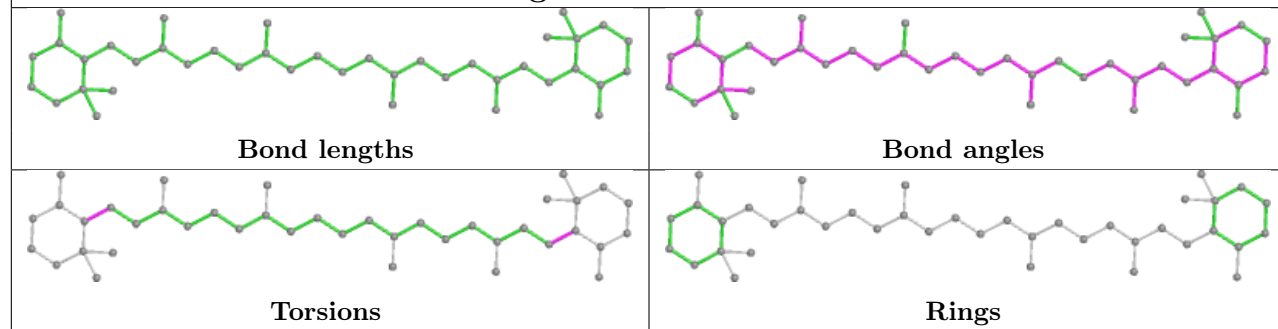


Rings

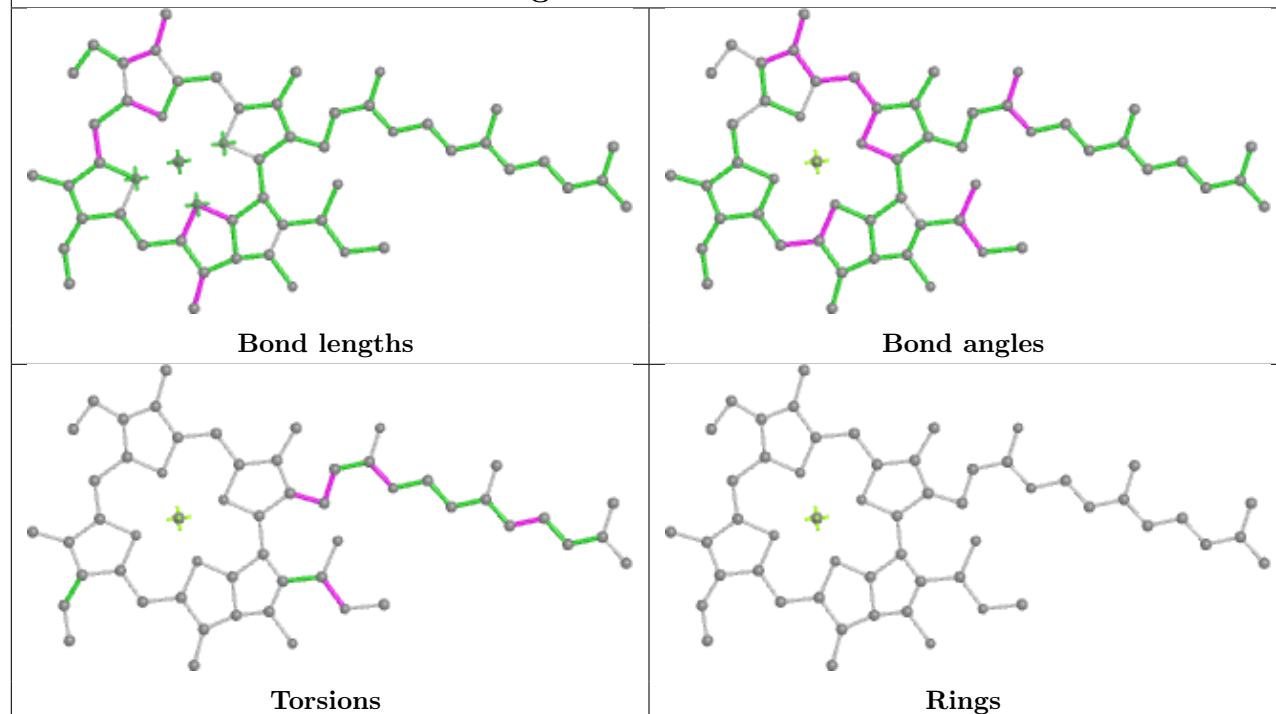
Ligand CLA 1 614



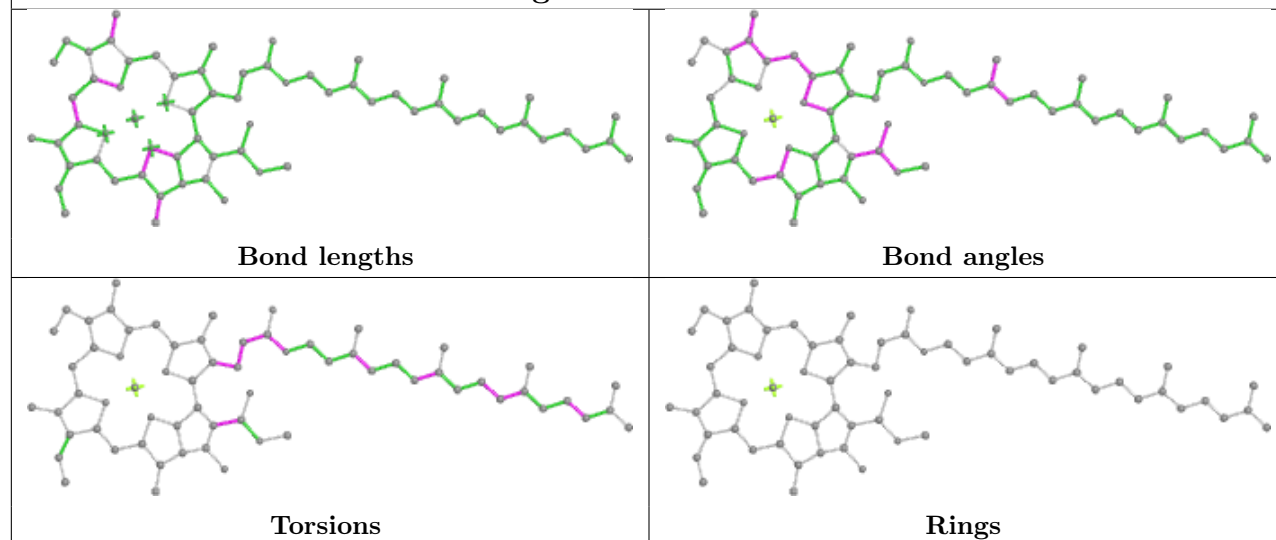
Ligand BCR K 202

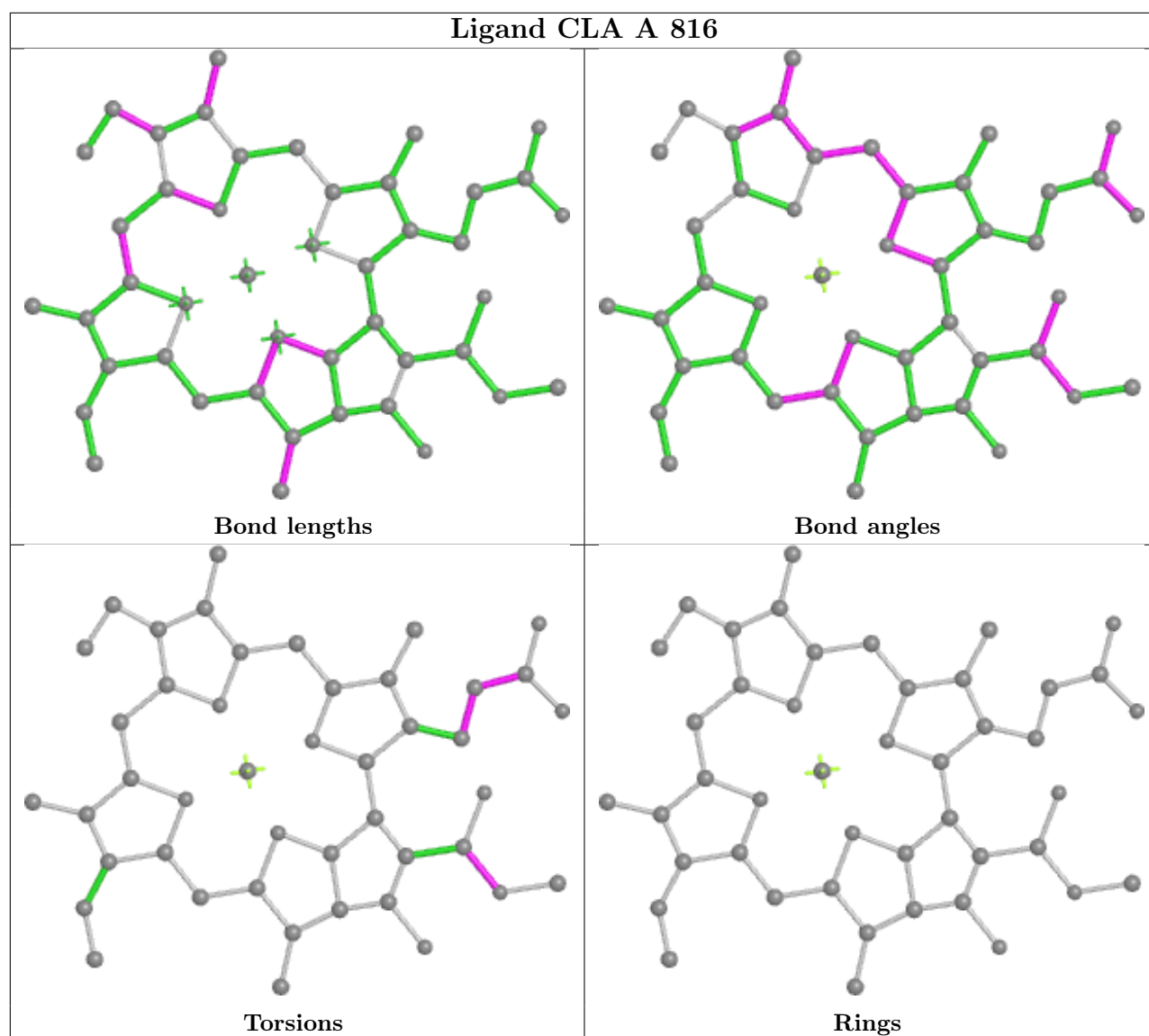


Ligand CLA A 811



Ligand CLA B 831





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.

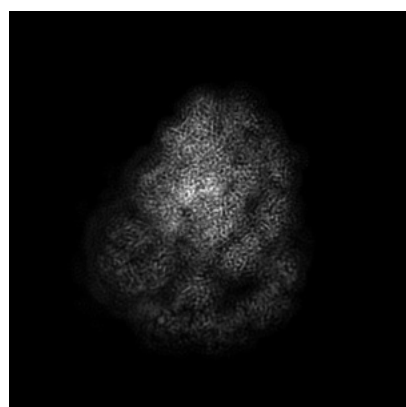
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35018. These allow visual inspection of the internal detail of the map and identification of artifacts.

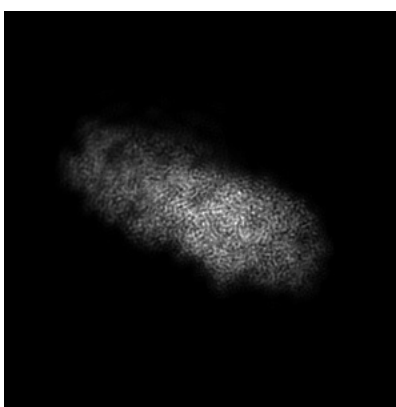
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

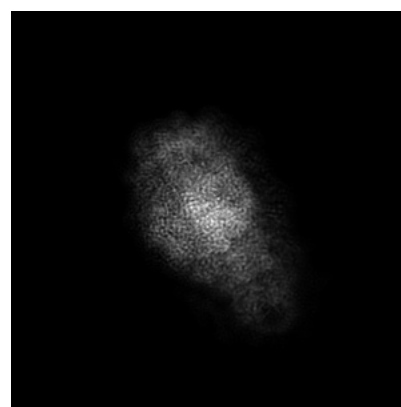
6.1.1 Primary map



X



Y

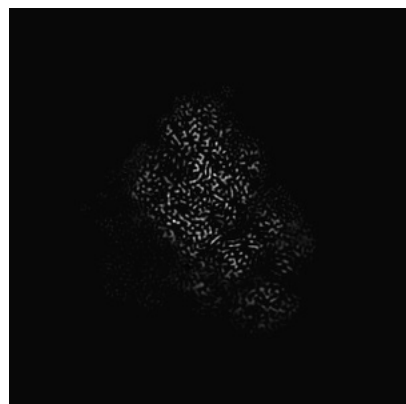


Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 160



Y Index: 160

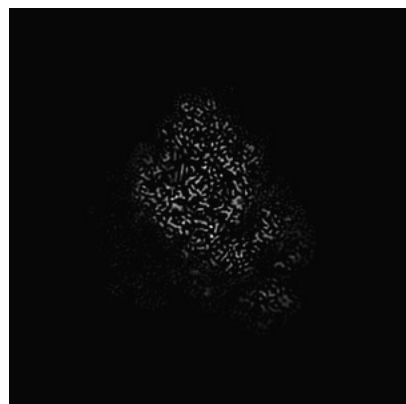


Z Index: 160

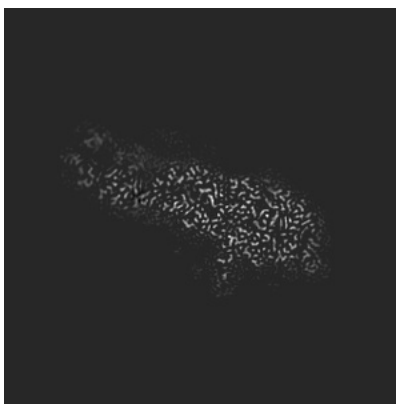
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 158



Y Index: 151

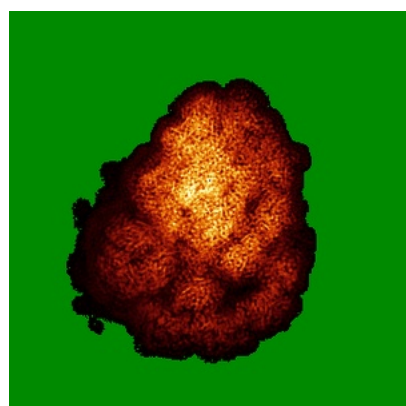


Z Index: 175

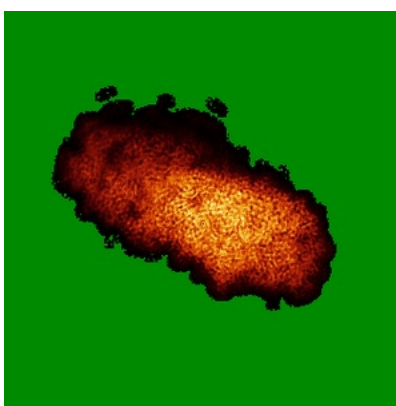
The images above show the largest variance slices of the map in three orthogonal directions.

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

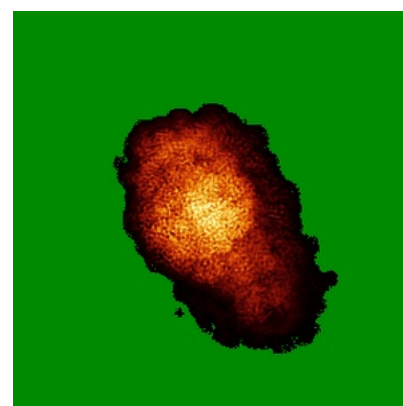
6.4.1 Primary map



X



Y

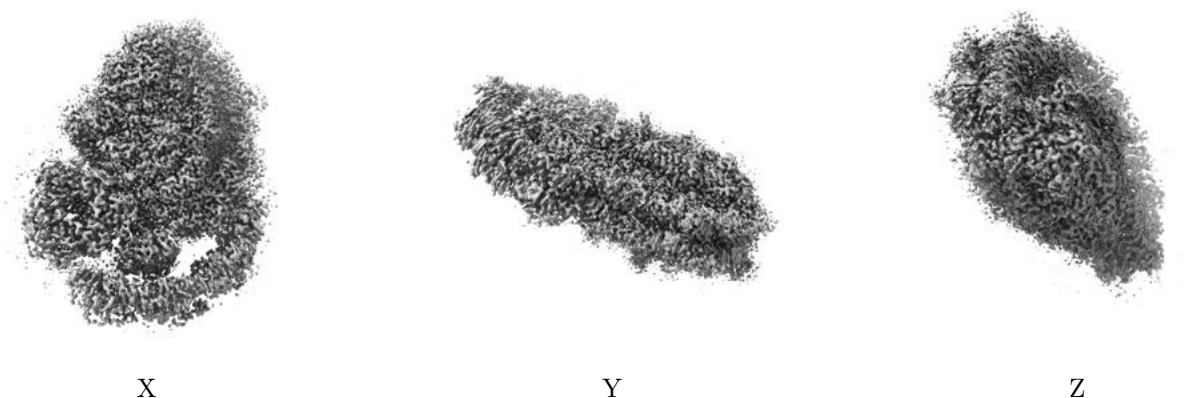


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0188. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

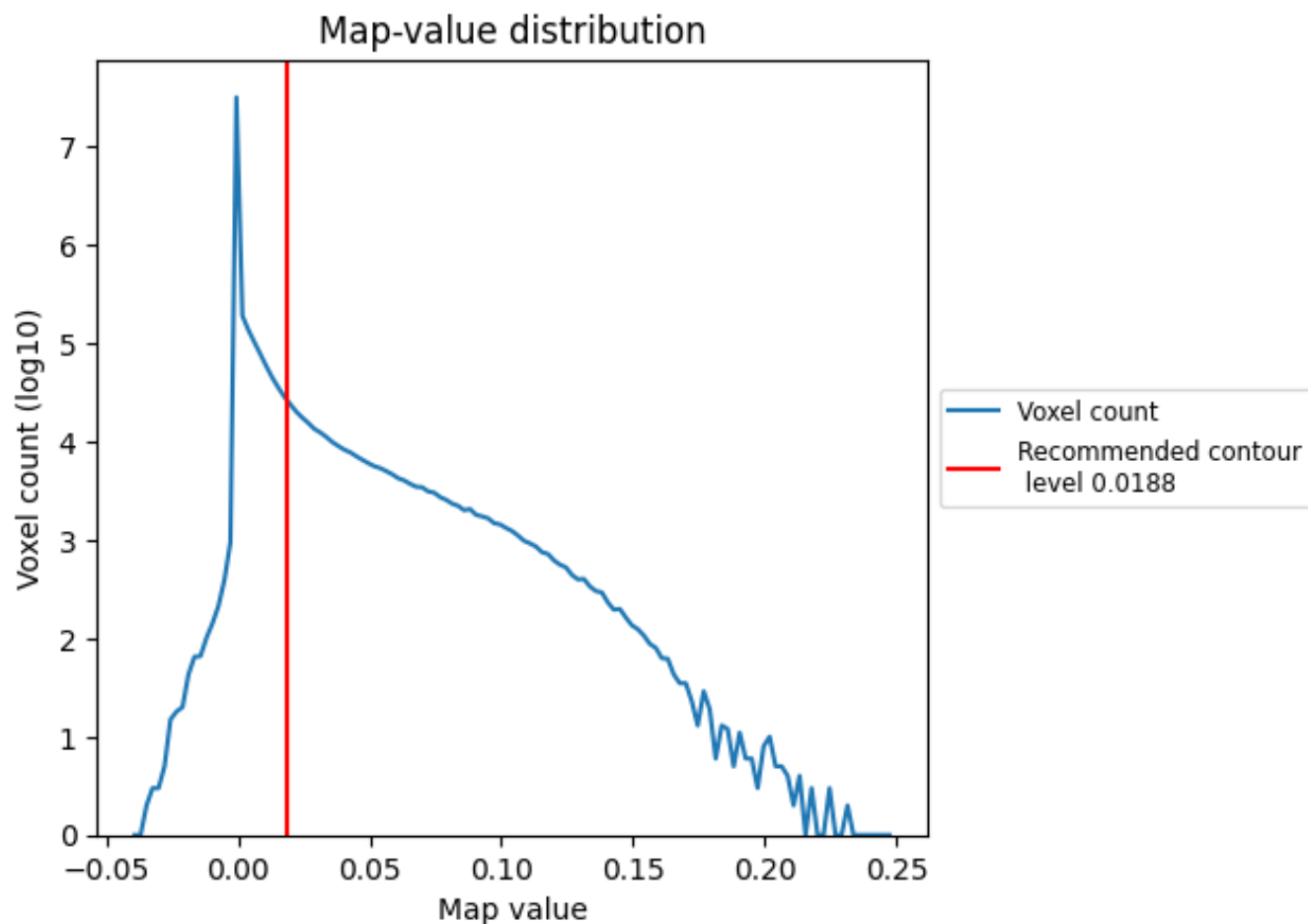
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

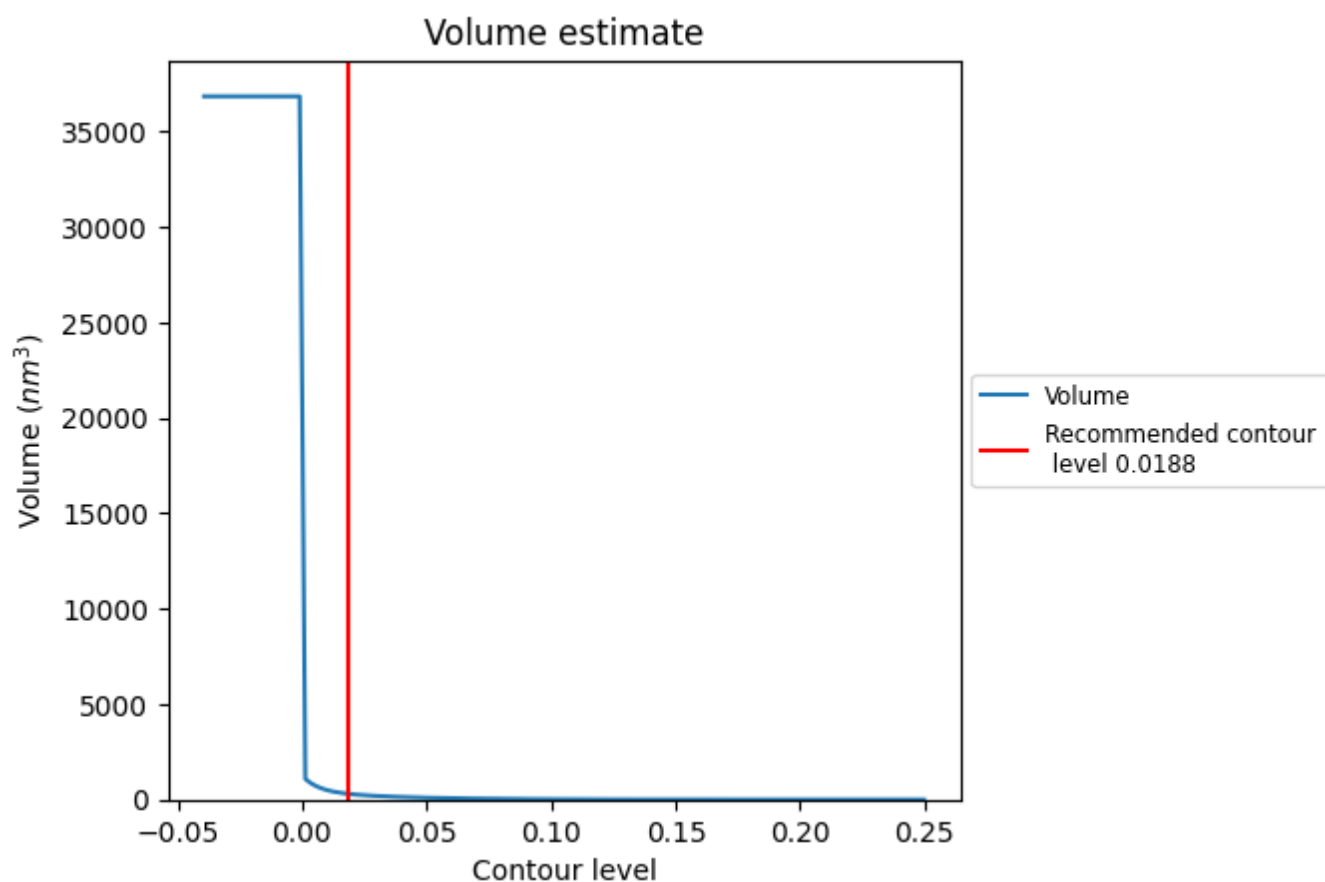
This section contains the results of statistical analysis of the map.

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.

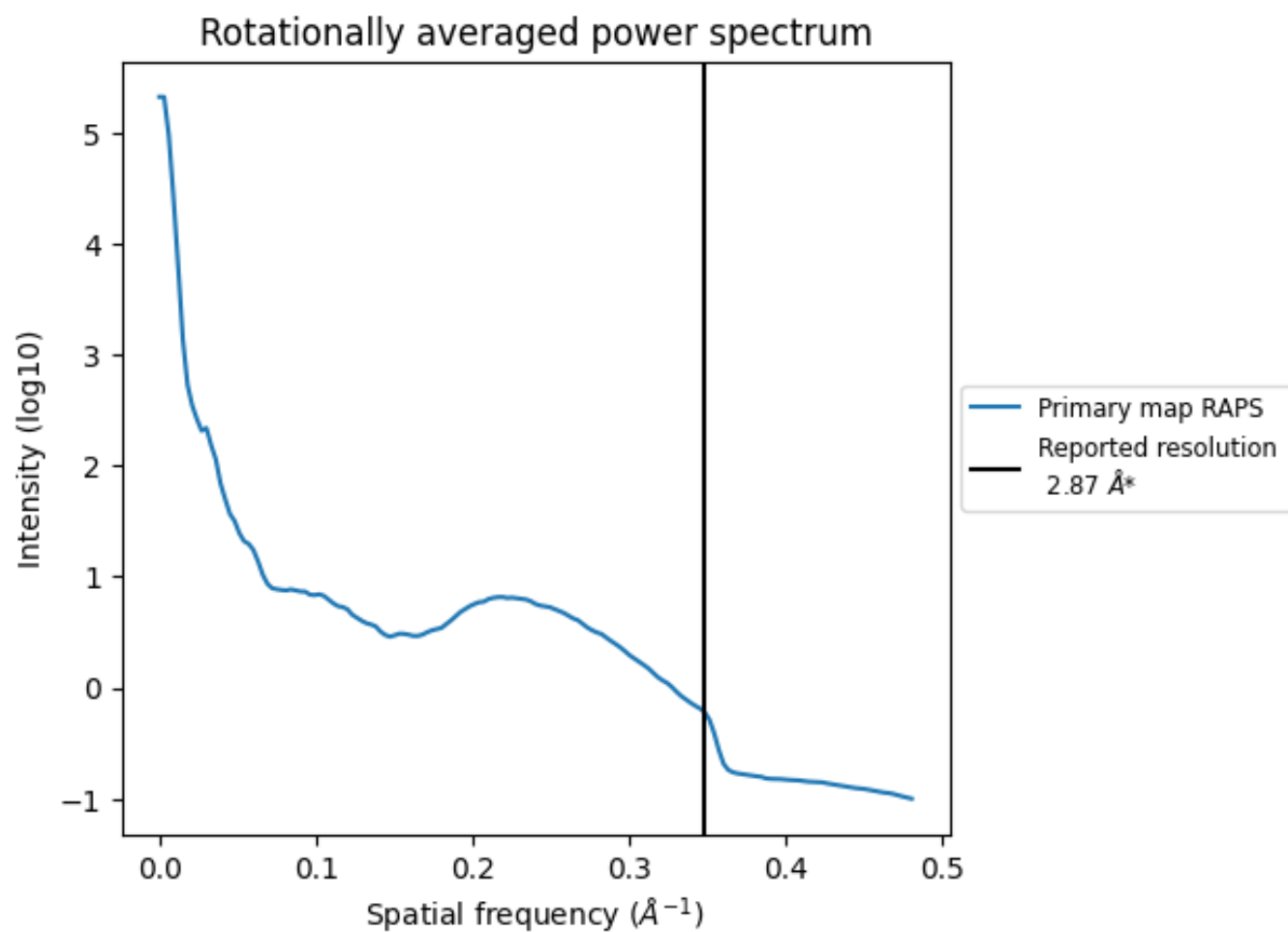
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 296 nm³; this corresponds to an approximate mass of 267 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 0.348 Å⁻¹

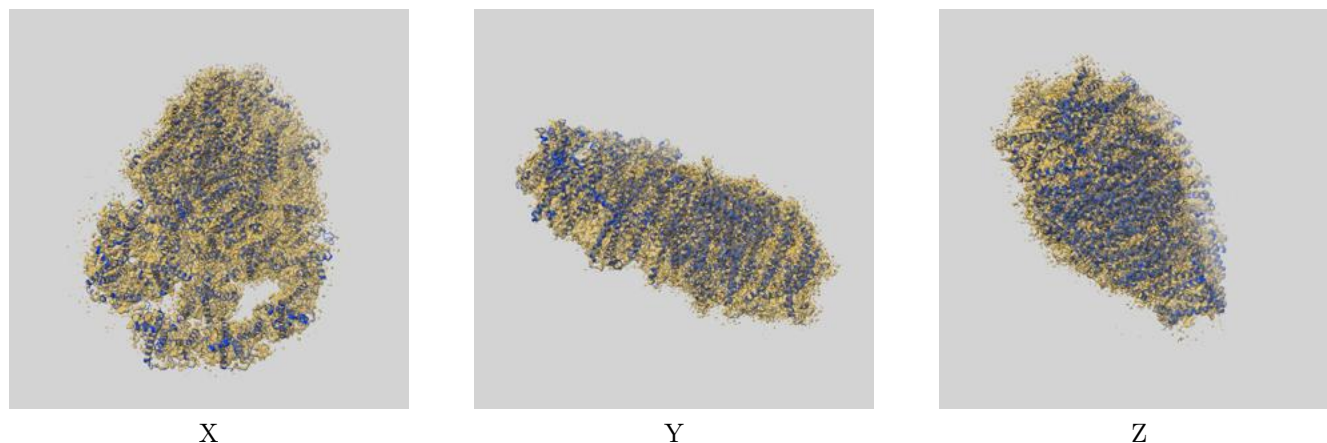
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

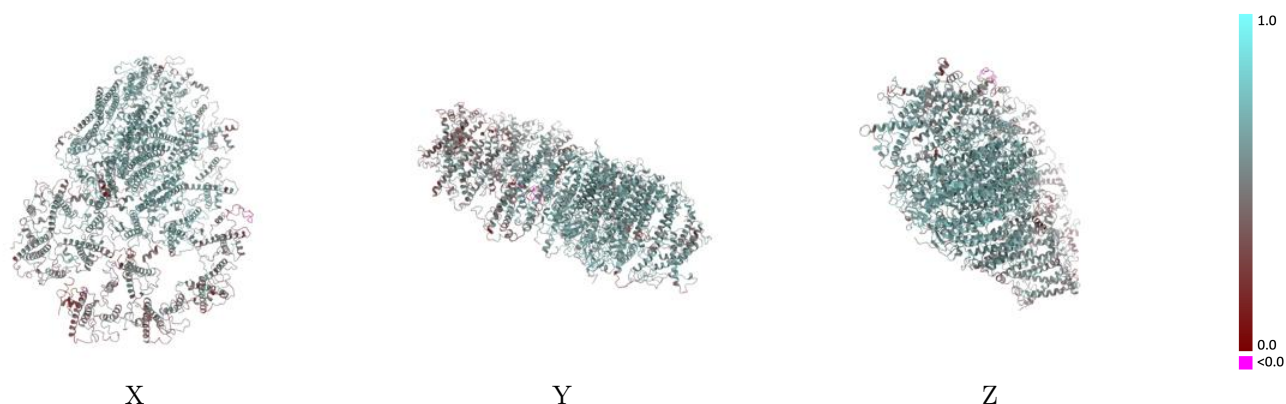
This section contains information regarding the fit between EMDB map EMD-35018 and PDB model 8HTU. Per-residue inclusion information can be found in section [3](#) on page [37](#).

9.1 Map-model overlay [i](#)



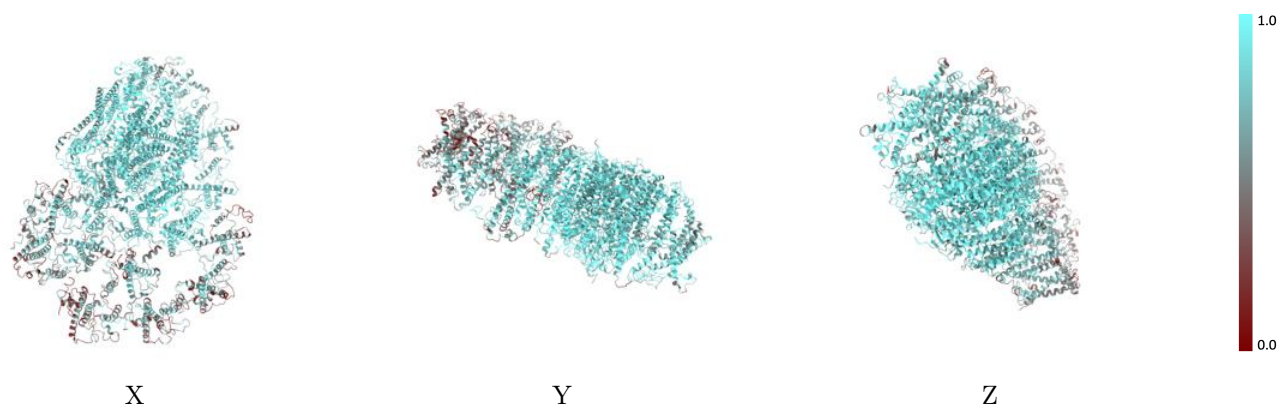
The images above show the 3D surface view of the map at the recommended contour level 0.0188 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



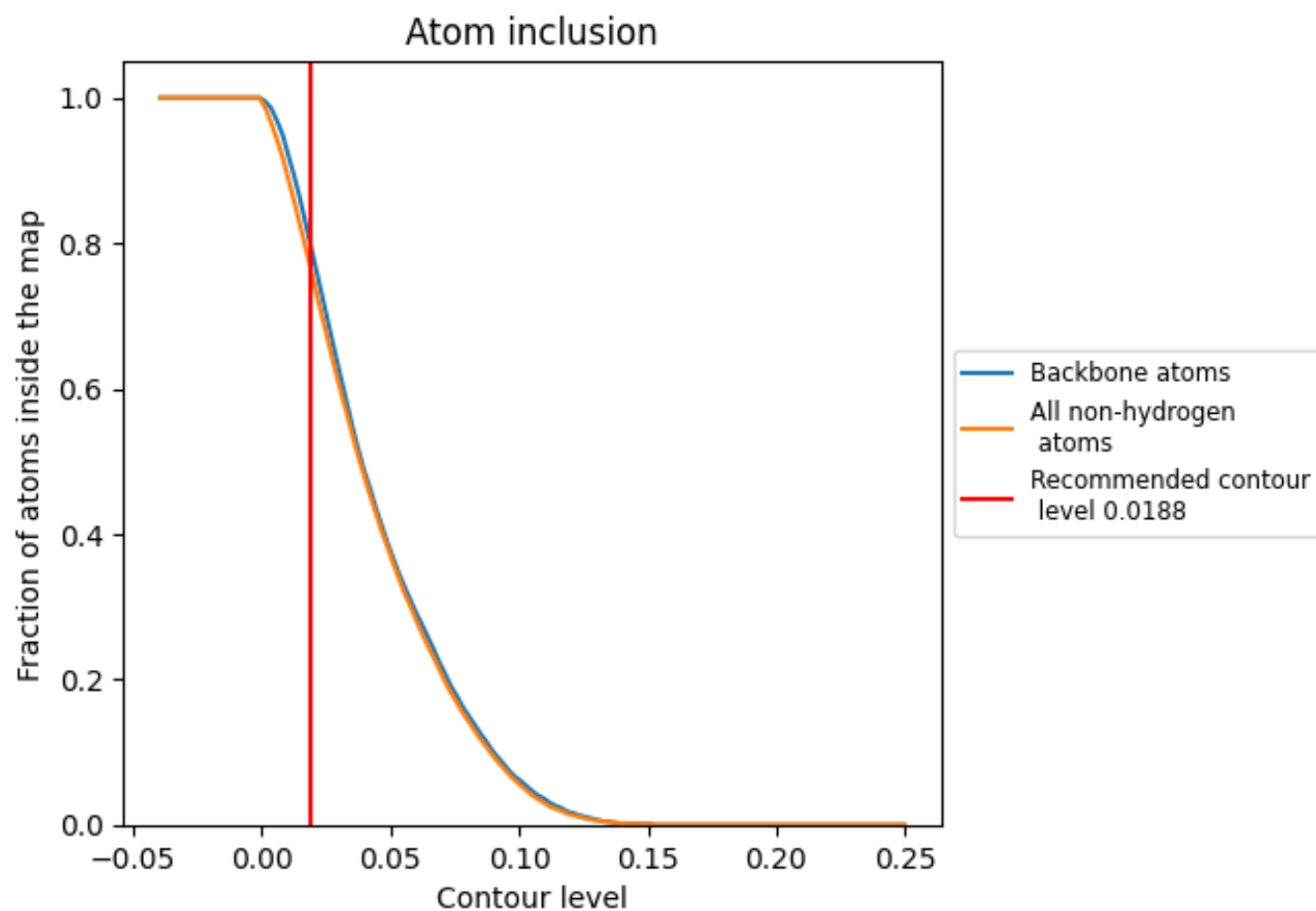
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0188).























































9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 77% 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 (0.0188) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7680	 0.5500
1	 0.7560	 0.5390
2	 0.8540	 0.5860
3	 0.8550	 0.5880
4	 0.7930	 0.5400
5	 0.5530	 0.4110
6	 0.5150	 0.4410
7	 0.4180	 0.3830
8	 0.5530	 0.4610
9	 0.6210	 0.4420
A	 0.9310	 0.6320
B	 0.9210	 0.6270
C	 0.9460	 0.6200
D	 0.8850	 0.5910
E	 0.8660	 0.6050
F	 0.8630	 0.5990
G	 0.7240	 0.5410
H	 0.7350	 0.5080
I	 0.9010	 0.5910
J	 0.8490	 0.5860
K	 0.8640	 0.5880
L	 0.8690	 0.5870
M	 0.7750	 0.5580
O	 0.7840	 0.4770
U	 0.6840	 0.5290
V	 0.5640	 0.4930
W	 0.6720	 0.5220

