



Full wwPDB EM Validation Report ⓘ

Jul 19, 2026 – 04:44 pm BST

PDB ID : 9S1M / pdb_00009s1m
EMDB ID : EMD-54456
Title : Cryo-EM structure of Posidonia oceanica L-PSI-LHCI-LHCII supercomplex
Authors : Capaldi, S.; Amelii, A.; Sanita, G.; Esposito, M.; Bassi, R.
Deposited on : 2025-07-18
Resolution : 3.31 Å(reported)
Based on initial model : 5ZJI

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.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

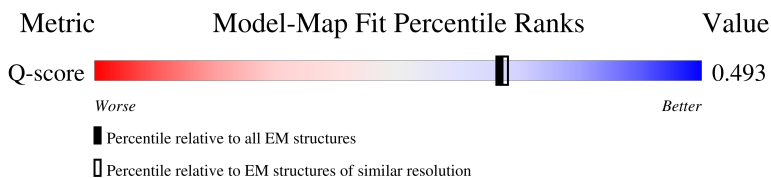
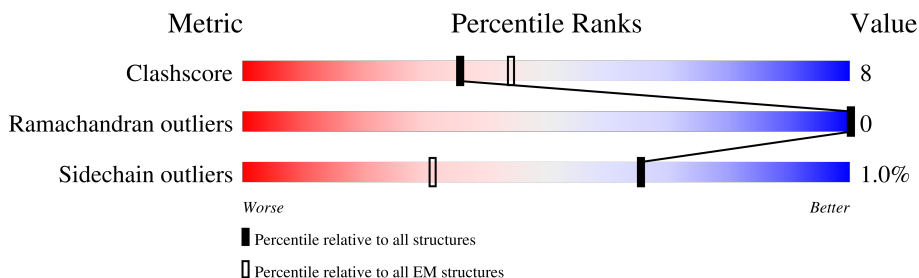
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.31 Å.

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



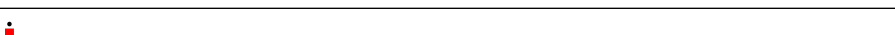
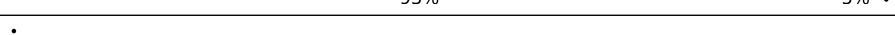
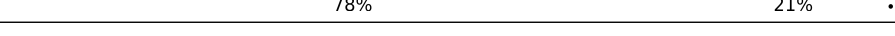
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14550 (2.81 - 3.81)

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	1	200	
1	5	200	
2	2	211	
3	3	232	

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Mol	Chain	Length	Quality of chain
4	4	200	 88% 10% .
4	6	200	 85% 14% .
5	A	750	 91% 6% .
6	B	734	 91% 9%
7	C	81	 84% 15% .
8	D	155	 77% 14% 10%
9	E	93	 66% . 32%
10	F	159	 78% 19% . .
11	G	100	 93% 5% .
12	H	95	 78% 21% .
13	I	36	 81% 8% 11%
14	J	42	 5% 74% 21% 5%
15	K	84	 10% 86% 10% 5%
16	L	170	 82% 13% 5%
17	O	89	 88% 12%
18	X	228	 33% 72% 24% .
18	Z	228	 36% 75% 20% .
19	Y	228	 25% 71% 28%

2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 49325 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 6 (Lhca1).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	198	Total	C	N	O	S	0	0
			1536	1004	256	271	5		
1	5	194	Total	C	N	O	S	0	0
			1504	981	252	266	5		

- Molecule 2 is a protein called Photosystem I chlorophyll a/b-binding protein 2 (Lhca2).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	203	Total	C	N	O	S	0	0
			1579	1031	257	285	6		

- Molecule 3 is a protein called Photosystem I chlorophyll a/b-binding protein 3-1 (Lhca3).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	213	Total	C	N	O	S	0	0
			1638	1074	263	295	6		

- Molecule 4 is a protein called Chlorophyll a-b binding protein 4 (Lhca4).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	198	Total	C	N	O	S	0	0
			1557	1017	254	283	3		
4	6	198	Total	C	N	O	S	0	0
			1557	1017	254	283	3		

- Molecule 5 is a protein called Photosystem I P700 chlorophyll a apoprotein A1 (PsaA).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	724	Total	C	N	O	S	0	0
			5684	3726	968	972	18		

- Molecule 6 is a protein called Photosystem I P700 chlorophyll a apoprotein A2 (PsaB).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	733	Total	C	N	O	S	0	0
			5858	3847	996	1002	13		

- Molecule 7 is a protein called Photosystem I iron-sulfur center (PsaC).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	80	Total	C	N	O	S	0	0
			614	380	106	117	11		

- Molecule 8 is a protein called Photosystem I reaction center subunit II-1, chloroplastic (PsaD1).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	140	Total	C	N	O	S	0	0
			1103	708	190	201	4		

- Molecule 9 is a protein called Photosystem I reaction center subunit IV B (PsaE2).

Mol	Chain	Residues	Atoms				AltConf	Trace
9	E	63	Total	C	N	O	0	0
			519	333	92	94		

- Molecule 10 is a protein called Photosystem I reaction center subunit III (PsaF).

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	155	Total	C	N	O	S	0	0
			1224	794	209	217	4		

- Molecule 11 is a protein called Photosystem I reaction center subunit V (PsaG).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	98	Total	C	N	O	S	0	0
			768	500	128	139	1		

- Molecule 12 is a protein called Photosystem I reaction center subunit VI-1 (PsaH).

Mol	Chain	Residues	Atoms				AltConf	Trace
12	H	94	Total	C	N	O	0	0
			736	483	114	139		

- Molecule 13 is a protein called Photosystem I reaction center subunit VIII (PsaI).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	32	Total	C	N	O	S	0	0
			246	167	39	39	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	40	Total	C	N	O		0	0
			319	216	49	54			

- Molecule 15 is a protein called Photosystem I reaction center subunit psaK (PsaK).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	80	Total	C	N	O	S	0	0
			566	360	97	105	4		

- Molecule 16 is a protein called Photosystem I reaction center subunit XI (PsaL).

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	162	Total	C	N	O	S	0	0
			1222	808	191	220	3		

- Molecule 17 is a protein called Photosystem I subunit O (PsaO).

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	89	Total	C	N	O	S	0	0
			716	481	116	117	2		

- Molecule 18 is a protein called Chlorophyll a-b binding protein 1 (Lhcb1).

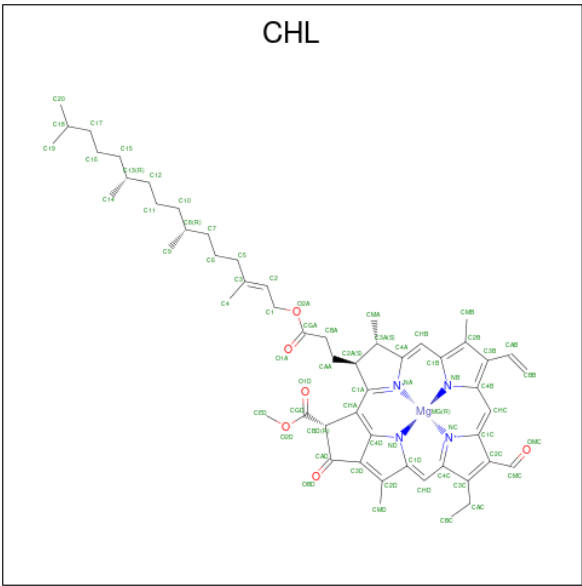
Mol	Chain	Residues	Atoms					AltConf	Trace
18	X	218	Total	C	N	O	S	0	0
			1659	1076	269	307	7		
18	Z	218	Total	C	N	O	S	0	0
			1659	1076	269	307	7		

- Molecule 19 is a protein called Chlorophyll a-b binding protein 2 (Lhcb2).

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Y	227	Total	C	N	O	P S	0	0
			1744	1130	286	321	1 6		

- Molecule 20 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆) (labeled as

"Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
20	1	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
20	1	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
20	2	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
20	2	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
20	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
20	2	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
20	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
20	3	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
20	4	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
20	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
20	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
20	4	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
20	5	1	Total	C	Mg	N	O	0
			55	44	1	4	6	

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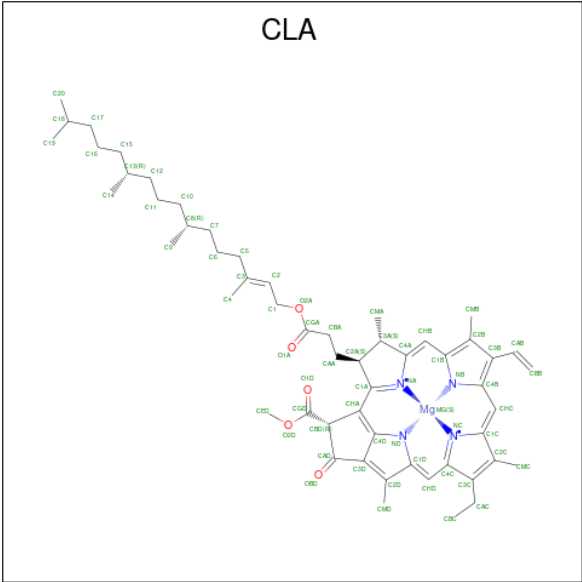
Mol	Chain	Residues	Atoms					AltConf
20	5	1	Total 41	C 32	Mg 1	N 4	O 4	0
20	6	1	Total 56	C 45	Mg 1	N 4	O 6	0
20	6	1	Total 46	C 35	Mg 1	N 4	O 6	0
20	6	1	Total 51	C 40	Mg 1	N 4	O 6	0
20	6	1	Total 41	C 32	Mg 1	N 4	O 4	0
20	X	1	Total 46	C 35	Mg 1	N 4	O 6	0
20	X	1	Total 42	C 33	Mg 1	N 4	O 4	0
20	X	1	Total 46	C 35	Mg 1	N 4	O 6	0
20	X	1	Total 46	C 35	Mg 1	N 4	O 6	0
20	X	1	Total 46	C 35	Mg 1	N 4	O 6	0
20	Y	1	Total 46	C 35	Mg 1	N 4	O 6	0
20	Y	1	Total 42	C 33	Mg 1	N 4	O 4	0
20	Y	1	Total 46	C 35	Mg 1	N 4	O 6	0
20	Y	1	Total 46	C 35	Mg 1	N 4	O 6	0
20	Y	1	Total 46	C 35	Mg 1	N 4	O 6	0
20	Y	1	Total 46	C 35	Mg 1	N 4	O 6	0
20	Y	1	Total 47	C 36	Mg 1	N 4	O 6	0
20	Z	1	Total 46	C 35	Mg 1	N 4	O 6	0
20	Z	1	Total 46	C 35	Mg 1	N 4	O 6	0
20	Z	1	Total 46	C 35	Mg 1	N 4	O 6	0
20	Z	1	Total 46	C 35	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
20	Z	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
20	Z	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

- Molecule 21 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
21	1	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
21	1	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
21	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	2	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
21	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
21	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	2	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
21	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
21	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
21	3	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
21	3	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
21	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
21	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
21	4	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
21	5	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
21	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	6	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	6	1	Total 54	C 44	Mg 1	N 4	O 5	0
21	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	6	1	Total 41	C 33	Mg 1	N 4	O 3	0
21	6	1	Total 57	C 47	Mg 1	N 4	O 5	0
21	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	6	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
21	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
21	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
21	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
21	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
21	B	1	Total 62	C 52	Mg 1	N 4	O 5	0
21	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 56	C 46	Mg 1	N 4	O 5	0
21	B	1	Total 43	C 35	Mg 1	N 4	O 3	0
21	B	1	Total 43	C 35	Mg 1	N 4	O 3	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	B	1	Total 42	C 34	Mg 1	N 4	O 3	0
21	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	F	1	Total 41	C 33	Mg 1	N 4	O 3	0
21	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	G	1	Total 42	C 34	Mg 1	N 4	O 3	0
21	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	H	1	Total 60	C 50	Mg 1	N 4	O 5	0

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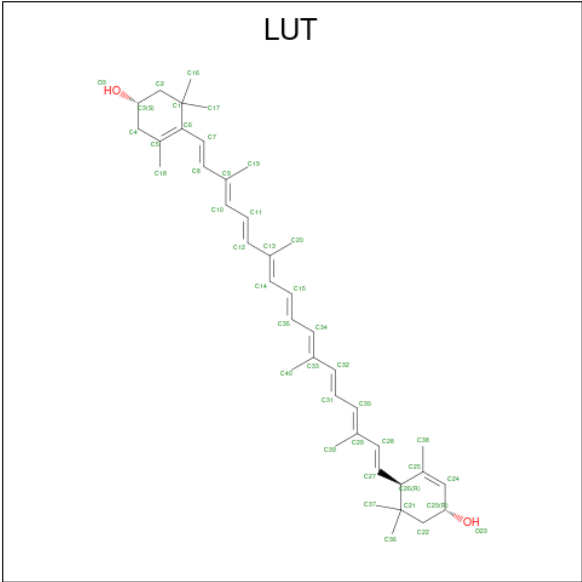
Mol	Chain	Residues	Atoms					AltConf
21	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
21	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
21	K	1	Total 37	C 31	Mg 1	N 4	O 1	0
21	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	K	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	K	1	Total 39	C 31	Mg 1	N 4	O 3	0
21	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	L	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	O	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	O	1	Total 62	C 52	Mg 1	N 4	O 5	0
21	O	1	Total 49	C 39	Mg 1	N 4	O 5	0
21	O	1	Total 38	C 30	Mg 1	N 4	O 3	0
21	X	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	X	1	Total 53	C 43	Mg 1	N 4	O 5	0
21	X	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	X	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	X	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	X	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	X	1	Total 45	C 35	Mg 1	N 4	O 5	0

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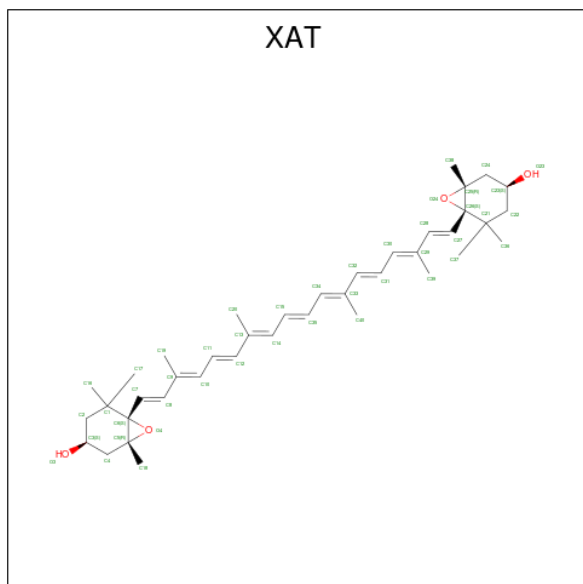
Mol	Chain	Residues	Atoms					AltConf
21	X	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	X	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	Y	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	Z	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	Z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	Z	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	Z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	Z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	Z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	Z	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

- Molecule 22 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂) (labeled as "Ligand of Interest" by depositor).



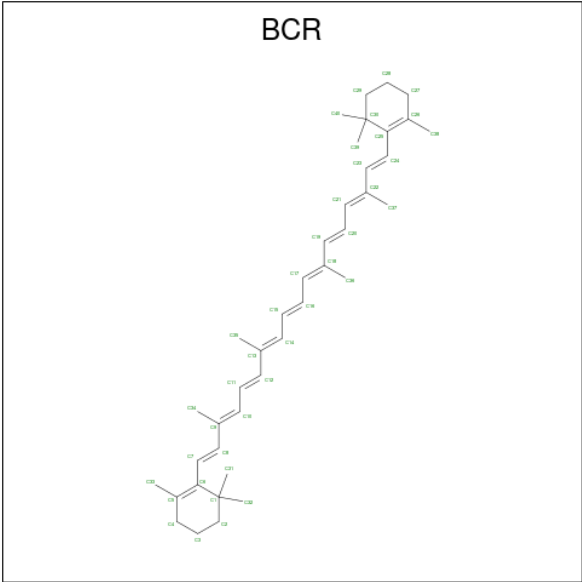
Mol	Chain	Residues	Atoms			AltConf
22	1	1	Total	C	O	0
			42	40	2	
22	2	1	Total	C	O	0
			42	40	2	
22	3	1	Total	C	O	0
			42	40	2	
22	4	1	Total	C	O	0
			42	40	2	
22	5	1	Total	C	O	0
			42	40	2	
22	5	1	Total	C	O	0
			42	40	2	
22	6	1	Total	C	O	0
			42	40	2	
22	F	1	Total	C	O	0
			42	40	2	
22	X	1	Total	C	O	0
			42	40	2	
22	X	1	Total	C	O	0
			42	40	2	
22	Y	1	Total	C	O	0
			42	40	2	
22	Y	1	Total	C	O	0
			42	40	2	
22	Z	1	Total	C	O	0
			42	40	2	
22	Z	1	Total	C	O	0
			42	40	2	

- Molecule 23 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'-TETRAHYDRO-BETA, BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: $C_{40}H_{56}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
23	1	1	Total	C	O	0
			44	40	4	
23	2	1	Total	C	O	0
			44	40	4	
23	3	1	Total	C	O	0
			44	40	4	
23	4	1	Total	C	O	0
			44	40	4	
23	5	1	Total	C	O	0
			44	40	4	
23	6	1	Total	C	O	0
			44	40	4	
23	O	1	Total	C	O	0
			44	40	4	

- Molecule 24 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



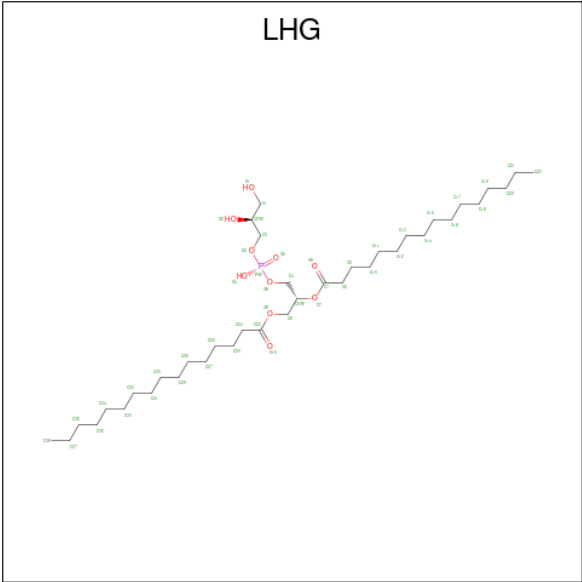
Mol	Chain	Residues	Atoms		AltConf
24	1	1	Total	C	0
			40	40	
24	2	1	Total	C	0
			40	40	
24	3	1	Total	C	0
			40	40	
24	4	1	Total	C	0
			40	40	
24	5	1	Total	C	0
			40	40	
24	6	1	Total	C	0
			40	40	
24	6	1	Total	C	0
			40	40	
24	A	1	Total	C	0
			40	40	
24	A	1	Total	C	0
			40	40	
24	A	1	Total	C	0
			40	40	
24	A	1	Total	C	0
			40	40	
24	A	1	Total	C	0
			40	40	
24	B	1	Total	C	0
			40	40	

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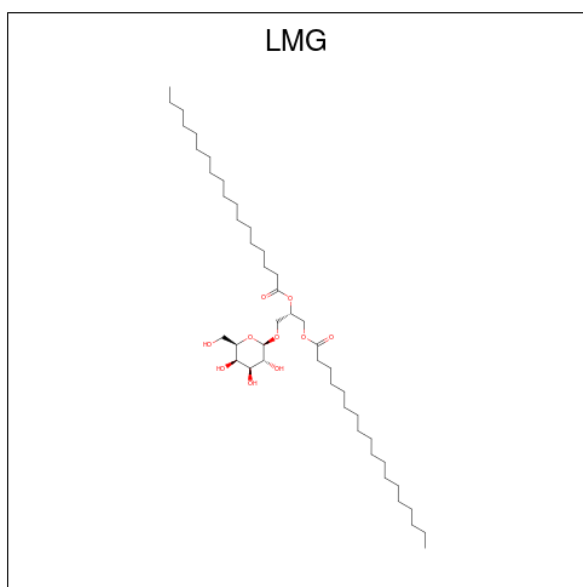
Mol	Chain	Residues	Atoms	AltConf
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	F	1	Total C 40 40	0
24	F	1	Total C 40 40	0
24	G	1	Total C 40 40	0
24	I	1	Total C 40 40	0
24	J	1	Total C 40 40	0
24	K	1	Total C 40 40	0
24	L	1	Total C 40 40	0
24	L	1	Total C 40 40	0
24	L	1	Total C 40 40	0
24	L	1	Total C 40 40	0
24	O	1	Total C 40 40	0
24	O	1	Total C 40 40	0
24	O	1	Total C 40 40	0

- Molecule 25 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
25	1	1	Total	C	O	P	0
			49	38	10	1	
25	1	1	Total	C	O	P	0
			49	38	10	1	
25	1	1	Total	C	O	P	0
			38	27	10	1	
25	2	1	Total	C	O	P	0
			37	26	10	1	
25	5	1	Total	C	O	P	0
			49	38	10	1	
25	A	1	Total	C	O	P	0
			49	38	10	1	
25	A	1	Total	C	O	P	0
			30	19	10	1	
25	X	1	Total	C	O	P	0
			37	26	10	1	
25	Y	1	Total	C	O	P	0
			35	24	10	1	
25	Z	1	Total	C	O	P	0
			32	21	10	1	

- Molecule 26 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).

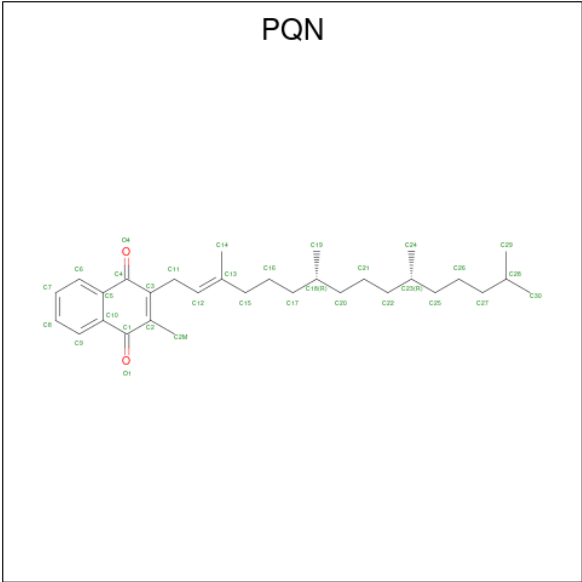


Mol	Chain	Residues	Atoms			AltConf
26	1	1	Total	C	O	0
			53	43	10	
26	1	1	Total	C	O	0
			49	39	10	
26	4	1	Total	C	O	0
			36	26	10	
26	5	1	Total	C	O	0
			53	43	10	
26	5	1	Total	C	O	0
			49	39	10	
26	6	1	Total	C	O	0
			36	26	10	
26	B	1	Total	C	O	0
			52	42	10	
26	F	1	Total	C	O	0
			47	37	10	
26	F	1	Total	C	O	0
			30	20	10	
26	G	1	Total	C	O	0
			50	40	10	

- Molecule 27 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).

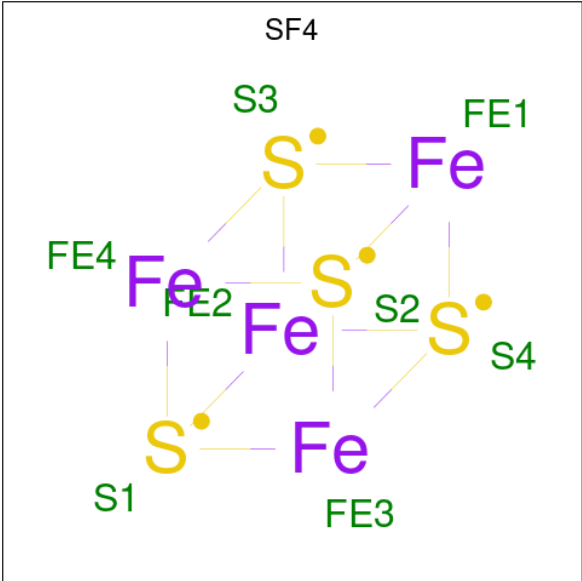


- Molecule 28 is PHYLLOQUINONE (CCD ID: PQN) (formula: $\text{C}_{31}\text{H}_{46}\text{O}_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 29 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



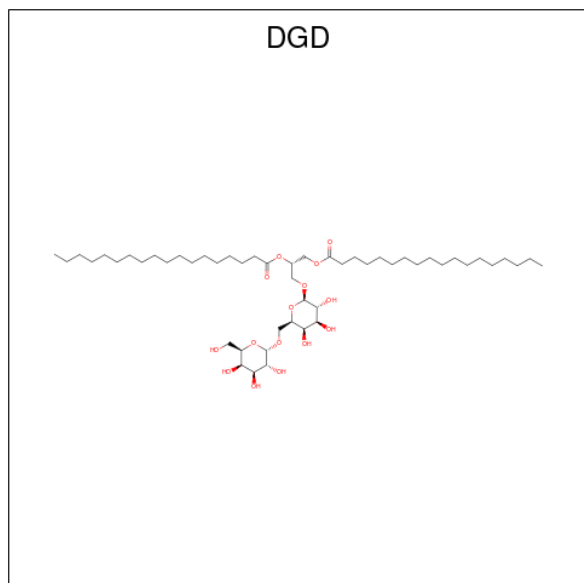
Mol	Chain	Residues	Atoms			AltConf
29	A	1	Total	Fe	S	0
			8	4	4	

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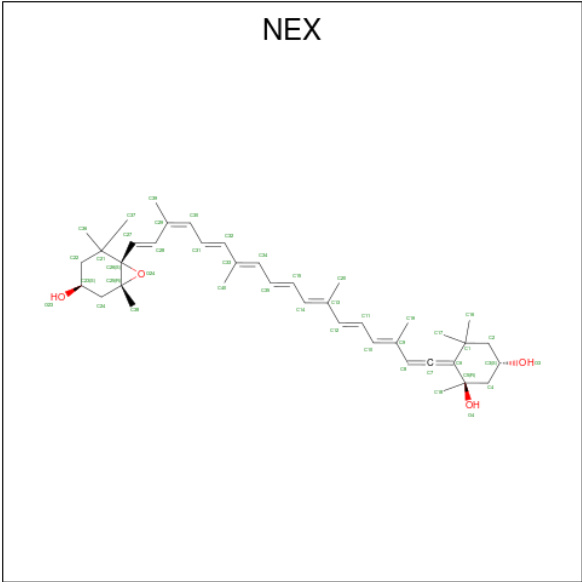
Mol	Chain	Residues	Atoms			AltConf
29	C	1	Total	Fe	S	0
			8	4	4	
29	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
30	B	1	Total	C	O	0
			61	46	15	

- Molecule 31 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: $C_{40}H_{56}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
31	X	1	Total	C	O	0
			44	40	4	
31	Y	1	Total	C	O	0
			44	40	4	
31	Z	1	Total	C	O	0
			44	40	4	

3 Residue-property plots [i](#)

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

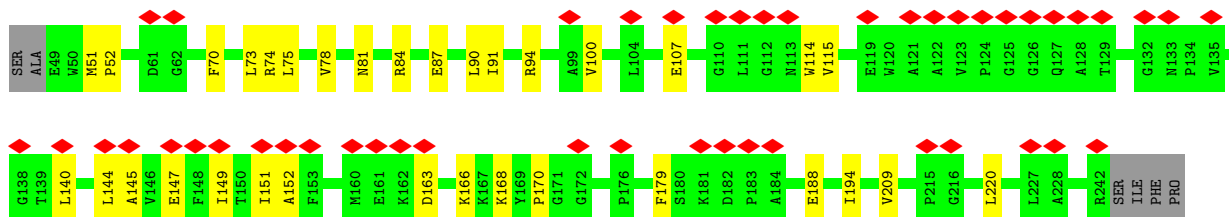
- Molecule 1: Chlorophyll a-b binding protein 6 (Lhca1)

Chain 1: 



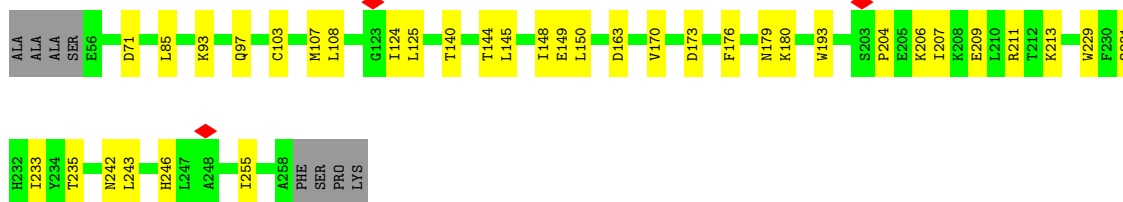
- Molecule 1: Chlorophyll a-b binding protein 6 (Lhca1)

Chain 5: 



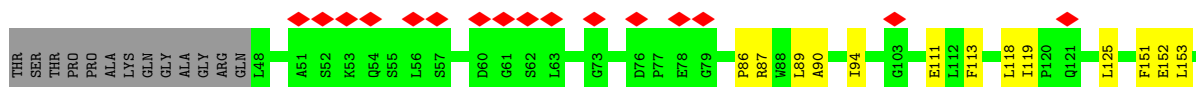
- Molecule 2: Photosystem I chlorophyll a/b-binding protein 2 (Lhca2)

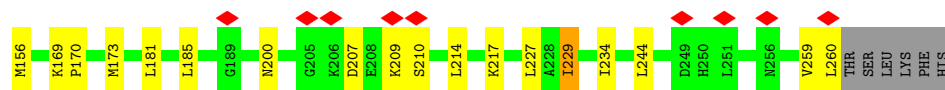
Chain 2: 



- Molecule 3: Photosystem I chlorophyll a/b-binding protein 3-1 (Lhca3)

Chain 3: 





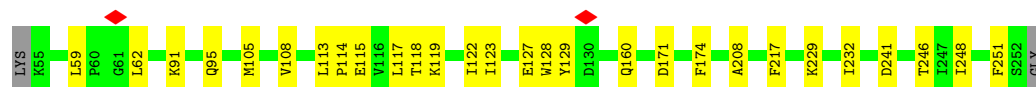
- Molecule 4: Chlorophyll a-b binding protein 4 (Lhca4)

Chain 4: 88% 10%



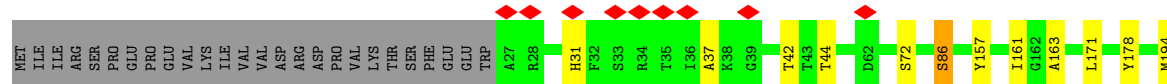
- Molecule 4: Chlorophyll a-b binding protein 4 (Lhca4)

Chain 6: 85% 14%



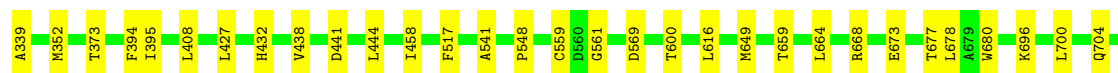
- Molecule 5: Photosystem I P700 chlorophyll a apoprotein A1 (PsaA)

Chain A: 91% 6%



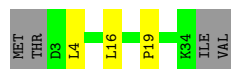
- Molecule 6: Photosystem I P700 chlorophyll a apoprotein A2 (PsaB)

Chain B: 91% 9%

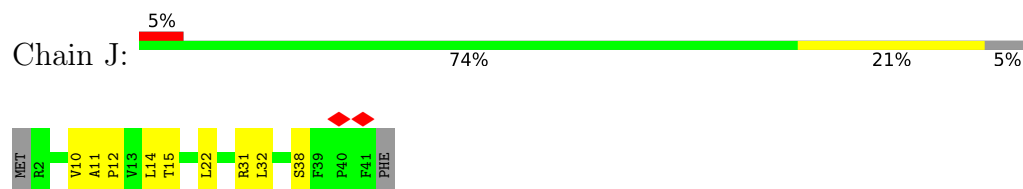


- Molecule 7: Photosystem I iron-sulfur center (PsaC)

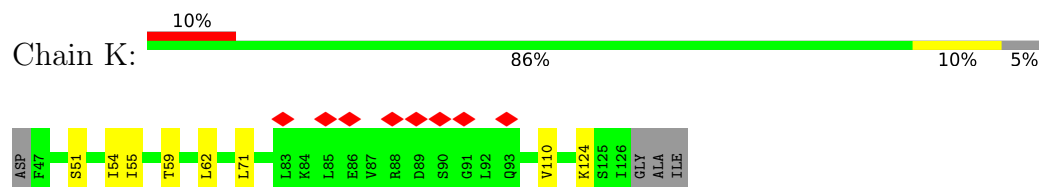
Chain C: 84% 15%



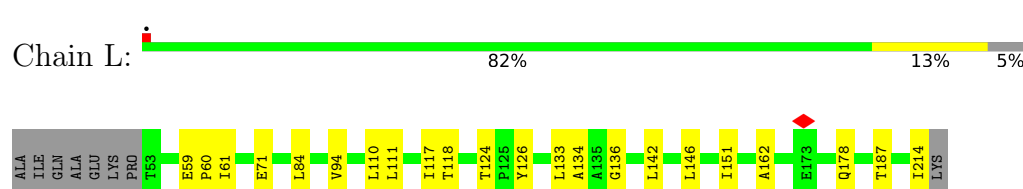
- Molecule 14: Photosystem I reaction center subunit IX



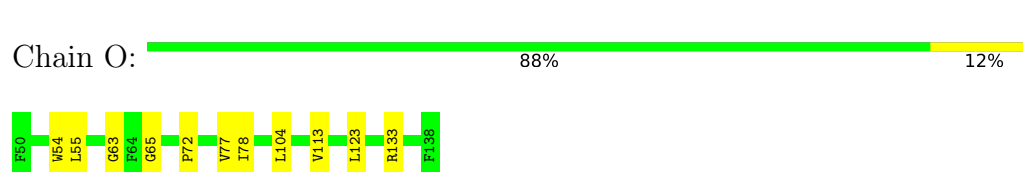
- Molecule 15: Photosystem I reaction center subunit psaK (PsaK)



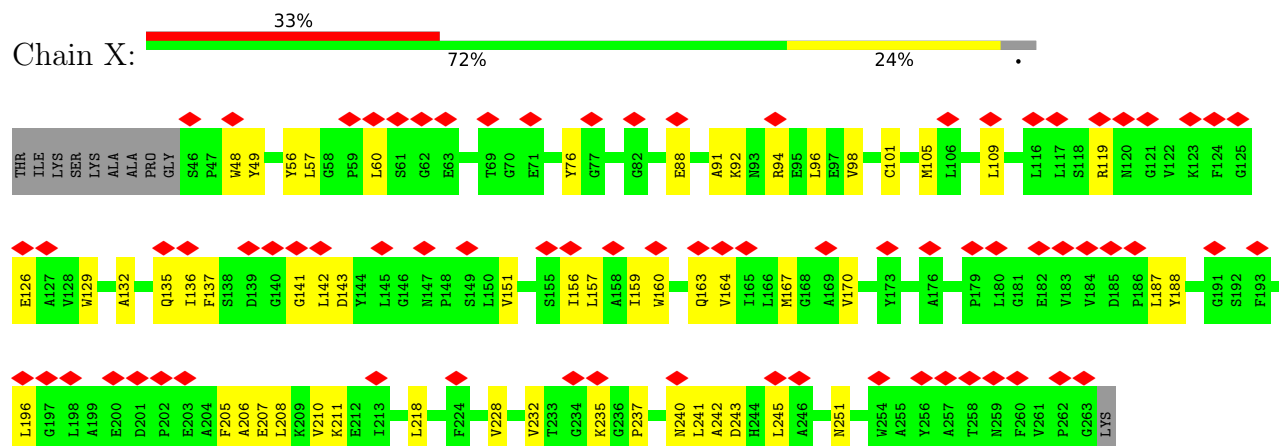
- Molecule 16: Photosystem I reaction center subunit XI (PsaL)



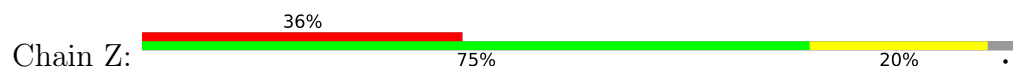
- Molecule 17: Photosystem I subunit O (PsaO)

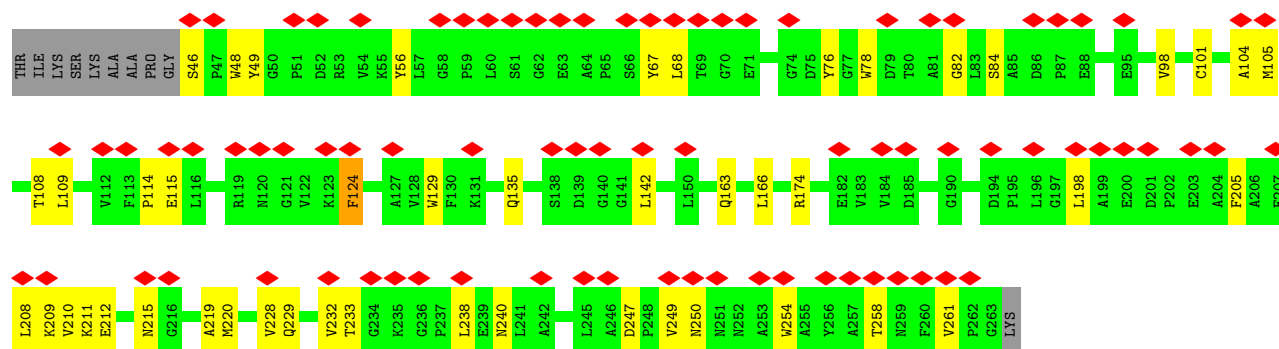


- Molecule 18: Chlorophyll a-b binding protein 1 (Lhcb1)

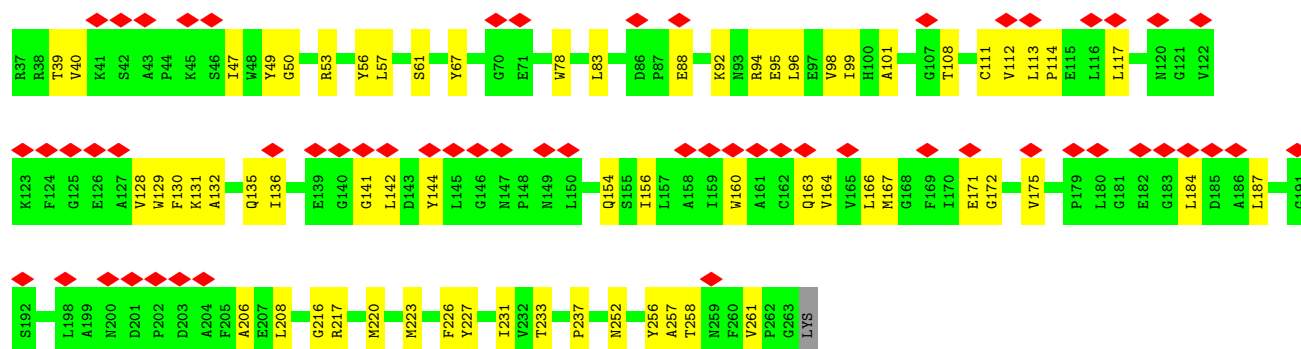


- Molecule 18: Chlorophyll a-b binding protein 1 (Lhcb1)





• Molecule 19: Chlorophyll a-b binding protein 2 (Lhcb2)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	37162	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	45.582	Depositor
Minimum map value	-16.918	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.985	Depositor
Recommended contour level	4.3	Depositor
Map size ($\text{\AA}$)	368.0, 368.0, 368.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.92, 0.92, 0.92	Depositor

5 Model quality

5.1 Standard geometry

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

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	1	0.16	0/1587	0.33	0/2166
1	5	0.13	0/1553	0.34	0/2119
2	2	0.15	0/1634	0.29	0/2236
3	3	0.15	0/1690	0.34	0/2292
4	4	0.17	0/1606	0.32	0/2191
4	6	0.15	0/1606	0.34	0/2191
5	A	0.20	0/5878	0.32	0/8020
6	B	0.21	0/6070	0.33	0/8291
7	C	0.20	0/626	0.40	0/849
8	D	0.16	0/1131	0.37	0/1530
9	E	0.16	0/531	0.27	0/721
10	F	0.17	0/1253	0.33	0/1691
11	G	0.15	0/788	0.33	0/1069
12	H	0.17	0/759	0.40	0/1030
13	I	0.16	0/252	0.31	0/343
14	J	0.15	0/328	0.36	0/448
15	K	0.15	0/572	0.35	0/772
16	L	0.15	0/1259	0.29	0/1723
17	O	0.15	0/746	0.30	0/1015
18	X	0.11	0/1710	0.31	0/2331
18	Z	0.12	0/1710	0.33	0/2331
19	Y	0.14	0/1784	0.34	0/2425
All	All	0.17	0/35073	0.33	0/47784

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1536	0	1523	18	0
1	5	1504	0	1491	29	0
2	2	1579	0	1524	26	0
3	3	1638	0	1602	23	0
4	4	1557	0	1519	15	0
4	6	1557	0	1519	22	0
5	A	5684	0	5539	35	0
6	B	5858	0	5635	48	0
7	C	614	0	593	11	0
8	D	1103	0	1114	14	0
9	E	519	0	512	4	0
10	F	1224	0	1257	23	0
11	G	768	0	748	4	0
12	H	736	0	723	18	0
13	I	246	0	265	2	0
14	J	319	0	330	8	0
15	K	566	0	596	5	0
16	L	1222	0	1224	15	0
17	O	716	0	683	9	0
18	X	1659	0	1595	49	0
18	Z	1659	0	1595	44	0
19	Y	1744	0	1688	47	0
20	1	96	0	68	3	0
20	2	226	0	150	8	0
20	3	47	0	31	1	0
20	4	194	0	138	5	0
20	5	96	0	68	3	0
20	6	194	0	138	7	0
20	X	226	0	151	9	0
20	Y	319	0	213	13	0
20	Z	272	0	182	13	0
21	1	628	0	553	12	0
21	2	504	0	433	12	0
21	3	601	0	463	10	0
21	4	502	0	418	6	0
21	5	574	0	461	12	0
21	6	533	0	425	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	A	2452	0	2391	61	0
21	B	2282	0	2215	50	0
21	F	41	0	29	0	0
21	G	132	0	97	2	0
21	H	60	0	59	2	0
21	J	84	0	62	4	0
21	K	167	0	116	3	0
21	L	215	0	197	10	0
21	O	199	0	161	9	0
21	X	413	0	309	20	0
21	Y	390	0	319	11	0
21	Z	336	0	263	19	0
22	1	42	0	56	4	0
22	2	42	0	56	4	0
22	3	42	0	56	6	0
22	4	42	0	56	4	0
22	5	84	0	112	9	0
22	6	42	0	56	3	0
22	F	42	0	56	3	0
22	X	84	0	112	16	0
22	Y	84	0	112	16	0
22	Z	84	0	112	13	0
23	1	44	0	56	1	0
23	2	44	0	56	0	0
23	3	44	0	56	2	0
23	4	44	0	56	1	0
23	5	44	0	56	1	0
23	6	44	0	56	2	0
23	O	44	0	56	4	0
24	1	40	0	56	0	0
24	2	40	0	56	2	0
24	3	40	0	56	2	0
24	4	40	0	56	2	0
24	5	40	0	56	1	0
24	6	80	0	112	5	0
24	A	240	0	336	16	0
24	B	280	0	392	17	0
24	F	80	0	112	2	0
24	G	40	0	56	2	0
24	I	40	0	56	1	0
24	J	40	0	56	4	0
24	K	40	0	56	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	L	160	0	224	15	0
24	O	120	0	168	6	0
25	1	136	0	194	8	0
25	2	37	0	44	2	0
25	5	49	0	74	2	0
25	A	79	0	104	3	0
25	X	37	0	44	3	0
25	Y	35	0	40	3	0
25	Z	32	0	34	2	0
26	1	102	0	150	1	0
26	4	36	0	42	0	0
26	5	102	0	150	2	0
26	6	36	0	42	1	0
26	B	52	0	77	3	0
26	F	77	0	97	1	0
26	G	50	0	70	1	0
27	4	35	0	46	1	0
27	6	35	0	46	0	0
27	A	35	0	46	0	0
27	F	35	0	46	0	0
27	G	35	0	46	0	0
28	A	33	0	46	0	0
28	B	33	0	46	4	0
29	A	8	0	0	1	0
29	C	16	0	0	0	0
30	B	61	0	83	2	0
31	X	44	0	56	1	0
31	Y	44	0	56	2	0
31	Z	44	0	56	3	0
All	All	49325	0	48144	762	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 (762) 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)
14:J:10:VAL:HG12	14:J:12:PRO:HD2	1.58	0.83
5:A:680:PHE:HA	21:A:802:CLA:HAB	1.60	0.82
21:B:821:CLA:HBA1	21:B:821:CLA:HBD	1.63	0.81
7:C:61:ASP:HB3	9:E:131:ASN:HD21	1.47	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:X:610:CLA:HED3	21:X:610:CLA:H2A	1.65	0.78
22:Y:616:LUT:H8	22:Y:616:LUT:H171	1.66	0.77
1:1:234:ASN:HD22	21:1:613:CLA:HED1	1.53	0.73
21:X:611:CLA:CGA	21:X:611:CLA:HBD	2.17	0.73
22:Z:314:LUT:H8	22:Z:314:LUT:H181	1.69	0.73
21:B:838:CLA:HAB	28:B:841:PQN:H192	1.72	0.72
1:5:100:VAL:HG11	22:5:615:LUT:H12	1.72	0.71
2:2:213:LYS:HZ1	21:2:611:CLA:HAA2	1.53	0.71
1:5:51:MET:HE2	4:6:160:GLN:HE21	1.55	0.71
12:H:103:ARG:HD3	16:L:151:ILE:HG12	1.73	0.71
22:X:614:LUT:H171	22:X:614:LUT:H8	1.73	0.71
22:3:615:LUT:H8	22:3:615:LUT:H171	1.71	0.71
21:O:206:CLA:HBD	21:O:206:CLA:HBA1	1.72	0.71
18:Z:174:ARG:HH12	20:Z:309:CHL:HED1	1.55	0.70
20:6:606:CHL:HBD	20:6:606:CHL:HBA1	1.73	0.69
19:Y:223:MET:HG2	22:Y:615:LUT:H12	1.75	0.69
15:K:124:LYS:HE3	15:K:124:LYS:HA	1.75	0.69
21:A:842:CLA:H43	6:B:438:VAL:HG22	1.74	0.68
4:4:122:ILE:HG13	4:4:123:ILE:HG23	1.74	0.68
2:2:213:LYS:NZ	21:2:611:CLA:HBD	2.09	0.68
22:5:619:LUT:H8	22:5:619:LUT:H181	1.76	0.68
11:G:154:VAL:HG22	26:G:206:LMG:H121	1.75	0.68
4:6:246:THR:HG23	4:6:248:ILE:H	1.59	0.67
3:3:259:VAL:HG13	3:3:260:LEU:HD12	1.77	0.67
6:B:262:HIS:HD2	6:B:264:GLN:H	1.43	0.66
12:H:83:SER:HB3	16:L:94:VAL:HG13	1.76	0.66
18:Z:247:ASP:HB2	18:Z:250:ASN:HB2	1.77	0.66
3:3:169:LYS:HD2	3:3:170:PRO:HD2	1.77	0.65
18:X:241:LEU:HG	18:X:245:LEU:HD23	1.76	0.65
19:Y:92:LYS:O	19:Y:96:LEU:HD12	1.95	0.65
19:Y:95:GLU:HG2	19:Y:187:LEU:HD21	1.78	0.65
5:A:42:THR:HG22	5:A:44:THR:H	1.62	0.65
20:4:304:CHL:HBA2	24:4:317:BCR:H21C	1.78	0.65
4:4:108:VAL:HG11	22:4:315:LUT:H12	1.79	0.65
21:A:824:CLA:HBB2	25:A:853:LHG:HC82	1.77	0.65
2:2:213:LYS:HZ1	21:2:611:CLA:HBD	1.62	0.65
16:L:59:GLU:HG2	16:L:60:PRO:HD2	1.80	0.64
2:2:103:CYS:O	2:2:107:MET:HG2	1.98	0.63
18:Z:208:LEU:HD22	21:Z:310:CLA:H3A	1.80	0.63
4:6:108:VAL:HG11	22:6:616:LUT:H12	1.80	0.63
16:L:124:THR:HG22	16:L:126:TYR:H	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2:609:CLA:HBB1	22:2:615:LUT:H32	1.79	0.63
1:5:51:MET:HE2	4:6:160:GLN:NE2	2.14	0.63
5:A:354:LEU:HD21	21:A:830:CLA:HBB1	1.81	0.63
21:3:617:CLA:HBB2	21:A:813:CLA:HMA2	1.81	0.63
6:B:458:ILE:HG21	10:F:152:SER:HB3	1.79	0.63
24:B:848:BCR:H10C	14:J:38:SER:O	2.00	0.62
8:D:160:HIS:HB3	8:D:161:PRO:HD3	1.81	0.62
22:F:301:LUT:H181	22:F:301:LUT:H8	1.81	0.62
12:H:90:SER:O	12:H:94:GLU:HG3	1.99	0.62
19:Y:166:LEU:HD21	31:Y:617:NEX:H34	1.82	0.62
6:B:30:ASP:HB3	21:B:828:CLA:HAA2	1.82	0.61
21:A:828:CLA:H171	24:J:103:BCR:H17C	1.81	0.61
18:Z:163:GLN:HG2	20:Z:307:CHL:HMA3	1.83	0.61
8:D:199:GLN:HE21	8:D:200:PRO:HD2	1.65	0.61
1:5:87:GLU:HB3	1:5:168:LYS:HG3	1.81	0.61
12:H:122:SER:HA	24:L:302:BCR:H322	1.82	0.61
20:4:305:CHL:HHC	20:4:305:CHL:HBB1	1.83	0.61
21:X:602:CLA:H2A	21:X:602:CLA:HED2	1.82	0.61
16:L:117:ILE:HG22	16:L:118:THR:HG23	1.82	0.61
10:F:83:LEU:HB2	10:F:140:LEU:HD12	1.83	0.60
18:Z:78:TRP:HZ2	22:Z:314:LUT:H162	1.66	0.60
4:6:105:MET:HE3	21:6:609:CLA:HBB1	1.84	0.60
17:O:63:GLY:HA3	23:O:208:XAT:H241	1.83	0.60
19:Y:130:PHE:HB2	20:Y:607:CHL:HMA3	1.84	0.60
19:Y:163:GLN:HG2	19:Y:167:MET:HE1	1.84	0.60
16:L:110:LEU:HD11	21:L:305:CLA:HBC3	1.84	0.60
25:2:617:LHG:HC81	24:3:601:BCR:HC42	1.83	0.60
3:3:111:GLU:HG3	3:3:244:LEU:HD23	1.84	0.60
23:O:208:XAT:H171	19:Y:257:ALA:HB1	1.84	0.60
18:X:208:LEU:HD21	21:X:609:CLA:HBA2	1.84	0.60
19:Y:101:ALA:HB1	19:Y:216:GLY:HA3	1.83	0.60
24:A:849:BCR:H352	24:A:849:BCR:H10C	1.84	0.59
18:X:205:PHE:HE1	21:X:609:CLA:HMA2	1.67	0.59
20:Z:302:CHL:HAC2	25:Z:317:LHG:HC42	1.84	0.59
21:B:809:CLA:H3A	24:L:302:BCR:HC31	1.84	0.59
18:X:159:ILE:O	18:X:163:GLN:HG2	2.02	0.59
22:Z:314:LUT:H181	22:Z:314:LUT:C8	2.32	0.59
1:1:177:LEU:HD23	22:1:615:LUT:H222	1.83	0.59
18:X:60:LEU:HD13	19:Y:172:GLY:HA3	1.85	0.59
18:X:109:LEU:HD11	22:X:614:LUT:H402	1.85	0.58
19:Y:108:THR:O	19:Y:112:VAL:HG22	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:659:THR:HA	21:B:802:CLA:HAB	1.86	0.58
18:X:101:CYS:O	18:X:105:MET:HG2	2.02	0.58
18:Z:115:GLU:HB3	18:Z:238:LEU:HD12	1.85	0.58
1:5:140:LEU:O	1:5:144:LEU:HD12	2.04	0.58
6:B:243:LEU:HD13	6:B:248:GLN:HE22	1.68	0.58
21:B:802:CLA:H191	21:B:839:CLA:H52	1.85	0.58
18:X:208:LEU:HD21	21:X:609:CLA:H3A	1.86	0.57
21:Z:303:CLA:H12	22:Z:314:LUT:H182	1.84	0.57
21:A:829:CLA:H2	24:A:846:BCR:HC7	1.86	0.57
19:Y:208:LEU:HD13	21:Y:610:CLA:H3A	1.86	0.57
18:Z:229:GLN:HE21	18:Z:240:ASN:HD22	1.50	0.57
21:2:609:CLA:CBB	22:2:615:LUT:H32	2.34	0.57
20:Y:609:CHL:HHC	20:Y:609:CHL:HBB1	1.86	0.57
26:1:619:LMG:H252	26:1:619:LMG:H212	1.87	0.57
6:B:68:VAL:HG11	6:B:124:TRP:HZ3	1.69	0.57
18:X:88:GLU:HG3	18:Z:67:TYR:HE1	1.70	0.57
21:X:618:CLA:HMA1	18:Z:249:VAL:HG22	1.86	0.57
2:2:246:HIS:HD2	21:2:612:CLA:HAA2	1.70	0.56
1:5:94:ARG:HB3	21:5:609:CLA:HBC2	1.87	0.56
17:O:104:LEU:HD12	21:O:203:CLA:H62	1.87	0.56
20:Z:309:CHL:HBA2	20:Z:309:CHL:HBD	1.87	0.56
3:3:200:ASN:HD21	21:3:610:CLA:HBD	1.69	0.56
21:A:821:CLA:H72	21:A:824:CLA:H42	1.87	0.56
18:X:48:TRP:HE1	18:X:207:GLU:HG2	1.70	0.56
24:A:845:BCR:H383	24:A:854:BCR:H10C	1.86	0.56
24:A:854:BCR:H382	24:A:854:BCR:H23C	1.88	0.56
20:Y:606:CHL:HHC	20:Y:606:CHL:HBB1	1.88	0.56
20:5:601:CHL:H8	21:5:612:CLA:H152	1.86	0.56
10:F:195:LYS:NZ	10:F:200:ASP:HB2	2.20	0.56
21:Z:313:CLA:H2A	21:Z:313:CLA:HED2	1.87	0.56
21:A:813:CLA:H43	24:A:846:BCR:H14C	1.89	0.55
22:X:615:LUT:H8	22:X:615:LUT:H161	1.87	0.55
21:1:612:CLA:H142	25:1:618:LHG:H282	1.87	0.55
22:5:619:LUT:H181	22:5:619:LUT:C8	2.35	0.55
20:X:607:CHL:HHC	20:X:607:CHL:HBB1	1.87	0.55
20:Z:309:CHL:HHC	20:Z:309:CHL:HBB1	1.87	0.55
19:Y:136:ILE:HD13	19:Y:142:LEU:HD12	1.89	0.55
2:2:145:LEU:O	2:2:149:GLU:HG3	2.07	0.55
16:L:142:LEU:HD22	24:L:306:BCR:H401	1.89	0.55
18:Z:46:SER:HB2	18:Z:49:TYR:HB2	1.87	0.55
18:Z:109:LEU:HD21	21:Z:312:CLA:HBB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Z:305:CLA:H11	31:Z:316:NEX:H363	1.88	0.55
1:5:87:GLU:O	1:5:91:ILE:HG12	2.07	0.55
22:F:301:LUT:H181	22:F:301:LUT:C8	2.37	0.55
15:K:51:SER:HA	15:K:54:ILE:HD12	1.89	0.55
20:5:601:CHL:H12	25:5:618:LHG:H161	1.89	0.54
6:B:131:THR:HG22	6:B:133:GLU:H	1.71	0.54
20:Z:307:CHL:HHC	20:Z:307:CHL:HBB1	1.90	0.54
5:A:205:LEU:HD13	24:A:846:BCR:H20C	1.89	0.54
7:C:28:MET:HE2	7:C:40:ALA:HB2	1.89	0.54
24:O:205:BCR:H14C	21:O:206:CLA:H11	1.90	0.54
18:Z:105:MET:HE1	21:Z:310:CLA:HMC2	1.88	0.54
14:J:31:ARG:HG2	21:J:102:CLA:HED3	1.90	0.54
1:5:78:VAL:HG12	1:5:81:ASN:H	1.72	0.54
1:5:166:LYS:HD3	1:5:170:PRO:HA	1.91	0.54
21:B:809:CLA:H62	24:L:302:BCR:H343	1.89	0.53
18:Z:56:TYR:HB3	18:Z:76:TYR:HB3	1.90	0.53
16:L:162:ALA:HB2	16:L:178:GLN:HG3	1.89	0.53
19:Y:88:GLU:CD	19:Y:88:GLU:H	2.16	0.53
6:B:292:ARG:HD3	11:G:105:PRO:HD3	1.89	0.53
21:H:201:CLA:H51	24:L:307:BCR:H353	1.90	0.53
18:X:218:LEU:HD21	21:X:610:CLA:HAC2	1.90	0.53
18:Z:211:LYS:HZ3	21:Z:312:CLA:HAA2	1.72	0.53
22:Z:315:LUT:C8	22:Z:315:LUT:H181	2.38	0.53
10:F:104:GLU:HG3	10:F:124:MET:HE1	1.91	0.53
19:Y:114:PRO:HA	19:Y:117:LEU:HD12	1.91	0.53
5:A:431:ARG:HG2	5:A:553:LEU:HD13	1.91	0.53
19:Y:88:GLU:O	19:Y:92:LYS:HG2	2.08	0.53
6:B:680:TRP:HD1	8:D:84:LEU:HD11	1.74	0.53
21:B:838:CLA:HAA1	21:B:838:CLA:HBD	1.91	0.53
3:3:214:LEU:HA	3:3:217:LYS:HE2	1.90	0.53
19:Y:154:GLN:HB2	20:Y:605:CHL:HAB	1.91	0.53
18:Z:48:TRP:HD1	18:Z:210:VAL:HG11	1.74	0.53
21:5:612:CLA:HAA1	21:5:612:CLA:HBD	1.90	0.53
5:A:439:ASN:ND2	6:B:678:LEU:HD21	2.24	0.52
21:L:305:CLA:HBD	21:L:305:CLA:HAA1	1.90	0.52
20:6:605:CHL:HHC	20:6:605:CHL:HBB1	1.92	0.52
18:X:126:GLU:HG3	18:X:135:GLN:HB2	1.92	0.52
22:Z:315:LUT:H181	22:Z:315:LUT:H8	1.91	0.52
3:3:118:LEU:H	3:3:118:LEU:HD12	1.73	0.52
5:A:537:HIS:HB3	21:A:837:CLA:HBB1	1.92	0.52
18:X:129:TRP:HB2	22:X:615:LUT:H221	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Z:310:CLA:CBB	22:Z:315:LUT:H32	2.39	0.52
1:1:66:GLY:HA3	1:1:194:ILE:HG21	1.90	0.52
5:A:473:ALA:HA	24:A:849:BCR:H272	1.90	0.52
5:A:531:PHE:CZ	24:A:849:BCR:H322	2.45	0.52
1:5:209:VAL:HG23	22:5:619:LUT:H162	1.91	0.52
10:F:115:ALA:HA	10:F:118:LEU:HD12	1.91	0.52
22:5:615:LUT:C8	22:5:615:LUT:H181	2.39	0.52
18:X:88:GLU:O	18:X:92:LYS:HG2	2.09	0.52
18:Z:135:GLN:HB2	18:Z:142:LEU:HD12	1.92	0.51
18:Z:220:MET:HE1	21:Z:303:CLA:HMC3	1.92	0.51
18:X:129:TRP:HZ3	18:X:237:PRO:HG3	1.76	0.51
21:B:828:CLA:HAA1	21:B:828:CLA:HBD	1.92	0.51
15:K:55:ILE:O	15:K:59:THR:HG22	2.10	0.51
23:O:208:XAT:H403	25:Y:618:LHG:H141	1.91	0.51
10:F:84:THR:O	10:F:141:CYS:HB3	2.10	0.51
21:O:202:CLA:HBD	21:O:202:CLA:HAA1	1.92	0.51
20:Y:601:CHL:C1D	25:Y:618:LHG:HC82	2.40	0.51
5:A:31:HIS:HA	5:A:37:ALA:HB2	1.91	0.51
21:Y:602:CLA:H3A	21:Y:602:CLA:H12	1.92	0.51
3:3:234:ILE:HG21	21:3:612:CLA:HAC2	1.92	0.51
18:X:91:ALA:HA	18:X:94:ARG:HE	1.75	0.51
21:Y:602:CLA:CBB	22:Y:615:LUT:H32	2.41	0.51
2:2:85:LEU:HD13	21:2:602:CLA:H42	1.92	0.51
4:4:113:LEU:HD13	21:4:303:CLA:HBC1	1.93	0.51
4:4:210:GLY:O	4:4:214:MET:HG2	2.10	0.51
5:A:688:GLY:HA3	6:B:569:ASP:HB2	1.91	0.51
21:A:828:CLA:H203	24:J:103:BCR:H17C	1.92	0.51
21:B:838:CLA:HBB2	28:B:841:PQN:H151	1.93	0.51
17:O:133:ARG:HG3	21:O:206:CLA:HED3	1.91	0.51
18:X:243:ASP:HB2	18:X:251:ASN:ND2	2.26	0.51
19:Y:128:VAL:HG12	19:Y:131:LYS:H	1.75	0.51
6:B:339:ALA:HB2	24:B:846:BCR:H372	1.93	0.51
20:2:605:CHL:HHC	20:2:605:CHL:HBB1	1.91	0.51
21:A:834:CLA:H51	24:L:308:BCR:H363	1.93	0.51
1:5:209:VAL:HG11	21:5:612:CLA:HAC2	1.92	0.51
19:Y:94:ARG:O	19:Y:98:VAL:HG23	2.11	0.51
10:F:107:LEU:HB2	10:F:120:ILE:HG21	1.93	0.50
24:O:205:BCR:H12C	21:O:206:CLA:H11	1.93	0.50
18:X:157:LEU:H	18:X:157:LEU:HD12	1.76	0.50
22:4:315:LUT:C8	22:4:315:LUT:H181	2.42	0.50
1:5:140:LEU:HD12	1:5:140:LEU:H	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:803:CLA:H201	21:B:808:CLA:H51	1.93	0.50
6:B:129:LEU:HD23	6:B:134:ASP:HB3	1.92	0.50
12:H:138:LEU:HD12	12:H:139:PRO:HD2	1.94	0.50
5:A:72:SER:OG	5:A:178:TYR:HB2	2.12	0.50
5:A:338:LEU:HG	5:A:421:ASN:HD21	1.77	0.50
6:B:668:ARG:HB2	28:B:841:PQN:H7	1.92	0.50
12:H:66:ASP:OD1	12:H:69:ASN:HB2	2.12	0.50
12:H:113:GLY:O	12:H:117:THR:HG22	2.12	0.50
20:4:306:CHL:OMC	20:4:314:CHL:HMC	2.12	0.50
20:6:605:CHL:HBA2	24:6:618:BCR:H21C	1.93	0.50
19:Y:83:LEU:HD22	21:Y:602:CLA:H2	1.92	0.50
19:Y:163:GLN:HG3	20:Y:606:CHL:HMA3	1.92	0.50
20:4:304:CHL:HHC	20:4:304:CHL:HBB1	1.93	0.50
22:5:615:LUT:H181	22:5:615:LUT:H8	1.93	0.50
1:1:103:ILE:HG13	23:1:616:XAT:H182	1.94	0.50
18:X:136:ILE:HB	18:X:142:LEU:HD22	1.91	0.50
7:C:55:GLU:HB3	7:C:63:LEU:HD13	1.93	0.50
5:A:573:CYS:HB3	29:A:850:SF4:S3	2.52	0.49
5:A:576:PRO:HD3	6:B:561:GLY:HA2	1.93	0.49
6:B:432:HIS:HD2	24:B:848:BCR:H23C	1.77	0.49
27:4:319:LMT:H5'	10:F:223:ILE:HD12	1.93	0.49
21:A:842:CLA:HMA1	21:B:801:CLA:H192	1.93	0.49
18:X:132:ALA:O	18:X:136:ILE:HG22	2.12	0.49
18:X:235:LYS:HB2	18:X:240:ASN:HD21	1.77	0.49
1:1:109:LEU:HB2	1:1:111:LEU:HD23	1.94	0.49
24:B:848:BCR:HC41	10:F:133:ASN:HD21	1.75	0.49
18:Z:114:PRO:HB3	18:Z:124:PHE:CE2	2.48	0.49
21:B:807:CLA:HAB	21:B:808:CLA:H42	1.94	0.49
10:F:199:ILE:HD11	14:J:14:LEU:HD23	1.94	0.49
1:1:176:PRO:HG2	1:1:177:LEU:HD22	1.94	0.49
21:6:602:CLA:O1A	21:6:602:CLA:H3A	2.13	0.49
6:B:257:LEU:HD13	21:B:816:CLA:HMB3	1.95	0.49
6:B:733:PHE:CE1	12:H:144:PRO:HG2	2.48	0.49
18:X:136:ILE:HG21	20:X:606:CHL:HBC1	1.94	0.49
2:2:207:ILE:O	2:2:211:ARG:HG3	2.13	0.49
6:B:293:THR:HG22	6:B:294:ASN:H	1.77	0.49
6:B:733:PHE:HE1	12:H:144:PRO:HG2	1.77	0.49
28:B:841:PQN:H142	24:B:847:BCR:H271	1.94	0.49
18:X:48:TRP:HA	18:X:48:TRP:CE3	2.48	0.49
2:2:206:LYS:O	2:2:209:GLU:HG3	2.12	0.49
17:O:113:VAL:HG21	21:O:203:CLA:H161	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Z:232:VAL:HG13	18:Z:233:THR:HG23	1.94	0.49
21:B:805:CLA:H92	21:B:805:CLA:H61	1.68	0.49
18:X:119:ARG:HH12	18:X:242:ALA:HB2	1.78	0.49
4:6:217:PHE:CZ	23:6:617:XAT:H10	2.47	0.48
5:A:86:SER:HB2	5:A:163:ALA:HB3	1.94	0.48
5:A:476:LEU:HB2	5:A:528:THR:HG23	1.94	0.48
8:D:88:GLN:HE21	12:H:73:GLN:HG2	1.78	0.48
20:X:608:CHL:HMB1	20:Z:302:CHL:HBA1	1.94	0.48
1:1:93:CYS:O	1:1:97:MET:HG3	2.14	0.48
3:3:207:ASP:HB3	3:3:210:SER:HB3	1.96	0.48
25:5:618:LHG:H292	25:5:618:LHG:H131	1.94	0.48
21:A:809:CLA:HAB	24:J:103:BCR:H352	1.95	0.48
6:B:548:PRO:HD2	7:C:62:PHE:CZ	2.49	0.48
21:B:825:CLA:H92	21:B:825:CLA:H62	1.71	0.48
7:C:61:ASP:HB3	9:E:131:ASN:ND2	2.22	0.48
10:F:204:ALA:O	10:F:208:ILE:HG13	2.12	0.48
20:X:605:CHL:HHC	20:X:605:CHL:HBB1	1.94	0.48
3:3:229:ILE:HG21	23:3:616:XAT:H12	1.96	0.48
21:L:304:CLA:H12	24:L:308:BCR:H332	1.95	0.48
19:Y:113:LEU:HG	19:Y:117:LEU:HD11	1.95	0.48
19:Y:132:ALA:HA	19:Y:135:GLN:HE21	1.78	0.48
21:B:809:CLA:HBA2	21:B:809:CLA:HBD	1.95	0.48
19:Y:184:LEU:HD12	19:Y:184:LEU:H	1.78	0.48
20:Y:608:CHL:HHC	20:Y:608:CHL:HBB1	1.96	0.48
18:Z:56:TYR:CD2	18:Z:78:TRP:HB2	2.47	0.48
21:A:802:CLA:H171	21:A:841:CLA:H51	1.95	0.48
16:L:61:ILE:HA	16:L:71:GLU:HG2	1.96	0.48
22:Y:615:LUT:C8	22:Y:615:LUT:H181	2.43	0.48
5:A:338:LEU:HG	5:A:421:ASN:ND2	2.28	0.48
1:5:107:GLU:HB3	1:5:220:LEU:HD12	1.96	0.48
20:6:607:CHL:HHC	20:6:607:CHL:HBB1	1.96	0.48
5:A:653:ALA:O	5:A:657:ILE:HG23	2.14	0.48
21:B:838:CLA:H11	21:L:301:CLA:HMC2	1.96	0.48
18:Z:108:THR:HG21	18:Z:219:ALA:HB1	1.96	0.48
6:B:309:ILE:HD11	6:B:320:LYS:NZ	2.28	0.48
21:B:838:CLA:H62	21:B:838:CLA:H41	1.68	0.48
8:D:150:VAL:HG22	8:D:156:VAL:HG12	1.96	0.48
20:1:601:CHL:HBA2	20:1:601:CHL:H3A	1.67	0.47
2:2:243:LEU:HD22	22:2:615:LUT:H172	1.95	0.47
20:6:605:CHL:HBA2	20:6:605:CHL:H3A	1.73	0.47
22:6:616:LUT:C8	22:6:616:LUT:H181	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:226:PHE:CE1	21:G:203:CLA:HBC1	2.49	0.47
21:B:824:CLA:H2	21:B:837:CLA:OBD	2.14	0.47
18:Z:228:VAL:HG11	21:Z:313:CLA:HBC3	1.96	0.47
20:6:606:CHL:HHB	20:6:606:CHL:HBB1	1.96	0.47
21:L:304:CLA:H62	21:L:304:CLA:H41	1.61	0.47
18:X:48:TRP:CH2	18:X:210:VAL:HG11	2.49	0.47
21:3:607:CLA:H3A	21:3:607:CLA:HBA2	1.61	0.47
21:A:804:CLA:H62	21:A:804:CLA:H41	1.66	0.47
21:B:804:CLA:HBA1	21:B:804:CLA:H3A	1.57	0.47
18:X:56:TYR:HB3	18:X:76:TYR:HB3	1.95	0.47
18:X:96:LEU:HD21	21:X:603:CLA:HAA1	1.96	0.47
19:Y:57:LEU:HB2	19:Y:61:SER:HB2	1.97	0.47
18:Z:114:PRO:HB3	18:Z:124:PHE:HE2	1.79	0.47
22:2:615:LUT:C8	22:2:615:LUT:H181	2.44	0.47
1:5:73:LEU:HB3	1:5:75:LEU:HG	1.96	0.47
4:6:115:GLU:OE1	4:6:232:ILE:HG12	2.14	0.47
6:B:722:ALA:HB2	21:B:826:CLA:HBB1	1.96	0.47
7:C:39:ILE:HG12	7:C:40:ALA:H	1.80	0.47
20:4:306:CHL:H3A	20:4:306:CHL:HBA2	1.31	0.47
21:6:602:CLA:H62	21:6:602:CLA:H41	1.69	0.47
18:X:156:ILE:HD11	18:Z:254:TRP:CG	2.49	0.47
4:4:246:THR:HG22	4:4:247:ILE:H	1.79	0.47
21:5:602:CLA:H62	21:5:602:CLA:H41	1.69	0.47
6:B:88:ALA:HB2	6:B:116:ALA:HB2	1.97	0.47
21:B:813:CLA:HED2	21:B:813:CLA:HAA1	1.95	0.47
19:Y:166:LEU:HD21	31:Y:617:NEX:H15	1.96	0.47
1:1:209:VAL:HG11	21:1:612:CLA:HAC2	1.97	0.47
2:2:93:LYS:O	2:2:97:GLN:HG2	2.15	0.47
21:3:612:CLA:C1B	22:3:615:LUT:H183	2.45	0.47
5:A:344:THR:HG21	5:A:419:ARG:HH22	1.80	0.47
21:2:613:CLA:HAA2	3:3:151:PHE:HD1	1.79	0.47
21:L:301:CLA:H152	24:L:308:BCR:H17C	1.97	0.47
21:A:810:CLA:HBA2	21:A:810:CLA:H3A	1.62	0.46
14:J:11:ALA:O	14:J:15:THR:HG22	2.15	0.46
21:Y:602:CLA:H101	21:Y:602:CLA:H13	1.40	0.46
1:5:74:ARG:HA	1:5:74:ARG:HD3	1.64	0.46
1:5:145:ALA:O	1:5:149:ILE:HG12	2.15	0.46
1:5:151:ILE:HG13	1:5:152:ALA:N	2.31	0.46
1:5:188:GLU:CD	1:5:188:GLU:H	2.24	0.46
18:X:48:TRP:CD2	18:X:210:VAL:HG21	2.51	0.46
19:Y:56:TYR:CD1	19:Y:78:TRP:HB2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Y:171:GLU:O	19:Y:175:VAL:HG23	2.15	0.46
1:1:74:ARG:HA	1:1:74:ARG:HD3	1.66	0.46
4:4:134:SER:HB3	4:4:136:TYR:CE1	2.49	0.46
21:5:604:CLA:H43	21:5:605:CLA:HBD	1.96	0.46
5:A:522:LEU:HD21	5:A:616:VAL:HA	1.97	0.46
17:O:77:VAL:HG23	17:O:78:ILE:HG23	1.97	0.46
18:X:196:LEU:HD11	22:X:614:LUT:H222	1.98	0.46
20:Y:601:CHL:HBA1	20:Y:601:CHL:H3A	1.50	0.46
20:Z:307:CHL:HBA2	20:Z:307:CHL:H3A	1.60	0.46
2:2:180:LYS:NZ	2:2:180:LYS:HB3	2.30	0.46
3:3:173:MET:HE3	3:3:173:MET:HB3	1.82	0.46
4:6:122:ILE:HG13	4:6:123:ILE:HG22	1.96	0.46
8:D:85:ARG:O	8:D:85:ARG:HG2	2.15	0.46
21:1:609:CLA:H61	21:1:609:CLA:H92	1.76	0.46
4:4:111:VAL:HG23	23:4:316:XAT:H182	1.98	0.46
21:B:839:CLA:HBC3	24:B:847:BCR:H21C	1.97	0.46
30:B:849:DGD:HB22	30:B:849:DGD:HG2	1.63	0.46
19:Y:141:GLY:HA3	19:Y:154:GLN:HE22	1.81	0.46
1:5:147:GLU:O	1:5:151:ILE:HG23	2.16	0.46
5:A:410:MET:HE2	5:A:410:MET:HB2	1.81	0.46
21:A:828:CLA:H102	21:A:842:CLA:H201	1.98	0.46
6:B:91:ILE:HB	6:B:112:PRO:HB2	1.97	0.46
6:B:129:LEU:HD22	6:B:135:LEU:HD23	1.96	0.46
6:B:159:PRO:HA	6:B:162:LYS:HE2	1.98	0.46
24:B:848:BCR:H393	24:B:848:BCR:H24C	1.72	0.46
21:A:818:CLA:H3A	21:A:818:CLA:HBA2	1.70	0.46
21:B:817:CLA:H3A	21:B:817:CLA:HBA2	1.65	0.46
12:H:118:LEU:HD12	12:H:118:LEU:HA	1.82	0.46
20:X:601:CHL:H3A	20:X:601:CHL:HBA1	1.34	0.46
20:Y:608:CHL:HBA2	20:Y:608:CHL:H3A	1.50	0.46
20:1:601:CHL:H12	25:1:618:LHG:H141	1.97	0.46
2:2:173:ASP:HB3	2:2:176:PHE:O	2.16	0.46
3:3:229:ILE:HG21	23:3:616:XAT:H14	1.98	0.46
21:6:601:CLA:HBB2	21:6:602:CLA:HBC2	1.96	0.46
22:X:615:LUT:H7	22:X:615:LUT:H181	1.68	0.46
21:Y:613:CLA:HAA1	21:Y:613:CLA:HBD	1.97	0.46
21:Z:310:CLA:H3A	21:Z:310:CLA:HBA2	1.65	0.46
2:2:231:GLN:O	2:2:235:THR:HG22	2.16	0.46
21:3:610:CLA:HBB1	22:3:615:LUT:H32	1.98	0.46
21:5:604:CLA:C3	21:5:605:CLA:HBD	2.46	0.46
4:6:113:LEU:HB3	4:6:114:PRO:HD3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:6:610:CLA:HBA1	21:6:610:CLA:HBD	1.98	0.46
12:H:130:LEU:HD21	24:L:302:BCR:H312	1.98	0.46
18:X:218:LEU:HA	25:X:617:LHG:H301	1.98	0.46
21:1:604:CLA:HAA1	21:1:604:CLA:HBD	1.98	0.46
6:B:517:PHE:HE1	24:B:848:BCR:H271	1.81	0.46
19:Y:129:TRP:HZ3	19:Y:237:PRO:HD3	1.81	0.46
21:A:830:CLA:HAA1	21:A:830:CLA:HBD	1.97	0.45
24:O:201:BCR:H24C	24:O:201:BCR:H371	1.81	0.45
21:X:604:CLA:HBB1	31:X:616:NEX:H27	1.98	0.45
20:Y:607:CHL:O2A	20:Y:607:CHL:HBD	2.16	0.45
1:5:179:PHE:HE1	22:5:615:LUT:H221	1.81	0.45
17:O:72:PRO:HG3	24:O:205:BCR:H19C	1.98	0.45
18:Z:166:LEU:HB3	31:Z:316:NEX:H401	1.97	0.45
2:2:229:TRP:O	2:2:233:ILE:HG22	2.16	0.45
21:2:610:CLA:HBC3	25:2:617:LHG:HC62	1.97	0.45
21:H:201:CLA:H102	21:H:201:CLA:H61	1.51	0.45
24:L:308:BCR:H24C	24:L:308:BCR:H371	1.85	0.45
19:Y:95:GLU:O	19:Y:99:ILE:HG12	2.17	0.45
20:2:601:CHL:HHC	20:2:601:CHL:HBB1	1.99	0.45
21:A:817:CLA:H61	21:A:817:CLA:H41	1.71	0.45
20:Z:302:CHL:HAC1	25:Z:317:LHG:HC31	1.98	0.45
25:1:620:LHG:HC81	25:1:620:LHG:HC5	1.40	0.45
21:A:802:CLA:CGA	21:A:802:CLA:H3A	2.47	0.45
21:A:832:CLA:H41	21:A:832:CLA:H62	1.66	0.45
12:H:130:LEU:HD23	12:H:130:LEU:HA	1.77	0.45
20:X:607:CHL:H3A	20:X:607:CHL:HBA2	1.47	0.45
22:Y:616:LUT:H171	22:Y:616:LUT:C8	2.43	0.45
20:Y:619:CHL:HBA1	20:Y:619:CHL:H3A	1.72	0.45
25:1:620:LHG:H241	25:1:620:LHG:HC62	1.29	0.45
3:3:181:LEU:O	3:3:185:LEU:HD23	2.16	0.45
4:4:133:LYS:HD3	4:4:133:LYS:N	2.32	0.45
1:5:168:LYS:HE2	1:5:168:LYS:HB2	1.74	0.45
6:B:208:ARG:O	6:B:212:PHE:HB3	2.17	0.45
21:B:804:CLA:H141	21:B:804:CLA:H162	1.81	0.45
26:B:850:LMG:H312	21:G:203:CLA:HBC2	1.99	0.45
8:D:116:ARG:H	8:D:116:ARG:HG2	1.66	0.45
10:F:220:ARG:C	10:F:220:ARG:HD2	2.42	0.45
23:O:208:XAT:H361	25:Y:618:LHG:HC81	1.99	0.45
18:X:143:ASP:HA	18:X:151:VAL:HB	1.99	0.45
18:X:218:LEU:HD22	25:X:617:LHG:H272	1.99	0.45
21:X:603:CLA:H3A	21:X:603:CLA:HBA1	1.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1:609:CLA:H143	22:1:615:LUT:H403	1.98	0.45
3:3:87:ARG:H	3:3:87:ARG:HG2	1.57	0.45
3:3:227:LEU:HD23	3:3:227:LEU:HA	1.82	0.45
21:5:611:CLA:HAA2	21:5:611:CLA:HED2	1.98	0.45
20:Y:608:CHL:HED3	20:Y:608:CHL:HBD	1.91	0.45
4:4:59:LEU:HD23	4:4:59:LEU:HA	1.88	0.45
8:D:102:GLU:HA	8:D:115:MET:O	2.17	0.45
18:X:105:MET:HE2	21:X:609:CLA:HMC2	1.97	0.45
19:Y:226:PHE:HZ	22:Y:616:LUT:H173	1.81	0.45
2:2:124:ILE:HB	2:2:125:LEU:HD22	1.99	0.45
21:A:816:CLA:HBA2	21:A:816:CLA:HBD	1.99	0.45
21:A:820:CLA:HBA2	21:A:820:CLA:H3A	1.64	0.45
18:X:48:TRP:HA	18:X:48:TRP:HE3	1.82	0.45
18:X:49:TYR:HE2	18:X:206:ALA:HB1	1.82	0.45
3:3:234:ILE:HD13	3:3:234:ILE:HA	1.86	0.45
22:3:615:LUT:H171	22:3:615:LUT:C8	2.45	0.45
21:B:812:CLA:H13	21:B:812:CLA:H102	1.87	0.45
8:D:88:GLN:NE2	12:H:73:GLN:HG2	2.32	0.45
14:J:22:LEU:HD11	21:J:101:CLA:C4B	2.47	0.45
24:J:103:BCR:H24C	24:J:103:BCR:H371	1.80	0.45
18:Z:198:LEU:H	18:Z:198:LEU:HD23	1.82	0.45
21:1:603:CLA:HED2	21:1:603:CLA:H43	1.97	0.44
25:1:618:LHG:H131	25:1:618:LHG:H292	1.99	0.44
22:3:615:LUT:H391	22:3:615:LUT:H31	1.80	0.44
5:A:531:PHE:HE2	24:A:849:BCR:H313	1.82	0.44
8:D:181:MET:HE2	8:D:181:MET:HA	1.99	0.44
1:1:113:ASN:HD21	1:1:116:LYS:HG2	1.83	0.44
5:A:42:THR:HG23	5:A:715:ARG:HG3	1.97	0.44
5:A:171:LEU:HD12	5:A:171:LEU:HA	1.79	0.44
24:B:842:BCR:H331	24:B:842:BCR:HC8	1.99	0.44
21:1:609:CLA:H62	21:1:609:CLA:H41	1.72	0.44
26:5:620:LMG:H331	12:H:96:PHE:HZ	1.82	0.44
6:B:704:GLN:HG3	30:B:849:DGD:HA31	1.98	0.44
14:J:32:LEU:HD22	21:J:102:CLA:HAA2	1.99	0.44
18:Z:211:LYS:HZ3	21:Z:312:CLA:HBD	1.81	0.44
21:3:609:CLA:H3A	21:3:609:CLA:HBA1	1.78	0.44
1:5:84:ARG:HA	1:5:87:GLU:OE2	2.17	0.44
4:6:171:ASP:HB3	4:6:174:PHE:O	2.17	0.44
21:A:818:CLA:HHC	21:A:818:CLA:HBB1	1.99	0.44
21:B:822:CLA:H93	21:B:822:CLA:H61	1.72	0.44
24:I:101:BCR:H372	24:L:308:BCR:H403	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:6:119:LYS:HA	4:6:119:LYS:HD2	1.84	0.44
5:A:342:LEU:HD23	5:A:342:LEU:HA	1.82	0.44
21:A:809:CLA:H92	25:A:851:LHG:H221	2.00	0.44
21:B:826:CLA:H92	21:B:826:CLA:H62	1.79	0.44
18:X:167:MET:O	18:X:170:VAL:HG12	2.15	0.44
18:Z:205:PHE:O	18:Z:209:LYS:HG2	2.17	0.44
20:2:607:CHL:HBA1	20:2:607:CHL:H3A	1.55	0.44
21:A:802:CLA:H92	21:A:802:CLA:H62	1.74	0.44
21:A:818:CLA:H42	21:A:827:CLA:HBB2	2.00	0.44
19:Y:227:TYR:O	19:Y:231:ILE:HG22	2.17	0.44
21:1:612:CLA:H41	25:1:618:LHG:H212	1.98	0.44
4:4:119:LYS:HD2	4:4:119:LYS:HA	1.74	0.44
21:6:612:CLA:HAA1	21:6:612:CLA:HBD	2.00	0.44
5:A:553:LEU:HD23	5:A:553:LEU:HA	1.85	0.44
21:A:812:CLA:HAC2	21:A:813:CLA:HAB	2.00	0.44
19:Y:111:CYS:SG	22:Y:615:LUT:H182	2.57	0.44
20:Z:308:CHL:HHB	20:Z:308:CHL:HBB1	1.98	0.44
2:2:173:ASP:HB2	2:2:179:ASN:HB2	2.00	0.44
21:2:604:CLA:HBA2	21:2:604:CLA:H122	1.99	0.44
21:6:610:CLA:HBB1	24:6:620:BCR:H10C	2.00	0.44
21:A:841:CLA:H3A	21:A:841:CLA:HBA2	1.78	0.44
19:Y:144:TYR:HE1	21:Y:604:CLA:HAA1	1.83	0.44
21:2:608:CLA:H3A	21:2:608:CLA:HBA2	1.58	0.44
21:A:826:CLA:H92	21:A:826:CLA:H61	1.75	0.44
10:F:87:LYS:HB2	10:F:88:GLU:OE1	2.17	0.44
21:X:603:CLA:HMA2	21:X:603:CLA:H2	1.99	0.44
21:Z:305:CLA:H3A	21:Z:305:CLA:HBA2	1.71	0.44
1:1:104:LEU:HD23	1:1:104:LEU:HA	1.83	0.43
20:2:607:CHL:HMB2	24:2:619:BCR:H402	1.99	0.43
1:5:52:PRO:HD2	20:5:601:CHL:O1D	2.18	0.43
21:A:837:CLA:H3A	21:A:837:CLA:HBA1	1.76	0.43
21:B:809:CLA:H92	21:B:809:CLA:H61	1.69	0.43
21:K:202:CLA:H2A	21:K:202:CLA:HED2	2.00	0.43
21:X:613:CLA:C1B	22:X:614:LUT:H183	2.48	0.43
1:5:163:ASP:HB3	1:5:166:LYS:HB3	1.99	0.43
21:A:804:CLA:HED1	14:J:15:THR:HG21	2.00	0.43
24:A:848:BCR:H24C	24:A:848:BCR:H371	1.83	0.43
21:B:811:CLA:HAC2	21:B:812:CLA:HAB	2.00	0.43
21:O:202:CLA:HBA1	21:O:202:CLA:H3A	1.65	0.43
22:X:615:LUT:H11	22:X:615:LUT:H191	1.89	0.43
1:1:100:VAL:HG11	22:1:615:LUT:H12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:3:608:CHL:H3A	20:3:608:CHL:HBA2	1.36	0.43
4:4:83:LEU:HD13	21:4:301:CLA:H42	2.01	0.43
21:5:612:CLA:H93	21:5:612:CLA:H111	1.87	0.43
4:6:59:LEU:HD23	4:6:62:LEU:HD11	1.99	0.43
5:A:157:TYR:O	5:A:161:ILE:HG12	2.17	0.43
5:A:576:PRO:HB3	6:B:559:CYS:SG	2.58	0.43
21:A:802:CLA:H112	21:A:802:CLA:H151	1.83	0.43
6:B:395:ILE:HG12	6:B:541:ALA:HB1	2.01	0.43
24:F:305:BCR:H24C	24:F:305:BCR:H371	1.86	0.43
15:K:71:LEU:HD12	21:K:204:CLA:C4A	2.48	0.43
21:X:602:CLA:HBA2	21:X:602:CLA:H3A	1.67	0.43
22:X:615:LUT:H161	22:X:615:LUT:C8	2.48	0.43
21:X:618:CLA:O2A	21:X:618:CLA:HBD	2.19	0.43
21:Y:603:CLA:H3A	21:Y:603:CLA:HBA1	1.53	0.43
22:1:615:LUT:C8	22:1:615:LUT:H181	2.49	0.43
22:5:615:LUT:H35	22:5:615:LUT:H401	1.87	0.43
21:A:803:CLA:H91	21:B:802:CLA:H112	2.00	0.43
21:A:804:CLA:HBB2	21:A:811:CLA:H112	1.99	0.43
21:A:808:CLA:H12	21:A:810:CLA:H2	1.99	0.43
21:A:832:CLA:H92	21:L:304:CLA:H11	2.00	0.43
7:C:15:THR:HA	7:C:28:MET:HE3	2.00	0.43
18:X:91:ALA:HA	18:X:94:ARG:NE	2.33	0.43
21:X:610:CLA:HBA2	21:X:610:CLA:H3A	1.57	0.43
22:X:614:LUT:H7	22:X:614:LUT:H181	1.75	0.43
22:Y:615:LUT:H181	22:Y:615:LUT:H8	2.00	0.43
18:Z:48:TRP:CD1	18:Z:210:VAL:HG11	2.53	0.43
22:3:615:LUT:H35	22:3:615:LUT:H401	1.82	0.43
7:C:61:ASP:CB	9:E:131:ASN:HD21	2.26	0.43
20:X:601:CHL:C1B	25:X:617:LHG:H122	2.47	0.43
18:Z:78:TRP:CZ2	22:Z:314:LUT:H162	2.52	0.43
1:1:67:ASP:OD1	1:1:67:ASP:C	2.62	0.43
2:2:163:ASP:HB2	2:2:170:VAL:HG21	2.01	0.43
5:A:438:LEU:HG	5:A:546:LEU:HB2	2.00	0.43
21:B:838:CLA:H112	21:B:838:CLA:H72	1.73	0.43
10:F:195:LYS:HB3	10:F:195:LYS:HE3	1.86	0.43
19:Y:113:LEU:HD22	21:Y:604:CLA:HBC3	2.00	0.43
18:Z:229:GLN:HE22	21:Z:313:CLA:C1A	2.30	0.43
18:Z:238:LEU:HD23	18:Z:238:LEU:HA	1.85	0.43
25:1:618:LHG:H162	21:4:313:CLA:HED1	2.01	0.43
2:2:150:LEU:HD23	2:2:150:LEU:HA	1.90	0.43
24:A:854:BCR:H24C	24:A:854:BCR:H392	1.69	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:B:850:LMG:HC8	26:B:850:LMG:H111	1.29	0.43
16:L:134:ALA:C	16:L:136:GLY:H	2.26	0.43
18:X:136:ILE:O	18:X:141:GLY:HA2	2.18	0.43
19:Y:233:THR:HG22	19:Y:256:TYR:HD1	1.83	0.43
18:Z:104:ALA:O	18:Z:108:THR:HG23	2.18	0.43
22:Z:315:LUT:H401	22:Z:315:LUT:H35	1.78	0.43
4:6:91:LYS:O	4:6:95:GLN:HG2	2.19	0.43
4:6:251:PHE:HE1	13:I:4:LEU:HD23	1.84	0.43
19:Y:56:TYR:CG	19:Y:78:TRP:HB2	2.54	0.43
22:Z:314:LUT:H15	22:Z:314:LUT:H201	1.87	0.43
3:3:209:LYS:HD2	3:3:209:LYS:HA	1.73	0.43
4:4:161:ASP:OD1	4:4:161:ASP:C	2.61	0.43
21:A:806:CLA:H193	24:A:845:BCR:H10C	2.01	0.43
21:A:819:CLA:H192	21:A:819:CLA:H161	1.74	0.43
24:A:847:BCR:H20C	24:A:847:BCR:H361	1.82	0.43
6:B:432:HIS:HB2	24:B:848:BCR:H392	2.01	0.43
21:B:809:CLA:H161	21:B:809:CLA:H192	1.80	0.43
17:O:55:LEU:HD12	17:O:55:LEU:HA	1.86	0.43
18:X:56:TYR:CZ	18:X:57:LEU:HG	2.54	0.43
19:Y:252:ASN:OD1	19:Y:252:ASN:C	2.61	0.43
18:Z:68:LEU:H	18:Z:68:LEU:HD23	1.84	0.43
1:1:244:ILE:HD12	1:1:244:ILE:HA	1.90	0.43
24:2:619:BCR:H19C	24:2:619:BCR:H373	2.00	0.43
21:6:612:CLA:H93	21:6:612:CLA:H61	1.90	0.43
5:A:680:PHE:CA	21:A:802:CLA:HAB	2.41	0.43
21:B:809:CLA:H93	24:L:302:BCR:H332	2.01	0.43
21:B:823:CLA:H112	21:B:823:CLA:H152	1.75	0.43
21:K:203:CLA:H3A	21:K:203:CLA:HBA1	1.46	0.43
16:L:117:ILE:HD11	16:L:214:ILE:HG23	2.00	0.43
19:Y:136:ILE:HD12	19:Y:136:ILE:HA	1.87	0.43
2:2:108:LEU:HD23	2:2:108:LEU:HA	1.82	0.42
2:2:193:TRP:HE1	20:2:614:CHL:C3D	2.31	0.42
21:4:308:CLA:CBB	22:4:315:LUT:H32	2.49	0.42
21:A:802:CLA:HBA2	6:B:427:LEU:HD23	2.00	0.42
12:H:145:ARG:NH2	12:H:148:LYS:HG2	2.34	0.42
6:B:696:LYS:HD2	7:C:79:LEU:HD13	2.01	0.42
21:B:816:CLA:HBA2	21:B:816:CLA:H3A	1.72	0.42
10:F:220:ARG:HD2	10:F:220:ARG:O	2.20	0.42
18:X:228:VAL:O	18:X:232:VAL:HG12	2.20	0.42
21:X:611:CLA:HBD	21:X:611:CLA:O1A	2.18	0.42
1:1:187:GLN:OE1	1:1:187:GLN:N	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:6:114:PRO:O	4:6:118:THR:HG22	2.20	0.42
5:A:708:VAL:CG1	10:F:180:ARG:HG3	2.50	0.42
24:B:842:BCR:H24C	24:B:842:BCR:H371	1.89	0.42
21:L:301:CLA:H121	21:L:301:CLA:H162	1.54	0.42
31:Z:316:NEX:C32	31:Z:316:NEX:H391	2.50	0.42
3:3:152:GLU:O	3:3:156:MET:HB2	2.19	0.42
21:A:819:CLA:H3A	21:A:819:CLA:HBA2	1.76	0.42
21:B:826:CLA:H3A	21:B:826:CLA:HBA2	1.44	0.42
11:G:167:PHE:CD1	11:G:167:PHE:N	2.88	0.42
17:O:54:TRP:H	17:O:54:TRP:CD1	2.36	0.42
1:1:90:LEU:HD13	1:1:90:LEU:HA	1.90	0.42
25:1:622:LHG:H311	21:B:840:CLA:H93	2.01	0.42
2:2:204:PRO:O	2:2:207:ILE:HG22	2.19	0.42
19:Y:160:TRP:O	19:Y:164:VAL:HG12	2.19	0.42
21:Y:602:CLA:H43	22:Y:615:LUT:H26	2.01	0.42
24:6:620:BCR:H24C	24:6:620:BCR:H371	1.88	0.42
5:A:360:LEU:HA	5:A:360:LEU:HD12	1.76	0.42
24:B:848:BCR:H372	10:F:161:PHE:CE1	2.54	0.42
10:F:182:TYR:O	10:F:186:ILE:HG23	2.19	0.42
24:F:302:BCR:H24C	24:F:302:BCR:H371	1.83	0.42
22:Y:616:LUT:H35	22:Y:616:LUT:H401	1.91	0.42
18:Z:142:LEU:HD21	21:Z:305:CLA:HAA2	2.01	0.42
18:Z:261:VAL:HG11	20:Z:301:CHL:HAA2	2.01	0.42
20:2:601:CHL:HMD1	24:3:601:BCR:HC21	2.01	0.42
3:3:90:ALA:O	3:3:94:ILE:HG13	2.19	0.42
21:3:603:CLA:H41	21:3:603:CLA:H61	1.80	0.42
4:4:200:LEU:HD23	4:4:204:GLU:HG3	2.02	0.42
24:5:617:BCR:H24C	24:5:617:BCR:H371	1.83	0.42
21:6:610:CLA:CBB	24:6:620:BCR:H10C	2.48	0.42
21:A:810:CLA:HHC	21:A:810:CLA:HBB1	2.02	0.42
25:A:853:LHG:H241	25:A:853:LHG:HC62	1.58	0.42
21:B:810:CLA:H92	24:B:843:BCR:H323	2.01	0.42
10:F:214:TRP:CD1	10:F:215:PRO:HD3	2.55	0.42
24:G:205:BCR:H371	24:G:205:BCR:H24C	1.80	0.42
18:X:137:PHE:CE2	18:Z:258:THR:HG21	2.54	0.42
19:Y:217:ARG:HA	19:Y:220:MET:HE3	2.01	0.42
22:Y:616:LUT:H7	22:Y:616:LUT:H181	1.75	0.42
2:2:246:HIS:CD2	21:2:612:CLA:HAA2	2.53	0.42
21:A:829:CLA:H162	21:A:829:CLA:H121	1.70	0.42
21:A:840:CLA:H143	21:J:101:CLA:HBC1	2.02	0.42
24:A:846:BCR:H24C	24:A:846:BCR:H371	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:X:98:VAL:HG21	18:X:187:LEU:HD13	2.02	0.42
18:X:187:LEU:HG	18:X:188:TYR:CD2	2.55	0.42
20:X:608:CHL:HHC	20:X:608:CHL:HBB1	2.00	0.42
22:X:615:LUT:H31	22:X:615:LUT:H391	1.88	0.42
21:1:603:CLA:H3A	21:1:603:CLA:HBA1	1.81	0.42
21:3:612:CLA:HBD	21:3:612:CLA:O1A	2.20	0.42
1:5:90:LEU:HD23	1:5:90:LEU:HA	1.83	0.42
4:6:115:GLU:HA	4:6:118:THR:HG22	2.02	0.42
4:6:127:GLU:HG3	4:6:128:TRP:N	2.34	0.42
19:Y:226:PHE:CZ	22:Y:616:LUT:H173	2.55	0.42
22:Y:615:LUT:H11	22:Y:615:LUT:H191	1.93	0.42
3:3:113:PHE:HB3	3:3:119:ILE:CD1	2.50	0.42
21:A:834:CLA:HAA1	21:A:834:CLA:HBD	2.02	0.42
21:B:813:CLA:HAB	21:B:827:CLA:H161	2.01	0.42
21:L:304:CLA:H62	21:L:304:CLA:H92	1.78	0.42
24:L:306:BCR:H20C	24:L:306:BCR:H361	1.90	0.42
18:X:211:LYS:HE3	21:X:611:CLA:HBA2	2.02	0.42
21:1:614:CLA:HED2	26:F:306:LMG:H292	2.01	0.41
4:6:229:LYS:HB2	4:6:229:LYS:HE3	1.88	0.41
21:L:301:CLA:H193	21:L:301:CLA:H161	1.81	0.41
18:Z:67:TYR:HE2	18:Z:82:GLY:HA2	1.85	0.41
18:Z:84:SER:HB3	21:Z:303:CLA:HBA1	2.02	0.41
21:Z:312:CLA:H3A	21:Z:312:CLA:HBA1	1.67	0.41
3:3:229:ILE:HD13	3:3:229:ILE:HA	1.93	0.41
4:6:113:LEU:O	4:6:117:LEU:HD22	2.20	0.41
5:A:194:MET:HE2	21:A:813:CLA:HBC2	2.02	0.41
21:A:801:CLA:H102	21:A:801:CLA:H62	1.94	0.41
24:A:848:BCR:H20C	24:A:848:BCR:H361	1.85	0.41
6:B:441:ASP:OD2	6:B:441:ASP:C	2.63	0.41
24:G:205:BCR:H361	24:G:205:BCR:H20C	1.85	0.41
19:Y:258:THR:O	19:Y:261:VAL:HG12	2.21	0.41
4:4:112:LEU:HD23	4:4:112:LEU:HA	1.88	0.41
21:4:313:CLA:HBA2	21:4:313:CLA:H3A	1.79	0.41
1:5:151:ILE:HD11	21:5:608:CLA:HBB1	2.02	0.41
4:6:127:GLU:HG2	4:6:129:TYR:CZ	2.56	0.41
20:6:605:CHL:H41	20:6:605:CHL:H62	1.68	0.41
5:A:360:LEU:HD13	21:A:827:CLA:H42	2.03	0.41
21:B:822:CLA:HMA1	21:B:840:CLA:HED3	2.03	0.41
24:B:847:BCR:H20C	24:B:847:BCR:H361	1.90	0.41
19:Y:50:GLY:O	19:Y:53:ARG:HD3	2.21	0.41
18:Z:109:LEU:HD12	22:Z:315:LUT:H401	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:4:311:CLA:H61	21:4:311:CLA:H93	1.76	0.41
24:4:317:BCR:H20C	24:4:317:BCR:H361	1.95	0.41
6:B:305:LEU:HD23	6:B:305:LEU:HA	1.83	0.41
7:C:62:PHE:HD2	8:D:184:ILE:HG21	1.85	0.41
9:E:92:ARG:CZ	9:E:92:ARG:HB2	2.51	0.41
12:H:108:LYS:HE2	12:H:108:LYS:HB2	1.80	0.41
21:Z:303:CLA:H3A	21:Z:303:CLA:HBA2	1.44	0.41
21:A:824:CLA:H93	21:A:826:CLA:H202	2.03	0.41
6:B:87:ILE:HD13	6:B:113:VAL:HG11	2.03	0.41
21:B:820:CLA:HBD	21:B:820:CLA:HAA1	2.03	0.41
21:O:203:CLA:H61	21:O:203:CLA:H101	1.60	0.41
22:X:614:LUT:H35	22:X:614:LUT:H401	1.79	0.41
19:Y:261:VAL:HG21	20:Y:619:CHL:HAA2	2.02	0.41
20:Z:302:CHL:HBA1	20:Z:302:CHL:H3A	1.88	0.41
1:1:119:GLU:OE2	1:1:119:GLU:HA	2.21	0.41
2:2:231:GLN:HE21	2:2:242:ASN:HD22	1.67	0.41
3:3:86:PRO:HA	3:3:89:LEU:HD12	2.03	0.41
4:6:217:PHE:CD2	23:6:617:XAT:H12	2.56	0.41
21:A:803:CLA:CAC	21:B:802:CLA:HMC2	2.51	0.41
6:B:517:PHE:CE1	24:B:848:BCR:H271	2.55	0.41
10:F:198:ILE:HG23	10:F:198:ILE:O	2.21	0.41
16:L:146:LEU:HB3	16:L:187:THR:HG22	2.02	0.41
18:X:109:LEU:HD21	22:X:614:LUT:H401	2.03	0.41
22:X:615:LUT:H35	22:X:615:LUT:H401	1.86	0.41
22:Y:615:LUT:H35	22:Y:615:LUT:H401	1.92	0.41
22:Z:314:LUT:H35	22:Z:314:LUT:H401	1.94	0.41
1:1:51:MET:HE2	1:1:54:GLN:HG3	2.02	0.41
2:2:231:GLN:NE2	2:2:242:ASN:HD22	2.19	0.41
3:3:153:LEU:HD12	3:3:153:LEU:HA	1.85	0.41
22:5:615:LUT:H31	22:5:615:LUT:H391	1.89	0.41
24:6:620:BCR:H10C	24:6:620:BCR:HC7	1.89	0.41
6:B:408:LEU:HD23	6:B:408:LEU:HA	1.85	0.41
21:B:831:CLA:HBA2	21:B:831:CLA:HBD	2.02	0.41
10:F:140:LEU:HD23	10:F:157:HIS:HE1	1.86	0.41
10:F:140:LEU:HD23	10:F:157:HIS:CE1	2.55	0.41
24:O:201:BCR:H20C	24:O:201:BCR:H361	1.85	0.41
19:Y:49:TYR:OH	19:Y:206:ALA:HB1	2.21	0.41
1:5:114:TRP:CD1	1:5:115:VAL:H	2.38	0.41
21:5:604:CLA:HAA1	21:5:604:CLA:HBD	2.02	0.41
21:A:805:CLA:HBB1	21:A:807:CLA:HBD	2.03	0.41
21:A:813:CLA:H61	21:A:813:CLA:H102	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:812:CLA:HBA1	21:B:812:CLA:H3A	1.40	0.41
8:D:101:LYS:HG3	8:D:103:GLN:HG2	2.02	0.41
24:L:306:BCR:H392	24:L:306:BCR:H23C	2.02	0.41
21:Z:303:CLA:H41	21:Z:303:CLA:H8	2.03	0.41
21:3:605:CLA:HBA2	21:3:605:CLA:H11	1.78	0.41
22:6:616:LUT:H181	22:6:616:LUT:H8	2.02	0.41
21:A:811:CLA:H13	21:A:811:CLA:H171	1.82	0.41
6:B:649:MET:HE2	6:B:649:MET:HB3	1.93	0.41
21:B:825:CLA:H143	24:B:846:BCR:H17C	2.03	0.41
26:B:850:LMG:HC92	26:B:850:LMG:H291	1.52	0.41
7:C:23:THR:HG21	7:C:47:ASP:O	2.21	0.41
22:F:301:LUT:H35	22:F:301:LUT:H401	1.93	0.41
24:O:204:BCR:H20C	24:O:204:BCR:H361	1.90	0.41
18:X:160:TRP:O	18:X:164:VAL:HG12	2.21	0.41
18:X:245:LEU:HD13	18:X:245:LEU:HA	1.91	0.41
20:Z:301:CHL:H3A	20:Z:301:CHL:HBA1	1.24	0.41
6:B:373:THR:HG22	21:B:826:CLA:HAB	2.03	0.40
6:B:668:ARG:HD2	6:B:700:LEU:O	2.21	0.40
21:B:839:CLA:H92	21:B:839:CLA:H61	1.80	0.40
10:F:214:TRP:CG	10:F:215:PRO:HD3	2.56	0.40
18:X:156:ILE:HD11	18:Z:254:TRP:CD1	2.55	0.40
19:Y:220:MET:SD	21:Y:602:CLA:HHC	2.61	0.40
18:Z:98:VAL:HA	18:Z:101:CYS:SG	2.61	0.40
18:Z:129:TRP:CD1	18:Z:129:TRP:H	2.38	0.40
22:Z:315:LUT:H15	22:Z:315:LUT:H201	1.98	0.40
4:4:164:ASN:HA	4:4:165:PRO:HD3	1.91	0.40
1:5:194:ILE:HD13	1:5:194:ILE:HA	1.94	0.40
21:5:613:CLA:HAA1	21:5:613:CLA:HBD	2.03	0.40
21:A:838:CLA:HMB2	21:A:839:CLA:C2D	2.51	0.40
11:G:72:PRO:HA	11:G:155:LEU:HD11	2.03	0.40
13:I:16:LEU:C	13:I:19:PRO:HD2	2.47	0.40
16:L:111:LEU:HD23	16:L:111:LEU:HA	1.94	0.40
24:L:307:BCR:H24C	24:L:307:BCR:H371	1.88	0.40
21:1:605:CLA:HBC2	20:1:606:CHL:HBC3	2.03	0.40
1:5:70:PHE:HE2	23:5:616:XAT:H383	1.86	0.40
21:A:817:CLA:HAA1	21:A:817:CLA:HBD	2.04	0.40
20:X:601:CHL:HHC	20:X:601:CHL:HBB1	2.04	0.40
21:X:611:CLA:HMB2	22:X:614:LUT:H403	2.03	0.40
2:2:144:THR:O	2:2:148:ILE:HG13	2.21	0.40
20:2:601:CHL:HBA1	20:2:601:CHL:H3A	1.83	0.40
20:2:605:CHL:HBB2	20:2:606:CHL:CBB	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:854:BCR:C19	15:K:110:VAL:HG11	2.51	0.40
6:B:673:GLU:O	6:B:677:THR:HG23	2.22	0.40
6:B:710:LEU:HD23	6:B:710:LEU:HA	1.86	0.40
21:B:802:CLA:CGA	21:B:802:CLA:H3A	2.48	0.40
24:B:845:BCR:H20C	24:B:845:BCR:H361	1.97	0.40
8:D:147:PHE:CZ	8:D:160:HIS:HB2	2.57	0.40
8:D:165:ILE:CD1	8:D:171:ASN:HD22	2.35	0.40
12:H:85:TYR:HE2	16:L:94:VAL:HG11	1.85	0.40
16:L:84:LEU:HD23	16:L:84:LEU:HA	1.95	0.40
17:O:65:GLY:HA3	17:O:123:LEU:HD23	2.03	0.40
22:X:615:LUT:H8	22:X:615:LUT:H171	2.03	0.40
18:Z:212:GLU:HA	18:Z:215:ASN:HD21	1.86	0.40
22:4:315:LUT:H181	22:4:315:LUT:H8	2.02	0.40
26:5:621:LMG:HC71	26:5:621:LMG:HC2	1.94	0.40
4:6:208:ALA:HB2	26:6:619:LMG:HC62	2.03	0.40
21:A:825:CLA:H93	21:A:825:CLA:H61	1.70	0.40
21:A:829:CLA:H161	21:A:829:CLA:H202	1.82	0.40
6:B:616:LEU:HD23	6:B:616:LEU:HA	1.95	0.40
22:Y:616:LUT:H11	22:Y:616:LUT:H191	1.93	0.40
22:Y:616:LUT:H31	22:Y:616:LUT:H391	1.93	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	1	196/200 (98%)	192 (98%)	4 (2%)	0	100	100
1	5	192/200 (96%)	187 (97%)	5 (3%)	0	100	100
2	2	201/211 (95%)	197 (98%)	4 (2%)	0	100	100
3	3	211/232 (91%)	204 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	4	196/200 (98%)	190 (97%)	6 (3%)	0	100	100
4	6	196/200 (98%)	188 (96%)	8 (4%)	0	100	100
5	A	722/750 (96%)	698 (97%)	24 (3%)	0	100	100
6	B	731/734 (100%)	704 (96%)	27 (4%)	0	100	100
7	C	78/81 (96%)	71 (91%)	7 (9%)	0	100	100
8	D	138/155 (89%)	129 (94%)	9 (6%)	0	100	100
9	E	61/93 (66%)	58 (95%)	3 (5%)	0	100	100
10	F	153/159 (96%)	147 (96%)	6 (4%)	0	100	100
11	G	96/100 (96%)	90 (94%)	6 (6%)	0	100	100
12	H	92/95 (97%)	86 (94%)	6 (6%)	0	100	100
13	I	30/36 (83%)	29 (97%)	1 (3%)	0	100	100
14	J	38/42 (90%)	37 (97%)	1 (3%)	0	100	100
15	K	78/84 (93%)	74 (95%)	4 (5%)	0	100	100
16	L	160/170 (94%)	154 (96%)	6 (4%)	0	100	100
17	O	87/89 (98%)	85 (98%)	2 (2%)	0	100	100
18	X	216/228 (95%)	211 (98%)	5 (2%)	0	100	100
18	Z	216/228 (95%)	212 (98%)	4 (2%)	0	100	100
19	Y	224/228 (98%)	214 (96%)	10 (4%)	0	100	100
All	All	4312/4515 (96%)	4157 (96%)	155 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	1	159/160 (99%)	158 (99%)	1 (1%)	78	80
1	5	155/160 (97%)	155 (100%)	0	100	100
2	2	164/169 (97%)	161 (98%)	3 (2%)	51	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	3	166/181 (92%)	164 (99%)	2 (1%)	63	74
4	4	166/167 (99%)	164 (99%)	2 (1%)	63	74
4	6	166/167 (99%)	165 (99%)	1 (1%)	78	80
5	A	582/608 (96%)	577 (99%)	5 (1%)	70	77
6	B	597/598 (100%)	589 (99%)	8 (1%)	61	73
7	C	70/71 (99%)	69 (99%)	1 (1%)	59	72
8	D	119/130 (92%)	117 (98%)	2 (2%)	53	70
9	E	58/79 (73%)	58 (100%)	0	100	100
10	F	128/132 (97%)	125 (98%)	3 (2%)	44	66
11	G	82/83 (99%)	82 (100%)	0	100	100
12	H	79/80 (99%)	79 (100%)	0	100	100
13	I	28/32 (88%)	28 (100%)	0	100	100
14	J	35/37 (95%)	35 (100%)	0	100	100
15	K	60/62 (97%)	59 (98%)	1 (2%)	53	70
16	L	128/134 (96%)	127 (99%)	1 (1%)	73	78
17	O	73/73 (100%)	73 (100%)	0	100	100
18	X	168/175 (96%)	168 (100%)	0	100	100
18	Z	168/175 (96%)	167 (99%)	1 (1%)	78	80
19	Y	174/175 (99%)	170 (98%)	4 (2%)	44	66
All	All	3525/3648 (97%)	3490 (99%)	35 (1%)	65	75

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	90	LEU
2	2	71	ASP
2	2	140	THR
2	2	255	ILE
3	3	125	LEU
3	3	229	ILE
4	4	247	ILE
4	4	250	THR
4	6	241	ASP
5	A	86	SER
5	A	247	LEU

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Mol	Chain	Res	Type
5	A	366	HIS
5	A	371	MET
5	A	749	VAL
6	B	257	LEU
6	B	258	LEU
6	B	285	LEU
6	B	352	MET
6	B	394	PHE
6	B	444	LEU
6	B	600	THR
6	B	664	LEU
7	C	65	VAL
8	D	67	LEU
8	D	131	LEU
10	F	80	ILE
10	F	104	GLU
10	F	213	ILE
15	K	62	LEU
16	L	133	LEU
19	Y	40	VAL
19	Y	47	ILE
19	Y	67	TYR
19	Y	156	ILE
18	Z	124	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	113	ASN
1	1	156	GLN
1	1	222	ASN
1	1	232	HIS
1	1	234	ASN
2	2	231	GLN
3	3	200	ASN
3	3	235	GLN
4	4	69	ASN
4	4	100	ASN
4	4	152	HIS
4	4	170	GLN
4	4	195	ASN
1	5	81	ASN

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Mol	Chain	Res	Type
1	5	196	ASN
1	5	232	HIS
4	6	66	ASN
4	6	76	ASN
4	6	152	HIS
4	6	160	GLN
4	6	245	ASN
5	A	50	HIS
5	A	113	GLN
5	A	121	GLN
5	A	177	HIS
5	A	213	HIS
5	A	216	HIS
5	A	307	HIS
5	A	439	ASN
5	A	542	HIS
5	A	729	HIS
6	B	53	GLN
6	B	89	HIS
6	B	95	HIS
6	B	114	ASN
6	B	170	ASN
6	B	178	HIS
6	B	193	HIS
6	B	196	HIS
6	B	210	ASN
6	B	248	GLN
6	B	262	HIS
6	B	289	HIS
6	B	368	GLN
6	B	399	ASN
6	B	432	HIS
6	B	439	HIS
6	B	467	HIS
6	B	627	ASN
6	B	641	ASN
6	B	689	ASN
8	D	180	ASN
8	D	199	GLN
9	E	131	ASN
9	E	132	ASN
10	F	133	ASN

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Mol	Chain	Res	Type
10	F	157	HIS
11	G	148	HIS
13	I	31	GLN
15	K	53	ASN
16	L	62	ASN
16	L	86	ASN
18	X	93	ASN
18	X	135	GLN
18	X	147	ASN
18	X	240	ASN
19	Y	63	GLN
19	Y	135	GLN
19	Y	163	GLN
19	Y	244	HIS
18	Z	147	ASN
18	Z	215	ASN
18	Z	229	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	$\# Z > 2$
19	TPO	Y	39	19	8,10,11	2.43	1 (12%)	10,14,16	1.26	1 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	TPO	Y	39	19	-	6/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	Y	39	TPO	P-OG1	6.72	1.72	1.59

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Y	39	TPO	OG1-P-O1P	-2.35	100.33	109.39

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	Y	39	TPO	N-CA-CB-CG2
19	Y	39	TPO	N-CA-CB-OG1
19	Y	39	TPO	C-CA-CB-CG2
19	Y	39	TPO	O-C-CA-CB
19	Y	39	TPO	CB-OG1-P-O3P
19	Y	39	TPO	CB-OG1-P-O2P

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](#)

318 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
21	CLA	B	822	6	64,68,73	1.29	8 (12%)	77,107,113	1.67	11 (14%)
21	CLA	2	612	-	59,63,73	1.33	8 (13%)	71,101,113	1.84	12 (16%)
21	CLA	B	821	6	59,63,73	1.32	8 (13%)	71,101,113	1.72	11 (15%)
21	CLA	G	202	-	49,53,73	1.42	8 (16%)	59,89,113	1.86	8 (13%)
21	CLA	B	809	-	69,73,73	1.23	7 (10%)	83,113,113	1.57	11 (13%)
21	CLA	A	824	5	59,63,73	1.33	8 (13%)	71,101,113	1.68	10 (14%)
21	CLA	A	803	-	69,73,73	1.21	7 (10%)	83,113,113	1.58	13 (15%)
21	CLA	1	602	1	65,69,73	1.26	8 (12%)	78,108,113	1.70	10 (12%)
21	CLA	X	609	18	49,53,73	1.41	7 (14%)	59,89,113	2.03	9 (15%)
21	CLA	L	304	16	64,68,73	1.28	8 (12%)	77,107,113	1.72	11 (14%)
26	LMG	5	620	-	53,53,55	0.18	0	61,61,63	0.14	0
24	BCR	4	317	-	41,41,41	0.13	0	56,56,56	0.30	0
21	CLA	A	832	5	60,64,73	1.32	8 (13%)	72,102,113	1.76	11 (15%)
20	CHL	Z	306	-	45,54,74	2.43	16 (35%)	35,90,114	3.18	16 (45%)
24	BCR	B	846	-	41,41,41	0.12	0	56,56,56	0.32	0
21	CLA	A	838	5	59,63,73	1.33	8 (13%)	71,101,113	1.75	10 (14%)
20	CHL	X	605	18	41,50,74	2.56	13 (31%)	30,85,114	3.45	15 (50%)
21	CLA	B	838	-	69,73,73	1.23	8 (11%)	83,113,113	1.66	10 (12%)
31	NEX	Y	617	-	38,46,46	0.39	1 (2%)	50,70,70	0.46	0
21	CLA	3	604	-	49,53,73	1.41	8 (16%)	59,89,113	1.83	9 (15%)
24	BCR	I	101	-	41,41,41	0.15	0	56,56,56	0.23	0
21	CLA	B	811	6	47,51,73	1.40	6 (12%)	56,86,113	1.86	8 (14%)
20	CHL	4	306	-	50,59,74	2.29	14 (28%)	41,96,114	3.04	19 (46%)
20	CHL	2	605	2	41,50,74	2.49	13 (31%)	30,85,114	3.55	13 (43%)
21	CLA	1	607	-	47,52,73	1.42	8 (17%)	56,88,113	1.74	6 (10%)
21	CLA	A	807	5	69,73,73	1.22	9 (13%)	83,113,113	1.73	11 (13%)
24	BCR	F	302	-	41,41,41	0.15	0	56,56,56	0.34	0
24	BCR	L	308	-	41,41,41	0.13	0	56,56,56	0.24	0
20	CHL	2	606	-	42,51,74	2.45	13 (30%)	31,86,114	3.29	15 (48%)
21	CLA	3	614	3	43,48,73	1.48	8 (18%)	51,83,113	1.75	7 (13%)
24	BCR	2	619	-	41,41,41	0.26	0	56,56,56	0.57	1 (1%)
24	BCR	B	843	-	41,41,41	0.18	0	56,56,56	0.55	0
21	CLA	3	602	3	64,68,73	1.29	8 (12%)	77,107,113	1.68	12 (15%)
26	LMG	F	306	-	47,47,55	0.21	0	55,55,63	0.18	0
21	CLA	A	816	-	49,53,73	1.42	8 (16%)	59,89,113	1.91	9 (15%)
26	LMG	1	621	-	49,49,55	0.19	0	57,57,63	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	Z	305	-	54,58,73	1.39	7 (12%)	65,95,113	1.78	7 (10%)
24	BCR	B	848	-	41,41,41	0.24	0	56,56,56	0.64	1 (1%)
21	CLA	A	825	-	69,73,73	1.22	8 (11%)	83,113,113	1.62	9 (10%)
25	LHG	A	853	21	29,29,48	0.38	0	32,35,54	0.33	0
21	CLA	6	614	4	54,58,73	1.38	8 (14%)	65,95,113	1.81	10 (15%)
21	CLA	O	202	25	54,58,73	1.39	8 (14%)	65,95,113	1.88	10 (15%)
26	LMG	1	619	-	53,53,55	0.18	0	61,61,63	0.17	0
21	CLA	A	830	5	69,73,73	1.24	7 (10%)	83,113,113	1.68	11 (13%)
24	BCR	A	849	-	41,41,41	0.19	0	56,56,56	0.53	1 (1%)
21	CLA	2	611	2	49,53,73	1.42	8 (16%)	59,89,113	1.87	8 (13%)
23	XAT	O	208	-	39,47,47	0.10	0	54,74,74	0.86	2 (3%)
21	CLA	B	804	6	69,73,73	1.24	9 (13%)	83,113,113	1.75	9 (10%)
21	CLA	B	825	6	66,70,73	1.27	7 (10%)	79,109,113	1.78	13 (16%)
21	CLA	Y	612	19	49,53,73	1.42	8 (16%)	59,89,113	1.81	7 (11%)
21	CLA	3	610	3	45,49,73	1.45	7 (15%)	54,84,113	1.90	9 (16%)
21	CLA	B	813	6	69,73,73	1.24	7 (10%)	83,113,113	1.68	10 (12%)
21	CLA	4	313	4	54,58,73	1.38	8 (14%)	65,95,113	1.84	10 (15%)
21	CLA	6	608	4	49,53,73	1.42	8 (16%)	59,89,113	1.82	8 (13%)
21	CLA	1	612	1	69,73,73	1.22	8 (11%)	83,113,113	1.66	12 (14%)
24	BCR	A	854	-	41,41,41	0.24	0	56,56,56	0.47	0
21	CLA	4	312	4	49,53,73	1.41	8 (16%)	59,89,113	1.83	8 (13%)
21	CLA	4	310	4	44,49,73	1.44	8 (18%)	52,84,113	1.85	4 (7%)
20	CHL	Z	309	18	45,54,74	2.44	15 (33%)	35,90,114	3.16	17 (48%)
21	CLA	A	805	5	49,53,73	1.41	7 (14%)	59,89,113	1.85	9 (15%)
21	CLA	3	613	-	43,48,73	1.47	8 (18%)	51,83,113	1.80	6 (11%)
29	SF4	A	850	6,5	0,12,12	-	-	-	-	-
21	CLA	A	821	-	69,73,73	1.23	8 (11%)	83,113,113	1.72	11 (13%)
21	CLA	B	835	-	54,58,73	1.40	8 (14%)	65,95,113	1.92	11 (16%)
21	CLA	Y	610	19	49,53,73	1.42	8 (16%)	59,89,113	1.79	8 (13%)
20	CHL	X	608	18	45,54,74	2.48	16 (35%)	35,90,114	3.10	16 (45%)
20	CHL	Y	606	19	45,54,74	2.51	15 (33%)	35,90,114	3.14	16 (45%)
24	BCR	L	302	-	41,41,41	0.14	0	56,56,56	0.27	0
21	CLA	4	308	4	58,62,73	1.33	7 (12%)	69,99,113	1.80	11 (15%)
21	CLA	J	102	-	46,50,73	1.41	8 (17%)	55,85,113	1.85	8 (14%)
21	CLA	B	839	6	69,73,73	1.23	8 (11%)	83,113,113	1.74	11 (13%)
21	CLA	X	611	18	49,53,73	1.41	7 (14%)	59,89,113	1.83	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	Z	313	-	50,54,73	1.41	8 (16%)	60,90,113	1.78	8 (13%)
21	CLA	A	842	-	69,73,73	1.22	8 (11%)	83,113,113	1.60	10 (12%)
20	CHL	X	606	18	45,54,74	2.48	16 (35%)	35,90,114	3.25	16 (45%)
21	CLA	A	810	5	54,58,73	1.39	7 (12%)	65,95,113	1.75	11 (16%)
21	CLA	Z	310	-	49,53,73	1.42	7 (14%)	59,89,113	1.79	9 (15%)
24	BCR	L	307	-	41,41,41	0.14	0	56,56,56	0.29	0
21	CLA	B	834	-	46,50,73	1.42	8 (17%)	55,85,113	1.88	7 (12%)
21	CLA	2	618	4	50,54,73	1.38	8 (16%)	60,90,113	1.80	9 (15%)
21	CLA	A	833	5	69,73,73	1.22	8 (11%)	83,113,113	1.73	12 (14%)
23	XAT	5	616	-	39,47,47	0.09	0	54,74,74	0.67	2 (3%)
20	CHL	4	314	-	40,49,74	2.41	11 (27%)	31,84,114	3.29	14 (45%)
24	BCR	5	617	-	41,41,41	0.10	0	56,56,56	0.23	0
21	CLA	K	203	15	50,54,73	1.39	7 (14%)	60,90,113	1.90	7 (11%)
22	LUT	1	615	-	42,43,43	1.65	8 (19%)	51,60,60	1.54	11 (21%)
21	CLA	A	840	5	69,73,73	1.21	7 (10%)	83,113,113	1.66	10 (12%)
21	CLA	B	805	6	69,73,73	1.21	8 (11%)	83,113,113	1.74	12 (14%)
22	LUT	5	619	-	42,43,43	1.64	8 (19%)	51,60,60	1.62	11 (21%)
21	CLA	F	304	10	45,49,73	1.45	8 (17%)	54,84,113	2.00	8 (14%)
24	BCR	B	844	-	41,41,41	0.13	0	56,56,56	0.33	0
27	LMT	4	319	-	36,36,36	0.11	0	47,47,47	0.16	0
21	CLA	6	613	4	49,53,73	1.41	7 (14%)	59,89,113	1.72	9 (15%)
21	CLA	2	602	2	69,73,73	1.23	8 (11%)	83,113,113	1.65	11 (13%)
21	CLA	B	824	-	54,58,73	1.39	6 (11%)	65,95,113	1.73	10 (15%)
21	CLA	4	309	-	64,68,73	1.28	8 (12%)	77,107,113	1.74	11 (14%)
21	CLA	3	611	-	47,51,73	1.42	8 (17%)	56,86,113	1.89	9 (16%)
24	BCR	A	846	-	41,41,41	0.16	0	56,56,56	0.56	1 (1%)
21	CLA	5	603	1	49,53,73	1.41	8 (16%)	59,89,113	1.91	7 (11%)
25	LHG	5	618	21	48,48,48	0.29	0	51,54,54	0.28	0
21	CLA	B	820	6	59,63,73	1.33	7 (11%)	71,101,113	1.71	11 (15%)
21	CLA	A	814	-	49,53,73	1.42	8 (16%)	59,89,113	1.86	8 (13%)
21	CLA	6	609	4	58,62,73	1.34	8 (13%)	69,99,113	1.79	9 (13%)
24	BCR	O	201	-	41,41,41	0.13	0	56,56,56	0.63	2 (3%)
21	CLA	A	808	5	54,58,73	1.39	8 (14%)	65,95,113	1.86	10 (15%)
21	CLA	5	608	1	49,53,73	1.42	6 (12%)	59,89,113	2.12	8 (13%)
24	BCR	6	618	-	41,41,41	0.13	0	56,56,56	0.37	0
24	BCR	F	305	-	41,41,41	0.13	0	56,56,56	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	LHG	A	851	-	48,48,48	0.29	0	51,54,54	0.29	0
21	CLA	Z	311	25	49,53,73	1.42	7 (14%)	59,89,113	1.73	8 (13%)
23	XAT	3	616	-	39,47,47	0.10	0	54,74,74	0.88	4 (7%)
27	LMT	6	621	-	36,36,36	0.11	0	47,47,47	0.19	0
21	CLA	4	302	4	49,53,73	1.42	8 (16%)	59,89,113	1.82	10 (16%)
21	CLA	A	820	5	49,53,73	1.41	8 (16%)	59,89,113	1.85	9 (15%)
25	LHG	1	620	-	48,48,48	0.30	0	51,54,54	0.30	0
22	LUT	2	615	-	42,43,43	1.65	8 (19%)	51,60,60	1.52	11 (21%)
20	CHL	4	305	-	45,54,74	2.42	15 (33%)	35,90,114	3.17	16 (45%)
21	CLA	B	829	6	47,51,73	1.41	7 (14%)	56,86,113	1.90	7 (12%)
20	CHL	Z	301	-	45,54,74	2.48	16 (35%)	35,90,114	3.34	17 (48%)
21	CLA	6	603	4	49,53,73	1.41	8 (16%)	59,89,113	1.79	9 (15%)
21	CLA	B	803	6	45,49,73	1.44	7 (15%)	54,84,113	1.91	10 (18%)
21	CLA	A	836	5	49,53,73	1.41	8 (16%)	59,89,113	1.90	8 (13%)
22	LUT	F	301	-	42,43,43	1.65	8 (19%)	51,60,60	1.60	11 (21%)
21	CLA	B	815	6	59,63,73	1.33	8 (13%)	71,101,113	1.80	9 (12%)
21	CLA	3	609	3	49,53,73	1.42	8 (16%)	59,89,113	1.89	9 (15%)
21	CLA	B	802	-	69,73,73	1.25	6 (8%)	83,113,113	1.55	14 (16%)
21	CLA	A	822	5	46,50,73	1.40	7 (15%)	55,85,113	1.73	6 (10%)
21	CLA	Y	614	19	49,53,73	1.41	8 (16%)	59,89,113	1.82	9 (15%)
21	CLA	6	610	-	49,53,73	1.43	7 (14%)	59,89,113	1.65	8 (13%)
21	CLA	5	605	-	43,48,73	1.42	7 (16%)	52,82,113	1.85	10 (19%)
21	CLA	1	614	1	49,53,73	1.41	8 (16%)	59,89,113	1.88	9 (15%)
31	NEX	X	616	-	38,46,46	0.41	1 (2%)	50,70,70	0.42	0
21	CLA	4	311	4	61,65,73	1.30	8 (13%)	73,103,113	1.73	10 (13%)
28	PQN	A	844	-	34,34,34	0.24	0	42,45,45	0.51	1 (2%)
21	CLA	X	610	25	49,53,73	1.41	7 (14%)	59,89,113	1.94	9 (15%)
21	CLA	3	607	3	49,53,73	1.41	8 (16%)	59,89,113	1.85	8 (13%)
21	CLA	5	607	-	47,52,73	1.44	7 (14%)	56,88,113	1.85	6 (10%)
21	CLA	5	611	1	49,53,73	1.42	8 (16%)	59,89,113	1.88	8 (13%)
21	CLA	B	830	6	47,51,73	1.40	8 (17%)	56,86,113	1.89	7 (12%)
21	CLA	5	612	1	69,73,73	1.23	8 (11%)	83,113,113	1.60	13 (15%)
20	CHL	2	607	-	50,59,74	2.31	15 (30%)	41,96,114	2.92	18 (43%)
21	CLA	L	301	-	69,73,73	1.22	8 (11%)	83,113,113	1.68	9 (10%)
29	SF4	C	101	7	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	L	303	16	49,53,73	1.41	8 (16%)	59,89,113	1.83	7 (11%)
21	CLA	1	613	1	49,53,73	1.40	6 (12%)	59,89,113	1.81	10 (16%)
20	CHL	Y	601	19	45,54,74	2.40	14 (31%)	35,90,114	3.19	17 (48%)
21	CLA	B	837	6	51,55,73	1.37	8 (15%)	61,91,113	1.86	10 (16%)
21	CLA	X	618	-	49,53,73	1.42	7 (14%)	59,89,113	1.73	10 (16%)
24	BCR	A	848	-	41,41,41	0.15	0	56,56,56	0.37	0
25	LHG	2	617	21	36,36,48	0.34	0	39,42,54	0.32	0
22	LUT	5	615	-	42,43,43	1.66	8 (19%)	51,60,60	1.58	8 (15%)
30	DGD	B	849	-	62,62,67	0.16	0	76,76,81	0.17	0
21	CLA	1	603	1	59,63,73	1.31	8 (13%)	71,101,113	1.80	12 (16%)
25	LHG	1	618	21	48,48,48	0.29	0	51,54,54	0.28	0
26	LMG	G	206	-	50,50,55	0.20	0	58,58,63	0.18	0
21	CLA	A	834	-	69,73,73	1.23	8 (11%)	83,113,113	1.68	10 (12%)
20	CHL	Y	608	-	45,54,74	2.45	15 (33%)	35,90,114	3.20	16 (45%)
21	CLA	K	201	15	42,45,73	1.52	8 (19%)	50,78,113	1.88	9 (18%)
21	CLA	B	840	25	69,73,73	1.23	8 (11%)	83,113,113	1.74	12 (14%)
20	CHL	X	607	-	45,54,74	2.51	15 (33%)	35,90,114	3.18	17 (48%)
21	CLA	6	604	-	49,53,73	1.41	8 (16%)	59,89,113	1.85	8 (13%)
21	CLA	4	307	4	49,53,73	1.42	8 (16%)	59,89,113	1.84	7 (11%)
22	LUT	Y	615	-	42,43,43	1.64	8 (19%)	51,60,60	1.54	9 (17%)
31	NEX	Z	316	-	38,46,46	0.37	1 (2%)	50,70,70	0.52	1 (2%)
21	CLA	3	612	3	47,52,73	1.44	8 (17%)	56,88,113	1.77	7 (12%)
21	CLA	5	609	1	49,53,73	1.41	8 (16%)	59,89,113	1.83	10 (16%)
21	CLA	B	814	6	59,63,73	1.34	8 (13%)	71,101,113	1.82	9 (12%)
21	CLA	B	808	6	59,63,73	1.33	8 (13%)	71,101,113	1.90	11 (15%)
26	LMG	6	619	-	36,36,55	0.20	0	44,44,63	0.17	0
21	CLA	2	610	25	45,49,73	1.46	8 (17%)	54,84,113	1.86	7 (12%)
21	CLA	A	841	5	69,73,73	1.22	8 (11%)	83,113,113	1.70	11 (13%)
21	CLA	L	305	-	49,53,73	1.42	8 (16%)	59,89,113	1.87	8 (13%)
21	CLA	O	207	17	40,46,73	1.47	8 (20%)	48,80,113	1.76	6 (12%)
20	CHL	2	614	2	42,51,74	2.45	13 (30%)	31,86,114	3.40	15 (48%)
21	CLA	B	826	6	64,68,73	1.26	8 (12%)	77,107,113	1.76	11 (14%)
25	LHG	X	617	21	36,36,48	0.34	0	39,42,54	0.31	0
24	BCR	A	847	-	41,41,41	0.14	0	56,56,56	0.38	0
21	CLA	A	835	5	49,53,73	1.42	6 (12%)	59,89,113	1.79	7 (11%)
20	CHL	Y	605	-	41,50,74	2.51	14 (34%)	30,85,114	3.35	15 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	LUT	6	616	-	42,43,43	1.64	8 (19%)	51,60,60	1.58	11 (21%)
22	LUT	Z	315	-	42,43,43	1.71	8 (19%)	51,60,60	1.93	10 (19%)
20	CHL	Y	607	-	45,54,74	2.50	16 (35%)	35,90,114	3.12	18 (51%)
21	CLA	A	809	5	59,63,73	1.33	8 (13%)	71,101,113	1.74	11 (15%)
24	BCR	O	204	-	41,41,41	0.14	0	56,56,56	0.20	0
21	CLA	O	203	-	66,70,73	1.25	7 (10%)	79,109,113	1.75	11 (13%)
21	CLA	B	817	6	64,68,73	1.27	8 (12%)	77,107,113	1.76	13 (16%)
20	CHL	Y	609	19	45,54,74	2.48	16 (35%)	35,90,114	3.19	16 (45%)
21	CLA	5	610	25	49,53,73	1.41	8 (16%)	59,89,113	1.90	8 (13%)
21	CLA	2	603	2	47,52,73	1.43	8 (17%)	56,88,113	1.77	7 (12%)
24	BCR	L	306	-	41,41,41	0.15	0	56,56,56	0.34	0
20	CHL	Y	619	-	46,55,74	2.42	14 (30%)	36,91,114	3.08	17 (47%)
22	LUT	Z	314	-	42,43,43	1.63	8 (19%)	51,60,60	1.55	10 (19%)
21	CLA	Y	603	-	49,53,73	1.42	8 (16%)	59,89,113	1.77	8 (13%)
25	LHG	Y	618	21	34,34,48	0.35	0	37,40,54	0.32	0
21	CLA	Z	304	-	49,53,73	1.42	8 (16%)	59,89,113	1.70	8 (13%)
21	CLA	A	815	5	46,50,73	1.41	8 (17%)	55,85,113	1.88	9 (16%)
21	CLA	A	828	-	69,73,73	1.22	7 (10%)	83,113,113	1.68	12 (14%)
24	BCR	J	103	-	41,41,41	0.14	0	56,56,56	0.29	0
21	CLA	A	801	5	69,73,73	1.22	8 (11%)	83,113,113	1.67	13 (15%)
21	CLA	3	617	5	59,63,73	1.32	7 (11%)	71,101,113	1.77	9 (12%)
21	CLA	B	831	6	69,73,73	1.23	8 (11%)	83,113,113	1.77	11 (13%)
24	BCR	G	205	-	41,41,41	0.12	0	56,56,56	0.31	0
21	CLA	Z	303	18	64,68,73	1.28	7 (10%)	77,107,113	1.84	10 (12%)
20	CHL	1	601	1	54,63,74	2.23	15 (27%)	46,101,114	2.76	16 (34%)
21	CLA	B	801	-	69,73,73	1.22	8 (11%)	83,113,113	1.70	12 (14%)
21	CLA	J	101	-	46,50,73	1.41	8 (17%)	55,85,113	1.88	7 (12%)
21	CLA	B	819	6	54,58,73	1.39	8 (14%)	65,95,113	1.80	10 (15%)
25	LHG	1	622	21	37,37,48	0.34	0	40,43,54	0.30	0
28	PQN	B	841	-	34,34,34	0.24	0	42,45,45	0.50	1 (2%)
21	CLA	6	611	-	44,49,73	1.44	8 (18%)	52,84,113	1.93	5 (9%)
21	CLA	A	819	5	69,73,73	1.23	8 (11%)	83,113,113	1.64	11 (13%)
21	CLA	B	810	6	58,62,73	1.34	9 (15%)	73,100,113	2.06	13 (17%)
21	CLA	Y	604	-	49,53,73	1.42	8 (16%)	59,89,113	1.78	7 (11%)
21	CLA	1	604	-	53,57,73	1.36	8 (15%)	62,93,113	1.82	7 (11%)
26	LMG	4	318	-	36,36,55	0.20	0	44,44,63	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	SF4	C	102	7	0,12,12	-	-	-		
21	CLA	A	827	5	69,73,73	1.23	8 (11%)	83,113,113	1.76	11 (13%)
21	CLA	H	201	12	64,68,73	1.27	7 (10%)	77,107,113	1.59	12 (15%)
22	LUT	Y	616	-	42,43,43	1.64	8 (19%)	51,60,60	1.60	11 (21%)
25	LHG	Z	317	21	31,31,48	0.36	0	34,37,54	0.33	0
21	CLA	B	833	6	64,68,73	1.30	8 (12%)	77,107,113	1.72	12 (15%)
22	LUT	4	315	-	42,43,43	1.66	8 (19%)	51,60,60	1.59	13 (25%)
21	CLA	Y	602	19	69,73,73	1.24	8 (11%)	83,113,113	1.69	9 (10%)
20	CHL	5	601	1	54,63,74	2.26	15 (27%)	46,101,114	2.71	17 (36%)
26	LMG	B	850	-	52,52,55	0.20	0	60,60,63	0.14	0
21	CLA	2	604	-	69,73,73	1.24	8 (11%)	83,113,113	1.65	13 (15%)
21	CLA	2	608	2	49,53,73	1.40	7 (14%)	59,89,113	1.81	8 (13%)
21	CLA	1	610	25	59,63,73	1.34	8 (13%)	71,101,113	1.78	9 (12%)
21	CLA	A	837	5	55,59,73	1.36	9 (16%)	66,96,113	1.99	11 (16%)
21	CLA	G	204	11	49,53,73	1.42	8 (16%)	59,89,113	1.90	9 (15%)
21	CLA	B	827	6	69,73,73	1.24	8 (11%)	83,113,113	1.69	11 (13%)
23	XAT	4	316	-	39,47,47	0.12	0	54,74,74	0.88	3 (5%)
21	CLA	Z	312	-	49,53,73	1.42	8 (16%)	59,89,113	1.77	8 (13%)
21	CLA	X	612	18	49,53,73	1.41	7 (14%)	59,89,113	1.74	10 (16%)
24	BCR	A	845	-	41,41,41	0.15	0	56,56,56	0.25	0
20	CHL	Z	308	-	41,50,74	2.50	14 (34%)	30,85,114	3.45	15 (50%)
20	CHL	5	606	1	40,49,74	2.54	13 (32%)	29,84,114	3.37	13 (44%)
21	CLA	A	831	5	54,58,73	1.39	8 (14%)	65,95,113	1.87	9 (13%)
24	BCR	O	205	-	41,41,41	0.11	0	56,56,56	0.22	0
21	CLA	5	613	1	49,53,73	1.42	7 (14%)	59,89,113	1.80	8 (13%)
27	LMT	F	303	-	36,36,36	0.12	0	47,47,47	0.46	0
21	CLA	B	832	-	49,53,73	1.41	8 (16%)	59,89,113	1.76	6 (10%)
26	LMG	F	307	-	30,30,55	0.21	0	38,38,63	0.16	0
21	CLA	4	303	-	49,53,73	1.40	7 (14%)	59,89,113	1.82	10 (16%)
21	CLA	X	603	-	57,61,73	1.35	8 (14%)	68,98,113	1.74	11 (16%)
24	BCR	B	847	-	41,41,41	0.13	0	56,56,56	0.29	0
21	CLA	X	604	-	49,53,73	1.42	7 (14%)	59,89,113	1.80	9 (15%)
20	CHL	Z	307	-	45,54,74	2.47	15 (33%)	35,90,114	3.26	16 (45%)
21	CLA	2	613	-	47,51,73	1.40	8 (17%)	56,86,113	1.82	7 (12%)
21	CLA	6	602	4	64,68,73	1.27	8 (12%)	77,107,113	1.72	10 (12%)
21	CLA	A	826	-	69,73,73	1.24	7 (10%)	83,113,113	1.65	12 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	Y	613	19	59,63,73	1.32	8 (13%)	71,101,113	1.69	12 (16%)
23	XAT	6	617	-	39,47,47	0.13	0	54,74,74	0.89	3 (5%)
24	BCR	B	845	-	41,41,41	0.13	0	56,56,56	0.34	0
21	CLA	A	839	5	54,58,73	1.38	8 (14%)	65,95,113	1.82	11 (16%)
20	CHL	6	606	-	45,54,74	2.44	15 (33%)	35,90,114	3.21	16 (45%)
24	BCR	6	620	-	41,41,41	0.18	0	56,56,56	0.47	0
21	CLA	B	836	6	69,73,73	1.23	8 (11%)	83,113,113	1.63	10 (12%)
21	CLA	B	828	6	60,64,73	1.31	7 (11%)	72,102,113	1.73	9 (12%)
21	CLA	A	829	5	69,73,73	1.23	8 (11%)	83,113,113	1.66	10 (12%)
21	CLA	A	813	5	69,73,73	1.21	7 (10%)	83,113,113	1.77	12 (14%)
21	CLA	K	202	-	49,53,73	1.41	8 (16%)	59,89,113	1.86	9 (15%)
21	CLA	1	605	-	43,48,73	1.42	8 (18%)	52,82,113	1.90	6 (11%)
21	CLA	2	609	2	59,63,73	1.33	8 (13%)	71,101,113	1.75	10 (14%)
20	CHL	4	304	-	55,64,74	2.22	15 (27%)	47,102,114	2.80	19 (40%)
21	CLA	O	206	-	53,57,73	1.36	8 (15%)	62,93,113	1.74	9 (14%)
22	LUT	3	615	-	42,43,43	1.61	8 (19%)	51,60,60	1.70	11 (21%)
21	CLA	1	608	1	69,73,73	1.23	8 (11%)	83,113,113	1.61	11 (13%)
23	XAT	2	616	-	39,47,47	0.10	0	54,74,74	0.75	3 (5%)
21	CLA	A	804	5	59,63,73	1.32	8 (13%)	71,101,113	1.85	13 (18%)
21	CLA	B	812	6	69,73,73	1.22	9 (13%)	83,113,113	1.71	10 (12%)
20	CHL	6	615	4	40,49,74	2.45	12 (30%)	31,84,114	3.27	14 (45%)
21	CLA	5	614	1	49,53,73	1.39	7 (14%)	59,89,113	1.85	8 (13%)
21	CLA	A	817	5	64,68,73	1.28	8 (12%)	77,107,113	1.69	13 (16%)
21	CLA	1	611	1	49,53,73	1.42	8 (16%)	59,89,113	1.87	9 (15%)
21	CLA	A	802	-	69,73,73	1.24	8 (11%)	83,113,113	1.72	12 (14%)
20	CHL	Z	302	18	45,54,74	2.47	15 (33%)	35,90,114	3.14	17 (48%)
21	CLA	X	602	18	49,53,73	1.42	8 (16%)	59,89,113	1.86	8 (13%)
21	CLA	X	613	18	49,53,73	1.42	8 (16%)	59,89,113	1.79	9 (15%)
21	CLA	B	807	-	69,73,73	1.21	8 (11%)	83,113,113	1.71	12 (14%)
20	CHL	1	606	1	40,49,74	2.47	13 (32%)	29,84,114	3.36	13 (44%)
24	BCR	3	601	-	41,41,41	0.12	0	56,56,56	0.26	0
20	CHL	6	607	-	50,59,74	2.32	14 (28%)	41,96,114	3.04	18 (43%)
20	CHL	2	601	2	46,55,74	2.38	14 (30%)	36,91,114	3.18	17 (47%)
21	CLA	3	606	-	44,49,73	1.44	8 (18%)	52,84,113	1.83	7 (13%)
21	CLA	B	816	-	63,67,73	1.27	6 (9%)	75,105,113	1.74	11 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CHL	3	608	-	46,55,74	2.38	13 (28%)	36,91,114	3.19	17 (47%)
23	XAT	1	616	-	39,47,47	0.11	0	54,74,74	0.86	3 (5%)
21	CLA	G	203	11	46,50,73	1.40	8 (17%)	55,85,113	1.88	8 (14%)
24	BCR	B	842	-	41,41,41	0.16	0	56,56,56	0.31	0
21	CLA	K	204	15	41,47,73	1.46	8 (19%)	49,81,113	1.92	7 (14%)
21	CLA	3	605	-	51,55,73	1.39	8 (15%)	61,91,113	1.88	11 (18%)
21	CLA	Y	611	25	49,53,73	1.42	8 (16%)	59,89,113	1.81	9 (15%)
21	CLA	B	823	-	69,73,73	1.23	8 (11%)	83,113,113	1.66	12 (14%)
21	CLA	B	818	-	59,63,73	1.34	8 (13%)	71,101,113	1.72	10 (14%)
21	CLA	B	806	6	56,60,73	1.36	8 (14%)	67,97,113	1.85	11 (16%)
21	CLA	6	601	4	50,54,73	1.39	8 (16%)	60,90,113	1.73	7 (11%)
21	CLA	4	301	4	64,68,73	1.27	8 (12%)	77,107,113	1.75	10 (12%)
27	LMT	G	201	-	36,36,36	0.10	0	47,47,47	0.16	0
26	LMG	5	621	-	49,49,55	0.19	0	57,57,63	0.14	0
21	CLA	6	612	4	61,65,73	1.31	8 (13%)	73,103,113	1.72	12 (16%)
24	BCR	K	205	-	41,41,41	0.12	0	56,56,56	0.21	0
21	CLA	5	604	-	53,57,73	1.37	7 (13%)	62,93,113	1.79	9 (14%)
21	CLA	A	812	5	58,62,73	1.33	8 (13%)	69,99,113	1.83	12 (17%)
21	CLA	3	603	3	59,63,73	1.33	8 (13%)	71,101,113	1.75	10 (14%)
21	CLA	5	602	1	65,69,73	1.27	8 (12%)	78,108,113	1.69	9 (11%)
21	CLA	A	811	5	69,73,73	1.23	8 (11%)	83,113,113	1.66	10 (12%)
22	LUT	X	614	-	42,43,43	1.67	8 (19%)	51,60,60	1.73	9 (17%)
21	CLA	A	823	-	45,49,73	1.44	8 (17%)	54,84,113	1.81	9 (16%)
22	LUT	X	615	-	42,43,43	1.65	8 (19%)	51,60,60	1.68	11 (21%)
21	CLA	1	609	1	63,67,73	1.29	8 (12%)	76,106,113	1.68	11 (14%)
21	CLA	A	818	5	63,67,73	1.27	8 (12%)	75,105,113	1.75	12 (16%)
20	CHL	6	605	-	55,64,74	2.23	15 (27%)	47,102,114	2.82	19 (40%)
20	CHL	X	601	18	45,54,74	2.48	16 (35%)	35,90,114	3.17	16 (45%)
21	CLA	A	843	-	61,65,73	1.30	8 (13%)	73,103,113	1.79	14 (19%)
21	CLA	A	806	5	69,73,73	1.22	8 (11%)	83,113,113	1.76	11 (13%)
27	LMT	A	852	-	36,36,36	0.12	0	47,47,47	0.24	0
24	BCR	1	617	-	41,41,41	0.12	0	56,56,56	0.24	0

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
21	CLA	B	822	6	-	18/33/109/115	-
21	CLA	2	612	-	-	10/27/103/115	-
21	CLA	B	821	6	-	12/27/103/115	-
21	CLA	G	202	-	-	7/15/91/115	-
21	CLA	B	809	-	-	17/39/115/115	-
21	CLA	A	824	5	-	13/27/103/115	-
21	CLA	A	803	-	-	15/39/115/115	-
21	CLA	1	602	1	-	10/35/111/115	-
21	CLA	X	609	18	-	7/15/91/115	-
21	CLA	L	304	16	-	11/33/109/115	-
26	LMG	5	620	-	-	10/48/68/70	0/1/1/1
24	BCR	4	317	-	-	0/29/63/63	0/2/2/2
21	CLA	A	832	5	-	7/29/105/115	-
20	CHL	Z	306	-	-	6/15/113/137	-
24	BCR	B	846	-	-	3/29/63/63	0/2/2/2
21	CLA	A	838	5	-	6/27/103/115	-
20	CHL	X	605	18	-	0/10/108/137	-
21	CLA	B	838	-	-	15/39/115/115	-
31	NEX	Y	617	-	-	3/27/83/83	0/3/3/3
21	CLA	3	604	-	-	5/15/91/115	-
24	BCR	I	101	-	-	0/29/63/63	0/2/2/2
21	CLA	B	811	6	-	5/13/89/115	-
20	CHL	4	306	-	-	6/21/119/137	-
20	CHL	2	605	2	-	5/10/108/137	-
21	CLA	1	607	-	-	1/13/89/115	-
21	CLA	A	807	5	-	21/39/115/115	-
24	BCR	F	302	-	-	0/29/63/63	0/2/2/2
24	BCR	L	308	-	-	6/29/63/63	0/2/2/2
20	CHL	2	606	-	-	9/12/110/137	-
21	CLA	3	614	3	-	0/8/84/115	-
24	BCR	2	619	-	-	14/29/63/63	0/2/2/2
24	BCR	B	843	-	-	3/29/63/63	0/2/2/2
21	CLA	3	602	3	-	10/33/109/115	-
26	LMG	F	306	-	-	9/42/62/70	0/1/1/1
21	CLA	A	816	-	-	4/15/91/115	-
26	LMG	1	621	-	-	8/44/64/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	Z	305	-	-	11/21/97/115	-
24	BCR	B	848	-	-	6/29/63/63	0/2/2/2
21	CLA	A	825	-	-	20/39/115/115	-
25	LHG	A	853	21	-	6/34/34/53	-
21	CLA	6	614	4	-	9/21/97/115	-
21	CLA	O	202	25	-	10/21/97/115	-
26	LMG	1	619	-	-	11/48/68/70	0/1/1/1
21	CLA	A	830	5	-	9/39/115/115	-
24	BCR	A	849	-	-	7/29/63/63	0/2/2/2
21	CLA	2	611	2	-	5/15/91/115	-
23	XAT	O	208	-	-	1/31/93/93	0/4/4/4
21	CLA	B	804	6	-	16/39/115/115	-
21	CLA	B	825	6	-	13/36/112/115	-
21	CLA	Y	612	19	-	5/15/91/115	-
21	CLA	3	610	3	-	3/10/86/115	-
21	CLA	B	813	6	-	18/39/115/115	-
21	CLA	4	313	4	-	7/21/97/115	-
21	CLA	6	608	4	-	5/15/91/115	-
21	CLA	1	612	1	-	19/39/115/115	-
24	BCR	A	854	-	-	3/29/63/63	0/2/2/2
21	CLA	4	312	4	-	5/15/91/115	-
21	CLA	4	310	4	-	2/10/86/115	-
20	CHL	Z	309	18	-	6/15/113/137	-
21	CLA	A	805	5	-	4/15/91/115	-
21	CLA	3	613	-	-	2/8/84/115	-
29	SF4	A	850	6,5	-	-	0/6/5/5
21	CLA	A	821	-	-	13/39/115/115	-
21	CLA	B	835	-	-	4/21/97/115	-
21	CLA	Y	610	19	-	10/15/91/115	-
20	CHL	X	608	18	-	5/15/113/137	-
20	CHL	Y	606	19	-	0/15/113/137	-
24	BCR	L	302	-	-	4/29/63/63	0/2/2/2
21	CLA	4	308	4	-	4/26/102/115	-
21	CLA	J	102	-	-	6/12/88/115	-
21	CLA	B	839	6	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	X	611	18	-	7/15/91/115	-
21	CLA	Z	313	-	-	9/17/93/115	-
21	CLA	A	842	-	-	10/39/115/115	-
20	CHL	X	606	18	-	6/15/113/137	-
21	CLA	A	810	5	-	6/21/97/115	-
21	CLA	Z	310	-	-	10/15/91/115	-
24	BCR	L	307	-	-	2/29/63/63	0/2/2/2
21	CLA	B	834	-	-	4/12/88/115	-
21	CLA	2	618	4	-	7/17/93/115	-
21	CLA	A	833	5	-	19/39/115/115	-
23	XAT	5	616	-	-	0/31/93/93	0/4/4/4
20	CHL	4	314	-	-	2/10/106/137	-
24	BCR	5	617	-	-	2/29/63/63	0/2/2/2
21	CLA	K	203	15	-	4/17/93/115	-
22	LUT	1	615	-	-	1/29/67/67	0/2/2/2
21	CLA	A	840	5	-	19/39/115/115	-
21	CLA	B	805	6	-	18/39/115/115	-
22	LUT	5	619	-	-	2/29/67/67	0/2/2/2
21	CLA	F	304	10	-	2/10/86/115	-
24	BCR	B	844	-	-	4/29/63/63	0/2/2/2
27	LMT	4	319	-	-	4/21/61/61	0/2/2/2
21	CLA	6	613	4	-	5/15/91/115	-
21	CLA	2	602	2	-	14/39/115/115	-
21	CLA	B	824	-	-	4/21/97/115	-
21	CLA	4	309	-	-	11/33/109/115	-
21	CLA	3	611	-	-	4/13/89/115	-
24	BCR	A	846	-	-	3/29/63/63	0/2/2/2
21	CLA	5	603	1	-	5/15/91/115	-
25	LHG	5	618	21	-	7/53/53/53	-
21	CLA	B	820	6	-	11/27/103/115	-
21	CLA	A	814	-	-	5/15/91/115	-
21	CLA	6	609	4	-	4/26/102/115	-
24	BCR	O	201	-	-	3/29/63/63	0/2/2/2
21	CLA	A	808	5	-	8/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	5	608	1	-	5/15/91/115	-
24	BCR	6	618	-	-	2/29/63/63	0/2/2/2
24	BCR	F	305	-	-	2/29/63/63	0/2/2/2
25	LHG	A	851	-	-	8/53/53/53	-
21	CLA	Z	311	25	-	6/15/91/115	-
23	XAT	3	616	-	-	0/31/93/93	0/4/4/4
27	LMT	6	621	-	-	4/21/61/61	0/2/2/2
21	CLA	4	302	4	-	5/15/91/115	-
21	CLA	A	820	5	-	7/15/91/115	-
25	LHG	1	620	-	-	11/53/53/53	-
22	LUT	2	615	-	-	1/29/67/67	0/2/2/2
20	CHL	4	305	-	-	6/15/113/137	-
21	CLA	B	829	6	-	5/13/89/115	-
20	CHL	Z	301	-	-	7/15/113/137	-
21	CLA	6	603	4	-	5/15/91/115	-
21	CLA	B	803	6	-	4/10/86/115	-
21	CLA	A	836	5	-	4/15/91/115	-
22	LUT	F	301	-	-	2/29/67/67	0/2/2/2
21	CLA	B	815	6	-	5/27/103/115	-
21	CLA	3	609	3	-	5/15/91/115	-
21	CLA	B	802	-	-	15/39/115/115	-
21	CLA	A	822	5	-	4/12/88/115	-
21	CLA	Y	614	19	-	6/15/91/115	-
21	CLA	6	610	-	-	5/15/91/115	-
21	CLA	5	605	-	-	2/10/82/115	-
21	CLA	1	614	1	-	8/15/91/115	-
31	NEX	X	616	-	-	2/27/83/83	0/3/3/3
21	CLA	4	311	4	-	12/30/106/115	-
28	PQN	A	844	-	-	6/23/43/43	0/2/2/2
21	CLA	X	610	25	-	9/15/91/115	-
21	CLA	3	607	3	-	7/15/91/115	-
21	CLA	5	607	-	-	3/13/89/115	-
21	CLA	5	611	1	-	7/15/91/115	-
21	CLA	B	830	6	-	2/13/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	5	612	1	-	19/39/115/115	-
20	CHL	2	607	-	-	5/21/119/137	-
21	CLA	L	301	-	-	16/39/115/115	-
29	SF4	C	101	7	-	-	0/6/5/5
21	CLA	L	303	16	-	6/15/91/115	-
21	CLA	1	613	1	-	4/15/91/115	-
20	CHL	Y	601	19	-	6/15/113/137	-
21	CLA	B	837	6	-	5/18/94/115	-
21	CLA	X	618	-	-	7/15/91/115	-
24	BCR	A	848	-	-	4/29/63/63	0/2/2/2
25	LHG	2	617	21	-	10/41/41/53	-
22	LUT	5	615	-	-	2/29/67/67	0/2/2/2
30	DGD	B	849	-	-	7/50/90/95	0/2/2/2
21	CLA	1	603	1	-	6/27/103/115	-
25	LHG	1	618	21	-	5/53/53/53	-
26	LMG	G	206	-	-	12/45/65/70	0/1/1/1
21	CLA	A	834	-	-	12/39/115/115	-
20	CHL	Y	608	-	-	8/15/113/137	-
21	CLA	K	201	15	-	0/4/76/115	-
21	CLA	B	840	25	-	25/39/115/115	-
20	CHL	X	607	-	-	3/15/113/137	-
21	CLA	6	604	-	-	4/15/91/115	-
21	CLA	4	307	4	-	4/15/91/115	-
22	LUT	Y	615	-	-	2/29/67/67	0/2/2/2
31	NEX	Z	316	-	-	5/27/83/83	0/3/3/3
21	CLA	3	612	3	-	2/13/89/115	-
21	CLA	5	609	1	-	8/15/91/115	-
21	CLA	B	814	6	-	9/27/103/115	-
21	CLA	B	808	6	-	7/27/103/115	-
26	LMG	6	619	-	-	10/31/51/70	0/1/1/1
21	CLA	2	610	25	-	2/10/86/115	-
21	CLA	A	841	5	-	16/39/115/115	-
21	CLA	L	305	-	-	6/15/91/115	-
21	CLA	O	207	17	-	1/6/78/115	-
20	CHL	2	614	2	-	2/12/110/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	B	826	6	-	13/33/109/115	-
25	LHG	X	617	21	-	11/41/41/53	-
24	BCR	A	847	-	-	2/29/63/63	0/2/2/2
21	CLA	A	835	5	-	3/15/91/115	-
20	CHL	Y	605	-	-	5/10/108/137	-
22	LUT	6	616	-	-	1/29/67/67	0/2/2/2
22	LUT	Z	315	-	-	4/29/67/67	0/2/2/2
20	CHL	Y	607	-	-	9/15/113/137	-
21	CLA	A	809	5	-	5/27/103/115	-
24	BCR	O	204	-	-	4/29/63/63	0/2/2/2
21	CLA	O	203	-	-	15/36/112/115	-
21	CLA	B	817	6	-	20/33/109/115	-
20	CHL	Y	609	19	-	4/15/113/137	-
21	CLA	5	610	25	-	3/15/91/115	-
21	CLA	2	603	2	-	3/13/89/115	-
24	BCR	L	306	-	-	4/29/63/63	0/2/2/2
20	CHL	Y	619	-	-	7/17/115/137	-
22	LUT	Z	314	-	-	2/29/67/67	0/2/2/2
21	CLA	Y	603	-	-	6/15/91/115	-
25	LHG	Y	618	21	-	9/39/39/53	-
21	CLA	Z	304	-	-	11/15/91/115	-
21	CLA	A	815	5	-	5/12/88/115	-
21	CLA	A	828	-	-	13/39/115/115	-
24	BCR	J	103	-	-	2/29/63/63	0/2/2/2
21	CLA	A	801	5	-	19/39/115/115	-
21	CLA	3	617	5	-	14/27/103/115	-
21	CLA	B	831	6	-	12/39/115/115	-
24	BCR	G	205	-	-	0/29/63/63	0/2/2/2
21	CLA	Z	303	18	-	19/33/109/115	-
20	CHL	1	601	1	-	7/25/123/137	-
21	CLA	B	801	-	-	13/39/115/115	-
21	CLA	J	101	-	-	0/12/88/115	-
21	CLA	B	819	6	-	7/21/97/115	-
25	LHG	1	622	21	-	4/42/42/53	-
28	PQN	B	841	-	-	8/23/43/43	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	6	611	-	-	0/10/86/115	-
21	CLA	A	819	5	-	18/39/115/115	-
21	CLA	B	810	6	-	9/25/101/115	-
21	CLA	Y	604	-	-	9/15/91/115	-
21	CLA	1	604	-	-	5/20/96/115	-
26	LMG	4	318	-	-	9/31/51/70	0/1/1/1
29	SF4	C	102	7	-	-	0/6/5/5
21	CLA	A	827	5	-	14/39/115/115	-
21	CLA	H	201	12	-	15/33/109/115	-
22	LUT	Y	616	-	-	0/29/67/67	0/2/2/2
25	LHG	Z	317	21	-	3/36/36/53	-
21	CLA	B	833	6	-	6/33/109/115	-
22	LUT	4	315	-	-	1/29/67/67	0/2/2/2
21	CLA	Y	602	19	-	28/39/115/115	-
20	CHL	5	601	1	-	5/25/123/137	-
26	LMG	B	850	-	-	12/47/67/70	0/1/1/1
21	CLA	2	604	-	-	17/39/115/115	-
21	CLA	2	608	2	-	6/15/91/115	-
21	CLA	1	610	25	-	6/27/103/115	-
21	CLA	A	837	5	-	8/23/99/115	-
21	CLA	G	204	11	-	7/15/91/115	-
21	CLA	B	827	6	-	18/39/115/115	-
23	XAT	4	316	-	-	0/31/93/93	0/4/4/4
21	CLA	Z	312	-	-	8/15/91/115	-
21	CLA	X	612	18	-	6/15/91/115	-
24	BCR	A	845	-	-	4/29/63/63	0/2/2/2
20	CHL	Z	308	-	-	5/10/108/137	-
20	CHL	5	606	1	-	1/8/106/137	-
21	CLA	A	831	5	-	5/21/97/115	-
24	BCR	O	205	-	-	2/29/63/63	0/2/2/2
21	CLA	5	613	1	-	2/15/91/115	-
27	LMT	F	303	-	-	6/21/61/61	0/2/2/2
21	CLA	B	832	-	-	3/15/91/115	-
26	LMG	F	307	-	-	3/25/45/70	0/1/1/1
21	CLA	4	303	-	-	5/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	X	603	-	-	12/25/101/115	-
24	BCR	B	847	-	-	0/29/63/63	0/2/2/2
21	CLA	X	604	-	-	7/15/91/115	-
20	CHL	Z	307	-	-	8/15/113/137	-
21	CLA	2	613	-	-	2/13/89/115	-
21	CLA	6	602	4	-	9/33/109/115	-
21	CLA	A	826	-	-	16/39/115/115	-
21	CLA	Y	613	19	-	8/27/103/115	-
23	XAT	6	617	-	-	0/31/93/93	0/4/4/4
24	BCR	B	845	-	-	0/29/63/63	0/2/2/2
21	CLA	A	839	5	-	4/21/97/115	-
20	CHL	6	606	-	-	8/15/113/137	-
24	BCR	6	620	-	-	11/29/63/63	0/2/2/2
21	CLA	B	836	6	-	11/39/115/115	-
21	CLA	B	828	6	-	13/29/105/115	-
21	CLA	A	829	5	-	16/39/115/115	-
21	CLA	A	813	5	-	22/39/115/115	-
21	CLA	K	202	-	-	3/15/91/115	-
21	CLA	1	605	-	-	3/10/82/115	-
21	CLA	2	609	2	-	8/27/103/115	-
20	CHL	4	304	-	-	14/27/125/137	-
21	CLA	O	206	-	-	7/20/96/115	-
22	LUT	3	615	-	-	2/29/67/67	0/2/2/2
21	CLA	1	608	1	-	17/39/115/115	-
23	XAT	2	616	-	-	0/31/93/93	0/4/4/4
21	CLA	A	804	5	-	12/27/103/115	-
21	CLA	B	812	6	-	19/39/115/115	-
20	CHL	6	615	4	-	0/10/106/137	-
21	CLA	5	614	1	-	9/15/91/115	-
21	CLA	A	817	5	-	16/33/109/115	-
21	CLA	1	611	1	-	4/15/91/115	-
21	CLA	A	802	-	-	9/39/115/115	-
20	CHL	Z	302	18	-	7/15/113/137	-
21	CLA	X	602	18	-	8/15/91/115	-
21	CLA	X	613	18	-	7/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	B	807	-	-	14/39/115/115	-
20	CHL	1	606	1	-	2/8/106/137	-
24	BCR	3	601	-	-	0/29/63/63	0/2/2/2
20	CHL	6	607	-	-	8/21/119/137	-
20	CHL	2	601	2	-	4/17/115/137	-
21	CLA	3	606	-	-	4/10/86/115	-
21	CLA	B	816	-	-	17/32/108/115	-
20	CHL	3	608	-	-	7/17/115/137	-
23	XAT	1	616	-	-	0/31/93/93	0/4/4/4
21	CLA	G	203	11	-	4/12/88/115	-
24	BCR	B	842	-	-	0/29/63/63	0/2/2/2
21	CLA	K	204	15	-	2/8/80/115	-
21	CLA	3	605	-	-	6/18/94/115	-
21	CLA	Y	611	25	-	2/15/91/115	-
21	CLA	B	823	-	-	21/39/115/115	-
21	CLA	B	818	-	-	12/27/103/115	-
21	CLA	B	806	6	-	5/24/100/115	-
21	CLA	6	601	4	-	6/17/93/115	-
21	CLA	4	301	4	-	6/33/109/115	-
27	LMT	G	201	-	-	2/21/61/61	0/2/2/2
26	LMG	5	621	-	-	7/44/64/70	0/1/1/1
21	CLA	6	612	4	-	12/30/106/115	-
24	BCR	K	205	-	-	4/29/63/63	0/2/2/2
21	CLA	5	604	-	-	6/20/96/115	-
21	CLA	A	812	5	-	10/26/102/115	-
21	CLA	3	603	3	-	12/27/103/115	-
21	CLA	5	602	1	-	14/35/111/115	-
21	CLA	A	811	5	-	12/39/115/115	-
22	LUT	X	614	-	-	0/29/67/67	0/2/2/2
21	CLA	A	823	-	-	1/10/86/115	-
22	LUT	X	615	-	-	3/29/67/67	0/2/2/2
21	CLA	1	609	1	-	7/31/107/115	-
21	CLA	A	818	5	-	15/32/108/115	-
20	CHL	6	605	-	-	10/27/125/137	-
20	CHL	X	601	18	-	9/15/113/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	A	843	-	-	12/30/106/115	-
21	CLA	A	806	5	-	22/39/115/115	-
27	LMT	A	852	-	-	4/21/61/61	0/2/2/2
24	BCR	1	617	-	-	0/29/63/63	0/2/2/2

All (2136) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	Y	606	CHL	C3B-C4B	7.20	1.47	1.41
20	X	605	CHL	CMC-C2C	7.19	1.56	1.44
20	X	607	CHL	CMC-C2C	7.19	1.56	1.44
20	5	606	CHL	CMC-C2C	7.17	1.56	1.44
20	X	606	CHL	CMC-C2C	7.16	1.56	1.44
20	Y	607	CHL	CMC-C2C	7.16	1.56	1.44
20	Y	605	CHL	CMC-C2C	7.15	1.56	1.44
20	X	601	CHL	CMC-C2C	7.15	1.56	1.44
20	Z	302	CHL	CMC-C2C	7.14	1.56	1.44
20	X	608	CHL	CMC-C2C	7.12	1.56	1.44
20	Y	606	CHL	CMC-C2C	7.11	1.56	1.44
20	Y	609	CHL	CMC-C2C	7.10	1.56	1.44
20	2	605	CHL	CMC-C2C	7.08	1.56	1.44
20	Z	307	CHL	C3B-C4B	7.07	1.47	1.41
20	2	614	CHL	CMC-C2C	7.07	1.56	1.44
20	6	606	CHL	CMC-C2C	7.06	1.56	1.44
20	X	605	CHL	C3B-C4B	7.06	1.47	1.41
20	Z	301	CHL	CMC-C2C	7.05	1.56	1.44
20	Z	307	CHL	CMC-C2C	7.04	1.56	1.44
20	5	601	CHL	CMC-C2C	7.04	1.56	1.44
20	X	607	CHL	C3B-C4B	7.03	1.47	1.41
20	Z	308	CHL	CMC-C2C	7.01	1.56	1.44
20	1	606	CHL	CMC-C2C	7.01	1.56	1.44
20	Y	619	CHL	CMC-C2C	7.01	1.56	1.44
20	2	606	CHL	CMC-C2C	7.01	1.56	1.44
20	Z	309	CHL	CMC-C2C	7.00	1.56	1.44
20	6	615	CHL	CMC-C2C	7.00	1.56	1.44
20	6	605	CHL	CMC-C2C	6.99	1.56	1.44
20	Y	607	CHL	C3B-C4B	6.99	1.46	1.41
20	Y	601	CHL	CMC-C2C	6.99	1.56	1.44
20	Y	619	CHL	C3B-C4B	6.97	1.46	1.41
20	2	601	CHL	CMC-C2C	6.96	1.56	1.44
20	Y	608	CHL	CMC-C2C	6.96	1.56	1.44
20	1	601	CHL	CMC-C2C	6.96	1.56	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	6	607	CHL	CMC-C2C	6.94	1.56	1.44
20	4	305	CHL	CMC-C2C	6.93	1.56	1.44
20	Z	306	CHL	CMC-C2C	6.93	1.56	1.44
20	3	608	CHL	CMC-C2C	6.91	1.56	1.44
20	4	304	CHL	CMC-C2C	6.91	1.56	1.44
20	4	305	CHL	C3B-C4B	6.91	1.46	1.41
20	2	607	CHL	CMC-C2C	6.90	1.56	1.44
20	Y	609	CHL	C3B-C4B	6.86	1.46	1.41
20	4	306	CHL	CMC-C2C	6.85	1.56	1.44
20	4	314	CHL	CMC-C2C	6.84	1.56	1.44
20	2	605	CHL	C3B-C4B	6.82	1.46	1.41
20	2	614	CHL	C3B-C4B	6.80	1.46	1.41
20	6	605	CHL	C3B-C4B	6.77	1.46	1.41
20	5	606	CHL	C3B-C4B	6.76	1.46	1.41
20	2	601	CHL	C3B-C4B	6.74	1.46	1.41
20	X	608	CHL	C3B-C4B	6.73	1.46	1.41
20	4	304	CHL	C3B-C4B	6.72	1.46	1.41
20	Z	302	CHL	C3B-C4B	6.71	1.46	1.41
20	Z	308	CHL	C3B-C4B	6.70	1.46	1.41
20	X	601	CHL	C3B-C4B	6.69	1.46	1.41
20	Y	605	CHL	C3B-C4B	6.68	1.46	1.41
20	Y	608	CHL	C3B-C4B	6.68	1.46	1.41
20	Z	309	CHL	C3B-C4B	6.64	1.46	1.41
20	2	606	CHL	C3B-C4B	6.63	1.46	1.41
20	Z	301	CHL	C3B-C4B	6.62	1.46	1.41
20	X	606	CHL	C3B-C4B	6.60	1.46	1.41
20	5	601	CHL	C3B-C4B	6.55	1.46	1.41
20	6	606	CHL	C3B-C4B	6.54	1.46	1.41
20	Z	306	CHL	C3B-C4B	6.54	1.46	1.41
20	Y	601	CHL	C3B-C4B	6.48	1.46	1.41
20	1	606	CHL	C3B-C4B	6.47	1.46	1.41
20	6	607	CHL	C3B-C4B	6.43	1.46	1.41
20	3	608	CHL	C3B-C4B	6.42	1.46	1.41
20	1	601	CHL	C3B-C4B	6.28	1.46	1.41
20	2	607	CHL	C3B-C4B	6.25	1.46	1.41
20	4	306	CHL	C3B-C4B	6.17	1.46	1.41
20	6	615	CHL	C4B-C3B	5.88	1.46	1.39
20	4	314	CHL	C4B-C3B	5.65	1.46	1.39
21	Y	612	CLA	MG-NA	5.04	2.18	2.06
21	2	611	CLA	MG-NA	5.02	2.18	2.06
21	3	611	CLA	MG-NA	5.00	2.18	2.06
21	3	605	CLA	MG-NA	5.00	2.18	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	3	603	CLA	MG-NA	5.00	2.18	2.06
21	B	804	CLA	MG-NA	4.99	2.18	2.06
21	1	610	CLA	MG-NA	4.99	2.18	2.06
21	X	611	CLA	MG-NA	4.98	2.18	2.06
21	J	102	CLA	MG-NA	4.98	2.18	2.06
21	O	202	CLA	MG-NA	4.98	2.18	2.06
21	Z	311	CLA	MG-NA	4.98	2.18	2.06
21	G	204	CLA	MG-NA	4.97	2.18	2.06
21	Y	604	CLA	MG-NA	4.97	2.18	2.06
21	4	313	CLA	MG-NA	4.97	2.18	2.06
21	6	603	CLA	MG-NA	4.97	2.18	2.06
21	4	302	CLA	MG-NA	4.97	2.18	2.06
21	5	604	CLA	MG-NA	4.97	2.18	2.06
21	B	808	CLA	MG-NA	4.97	2.18	2.06
21	A	815	CLA	MG-NA	4.96	2.18	2.06
21	Y	602	CLA	MG-NA	4.96	2.18	2.06
21	4	307	CLA	MG-NA	4.96	2.18	2.06
21	A	808	CLA	MG-NA	4.95	2.18	2.06
21	A	811	CLA	MG-NA	4.95	2.18	2.06
21	O	203	CLA	MG-NA	4.95	2.18	2.06
21	2	610	CLA	MG-NA	4.95	2.18	2.06
21	1	605	CLA	MG-NA	4.95	2.18	2.06
21	Y	611	CLA	MG-NA	4.95	2.18	2.06
21	B	839	CLA	MG-NA	4.94	2.18	2.06
21	G	202	CLA	MG-NA	4.94	2.18	2.06
21	5	613	CLA	MG-NA	4.94	2.18	2.06
21	A	839	CLA	MG-NA	4.94	2.18	2.06
21	J	101	CLA	MG-NA	4.94	2.18	2.06
21	Z	313	CLA	MG-NA	4.94	2.18	2.06
21	B	834	CLA	MG-NA	4.94	2.18	2.06
21	A	834	CLA	MG-NA	4.94	2.18	2.06
21	4	310	CLA	MG-NA	4.94	2.18	2.06
21	X	618	CLA	MG-NA	4.94	2.18	2.06
21	3	602	CLA	MG-NA	4.94	2.18	2.06
21	6	612	CLA	MG-NA	4.94	2.18	2.06
21	L	305	CLA	MG-NA	4.93	2.18	2.06
21	X	603	CLA	MG-NA	4.93	2.18	2.06
21	A	817	CLA	MG-NA	4.93	2.18	2.06
21	B	838	CLA	MG-NA	4.93	2.18	2.06
21	5	605	CLA	MG-NA	4.93	2.18	2.06
21	B	819	CLA	MG-NA	4.93	2.18	2.06
21	B	831	CLA	MG-NA	4.93	2.18	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	827	CLA	MG-NA	4.92	2.18	2.06
21	Z	305	CLA	MG-NA	4.92	2.18	2.06
21	6	611	CLA	MG-NA	4.92	2.18	2.06
21	K	204	CLA	MG-NA	4.92	2.18	2.06
21	B	818	CLA	MG-NA	4.92	2.18	2.06
21	5	611	CLA	MG-NA	4.92	2.18	2.06
21	2	613	CLA	MG-NA	4.92	2.18	2.06
21	3	610	CLA	MG-NA	4.92	2.18	2.06
21	A	838	CLA	MG-NA	4.92	2.18	2.06
21	A	829	CLA	MG-NA	4.92	2.18	2.06
21	A	843	CLA	MG-NA	4.92	2.18	2.06
21	A	807	CLA	MG-NA	4.92	2.17	2.06
21	A	816	CLA	MG-NA	4.92	2.17	2.06
21	Y	614	CLA	MG-NA	4.92	2.17	2.06
21	A	825	CLA	MG-NA	4.92	2.17	2.06
21	L	303	CLA	MG-NA	4.92	2.17	2.06
21	3	613	CLA	MG-NA	4.91	2.17	2.06
21	2	612	CLA	MG-NA	4.91	2.17	2.06
21	3	617	CLA	MG-NA	4.91	2.17	2.06
21	6	608	CLA	MG-NA	4.91	2.17	2.06
21	X	613	CLA	MG-NA	4.91	2.17	2.06
21	6	602	CLA	MG-NA	4.91	2.17	2.06
21	B	814	CLA	MG-NA	4.91	2.17	2.06
21	Z	312	CLA	MG-NA	4.91	2.17	2.06
21	1	611	CLA	MG-NA	4.91	2.17	2.06
21	X	602	CLA	MG-NA	4.91	2.17	2.06
21	X	612	CLA	MG-NA	4.91	2.17	2.06
21	B	810	CLA	MG-NA	4.91	2.17	2.06
21	B	835	CLA	MG-NA	4.91	2.17	2.06
21	L	301	CLA	MG-NA	4.91	2.17	2.06
21	F	304	CLA	MG-NA	4.90	2.17	2.06
21	A	804	CLA	MG-NA	4.90	2.17	2.06
21	B	815	CLA	MG-NA	4.90	2.17	2.06
21	Y	613	CLA	MG-NA	4.90	2.17	2.06
21	6	613	CLA	MG-NA	4.90	2.17	2.06
21	4	301	CLA	MG-NA	4.90	2.17	2.06
21	1	612	CLA	MG-NA	4.90	2.17	2.06
21	X	604	CLA	MG-NA	4.90	2.17	2.06
21	3	607	CLA	MG-NA	4.90	2.17	2.06
21	2	603	CLA	MG-NA	4.90	2.17	2.06
21	B	833	CLA	MG-NA	4.89	2.17	2.06
21	L	304	CLA	MG-NA	4.89	2.17	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	602	CLA	MG-NA	4.89	2.17	2.06
21	B	807	CLA	MG-NA	4.89	2.17	2.06
21	A	841	CLA	MG-NA	4.89	2.17	2.06
21	1	602	CLA	MG-NA	4.89	2.17	2.06
21	6	604	CLA	MG-NA	4.89	2.17	2.06
21	A	842	CLA	MG-NA	4.89	2.17	2.06
21	B	840	CLA	MG-NA	4.89	2.17	2.06
21	3	612	CLA	MG-NA	4.89	2.17	2.06
21	5	603	CLA	MG-NA	4.89	2.17	2.06
21	6	610	CLA	MG-NA	4.89	2.17	2.06
21	6	614	CLA	MG-NA	4.89	2.17	2.06
21	B	825	CLA	MG-NA	4.89	2.17	2.06
21	X	610	CLA	MG-NA	4.88	2.17	2.06
21	B	821	CLA	MG-NA	4.88	2.17	2.06
21	3	609	CLA	MG-NA	4.88	2.17	2.06
21	B	806	CLA	MG-NA	4.88	2.17	2.06
21	B	805	CLA	MG-NA	4.88	2.17	2.06
21	A	801	CLA	MG-NA	4.88	2.17	2.06
21	3	614	CLA	MG-NA	4.88	2.17	2.06
21	A	809	CLA	MG-NA	4.88	2.17	2.06
21	A	812	CLA	MG-NA	4.88	2.17	2.06
21	6	601	CLA	MG-NA	4.88	2.17	2.06
21	3	606	CLA	MG-NA	4.88	2.17	2.06
21	A	821	CLA	MG-NA	4.88	2.17	2.06
21	5	609	CLA	MG-NA	4.87	2.17	2.06
21	B	812	CLA	MG-NA	4.87	2.17	2.06
21	2	604	CLA	MG-NA	4.87	2.17	2.06
21	4	311	CLA	MG-NA	4.87	2.17	2.06
21	Z	310	CLA	MG-NA	4.87	2.17	2.06
21	A	802	CLA	MG-NA	4.87	2.17	2.06
21	K	201	CLA	MG-NA	4.87	2.17	2.06
21	A	833	CLA	MG-NA	4.87	2.17	2.06
21	A	830	CLA	MG-NA	4.87	2.17	2.06
21	B	828	CLA	MG-NA	4.87	2.17	2.06
21	A	823	CLA	MG-NA	4.87	2.17	2.06
21	1	603	CLA	MG-NA	4.86	2.17	2.06
21	B	823	CLA	MG-NA	4.86	2.17	2.06
21	Y	610	CLA	MG-NA	4.86	2.17	2.06
21	Z	304	CLA	MG-NA	4.86	2.17	2.06
21	A	810	CLA	MG-NA	4.86	2.17	2.06
21	O	207	CLA	MG-NA	4.86	2.17	2.06
21	Y	603	CLA	MG-NA	4.86	2.17	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	830	CLA	MG-NA	4.86	2.17	2.06
21	K	202	CLA	MG-NA	4.86	2.17	2.06
21	4	309	CLA	MG-NA	4.85	2.17	2.06
21	A	824	CLA	MG-NA	4.85	2.17	2.06
21	3	604	CLA	MG-NA	4.85	2.17	2.06
21	B	837	CLA	MG-NA	4.85	2.17	2.06
21	K	203	CLA	MG-NA	4.85	2.17	2.06
21	5	612	CLA	MG-NA	4.85	2.17	2.06
21	A	806	CLA	MG-NA	4.84	2.17	2.06
21	B	832	CLA	MG-NA	4.84	2.17	2.06
21	2	618	CLA	MG-NA	4.84	2.17	2.06
21	5	610	CLA	MG-NA	4.84	2.17	2.06
21	A	813	CLA	MG-NA	4.84	2.17	2.06
21	A	820	CLA	MG-NA	4.84	2.17	2.06
20	X	608	CHL	C1D-C2D	4.84	1.45	1.39
21	A	831	CLA	MG-NA	4.84	2.17	2.06
21	1	614	CLA	MG-NA	4.84	2.17	2.06
21	G	203	CLA	MG-NA	4.84	2.17	2.06
21	5	602	CLA	MG-NA	4.84	2.17	2.06
21	A	837	CLA	MG-NA	4.83	2.17	2.06
21	B	802	CLA	MG-NA	4.83	2.17	2.06
21	B	829	CLA	MG-NA	4.83	2.17	2.06
21	2	608	CLA	MG-NA	4.83	2.17	2.06
21	A	826	CLA	MG-NA	4.83	2.17	2.06
21	B	836	CLA	MG-NA	4.83	2.17	2.06
21	A	814	CLA	MG-NA	4.82	2.17	2.06
21	A	819	CLA	MG-NA	4.82	2.17	2.06
21	B	820	CLA	MG-NA	4.82	2.17	2.06
21	A	836	CLA	MG-NA	4.82	2.17	2.06
21	B	817	CLA	MG-NA	4.82	2.17	2.06
21	B	822	CLA	MG-NA	4.82	2.17	2.06
21	4	312	CLA	MG-NA	4.82	2.17	2.06
21	B	801	CLA	MG-NA	4.82	2.17	2.06
21	4	303	CLA	MG-NA	4.81	2.17	2.06
21	B	809	CLA	MG-NA	4.81	2.17	2.06
21	6	609	CLA	MG-NA	4.81	2.17	2.06
21	A	835	CLA	MG-NA	4.81	2.17	2.06
21	1	609	CLA	MG-NA	4.81	2.17	2.06
21	A	828	CLA	MG-NA	4.81	2.17	2.06
21	B	811	CLA	MG-NA	4.81	2.17	2.06
21	1	607	CLA	MG-NA	4.80	2.17	2.06
21	1	604	CLA	MG-NA	4.80	2.17	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	832	CLA	MG-NA	4.80	2.17	2.06
21	2	609	CLA	MG-NA	4.80	2.17	2.06
21	1	608	CLA	MG-NA	4.80	2.17	2.06
21	5	607	CLA	MG-NA	4.80	2.17	2.06
21	1	613	CLA	MG-NA	4.79	2.17	2.06
21	5	614	CLA	MG-NA	4.79	2.17	2.06
21	4	308	CLA	MG-NA	4.79	2.17	2.06
21	B	813	CLA	MG-NA	4.79	2.17	2.06
21	B	826	CLA	MG-NA	4.79	2.17	2.06
21	A	840	CLA	MG-NA	4.79	2.17	2.06
21	H	201	CLA	MG-NA	4.79	2.17	2.06
21	A	827	CLA	MG-NA	4.79	2.17	2.06
20	Z	307	CHL	C1D-C2D	4.79	1.45	1.39
21	O	206	CLA	MG-NA	4.78	2.17	2.06
21	A	822	CLA	MG-NA	4.78	2.17	2.06
21	A	818	CLA	MG-NA	4.78	2.17	2.06
20	X	605	CHL	C1D-C2D	4.77	1.45	1.39
20	Z	302	CHL	C1D-C2D	4.77	1.45	1.39
21	X	609	CLA	MG-NA	4.77	2.17	2.06
21	Z	303	CLA	MG-NA	4.77	2.17	2.06
20	X	606	CHL	C1D-C2D	4.76	1.45	1.39
21	B	816	CLA	MG-NA	4.74	2.17	2.06
21	B	824	CLA	MG-NA	4.74	2.17	2.06
21	A	805	CLA	MG-NA	4.74	2.17	2.06
21	B	803	CLA	MG-NA	4.73	2.17	2.06
20	X	607	CHL	C1D-C2D	4.72	1.45	1.39
21	5	608	CLA	MG-NA	4.72	2.17	2.06
20	Y	608	CHL	C1D-C2D	4.71	1.45	1.39
21	A	803	CLA	MG-NA	4.71	2.17	2.06
20	X	607	CHL	C1C-NC	4.71	1.39	1.35
20	Y	605	CHL	C1C-NC	4.70	1.39	1.35
20	Z	301	CHL	C1D-C2D	4.70	1.45	1.39
20	Y	606	CHL	C1C-NC	4.70	1.39	1.35
20	5	606	CHL	C1D-C2D	4.70	1.45	1.39
20	2	605	CHL	C1D-C2D	4.68	1.45	1.39
20	Y	607	CHL	C1D-C2D	4.68	1.45	1.39
20	Y	605	CHL	C1D-C2D	4.67	1.45	1.39
20	5	606	CHL	C1C-NC	4.66	1.39	1.35
20	Z	302	CHL	C1C-NC	4.65	1.39	1.35
20	Y	619	CHL	C1D-C2D	4.65	1.45	1.39
20	X	605	CHL	C1C-NC	4.65	1.39	1.35
20	Y	609	CHL	C1D-C2D	4.64	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	2	607	CHL	C1D-C2D	4.64	1.45	1.39
20	Z	301	CHL	C1C-NC	4.63	1.39	1.35
20	Z	308	CHL	C1D-C2D	4.62	1.45	1.39
20	3	608	CHL	C1C-NC	4.62	1.39	1.35
20	Y	606	CHL	C1D-C2D	4.61	1.45	1.39
20	4	314	CHL	C1C-NC	4.61	1.39	1.35
20	Z	306	CHL	C1D-C2D	4.60	1.45	1.39
20	X	601	CHL	C1D-C2D	4.59	1.45	1.39
20	Y	607	CHL	C1C-NC	4.59	1.39	1.35
20	X	606	CHL	C1C-NC	4.58	1.39	1.35
20	6	605	CHL	C1D-C2D	4.57	1.45	1.39
20	2	601	CHL	C1D-C2D	4.57	1.45	1.39
20	3	608	CHL	C1D-C2D	4.56	1.45	1.39
20	1	601	CHL	C1C-NC	4.56	1.39	1.35
20	6	615	CHL	C1D-C2D	4.56	1.45	1.39
20	5	601	CHL	C1D-C2D	4.55	1.45	1.39
20	2	614	CHL	C1D-C2D	4.54	1.45	1.39
20	2	606	CHL	C1D-C2D	4.54	1.45	1.39
20	X	601	CHL	C1C-NC	4.54	1.39	1.35
20	6	615	CHL	C1C-NC	4.53	1.39	1.35
20	4	314	CHL	C1D-C2D	4.53	1.45	1.39
20	6	606	CHL	C1D-C2D	4.50	1.45	1.39
20	Y	619	CHL	C1C-NC	4.50	1.39	1.35
20	Z	309	CHL	C1D-C2D	4.49	1.45	1.39
20	X	608	CHL	C1B-C2B	4.49	1.45	1.39
20	Y	609	CHL	C1C-NC	4.49	1.39	1.35
20	5	601	CHL	C1C-NC	4.49	1.39	1.35
20	Z	308	CHL	C1C-NC	4.48	1.39	1.35
20	4	304	CHL	C1D-C2D	4.48	1.45	1.39
20	X	606	CHL	C1B-C2B	4.47	1.45	1.39
20	2	601	CHL	C1C-NC	4.47	1.39	1.35
20	4	306	CHL	C1C-NC	4.46	1.39	1.35
22	Z	315	LUT	C34-C33	4.44	1.41	1.35
20	Z	308	CHL	C1B-C2B	4.43	1.44	1.39
20	Z	302	CHL	C1B-C2B	4.42	1.44	1.39
20	X	601	CHL	C1B-C2B	4.42	1.44	1.39
20	X	605	CHL	C1B-C2B	4.41	1.44	1.39
20	5	601	CHL	C1B-C2B	4.41	1.44	1.39
20	Z	307	CHL	C1C-NC	4.40	1.39	1.35
20	5	606	CHL	C1B-C2B	4.39	1.44	1.39
20	6	607	CHL	C1D-C2D	4.39	1.44	1.39
20	2	605	CHL	C1C-NC	4.39	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	2	614	CHL	C1C-NC	4.39	1.39	1.35
20	6	615	CHL	C1B-C2B	4.38	1.44	1.39
20	4	305	CHL	C1D-C2D	4.38	1.44	1.39
20	1	606	CHL	C1C-NC	4.38	1.39	1.35
20	Y	605	CHL	C1B-C2B	4.38	1.44	1.39
20	6	607	CHL	C1B-C2B	4.37	1.44	1.39
20	2	606	CHL	C1C-NC	4.37	1.39	1.35
20	Y	607	CHL	C1B-C2B	4.37	1.44	1.39
20	Y	608	CHL	C1B-C2B	4.36	1.44	1.39
20	Y	609	CHL	C1B-C2B	4.36	1.44	1.39
20	Y	601	CHL	C1D-C2D	4.36	1.44	1.39
20	Z	306	CHL	C1C-NC	4.36	1.39	1.35
20	6	607	CHL	C1C-NC	4.35	1.39	1.35
20	Y	608	CHL	C1C-NC	4.35	1.39	1.35
20	X	607	CHL	C1B-C2B	4.35	1.44	1.39
20	1	606	CHL	C1D-C2D	4.35	1.44	1.39
20	4	306	CHL	C1D-C2D	4.35	1.44	1.39
20	X	608	CHL	C1C-NC	4.35	1.39	1.35
20	Y	601	CHL	C1C-NC	4.34	1.39	1.35
20	Z	301	CHL	C1B-C2B	4.34	1.44	1.39
20	2	607	CHL	C1C-NC	4.34	1.39	1.35
20	1	601	CHL	C1D-C2D	4.33	1.44	1.39
20	3	608	CHL	C1B-C2B	4.32	1.44	1.39
20	6	606	CHL	C1B-C2B	4.32	1.44	1.39
20	Y	606	CHL	C1B-C2B	4.31	1.44	1.39
22	Z	315	LUT	C10-C9	4.31	1.41	1.35
20	6	605	CHL	C1B-C2B	4.31	1.44	1.39
22	Z	315	LUT	C14-C13	4.31	1.41	1.35
22	Z	315	LUT	C30-C29	4.30	1.41	1.35
20	4	314	CHL	C1B-C2B	4.30	1.44	1.39
20	Y	601	CHL	C1B-C2B	4.30	1.44	1.39
20	Z	306	CHL	C1B-C2B	4.29	1.44	1.39
20	6	606	CHL	C1C-NC	4.28	1.39	1.35
20	Z	309	CHL	C1C-NC	4.27	1.39	1.35
20	Y	619	CHL	C1B-C2B	4.27	1.44	1.39
20	2	614	CHL	C1B-C2B	4.26	1.44	1.39
20	2	606	CHL	C1B-C2B	4.26	1.44	1.39
20	Z	307	CHL	C1B-C2B	4.26	1.44	1.39
20	1	606	CHL	C1B-C2B	4.25	1.44	1.39
20	6	605	CHL	C1C-NC	4.22	1.39	1.35
20	Z	309	CHL	C1B-C2B	4.20	1.44	1.39
20	2	607	CHL	C1B-C2B	4.20	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	601	CHL	C1B-C2B	4.20	1.44	1.39
20	2	605	CHL	C1B-C2B	4.19	1.44	1.39
20	4	305	CHL	C1B-C2B	4.19	1.44	1.39
22	X	614	LUT	C30-C29	4.19	1.41	1.35
20	2	601	CHL	C1B-C2B	4.19	1.44	1.39
20	4	304	CHL	C1C-NC	4.17	1.38	1.35
20	4	304	CHL	C1B-C2B	4.16	1.44	1.39
22	X	614	LUT	C34-C33	4.15	1.41	1.35
22	X	614	LUT	C14-C13	4.12	1.41	1.35
22	X	615	LUT	C14-C13	4.09	1.41	1.35
22	X	615	LUT	C30-C29	4.08	1.41	1.35
22	X	615	LUT	C34-C33	4.06	1.41	1.35
22	X	614	LUT	C10-C9	4.05	1.41	1.35
22	5	615	LUT	C30-C29	4.05	1.41	1.35
22	4	315	LUT	C34-C33	4.04	1.41	1.35
22	5	615	LUT	C14-C13	4.04	1.41	1.35
22	F	301	LUT	C34-C33	4.03	1.41	1.35
20	4	305	CHL	C1C-NC	4.01	1.38	1.35
22	Y	616	LUT	C34-C33	4.01	1.41	1.35
22	1	615	LUT	C34-C33	3.99	1.41	1.35
20	4	306	CHL	C1B-C2B	3.98	1.44	1.39
22	Y	616	LUT	C14-C13	3.98	1.41	1.35
22	Y	615	LUT	C10-C9	3.98	1.41	1.35
22	5	615	LUT	C34-C33	3.98	1.41	1.35
22	5	615	LUT	C10-C9	3.97	1.41	1.35
22	2	615	LUT	C34-C33	3.97	1.41	1.35
22	4	315	LUT	C14-C13	3.96	1.41	1.35
22	5	619	LUT	C14-C13	3.95	1.41	1.35
22	6	616	LUT	C10-C9	3.95	1.41	1.35
22	Y	615	LUT	C34-C33	3.94	1.41	1.35
22	6	616	LUT	C14-C13	3.93	1.41	1.35
22	Y	616	LUT	C30-C29	3.92	1.41	1.35
22	6	616	LUT	C34-C33	3.91	1.41	1.35
22	X	615	LUT	C10-C9	3.91	1.41	1.35
22	Y	615	LUT	C30-C29	3.91	1.41	1.35
22	F	301	LUT	C30-C29	3.90	1.40	1.35
22	3	615	LUT	C14-C13	3.89	1.40	1.35
22	Y	615	LUT	C14-C13	3.89	1.40	1.35
22	2	615	LUT	C30-C29	3.89	1.40	1.35
22	5	619	LUT	C34-C33	3.89	1.40	1.35
22	2	615	LUT	C14-C13	3.89	1.40	1.35
22	F	301	LUT	C10-C9	3.89	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	4	306	CHL	C3B-C2B	-3.88	1.35	1.40
20	4	314	CHL	CAB-C3B	-3.88	1.43	1.51
22	3	615	LUT	C30-C29	3.87	1.40	1.35
22	Z	314	LUT	C34-C33	3.87	1.40	1.35
22	5	619	LUT	C30-C29	3.86	1.40	1.35
22	1	615	LUT	C30-C29	3.85	1.40	1.35
22	4	315	LUT	C30-C29	3.85	1.40	1.35
22	1	615	LUT	C14-C13	3.85	1.40	1.35
22	Y	616	LUT	C10-C9	3.85	1.40	1.35
22	6	616	LUT	C30-C29	3.85	1.40	1.35
22	Z	314	LUT	C30-C29	3.84	1.40	1.35
22	5	619	LUT	C10-C9	3.84	1.40	1.35
22	Z	314	LUT	C14-C13	3.81	1.40	1.35
22	2	615	LUT	C10-C9	3.81	1.40	1.35
20	X	605	CHL	C4C-NC	3.81	1.38	1.35
20	Z	308	CHL	C4C-NC	3.81	1.38	1.35
22	4	315	LUT	C10-C9	3.80	1.40	1.35
22	F	301	LUT	C14-C13	3.80	1.40	1.35
20	6	615	CHL	CAB-C3B	-3.80	1.43	1.51
20	X	606	CHL	C4C-NC	3.79	1.38	1.35
20	Y	605	CHL	C4C-NC	3.79	1.38	1.35
22	3	615	LUT	C34-C33	3.78	1.40	1.35
22	1	615	LUT	C10-C9	3.78	1.40	1.35
20	Y	606	CHL	C4C-NC	3.78	1.38	1.35
20	1	601	CHL	C4C-NC	3.77	1.38	1.35
22	Z	314	LUT	C10-C9	3.77	1.40	1.35
20	6	615	CHL	C4C-NC	3.76	1.38	1.35
20	Y	609	CHL	C4C-NC	3.75	1.38	1.35
22	3	615	LUT	C10-C9	3.75	1.40	1.35
20	Z	306	CHL	C4C-NC	3.74	1.38	1.35
20	1	601	CHL	C3B-C2B	-3.73	1.35	1.40
20	2	605	CHL	C4C-NC	3.73	1.38	1.35
20	Z	301	CHL	C4C-NC	3.73	1.38	1.35
20	Y	608	CHL	C4C-NC	3.72	1.38	1.35
20	5	606	CHL	C4C-NC	3.71	1.38	1.35
20	X	607	CHL	C4C-NC	3.70	1.38	1.35
20	4	304	CHL	C3B-C2B	-3.70	1.35	1.40
20	Z	302	CHL	C4C-NC	3.70	1.38	1.35
20	Z	301	CHL	CHA-CBD	3.69	1.55	1.51
20	2	606	CHL	C3B-C2B	-3.69	1.35	1.40
20	Z	307	CHL	C4C-NC	3.68	1.38	1.35
20	Y	607	CHL	C4C-NC	3.67	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	X	601	CHL	C4C-NC	3.66	1.38	1.35
20	2	614	CHL	C4C-NC	3.64	1.38	1.35
20	X	607	CHL	CHA-CBD	3.64	1.55	1.51
20	6	607	CHL	C3B-C2B	-3.63	1.35	1.40
20	X	608	CHL	C4C-NC	3.63	1.38	1.35
20	3	608	CHL	C3B-C2B	-3.61	1.35	1.40
20	4	305	CHL	C3B-C2B	-3.61	1.35	1.40
20	6	606	CHL	C4C-NC	3.61	1.38	1.35
20	2	606	CHL	C4C-NC	3.60	1.38	1.35
20	X	601	CHL	CHA-CBD	3.60	1.55	1.51
20	3	608	CHL	C4C-NC	3.60	1.38	1.35
20	Z	309	CHL	C3B-C2B	-3.59	1.35	1.40
20	2	607	CHL	C3B-C2B	-3.59	1.35	1.40
20	2	601	CHL	C3B-C2B	-3.59	1.35	1.40
20	5	601	CHL	C4C-NC	3.58	1.38	1.35
20	X	605	CHL	CHA-CBD	3.58	1.55	1.51
20	1	606	CHL	C4C-NC	3.57	1.38	1.35
20	5	601	CHL	C3B-C2B	-3.57	1.35	1.40
20	5	606	CHL	CHA-CBD	3.57	1.55	1.51
20	Y	619	CHL	C3B-C2B	-3.57	1.35	1.40
20	Y	601	CHL	C4C-NC	3.56	1.38	1.35
20	Z	308	CHL	CHA-CBD	3.56	1.55	1.51
20	6	607	CHL	CHA-CBD	3.55	1.55	1.51
20	Y	619	CHL	C4C-NC	3.55	1.38	1.35
20	2	601	CHL	C4C-NC	3.55	1.38	1.35
20	2	605	CHL	C3B-C2B	-3.54	1.35	1.40
20	X	608	CHL	CHA-CBD	3.53	1.55	1.51
20	4	314	CHL	C4C-NC	3.53	1.38	1.35
20	6	606	CHL	C3B-C2B	-3.53	1.35	1.40
20	1	606	CHL	C3B-C2B	-3.53	1.35	1.40
20	Z	307	CHL	C3B-C2B	-3.52	1.35	1.40
20	6	605	CHL	C4C-NC	3.52	1.38	1.35
20	Y	607	CHL	CHA-CBD	3.52	1.55	1.51
20	2	607	CHL	C4C-NC	3.52	1.38	1.35
20	Y	601	CHL	C3B-C2B	-3.52	1.35	1.40
20	4	305	CHL	C4C-NC	3.51	1.38	1.35
20	6	605	CHL	C3B-C2B	-3.51	1.35	1.40
20	Z	309	CHL	C4C-NC	3.50	1.38	1.35
20	Y	606	CHL	CHA-CBD	3.49	1.55	1.51
20	Y	609	CHL	C3B-C2B	-3.49	1.35	1.40
20	6	607	CHL	C4C-NC	3.49	1.38	1.35
20	Y	605	CHL	CHA-CBD	3.48	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	Z	308	CHL	O2D-CGD	3.48	1.41	1.33
20	X	605	CHL	O2D-CGD	3.48	1.41	1.33
20	Y	605	CHL	O2D-CGD	3.48	1.41	1.33
20	Z	302	CHL	O2D-CGD	3.48	1.41	1.33
20	X	608	CHL	O2D-CGD	3.47	1.41	1.33
20	X	607	CHL	O2D-CGD	3.47	1.41	1.33
20	Y	606	CHL	O2D-CGD	3.47	1.41	1.33
20	Y	607	CHL	O2D-CGD	3.47	1.41	1.33
20	Z	306	CHL	C3B-C2B	-3.46	1.35	1.40
20	Z	308	CHL	C3B-C2B	-3.46	1.35	1.40
20	Z	306	CHL	O2D-CGD	3.46	1.41	1.33
20	4	306	CHL	C4C-NC	3.46	1.38	1.35
20	Y	609	CHL	O2D-CGD	3.46	1.41	1.33
20	Z	309	CHL	CHA-CBD	3.46	1.55	1.51
20	6	606	CHL	CHA-CBD	3.46	1.55	1.51
20	4	304	CHL	C4C-NC	3.45	1.38	1.35
20	6	605	CHL	O2D-CGD	3.45	1.41	1.33
20	6	606	CHL	O2D-CGD	3.45	1.41	1.33
20	X	606	CHL	O2D-CGD	3.45	1.41	1.33
20	Y	608	CHL	O2D-CGD	3.44	1.41	1.33
20	Z	301	CHL	O2D-CGD	3.44	1.41	1.33
20	Y	608	CHL	CHA-CBD	3.44	1.55	1.51
20	3	608	CHL	CHA-CBD	3.43	1.55	1.51
20	X	601	CHL	O2D-CGD	3.43	1.41	1.33
20	4	306	CHL	CHA-CBD	3.43	1.55	1.51
20	Y	607	CHL	C3B-C2B	-3.42	1.35	1.40
20	Z	307	CHL	O2D-CGD	3.42	1.41	1.33
20	Y	619	CHL	O2D-CGD	3.42	1.41	1.33
20	2	614	CHL	O2D-CGD	3.42	1.41	1.33
20	2	605	CHL	O2D-CGD	3.41	1.41	1.33
20	Y	619	CHL	CHA-CBD	3.41	1.55	1.51
20	Y	609	CHL	CHA-CBD	3.41	1.55	1.51
20	2	614	CHL	C3B-C2B	-3.41	1.35	1.40
20	5	601	CHL	CHA-CBD	3.41	1.55	1.51
20	5	606	CHL	O2D-CGD	3.41	1.41	1.30
20	2	606	CHL	O2D-CGD	3.40	1.41	1.33
20	1	606	CHL	CHA-CBD	3.40	1.55	1.51
20	6	615	CHL	CHA-CBD	3.39	1.55	1.51
20	Y	608	CHL	C3B-C2B	-3.39	1.35	1.40
20	Y	606	CHL	C3B-C2B	-3.39	1.35	1.40
20	5	606	CHL	C3B-C2B	-3.39	1.35	1.40
20	X	607	CHL	C3B-C2B	-3.38	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	6	615	CHL	O2D-CGD	3.38	1.41	1.30
20	2	614	CHL	CHA-CBD	3.38	1.55	1.51
20	2	606	CHL	CHA-CBD	3.38	1.55	1.51
20	X	605	CHL	C3B-C2B	-3.38	1.35	1.40
20	4	314	CHL	O2D-CGD	3.38	1.41	1.30
20	Z	309	CHL	O2D-CGD	3.37	1.41	1.33
20	4	305	CHL	O2D-CGD	3.37	1.41	1.33
20	4	304	CHL	O2D-CGD	3.37	1.41	1.33
20	Z	302	CHL	C3B-C2B	-3.37	1.35	1.40
20	X	607	CHL	O2A-CGA	3.37	1.42	1.30
20	Z	306	CHL	O2A-CGA	3.37	1.42	1.30
20	Z	302	CHL	O2A-CGA	3.36	1.42	1.30
20	Z	301	CHL	O2A-CGA	3.36	1.42	1.30
20	1	601	CHL	CHA-CBD	3.36	1.55	1.51
20	4	314	CHL	CHA-CBD	3.36	1.55	1.51
20	X	606	CHL	CHA-CBD	3.36	1.55	1.51
20	Z	309	CHL	O2A-CGA	3.36	1.42	1.30
20	Y	608	CHL	O2A-CGA	3.36	1.42	1.30
20	X	601	CHL	O2A-CGA	3.36	1.42	1.30
20	6	606	CHL	O2A-CGA	3.35	1.42	1.30
20	X	608	CHL	O2A-CGA	3.35	1.42	1.30
20	Z	307	CHL	O2A-CGA	3.35	1.42	1.30
20	Z	306	CHL	CHA-CBD	3.35	1.55	1.51
20	Y	609	CHL	O2A-CGA	3.35	1.42	1.30
20	X	606	CHL	O2A-CGA	3.34	1.42	1.30
20	Y	605	CHL	C3B-C2B	-3.34	1.35	1.40
20	4	305	CHL	O2A-CGA	3.34	1.42	1.30
20	Y	606	CHL	O2A-CGA	3.34	1.42	1.30
20	2	607	CHL	CHA-CBD	3.34	1.55	1.51
20	1	606	CHL	O2D-CGD	3.34	1.41	1.30
20	2	607	CHL	O2D-CGD	3.33	1.41	1.33
20	X	601	CHL	C3B-C2B	-3.33	1.35	1.40
20	Y	601	CHL	O2A-CGA	3.33	1.41	1.30
20	Y	607	CHL	O2A-CGA	3.32	1.41	1.30
20	Y	601	CHL	O2D-CGD	3.32	1.41	1.33
20	Z	301	CHL	C3B-C2B	-3.32	1.35	1.40
20	3	608	CHL	O2D-CGD	3.32	1.41	1.33
20	Z	302	CHL	CHA-CBD	3.31	1.55	1.51
20	6	607	CHL	O2D-CGD	3.31	1.41	1.33
20	5	601	CHL	O2D-CGD	3.31	1.41	1.30
20	X	606	CHL	C3B-C2B	-3.30	1.35	1.40
20	2	601	CHL	O2D-CGD	3.29	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	6	605	CHL	CHA-CBD	3.28	1.55	1.51
20	X	608	CHL	C3B-C2B	-3.28	1.35	1.40
20	1	601	CHL	O2D-CGD	3.28	1.41	1.30
20	4	306	CHL	O2D-CGD	3.28	1.41	1.33
20	Y	601	CHL	CHA-CBD	3.27	1.55	1.51
20	4	304	CHL	CHA-CBD	3.26	1.55	1.51
20	2	601	CHL	CHA-CBD	3.25	1.55	1.51
20	2	605	CHL	CHA-CBD	3.25	1.55	1.51
20	Z	307	CHL	CHA-CBD	3.22	1.55	1.51
20	4	305	CHL	CHA-CBD	3.11	1.55	1.51
20	1	601	CHL	O2A-CGA	3.07	1.42	1.33
20	4	304	CHL	O2A-CGA	3.04	1.42	1.33
20	5	601	CHL	O2A-CGA	3.04	1.42	1.33
21	B	820	CLA	C1D-ND	-3.03	1.34	1.37
21	B	813	CLA	C1D-ND	-3.02	1.34	1.37
20	6	605	CHL	O2A-CGA	3.01	1.42	1.33
21	B	836	CLA	C1D-ND	-3.01	1.34	1.37
20	6	607	CHL	O2A-CGA	3.00	1.42	1.33
21	B	835	CLA	C1D-ND	-3.00	1.34	1.37
21	A	822	CLA	C1D-ND	-2.99	1.34	1.37
21	B	829	CLA	C1D-ND	-2.99	1.34	1.37
21	A	802	CLA	C1D-ND	-2.98	1.34	1.37
20	2	607	CHL	O2A-CGA	2.98	1.42	1.33
21	A	835	CLA	C1D-ND	-2.96	1.34	1.37
20	4	306	CHL	O2A-CGA	2.96	1.42	1.33
21	A	830	CLA	C1D-ND	-2.94	1.34	1.37
21	A	818	CLA	C1D-ND	-2.94	1.34	1.37
21	A	826	CLA	C1D-ND	-2.94	1.34	1.37
21	A	810	CLA	C1D-ND	-2.93	1.34	1.37
21	A	831	CLA	C1D-ND	-2.93	1.34	1.37
21	B	809	CLA	C1D-ND	-2.93	1.34	1.37
21	A	824	CLA	C1D-ND	-2.92	1.34	1.37
22	2	615	LUT	C8-C9	-2.92	1.39	1.45
21	B	822	CLA	C1D-ND	-2.92	1.34	1.37
21	4	307	CLA	C1D-ND	-2.92	1.34	1.37
21	B	804	CLA	C1D-ND	-2.92	1.34	1.37
21	B	818	CLA	C1D-ND	-2.91	1.34	1.37
21	A	842	CLA	C1D-ND	-2.91	1.34	1.37
21	5	608	CLA	C1D-ND	-2.91	1.34	1.37
22	Z	314	LUT	C8-C9	-2.91	1.39	1.45
21	B	803	CLA	C1D-ND	-2.91	1.34	1.37
21	B	824	CLA	C1D-ND	-2.91	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	6	608	CLA	C1D-ND	-2.91	1.34	1.37
21	A	832	CLA	C1D-ND	-2.90	1.34	1.37
21	A	837	CLA	C1D-ND	-2.90	1.34	1.37
21	B	828	CLA	C1D-ND	-2.90	1.34	1.37
21	A	821	CLA	C1D-ND	-2.89	1.34	1.37
21	A	827	CLA	C1D-ND	-2.89	1.34	1.37
21	3	609	CLA	C1D-ND	-2.89	1.34	1.37
21	B	802	CLA	C1D-ND	-2.89	1.34	1.37
22	4	315	LUT	C8-C9	-2.89	1.39	1.45
21	B	815	CLA	C1D-ND	-2.89	1.34	1.37
21	1	614	CLA	C1D-ND	-2.89	1.34	1.37
21	A	841	CLA	C1D-ND	-2.89	1.34	1.37
21	B	802	CLA	C1B-NB	-2.88	1.34	1.37
21	L	304	CLA	C1D-ND	-2.87	1.34	1.37
21	A	807	CLA	C1D-ND	-2.87	1.34	1.37
21	B	801	CLA	C1D-ND	-2.87	1.34	1.37
21	A	806	CLA	C1D-ND	-2.86	1.34	1.37
21	B	816	CLA	C1D-ND	-2.86	1.34	1.37
21	4	308	CLA	C1D-ND	-2.86	1.34	1.37
21	B	840	CLA	C1D-ND	-2.86	1.34	1.37
21	B	839	CLA	C1D-ND	-2.86	1.34	1.37
21	A	828	CLA	C1D-ND	-2.86	1.34	1.37
21	A	820	CLA	C1D-ND	-2.85	1.34	1.37
21	A	801	CLA	C1D-ND	-2.85	1.34	1.37
21	B	832	CLA	C1D-ND	-2.85	1.34	1.37
21	1	605	CLA	C1D-ND	-2.85	1.34	1.37
21	A	809	CLA	C1D-ND	-2.85	1.34	1.37
21	B	811	CLA	C1D-ND	-2.85	1.34	1.37
21	B	812	CLA	C1D-ND	-2.85	1.34	1.37
21	B	833	CLA	C1D-ND	-2.85	1.34	1.37
21	B	808	CLA	C1D-ND	-2.85	1.34	1.37
22	1	615	LUT	C8-C9	-2.85	1.39	1.45
21	A	813	CLA	C1D-ND	-2.84	1.34	1.37
21	A	838	CLA	C1D-ND	-2.84	1.34	1.37
21	1	608	CLA	C1D-ND	-2.84	1.34	1.37
21	A	814	CLA	C1D-ND	-2.84	1.34	1.37
21	B	827	CLA	C1D-ND	-2.84	1.34	1.37
20	3	608	CHL	O2A-CGA	2.84	1.42	1.33
20	2	601	CHL	O2A-CGA	2.84	1.42	1.33
21	B	810	CLA	C1D-ND	-2.83	1.34	1.37
22	F	301	LUT	C8-C9	-2.83	1.39	1.45
20	Y	619	CHL	O2A-CGA	2.83	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	825	CLA	C1D-ND	-2.83	1.34	1.37
21	X	609	CLA	C1D-ND	-2.83	1.34	1.37
21	A	805	CLA	C1D-ND	-2.83	1.34	1.37
21	B	838	CLA	C1D-ND	-2.83	1.34	1.37
21	1	607	CLA	C1D-ND	-2.82	1.34	1.37
21	1	613	CLA	C1D-ND	-2.82	1.34	1.37
21	4	312	CLA	C1D-ND	-2.82	1.34	1.37
21	Y	602	CLA	C1D-ND	-2.82	1.34	1.37
21	L	303	CLA	C1D-ND	-2.82	1.34	1.37
21	B	821	CLA	C1D-ND	-2.82	1.34	1.37
21	A	829	CLA	C1D-ND	-2.82	1.34	1.37
21	3	617	CLA	C1D-ND	-2.82	1.34	1.37
21	A	843	CLA	C1D-ND	-2.82	1.34	1.37
21	1	602	CLA	C1D-ND	-2.81	1.34	1.37
21	6	609	CLA	C1D-ND	-2.81	1.34	1.37
21	A	840	CLA	C1D-ND	-2.81	1.34	1.37
21	B	805	CLA	C1D-ND	-2.81	1.34	1.37
22	5	615	LUT	C8-C9	-2.81	1.39	1.45
21	6	612	CLA	C1D-ND	-2.81	1.34	1.37
21	5	610	CLA	C1D-ND	-2.81	1.34	1.37
21	6	602	CLA	C1D-ND	-2.81	1.34	1.37
22	3	615	LUT	C8-C9	-2.81	1.39	1.45
20	Z	301	CHL	C1A-CHA	2.80	1.43	1.40
21	B	826	CLA	C1D-ND	-2.80	1.34	1.37
21	Z	303	CLA	C1D-ND	-2.80	1.34	1.37
21	2	602	CLA	C1D-ND	-2.80	1.34	1.37
22	6	616	LUT	C8-C9	-2.80	1.39	1.45
21	B	814	CLA	C1D-ND	-2.80	1.34	1.37
21	A	817	CLA	C1D-ND	-2.79	1.34	1.37
21	A	825	CLA	C1D-ND	-2.79	1.34	1.37
21	2	608	CLA	C1D-ND	-2.79	1.34	1.37
21	2	612	CLA	C1D-ND	-2.79	1.34	1.37
21	1	612	CLA	C1D-ND	-2.79	1.34	1.37
21	A	819	CLA	C1D-ND	-2.79	1.34	1.37
21	Y	610	CLA	C1D-ND	-2.79	1.34	1.37
21	4	311	CLA	C1D-ND	-2.78	1.34	1.37
21	B	834	CLA	C1D-ND	-2.78	1.34	1.37
21	L	301	CLA	C1D-ND	-2.78	1.34	1.37
21	4	309	CLA	C1D-ND	-2.78	1.34	1.37
21	Z	304	CLA	C1D-ND	-2.78	1.34	1.37
21	A	834	CLA	C1D-ND	-2.78	1.34	1.37
21	4	301	CLA	C1D-ND	-2.78	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	830	CLA	C1D-ND	-2.78	1.34	1.37
21	A	833	CLA	C1D-ND	-2.78	1.34	1.37
21	B	806	CLA	C1D-ND	-2.78	1.34	1.37
22	5	619	LUT	C8-C9	-2.78	1.40	1.45
22	X	614	LUT	C8-C9	-2.77	1.40	1.45
22	X	615	LUT	C8-C9	-2.77	1.40	1.45
21	2	618	CLA	C1D-ND	-2.77	1.34	1.37
21	A	808	CLA	C1D-ND	-2.77	1.34	1.37
22	Y	616	LUT	C8-C9	-2.77	1.40	1.45
21	A	812	CLA	C1D-ND	-2.76	1.34	1.37
21	5	602	CLA	C1D-ND	-2.76	1.34	1.37
21	6	614	CLA	C1D-ND	-2.76	1.34	1.37
21	4	303	CLA	C1D-ND	-2.76	1.34	1.37
21	B	837	CLA	C1D-ND	-2.76	1.34	1.37
21	4	302	CLA	C1D-ND	-2.76	1.34	1.37
21	F	304	CLA	C1D-ND	-2.76	1.34	1.37
21	G	202	CLA	C1D-ND	-2.76	1.34	1.37
21	G	204	CLA	C1D-ND	-2.75	1.34	1.37
21	K	202	CLA	C1D-ND	-2.75	1.34	1.37
21	Y	611	CLA	C1D-ND	-2.75	1.34	1.37
21	A	823	CLA	C1D-ND	-2.75	1.34	1.37
21	A	803	CLA	C1D-ND	-2.75	1.34	1.37
21	A	836	CLA	C1D-ND	-2.75	1.34	1.37
21	O	202	CLA	C1D-ND	-2.75	1.34	1.37
21	B	823	CLA	C1D-ND	-2.75	1.34	1.37
21	O	206	CLA	C1D-ND	-2.75	1.34	1.37
21	3	602	CLA	C1D-ND	-2.74	1.34	1.37
21	B	817	CLA	C1D-ND	-2.74	1.34	1.37
21	1	610	CLA	C1D-ND	-2.74	1.34	1.37
21	A	816	CLA	C1D-ND	-2.74	1.34	1.37
21	A	815	CLA	C1D-ND	-2.74	1.34	1.37
21	2	609	CLA	C1D-ND	-2.74	1.34	1.37
21	A	804	CLA	C1D-ND	-2.74	1.34	1.37
21	A	839	CLA	C1D-ND	-2.74	1.34	1.37
21	B	831	CLA	C1D-ND	-2.74	1.34	1.37
21	K	203	CLA	C1D-ND	-2.74	1.34	1.37
21	X	602	CLA	C1D-ND	-2.73	1.34	1.37
21	6	604	CLA	C1D-ND	-2.73	1.34	1.37
21	3	607	CLA	C1D-ND	-2.72	1.34	1.37
21	3	612	CLA	C1D-ND	-2.72	1.34	1.37
21	2	604	CLA	C1D-ND	-2.72	1.34	1.37
21	3	614	CLA	C1D-ND	-2.72	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	3	610	CLA	C1D-ND	-2.72	1.34	1.37
20	X	606	CHL	C1A-CHA	2.72	1.43	1.40
21	Z	310	CLA	C1D-ND	-2.72	1.34	1.37
21	O	207	CLA	C1D-ND	-2.72	1.34	1.37
22	Y	615	LUT	C8-C9	-2.71	1.40	1.45
21	1	611	CLA	C1D-ND	-2.71	1.34	1.37
21	5	614	CLA	C1D-ND	-2.71	1.34	1.37
21	6	611	CLA	C1D-ND	-2.71	1.34	1.37
21	X	613	CLA	C1D-ND	-2.71	1.34	1.37
21	6	610	CLA	C1D-ND	-2.71	1.34	1.37
21	5	612	CLA	C1D-ND	-2.71	1.34	1.37
21	3	604	CLA	C1D-ND	-2.70	1.34	1.37
21	L	305	CLA	C1D-ND	-2.70	1.34	1.37
21	3	606	CLA	C1D-ND	-2.70	1.34	1.37
21	1	609	CLA	C1D-ND	-2.70	1.34	1.37
21	K	204	CLA	C1D-ND	-2.70	1.34	1.37
21	G	203	CLA	C1D-ND	-2.69	1.34	1.37
21	B	807	CLA	C1D-ND	-2.69	1.34	1.37
21	2	610	CLA	C1D-ND	-2.69	1.34	1.37
21	5	607	CLA	C1D-ND	-2.69	1.34	1.37
20	X	601	CHL	C2C-C3C	2.69	1.38	1.36
21	2	603	CLA	C1D-ND	-2.69	1.34	1.37
21	4	313	CLA	C1D-ND	-2.69	1.34	1.37
21	3	605	CLA	C1D-ND	-2.69	1.34	1.37
21	B	819	CLA	C1D-ND	-2.68	1.34	1.37
21	1	604	CLA	C1D-ND	-2.68	1.34	1.37
21	Z	312	CLA	C1D-ND	-2.68	1.34	1.37
20	X	606	CHL	C2C-C3C	2.68	1.38	1.36
21	6	603	CLA	C1D-ND	-2.68	1.34	1.37
21	H	201	CLA	C1D-ND	-2.68	1.34	1.37
21	Y	612	CLA	C1D-ND	-2.67	1.34	1.37
20	Y	609	CHL	C2C-C3C	2.67	1.38	1.36
20	X	605	CHL	C1A-CHA	2.67	1.43	1.40
21	Y	614	CLA	C1D-ND	-2.67	1.34	1.37
21	X	604	CLA	C1D-ND	-2.67	1.34	1.37
21	X	603	CLA	C1D-ND	-2.66	1.34	1.37
21	2	613	CLA	C1D-ND	-2.66	1.34	1.37
20	6	607	CHL	C1A-CHA	2.66	1.43	1.40
21	4	310	CLA	C1D-ND	-2.66	1.34	1.37
21	Z	313	CLA	C1D-ND	-2.66	1.34	1.37
21	5	611	CLA	C1D-ND	-2.66	1.34	1.37
21	5	604	CLA	C1D-ND	-2.65	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	X	608	CHL	C1A-CHA	2.65	1.43	1.40
20	Z	309	CHL	C1A-CHA	2.65	1.43	1.40
20	X	608	CHL	C2C-C3C	2.65	1.38	1.36
20	X	607	CHL	C1A-CHA	2.64	1.43	1.40
21	1	603	CLA	C1D-ND	-2.64	1.34	1.37
21	6	601	CLA	C1D-ND	-2.64	1.34	1.37
21	J	102	CLA	C1D-ND	-2.64	1.34	1.37
21	X	610	CLA	C1D-ND	-2.64	1.34	1.37
21	Y	603	CLA	C1D-ND	-2.64	1.34	1.37
21	6	613	CLA	C1D-ND	-2.64	1.34	1.37
21	5	609	CLA	C1D-ND	-2.64	1.34	1.37
21	Y	613	CLA	C1D-ND	-2.63	1.34	1.37
21	5	613	CLA	C1D-ND	-2.63	1.34	1.37
21	Z	305	CLA	C1D-ND	-2.63	1.34	1.37
21	A	811	CLA	C1D-ND	-2.63	1.34	1.37
22	Z	315	LUT	C8-C9	-2.62	1.40	1.45
21	3	603	CLA	C1D-ND	-2.62	1.34	1.37
21	O	203	CLA	C1D-ND	-2.62	1.34	1.37
21	5	603	CLA	C1D-ND	-2.62	1.34	1.37
21	J	101	CLA	C1D-ND	-2.62	1.34	1.37
20	2	614	CHL	C1A-CHA	2.62	1.43	1.40
20	2	605	CHL	C1A-CHA	2.61	1.43	1.40
20	6	606	CHL	C1A-CHA	2.61	1.43	1.40
20	X	601	CHL	C1A-CHA	2.61	1.43	1.40
20	Y	606	CHL	C1A-CHA	2.60	1.43	1.40
21	2	611	CLA	C1D-ND	-2.59	1.34	1.37
20	5	606	CHL	C1A-CHA	2.59	1.43	1.40
21	5	605	CLA	C1D-ND	-2.59	1.34	1.37
20	X	605	CHL	C2C-C3C	2.59	1.38	1.36
21	Z	311	CLA	C1D-ND	-2.58	1.34	1.37
21	X	609	CLA	C3B-C4B	2.58	1.48	1.42
20	1	606	CHL	C1A-CHA	2.58	1.43	1.40
21	Y	604	CLA	C1D-ND	-2.57	1.34	1.37
20	4	304	CHL	C2-C3	2.57	1.39	1.33
20	3	608	CHL	C1A-CHA	2.57	1.43	1.40
21	X	618	CLA	C1D-ND	-2.56	1.34	1.37
20	Y	607	CHL	C1A-CHA	2.56	1.43	1.40
20	4	306	CHL	C1A-CHA	2.55	1.43	1.40
21	3	613	CLA	C1D-ND	-2.55	1.34	1.37
21	X	612	CLA	C1D-ND	-2.55	1.34	1.37
21	Z	310	CLA	C3B-C4B	2.55	1.48	1.42
21	X	611	CLA	C1D-ND	-2.55	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	Z	308	CHL	C1A-CHA	2.54	1.43	1.40
21	K	201	CLA	C1D-ND	-2.54	1.34	1.37
20	4	305	CHL	C2C-C3C	2.53	1.38	1.36
20	Y	607	CHL	C2C-C3C	2.53	1.38	1.36
20	6	605	CHL	C2-C3	2.53	1.39	1.33
21	6	610	CLA	C3B-C4B	2.53	1.48	1.42
20	1	601	CHL	C2-C3	2.53	1.39	1.33
20	2	606	CHL	MG-NB	2.52	2.10	2.05
20	Y	606	CHL	MG-NB	2.51	2.10	2.05
21	5	607	CLA	C3B-C4B	2.51	1.48	1.42
20	X	605	CHL	MG-NB	2.50	2.10	2.05
21	3	614	CLA	C3B-C4B	2.50	1.48	1.42
21	A	814	CLA	C3B-C4B	2.50	1.48	1.42
21	Z	303	CLA	C3B-C4B	2.50	1.48	1.42
21	5	608	CLA	C3B-C4B	2.50	1.48	1.42
20	1	601	CHL	C1A-CHA	2.50	1.42	1.40
21	B	829	CLA	C1B-NB	-2.49	1.34	1.37
20	5	601	CHL	C2-C3	2.49	1.39	1.33
31	X	616	NEX	C1-C6	-2.49	1.50	1.54
21	X	613	CLA	C3B-C4B	2.49	1.48	1.42
21	3	611	CLA	C1D-ND	-2.49	1.34	1.37
20	Y	606	CHL	CBA-CGA	2.49	1.56	1.50
21	Z	312	CLA	C3B-C4B	2.49	1.48	1.42
21	X	618	CLA	C3B-C4B	2.49	1.48	1.42
21	B	833	CLA	C3B-C4B	2.49	1.48	1.42
20	Z	307	CHL	C1A-CHA	2.48	1.42	1.40
21	B	830	CLA	C3B-C4B	2.48	1.48	1.42
21	O	207	CLA	C3B-C4B	2.48	1.48	1.42
20	6	606	CHL	C2C-C3C	2.48	1.38	1.36
21	3	611	CLA	C3B-C4B	2.48	1.48	1.42
21	2	609	CLA	C3B-C4B	2.48	1.48	1.42
21	A	826	CLA	C3B-C4B	2.48	1.48	1.42
20	Z	308	CHL	MG-NB	2.48	2.10	2.05
22	1	615	LUT	C32-C33	-2.47	1.40	1.45
20	5	601	CHL	C1A-CHA	2.47	1.42	1.40
21	5	608	CLA	CHC-C1C	2.47	1.43	1.38
20	Y	607	CHL	MG-NB	2.47	2.10	2.05
21	B	802	CLA	CHC-C1C	2.47	1.43	1.38
21	Z	311	CLA	C3B-C4B	2.47	1.48	1.42
21	Y	602	CLA	C3B-C4B	2.47	1.48	1.42
21	X	609	CLA	CHC-C1C	2.47	1.43	1.38
20	Y	605	CHL	MG-NB	2.46	2.10	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	824	CLA	C3B-C4B	2.46	1.48	1.42
21	X	612	CLA	C3B-C4B	2.46	1.48	1.42
21	3	604	CLA	C3B-C4B	2.46	1.48	1.42
20	Y	601	CHL	C1A-CHA	2.46	1.42	1.40
21	4	302	CLA	CHB-C1B	-2.46	1.33	1.39
20	2	606	CHL	C1A-CHA	2.46	1.42	1.40
21	A	802	CLA	CHC-C1C	2.46	1.43	1.38
20	Z	301	CHL	CBA-CGA	2.46	1.56	1.50
21	A	816	CLA	C3B-C4B	2.45	1.48	1.42
21	A	825	CLA	CHB-C1B	-2.45	1.33	1.39
21	5	611	CLA	C3B-C4B	2.45	1.48	1.42
21	6	609	CLA	C3B-C4B	2.45	1.48	1.42
21	B	813	CLA	C3B-C4B	2.45	1.48	1.42
21	B	822	CLA	C3B-C4B	2.45	1.48	1.42
21	K	201	CLA	C3B-C4B	2.45	1.48	1.42
21	Z	303	CLA	CHC-C1C	2.45	1.43	1.38
21	1	611	CLA	C3B-C4B	2.45	1.48	1.42
21	B	822	CLA	CHC-C1C	2.45	1.43	1.38
21	X	611	CLA	C3B-C4B	2.45	1.48	1.42
21	6	611	CLA	C3B-C4B	2.45	1.48	1.42
21	B	802	CLA	C3B-C4B	2.45	1.48	1.42
21	A	826	CLA	CHB-C1B	-2.45	1.33	1.39
20	Y	619	CHL	MG-NB	2.45	2.10	2.05
21	3	605	CLA	C3B-C4B	2.44	1.48	1.42
21	6	613	CLA	C3B-C4B	2.44	1.48	1.42
21	1	609	CLA	C3B-C4B	2.44	1.48	1.42
21	H	201	CLA	C3B-C4B	2.44	1.48	1.42
20	6	606	CHL	CBA-CGA	2.44	1.56	1.50
21	B	823	CLA	CHB-C1B	-2.44	1.33	1.39
20	Z	302	CHL	CBA-CGA	2.44	1.56	1.50
22	4	315	LUT	C32-C33	-2.44	1.40	1.45
21	Z	304	CLA	C3B-C4B	2.44	1.48	1.42
21	5	604	CLA	C3B-C4B	2.44	1.48	1.42
20	Y	609	CHL	MG-NB	2.44	2.10	2.05
21	B	832	CLA	C3B-C4B	2.44	1.48	1.42
21	Y	603	CLA	C3B-C4B	2.44	1.48	1.42
20	X	607	CHL	MG-NB	2.44	2.10	2.05
20	Y	608	CHL	MG-NB	2.43	2.10	2.05
21	A	836	CLA	C3B-C4B	2.43	1.48	1.42
20	X	607	CHL	CBA-CGA	2.43	1.56	1.50
21	1	608	CLA	C3B-C4B	2.43	1.48	1.42
20	Y	605	CHL	C1A-CHA	2.43	1.42	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	5	610	CLA	C3B-C4B	2.43	1.48	1.42
20	4	305	CHL	MG-NB	2.43	2.10	2.05
22	6	616	LUT	C32-C33	-2.43	1.40	1.45
20	4	314	CHL	C1A-CHA	2.43	1.42	1.40
20	6	607	CHL	MG-NB	2.43	2.10	2.05
21	B	814	CLA	C3B-C4B	2.43	1.48	1.42
20	X	608	CHL	CBA-CGA	2.43	1.56	1.50
21	5	605	CLA	C3B-C4B	2.43	1.48	1.42
21	5	609	CLA	C3B-C4B	2.43	1.48	1.42
21	B	829	CLA	C3B-C4B	2.43	1.48	1.42
20	Z	306	CHL	C1A-CHA	2.43	1.42	1.40
21	A	830	CLA	C3B-C4B	2.42	1.48	1.42
20	X	601	CHL	MG-NB	2.42	2.10	2.05
21	1	611	CLA	CHB-C1B	-2.42	1.34	1.39
21	B	833	CLA	CHC-C1C	2.42	1.43	1.38
21	G	202	CLA	C3B-C4B	2.42	1.48	1.42
21	X	602	CLA	C3B-C4B	2.42	1.48	1.42
21	3	606	CLA	C3B-C4B	2.42	1.48	1.42
20	Z	306	CHL	CBA-CGA	2.42	1.56	1.50
20	2	605	CHL	MG-NB	2.42	2.10	2.05
22	F	301	LUT	C12-C13	-2.42	1.40	1.45
21	2	610	CLA	C3B-C4B	2.42	1.48	1.42
21	X	604	CLA	C3B-C4B	2.42	1.48	1.42
22	Z	314	LUT	C12-C13	-2.42	1.40	1.45
21	A	828	CLA	C3B-C4B	2.42	1.48	1.42
20	2	601	CHL	C1A-CHA	2.42	1.42	1.40
21	J	102	CLA	C3B-C4B	2.42	1.48	1.42
21	A	832	CLA	C3B-C4B	2.42	1.48	1.42
21	Y	612	CLA	C3B-C4B	2.42	1.48	1.42
21	A	808	CLA	C3B-C4B	2.42	1.48	1.42
21	F	304	CLA	C3B-C4B	2.42	1.48	1.42
21	A	806	CLA	CHB-C1B	-2.42	1.34	1.39
21	Z	310	CLA	CHC-C1C	2.42	1.43	1.38
21	B	838	CLA	CHB-C1B	-2.42	1.34	1.39
20	4	304	CHL	MG-NB	2.41	2.10	2.05
22	Z	314	LUT	C32-C33	-2.41	1.40	1.45
21	2	611	CLA	CHB-C1B	-2.41	1.34	1.39
20	6	615	CHL	C1A-CHA	2.41	1.42	1.40
21	2	602	CLA	C3B-C4B	2.41	1.48	1.42
20	Z	309	CHL	CBA-CGA	2.41	1.56	1.50
21	K	204	CLA	C3B-C4B	2.41	1.48	1.42
20	Y	606	CHL	C2C-C3C	2.41	1.38	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	5	602	CLA	C3B-C4B	2.41	1.48	1.42
21	A	803	CLA	C3B-C4B	2.41	1.48	1.42
21	2	611	CLA	C3B-C4B	2.41	1.48	1.42
21	A	838	CLA	C3B-C4B	2.41	1.48	1.42
21	1	610	CLA	C3B-C4B	2.41	1.48	1.42
22	2	615	LUT	C12-C13	-2.41	1.40	1.45
22	F	301	LUT	C28-C29	-2.41	1.40	1.45
21	3	613	CLA	C3B-C4B	2.41	1.48	1.42
21	5	613	CLA	C3B-C4B	2.41	1.48	1.42
21	B	814	CLA	CHC-C1C	2.41	1.43	1.38
21	Z	305	CLA	C3B-C4B	2.41	1.48	1.42
21	B	814	CLA	CHB-C1B	-2.41	1.34	1.39
20	Z	306	CHL	MG-NB	2.41	2.10	2.05
20	2	607	CHL	C1A-CHA	2.41	1.42	1.40
21	3	612	CLA	C3B-C4B	2.41	1.48	1.42
20	Y	609	CHL	C1A-CHA	2.41	1.42	1.40
21	4	309	CLA	C3B-C4B	2.41	1.48	1.42
20	X	601	CHL	CBA-CGA	2.41	1.56	1.50
21	3	609	CLA	C3B-C4B	2.40	1.48	1.42
21	3	607	CLA	C3B-C4B	2.40	1.48	1.42
20	Y	608	CHL	C1A-CHA	2.40	1.42	1.40
22	1	615	LUT	C12-C13	-2.40	1.40	1.45
21	G	204	CLA	C3B-C4B	2.40	1.48	1.42
20	Y	607	CHL	CBA-CGA	2.40	1.56	1.50
21	L	303	CLA	C3B-C4B	2.40	1.48	1.42
21	5	603	CLA	C3B-C4B	2.40	1.48	1.42
21	4	312	CLA	C3B-C4B	2.40	1.48	1.42
20	Z	307	CHL	MG-NB	2.40	2.10	2.05
21	2	613	CLA	C3B-C4B	2.40	1.48	1.42
21	L	305	CLA	C3B-C4B	2.40	1.48	1.42
21	G	203	CLA	C3B-C4B	2.40	1.48	1.42
22	4	315	LUT	C12-C13	-2.39	1.40	1.45
21	Y	613	CLA	C3B-C4B	2.39	1.48	1.42
20	X	607	CHL	C2C-C3C	2.39	1.38	1.36
21	4	301	CLA	C3B-C4B	2.39	1.48	1.42
22	2	615	LUT	C32-C33	-2.39	1.40	1.45
21	X	610	CLA	C3B-C4B	2.39	1.48	1.42
22	F	301	LUT	C32-C33	-2.39	1.40	1.45
21	4	310	CLA	CHB-C1B	-2.39	1.34	1.39
20	Y	605	CHL	C2C-C3C	2.39	1.38	1.36
22	2	615	LUT	C28-C29	-2.39	1.40	1.45
21	B	829	CLA	CHB-C1B	-2.39	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	819	CLA	C3B-C4B	2.39	1.48	1.42
22	Y	615	LUT	C32-C33	-2.39	1.40	1.45
20	4	314	CHL	MG-NB	2.39	2.10	2.05
21	2	609	CLA	CHC-C1C	2.39	1.43	1.38
21	B	811	CLA	C1B-NB	-2.39	1.34	1.37
21	B	820	CLA	CHC-C1C	2.39	1.43	1.38
21	3	602	CLA	C3B-C4B	2.39	1.48	1.42
21	X	603	CLA	C3B-C4B	2.39	1.48	1.42
21	A	835	CLA	CHC-C1C	2.39	1.43	1.38
21	X	613	CLA	CHC-C1C	2.39	1.43	1.38
21	Y	604	CLA	C3B-C4B	2.39	1.48	1.42
20	5	606	CHL	MG-NB	2.39	2.10	2.05
21	B	812	CLA	CHB-C1B	-2.39	1.34	1.39
21	A	825	CLA	C3B-C4B	2.39	1.48	1.42
21	Y	611	CLA	C3B-C4B	2.39	1.48	1.42
20	6	605	CHL	MG-NB	2.39	2.10	2.05
20	Y	601	CHL	CBA-CGA	2.39	1.56	1.50
21	A	821	CLA	C3B-C4B	2.38	1.48	1.42
20	Y	608	CHL	C2C-C3C	2.38	1.38	1.36
21	3	610	CLA	C3B-C4B	2.38	1.48	1.42
21	B	811	CLA	C3B-C4B	2.38	1.48	1.42
21	5	612	CLA	C3B-C4B	2.38	1.48	1.42
21	Z	313	CLA	C3B-C4B	2.38	1.48	1.42
21	2	612	CLA	C3B-C4B	2.38	1.48	1.42
21	K	202	CLA	C3B-C4B	2.38	1.48	1.42
20	Y	608	CHL	CBA-CGA	2.38	1.56	1.50
21	Y	614	CLA	C3B-C4B	2.38	1.48	1.42
21	B	805	CLA	CHB-C1B	-2.38	1.34	1.39
21	L	305	CLA	CHB-C1B	-2.38	1.34	1.39
21	4	303	CLA	CHB-C1B	-2.38	1.34	1.39
21	A	835	CLA	C3B-C4B	2.38	1.48	1.42
21	3	603	CLA	CHB-C1B	-2.38	1.34	1.39
21	Y	610	CLA	C3B-C4B	2.38	1.48	1.42
20	Z	302	CHL	MG-NB	2.38	2.10	2.05
21	6	603	CLA	CHB-C1B	-2.38	1.34	1.39
21	O	202	CLA	C3B-C4B	2.38	1.48	1.42
22	1	615	LUT	C28-C29	-2.38	1.40	1.45
21	4	308	CLA	C3B-C4B	2.38	1.48	1.42
21	B	806	CLA	C3B-C4B	2.38	1.48	1.42
21	K	204	CLA	CHC-C1C	2.37	1.43	1.38
21	4	307	CLA	CHB-C1B	-2.37	1.34	1.39
21	B	816	CLA	C1B-NB	-2.37	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	813	CLA	CHC-C1C	2.37	1.43	1.38
20	X	606	CHL	CBA-CGA	2.37	1.56	1.50
21	6	614	CLA	C3B-C4B	2.37	1.48	1.42
21	1	608	CLA	CHB-C1B	-2.37	1.34	1.39
21	A	831	CLA	CHB-C1B	-2.37	1.34	1.39
21	B	830	CLA	CHC-C1C	2.37	1.43	1.38
20	3	608	CHL	MG-NB	2.37	2.10	2.05
20	4	306	CHL	MG-NB	2.37	2.10	2.05
21	B	823	CLA	C3B-C4B	2.37	1.48	1.42
21	A	819	CLA	CHB-C1B	-2.37	1.34	1.39
21	B	837	CLA	CHB-C1B	-2.37	1.34	1.39
20	Z	302	CHL	C2C-C3C	2.37	1.38	1.36
21	O	207	CLA	CHC-C1C	2.37	1.43	1.38
21	A	808	CLA	CHC-C1C	2.37	1.43	1.38
21	A	822	CLA	CHC-C1C	2.37	1.43	1.38
21	A	805	CLA	CHC-C1C	2.36	1.43	1.38
21	B	836	CLA	C3B-C4B	2.36	1.48	1.42
21	6	604	CLA	C3B-C4B	2.36	1.48	1.42
21	B	840	CLA	C3B-C4B	2.36	1.48	1.42
20	Y	609	CHL	CBA-CGA	2.36	1.56	1.50
21	B	834	CLA	C3B-C4B	2.36	1.48	1.42
20	6	615	CHL	MG-NB	2.36	2.10	2.05
20	4	306	CHL	C3B-CAB	-2.36	1.43	1.47
21	1	604	CLA	CHB-C1B	-2.36	1.34	1.39
21	A	827	CLA	CHB-C1B	-2.36	1.34	1.39
21	A	830	CLA	CHC-C1C	2.36	1.43	1.38
21	A	815	CLA	C3B-C4B	2.36	1.48	1.42
21	3	611	CLA	MG-NB	2.36	2.10	2.05
20	6	606	CHL	MG-NB	2.36	2.10	2.05
21	B	832	CLA	CHC-C1C	2.36	1.43	1.38
21	B	804	CLA	CHB-C1B	-2.36	1.34	1.39
20	2	601	CHL	MG-NB	2.36	2.10	2.05
21	1	605	CLA	C3B-C4B	2.36	1.48	1.42
22	Y	616	LUT	C32-C33	-2.36	1.40	1.45
21	4	301	CLA	CHB-C1B	-2.36	1.34	1.39
21	2	603	CLA	CHB-C1B	-2.36	1.34	1.39
21	1	603	CLA	CHB-C1B	-2.36	1.34	1.39
21	2	604	CLA	C3B-C4B	2.35	1.48	1.42
21	4	302	CLA	C3B-C4B	2.35	1.48	1.42
20	Y	619	CHL	C1A-CHA	2.35	1.42	1.40
21	A	808	CLA	CHB-C1B	-2.35	1.34	1.39
21	A	805	CLA	C3B-C4B	2.35	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	803	CLA	CHB-C1B	-2.35	1.34	1.39
21	B	808	CLA	CHB-C1B	-2.35	1.34	1.39
21	1	613	CLA	C3B-C4B	2.35	1.48	1.42
20	X	606	CHL	MG-NB	2.35	2.10	2.05
22	3	615	LUT	C28-C29	-2.35	1.40	1.45
21	3	605	CLA	CHB-C1B	-2.35	1.34	1.39
21	A	804	CLA	CHB-C1B	-2.35	1.34	1.39
21	1	607	CLA	C3B-C4B	2.35	1.48	1.42
21	B	801	CLA	C3B-C4B	2.35	1.48	1.42
22	3	615	LUT	C12-C13	-2.35	1.40	1.45
21	B	833	CLA	CHB-C1B	-2.35	1.34	1.39
21	5	602	CLA	CHB-C1B	-2.35	1.34	1.39
21	B	828	CLA	CHB-C1B	-2.35	1.34	1.39
21	J	101	CLA	C3B-C4B	2.35	1.48	1.42
20	Z	301	CHL	MG-NB	2.35	2.10	2.05
20	2	606	CHL	C2C-C3C	2.35	1.38	1.36
21	F	304	CLA	CHB-C1B	-2.35	1.34	1.39
21	B	815	CLA	C1B-NB	-2.35	1.34	1.37
21	3	603	CLA	C3B-C4B	2.35	1.48	1.42
21	A	813	CLA	CHB-C1B	-2.35	1.34	1.39
21	6	601	CLA	C3B-C4B	2.35	1.48	1.42
21	O	206	CLA	C3B-C4B	2.35	1.48	1.42
21	4	313	CLA	CHB-C1B	-2.35	1.34	1.39
21	A	837	CLA	CHB-C1B	-2.35	1.34	1.39
22	5	619	LUT	C12-C13	-2.35	1.40	1.45
21	Y	611	CLA	CHC-C1C	2.35	1.43	1.38
21	B	835	CLA	C3B-C4B	2.34	1.48	1.42
21	6	608	CLA	C3B-C4B	2.34	1.48	1.42
22	Y	616	LUT	C12-C13	-2.34	1.40	1.45
21	A	840	CLA	C1B-NB	-2.34	1.34	1.37
21	B	808	CLA	C3B-C4B	2.34	1.48	1.42
21	K	201	CLA	CHB-C1B	-2.34	1.34	1.39
21	B	806	CLA	CHB-C1B	-2.34	1.34	1.39
21	5	614	CLA	C3B-C4B	2.34	1.48	1.42
21	5	612	CLA	CHB-C1B	-2.34	1.34	1.39
20	Z	307	CHL	CBA-CGA	2.34	1.56	1.50
21	B	826	CLA	C3B-C4B	2.34	1.48	1.42
20	2	607	CHL	MG-NB	2.34	2.10	2.05
21	K	202	CLA	CHC-C1C	2.34	1.43	1.38
21	6	604	CLA	CHB-C1B	-2.34	1.34	1.39
21	G	204	CLA	CHB-C1B	-2.34	1.34	1.39
21	O	203	CLA	C3B-C4B	2.34	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	6	616	LUT	C12-C13	-2.34	1.40	1.45
21	A	807	CLA	CHB-C1B	-2.34	1.34	1.39
21	A	829	CLA	CHB-C1B	-2.34	1.34	1.39
21	H	201	CLA	CHB-C1B	-2.34	1.34	1.39
21	4	303	CLA	C3B-C4B	2.34	1.48	1.42
21	2	603	CLA	C3B-C4B	2.34	1.48	1.42
21	4	310	CLA	C3B-C4B	2.34	1.48	1.42
21	5	603	CLA	CHB-C1B	-2.34	1.34	1.39
20	1	606	CHL	MG-NB	2.34	2.10	2.05
22	5	619	LUT	C32-C33	-2.34	1.40	1.45
21	Y	602	CLA	CHC-C1C	2.34	1.43	1.38
20	2	607	CHL	C2C-C3C	2.34	1.38	1.36
21	L	301	CLA	C3B-C4B	2.34	1.48	1.42
21	A	835	CLA	CHB-C1B	-2.34	1.34	1.39
21	X	612	CLA	MG-NB	2.34	2.10	2.05
21	A	806	CLA	CHC-C1C	2.34	1.43	1.38
21	X	618	CLA	CHC-C1C	2.34	1.43	1.38
21	2	608	CLA	C3B-C4B	2.34	1.48	1.42
21	2	602	CLA	CHB-C1B	-2.33	1.34	1.39
20	Z	301	CHL	C2C-C3C	2.33	1.38	1.36
21	A	806	CLA	C3B-C4B	2.33	1.48	1.42
31	Y	617	NEX	C1-C6	-2.33	1.50	1.54
20	X	608	CHL	MG-NB	2.33	2.10	2.05
21	X	618	CLA	MG-NB	2.33	2.10	2.05
21	3	602	CLA	CHB-C1B	-2.33	1.34	1.39
21	B	803	CLA	CHC-C1C	2.33	1.43	1.38
21	B	831	CLA	C3B-C4B	2.33	1.48	1.42
21	Y	612	CLA	CHB-C1B	-2.33	1.34	1.39
21	B	808	CLA	C1B-NB	-2.33	1.34	1.37
20	4	305	CHL	CBA-CGA	2.33	1.56	1.50
21	3	609	CLA	CHC-C1C	2.33	1.43	1.38
21	Z	304	CLA	CHC-C1C	2.33	1.43	1.38
21	B	803	CLA	C3B-C4B	2.33	1.48	1.42
21	B	815	CLA	CHB-C1B	-2.33	1.34	1.39
21	A	843	CLA	C3B-C4B	2.33	1.48	1.42
21	6	610	CLA	CHB-C1B	-2.33	1.34	1.39
21	B	811	CLA	CHB-C1B	-2.33	1.34	1.39
21	A	826	CLA	CHC-C1C	2.33	1.43	1.38
21	A	820	CLA	C3B-C4B	2.33	1.48	1.42
21	1	602	CLA	CHB-C1B	-2.33	1.34	1.39
21	3	606	CLA	CHB-C1B	-2.33	1.34	1.39
20	Z	309	CHL	MG-NB	2.33	2.10	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	818	CLA	CHB-C1B	-2.33	1.34	1.39
21	A	838	CLA	CHB-C1B	-2.33	1.34	1.39
21	A	833	CLA	CHB-C1B	-2.33	1.34	1.39
21	B	827	CLA	CHB-C1B	-2.33	1.34	1.39
21	1	613	CLA	CHC-C1C	2.33	1.43	1.38
21	B	829	CLA	CHC-C1C	2.33	1.43	1.38
21	2	604	CLA	CHB-C1B	-2.33	1.34	1.39
21	2	618	CLA	CHB-C1B	-2.33	1.34	1.39
21	5	607	CLA	CHC-C1C	2.33	1.43	1.38
21	1	604	CLA	C3B-C4B	2.33	1.48	1.42
22	3	615	LUT	C32-C33	-2.33	1.40	1.45
22	5	615	LUT	C12-C13	-2.33	1.40	1.45
22	Y	615	LUT	C12-C13	-2.32	1.41	1.45
21	Y	602	CLA	CHB-C1B	-2.32	1.34	1.39
21	X	612	CLA	CHC-C1C	2.32	1.43	1.38
21	6	612	CLA	CHB-C1B	-2.32	1.34	1.39
21	A	836	CLA	CHC-C1C	2.32	1.43	1.38
21	A	811	CLA	CHB-C1B	-2.32	1.34	1.39
21	K	201	CLA	CHC-C1C	2.32	1.43	1.38
21	3	613	CLA	CHB-C1B	-2.32	1.34	1.39
20	5	606	CHL	C2C-C3C	2.32	1.38	1.36
21	4	312	CLA	CHB-C1B	-2.32	1.34	1.39
21	A	805	CLA	CHB-C1B	-2.32	1.34	1.39
21	A	810	CLA	CHC-C1C	2.32	1.43	1.38
21	B	818	CLA	C3B-C4B	2.32	1.48	1.42
21	Y	614	CLA	CHB-C1B	-2.32	1.34	1.39
20	5	601	CHL	MG-NB	2.32	2.10	2.05
20	6	607	CHL	C2-C3	2.32	1.39	1.32
21	B	836	CLA	C1B-NB	-2.32	1.34	1.37
21	A	814	CLA	CHC-C1C	2.32	1.43	1.38
21	A	831	CLA	C3B-C4B	2.32	1.48	1.42
21	B	825	CLA	C3B-C4B	2.32	1.48	1.42
21	A	815	CLA	CHC-C1C	2.32	1.43	1.38
21	1	609	CLA	CHB-C1B	-2.32	1.34	1.39
21	4	308	CLA	CHC-C1C	2.32	1.43	1.38
21	F	304	CLA	CHC-C1C	2.32	1.43	1.38
21	Z	312	CLA	CHC-C1C	2.32	1.43	1.38
21	B	812	CLA	C1B-NB	-2.32	1.34	1.37
21	3	604	CLA	CHB-C1B	-2.32	1.34	1.39
21	A	812	CLA	CHB-C1B	-2.32	1.34	1.39
20	Z	306	CHL	C2C-C3C	2.32	1.38	1.36
21	K	203	CLA	C3B-C4B	2.32	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	3	611	CLA	CHB-C1B	-2.32	1.34	1.39
21	A	840	CLA	C3B-C4B	2.32	1.48	1.42
20	Y	601	CHL	MG-NB	2.32	2.10	2.05
21	6	610	CLA	CHC-C1C	2.32	1.43	1.38
20	6	605	CHL	C1A-CHA	2.32	1.42	1.40
21	2	610	CLA	CHB-C1B	-2.32	1.34	1.39
21	A	819	CLA	C3B-C4B	2.32	1.48	1.42
21	B	826	CLA	CHC-C1C	2.32	1.43	1.38
21	5	603	CLA	CHC-C1C	2.32	1.43	1.38
21	A	828	CLA	CHC-C1C	2.31	1.43	1.38
21	B	836	CLA	CHC-C1C	2.31	1.43	1.38
21	B	819	CLA	CHB-C1B	-2.31	1.34	1.39
21	Z	311	CLA	CHB-C1B	-2.31	1.34	1.39
21	A	809	CLA	C3B-C4B	2.31	1.48	1.42
21	A	828	CLA	CHB-C1B	-2.31	1.34	1.39
21	Z	305	CLA	CHB-C1B	-2.31	1.34	1.39
21	6	609	CLA	CHC-C1C	2.31	1.43	1.38
21	6	611	CLA	CHC-C1C	2.31	1.43	1.38
21	2	608	CLA	CHB-C1B	-2.31	1.34	1.39
21	B	816	CLA	CHB-C1B	-2.31	1.34	1.39
21	1	604	CLA	CHC-C1C	2.31	1.43	1.38
22	6	616	LUT	C28-C29	-2.31	1.41	1.45
21	X	604	CLA	CHB-C1B	-2.31	1.34	1.39
21	A	827	CLA	CHC-C1C	2.31	1.43	1.38
21	B	806	CLA	CHC-C1C	2.31	1.43	1.38
21	A	811	CLA	C3B-C4B	2.31	1.48	1.42
21	A	816	CLA	CHC-C1C	2.31	1.43	1.38
21	2	602	CLA	CHC-C1C	2.31	1.43	1.38
21	5	610	CLA	CHC-C1C	2.31	1.43	1.38
21	5	602	CLA	CHC-C1C	2.31	1.43	1.38
21	1	614	CLA	C3B-C4B	2.31	1.48	1.42
21	3	617	CLA	C3B-C4B	2.31	1.48	1.42
21	B	837	CLA	C3B-C4B	2.31	1.48	1.42
21	A	843	CLA	CHB-C1B	-2.31	1.34	1.39
21	A	838	CLA	C1B-NB	-2.31	1.34	1.37
21	B	824	CLA	C1B-NB	-2.31	1.34	1.37
21	3	611	CLA	CHC-C1C	2.31	1.43	1.38
21	A	802	CLA	C3B-C4B	2.31	1.48	1.42
21	B	820	CLA	C3B-C4B	2.31	1.48	1.42
21	A	816	CLA	CHB-C1B	-2.31	1.34	1.39
21	A	804	CLA	C3B-C4B	2.31	1.48	1.42
21	4	312	CLA	CHC-C1C	2.31	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	837	CLA	CHC-C1C	2.31	1.43	1.38
21	B	835	CLA	CHC-C1C	2.31	1.43	1.38
21	2	613	CLA	CHB-C1B	-2.31	1.34	1.39
21	A	821	CLA	CHB-C1B	-2.31	1.34	1.39
21	A	832	CLA	CHB-C1B	-2.31	1.34	1.39
20	6	605	CHL	C2C-C3C	2.31	1.38	1.36
22	4	315	LUT	C28-C29	-2.31	1.41	1.45
21	3	614	CLA	CHC-C1C	2.31	1.43	1.38
21	G	202	CLA	CHC-C1C	2.31	1.43	1.38
21	Z	311	CLA	CHC-C1C	2.31	1.43	1.38
21	B	809	CLA	C3B-C4B	2.30	1.48	1.42
21	B	831	CLA	CHB-C1B	-2.30	1.34	1.39
21	2	611	CLA	MG-NB	2.30	2.10	2.05
21	5	608	CLA	C1B-NB	-2.30	1.35	1.37
20	Z	302	CHL	C1A-CHA	2.30	1.42	1.40
21	B	835	CLA	CHB-C1B	-2.30	1.34	1.39
21	A	831	CLA	C1B-NB	-2.30	1.35	1.37
21	B	824	CLA	CHB-C1B	-2.30	1.34	1.39
21	G	203	CLA	CHC-C1C	2.30	1.43	1.38
21	4	311	CLA	C3B-C4B	2.30	1.48	1.42
21	A	830	CLA	CHB-C1B	-2.30	1.34	1.39
21	A	832	CLA	CHC-C1C	2.30	1.43	1.38
21	A	814	CLA	CHB-C1B	-2.30	1.34	1.39
21	X	603	CLA	CHB-C1B	-2.30	1.34	1.39
21	A	842	CLA	CHB-C1B	-2.30	1.34	1.39
21	K	202	CLA	CHB-C1B	-2.30	1.34	1.39
21	L	301	CLA	CHB-C1B	-2.30	1.34	1.39
21	G	204	CLA	CHC-C1C	2.30	1.43	1.38
22	Z	314	LUT	C28-C29	-2.30	1.41	1.45
21	2	618	CLA	C3B-C4B	2.30	1.48	1.42
21	A	822	CLA	C3B-C4B	2.30	1.48	1.42
20	2	607	CHL	C2-C3	2.30	1.39	1.32
22	X	614	LUT	C32-C33	-2.30	1.41	1.45
21	A	837	CLA	C3B-C4B	2.30	1.48	1.42
21	3	605	CLA	CHC-C1C	2.30	1.43	1.38
21	5	611	CLA	CHB-C1B	-2.30	1.34	1.39
21	L	303	CLA	CHB-C1B	-2.30	1.34	1.39
21	X	611	CLA	MG-NB	2.30	2.10	2.05
21	5	604	CLA	CHC-C1C	2.29	1.43	1.38
21	A	809	CLA	CHB-C1B	-2.29	1.34	1.39
21	B	834	CLA	CHB-C1B	-2.29	1.34	1.39
21	Z	304	CLA	CHB-C1B	-2.29	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	824	CLA	CHC-C1C	2.29	1.43	1.38
21	B	821	CLA	CHB-C1B	-2.29	1.34	1.39
21	3	607	CLA	CHC-C1C	2.29	1.43	1.38
21	5	610	CLA	CHB-C1B	-2.29	1.34	1.39
21	A	841	CLA	CHB-C1B	-2.29	1.34	1.39
21	Y	603	CLA	CHB-C1B	-2.29	1.34	1.39
22	5	619	LUT	C28-C29	-2.29	1.41	1.45
21	6	611	CLA	CHB-C1B	-2.29	1.34	1.39
21	B	809	CLA	C1B-NB	-2.29	1.35	1.37
21	A	801	CLA	CHC-C1C	2.29	1.43	1.38
21	X	602	CLA	CHC-C1C	2.29	1.43	1.38
21	3	607	CLA	CHB-C1B	-2.29	1.34	1.39
21	B	817	CLA	CHB-C1B	-2.29	1.34	1.39
21	A	833	CLA	C3B-C4B	2.29	1.48	1.42
20	2	614	CHL	C2C-C3C	2.29	1.38	1.36
21	L	304	CLA	C3B-C4B	2.29	1.48	1.42
21	1	610	CLA	CHB-C1B	-2.29	1.34	1.39
21	A	840	CLA	CHB-C1B	-2.29	1.34	1.39
21	Z	311	CLA	MG-NB	2.29	2.10	2.05
21	5	613	CLA	CHB-C1B	-2.29	1.34	1.39
21	A	815	CLA	CHB-C1B	-2.29	1.34	1.39
21	B	824	CLA	CHC-C1C	2.29	1.43	1.38
20	Z	307	CHL	C2C-C3C	2.29	1.38	1.36
21	2	613	CLA	CHC-C1C	2.29	1.43	1.38
21	B	828	CLA	C3B-C4B	2.29	1.48	1.42
21	A	836	CLA	CHB-C1B	-2.29	1.34	1.39
21	A	842	CLA	C3B-C4B	2.29	1.48	1.42
21	X	611	CLA	CHB-C1B	-2.29	1.34	1.39
21	1	611	CLA	CHC-C1C	2.29	1.43	1.38
21	B	809	CLA	CHC-C1C	2.29	1.43	1.38
21	3	604	CLA	CHC-C1C	2.28	1.43	1.38
21	5	614	CLA	CHC-C1C	2.28	1.43	1.38
21	1	612	CLA	CHB-C1B	-2.28	1.34	1.39
21	X	602	CLA	CHB-C1B	-2.28	1.34	1.39
21	B	833	CLA	C1B-NB	-2.28	1.35	1.37
21	6	601	CLA	CHC-C1C	2.28	1.43	1.38
21	4	309	CLA	CHB-C1B	-2.28	1.34	1.39
21	A	812	CLA	C3B-C4B	2.28	1.48	1.42
21	A	839	CLA	C3B-C4B	2.28	1.48	1.42
21	A	813	CLA	C1B-NB	-2.28	1.35	1.37
22	5	615	LUT	C32-C33	-2.28	1.41	1.45
21	6	603	CLA	C3B-C4B	2.28	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	801	CLA	C3B-C4B	2.28	1.48	1.42
21	1	614	CLA	CHC-C1C	2.28	1.43	1.38
21	4	313	CLA	C1B-NB	-2.28	1.35	1.37
21	B	838	CLA	C1B-NB	-2.28	1.35	1.37
21	1	602	CLA	C3B-C4B	2.28	1.48	1.42
21	A	817	CLA	C3B-C4B	2.28	1.48	1.42
21	B	818	CLA	CHB-C1B	-2.28	1.34	1.39
21	5	612	CLA	CHC-C1C	2.28	1.43	1.38
21	Z	313	CLA	CHC-C1C	2.28	1.43	1.38
21	Y	603	CLA	CHC-C1C	2.28	1.43	1.38
21	A	810	CLA	C3B-C4B	2.28	1.48	1.42
21	A	823	CLA	CHB-C1B	-2.28	1.34	1.39
21	5	609	CLA	CHB-C1B	-2.28	1.34	1.39
20	4	305	CHL	C1A-CHA	2.28	1.42	1.40
20	4	306	CHL	C2-C3	2.28	1.38	1.32
21	A	817	CLA	CHB-C1B	-2.28	1.34	1.39
21	4	307	CLA	C3B-C4B	2.28	1.48	1.42
21	B	815	CLA	C3B-C4B	2.28	1.48	1.42
21	G	202	CLA	CHB-C1B	-2.28	1.34	1.39
21	A	809	CLA	CHC-C1C	2.28	1.43	1.38
21	B	811	CLA	CHC-C1C	2.28	1.43	1.38
21	A	834	CLA	C1B-NB	-2.28	1.35	1.37
21	B	832	CLA	C1B-NB	-2.28	1.35	1.37
21	6	608	CLA	CHB-C1B	-2.28	1.34	1.39
21	Y	604	CLA	CHB-C1B	-2.28	1.34	1.39
21	B	805	CLA	C1B-NB	-2.28	1.35	1.37
21	5	602	CLA	C1B-NB	-2.28	1.35	1.37
21	A	826	CLA	C1B-NB	-2.28	1.35	1.37
21	A	834	CLA	CHB-C1B	-2.28	1.34	1.39
21	B	836	CLA	CHB-C1B	-2.28	1.34	1.39
21	Y	613	CLA	CHB-C1B	-2.28	1.34	1.39
21	A	824	CLA	C3B-C4B	2.27	1.48	1.42
20	1	606	CHL	C2C-C3C	2.27	1.38	1.36
21	B	830	CLA	CHB-C1B	-2.27	1.34	1.39
21	A	827	CLA	C3B-C4B	2.27	1.48	1.42
21	6	612	CLA	C1B-NB	-2.27	1.35	1.37
21	Z	313	CLA	MG-NB	2.27	2.10	2.05
21	2	612	CLA	CHC-C1C	2.27	1.43	1.38
21	B	834	CLA	CHC-C1C	2.27	1.43	1.38
21	6	602	CLA	C3B-C4B	2.27	1.48	1.42
21	6	609	CLA	CHB-C1B	-2.27	1.34	1.39
21	B	818	CLA	CHC-C1C	2.27	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	603	CLA	C3B-C4B	2.27	1.48	1.42
21	1	612	CLA	C3B-C4B	2.27	1.48	1.42
21	A	802	CLA	CHB-C1B	-2.27	1.34	1.39
21	B	801	CLA	CHB-C1B	-2.27	1.34	1.39
21	B	825	CLA	CHB-C1B	-2.27	1.34	1.39
21	3	610	CLA	CHC-C1C	2.27	1.43	1.38
21	B	807	CLA	MG-NB	2.27	2.10	2.05
21	A	824	CLA	CHB-C1B	-2.27	1.34	1.39
21	B	817	CLA	C3B-C4B	2.27	1.48	1.42
21	3	606	CLA	CHC-C1C	2.27	1.43	1.38
21	Z	305	CLA	CHC-C1C	2.27	1.43	1.38
21	J	102	CLA	CHB-C1B	-2.27	1.34	1.39
21	6	602	CLA	CHC-C1C	2.27	1.43	1.38
21	O	203	CLA	CHC-C1C	2.27	1.43	1.38
21	O	202	CLA	CHB-C1B	-2.27	1.34	1.39
21	B	819	CLA	CHC-C1C	2.27	1.43	1.38
21	X	604	CLA	CHC-C1C	2.27	1.43	1.38
21	G	203	CLA	CHB-C1B	-2.27	1.34	1.39
21	3	612	CLA	CHB-C1B	-2.27	1.34	1.39
22	Y	616	LUT	C28-C29	-2.27	1.41	1.45
21	A	807	CLA	CHC-C1C	2.27	1.43	1.38
21	3	609	CLA	CHB-C1B	-2.27	1.34	1.39
21	A	840	CLA	CHC-C1C	2.27	1.43	1.38
21	B	823	CLA	C1B-NB	-2.27	1.35	1.37
21	B	805	CLA	CHC-C1C	2.27	1.43	1.38
21	4	302	CLA	MG-NB	2.27	2.10	2.05
21	4	313	CLA	C3B-C4B	2.27	1.48	1.42
21	A	829	CLA	C3B-C4B	2.27	1.48	1.42
21	4	311	CLA	CHB-C1B	-2.27	1.34	1.39
21	3	602	CLA	CHC-C1C	2.27	1.43	1.38
21	A	809	CLA	C1B-NB	-2.27	1.35	1.37
21	B	814	CLA	C1B-NB	-2.27	1.35	1.37
22	X	615	LUT	C12-C13	-2.27	1.41	1.45
21	K	204	CLA	CHB-C1B	-2.27	1.34	1.39
21	6	601	CLA	CHB-C1B	-2.26	1.34	1.39
21	X	618	CLA	CHB-C1B	-2.26	1.34	1.39
21	B	840	CLA	CHC-C1C	2.26	1.43	1.38
20	Y	619	CHL	C2C-C3C	2.26	1.38	1.36
21	1	609	CLA	CHC-C1C	2.26	1.43	1.38
21	1	612	CLA	CHC-C1C	2.26	1.43	1.38
21	A	821	CLA	CHC-C1C	2.26	1.43	1.38
21	X	610	CLA	MG-NB	2.26	2.10	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	839	CLA	CHB-C1B	-2.26	1.34	1.39
21	B	827	CLA	C3B-C4B	2.26	1.48	1.42
21	J	102	CLA	CHC-C1C	2.26	1.43	1.38
21	A	820	CLA	CHB-C1B	-2.26	1.34	1.39
21	A	839	CLA	CHB-C1B	-2.26	1.34	1.39
21	Z	313	CLA	CHB-C1B	-2.26	1.34	1.39
21	B	805	CLA	C3B-C4B	2.26	1.48	1.42
20	1	601	CHL	MG-NB	2.26	2.10	2.05
21	J	101	CLA	CHC-C1C	2.26	1.43	1.38
21	2	609	CLA	CHB-C1B	-2.26	1.34	1.39
21	B	809	CLA	CHB-C1B	-2.26	1.34	1.39
21	6	612	CLA	C3B-C4B	2.26	1.48	1.42
21	3	613	CLA	MG-NB	2.26	2.10	2.05
21	Z	305	CLA	MG-NB	2.26	2.10	2.05
21	B	817	CLA	C1B-NB	-2.26	1.35	1.37
22	X	615	LUT	C32-C33	-2.26	1.41	1.45
21	A	811	CLA	MG-NB	2.26	2.10	2.05
21	K	203	CLA	CHB-C1B	-2.26	1.34	1.39
21	A	807	CLA	C3B-C4B	2.26	1.48	1.42
21	3	603	CLA	MG-NB	2.26	2.10	2.05
21	6	602	CLA	CHB-C1B	-2.26	1.34	1.39
21	A	841	CLA	CHC-C1C	2.26	1.43	1.38
21	5	609	CLA	MG-NB	2.26	2.10	2.05
21	5	613	CLA	MG-NB	2.26	2.10	2.05
21	A	835	CLA	C1B-NB	-2.26	1.35	1.37
20	Z	308	CHL	C2C-C3C	2.26	1.38	1.36
21	4	307	CLA	CHC-C1C	2.26	1.43	1.38
21	Y	614	CLA	CHC-C1C	2.26	1.43	1.38
20	4	304	CHL	C1A-CHA	2.26	1.42	1.40
21	2	603	CLA	CHC-C1C	2.26	1.43	1.38
21	3	617	CLA	CHC-C1C	2.26	1.43	1.38
21	3	617	CLA	CHB-C1B	-2.26	1.34	1.39
21	6	603	CLA	MG-NB	2.26	2.10	2.05
21	B	815	CLA	CHC-C1C	2.26	1.43	1.38
21	B	810	CLA	CHB-C1B	-2.26	1.34	1.39
22	Y	615	LUT	C28-C29	-2.26	1.41	1.45
21	B	821	CLA	C3B-C4B	2.26	1.48	1.42
21	6	613	CLA	CHC-C1C	2.26	1.43	1.38
21	A	813	CLA	C3B-C4B	2.25	1.48	1.42
21	B	831	CLA	CHC-C1C	2.25	1.43	1.38
21	H	201	CLA	CHC-C1C	2.25	1.43	1.38
21	X	610	CLA	CHB-C1B	-2.25	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	O	206	CLA	CHB-C1B	-2.25	1.34	1.39
21	A	829	CLA	CHC-C1C	2.25	1.43	1.38
22	X	615	LUT	C28-C29	-2.25	1.41	1.45
21	B	816	CLA	CHC-C1C	2.25	1.43	1.38
21	1	610	CLA	CHC-C1C	2.25	1.43	1.38
21	5	611	CLA	CHC-C1C	2.25	1.43	1.38
22	5	615	LUT	C28-C29	-2.25	1.41	1.45
21	A	803	CLA	CHC-C1C	2.25	1.43	1.38
21	J	101	CLA	CHB-C1B	-2.25	1.34	1.39
21	2	610	CLA	CHC-C1C	2.25	1.43	1.38
21	B	823	CLA	CHC-C1C	2.25	1.43	1.38
21	6	610	CLA	MG-NB	2.25	2.10	2.05
21	Y	612	CLA	MG-NB	2.25	2.10	2.05
21	B	820	CLA	C1B-NB	-2.25	1.35	1.37
21	3	614	CLA	CHB-C1B	-2.25	1.34	1.39
21	A	806	CLA	C1B-NB	-2.25	1.35	1.37
21	B	826	CLA	CHB-C1B	-2.25	1.34	1.39
21	1	605	CLA	CHC-C1C	2.25	1.43	1.38
21	5	605	CLA	CHC-C1C	2.25	1.43	1.38
21	B	817	CLA	CHC-C1C	2.25	1.43	1.38
21	B	828	CLA	CHC-C1C	2.25	1.43	1.38
21	Y	610	CLA	CHC-C1C	2.25	1.43	1.38
21	B	804	CLA	C3B-C4B	2.25	1.48	1.42
21	3	610	CLA	CHB-C1B	-2.25	1.34	1.39
21	5	604	CLA	MG-NB	2.25	2.10	2.05
21	L	303	CLA	C1B-NB	-2.25	1.35	1.37
21	B	840	CLA	CHB-C1B	-2.25	1.34	1.39
21	A	818	CLA	C1B-NB	-2.25	1.35	1.37
21	B	827	CLA	C1B-NB	-2.25	1.35	1.37
21	B	803	CLA	CHB-C1B	-2.25	1.34	1.39
21	A	831	CLA	CHC-C1C	2.24	1.43	1.38
21	X	613	CLA	CHB-C1B	-2.24	1.34	1.39
21	B	837	CLA	CHC-C1C	2.24	1.43	1.38
21	Z	312	CLA	CHB-C1B	-2.24	1.34	1.39
21	B	810	CLA	CHC-C1C	2.24	1.43	1.38
21	1	614	CLA	CHB-C1B	-2.24	1.34	1.39
21	6	614	CLA	CHB-C1B	-2.24	1.34	1.39
21	6	601	CLA	C1B-NB	-2.24	1.35	1.37
20	1	601	CHL	C3B-CAB	-2.24	1.43	1.47
21	4	307	CLA	C1B-NB	-2.24	1.35	1.37
21	5	613	CLA	CHC-C1C	2.24	1.43	1.38
21	B	813	CLA	C1B-NB	-2.24	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	L	305	CLA	MG-NB	2.24	2.10	2.05
21	4	311	CLA	CHC-C1C	2.24	1.43	1.38
21	Y	604	CLA	MG-NB	2.24	2.10	2.05
21	1	605	CLA	CHB-C1B	-2.24	1.34	1.39
21	A	823	CLA	C3B-C4B	2.24	1.48	1.42
21	B	812	CLA	C3B-C4B	2.24	1.48	1.42
21	Y	611	CLA	CHB-C1B	-2.24	1.34	1.39
21	4	309	CLA	CHC-C1C	2.24	1.43	1.38
21	6	613	CLA	CHB-C1B	-2.24	1.34	1.39
21	1	608	CLA	CHC-C1C	2.24	1.43	1.38
21	A	843	CLA	CHC-C1C	2.24	1.43	1.38
21	3	604	CLA	MG-NB	2.24	2.10	2.05
21	4	303	CLA	CHC-C1C	2.24	1.43	1.38
21	5	609	CLA	CHC-C1C	2.24	1.43	1.38
21	A	820	CLA	CHC-C1C	2.24	1.43	1.38
21	X	610	CLA	CHC-C1C	2.24	1.43	1.38
21	4	310	CLA	CHC-C1C	2.24	1.43	1.38
21	K	203	CLA	CHC-C1C	2.24	1.43	1.38
21	B	807	CLA	CHB-C1B	-2.23	1.34	1.39
21	A	807	CLA	C1B-NB	-2.23	1.35	1.37
21	1	607	CLA	CHB-C1B	-2.23	1.34	1.39
21	B	839	CLA	C3B-C4B	2.23	1.48	1.42
21	B	838	CLA	CHC-C1C	2.23	1.43	1.38
21	A	825	CLA	CHC-C1C	2.23	1.43	1.38
21	6	604	CLA	CHC-C1C	2.23	1.43	1.38
21	A	817	CLA	CHC-C1C	2.23	1.43	1.38
21	5	604	CLA	CHB-C1B	-2.23	1.34	1.39
21	3	611	CLA	MG-NC	2.23	2.11	2.06
21	2	604	CLA	CHC-C1C	2.23	1.43	1.38
20	2	614	CHL	MG-NB	2.23	2.10	2.05
21	5	607	CLA	MG-NB	2.23	2.10	2.05
21	A	829	CLA	C1B-NB	-2.23	1.35	1.37
21	O	206	CLA	CHC-C1C	2.23	1.43	1.38
21	Y	613	CLA	CHC-C1C	2.23	1.43	1.38
21	L	304	CLA	CHB-C1B	-2.23	1.34	1.39
21	A	834	CLA	C3B-C4B	2.23	1.48	1.42
21	A	841	CLA	C3B-C4B	2.23	1.48	1.42
21	A	810	CLA	C1B-NB	-2.23	1.35	1.37
21	B	835	CLA	C1B-NB	-2.23	1.35	1.37
21	B	801	CLA	CHC-C1C	2.23	1.43	1.38
21	L	304	CLA	CHC-C1C	2.23	1.43	1.38
21	6	604	CLA	MG-NB	2.23	2.10	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	839	CLA	C1B-NB	-2.22	1.35	1.37
21	B	825	CLA	CHC-C1C	2.22	1.43	1.38
21	L	303	CLA	CHC-C1C	2.22	1.43	1.38
21	X	611	CLA	CHC-C1C	2.22	1.43	1.38
21	Y	613	CLA	MG-NB	2.22	2.10	2.05
21	A	836	CLA	C1B-NB	-2.22	1.35	1.37
21	3	603	CLA	CHC-C1C	2.22	1.43	1.38
21	K	201	CLA	MG-NB	2.22	2.10	2.05
21	5	614	CLA	CHB-C1B	-2.22	1.34	1.39
21	6	608	CLA	CHC-C1C	2.22	1.43	1.38
21	4	301	CLA	CHC-C1C	2.22	1.43	1.38
21	1	613	CLA	CHB-C1B	-2.22	1.34	1.39
21	O	203	CLA	CHB-C1B	-2.22	1.34	1.39
21	A	822	CLA	CHB-C1B	-2.22	1.34	1.39
21	3	613	CLA	CHC-C1C	2.22	1.43	1.38
21	A	819	CLA	C1B-NB	-2.22	1.35	1.37
21	3	610	CLA	MG-NB	2.22	2.10	2.05
21	B	821	CLA	CHC-C1C	2.22	1.43	1.38
21	B	807	CLA	C3B-C4B	2.22	1.48	1.42
21	2	611	CLA	CHC-C1C	2.22	1.43	1.38
21	A	808	CLA	C1B-NB	-2.22	1.35	1.37
21	A	837	CLA	C1B-NB	-2.22	1.35	1.37
21	X	603	CLA	CHC-C1C	2.22	1.43	1.38
21	3	606	CLA	MG-NB	2.21	2.10	2.05
21	Z	303	CLA	CHB-C1B	-2.21	1.34	1.39
21	Y	604	CLA	CHC-C1C	2.21	1.43	1.38
21	5	605	CLA	MG-NB	2.21	2.10	2.05
21	A	801	CLA	CHB-C1B	-2.21	1.34	1.39
21	B	822	CLA	CHB-C1B	-2.21	1.34	1.39
21	B	825	CLA	C1B-NB	-2.21	1.35	1.37
21	6	613	CLA	MG-NB	2.21	2.10	2.05
21	B	837	CLA	MG-NB	2.21	2.10	2.05
21	3	603	CLA	MG-NC	2.21	2.11	2.06
21	4	302	CLA	CHC-C1C	2.21	1.43	1.38
21	B	838	CLA	C3B-C4B	2.21	1.47	1.42
21	5	608	CLA	CHB-C1B	-2.21	1.34	1.39
21	H	201	CLA	C1B-NB	-2.21	1.35	1.37
21	K	203	CLA	MG-NB	2.21	2.10	2.05
21	B	820	CLA	CHB-C1B	-2.21	1.34	1.39
21	2	608	CLA	CHC-C1C	2.21	1.43	1.38
21	A	804	CLA	CHC-C1C	2.21	1.43	1.38
21	A	811	CLA	CHC-C1C	2.21	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	5	605	CLA	CHB-C1B	-2.21	1.34	1.39
21	3	605	CLA	MG-NB	2.20	2.10	2.05
21	3	612	CLA	CHC-C1C	2.20	1.43	1.38
21	B	808	CLA	CHC-C1C	2.20	1.43	1.38
21	1	604	CLA	C1B-NB	-2.20	1.35	1.37
21	2	613	CLA	MG-NB	2.20	2.10	2.05
21	G	204	CLA	MG-NB	2.20	2.10	2.05
21	A	802	CLA	C1B-NB	-2.20	1.35	1.37
21	B	831	CLA	C1B-NB	-2.20	1.35	1.37
21	6	612	CLA	CHC-C1C	2.20	1.43	1.38
21	2	602	CLA	MG-NB	2.20	2.10	2.05
21	A	832	CLA	C1B-NB	-2.20	1.35	1.37
21	L	301	CLA	CHC-C1C	2.20	1.43	1.38
21	1	602	CLA	MG-NB	2.20	2.10	2.05
21	B	839	CLA	CHC-C1C	2.20	1.43	1.38
21	G	202	CLA	MG-NB	2.20	2.10	2.05
22	Z	315	LUT	C32-C33	-2.20	1.41	1.45
21	B	813	CLA	CHB-C1B	-2.20	1.34	1.39
21	Y	610	CLA	MG-NB	2.20	2.10	2.05
21	A	828	CLA	MG-NB	2.20	2.10	2.05
21	2	610	CLA	MG-NB	2.20	2.10	2.05
21	X	612	CLA	CHB-C1B	-2.20	1.34	1.39
21	B	801	CLA	MG-NB	2.20	2.10	2.05
20	Z	309	CHL	C2C-C3C	2.19	1.38	1.36
21	A	839	CLA	CHC-C1C	2.19	1.43	1.38
21	B	810	CLA	C3B-C2B	-2.19	1.35	1.44
21	B	834	CLA	MG-NB	2.19	2.10	2.05
21	A	812	CLA	C1B-NB	-2.19	1.35	1.37
21	A	825	CLA	C1B-NB	-2.19	1.35	1.37
21	A	841	CLA	C1B-NB	-2.19	1.35	1.37
21	Y	610	CLA	CHB-C1B	-2.19	1.34	1.39
21	X	604	CLA	MG-NB	2.19	2.10	2.05
21	B	804	CLA	CHC-C1C	2.19	1.43	1.38
22	Z	315	LUT	C28-C29	-2.19	1.41	1.45
21	4	303	CLA	MG-NB	2.19	2.10	2.05
21	1	607	CLA	CHC-C1C	2.19	1.43	1.38
21	K	204	CLA	MG-NB	2.19	2.10	2.05
21	Y	612	CLA	MG-NC	2.19	2.11	2.06
22	X	614	LUT	C12-C13	-2.19	1.41	1.45
21	2	611	CLA	MG-NC	2.19	2.11	2.06
21	O	202	CLA	MG-NC	2.19	2.11	2.06
22	X	614	LUT	C28-C29	-2.19	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	3	613	CLA	MG-NC	2.19	2.11	2.06
21	5	607	CLA	CHB-C1B	-2.19	1.34	1.39
21	A	817	CLA	C1B-NB	-2.19	1.35	1.37
21	A	818	CLA	CHC-C1C	2.19	1.43	1.38
21	B	804	CLA	C1B-NB	-2.19	1.35	1.37
21	J	101	CLA	MG-NB	2.19	2.10	2.05
21	A	822	CLA	C1B-NB	-2.19	1.35	1.37
21	F	304	CLA	C1B-NB	-2.18	1.35	1.37
21	Z	303	CLA	C1B-NB	-2.18	1.35	1.37
21	Y	614	CLA	MG-NB	2.18	2.10	2.05
31	Z	316	NEX	C1-C6	-2.18	1.50	1.54
20	5	601	CHL	C3B-CAB	-2.18	1.43	1.47
21	3	617	CLA	C1B-NB	-2.18	1.35	1.37
21	A	820	CLA	C1B-NB	-2.18	1.35	1.37
21	6	608	CLA	MG-NB	2.18	2.10	2.05
21	L	305	CLA	C1B-NB	-2.18	1.35	1.37
21	J	102	CLA	MG-NB	2.18	2.10	2.05
21	L	301	CLA	MG-NB	2.18	2.10	2.05
21	A	810	CLA	CHB-C1B	-2.18	1.34	1.39
21	2	618	CLA	CHC-C1C	2.18	1.43	1.38
21	1	612	CLA	C1B-NB	-2.18	1.35	1.37
21	O	207	CLA	CHB-C1B	-2.18	1.34	1.39
21	L	304	CLA	C1B-NB	-2.18	1.35	1.37
21	O	202	CLA	CHC-C1C	2.18	1.43	1.38
20	5	601	CHL	C2C-C3C	2.18	1.38	1.36
21	O	202	CLA	MG-NB	2.18	2.10	2.05
21	4	310	CLA	C1B-NB	-2.18	1.35	1.37
21	A	830	CLA	C1B-NB	-2.18	1.35	1.37
21	6	611	CLA	MG-NB	2.18	2.10	2.05
21	4	310	CLA	MG-NC	2.18	2.11	2.06
21	A	805	CLA	C1B-NB	-2.18	1.35	1.37
21	Z	310	CLA	CHB-C1B	-2.18	1.34	1.39
21	A	842	CLA	MG-NB	2.18	2.10	2.05
20	3	608	CHL	C3B-CAB	-2.18	1.43	1.47
21	A	838	CLA	CHC-C1C	2.18	1.42	1.38
21	Z	310	CLA	MG-NB	2.18	2.10	2.05
21	B	832	CLA	CHB-C1B	-2.18	1.34	1.39
21	A	827	CLA	C1B-NB	-2.17	1.35	1.37
21	2	604	CLA	MG-NB	2.17	2.10	2.05
21	3	614	CLA	MG-NB	2.17	2.10	2.05
21	X	613	CLA	MG-NB	2.17	2.10	2.05
21	B	827	CLA	CHC-C1C	2.17	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	5	612	CLA	MG-NB	2.17	2.10	2.05
21	1	603	CLA	CHC-C1C	2.17	1.42	1.38
21	1	611	CLA	MG-NB	2.17	2.10	2.05
21	Y	612	CLA	CHC-C1C	2.17	1.42	1.38
21	A	803	CLA	C1B-NB	-2.17	1.35	1.37
21	4	312	CLA	MG-NB	2.17	2.10	2.05
21	2	612	CLA	C1B-NB	-2.17	1.35	1.37
21	X	602	CLA	MG-NB	2.17	2.10	2.05
21	A	814	CLA	C1B-NB	-2.17	1.35	1.37
21	B	821	CLA	MG-NB	2.17	2.10	2.05
21	A	824	CLA	C1B-NB	-2.17	1.35	1.37
21	5	611	CLA	MG-NB	2.17	2.10	2.05
21	A	818	CLA	C3B-C4B	2.17	1.47	1.42
21	A	812	CLA	CHC-C1C	2.17	1.42	1.38
21	2	612	CLA	CHB-C1B	-2.17	1.34	1.39
21	4	313	CLA	CHC-C1C	2.17	1.42	1.38
21	A	823	CLA	CHC-C1C	2.17	1.42	1.38
21	4	308	CLA	CHB-C1B	-2.16	1.34	1.39
21	6	603	CLA	CHC-C1C	2.16	1.42	1.38
21	B	807	CLA	MG-NC	2.16	2.11	2.06
21	6	608	CLA	C1B-NB	-2.16	1.35	1.37
20	2	607	CHL	C3B-CAB	-2.16	1.43	1.47
21	X	618	CLA	MG-NC	2.16	2.11	2.06
21	4	303	CLA	C1B-NB	-2.16	1.35	1.37
21	B	831	CLA	MG-NC	2.16	2.11	2.06
21	B	806	CLA	C1B-NB	-2.16	1.35	1.37
21	A	816	CLA	MG-NB	2.16	2.10	2.05
21	Y	604	CLA	MG-NC	2.16	2.11	2.06
21	Y	611	CLA	MG-NC	2.16	2.11	2.06
21	B	807	CLA	CHC-C1C	2.16	1.42	1.38
21	B	814	CLA	MG-NB	2.16	2.10	2.05
21	B	816	CLA	C3B-C4B	2.16	1.47	1.42
21	X	611	CLA	MG-NC	2.16	2.11	2.06
21	B	810	CLA	C4B-C3B	2.16	1.48	1.43
21	3	602	CLA	MG-NB	2.16	2.10	2.05
21	3	606	CLA	C1B-NB	-2.16	1.35	1.37
21	6	611	CLA	MG-NC	2.16	2.11	2.06
21	Y	602	CLA	MG-NB	2.16	2.10	2.05
21	B	819	CLA	C1B-NB	-2.15	1.35	1.37
21	6	614	CLA	MG-NB	2.15	2.10	2.05
21	F	304	CLA	MG-NB	2.15	2.10	2.05
21	6	614	CLA	CHC-C1C	2.15	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	833	CLA	CHC-C1C	2.15	1.42	1.38
21	A	819	CLA	CHC-C1C	2.15	1.42	1.38
21	5	605	CLA	MG-NC	2.15	2.11	2.06
21	2	603	CLA	C1B-NB	-2.15	1.35	1.37
21	X	612	CLA	MG-NC	2.15	2.11	2.06
21	4	309	CLA	MG-NB	2.15	2.10	2.05
21	A	843	CLA	C1B-NB	-2.15	1.35	1.37
21	Z	311	CLA	MG-NC	2.15	2.11	2.06
21	Z	312	CLA	MG-NB	2.15	2.10	2.05
20	1	606	CHL	C3B-CAB	-2.15	1.43	1.47
21	L	305	CLA	CHC-C1C	2.15	1.42	1.38
21	5	613	CLA	MG-NC	2.15	2.11	2.06
21	G	202	CLA	C1B-NB	-2.15	1.35	1.37
21	Z	305	CLA	MG-NC	2.15	2.11	2.06
21	3	607	CLA	MG-NB	2.15	2.10	2.05
21	A	825	CLA	MG-NB	2.15	2.10	2.05
21	B	839	CLA	MG-NC	2.15	2.11	2.06
21	1	608	CLA	MG-NB	2.15	2.10	2.05
21	3	612	CLA	MG-NB	2.15	2.10	2.05
21	X	603	CLA	MG-NB	2.15	2.10	2.05
21	Y	603	CLA	C1B-NB	-2.15	1.35	1.37
21	B	834	CLA	MG-NC	2.15	2.11	2.06
21	4	301	CLA	C1B-NB	-2.14	1.35	1.37
21	A	833	CLA	C1B-NB	-2.14	1.35	1.37
21	K	202	CLA	MG-NB	2.14	2.10	2.05
21	B	812	CLA	CHC-C1C	2.14	1.42	1.38
21	6	604	CLA	C1B-NB	-2.14	1.35	1.37
21	A	829	CLA	MG-NB	2.14	2.10	2.05
21	B	823	CLA	MG-NB	2.14	2.10	2.05
21	2	603	CLA	MG-NB	2.14	2.10	2.05
21	1	611	CLA	C1B-NB	-2.14	1.35	1.37
21	6	603	CLA	MG-NC	2.14	2.11	2.06
21	4	311	CLA	MG-NB	2.14	2.10	2.05
21	A	842	CLA	CHC-C1C	2.14	1.42	1.38
21	B	810	CLA	MG-NB	2.14	2.10	2.05
21	1	611	CLA	MG-NC	2.14	2.11	2.06
21	2	613	CLA	MG-NC	2.14	2.11	2.06
21	A	813	CLA	CHC-C1C	2.14	1.42	1.38
21	B	830	CLA	MG-NB	2.14	2.10	2.05
21	6	602	CLA	C1B-NB	-2.14	1.35	1.37
21	A	834	CLA	CHC-C1C	2.14	1.42	1.38
21	1	610	CLA	MG-NC	2.14	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	2	606	CHL	C3B-CAB	-2.14	1.43	1.47
21	Y	614	CLA	MG-NC	2.14	2.11	2.06
21	X	609	CLA	CHB-C1B	-2.14	1.34	1.39
21	1	605	CLA	MG-NB	2.14	2.10	2.05
21	B	821	CLA	MG-NC	2.14	2.11	2.06
21	4	302	CLA	MG-NC	2.14	2.11	2.06
21	A	839	CLA	C1B-NB	-2.14	1.35	1.37
21	B	828	CLA	C1B-NB	-2.14	1.35	1.37
21	A	815	CLA	MG-NB	2.13	2.10	2.05
21	A	839	CLA	MG-NB	2.13	2.10	2.05
21	Y	603	CLA	MG-NB	2.13	2.10	2.05
21	6	612	CLA	MG-NC	2.13	2.11	2.06
21	6	610	CLA	MG-NC	2.13	2.11	2.06
21	A	804	CLA	MG-NB	2.13	2.10	2.05
21	O	203	CLA	MG-NB	2.13	2.10	2.05
21	1	610	CLA	C1B-NB	-2.13	1.35	1.37
21	A	816	CLA	C1B-NB	-2.13	1.35	1.37
21	A	816	CLA	MG-NC	2.13	2.11	2.06
21	1	604	CLA	MG-NB	2.13	2.10	2.05
21	6	601	CLA	MG-NC	2.13	2.11	2.06
21	B	830	CLA	C1B-NB	-2.13	1.35	1.37
21	A	821	CLA	C1B-NB	-2.13	1.35	1.37
21	G	202	CLA	MG-NC	2.13	2.11	2.06
21	1	613	CLA	MG-NB	2.13	2.10	2.05
21	3	614	CLA	MG-NC	2.13	2.11	2.06
21	2	611	CLA	C1B-NB	-2.13	1.35	1.37
21	B	806	CLA	MG-NB	2.13	2.10	2.05
21	J	101	CLA	MG-NC	2.13	2.11	2.06
21	A	819	CLA	MG-NB	2.13	2.10	2.05
21	A	825	CLA	MG-NC	2.13	2.11	2.06
21	K	201	CLA	MG-NC	2.13	2.11	2.06
21	5	612	CLA	C1B-NB	-2.13	1.35	1.37
20	6	607	CHL	C3B-CAB	-2.13	1.43	1.47
21	B	826	CLA	MG-NB	2.13	2.10	2.05
20	2	605	CHL	C3B-CAB	-2.13	1.43	1.47
21	3	605	CLA	MG-NC	2.12	2.11	2.06
21	A	803	CLA	MG-NB	2.12	2.10	2.05
21	Y	602	CLA	C1B-NB	-2.12	1.35	1.37
21	Y	611	CLA	C1B-NB	-2.12	1.35	1.37
21	A	823	CLA	MG-NB	2.12	2.10	2.05
21	L	303	CLA	MG-NB	2.12	2.10	2.05
21	3	610	CLA	MG-NC	2.12	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	609	CLA	MG-NB	2.12	2.10	2.05
21	1	609	CLA	C1B-NB	-2.12	1.35	1.37
21	2	610	CLA	MG-NC	2.12	2.11	2.06
21	5	604	CLA	MG-NC	2.12	2.11	2.06
21	B	840	CLA	MG-NB	2.12	2.10	2.05
21	J	102	CLA	MG-NC	2.12	2.11	2.06
21	3	609	CLA	C1B-NB	-2.12	1.35	1.37
21	B	838	CLA	MG-NC	2.12	2.11	2.06
21	X	610	CLA	MG-NC	2.12	2.11	2.06
21	A	841	CLA	MG-NC	2.12	2.11	2.06
21	4	310	CLA	MG-NB	2.12	2.10	2.05
21	1	610	CLA	MG-NB	2.12	2.10	2.05
21	G	203	CLA	MG-NB	2.12	2.10	2.05
21	2	609	CLA	C1B-NB	-2.12	1.35	1.37
21	A	801	CLA	C1B-NB	-2.12	1.35	1.37
21	A	828	CLA	C1B-NB	-2.12	1.35	1.37
21	B	826	CLA	C1B-NB	-2.12	1.35	1.37
21	K	202	CLA	MG-NC	2.12	2.11	2.06
21	4	313	CLA	MG-NB	2.12	2.10	2.05
21	A	823	CLA	MG-NC	2.12	2.11	2.06
21	B	818	CLA	MG-NC	2.12	2.11	2.06
21	2	608	CLA	MG-NB	2.12	2.10	2.05
21	2	618	CLA	C1B-NB	-2.11	1.35	1.37
21	5	614	CLA	MG-NB	2.11	2.10	2.05
21	A	831	CLA	MG-NB	2.11	2.10	2.05
21	B	823	CLA	MG-NC	2.11	2.11	2.06
21	1	603	CLA	C1B-NB	-2.11	1.35	1.37
21	5	611	CLA	MG-NC	2.11	2.11	2.06
21	4	307	CLA	MG-NB	2.11	2.10	2.05
21	4	301	CLA	MG-NB	2.11	2.10	2.05
21	2	602	CLA	C1B-NB	-2.11	1.35	1.37
21	B	810	CLA	C1B-NB	-2.11	1.35	1.37
21	5	612	CLA	MG-NC	2.11	2.11	2.06
21	3	607	CLA	MG-NC	2.11	2.11	2.06
21	B	819	CLA	MG-NC	2.11	2.11	2.06
21	A	802	CLA	C3D-C4D	-2.11	1.39	1.44
21	O	203	CLA	MG-NC	2.11	2.11	2.06
21	2	608	CLA	C1B-NB	-2.11	1.35	1.37
21	A	823	CLA	C1B-NB	-2.11	1.35	1.37
21	B	804	CLA	MG-NC	2.11	2.11	2.06
21	1	602	CLA	CHC-C1C	2.11	1.42	1.38
21	5	603	CLA	C1B-NB	-2.11	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	X	603	CLA	MG-NC	2.11	2.11	2.06
21	Z	313	CLA	MG-NC	2.11	2.11	2.06
21	B	818	CLA	C1B-NB	-2.11	1.35	1.37
21	B	821	CLA	C1B-NB	-2.11	1.35	1.37
21	B	822	CLA	C1B-NB	-2.11	1.35	1.37
21	A	811	CLA	MG-NC	2.11	2.11	2.06
21	G	203	CLA	MG-NC	2.11	2.11	2.06
21	6	613	CLA	MG-NC	2.11	2.11	2.06
21	A	842	CLA	MG-NC	2.11	2.11	2.06
21	1	607	CLA	MG-NB	2.11	2.10	2.05
21	Z	304	CLA	MG-NB	2.11	2.10	2.05
21	G	204	CLA	MG-NC	2.11	2.11	2.06
21	O	207	CLA	MG-NB	2.11	2.10	2.05
21	L	301	CLA	MG-NC	2.11	2.11	2.06
21	Y	603	CLA	MG-NC	2.11	2.11	2.06
21	A	815	CLA	C1B-NB	-2.11	1.35	1.37
21	A	817	CLA	MG-NB	2.11	2.10	2.05
21	A	839	CLA	MG-NC	2.11	2.11	2.06
21	2	618	CLA	MG-NB	2.11	2.10	2.05
21	3	612	CLA	MG-NC	2.10	2.11	2.06
21	O	207	CLA	MG-NC	2.10	2.11	2.06
21	Y	602	CLA	MG-NC	2.10	2.11	2.06
21	K	202	CLA	C1B-NB	-2.10	1.35	1.37
21	Y	614	CLA	C1B-NB	-2.10	1.35	1.37
20	2	601	CHL	C3B-CAB	-2.10	1.43	1.47
21	O	206	CLA	MG-NB	2.10	2.10	2.05
20	6	606	CHL	C3B-CAB	-2.10	1.43	1.47
21	3	605	CLA	C1B-NB	-2.10	1.35	1.37
21	B	804	CLA	MG-NB	2.10	2.10	2.05
21	L	305	CLA	MG-NC	2.10	2.11	2.06
21	2	610	CLA	C1B-NB	-2.10	1.35	1.37
21	B	831	CLA	MG-NB	2.10	2.10	2.05
21	6	612	CLA	MG-NB	2.10	2.09	2.05
21	G	204	CLA	C1B-NB	-2.10	1.35	1.37
21	A	843	CLA	MG-NB	2.10	2.09	2.05
21	B	805	CLA	MG-NB	2.10	2.09	2.05
21	6	602	CLA	MG-NC	2.10	2.11	2.06
21	B	802	CLA	CHB-C1B	-2.10	1.34	1.39
21	X	602	CLA	MG-NC	2.10	2.11	2.06
21	B	825	CLA	MG-NC	2.10	2.11	2.06
21	3	603	CLA	C1B-NB	-2.10	1.35	1.37
21	Z	304	CLA	C1B-NB	-2.10	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	827	CLA	MG-NB	2.09	2.09	2.05
21	3	602	CLA	C1B-NB	-2.09	1.35	1.37
21	3	609	CLA	MG-NB	2.09	2.09	2.05
21	X	604	CLA	MG-NC	2.09	2.11	2.06
21	O	207	CLA	C1B-NB	-2.09	1.35	1.37
21	A	833	CLA	MG-NC	2.09	2.11	2.06
21	Y	610	CLA	MG-NC	2.09	2.11	2.06
21	B	803	CLA	MG-NB	2.09	2.09	2.05
21	B	838	CLA	MG-NB	2.09	2.09	2.05
21	4	311	CLA	C1B-NB	-2.09	1.35	1.37
21	X	603	CLA	C1B-NB	-2.09	1.35	1.37
21	1	612	CLA	MG-NB	2.09	2.09	2.05
20	4	304	CHL	C3B-CAB	-2.09	1.43	1.47
21	1	605	CLA	MG-NC	2.09	2.11	2.06
21	1	605	CLA	C1B-NB	-2.09	1.35	1.37
21	B	834	CLA	C1B-NB	-2.09	1.35	1.37
21	2	603	CLA	MG-NC	2.09	2.11	2.06
21	2	604	CLA	MG-NC	2.09	2.11	2.06
21	4	311	CLA	MG-NC	2.09	2.11	2.06
21	1	603	CLA	MG-NB	2.09	2.09	2.05
21	5	602	CLA	MG-NC	2.09	2.11	2.06
21	5	603	CLA	MG-NC	2.09	2.11	2.06
21	6	604	CLA	MG-NC	2.09	2.11	2.06
21	A	813	CLA	MG-NB	2.09	2.09	2.05
21	A	834	CLA	MG-NB	2.09	2.09	2.05
21	A	843	CLA	MG-NC	2.09	2.11	2.06
21	3	602	CLA	MG-NC	2.09	2.11	2.06
21	1	607	CLA	C1B-NB	-2.09	1.35	1.37
21	A	807	CLA	MG-NB	2.08	2.09	2.05
21	A	817	CLA	MG-NC	2.08	2.11	2.06
21	A	802	CLA	MG-NC	2.08	2.11	2.06
20	4	304	CHL	C2C-C3C	2.08	1.38	1.36
21	5	603	CLA	MG-NB	2.08	2.09	2.05
21	4	313	CLA	MG-NC	2.08	2.11	2.06
21	B	814	CLA	MG-NC	2.08	2.11	2.06
21	A	824	CLA	MG-NC	2.08	2.11	2.06
20	Y	601	CHL	C3B-CAB	-2.08	1.43	1.47
21	6	614	CLA	MG-NC	2.08	2.11	2.06
21	Z	312	CLA	MG-NC	2.08	2.11	2.06
20	1	601	CHL	C2C-C3C	2.08	1.38	1.36
21	5	610	CLA	MG-NB	2.08	2.09	2.05
21	A	821	CLA	MG-NC	2.08	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	6	609	CLA	MG-NB	2.08	2.09	2.05
21	3	607	CLA	C1B-NB	-2.08	1.35	1.37
21	A	829	CLA	MG-NC	2.08	2.11	2.06
21	A	838	CLA	MG-NC	2.08	2.11	2.06
21	X	609	CLA	MG-NB	2.08	2.09	2.05
21	Z	304	CLA	MG-NC	2.08	2.11	2.06
20	Z	309	CHL	C3B-CAB	-2.08	1.43	1.47
21	4	302	CLA	C1B-NB	-2.08	1.35	1.37
21	A	801	CLA	MG-NB	2.08	2.09	2.05
21	X	613	CLA	MG-NC	2.08	2.11	2.06
21	X	602	CLA	C1B-NB	-2.08	1.35	1.37
21	1	609	CLA	MG-NC	2.08	2.11	2.06
21	4	307	CLA	MG-NC	2.08	2.11	2.06
21	A	834	CLA	MG-NC	2.08	2.11	2.06
20	2	601	CHL	C2C-C3C	2.08	1.38	1.36
21	B	815	CLA	MG-NC	2.08	2.11	2.06
21	2	604	CLA	C1B-NB	-2.07	1.35	1.37
21	4	309	CLA	MG-NC	2.07	2.11	2.06
21	B	827	CLA	MG-NC	2.07	2.11	2.06
21	B	837	CLA	MG-NC	2.07	2.11	2.06
21	O	202	CLA	C1B-NB	-2.07	1.35	1.37
21	Y	611	CLA	MG-NB	2.07	2.09	2.05
21	A	814	CLA	MG-NB	2.07	2.09	2.05
21	B	835	CLA	MG-NB	2.07	2.09	2.05
21	A	809	CLA	MG-NC	2.07	2.11	2.06
21	2	612	CLA	MG-NC	2.07	2.11	2.06
21	B	840	CLA	MG-NC	2.07	2.11	2.06
21	5	611	CLA	C1B-NB	-2.07	1.35	1.37
21	B	817	CLA	MG-NB	2.07	2.09	2.05
20	Z	301	CHL	C3B-CAB	-2.07	1.43	1.47
21	6	603	CLA	C1B-NB	-2.07	1.35	1.37
21	B	840	CLA	C1B-NB	-2.07	1.35	1.37
21	A	812	CLA	MG-NC	2.07	2.11	2.06
21	Y	613	CLA	C1B-NB	-2.07	1.35	1.37
21	B	828	CLA	MG-NB	2.07	2.09	2.05
21	A	830	CLA	MG-NB	2.07	2.09	2.05
20	X	606	CHL	C3B-CAB	-2.07	1.43	1.47
21	B	835	CLA	MG-NC	2.07	2.11	2.06
21	B	810	CLA	MG-NC	2.06	2.11	2.06
21	B	819	CLA	MG-NB	2.06	2.09	2.05
21	B	822	CLA	MG-NB	2.06	2.09	2.05
21	B	803	CLA	C1B-NB	-2.06	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4	308	CLA	MG-NB	2.06	2.09	2.05
21	1	614	CLA	C1B-NB	-2.06	1.35	1.37
21	A	815	CLA	MG-NC	2.06	2.11	2.06
21	A	826	CLA	MG-NC	2.06	2.11	2.06
21	5	609	CLA	MG-NC	2.06	2.11	2.06
21	A	804	CLA	MG-NC	2.06	2.11	2.06
21	A	820	CLA	MG-NC	2.06	2.11	2.06
21	3	614	CLA	C1B-NB	-2.06	1.35	1.37
21	4	308	CLA	C1B-NB	-2.06	1.35	1.37
21	A	842	CLA	C1B-NB	-2.06	1.35	1.37
21	B	818	CLA	MG-NB	2.06	2.09	2.05
21	2	612	CLA	MG-NB	2.06	2.09	2.05
21	6	609	CLA	C1B-NB	-2.06	1.35	1.37
21	A	841	CLA	MG-NB	2.06	2.09	2.05
21	1	604	CLA	MG-NC	2.06	2.11	2.06
21	3	604	CLA	MG-NC	2.06	2.11	2.06
21	3	606	CLA	MG-NC	2.06	2.11	2.06
21	5	610	CLA	C1B-NB	-2.06	1.35	1.37
21	J	101	CLA	C1B-NB	-2.06	1.35	1.37
21	Z	312	CLA	C1B-NB	-2.06	1.35	1.37
21	B	806	CLA	MG-NC	2.06	2.11	2.06
20	Z	306	CHL	C3B-CAB	-2.06	1.43	1.47
21	F	304	CLA	MG-NC	2.06	2.11	2.06
21	A	833	CLA	MG-NB	2.06	2.09	2.05
21	3	617	CLA	MG-NC	2.06	2.11	2.06
20	Y	607	CHL	C3B-CAB	-2.06	1.43	1.47
21	B	815	CLA	MG-NB	2.06	2.09	2.05
21	B	833	CLA	MG-NB	2.06	2.09	2.05
21	1	608	CLA	C1B-NB	-2.06	1.35	1.37
21	K	204	CLA	MG-NC	2.06	2.11	2.06
21	4	312	CLA	MG-NC	2.05	2.11	2.06
21	B	808	CLA	MG-NC	2.05	2.11	2.06
20	6	605	CHL	C3B-CAB	-2.05	1.43	1.47
21	A	818	CLA	C3D-C4D	-2.05	1.39	1.44
21	1	603	CLA	MG-NC	2.05	2.11	2.06
21	B	808	CLA	MG-NB	2.05	2.09	2.05
21	B	812	CLA	MG-NB	2.05	2.09	2.05
21	B	801	CLA	MG-NC	2.05	2.11	2.06
21	2	602	CLA	MG-NC	2.05	2.11	2.06
20	Y	605	CHL	C3B-CAB	-2.05	1.43	1.47
20	Y	619	CHL	C3B-CAB	-2.05	1.43	1.47
21	K	203	CLA	MG-NC	2.05	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	6	601	CLA	MG-NB	2.05	2.09	2.05
21	B	836	CLA	C3D-C4D	-2.05	1.39	1.44
21	O	206	CLA	C1B-NB	-2.05	1.35	1.37
21	5	607	CLA	MG-NC	2.05	2.11	2.06
21	A	838	CLA	MG-NB	2.05	2.09	2.05
21	L	304	CLA	MG-NC	2.05	2.11	2.06
20	2	605	CHL	CAC-C3C	2.05	1.53	1.50
21	A	806	CLA	MG-NB	2.05	2.09	2.05
21	L	303	CLA	MG-NC	2.05	2.11	2.06
21	1	602	CLA	MG-NC	2.04	2.11	2.06
21	6	609	CLA	MG-NC	2.04	2.11	2.06
21	A	808	CLA	MG-NB	2.04	2.09	2.05
21	H	201	CLA	MG-NB	2.04	2.09	2.05
21	A	836	CLA	MG-NC	2.04	2.11	2.06
21	5	614	CLA	C1B-NB	-2.04	1.35	1.37
21	G	203	CLA	C1B-NB	-2.04	1.35	1.37
21	A	821	CLA	MG-NB	2.04	2.09	2.05
21	6	602	CLA	MG-NB	2.04	2.09	2.05
21	A	811	CLA	C1B-NB	-2.04	1.35	1.37
20	5	606	CHL	C3B-CAB	-2.04	1.43	1.47
20	2	614	CHL	C3B-CAB	-2.04	1.43	1.47
20	4	305	CHL	C3B-CAB	-2.04	1.43	1.47
20	6	615	CHL	C2C-C3C	2.04	1.38	1.36
21	Y	610	CLA	C1B-NB	-2.04	1.35	1.37
21	6	608	CLA	MG-NC	2.04	2.11	2.06
21	A	810	CLA	MG-NC	2.04	2.11	2.06
21	A	805	CLA	MG-NB	2.04	2.09	2.05
21	4	312	CLA	C1B-NB	-2.04	1.35	1.37
21	A	812	CLA	MG-NB	2.04	2.09	2.05
21	Z	303	CLA	MG-NB	2.04	2.09	2.05
20	Y	605	CHL	O1D-CGD	2.04	1.26	1.21
21	3	612	CLA	C1B-NB	-2.04	1.35	1.37
21	B	830	CLA	MG-NC	2.03	2.11	2.06
21	A	807	CLA	MG-NC	2.03	2.11	2.06
21	3	604	CLA	C1B-NB	-2.03	1.35	1.37
21	O	206	CLA	MG-NC	2.03	2.11	2.06
21	A	809	CLA	MG-NB	2.03	2.09	2.05
21	A	837	CLA	MG-NC	2.03	2.11	2.06
21	B	805	CLA	MG-NC	2.03	2.11	2.06
21	K	204	CLA	C1B-NB	-2.03	1.35	1.37
21	1	614	CLA	MG-NB	2.03	2.09	2.05
20	Z	301	CHL	O1D-CGD	2.03	1.26	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	837	CLA	MG-NB	2.03	2.09	2.05
21	2	609	CLA	MG-NC	2.03	2.11	2.06
21	A	836	CLA	MG-NB	2.03	2.09	2.05
20	X	605	CHL	O1D-CGD	2.03	1.26	1.21
21	4	301	CLA	MG-NC	2.03	2.11	2.06
21	Z	310	CLA	MG-NC	2.03	2.11	2.06
20	Y	609	CHL	C3B-CAB	-2.03	1.43	1.47
21	A	832	CLA	MG-NB	2.03	2.09	2.05
21	1	608	CLA	MG-NC	2.03	2.11	2.06
21	1	602	CLA	C1B-NB	-2.03	1.35	1.37
21	4	309	CLA	C1B-NB	-2.03	1.35	1.37
20	Y	606	CHL	O1D-CGD	2.03	1.26	1.21
21	1	612	CLA	MG-NC	2.03	2.11	2.06
21	A	819	CLA	MG-NC	2.03	2.11	2.06
21	3	613	CLA	CAA-C2A	2.03	1.57	1.53
21	A	818	CLA	MG-NC	2.03	2.11	2.06
21	B	832	CLA	MG-NC	2.03	2.11	2.06
21	L	304	CLA	MG-NB	2.02	2.09	2.05
20	X	608	CHL	O1D-CGD	2.02	1.26	1.21
21	B	820	CLA	MG-NC	2.02	2.11	2.06
21	5	602	CLA	MG-NB	2.02	2.09	2.05
20	Z	308	CHL	O1D-CGD	2.02	1.26	1.21
21	A	808	CLA	MG-NC	2.02	2.11	2.06
21	A	827	CLA	MG-NC	2.02	2.11	2.06
21	A	804	CLA	C1B-NB	-2.02	1.35	1.37
21	K	201	CLA	C1B-NB	-2.02	1.35	1.37
21	A	807	CLA	C3D-C4D	-2.02	1.39	1.44
20	Y	609	CHL	O1D-CGD	2.02	1.26	1.21
21	X	609	CLA	C1B-NB	-2.02	1.35	1.37
21	2	609	CLA	MG-NB	2.02	2.09	2.05
21	B	839	CLA	MG-NB	2.02	2.09	2.05
20	Z	307	CHL	C3B-CAB	-2.02	1.43	1.47
21	3	609	CLA	MG-NC	2.02	2.11	2.06
21	B	807	CLA	C1B-NB	-2.02	1.35	1.37
21	B	837	CLA	C1B-NB	-2.02	1.35	1.37
21	Y	612	CLA	C1B-NB	-2.02	1.35	1.37
20	X	608	CHL	C3B-CAB	-2.02	1.43	1.47
20	Z	308	CHL	C3B-CAB	-2.02	1.43	1.47
20	X	606	CHL	O1D-CGD	2.02	1.26	1.21
21	B	833	CLA	MG-NC	2.02	2.11	2.06
20	Z	302	CHL	O1D-CGD	2.02	1.26	1.21
21	A	801	CLA	MG-NC	2.02	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	Y	607	CHL	O1D-CGD	2.02	1.26	1.21
21	B	826	CLA	MG-NC	2.02	2.11	2.06
21	A	820	CLA	MG-NB	2.01	2.09	2.05
21	A	824	CLA	MG-NB	2.01	2.09	2.05
21	B	836	CLA	MG-NC	2.01	2.11	2.06
20	X	601	CHL	C3B-CAB	-2.01	1.43	1.47
20	Y	608	CHL	O1D-CGD	2.01	1.26	1.21
21	5	609	CLA	C1B-NB	-2.01	1.35	1.37
21	J	102	CLA	C1B-NB	-2.01	1.35	1.37
21	5	610	CLA	MG-NC	2.01	2.11	2.06
21	B	817	CLA	MG-NC	2.01	2.11	2.06
20	X	601	CHL	O1D-CGD	2.01	1.26	1.21
21	1	607	CLA	MG-NC	2.01	2.11	2.06
21	B	812	CLA	C3D-C4D	-2.01	1.39	1.44
21	Y	604	CLA	C1B-NB	-2.01	1.35	1.37
21	B	832	CLA	MG-NB	2.01	2.09	2.05
21	6	611	CLA	C1B-NB	-2.01	1.35	1.37
21	X	613	CLA	C1B-NB	-2.01	1.35	1.37
21	A	831	CLA	MG-NC	2.01	2.11	2.06
21	A	814	CLA	MG-NC	2.01	2.11	2.06
21	B	809	CLA	C3D-C4D	-2.01	1.39	1.44
21	2	613	CLA	C1B-NB	-2.01	1.35	1.37
21	L	301	CLA	C1B-NB	-2.01	1.35	1.37
21	A	837	CLA	C3D-C4D	-2.01	1.39	1.44
21	2	618	CLA	MG-NC	2.01	2.11	2.06
21	B	804	CLA	C3D-C4D	-2.01	1.39	1.44
21	Z	313	CLA	C1B-NB	-2.01	1.35	1.37
22	Z	315	LUT	C12-C13	-2.00	1.41	1.45
21	A	832	CLA	C3D-C4D	-2.00	1.39	1.44
21	A	840	CLA	MG-NC	2.00	2.11	2.06
20	Z	306	CHL	O1D-CGD	2.00	1.26	1.21
21	B	822	CLA	C3D-C4D	-2.00	1.39	1.44
21	B	829	CLA	C3D-C4D	-2.00	1.39	1.44
21	B	801	CLA	C1B-NB	-2.00	1.35	1.37
21	A	806	CLA	C3D-C4D	-2.00	1.39	1.44
20	X	607	CHL	O1D-CGD	2.00	1.26	1.21
21	B	812	CLA	MG-NC	2.00	2.11	2.06
21	A	822	CLA	MG-NC	2.00	2.11	2.06
21	A	827	CLA	C3D-C4D	-2.00	1.39	1.44
21	Y	613	CLA	MG-NC	2.00	2.11	2.06
21	3	611	CLA	C1B-NB	-2.00	1.35	1.37
21	1	614	CLA	MG-NC	2.00	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	813	CLA	C3D-C4D	-2.00	1.39	1.44
21	6	614	CLA	C1B-NB	-2.00	1.35	1.37

All (2611) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2	605	CHL	C1B-CHB-C4A	13.88	129.89	121.39
20	1	601	CHL	C1B-CHB-C4A	13.04	129.38	121.39
20	6	615	CHL	C1B-CHB-C4A	12.95	129.33	121.39
20	4	314	CHL	C1B-CHB-C4A	12.93	129.31	121.39
20	5	606	CHL	C1B-CHB-C4A	12.87	129.27	121.39
20	X	606	CHL	C1B-CHB-C4A	12.83	129.25	121.39
20	Y	609	CHL	C1B-CHB-C4A	12.77	129.22	121.39
20	1	606	CHL	C1B-CHB-C4A	12.77	129.21	121.39
20	3	608	CHL	C1B-CHB-C4A	12.69	129.16	121.39
20	Y	608	CHL	C1B-CHB-C4A	12.67	129.16	121.39
20	X	601	CHL	C1B-CHB-C4A	12.66	129.15	121.39
20	Z	307	CHL	C1B-CHB-C4A	12.66	129.15	121.39
20	4	306	CHL	C1B-CHB-C4A	12.66	129.15	121.39
20	2	614	CHL	C1B-CHB-C4A	12.62	129.12	121.39
20	Z	301	CHL	C1B-CHB-C4A	12.62	129.12	121.39
20	6	605	CHL	C1B-CHB-C4A	12.60	129.11	121.39
20	6	606	CHL	C1B-CHB-C4A	12.58	129.10	121.39
20	6	607	CHL	C1B-CHB-C4A	12.57	129.09	121.39
20	X	605	CHL	C1B-CHB-C4A	12.54	129.07	121.39
20	X	607	CHL	C1B-CHB-C4A	12.53	129.06	121.39
20	Y	606	CHL	C1B-CHB-C4A	12.49	129.04	121.39
20	Z	308	CHL	C1B-CHB-C4A	12.49	129.04	121.39
20	Z	302	CHL	C1B-CHB-C4A	12.42	129.00	121.39
20	Z	306	CHL	C1B-CHB-C4A	12.41	128.99	121.39
20	2	601	CHL	C1B-CHB-C4A	12.37	128.97	121.39
20	Y	601	CHL	C1B-CHB-C4A	12.34	128.95	121.39
20	5	601	CHL	C1B-CHB-C4A	12.33	128.94	121.39
20	4	305	CHL	C1B-CHB-C4A	12.32	128.94	121.39
20	Z	309	CHL	C1B-CHB-C4A	12.31	128.93	121.39
20	4	304	CHL	C1B-CHB-C4A	12.22	128.88	121.39
20	2	606	CHL	C1B-CHB-C4A	12.20	128.87	121.39
20	Y	607	CHL	C1B-CHB-C4A	12.18	128.85	121.39
21	5	608	CLA	C4A-NA-C1A	12.06	112.13	106.71
20	2	607	CHL	C1B-CHB-C4A	12.02	128.75	121.39
20	Y	619	CHL	C1B-CHB-C4A	11.99	128.74	121.39
20	Y	605	CHL	C1B-CHB-C4A	11.91	128.68	121.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	X	608	CHL	C1B-CHB-C4A	11.79	128.62	121.39
21	X	609	CLA	C4A-NA-C1A	11.26	111.77	106.71
21	Z	303	CLA	C4A-NA-C1A	11.10	111.70	106.71
21	A	806	CLA	C4A-NA-C1A	10.99	111.65	106.71
21	B	831	CLA	C4A-NA-C1A	10.98	111.64	106.71
21	6	611	CLA	C4A-NA-C1A	10.98	111.64	106.71
21	B	808	CLA	C4A-NA-C1A	10.97	111.64	106.71
21	X	610	CLA	C4A-NA-C1A	10.91	111.61	106.71
21	A	813	CLA	C4A-NA-C1A	10.91	111.61	106.71
21	B	805	CLA	C4A-NA-C1A	10.91	111.61	106.71
21	B	804	CLA	C4A-NA-C1A	10.90	111.61	106.71
21	A	807	CLA	C4A-NA-C1A	10.77	111.55	106.71
21	B	840	CLA	C4A-NA-C1A	10.76	111.54	106.71
21	A	804	CLA	C4A-NA-C1A	10.70	111.52	106.71
21	2	612	CLA	C4A-NA-C1A	10.69	111.51	106.71
21	A	837	CLA	C4A-NA-C1A	10.68	111.51	106.71
21	A	816	CLA	C4A-NA-C1A	10.67	111.50	106.71
21	5	603	CLA	C4A-NA-C1A	10.65	111.49	106.71
21	B	814	CLA	C4A-NA-C1A	10.62	111.48	106.71
21	O	203	CLA	C4A-NA-C1A	10.62	111.48	106.71
21	B	839	CLA	C4A-NA-C1A	10.61	111.48	106.71
21	K	203	CLA	C4A-NA-C1A	10.59	111.47	106.71
21	F	304	CLA	C4A-NA-C1A	10.56	111.45	106.71
21	B	835	CLA	C4A-NA-C1A	10.53	111.44	106.71
21	O	202	CLA	C4A-NA-C1A	10.51	111.43	106.71
21	B	807	CLA	C4A-NA-C1A	10.49	111.42	106.71
21	A	827	CLA	C4A-NA-C1A	10.47	111.42	106.71
21	5	607	CLA	C4A-NA-C1A	10.47	111.41	106.71
21	1	614	CLA	C4A-NA-C1A	10.46	111.41	106.71
21	3	611	CLA	C4A-NA-C1A	10.45	111.41	106.71
21	G	204	CLA	C4A-NA-C1A	10.42	111.39	106.71
21	B	812	CLA	C4A-NA-C1A	10.41	111.38	106.71
21	4	310	CLA	C4A-NA-C1A	10.38	111.37	106.71
21	X	602	CLA	C4A-NA-C1A	10.36	111.36	106.71
21	4	313	CLA	C4A-NA-C1A	10.35	111.36	106.71
21	A	836	CLA	C4A-NA-C1A	10.35	111.36	106.71
21	B	801	CLA	C4A-NA-C1A	10.34	111.35	106.71
21	6	604	CLA	C4A-NA-C1A	10.32	111.34	106.71
21	Y	602	CLA	C4A-NA-C1A	10.31	111.34	106.71
21	5	611	CLA	C4A-NA-C1A	10.31	111.34	106.71
21	L	301	CLA	C4A-NA-C1A	10.30	111.34	106.71
21	A	821	CLA	C4A-NA-C1A	10.29	111.33	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	G	202	CLA	C4A-NA-C1A	10.29	111.33	106.71
21	B	829	CLA	C4A-NA-C1A	10.27	111.33	106.71
21	A	812	CLA	C4A-NA-C1A	10.27	111.32	106.71
21	L	305	CLA	C4A-NA-C1A	10.25	111.31	106.71
21	A	841	CLA	C4A-NA-C1A	10.24	111.31	106.71
21	2	611	CLA	C4A-NA-C1A	10.24	111.31	106.71
21	3	609	CLA	C4A-NA-C1A	10.23	111.31	106.71
21	1	603	CLA	C4A-NA-C1A	10.23	111.30	106.71
21	5	610	CLA	C4A-NA-C1A	10.22	111.30	106.71
21	B	815	CLA	C4A-NA-C1A	10.22	111.30	106.71
21	A	833	CLA	C4A-NA-C1A	10.22	111.30	106.71
21	4	301	CLA	C4A-NA-C1A	10.21	111.30	106.71
21	1	611	CLA	C4A-NA-C1A	10.18	111.28	106.71
21	1	604	CLA	C4A-NA-C1A	10.17	111.28	106.71
21	B	825	CLA	C4A-NA-C1A	10.16	111.27	106.71
21	5	614	CLA	C4A-NA-C1A	10.15	111.27	106.71
21	B	810	CLA	C4A-NA-C1A	10.14	111.27	106.71
21	A	814	CLA	C4A-NA-C1A	10.14	111.26	106.71
21	A	831	CLA	C4A-NA-C1A	10.13	111.26	106.71
21	6	614	CLA	C4A-NA-C1A	10.09	111.24	106.71
21	B	826	CLA	C4A-NA-C1A	10.09	111.24	106.71
21	K	202	CLA	C4A-NA-C1A	10.09	111.24	106.71
21	A	820	CLA	C4A-NA-C1A	10.07	111.23	106.71
21	6	609	CLA	C4A-NA-C1A	10.06	111.23	106.71
21	B	830	CLA	C4A-NA-C1A	10.06	111.23	106.71
21	A	802	CLA	C4A-NA-C1A	10.06	111.23	106.71
21	3	605	CLA	C4A-NA-C1A	10.05	111.22	106.71
21	3	617	CLA	C4A-NA-C1A	10.04	111.22	106.71
21	1	602	CLA	C4A-NA-C1A	10.03	111.22	106.71
21	3	606	CLA	C4A-NA-C1A	10.02	111.21	106.71
21	1	610	CLA	C4A-NA-C1A	10.02	111.21	106.71
21	3	612	CLA	C4A-NA-C1A	10.01	111.21	106.71
21	4	303	CLA	C4A-NA-C1A	10.01	111.21	106.71
21	B	817	CLA	C4A-NA-C1A	10.01	111.21	106.71
21	B	811	CLA	C4A-NA-C1A	10.01	111.21	106.71
21	K	201	CLA	C4A-NA-C1A	10.00	111.20	106.71
21	B	806	CLA	C4A-NA-C1A	9.99	111.20	106.71
21	B	827	CLA	C4A-NA-C1A	9.99	111.20	106.71
21	1	612	CLA	C4A-NA-C1A	9.97	111.19	106.71
21	A	834	CLA	C4A-NA-C1A	9.97	111.19	106.71
21	4	309	CLA	C4A-NA-C1A	9.96	111.19	106.71
21	A	815	CLA	C4A-NA-C1A	9.96	111.18	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	834	CLA	C4A-NA-C1A	9.96	111.18	106.71
21	Y	614	CLA	C4A-NA-C1A	9.96	111.18	106.71
21	3	607	CLA	C4A-NA-C1A	9.95	111.18	106.71
21	A	808	CLA	C4A-NA-C1A	9.95	111.18	106.71
21	A	839	CLA	C4A-NA-C1A	9.93	111.17	106.71
21	5	602	CLA	C4A-NA-C1A	9.92	111.17	106.71
21	A	843	CLA	C4A-NA-C1A	9.92	111.17	106.71
21	5	609	CLA	C4A-NA-C1A	9.91	111.16	106.71
21	Z	305	CLA	C4A-NA-C1A	9.91	111.16	106.71
21	3	603	CLA	C4A-NA-C1A	9.91	111.16	106.71
21	3	604	CLA	C4A-NA-C1A	9.88	111.15	106.71
21	5	604	CLA	C4A-NA-C1A	9.88	111.15	106.71
21	4	308	CLA	C4A-NA-C1A	9.87	111.14	106.71
21	Z	313	CLA	C4A-NA-C1A	9.87	111.14	106.71
21	4	307	CLA	C4A-NA-C1A	9.86	111.14	106.71
21	5	613	CLA	C4A-NA-C1A	9.86	111.14	106.71
21	A	840	CLA	C4A-NA-C1A	9.85	111.14	106.71
21	6	602	CLA	C4A-NA-C1A	9.84	111.13	106.71
21	B	813	CLA	C4A-NA-C1A	9.84	111.13	106.71
21	B	837	CLA	C4A-NA-C1A	9.81	111.12	106.71
21	L	303	CLA	C4A-NA-C1A	9.81	111.11	106.71
21	A	811	CLA	C4A-NA-C1A	9.78	111.11	106.71
21	1	605	CLA	C4A-NA-C1A	9.78	111.10	106.71
21	J	101	CLA	C4A-NA-C1A	9.76	111.09	106.71
21	A	829	CLA	C4A-NA-C1A	9.76	111.09	106.71
21	A	805	CLA	C4A-NA-C1A	9.75	111.09	106.71
21	B	833	CLA	C4A-NA-C1A	9.75	111.09	106.71
21	B	819	CLA	C4A-NA-C1A	9.74	111.09	106.71
21	G	203	CLA	C4A-NA-C1A	9.74	111.09	106.71
21	2	613	CLA	C4A-NA-C1A	9.73	111.08	106.71
21	4	311	CLA	C4A-NA-C1A	9.73	111.08	106.71
21	2	608	CLA	C4A-NA-C1A	9.73	111.08	106.71
21	3	610	CLA	C4A-NA-C1A	9.72	111.08	106.71
21	3	613	CLA	C4A-NA-C1A	9.72	111.08	106.71
21	2	603	CLA	C4A-NA-C1A	9.72	111.07	106.71
21	2	604	CLA	C4A-NA-C1A	9.72	111.07	106.71
21	4	312	CLA	C4A-NA-C1A	9.72	111.07	106.71
21	A	809	CLA	C4A-NA-C1A	9.71	111.07	106.71
21	A	832	CLA	C4A-NA-C1A	9.71	111.07	106.71
21	A	828	CLA	C4A-NA-C1A	9.71	111.07	106.71
21	Y	612	CLA	C4A-NA-C1A	9.69	111.06	106.71
21	B	838	CLA	C4A-NA-C1A	9.67	111.05	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	6	608	CLA	C4A-NA-C1A	9.66	111.05	106.71
21	K	204	CLA	C4A-NA-C1A	9.65	111.05	106.71
21	6	612	CLA	C4A-NA-C1A	9.64	111.04	106.71
21	2	602	CLA	C4A-NA-C1A	9.63	111.04	106.71
21	1	607	CLA	C4A-NA-C1A	9.63	111.03	106.71
21	B	828	CLA	C4A-NA-C1A	9.63	111.03	106.71
21	B	803	CLA	C4A-NA-C1A	9.62	111.03	106.71
21	Y	610	CLA	C4A-NA-C1A	9.62	111.03	106.71
21	B	821	CLA	C4A-NA-C1A	9.60	111.02	106.71
21	A	801	CLA	C4A-NA-C1A	9.59	111.02	106.71
21	6	603	CLA	C4A-NA-C1A	9.59	111.02	106.71
21	A	830	CLA	C4A-NA-C1A	9.58	111.01	106.71
21	A	838	CLA	C4A-NA-C1A	9.58	111.01	106.71
21	1	613	CLA	C4A-NA-C1A	9.57	111.01	106.71
21	Y	604	CLA	C4A-NA-C1A	9.57	111.01	106.71
21	2	609	CLA	C4A-NA-C1A	9.49	110.97	106.71
21	2	618	CLA	C4A-NA-C1A	9.49	110.97	106.71
21	4	302	CLA	C4A-NA-C1A	9.48	110.97	106.71
21	B	823	CLA	C4A-NA-C1A	9.48	110.97	106.71
21	3	602	CLA	C4A-NA-C1A	9.45	110.96	106.71
21	A	817	CLA	C4A-NA-C1A	9.40	110.93	106.71
21	Y	603	CLA	C4A-NA-C1A	9.40	110.93	106.71
21	1	609	CLA	C4A-NA-C1A	9.39	110.93	106.71
21	L	304	CLA	C4A-NA-C1A	9.39	110.93	106.71
21	A	818	CLA	C4A-NA-C1A	9.37	110.92	106.71
21	2	610	CLA	C4A-NA-C1A	9.37	110.92	106.71
21	X	613	CLA	C4A-NA-C1A	9.37	110.92	106.71
21	X	604	CLA	C4A-NA-C1A	9.37	110.92	106.71
21	5	612	CLA	C4A-NA-C1A	9.35	110.91	106.71
21	A	826	CLA	C4A-NA-C1A	9.35	110.91	106.71
21	Z	312	CLA	C4A-NA-C1A	9.33	110.90	106.71
21	1	608	CLA	C4A-NA-C1A	9.33	110.90	106.71
21	A	819	CLA	C4A-NA-C1A	9.32	110.89	106.71
21	X	611	CLA	C4A-NA-C1A	9.29	110.88	106.71
21	J	102	CLA	C4A-NA-C1A	9.29	110.88	106.71
21	Y	611	CLA	C4A-NA-C1A	9.18	110.83	106.71
21	A	825	CLA	C4A-NA-C1A	9.14	110.81	106.71
21	X	603	CLA	C4A-NA-C1A	9.12	110.81	106.71
21	6	601	CLA	C4A-NA-C1A	9.10	110.80	106.71
21	Y	613	CLA	C4A-NA-C1A	9.10	110.80	106.71
21	A	835	CLA	C4A-NA-C1A	9.10	110.80	106.71
21	5	605	CLA	C4A-NA-C1A	9.09	110.79	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	822	CLA	C4A-NA-C1A	9.09	110.79	106.71
21	B	836	CLA	C4A-NA-C1A	9.08	110.79	106.71
21	B	818	CLA	C4A-NA-C1A	8.98	110.74	106.71
21	A	810	CLA	C4A-NA-C1A	8.97	110.74	106.71
21	A	823	CLA	C4A-NA-C1A	8.97	110.74	106.71
21	B	816	CLA	C4A-NA-C1A	8.95	110.73	106.71
21	X	618	CLA	C4A-NA-C1A	8.93	110.72	106.71
21	O	207	CLA	C4A-NA-C1A	8.93	110.72	106.71
21	B	832	CLA	C4A-NA-C1A	8.89	110.70	106.71
21	B	824	CLA	C4A-NA-C1A	8.87	110.69	106.71
21	Z	311	CLA	C4A-NA-C1A	8.85	110.69	106.71
21	B	820	CLA	C4A-NA-C1A	8.76	110.64	106.71
21	A	824	CLA	C4A-NA-C1A	8.74	110.63	106.71
21	3	614	CLA	C4A-NA-C1A	8.73	110.63	106.71
21	Z	310	CLA	C4A-NA-C1A	8.63	110.59	106.71
21	O	206	CLA	C4A-NA-C1A	8.60	110.57	106.71
21	A	842	CLA	C4A-NA-C1A	8.53	110.54	106.71
21	B	809	CLA	C4A-NA-C1A	8.52	110.54	106.71
21	A	822	CLA	C4A-NA-C1A	8.51	110.53	106.71
21	Z	304	CLA	C4A-NA-C1A	8.51	110.53	106.71
21	6	613	CLA	C4A-NA-C1A	8.49	110.52	106.71
21	X	612	CLA	C4A-NA-C1A	8.41	110.49	106.71
21	A	803	CLA	C4A-NA-C1A	8.16	110.37	106.71
21	B	810	CLA	CAB-C3B-C4B	7.90	137.40	125.37
21	6	610	CLA	C4A-NA-C1A	7.85	110.23	106.71
21	H	201	CLA	C4A-NA-C1A	7.40	110.03	106.71
20	Z	301	CHL	C4D-CHA-CBD	-6.77	101.91	108.89
21	B	802	CLA	C4A-NA-C1A	6.75	109.74	106.71
20	2	601	CHL	O2D-CGD-CBD	6.70	119.49	111.00
22	Z	315	LUT	C15-C35-C34	6.29	136.37	123.47
20	Y	601	CHL	O2D-CGD-CBD	6.02	118.63	111.00
20	X	606	CHL	O2D-CGD-CBD	5.89	118.45	111.00
20	X	607	CHL	O2D-CGD-CBD	5.83	118.39	111.00
20	4	305	CHL	O2D-CGD-CBD	5.82	118.38	111.00
20	2	605	CHL	O2D-CGD-CBD	5.82	118.36	111.00
20	6	606	CHL	O2D-CGD-CBD	5.79	118.33	111.00
20	Z	308	CHL	O2D-CGD-CBD	5.77	118.31	111.00
20	X	601	CHL	O2D-CGD-CBD	5.77	118.31	111.00
20	X	608	CHL	O2D-CGD-CBD	5.77	118.31	111.00
20	Y	609	CHL	O2D-CGD-CBD	5.77	118.30	111.00
20	Z	307	CHL	O2D-CGD-CBD	5.74	118.27	111.00
20	Z	306	CHL	O2D-CGD-CBD	5.73	118.26	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	6	607	CHL	O2D-CGD-CBD	5.67	118.19	111.00
20	X	605	CHL	O2D-CGD-CBD	5.67	118.17	111.00
20	3	608	CHL	O2D-CGD-CBD	5.64	118.14	111.00
20	Y	606	CHL	O2D-CGD-CBD	5.61	118.11	111.00
20	4	306	CHL	O2D-CGD-CBD	5.58	118.07	111.00
20	2	607	CHL	O2D-CGD-CBD	5.57	118.06	111.00
20	Y	605	CHL	O2D-CGD-CBD	5.51	117.98	111.00
20	Z	307	CHL	C4D-CHA-CBD	-5.48	103.24	108.89
20	2	614	CHL	O2D-CGD-CBD	5.47	117.93	111.00
22	X	614	LUT	C15-C35-C34	5.44	134.63	123.47
20	X	606	CHL	C4D-CHA-CBD	-5.42	103.30	108.89
20	4	304	CHL	O2D-CGD-CBD	5.41	117.85	111.00
20	Y	608	CHL	O2D-CGD-CBD	5.37	117.80	111.00
20	2	606	CHL	O2D-CGD-CBD	5.37	117.80	111.00
20	Z	309	CHL	C4D-CHA-CBD	-5.32	103.41	108.89
20	Z	301	CHL	O2D-CGD-CBD	5.29	117.69	111.00
20	1	606	CHL	CAA-C2A-C3A	-5.28	103.78	116.10
20	6	605	CHL	O2D-CGD-CBD	5.23	117.62	111.00
20	X	605	CHL	CAA-C2A-C3A	-5.23	103.91	116.10
20	Z	308	CHL	CAA-C2A-C3A	-5.22	103.91	116.10
20	Y	605	CHL	CAA-C2A-C3A	-5.19	103.98	116.10
20	2	605	CHL	C4D-CHA-CBD	-5.19	103.54	108.89
20	5	606	CHL	CAA-C2A-C3A	-5.14	104.10	116.10
20	Y	619	CHL	O2D-CGD-CBD	5.14	117.51	111.00
20	Y	607	CHL	O2D-CGD-CBD	5.09	117.45	111.00
20	Z	302	CHL	O2D-CGD-CBD	4.99	117.32	111.00
20	2	614	CHL	C4D-CHA-CBD	-4.92	103.82	108.89
21	B	806	CLA	O2D-CGD-CBD	4.86	119.90	111.27
20	6	607	CHL	C4D-CHA-CBD	-4.83	103.91	108.89
20	5	606	CHL	C4D-CHA-CBD	-4.82	103.92	108.89
20	4	306	CHL	C4D-CHA-CBD	-4.76	103.98	108.89
20	Z	309	CHL	O2D-CGD-CBD	4.73	117.00	111.00
22	3	615	LUT	C15-C35-C34	4.70	133.11	123.47
23	O	208	XAT	O24-C25-C24	-4.67	109.87	113.38
20	Z	306	CHL	C3D-C4D-CHA	4.64	115.60	108.54
20	2	614	CHL	C3D-C4D-CHA	4.62	115.56	108.54
20	1	606	CHL	C3D-C4D-CHA	4.61	115.55	108.54
20	1	601	CHL	C3D-C4D-CHA	4.61	115.54	108.54
20	Y	605	CHL	C3D-C4D-CHA	4.58	115.51	108.54
20	6	606	CHL	C3D-C4D-CHA	4.57	115.49	108.54
20	6	615	CHL	C3D-C4D-CHA	4.57	115.48	108.54
20	Y	608	CHL	C4D-CHA-CBD	-4.57	104.18	108.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	831	CLA	O2D-CGD-CBD	4.56	119.38	111.27
20	Y	607	CHL	C3D-C4D-CHA	4.56	115.48	108.54
20	6	607	CHL	C3D-C4D-CHA	4.55	115.46	108.54
20	X	608	CHL	C3D-C4D-CHA	4.55	115.45	108.54
20	X	601	CHL	C3D-C4D-CHA	4.52	115.42	108.54
20	4	305	CHL	C3D-C4D-CHA	4.52	115.41	108.54
20	2	607	CHL	C3D-C4D-CHA	4.52	115.41	108.54
20	3	608	CHL	C3D-C4D-CHA	4.52	115.41	108.54
20	X	607	CHL	C3D-C4D-CHA	4.52	115.40	108.54
20	Y	601	CHL	C3D-C4D-CHA	4.51	115.39	108.54
20	Z	308	CHL	C3D-C4D-CHA	4.51	115.39	108.54
22	Z	315	LUT	C39-C29-C30	-4.50	116.62	122.92
20	X	605	CHL	C4D-CHA-CBD	-4.50	104.25	108.89
20	Z	309	CHL	C3D-C4D-CHA	4.50	115.38	108.54
20	2	606	CHL	C3D-C4D-CHA	4.49	115.37	108.54
20	Y	609	CHL	C3D-C4D-CHA	4.49	115.37	108.54
20	1	606	CHL	C4D-CHA-CBD	-4.49	104.27	108.89
20	5	601	CHL	C3D-C4D-CHA	4.48	115.35	108.54
20	4	314	CHL	C3D-C4D-CHA	4.48	115.35	108.54
20	4	306	CHL	C3D-C4D-CHA	4.47	115.34	108.54
20	X	605	CHL	C3D-C4D-CHA	4.47	115.33	108.54
20	Y	606	CHL	C3D-C4D-CHA	4.46	115.33	108.54
21	B	826	CLA	O2D-CGD-CBD	4.46	119.20	111.27
20	X	601	CHL	C4D-CHA-CBD	-4.44	104.31	108.89
21	B	802	CLA	C3B-C4B-NB	-4.42	106.41	110.52
20	Z	302	CHL	C3D-C4D-CHA	4.42	115.26	108.54
21	A	827	CLA	O2D-CGD-CBD	4.42	119.11	111.27
20	2	601	CHL	C3D-C4D-CHA	4.41	115.25	108.54
20	6	605	CHL	C3D-C4D-CHA	4.41	115.24	108.54
21	A	842	CLA	O2D-CGD-CBD	4.41	119.10	111.27
20	Y	619	CHL	C3D-C4D-CHA	4.41	115.24	108.54
20	2	605	CHL	C3D-C4D-CHA	4.40	115.23	108.54
22	Z	315	LUT	C32-C33-C34	4.40	125.69	118.94
20	X	608	CHL	C4D-CHA-CBD	-4.36	104.39	108.89
21	5	608	CLA	CHD-C1D-ND	-4.36	120.44	124.45
20	Y	608	CHL	C3D-C4D-CHA	4.36	115.17	108.54
20	2	614	CHL	CAA-C2A-C3A	-4.35	103.39	114.26
20	4	304	CHL	C3D-C4D-CHA	4.34	115.14	108.54
20	X	606	CHL	C3D-C4D-CHA	4.33	115.13	108.54
21	X	609	CLA	O2D-CGD-CBD	4.33	118.95	111.27
20	4	304	CHL	C4D-CHA-CBD	-4.32	104.43	108.89
21	A	833	CLA	O2D-CGD-CBD	4.32	118.94	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3	615	LUT	C39-C29-C30	-4.31	116.88	122.92
21	L	304	CLA	O2D-CGD-CBD	4.30	118.91	111.27
20	5	606	CHL	C3D-C4D-CHA	4.30	115.07	108.54
21	L	301	CLA	O2D-CGD-CBD	4.29	118.89	111.27
20	Y	607	CHL	C4D-CHA-CBD	-4.28	104.47	108.89
21	A	802	CLA	O2D-CGD-CBD	4.28	118.88	111.27
20	3	608	CHL	C4D-CHA-CBD	-4.28	104.48	108.89
21	B	837	CLA	O2D-CGD-CBD	4.28	118.86	111.27
22	Z	315	LUT	C28-C29-C30	4.27	125.49	118.94
22	5	619	LUT	C19-C9-C10	-4.25	116.97	122.92
20	4	305	CHL	C4D-CHA-CBD	-4.24	104.52	108.89
20	5	601	CHL	C4D-CHA-CBD	-4.24	104.52	108.89
20	Z	306	CHL	C4D-CHA-CBD	-4.24	104.52	108.89
20	6	605	CHL	C4D-CHA-CBD	-4.23	104.53	108.89
20	2	601	CHL	C4D-CHA-CBD	-4.23	104.53	108.89
22	X	615	LUT	C15-C35-C34	4.23	132.14	123.47
20	Z	307	CHL	C3D-C4D-CHA	4.23	114.97	108.54
20	Z	302	CHL	C4D-CHA-CBD	-4.22	104.54	108.89
21	B	804	CLA	O2D-CGD-CBD	4.22	118.76	111.27
21	A	840	CLA	O2D-CGD-CBD	4.21	118.76	111.27
20	4	314	CHL	CBC-CAC-C3C	-4.21	106.72	112.88
22	5	619	LUT	C35-C15-C14	4.20	132.09	123.47
21	B	819	CLA	O2D-CGD-CBD	4.20	118.73	111.27
20	Z	301	CHL	C3D-C4D-CHA	4.18	114.90	108.54
21	B	815	CLA	O2D-CGD-CBD	4.18	118.70	111.27
20	6	606	CHL	C4D-CHA-CBD	-4.18	104.58	108.89
21	B	816	CLA	O2D-CGD-CBD	4.18	118.70	111.27
20	Y	619	CHL	C4D-CHA-CBD	-4.17	104.59	108.89
20	4	314	CHL	C4D-CHA-CBD	-4.16	104.60	108.89
21	L	305	CLA	O2D-CGD-CBD	4.16	118.66	111.27
21	B	807	CLA	O2D-CGD-CBD	4.15	118.65	111.27
21	A	826	CLA	O2D-CGD-CBD	4.15	118.64	111.27
22	F	301	LUT	C19-C9-C10	-4.15	117.11	122.92
21	B	810	CLA	C3B-C4B-NB	-4.15	107.45	110.23
21	A	829	CLA	O2D-CGD-CBD	4.14	118.63	111.27
20	2	607	CHL	C4D-CHA-CBD	-4.14	104.62	108.89
21	A	841	CLA	O2D-CGD-CBD	4.14	118.62	111.27
21	4	307	CLA	O2D-CGD-CBD	4.13	118.61	111.27
20	6	615	CHL	CAA-C2A-C3A	-4.13	103.94	114.26
21	L	303	CLA	O2D-CGD-CBD	4.12	118.59	111.27
20	2	606	CHL	C4D-CHA-CBD	-4.12	104.64	108.89
20	Y	601	CHL	C4D-CHA-CBD	-4.11	104.65	108.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	Z	315	LUT	C19-C9-C10	-4.10	117.17	122.92
21	J	101	CLA	O2D-CGD-CBD	4.10	118.56	111.27
21	A	832	CLA	O2D-CGD-CBD	4.10	118.55	111.27
21	6	609	CLA	O2D-CGD-CBD	4.10	118.55	111.27
21	O	202	CLA	O2D-CGD-CBD	4.10	118.55	111.27
20	3	608	CHL	CBC-CAC-C3C	-4.08	106.90	112.88
20	6	615	CHL	C4D-CHA-CBD	-4.08	104.68	108.89
22	X	615	LUT	C19-C9-C10	-4.08	117.21	122.92
21	A	808	CLA	O2D-CGD-CBD	4.07	118.50	111.27
22	X	615	LUT	C39-C29-C30	-4.07	117.22	122.92
22	6	616	LUT	C15-C35-C34	4.07	131.81	123.47
21	B	830	CLA	O2D-CGD-CBD	4.07	118.49	111.27
21	A	835	CLA	O2D-CGD-CBD	4.06	118.49	111.27
20	X	607	CHL	C4D-CHA-CBD	-4.06	104.70	108.89
20	4	314	CHL	CAA-C2A-C3A	-4.06	104.12	114.26
20	Z	308	CHL	C4D-CHA-CBD	-4.06	104.71	108.89
20	6	607	CHL	CBC-CAC-C3C	-4.06	106.94	112.88
21	Y	611	CLA	O2D-CGD-CBD	4.06	118.47	111.27
20	Y	609	CHL	C4D-CHA-CBD	-4.05	104.71	108.89
21	B	835	CLA	O2D-CGD-CBD	4.05	118.47	111.27
22	1	615	LUT	C15-C35-C34	4.05	131.78	123.47
21	3	617	CLA	O2D-CGD-CBD	4.05	118.47	111.27
20	1	601	CHL	C4D-CHA-CBD	-4.05	104.72	108.89
21	J	102	CLA	O2D-CGD-CBD	4.04	118.45	111.27
22	5	615	LUT	C15-C35-C34	4.04	131.75	123.47
21	A	813	CLA	O2D-CGD-CBD	4.03	118.44	111.27
21	A	825	CLA	O2D-CGD-CBD	4.03	118.43	111.27
21	2	609	CLA	O2D-CGD-CBD	4.03	118.42	111.27
20	Y	605	CHL	C4D-CHA-CBD	-4.02	104.74	108.89
22	Y	615	LUT	C19-C9-C10	-4.02	117.29	122.92
21	A	806	CLA	O2D-CGD-CBD	4.02	118.42	111.27
23	6	617	XAT	C7-C8-C9	4.02	131.76	125.53
21	3	605	CLA	O2D-CGD-CBD	4.01	118.39	111.27
21	6	602	CLA	O2D-CGD-CBD	4.01	118.39	111.27
22	Y	616	LUT	C19-C9-C10	-4.00	117.31	122.92
22	Z	314	LUT	C19-C9-C10	-4.00	117.32	122.92
20	Y	606	CHL	C4D-CHA-CBD	-4.00	104.77	108.89
21	B	818	CLA	O2D-CGD-CBD	4.00	118.37	111.27
21	B	811	CLA	O2D-CGD-CBD	4.00	118.37	111.27
21	B	827	CLA	O2D-CGD-CBD	3.99	118.37	111.27
22	5	615	LUT	C39-C29-C30	-3.99	117.34	122.92
21	B	831	CLA	O2D-CGD-CBD	3.98	118.34	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	1	611	CLA	O2D-CGD-CBD	3.98	118.34	111.27
21	A	823	CLA	O2D-CGD-CBD	3.98	118.33	111.27
22	4	315	LUT	C15-C35-C34	3.98	131.62	123.47
21	2	613	CLA	O2D-CGD-CBD	3.97	118.33	111.27
21	B	825	CLA	O2D-CGD-CBD	3.97	118.32	111.27
22	5	615	LUT	C19-C9-C10	-3.97	117.37	122.92
21	B	802	CLA	O2D-CGD-CBD	3.97	118.31	111.27
21	2	608	CLA	O2D-CGD-CBD	3.96	118.31	111.27
21	1	604	CLA	O2D-CGD-CBD	3.96	118.30	111.27
20	2	605	CHL	CAA-C2A-C3A	-3.96	104.38	114.26
22	Z	315	LUT	C40-C33-C34	-3.95	117.39	122.92
22	X	614	LUT	C39-C29-C30	-3.95	117.39	122.92
21	3	611	CLA	O2D-CGD-CBD	3.95	118.28	111.27
21	B	822	CLA	O2D-CGD-CBD	3.94	118.27	111.27
21	5	609	CLA	O2D-CGD-CBD	3.94	118.27	111.27
21	A	818	CLA	O2D-CGD-CBD	3.94	118.26	111.27
21	6	613	CLA	O2D-CGD-CBD	3.94	118.26	111.27
21	B	823	CLA	O2D-CGD-CBD	3.94	118.26	111.27
21	4	312	CLA	O2D-CGD-CBD	3.93	118.25	111.27
20	Z	301	CHL	OBD-CAD-CBD	-3.93	120.05	125.82
21	5	608	CLA	O2D-CGD-CBD	3.93	118.25	111.27
22	6	616	LUT	C39-C29-C30	-3.93	117.42	122.92
21	Z	310	CLA	O2D-CGD-CBD	3.93	118.24	111.27
21	K	203	CLA	O2D-CGD-CBD	3.92	118.24	111.27
21	B	813	CLA	C3B-C4B-NB	-3.92	106.88	110.52
21	O	203	CLA	O2D-CGD-CBD	3.92	118.23	111.27
22	Y	615	LUT	C39-C29-C30	-3.91	117.44	122.92
21	G	202	CLA	O2D-CGD-CBD	3.91	118.21	111.27
21	A	804	CLA	O2D-CGD-CBD	3.91	118.21	111.27
22	1	615	LUT	C19-C9-C10	-3.91	117.45	122.92
22	X	614	LUT	C19-C9-C10	-3.90	117.46	122.92
21	B	820	CLA	O2D-CGD-CBD	3.90	118.20	111.27
20	6	605	CHL	CBC-CAC-C3C	-3.90	107.17	112.88
21	X	602	CLA	O2D-CGD-CBD	3.90	118.19	111.27
21	Z	310	CLA	CHD-C1D-ND	-3.89	120.88	124.45
21	1	612	CLA	O2D-CGD-CBD	3.89	118.19	111.27
22	Y	616	LUT	C39-C29-C30	-3.89	117.48	122.92
21	A	820	CLA	O2D-CGD-CBD	3.89	118.18	111.27
21	K	204	CLA	CBD-CHA-C1A	3.89	133.08	128.50
22	3	615	LUT	C19-C9-C10	-3.88	117.48	122.92
21	Y	612	CLA	O2D-CGD-CBD	3.88	118.17	111.27
21	A	809	CLA	O2D-CGD-CBD	3.88	118.17	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	819	CLA	O2D-CGD-CBD	3.88	118.17	111.27
21	Z	313	CLA	O2D-CGD-CBD	3.88	118.17	111.27
21	1	610	CLA	O2D-CGD-CBD	3.88	118.16	111.27
21	2	610	CLA	O2D-CGD-CBD	3.88	118.16	111.27
21	B	834	CLA	O2D-CGD-CBD	3.88	118.16	111.27
21	A	837	CLA	C4-C3-C5	-3.87	111.56	115.98
21	B	839	CLA	O2D-CGD-CBD	3.87	118.15	111.27
22	X	614	LUT	C32-C33-C34	3.87	124.88	118.94
21	A	834	CLA	O2D-CGD-CBD	3.87	118.14	111.27
21	B	829	CLA	O2D-CGD-CBD	3.86	118.13	111.27
21	1	614	CLA	O2D-CGD-CBD	3.86	118.13	111.27
21	A	821	CLA	O2D-CGD-CBD	3.86	118.13	111.27
21	A	811	CLA	O2D-CGD-CBD	3.86	118.12	111.27
21	B	836	CLA	O2D-CGD-CBD	3.86	118.12	111.27
21	A	836	CLA	O2D-CGD-CBD	3.85	118.12	111.27
21	4	309	CLA	O2D-CGD-CBD	3.85	118.11	111.27
20	Z	307	CHL	CBC-CAC-C3C	-3.85	107.25	112.88
21	4	311	CLA	O2D-CGD-CBD	3.84	118.10	111.27
21	4	301	CLA	O2D-CGD-CBD	3.84	118.09	111.27
21	A	812	CLA	O2D-CGD-CBD	3.84	118.09	111.27
21	A	810	CLA	O2D-CGD-CBD	3.83	118.08	111.27
21	X	618	CLA	O2D-CGD-CBD	3.83	118.07	111.27
21	1	613	CLA	O2D-CGD-CBD	3.83	118.07	111.27
21	A	824	CLA	O2D-CGD-CBD	3.83	118.07	111.27
21	5	610	CLA	O2D-CGD-CBD	3.83	118.07	111.27
22	6	616	LUT	C19-C9-C10	-3.83	117.56	122.92
21	5	611	CLA	O2D-CGD-CBD	3.83	118.07	111.27
20	4	304	CHL	CMA-C3A-C4A	-3.83	106.00	114.38
21	A	839	CLA	O2D-CGD-CBD	3.83	118.06	111.27
22	Z	314	LUT	C35-C15-C14	3.82	131.30	123.47
21	A	838	CLA	O2D-CGD-CBD	3.82	118.06	111.27
21	F	304	CLA	O2D-CGD-CBD	3.82	118.06	111.27
21	Y	604	CLA	O2D-CGD-CBD	3.82	118.05	111.27
22	X	614	LUT	C40-C33-C34	-3.81	117.58	122.92
21	1	608	CLA	O2D-CGD-CBD	3.81	118.04	111.27
22	2	615	LUT	C19-C9-C10	-3.81	117.59	122.92
21	6	608	CLA	O2D-CGD-CBD	3.81	118.03	111.27
21	1	605	CLA	O2D-CGD-CBD	3.81	118.03	111.27
21	B	808	CLA	O2D-CGD-CBD	3.81	118.03	111.27
20	X	608	CHL	CBC-CAC-C3C	-3.80	107.31	112.88
23	1	616	XAT	C7-C8-C9	3.80	131.43	125.53
22	5	619	LUT	C39-C29-C30	-3.79	117.61	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	832	CLA	O2D-CGD-CBD	3.79	118.01	111.27
21	G	203	CLA	O2D-CGD-CBD	3.79	118.01	111.27
21	A	802	CLA	C3B-C4B-NB	-3.79	107.00	110.52
21	X	603	CLA	O2D-CGD-CBD	3.78	117.99	111.27
21	Z	305	CLA	O2D-CGD-CBD	3.78	117.99	111.27
20	Y	601	CHL	CBC-CAC-C3C	-3.78	107.35	112.88
21	3	610	CLA	O2D-CGD-CBD	3.78	117.98	111.27
22	4	315	LUT	C39-C29-C30	-3.77	117.64	122.92
21	A	830	CLA	O2D-CGD-CBD	3.77	117.97	111.27
21	6	612	CLA	O2D-CGD-CBD	3.77	117.97	111.27
21	Y	610	CLA	O2D-CGD-CBD	3.77	117.97	111.27
21	3	603	CLA	O2D-CGD-CBD	3.77	117.97	111.27
22	Z	314	LUT	C39-C29-C30	-3.76	117.65	122.92
21	B	838	CLA	O2D-CGD-CBD	3.76	117.95	111.27
21	H	201	CLA	O2D-CGD-CBD	3.76	117.95	111.27
21	B	812	CLA	O2D-CGD-CBD	3.76	117.95	111.27
21	Y	603	CLA	O2D-CGD-CBD	3.76	117.95	111.27
21	B	828	CLA	O2D-CGD-CBD	3.76	117.94	111.27
20	Z	309	CHL	CAA-C2A-C3A	-3.75	102.50	112.78
21	G	204	CLA	O2D-CGD-CBD	3.75	117.93	111.27
21	5	608	CLA	C3B-C4B-NB	-3.75	107.04	110.52
21	6	610	CLA	O2D-CGD-CBD	3.74	117.92	111.27
21	2	612	CLA	O2D-CGD-CBD	3.74	117.92	111.27
20	2	606	CHL	CAA-C2A-C3A	-3.74	104.92	114.26
20	4	306	CHL	CBC-CAC-C3C	-3.74	107.41	112.88
21	2	611	CLA	O2D-CGD-CBD	3.74	117.91	111.27
21	A	827	CLA	C3B-C4B-NB	-3.74	107.05	110.52
21	A	826	CLA	C3B-C4B-NB	-3.74	107.05	110.52
20	5	601	CHL	CBC-CAC-C3C	-3.74	107.41	112.88
23	4	316	XAT	C7-C8-C9	3.73	131.32	125.53
21	A	835	CLA	C3B-C4B-NB	-3.73	107.06	110.52
21	Y	614	CLA	O2D-CGD-CBD	3.72	117.89	111.27
21	X	611	CLA	CHD-C1D-ND	-3.72	121.04	124.45
22	Y	615	LUT	C35-C15-C14	3.71	131.08	123.47
22	4	315	LUT	C19-C9-C10	-3.71	117.72	122.92
21	4	313	CLA	O2D-CGD-CBD	3.71	117.86	111.27
21	4	308	CLA	O2D-CGD-CBD	3.71	117.85	111.27
21	2	609	CLA	C3B-C4B-NB	-3.70	107.08	110.52
22	1	615	LUT	C39-C29-C30	-3.70	117.74	122.92
21	X	610	CLA	O2D-CGD-CBD	3.70	117.85	111.27
21	A	830	CLA	C3B-C4B-NB	-3.70	107.08	110.52
20	Y	619	CHL	CMA-C3A-C4A	-3.70	106.28	114.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2	601	CHL	CBC-CAC-C3C	-3.69	107.47	112.88
21	5	602	CLA	O2D-CGD-CBD	3.69	117.83	111.27
21	A	828	CLA	O2D-CGD-CBD	3.69	117.83	111.27
22	2	615	LUT	C39-C29-C30	-3.69	117.75	122.92
20	X	607	CHL	CBC-CAC-C3C	-3.69	107.48	112.88
21	2	618	CLA	O2D-CGD-CBD	3.69	117.82	111.27
21	3	604	CLA	O2D-CGD-CBD	3.69	117.82	111.27
21	A	803	CLA	O2D-CGD-CBD	3.69	117.82	111.27
21	A	822	CLA	O2D-CGD-CBD	3.69	117.82	111.27
21	B	833	CLA	C3B-C4B-NB	-3.69	107.10	110.52
21	5	603	CLA	O2D-CGD-CBD	3.68	117.81	111.27
21	B	829	CLA	C3B-C4B-NB	-3.68	107.10	110.52
20	6	606	CHL	CBC-CAC-C3C	-3.68	107.50	112.88
20	Y	607	CHL	CBC-CAC-C3C	-3.68	107.50	112.88
21	1	609	CLA	O2D-CGD-CBD	3.67	117.80	111.27
21	B	817	CLA	O2D-CGD-CBD	3.67	117.79	111.27
20	Y	619	CHL	CBC-CAC-C3C	-3.66	107.52	112.88
21	5	613	CLA	O2D-CGD-CBD	3.65	117.76	111.27
21	B	822	CLA	C3B-C4B-NB	-3.65	107.13	110.52
21	A	816	CLA	O2D-CGD-CBD	3.65	117.76	111.27
20	X	606	CHL	CBC-CAC-C3C	-3.65	107.54	112.88
21	X	609	CLA	CHD-C1D-ND	-3.65	121.10	124.45
21	B	813	CLA	O2D-CGD-CBD	3.65	117.75	111.27
21	B	816	CLA	C3B-C4B-NB	-3.65	107.13	110.52
20	4	314	CHL	CAB-C3B-C2B	-3.64	117.56	124.69
21	B	820	CLA	C3B-C4B-NB	-3.64	107.14	110.52
23	3	616	XAT	O24-C25-C24	-3.63	110.65	113.38
20	Y	609	CHL	CBC-CAC-C3C	-3.63	107.56	112.88
21	6	601	CLA	O2D-CGD-CBD	3.63	117.72	111.27
21	3	605	CLA	CHD-C1D-ND	-3.63	121.12	124.45
21	A	837	CLA	C3B-C4B-NB	-3.63	107.15	110.52
20	6	615	CHL	CAB-C3B-C2B	-3.62	117.59	124.69
21	X	612	CLA	O2D-CGD-CBD	3.62	117.70	111.27
20	5	601	CHL	OBD-CAD-CBD	-3.62	120.52	125.82
21	A	801	CLA	O2D-CGD-CBD	3.62	117.69	111.27
21	A	805	CLA	O2D-CGD-CBD	3.61	117.69	111.27
20	X	601	CHL	CBC-CAC-C3C	-3.61	107.59	112.88
21	B	803	CLA	O2D-CGD-CBD	3.61	117.69	111.27
21	B	814	CLA	O2D-CGD-CBD	3.61	117.69	111.27
21	A	832	CLA	C3B-C4B-NB	-3.61	107.17	110.52
21	B	818	CLA	C3B-C4B-NB	-3.61	107.17	110.52
21	B	835	CLA	C3B-C4B-NB	-3.61	107.17	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	817	CLA	C3B-C4B-NB	-3.61	107.17	110.52
22	3	615	LUT	C40-C33-C34	-3.61	117.87	122.92
20	3	608	CHL	OBD-CAD-CBD	-3.61	120.53	125.82
21	A	808	CLA	C3B-C4B-NB	-3.60	107.17	110.52
20	Y	608	CHL	CBC-CAC-C3C	-3.60	107.61	112.88
21	A	821	CLA	C3B-C4B-NB	-3.60	107.18	110.52
22	Y	616	LUT	C15-C35-C34	3.60	130.84	123.47
20	2	607	CHL	CMA-C3A-C4A	-3.59	106.50	114.38
21	H	201	CLA	CHD-C1D-ND	-3.59	121.15	124.45
21	X	613	CLA	O2D-CGD-CBD	3.59	117.65	111.27
22	F	301	LUT	C39-C29-C30	-3.59	117.89	122.92
21	2	604	CLA	O2D-CGD-CBD	3.59	117.65	111.27
21	A	837	CLA	O2D-CGD-CBD	3.59	117.64	111.27
21	2	602	CLA	O2D-CGD-CBD	3.59	117.64	111.27
21	B	809	CLA	O2D-CGD-CBD	3.58	117.64	111.27
21	B	808	CLA	C3B-C4B-NB	-3.58	107.19	110.52
21	5	612	CLA	O2D-CGD-CBD	3.58	117.62	111.27
21	B	830	CLA	C3B-C4B-NB	-3.57	107.20	110.52
20	5	601	CHL	CMA-C3A-C4A	-3.57	106.56	114.38
20	Y	601	CHL	CMA-C3A-C4A	-3.57	106.56	114.38
21	B	833	CLA	O2D-CGD-CBD	3.57	117.61	111.27
21	A	822	CLA	C3B-C4B-NB	-3.57	107.20	110.52
21	B	801	CLA	O2D-CGD-CBD	3.57	117.61	111.27
20	4	304	CHL	CBC-CAC-C3C	-3.57	107.66	112.88
21	O	206	CLA	O2D-CGD-CBD	3.57	117.60	111.27
20	3	608	CHL	CMA-C3A-C4A	-3.56	106.57	114.38
21	B	832	CLA	C3B-C4B-NB	-3.56	107.21	110.52
21	B	828	CLA	C3B-C4B-NB	-3.56	107.21	110.52
21	B	824	CLA	O2D-CGD-CBD	3.56	117.59	111.27
21	A	818	CLA	C3B-C4B-NB	-3.56	107.22	110.52
21	B	809	CLA	C3B-C4B-NB	-3.55	107.22	110.52
21	3	607	CLA	O2D-CGD-CBD	3.55	117.58	111.27
22	F	301	LUT	C15-C35-C34	3.55	130.74	123.47
21	O	207	CLA	C3B-C4B-NB	-3.55	107.22	110.52
21	X	609	CLA	C3B-C4B-NB	-3.55	107.22	110.52
21	B	840	CLA	O2D-CGD-CBD	3.54	117.57	111.27
21	A	824	CLA	C3B-C4B-NB	-3.54	107.23	110.52
21	Z	303	CLA	O2D-CGD-CBD	3.54	117.56	111.27
21	4	303	CLA	O2D-CGD-CBD	3.54	117.55	111.27
20	Y	605	CHL	CBC-CAC-C3C	-3.54	107.70	112.88
21	5	607	CLA	CHD-C1D-ND	-3.54	121.20	124.45
20	2	607	CHL	CBC-CAC-C3C	-3.54	107.70	112.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	3	609	CLA	O2D-CGD-CBD	3.53	117.55	111.27
21	3	617	CLA	C3B-C4B-NB	-3.53	107.24	110.52
21	A	810	CLA	C3B-C4B-NB	-3.53	107.24	110.52
21	5	604	CLA	O2D-CGD-CBD	3.53	117.54	111.27
21	Y	613	CLA	O2D-CGD-CBD	3.53	117.54	111.27
21	A	815	CLA	O2D-CGD-CBD	3.53	117.53	111.27
21	Y	602	CLA	O2D-CGD-CBD	3.53	117.53	111.27
21	Z	312	CLA	O2D-CGD-CBD	3.53	117.53	111.27
21	1	602	CLA	O2D-CGD-CBD	3.53	117.53	111.27
21	H	201	CLA	C3B-C4B-NB	-3.52	107.25	110.52
20	6	606	CHL	CAA-C2A-C3A	-3.52	103.14	112.78
21	5	610	CLA	CHD-C1D-ND	-3.52	121.22	124.45
21	Z	311	CLA	O2D-CGD-CBD	3.51	117.51	111.27
20	2	606	CHL	CMA-C3A-C4A	-3.51	106.68	114.38
21	B	831	CLA	C3B-C4B-NB	-3.51	107.26	110.52
21	A	805	CLA	C3B-C4B-NB	-3.51	107.26	110.52
21	L	304	CLA	C3B-C4B-NB	-3.51	107.26	110.52
21	X	604	CLA	O2D-CGD-CBD	3.51	117.50	111.27
21	6	614	CLA	O2D-CGD-CBD	3.50	117.49	111.27
21	5	605	CLA	O2D-CGD-CBD	3.50	117.49	111.27
21	A	828	CLA	C3B-C4B-NB	-3.50	107.27	110.52
20	1	601	CHL	CBC-CAC-C3C	-3.50	107.75	112.88
20	Y	619	CHL	CAA-C2A-C3A	-3.50	103.19	112.78
21	6	604	CLA	O2D-CGD-CBD	3.50	117.49	111.27
21	A	806	CLA	C3B-C4B-NB	-3.50	107.27	110.52
20	6	607	CHL	CMA-C3A-C4A	-3.50	106.72	114.38
21	B	806	CLA	C3B-C4B-NB	-3.50	107.27	110.52
21	A	814	CLA	C3B-C4B-NB	-3.50	107.27	110.52
21	B	836	CLA	C3B-C4B-NB	-3.50	107.27	110.52
20	1	601	CHL	CMA-C3A-C4A	-3.49	106.73	114.38
21	B	810	CLA	O2D-CGD-CBD	3.49	117.46	111.27
20	2	601	CHL	CMA-C3A-C4A	-3.48	106.75	114.38
21	B	814	CLA	C3B-C4B-NB	-3.48	107.28	110.52
21	A	836	CLA	C3B-C4B-NB	-3.48	107.29	110.52
20	4	314	CHL	CMA-C3A-C4A	-3.48	106.76	114.38
21	Z	303	CLA	C3B-C4B-NB	-3.48	107.29	110.52
21	5	614	CLA	O2D-CGD-CBD	3.47	117.44	111.27
20	Z	306	CHL	CMA-C3A-C4A	-3.47	106.77	114.38
21	4	308	CLA	C3B-C4B-NB	-3.47	107.30	110.52
22	F	301	LUT	C35-C15-C14	3.47	130.58	123.47
21	B	803	CLA	C3B-C4B-NB	-3.47	107.30	110.52
20	Z	301	CHL	CBC-CAC-C3C	-3.46	107.81	112.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2	614	CHL	CBC-CAC-C3C	-3.46	107.81	112.88
21	3	614	CLA	C3B-C4B-NB	-3.46	107.31	110.52
20	2	605	CHL	CMA-C3A-C4A	-3.46	106.80	114.38
21	B	807	CLA	O2A-CGA-CBA	3.46	122.75	111.91
21	4	309	CLA	CHD-C1D-ND	-3.45	121.28	124.45
20	6	605	CHL	OBD-CAD-CBD	-3.45	120.76	125.82
20	5	606	CHL	CBC-CAC-C3C	-3.45	107.83	112.88
20	Z	308	CHL	CBC-CAC-C3C	-3.45	107.83	112.88
20	4	306	CHL	CAA-C2A-C3A	-3.45	103.34	112.78
21	A	831	CLA	C3B-C4B-NB	-3.45	107.32	110.52
22	Z	315	LUT	C30-C31-C32	3.45	133.97	123.22
20	6	605	CHL	CMA-C3A-C4A	-3.45	106.83	114.38
20	Z	309	CHL	CBC-CAC-C3C	-3.44	107.84	112.88
20	Z	306	CHL	CBC-CAC-C3C	-3.44	107.84	112.88
21	4	302	CLA	O2D-CGD-CBD	3.44	117.39	111.27
23	4	316	XAT	O24-C25-C24	-3.44	110.80	113.38
21	1	614	CLA	C3B-C4B-NB	-3.44	107.32	110.52
21	A	801	CLA	C3B-C4B-NB	-3.44	107.32	110.52
21	B	826	CLA	C3B-C4B-NB	-3.44	107.33	110.52
21	A	840	CLA	C3B-C4B-NB	-3.44	107.33	110.52
21	3	609	CLA	C3B-C4B-NB	-3.43	107.33	110.52
24	B	848	BCR	C23-C24-C25	3.43	136.84	127.20
21	B	821	CLA	O2D-CGD-CBD	3.43	117.36	111.27
22	3	615	LUT	C32-C33-C34	3.43	124.20	118.94
20	4	305	CHL	CMA-C3A-C4A	-3.42	106.88	114.38
22	X	615	LUT	C40-C33-C34	-3.42	118.13	122.92
21	X	604	CLA	CHD-C1D-ND	-3.42	121.31	124.45
21	Y	611	CLA	C3B-C4B-NB	-3.42	107.34	110.52
21	A	814	CLA	O2D-CGD-CBD	3.42	117.35	111.27
20	Y	609	CHL	CMA-C3A-C4A	-3.42	106.89	114.38
21	2	612	CLA	C3B-C4B-NB	-3.42	107.34	110.52
21	B	811	CLA	C3B-C4B-NB	-3.42	107.34	110.52
21	A	803	CLA	C3B-C4B-NB	-3.42	107.35	110.52
21	B	825	CLA	C3B-C4B-NB	-3.41	107.35	110.52
21	Z	310	CLA	C3B-C4B-NB	-3.41	107.35	110.52
20	X	605	CHL	CMA-C3A-C4A	-3.41	106.90	114.38
21	2	602	CLA	C3B-C4B-NB	-3.41	107.35	110.52
21	B	815	CLA	C3B-C4B-NB	-3.41	107.35	110.52
20	2	614	CHL	CMA-C3A-C4A	-3.41	106.91	114.38
21	A	812	CLA	C3B-C4B-NB	-3.41	107.35	110.52
21	A	820	CLA	C3B-C4B-NB	-3.41	107.35	110.52
21	K	202	CLA	O2D-CGD-CBD	3.41	117.32	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	843	CLA	CHD-C1D-ND	-3.40	121.33	124.45
21	B	838	CLA	O2A-CGA-CBA	3.40	122.58	111.91
21	A	829	CLA	C3B-C4B-NB	-3.40	107.36	110.52
21	6	602	CLA	C3B-C4B-NB	-3.40	107.36	110.52
21	B	827	CLA	C3B-C4B-NB	-3.40	107.36	110.52
22	5	619	LUT	C20-C13-C14	-3.40	118.16	122.92
21	A	815	CLA	C3B-C4B-NB	-3.40	107.36	110.52
21	3	607	CLA	C3B-C4B-NB	-3.40	107.36	110.52
21	B	837	CLA	C3B-C4B-NB	-3.39	107.37	110.52
21	A	841	CLA	C3B-C4B-NB	-3.39	107.37	110.52
20	4	305	CHL	CAA-C2A-C3A	-3.39	103.50	112.78
20	1	606	CHL	CMA-C3A-C4A	-3.39	106.96	114.38
21	B	825	CLA	O2A-CGA-CBA	3.39	122.53	111.91
21	6	609	CLA	C3B-C4B-NB	-3.38	107.38	110.52
22	5	615	LUT	C40-C33-C34	-3.38	118.18	122.92
22	2	615	LUT	C15-C35-C34	3.38	130.40	123.47
21	4	301	CLA	C3B-C4B-NB	-3.38	107.38	110.52
21	A	809	CLA	C3B-C4B-NB	-3.38	107.38	110.52
22	F	301	LUT	C20-C13-C14	-3.38	118.19	122.92
21	1	613	CLA	C3B-C4B-NB	-3.38	107.38	110.52
20	Y	608	CHL	OMC-CMC-C2C	-3.38	119.61	125.03
21	O	206	CLA	CHD-C1D-ND	-3.38	121.35	124.45
21	5	610	CLA	C3B-C4B-NB	-3.38	107.38	110.52
21	B	819	CLA	C3B-C4B-NB	-3.38	107.38	110.52
20	X	605	CHL	CBC-CAC-C3C	-3.38	107.94	112.88
20	Z	301	CHL	CMA-C3A-C4A	-3.37	106.99	114.38
21	B	834	CLA	C3B-C4B-NB	-3.37	107.39	110.52
21	Z	303	CLA	CHD-C1D-ND	-3.37	121.36	124.45
20	5	601	CHL	C1-C2-C3	3.37	131.87	126.04
21	A	833	CLA	C3B-C4B-NB	-3.37	107.39	110.52
21	4	307	CLA	C3B-C4B-NB	-3.37	107.39	110.52
21	G	203	CLA	C3B-C4B-NB	-3.36	107.39	110.52
20	6	607	CHL	CAA-C2A-C3A	-3.36	103.58	112.78
20	Z	307	CHL	CMA-C3A-C4A	-3.36	107.02	114.38
20	4	304	CHL	C1-C2-C3	3.36	131.85	126.04
21	X	611	CLA	O2D-CGD-CBD	3.36	117.23	111.27
20	4	305	CHL	CBC-CAC-C3C	-3.36	107.96	112.88
20	Z	301	CHL	CAA-C2A-C3A	-3.35	103.60	112.78
20	Y	606	CHL	CBC-CAC-C3C	-3.35	107.97	112.88
20	Z	302	CHL	CMA-C3A-C4A	-3.35	107.05	114.38
21	A	817	CLA	C3B-C4B-NB	-3.34	107.41	110.52
20	6	606	CHL	CMA-C3A-C4A	-3.34	107.05	114.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	838	CLA	O2A-CGA-CBA	3.34	122.38	111.91
21	X	610	CLA	CHD-C1D-ND	-3.34	121.39	124.45
21	B	838	CLA	C3B-C4B-NB	-3.33	107.42	110.52
21	O	206	CLA	C3B-C4B-NB	-3.33	107.42	110.52
20	4	306	CHL	CMA-C3A-C4A	-3.33	107.08	114.38
20	6	615	CHL	CMA-C3A-C4A	-3.33	107.08	114.38
20	Y	607	CHL	CAA-C2A-C3A	-3.33	103.65	112.78
21	A	819	CLA	C3B-C4B-NB	-3.33	107.42	110.52
20	6	615	CHL	CBC-CAC-C3C	-3.33	108.00	112.88
21	A	838	CLA	C3B-C4B-NB	-3.33	107.43	110.52
21	X	604	CLA	C3B-C4B-NB	-3.33	107.43	110.52
20	Z	307	CHL	CAA-C2A-C3A	-3.33	103.67	112.78
20	X	607	CHL	CMA-C3A-C4A	-3.32	107.10	114.38
21	1	604	CLA	C3B-C4B-NB	-3.32	107.44	110.52
21	5	602	CLA	C3B-C4B-NB	-3.32	107.44	110.52
21	2	610	CLA	C3B-C4B-NB	-3.32	107.44	110.52
21	A	839	CLA	C3B-C4B-NB	-3.31	107.44	110.52
21	1	609	CLA	C3B-C4B-NB	-3.31	107.44	110.52
21	A	817	CLA	O2D-CGD-CBD	3.31	117.15	111.27
21	A	826	CLA	CHD-C1D-ND	-3.31	121.41	124.45
21	F	304	CLA	C3B-C4B-NB	-3.31	107.44	110.52
21	A	816	CLA	C3B-C4B-NB	-3.31	107.45	110.52
21	X	613	CLA	C3B-C4B-NB	-3.30	107.45	110.52
21	Z	304	CLA	C3B-C4B-NB	-3.30	107.45	110.52
21	Z	304	CLA	O2D-CGD-CBD	3.30	117.13	111.27
20	Z	302	CHL	CBC-CAC-C3C	-3.30	108.05	112.88
21	B	804	CLA	C3B-C4B-NB	-3.30	107.45	110.52
21	1	612	CLA	C3B-C4B-NB	-3.30	107.45	110.52
21	K	201	CLA	C3B-C4B-NB	-3.30	107.45	110.52
21	3	602	CLA	C3B-C4B-NB	-3.30	107.46	110.52
22	2	615	LUT	C35-C15-C14	3.30	130.23	123.47
21	K	204	CLA	C3B-C4B-NB	-3.30	107.46	110.52
20	Y	608	CHL	CMA-C3A-C4A	-3.30	107.16	114.38
21	B	840	CLA	C3B-C4B-NB	-3.30	107.46	110.52
21	Y	602	CLA	C3B-C4B-NB	-3.29	107.46	110.52
20	4	306	CHL	C1-C2-C3	3.29	132.07	126.75
21	1	610	CLA	C3B-C4B-NB	-3.29	107.47	110.52
21	5	603	CLA	C3B-C4B-NB	-3.28	107.47	110.52
20	Y	609	CHL	CAA-C2A-C3A	-3.28	103.79	112.78
21	6	608	CLA	C3B-C4B-NB	-3.28	107.47	110.52
21	4	312	CLA	C3B-C4B-NB	-3.28	107.47	110.52
22	6	616	LUT	C40-C33-C34	-3.28	118.33	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	5	601	CHL	CAA-C2A-C3A	-3.28	103.80	112.78
20	2	606	CHL	OBD-CAD-CBD	-3.28	121.02	125.82
21	3	605	CLA	C3B-C4B-NB	-3.28	107.47	110.52
21	B	812	CLA	C3B-C4B-NB	-3.28	107.47	110.52
23	5	616	XAT	O24-C25-C24	-3.28	110.92	113.38
21	A	843	CLA	O2D-CGD-CBD	3.27	117.08	111.27
20	1	601	CHL	C1-C2-C3	3.27	131.70	126.04
21	2	618	CLA	C3B-C4B-NB	-3.27	107.48	110.52
22	Z	314	LUT	C20-C13-C14	-3.27	118.34	122.92
21	K	202	CLA	C3B-C4B-NB	-3.27	107.48	110.52
21	1	609	CLA	O2A-CGA-CBA	3.27	122.16	111.91
21	B	801	CLA	C3B-C4B-NB	-3.27	107.48	110.52
21	3	610	CLA	C3B-C4B-NB	-3.27	107.49	110.52
20	5	606	CHL	CMA-C3A-C4A	-3.26	107.23	114.38
21	A	804	CLA	C3B-C4B-NB	-3.26	107.49	110.52
20	Z	309	CHL	CMA-C3A-C4A	-3.26	107.23	114.38
21	2	603	CLA	C3B-C4B-NB	-3.26	107.49	110.52
21	B	839	CLA	O2A-CGA-CBA	3.26	122.14	111.91
20	6	606	CHL	OBD-CAD-CBD	-3.26	121.04	125.82
21	O	206	CLA	O2A-CGA-CBA	3.26	122.13	111.91
20	Y	601	CHL	CAA-C2A-C3A	-3.26	103.86	112.78
20	Z	306	CHL	CAA-C2A-C3A	-3.26	103.86	112.78
21	B	839	CLA	C3B-C4B-NB	-3.26	107.49	110.52
21	5	611	CLA	CHD-C1D-ND	-3.26	121.46	124.45
21	K	203	CLA	CHD-C1D-ND	-3.26	121.46	124.45
21	1	603	CLA	C3B-C4B-NB	-3.26	107.50	110.52
20	2	606	CHL	CBC-CAC-C3C	-3.25	108.11	112.88
21	5	607	CLA	C3B-C4B-NB	-3.25	107.50	110.52
21	5	611	CLA	C3B-C4B-NB	-3.25	107.50	110.52
20	2	607	CHL	CAA-C2A-C3A	-3.25	103.89	112.78
21	3	604	CLA	C3B-C4B-NB	-3.24	107.50	110.52
21	J	102	CLA	C3B-C4B-NB	-3.24	107.50	110.52
21	Z	312	CLA	C3B-C4B-NB	-3.24	107.50	110.52
21	A	823	CLA	C3B-C4B-NB	-3.24	107.51	110.52
21	4	309	CLA	C3B-C4B-NB	-3.24	107.51	110.52
21	Y	612	CLA	CHD-C1D-ND	-3.24	121.48	124.45
20	4	304	CHL	OBD-CAD-CBD	-3.24	121.07	125.82
21	A	813	CLA	C3B-C4B-NB	-3.24	107.51	110.52
21	B	805	CLA	C3B-C4B-NB	-3.24	107.51	110.52
21	Y	603	CLA	C3B-C4B-NB	-3.23	107.52	110.52
21	B	816	CLA	O2A-CGA-CBA	3.23	122.05	111.91
21	A	837	CLA	CHD-C1D-ND	-3.23	121.48	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	6	611	CLA	C3B-C4B-NB	-3.23	107.52	110.52
20	4	306	CHL	OBD-CAD-CBD	-3.23	121.08	125.82
22	Y	615	LUT	C15-C35-C34	3.23	130.09	123.47
21	1	611	CLA	C3B-C4B-NB	-3.23	107.52	110.52
21	5	605	CLA	C3B-C4B-NB	-3.23	107.52	110.52
21	1	607	CLA	C3B-C4B-NB	-3.23	107.52	110.52
21	A	839	CLA	O2A-CGA-CBA	3.23	122.04	111.91
21	2	609	CLA	CHD-C1D-ND	-3.23	121.49	124.45
21	A	807	CLA	C3B-C4B-NB	-3.23	107.52	110.52
21	L	303	CLA	C3B-C4B-NB	-3.23	107.52	110.52
20	2	601	CHL	CAA-C2A-C3A	-3.23	103.95	112.78
21	4	311	CLA	C3B-C4B-NB	-3.22	107.53	110.52
21	2	611	CLA	CHD-C1D-ND	-3.22	121.49	124.45
21	1	608	CLA	C3B-C4B-NB	-3.22	107.53	110.52
21	6	610	CLA	C3B-C4B-NB	-3.22	107.53	110.52
21	L	301	CLA	C3B-C4B-NB	-3.21	107.53	110.52
21	B	824	CLA	C3B-C4B-NB	-3.21	107.53	110.52
21	A	825	CLA	C3B-C4B-NB	-3.21	107.53	110.52
20	Z	308	CHL	CMA-C3A-C4A	-3.21	107.34	114.38
21	2	609	CLA	O2A-CGA-CBA	3.21	121.98	111.91
21	3	612	CLA	C3B-C4B-NB	-3.21	107.54	110.52
21	A	843	CLA	C3B-C4B-NB	-3.21	107.54	110.52
21	G	204	CLA	C3B-C4B-NB	-3.21	107.54	110.52
21	A	842	CLA	O2A-CGA-CBA	3.21	121.97	111.91
21	3	602	CLA	O2D-CGD-CBD	3.21	116.97	111.27
21	B	806	CLA	O2A-CGA-CBA	3.21	121.97	111.91
21	1	605	CLA	C3B-C4B-NB	-3.20	107.54	110.52
21	B	829	CLA	CHD-C1D-ND	-3.20	121.51	124.45
20	Y	607	CHL	CMA-C3A-C4A	-3.20	107.36	114.38
21	J	101	CLA	CHD-C1D-ND	-3.20	121.51	124.45
21	4	311	CLA	O2A-CGA-CBA	3.20	121.96	111.91
22	Y	615	LUT	C20-C13-C14	-3.20	118.44	122.92
21	B	823	CLA	C3B-C4B-NB	-3.20	107.55	110.52
21	J	101	CLA	C3B-C4B-NB	-3.20	107.55	110.52
21	B	827	CLA	O2A-CGA-CBA	3.20	121.95	111.91
21	B	821	CLA	C3B-C4B-NB	-3.20	107.55	110.52
20	X	608	CHL	CMA-C3A-C4A	-3.20	107.37	114.38
21	A	818	CLA	O2A-CGA-CBA	3.20	121.94	111.91
21	5	612	CLA	C3B-C4B-NB	-3.20	107.55	110.52
21	A	807	CLA	O2A-CGA-CBA	3.20	121.94	111.91
21	A	834	CLA	C3B-C4B-NB	-3.19	107.55	110.52
21	6	611	CLA	CHD-C1D-ND	-3.19	121.52	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2	614	CHL	OBD-CAD-CBD	-3.19	121.14	125.82
21	6	613	CLA	C3B-C4B-NB	-3.19	107.56	110.52
21	4	308	CLA	CHD-C1D-ND	-3.19	121.52	124.45
21	6	603	CLA	O2D-CGD-CBD	3.19	116.93	111.27
21	1	602	CLA	O2A-CGA-CBA	3.19	121.91	111.91
21	2	604	CLA	C3B-C4B-NB	-3.19	107.56	110.52
21	A	807	CLA	O2D-CGD-CBD	3.18	116.93	111.27
20	Y	601	CHL	OBD-CAD-CBD	-3.18	121.15	125.82
20	1	601	CHL	CAA-C2A-C3A	-3.18	104.07	112.78
21	4	310	CLA	C3B-C4B-NB	-3.18	107.56	110.52
21	4	313	CLA	C3B-C4B-NB	-3.18	107.56	110.52
21	6	601	CLA	C3B-C4B-NB	-3.18	107.56	110.52
21	A	812	CLA	O2A-CGA-CBA	3.18	121.88	111.91
21	6	614	CLA	C3B-C4B-NB	-3.18	107.57	110.52
21	B	808	CLA	O2A-CGA-CBA	3.18	121.88	111.91
21	K	203	CLA	C3B-C4B-NB	-3.17	107.57	110.52
20	X	606	CHL	CAA-C2A-C3A	-3.17	104.09	112.78
21	1	603	CLA	O2D-CGD-CBD	3.17	116.91	111.27
21	X	618	CLA	C3B-C4B-NB	-3.17	107.57	110.52
20	X	608	CHL	CAA-C2A-C3A	-3.17	104.10	112.78
21	X	602	CLA	C3B-C4B-NB	-3.17	107.58	110.52
21	2	613	CLA	C3B-C4B-NB	-3.16	107.58	110.52
21	1	610	CLA	O2A-CGA-CBA	3.16	121.84	111.91
21	B	805	CLA	O2D-CGD-CBD	3.16	116.89	111.27
20	4	305	CHL	C1A-CHA-C4D	3.16	124.26	118.98
21	O	203	CLA	C3B-C4B-NB	-3.16	107.58	110.52
20	Y	606	CHL	C1C-CHC-C4B	3.16	126.20	115.73
21	B	822	CLA	O2A-CGA-CBA	3.16	121.83	111.91
21	6	612	CLA	C3B-C4B-NB	-3.16	107.58	110.52
21	6	614	CLA	O2A-CGA-CBA	3.16	121.83	111.91
21	2	612	CLA	O2A-CGA-CBA	3.16	121.83	111.91
21	O	202	CLA	C3B-C4B-NB	-3.16	107.58	110.52
20	Y	608	CHL	CAA-C2A-C3A	-3.16	104.13	112.78
21	B	837	CLA	O2A-CGA-CBA	3.16	121.82	111.91
20	Z	306	CHL	OMC-CMC-C2C	-3.16	119.97	125.03
21	A	833	CLA	O2A-CGA-CBA	3.16	121.82	111.91
20	Y	606	CHL	CMA-C3A-C4A	-3.16	107.46	114.38
21	3	606	CLA	C3B-C4B-NB	-3.16	107.59	110.52
21	A	819	CLA	O2A-CGA-CBA	3.16	121.81	111.91
21	B	803	CLA	CHD-C1D-ND	-3.15	121.56	124.45
21	A	842	CLA	C3B-C4B-NB	-3.15	107.59	110.52
20	2	601	CHL	C1C-CHC-C4B	3.15	126.17	115.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	Y	616	LUT	C35-C15-C14	3.15	129.93	123.47
21	G	202	CLA	C3B-C4B-NB	-3.15	107.59	110.52
22	1	615	LUT	C40-C33-C34	-3.15	118.51	122.92
21	A	830	CLA	O2A-CGA-CBA	3.15	121.80	111.91
20	Y	608	CHL	OBD-CAD-CBD	-3.15	121.20	125.82
21	B	807	CLA	C3B-C4B-NB	-3.15	107.59	110.52
21	B	835	CLA	O2A-CGA-CBA	3.15	121.78	111.91
20	X	605	CHL	C1C-CHC-C4B	3.15	126.15	115.73
21	1	608	CLA	O2A-CGA-CBA	3.15	121.78	111.91
21	5	614	CLA	C3B-C4B-NB	-3.15	107.60	110.52
21	2	610	CLA	CHD-C1D-ND	-3.14	121.56	124.45
21	B	810	CLA	C1-C2-C3	3.14	131.48	126.04
20	X	607	CHL	CAA-C2A-C3A	-3.14	104.17	112.78
20	Z	308	CHL	OBD-CAD-CBD	-3.14	121.21	125.82
20	1	601	CHL	O2A-CGA-CBA	3.14	121.77	111.91
22	Y	616	LUT	C40-C33-C34	-3.14	118.53	122.92
21	6	609	CLA	O2A-CGA-CBA	3.14	121.75	111.91
20	X	607	CHL	C1C-CHC-C4B	3.14	126.12	115.73
20	Z	309	CHL	C1C-CHC-C4B	3.14	126.12	115.73
21	2	608	CLA	C3B-C4B-NB	-3.14	107.61	110.52
20	X	606	CHL	CMA-C3A-C4A	-3.14	107.51	114.38
22	X	615	LUT	C32-C33-C34	3.13	123.75	118.94
21	A	808	CLA	O2A-CGA-CBA	3.13	121.74	111.91
21	4	303	CLA	C3B-C4B-NB	-3.13	107.61	110.52
21	1	602	CLA	C3B-C4B-NB	-3.13	107.61	110.52
22	4	315	LUT	C40-C33-C34	-3.13	118.54	122.92
20	Y	607	CHL	CHA-C1A-C2A	-3.13	125.96	133.31
21	A	811	CLA	C3B-C4B-NB	-3.13	107.61	110.52
20	3	608	CHL	CAA-C2A-C3A	-3.13	104.22	112.78
22	X	615	LUT	C20-C13-C14	-3.13	118.55	122.92
21	Y	613	CLA	C3B-C4B-NB	-3.12	107.62	110.52
21	A	825	CLA	CHD-C1D-ND	-3.12	121.58	124.45
21	3	614	CLA	CHD-C1D-ND	-3.12	121.59	124.45
20	X	608	CHL	C1C-CHC-C4B	3.12	126.07	115.73
21	Y	602	CLA	O2A-CGA-CBA	3.12	121.70	111.91
22	3	615	LUT	C28-C29-C30	3.12	123.72	118.94
22	Z	315	LUT	C20-C13-C14	-3.12	118.56	122.92
21	Y	614	CLA	C3B-C4B-NB	-3.12	107.62	110.52
20	2	605	CHL	C1A-CHA-C4D	3.12	124.18	118.98
21	B	812	CLA	O2A-CGA-CBA	3.12	121.69	111.91
21	6	609	CLA	CHD-C1D-ND	-3.12	121.59	124.45
21	A	837	CLA	O2A-CGA-CBA	3.12	121.69	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	Z	308	CHL	C1C-CHC-C4B	3.11	126.04	115.73
22	5	615	LUT	C20-C13-C14	-3.11	118.56	122.92
21	B	813	CLA	CHD-C1D-ND	-3.11	121.59	124.45
21	4	302	CLA	C3B-C4B-NB	-3.11	107.63	110.52
21	B	822	CLA	CHD-C1D-ND	-3.11	121.59	124.45
21	X	603	CLA	C3B-C4B-NB	-3.11	107.63	110.52
21	A	834	CLA	O2A-CGA-CBA	3.11	121.66	111.91
21	B	840	CLA	O2A-CGA-CBA	3.11	121.66	111.91
21	X	612	CLA	C3B-C4B-NB	-3.10	107.64	110.52
20	Y	619	CHL	C1C-CHC-C4B	3.10	126.01	115.73
21	A	831	CLA	CHD-C1D-ND	-3.10	121.60	124.45
22	2	615	LUT	C20-C13-C14	-3.10	118.58	122.92
22	5	619	LUT	C12-C13-C14	3.10	123.70	118.94
21	A	810	CLA	O2A-CGA-CBA	3.10	121.64	111.91
20	2	605	CHL	CHA-C1A-C2A	-3.10	126.03	133.31
20	5	606	CHL	C1C-CHC-C4B	3.10	126.00	115.73
21	B	815	CLA	CHD-C1D-ND	-3.10	121.61	124.45
21	A	803	CLA	O2A-CGA-CBA	3.10	121.63	111.91
22	Y	616	LUT	C20-C13-C14	-3.10	118.58	122.92
21	A	829	CLA	O2A-CGA-CBA	3.10	121.62	111.91
20	4	304	CHL	CAA-C2A-C3A	-3.10	104.30	112.78
21	4	301	CLA	O2A-CGA-CBA	3.10	121.62	111.91
21	A	808	CLA	CHD-C1D-ND	-3.09	121.61	124.45
21	B	836	CLA	O2A-CGA-CBA	3.09	121.62	111.91
20	2	601	CHL	OBD-CAD-CBD	-3.09	121.28	125.82
21	3	609	CLA	CHD-C1D-ND	-3.09	121.61	124.45
21	B	835	CLA	CHD-C1D-ND	-3.09	121.61	124.45
21	B	824	CLA	O2A-CGA-CBA	3.09	121.62	111.91
20	5	601	CHL	C1C-CHC-C4B	3.09	125.98	115.73
20	Z	302	CHL	C1C-CHC-C4B	3.09	125.98	115.73
21	3	602	CLA	CHD-C1D-ND	-3.09	121.61	124.45
20	2	614	CHL	C4C-CHD-C1D	3.09	125.97	115.73
21	B	801	CLA	O2A-CGA-CBA	3.09	121.60	111.91
20	6	605	CHL	C1-C2-C3	3.09	131.38	126.04
21	1	604	CLA	O2A-CGA-CBA	3.09	121.60	111.91
20	6	607	CHL	C1-C2-C3	3.08	131.74	126.75
21	B	833	CLA	O2A-CGA-CBA	3.08	121.58	111.91
21	A	824	CLA	O2A-CGA-CBA	3.08	121.58	111.91
22	F	301	LUT	C39-C29-C28	3.08	122.93	118.08
21	5	604	CLA	C3B-C4B-NB	-3.08	107.66	110.52
21	L	304	CLA	O2A-CGA-CBA	3.08	121.57	111.91
21	3	610	CLA	CHD-C1D-ND	-3.08	121.62	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	6	612	CLA	O2A-CGA-CBA	3.08	121.57	111.91
22	X	615	LUT	C35-C15-C14	3.08	129.78	123.47
21	B	820	CLA	O2A-CGA-CBA	3.08	121.56	111.91
22	5	619	LUT	C40-C33-C34	-3.07	118.62	122.92
21	3	611	CLA	C3B-C4B-NB	-3.07	107.66	110.52
20	6	607	CHL	C1C-CHC-C4B	3.07	125.91	115.73
21	Y	612	CLA	C3B-C4B-NB	-3.07	107.66	110.52
21	A	828	CLA	CHD-C1D-ND	-3.07	121.63	124.45
21	Y	610	CLA	C3B-C4B-NB	-3.07	107.67	110.52
21	K	204	CLA	CHD-C1D-ND	-3.07	121.63	124.45
21	4	313	CLA	O2A-CGA-CBA	3.07	121.55	111.91
20	Y	619	CHL	OBD-CAD-CBD	-3.07	121.32	125.82
21	Z	305	CLA	O2A-CGA-CBA	3.07	121.54	111.91
21	B	828	CLA	O2A-CGA-CBA	3.07	121.54	111.91
20	4	305	CHL	C1C-CHC-C4B	3.07	125.89	115.73
20	6	606	CHL	C1C-CHC-C4B	3.07	125.89	115.73
20	2	605	CHL	OBD-CAD-CBD	-3.07	121.33	125.82
20	Y	601	CHL	C1C-CHC-C4B	3.07	125.89	115.73
21	A	813	CLA	CHD-C1D-ND	-3.06	121.64	124.45
21	A	821	CLA	CHD-C1D-ND	-3.06	121.64	124.45
22	2	615	LUT	C40-C33-C34	-3.06	118.63	122.92
21	6	604	CLA	C3B-C4B-NB	-3.06	107.67	110.52
21	G	204	CLA	CHD-C1D-ND	-3.06	121.64	124.45
20	2	605	CHL	C1C-CHC-C4B	3.06	125.87	115.73
21	3	602	CLA	O2A-CGA-CBA	3.06	121.51	111.91
21	Y	602	CLA	CHD-C1D-ND	-3.06	121.64	124.45
21	2	602	CLA	O2A-CGA-CBA	3.06	121.51	111.91
21	F	304	CLA	CHD-C1D-ND	-3.06	121.64	124.45
20	6	615	CHL	C1C-CHC-C4B	3.06	125.86	115.73
21	A	821	CLA	O2A-CGA-CBA	3.06	121.50	111.91
22	F	301	LUT	C12-C13-C14	3.06	123.63	118.94
21	B	810	CLA	O2A-CGA-CBA	3.06	121.50	111.91
21	3	606	CLA	CHD-C1D-ND	-3.05	121.65	124.45
21	A	828	CLA	O2A-CGA-CBA	3.05	121.49	111.91
21	6	602	CLA	O2A-CGA-CBA	3.05	121.49	111.91
21	O	203	CLA	O2A-CGA-CBA	3.05	121.48	111.91
21	Z	311	CLA	C3B-C4B-NB	-3.05	107.69	110.52
21	X	610	CLA	C3B-C4B-NB	-3.05	107.69	110.52
23	1	616	XAT	O4-C5-C4	-3.05	111.09	113.38
22	X	614	LUT	C20-C13-C14	-3.05	118.65	122.92
21	B	817	CLA	O2A-CGA-CBA	3.05	121.46	111.91
20	1	601	CHL	C1C-CHC-C4B	3.04	125.81	115.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	Y	607	CHL	C1C-CHC-C4B	3.04	125.81	115.73
20	Y	605	CHL	CMA-C3A-C4A	-3.04	107.71	114.38
21	A	818	CLA	C12-C11-C10	-3.04	102.86	113.62
21	B	823	CLA	O2A-CGA-CBA	3.04	121.45	111.91
21	B	826	CLA	O2A-CGA-CBA	3.04	121.45	111.91
21	3	603	CLA	C3B-C4B-NB	-3.04	107.69	110.52
21	B	814	CLA	CHD-C1D-ND	-3.04	121.66	124.45
23	6	617	XAT	O24-C25-C24	-3.04	111.10	113.38
21	A	841	CLA	O2A-CGA-CBA	3.04	121.44	111.91
21	B	818	CLA	O2A-CGA-CBA	3.04	121.44	111.91
22	5	615	LUT	C32-C33-C34	3.04	123.60	118.94
20	6	605	CHL	CAA-C2A-C3A	-3.04	104.46	112.78
21	A	806	CLA	O2A-CGA-CBA	3.04	121.44	111.91
20	Z	302	CHL	CAA-C2A-C3A	-3.04	104.46	112.78
21	A	801	CLA	CHD-C1D-ND	-3.04	121.66	124.45
20	X	601	CHL	C4C-CHD-C1D	3.04	125.79	115.73
20	6	615	CHL	C4C-CHD-C1D	3.03	125.78	115.73
20	6	605	CHL	C1C-CHC-C4B	3.03	125.78	115.73
21	5	613	CLA	C3B-C4B-NB	-3.03	107.70	110.52
22	Y	615	LUT	C40-C33-C34	-3.03	118.67	122.92
20	Y	605	CHL	C1C-CHC-C4B	3.03	125.78	115.73
20	Y	608	CHL	C4C-CHD-C1D	3.03	125.77	115.73
20	1	606	CHL	C1C-CHC-C4B	3.03	125.77	115.73
21	6	608	CLA	CHD-C1D-ND	-3.03	121.67	124.45
21	A	827	CLA	O2A-CGA-CBA	3.03	121.42	111.91
21	Y	611	CLA	CHD-C1D-ND	-3.03	121.67	124.45
21	Y	604	CLA	C3B-C4B-NB	-3.02	107.71	110.52
21	Z	305	CLA	C3B-C4B-NB	-3.02	107.71	110.52
22	5	615	LUT	C35-C15-C14	3.02	129.67	123.47
22	6	616	LUT	C20-C13-C14	-3.02	118.69	122.92
21	A	803	CLA	CHD-C1D-ND	-3.02	121.68	124.45
21	B	809	CLA	O2A-CGA-CBA	3.02	121.39	111.91
20	6	606	CHL	C1A-CHA-C4D	3.02	124.02	118.98
20	2	606	CHL	C1C-CHC-C4B	3.01	125.72	115.73
21	6	613	CLA	CHD-C1D-ND	-3.01	121.68	124.45
20	3	608	CHL	C3C-C4C-NC	-3.01	108.36	115.01
21	Y	613	CLA	C1-C2-C3	3.01	131.25	126.04
20	Y	619	CHL	O1D-CGD-CBD	-3.01	119.72	124.74
21	6	603	CLA	C3B-C4B-NB	-3.01	107.72	110.52
20	2	605	CHL	C4C-CHD-C1D	3.01	125.70	115.73
20	1	606	CHL	CBC-CAC-C3C	-3.01	108.47	112.88
20	Z	306	CHL	C4C-CHD-C1D	3.01	125.70	115.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	836	CLA	CHD-C1D-ND	-3.01	121.69	124.45
22	F	301	LUT	C40-C33-C34	-3.01	118.71	122.92
21	B	814	CLA	O2A-CGA-CBA	3.01	121.34	111.91
21	4	308	CLA	O2A-CGA-CBA	3.01	121.34	111.91
21	A	827	CLA	CHD-C1D-ND	-3.01	121.69	124.45
20	1	606	CHL	C4C-CHD-C1D	3.01	125.69	115.73
21	B	815	CLA	O2A-CGA-CBA	3.00	121.33	111.91
21	B	816	CLA	C12-C11-C10	-3.00	103.00	113.62
21	1	612	CLA	O2A-CGA-CBA	3.00	121.33	111.91
20	3	608	CHL	C4C-CHD-C1D	3.00	125.67	115.73
20	4	305	CHL	CHA-C1A-C2A	-3.00	126.26	133.31
20	Z	307	CHL	C1C-CHC-C4B	3.00	125.67	115.73
21	A	825	CLA	O2A-CGA-CBA	3.00	121.32	111.91
21	X	611	CLA	C3B-C4B-NB	-3.00	107.73	110.52
20	Z	301	CHL	C4C-CHD-C1D	3.00	125.66	115.73
20	2	607	CHL	O2A-CGA-CBA	3.00	121.31	111.91
21	X	612	CLA	CHD-C1D-ND	-3.00	121.70	124.45
20	Y	606	CHL	CAA-C2A-C3A	-2.99	104.58	112.78
21	B	821	CLA	O2A-CGA-CBA	2.99	121.30	111.91
21	2	611	CLA	C3B-C4B-NB	-2.99	107.74	110.52
20	Z	307	CHL	OBD-CAD-CBD	-2.99	121.43	125.82
20	Y	609	CHL	C1C-CHC-C4B	2.99	125.64	115.73
21	G	203	CLA	CHD-C1D-ND	-2.99	121.70	124.45
20	2	614	CHL	C3C-C4C-NC	-2.99	108.41	115.01
20	5	601	CHL	C4C-CHD-C1D	2.99	125.64	115.73
21	A	831	CLA	O2A-CGA-CBA	2.99	121.28	111.91
21	A	811	CLA	O2A-CGA-CBA	2.98	121.27	111.91
21	3	603	CLA	O2A-CGA-CBA	2.98	121.27	111.91
21	X	618	CLA	CHD-C1D-ND	-2.98	121.71	124.45
21	B	831	CLA	CHD-C1D-ND	-2.98	121.71	124.45
21	2	608	CLA	CHD-C1D-ND	-2.98	121.72	124.45
20	Z	302	CHL	C3C-C4C-NC	-2.98	108.44	115.01
20	Y	609	CHL	C4C-CHD-C1D	2.98	125.60	115.73
20	X	601	CHL	CAA-C2A-C3A	-2.98	104.62	112.78
21	A	811	CLA	CHD-C1D-ND	-2.98	121.72	124.45
21	5	602	CLA	O2A-CGA-CBA	2.98	121.26	111.91
20	X	606	CHL	C4C-CHD-C1D	2.98	125.60	115.73
20	4	306	CHL	C4C-CHD-C1D	2.98	125.59	115.73
21	2	604	CLA	O2A-CGA-CBA	2.98	121.25	111.91
20	1	601	CHL	C4C-CHD-C1D	2.97	125.58	115.73
21	B	805	CLA	O2A-CGA-CBA	2.97	121.24	111.91
20	2	607	CHL	C1C-CHC-C4B	2.97	125.58	115.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	Z	302	CHL	O1D-CGD-CBD	-2.97	119.79	124.74
20	X	608	CHL	C3C-C4C-NC	-2.97	108.45	115.01
21	3	613	CLA	C3B-C4B-NB	-2.97	107.76	110.52
20	6	607	CHL	C3C-C4C-NC	-2.97	108.45	115.01
20	X	601	CHL	CMA-C3A-C4A	-2.97	107.88	114.38
20	4	304	CHL	C1C-CHC-C4B	2.97	125.56	115.73
20	Z	301	CHL	O1D-CGD-CBD	-2.97	119.80	124.74
20	Z	307	CHL	C4C-CHD-C1D	2.97	125.56	115.73
20	Z	308	CHL	C4C-CHD-C1D	2.97	125.56	115.73
21	A	805	CLA	CHD-C1D-ND	-2.97	121.73	124.45
22	Z	315	LUT	C8-C9-C10	2.97	123.49	118.94
21	4	309	CLA	O2A-CGA-CBA	2.96	121.21	111.91
20	X	607	CHL	C4C-CHD-C1D	2.96	125.54	115.73
20	5	606	CHL	C4C-CHD-C1D	2.96	125.54	115.73
20	6	607	CHL	O2A-CGA-CBA	2.96	121.20	111.91
20	Z	307	CHL	C3C-C4C-NC	-2.96	108.48	115.01
21	A	801	CLA	O2A-CGA-CBA	2.96	121.19	111.91
21	A	813	CLA	O2A-CGA-CBA	2.96	121.19	111.91
22	Z	314	LUT	C40-C33-C34	-2.96	118.78	122.92
21	A	804	CLA	O2A-CGA-CBA	2.96	121.19	111.91
20	4	306	CHL	C1C-CHC-C4B	2.96	125.52	115.73
20	4	314	CHL	C4C-CHD-C1D	2.96	125.52	115.73
21	A	840	CLA	O2A-CGA-CBA	2.95	121.18	111.91
21	5	609	CLA	C3B-C4B-NB	-2.95	107.78	110.52
21	1	611	CLA	CHD-C1D-ND	-2.95	121.74	124.45
21	B	824	CLA	CHD-C1D-ND	-2.95	121.74	124.45
20	Z	301	CHL	C1C-CHC-C4B	2.95	125.51	115.73
21	A	812	CLA	CHD-C1D-ND	-2.95	121.74	124.45
20	Y	608	CHL	C3C-C4C-NC	-2.95	108.50	115.01
21	B	810	CLA	CHD-C1D-ND	-2.95	121.74	124.45
20	X	601	CHL	C1C-CHC-C4B	2.95	125.50	115.73
20	X	606	CHL	C1C-CHC-C4B	2.95	125.50	115.73
20	4	314	CHL	C3C-C4C-NC	-2.95	108.50	115.01
20	2	601	CHL	C1A-CHA-C4D	2.95	123.90	118.98
20	Z	306	CHL	C3C-C4C-NC	-2.95	108.51	115.01
21	1	610	CLA	C1-C2-C3	2.94	131.13	126.04
20	2	614	CHL	C1C-CHC-C4B	2.94	125.48	115.73
20	5	601	CHL	C3C-C4C-NC	-2.94	108.52	115.01
21	A	832	CLA	CHD-C1D-ND	-2.94	121.75	124.45
20	Y	605	CHL	CMA-C3A-C2A	-2.94	109.23	116.10
21	L	305	CLA	C3B-C4B-NB	-2.94	107.79	110.52
20	Y	606	CHL	C4C-CHD-C1D	2.94	125.47	115.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	304	CHL	O1D-CGD-CBD	-2.94	119.84	124.74
20	Y	619	CHL	C3C-C4C-NC	-2.93	108.54	115.01
20	X	605	CHL	C4C-CHD-C1D	2.93	125.44	115.73
21	Z	303	CLA	O2A-CGA-CBA	2.93	121.11	111.91
21	A	838	CLA	CHD-C1D-ND	-2.93	121.76	124.45
20	Z	307	CHL	OMC-CMC-C2C	-2.93	120.33	125.03
20	1	601	CHL	C3C-C4C-NC	-2.93	108.54	115.01
20	2	601	CHL	C3C-C4C-NC	-2.93	108.54	115.01
20	Z	309	CHL	C4C-CHD-C1D	2.93	125.44	115.73
20	X	608	CHL	C1A-CHA-C4D	2.93	123.87	118.98
21	3	611	CLA	CHD-C1D-ND	-2.93	121.76	124.45
20	5	606	CHL	C3C-C4C-NC	-2.93	108.55	115.01
21	O	202	CLA	O2A-CGA-CBA	2.93	121.09	111.91
21	A	802	CLA	O2A-CGA-CBA	2.93	121.09	111.91
20	4	314	CHL	C1C-CHC-C4B	2.92	125.42	115.73
20	X	605	CHL	C3C-C4C-NC	-2.92	108.56	115.01
20	Z	301	CHL	C3C-C4C-NC	-2.92	108.56	115.01
20	X	606	CHL	C1A-CHA-C4D	2.92	123.86	118.98
20	X	607	CHL	C3C-C4C-NC	-2.92	108.56	115.01
21	B	818	CLA	CHD-C1D-ND	-2.92	121.77	124.45
20	Y	601	CHL	C1A-CHA-C4D	2.92	123.85	118.98
20	Z	302	CHL	C4C-CHD-C1D	2.92	125.40	115.73
20	Z	302	CHL	C1A-CHA-C4D	2.92	123.85	118.98
21	B	833	CLA	CHD-C1D-ND	-2.92	121.77	124.45
20	5	606	CHL	OBD-CAD-CBD	-2.91	121.55	125.82
21	A	833	CLA	C1-C2-C3	2.91	131.08	126.04
20	6	605	CHL	O1D-CGD-CBD	-2.91	119.89	124.74
21	5	605	CLA	CHD-C1D-ND	-2.91	121.78	124.45
21	B	831	CLA	O2A-CGA-CBA	2.91	121.05	111.91
21	B	810	CLA	CAB-C3B-C2B	-2.91	116.04	123.59
20	6	605	CHL	C3C-C4C-NC	-2.91	108.59	115.01
21	1	608	CLA	CHD-C1D-ND	-2.91	121.78	124.45
21	2	603	CLA	CHD-C1D-ND	-2.91	121.78	124.45
28	B	841	PQN	C11-C3-C4	-2.91	115.39	118.50
20	Y	606	CHL	C3C-C4C-NC	-2.91	108.60	115.01
20	6	605	CHL	C4C-CHD-C1D	2.91	125.36	115.73
21	Z	312	CLA	CHD-C1D-ND	-2.91	121.78	124.45
21	1	613	CLA	CHD-C1D-ND	-2.90	121.79	124.45
20	1	606	CHL	CMA-C3A-C2A	-2.90	109.32	116.10
20	4	304	CHL	C4C-CHD-C1D	2.90	125.35	115.73
21	1	607	CLA	CHD-C1D-ND	-2.90	121.79	124.45
21	B	825	CLA	C4-C3-C5	-2.90	110.39	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	6	616	LUT	C32-C33-C34	2.90	123.39	118.94
21	B	834	CLA	CHD-C1D-ND	-2.90	121.79	124.45
21	X	613	CLA	CHD-C1D-ND	-2.90	121.79	124.45
20	Z	309	CHL	C3C-C4C-NC	-2.89	108.63	115.01
20	6	607	CHL	C4C-CHD-C1D	2.89	125.31	115.73
28	A	844	PQN	C11-C3-C4	-2.89	115.41	118.50
21	L	301	CLA	O2A-CGA-CBA	2.89	120.98	111.91
20	1	601	CHL	C1A-CHA-C4D	2.89	123.81	118.98
20	X	606	CHL	OBD-CAD-CBD	-2.89	121.59	125.82
20	4	305	CHL	OBD-CAD-CBD	-2.89	121.59	125.82
20	Y	607	CHL	C4C-CHD-C1D	2.89	125.29	115.73
20	X	606	CHL	C3C-C4C-NC	-2.88	108.65	115.01
20	Z	308	CHL	CMA-C3A-C2A	-2.88	109.37	116.10
22	4	315	LUT	C20-C13-C14	-2.88	118.89	122.92
21	A	804	CLA	CHD-C1D-ND	-2.88	121.81	124.45
24	O	201	BCR	C7-C8-C9	2.88	130.59	126.23
20	5	606	CHL	C1A-CHA-C4D	2.88	123.78	118.98
20	X	607	CHL	OBD-CAD-CBD	-2.88	121.60	125.82
20	Y	609	CHL	OBD-CAD-CBD	-2.88	121.60	125.82
22	5	619	LUT	C39-C29-C28	2.88	122.61	118.08
21	B	804	CLA	O2A-CGA-CBA	2.88	120.94	111.91
20	4	306	CHL	C3C-C4C-NC	-2.88	108.66	115.01
21	A	817	CLA	CHD-C1D-ND	-2.87	121.81	124.45
20	2	601	CHL	C4C-CHD-C1D	2.87	125.25	115.73
20	Y	606	CHL	C1A-CHA-C4D	2.87	123.78	118.98
21	5	604	CLA	O2A-CGA-CBA	2.87	120.93	111.91
20	Y	619	CHL	C4C-CHD-C1D	2.87	125.25	115.73
20	Y	601	CHL	C3C-C4C-NC	-2.87	108.67	115.01
21	1	605	CLA	CHD-C1D-ND	-2.87	121.81	124.45
21	B	819	CLA	O2A-CGA-CBA	2.87	120.92	111.91
20	X	601	CHL	C3C-C4C-NC	-2.87	108.67	115.01
22	Z	314	LUT	C15-C35-C34	2.87	129.36	123.47
21	4	312	CLA	CHD-C1D-ND	-2.87	121.82	124.45
20	2	607	CHL	C3C-C4C-NC	-2.87	108.68	115.01
20	6	606	CHL	C3C-C4C-NC	-2.87	108.68	115.01
20	1	606	CHL	C3C-C4C-NC	-2.87	108.68	115.01
20	2	606	CHL	C4C-CHD-C1D	2.87	125.23	115.73
20	Y	605	CHL	C4C-CHD-C1D	2.87	125.23	115.73
21	Z	313	CLA	C3B-C4B-NB	-2.87	107.86	110.52
20	Y	601	CHL	C4C-CHD-C1D	2.87	125.22	115.73
23	2	616	XAT	C7-C8-C9	2.87	129.98	125.53
21	A	806	CLA	CHD-C1D-ND	-2.87	121.82	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	X	603	CLA	O2A-CGA-CBA	2.87	120.90	111.91
21	A	825	CLA	C1-C2-C3	2.86	131.00	126.04
21	B	808	CLA	CHD-C1D-ND	-2.86	121.82	124.45
21	Z	304	CLA	CHD-C1D-ND	-2.86	121.82	124.45
20	3	608	CHL	C1C-CHC-C4B	2.86	125.20	115.73
20	Y	605	CHL	C3C-C4C-NC	-2.86	108.70	115.01
22	1	615	LUT	C20-C13-C14	-2.86	118.92	122.92
21	A	814	CLA	CHD-C1D-ND	-2.86	121.83	124.45
23	3	616	XAT	C7-C8-C9	2.86	129.96	125.53
21	5	609	CLA	CHD-C1D-ND	-2.86	121.83	124.45
21	X	603	CLA	CHD-C1D-ND	-2.86	121.83	124.45
20	Y	607	CHL	C3C-C4C-NC	-2.86	108.71	115.01
20	Z	308	CHL	C1A-CHA-C4D	2.86	123.75	118.98
21	1	603	CLA	O2A-CGA-CBA	2.85	120.86	111.91
21	B	823	CLA	C1-C2-C3	2.85	130.98	126.04
20	4	314	CHL	C1A-CHA-C4D	2.85	123.74	118.98
21	3	607	CLA	CHD-C1D-ND	-2.85	121.83	124.45
22	Z	314	LUT	C12-C13-C14	2.85	123.32	118.94
20	Z	308	CHL	C3C-C4C-NC	-2.85	108.72	115.01
22	6	616	LUT	C35-C15-C14	2.85	129.31	123.47
21	A	815	CLA	CHD-C1D-ND	-2.85	121.84	124.45
21	A	842	CLA	CHD-C1D-ND	-2.85	121.84	124.45
20	6	615	CHL	C3C-C4C-NC	-2.84	108.73	115.01
22	5	619	LUT	C15-C35-C34	2.84	129.30	123.47
20	2	607	CHL	C4C-CHD-C1D	2.84	125.15	115.73
21	A	809	CLA	O2A-CGA-CBA	2.84	120.83	111.91
21	J	102	CLA	CHD-C1D-ND	-2.84	121.84	124.45
21	B	801	CLA	CHD-C1D-ND	-2.84	121.85	124.45
20	2	606	CHL	C3C-C4C-NC	-2.84	108.75	115.01
20	Y	609	CHL	C1A-CHA-C4D	2.84	123.72	118.98
21	B	830	CLA	CHD-C1D-ND	-2.84	121.85	124.45
21	A	823	CLA	CMA-C3A-C2A	-2.84	109.48	116.10
21	Y	613	CLA	O2A-CGA-CBA	2.83	120.80	111.91
20	3	608	CHL	C1A-CHA-C4D	2.83	123.71	118.98
20	6	615	CHL	C1A-CHA-C4D	2.83	123.71	118.98
22	Z	314	LUT	C39-C29-C28	2.83	122.54	118.08
20	2	607	CHL	C1-C2-C3	2.83	131.33	126.75
20	Y	609	CHL	C3C-C4C-NC	-2.83	108.76	115.01
20	4	304	CHL	C3C-C4C-NC	-2.83	108.77	115.01
21	B	836	CLA	CHD-C1D-ND	-2.83	121.86	124.45
20	Y	606	CHL	OBD-CAD-CBD	-2.83	121.67	125.82
21	4	302	CLA	CHD-C1D-ND	-2.83	121.86	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	X	607	CHL	C1A-CHA-C4D	2.83	123.70	118.98
20	4	304	CHL	O2A-CGA-CBA	2.82	120.77	111.91
20	6	605	CHL	O2A-CGA-CBA	2.82	120.76	111.91
22	4	315	LUT	C35-C15-C14	2.82	129.25	123.47
21	1	603	CLA	CHD-C1D-ND	-2.82	121.86	124.45
22	3	615	LUT	C20-C13-C14	-2.82	118.97	122.92
20	5	606	CHL	CMA-C3A-C2A	-2.81	109.53	116.10
20	2	607	CHL	C1A-CHA-C4D	2.81	123.68	118.98
21	2	604	CLA	C1-C2-C3	2.81	130.91	126.04
20	2	606	CHL	C1A-CHA-C4D	2.81	123.67	118.98
21	B	818	CLA	C1-C2-C3	2.81	130.90	126.04
20	X	606	CHL	CHA-C1A-C2A	-2.81	126.71	133.31
22	1	615	LUT	C39-C29-C28	2.81	122.50	118.08
21	2	602	CLA	C1-C2-C3	2.81	130.90	126.04
20	Z	301	CHL	CHA-C1A-C2A	-2.81	126.72	133.31
20	4	305	CHL	C3C-C4C-NC	-2.80	108.82	115.01
21	L	304	CLA	C1-C2-C3	2.80	130.89	126.04
21	A	824	CLA	CHD-C1D-ND	-2.80	121.88	124.45
21	B	812	CLA	CHD-C1D-ND	-2.80	121.88	124.45
21	L	301	CLA	CHD-C1D-ND	-2.80	121.88	124.45
20	4	306	CHL	OMC-CMC-C2C	-2.80	120.54	125.03
21	O	207	CLA	CHD-C1D-ND	-2.80	121.88	124.45
21	A	834	CLA	CHD-C1D-ND	-2.80	121.88	124.45
21	4	310	CLA	CHD-C1D-ND	-2.80	121.88	124.45
21	2	618	CLA	CHD-C1D-ND	-2.80	121.88	124.45
20	X	608	CHL	C4C-CHD-C1D	2.80	125.00	115.73
20	X	605	CHL	OBD-CAD-CBD	-2.80	121.72	125.82
20	X	601	CHL	OBD-CAD-CBD	-2.80	121.72	125.82
20	6	606	CHL	C4C-CHD-C1D	2.79	124.99	115.73
21	3	617	CLA	CHD-C1D-ND	-2.79	121.89	124.45
21	B	804	CLA	CHD-C1D-ND	-2.79	121.89	124.45
21	B	828	CLA	CHD-C1D-ND	-2.79	121.89	124.45
21	L	303	CLA	CHD-C1D-ND	-2.79	121.89	124.45
20	Z	306	CHL	C1C-CHC-C4B	2.79	124.97	115.73
21	Z	311	CLA	CHD-C1D-ND	-2.79	121.89	124.45
21	A	803	CLA	C1-C2-C3	2.79	130.86	126.04
21	A	826	CLA	O2A-CGA-CBA	2.79	120.65	111.91
21	B	823	CLA	CHD-C1D-ND	-2.79	121.89	124.45
21	A	840	CLA	CHD-C1D-ND	-2.78	121.89	124.45
21	B	832	CLA	CHD-C1D-ND	-2.78	121.89	124.45
21	2	610	CLA	CMA-C3A-C2A	-2.78	109.60	116.10
21	L	304	CLA	CHD-C1D-ND	-2.78	121.90	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	Z	309	CHL	O1D-CGD-CBD	-2.78	120.11	124.74
20	Z	309	CHL	OBD-CAD-CBD	-2.78	121.74	125.82
21	4	313	CLA	CHD-C1D-ND	-2.78	121.90	124.45
21	B	803	CLA	CMA-C3A-C2A	-2.78	109.61	116.10
23	3	616	XAT	O4-C5-C4	-2.78	111.29	113.38
20	Y	607	CHL	OBD-CAD-CBD	-2.78	121.75	125.82
21	A	811	CLA	C1-C2-C3	2.78	130.85	126.04
21	2	602	CLA	CHD-C1D-ND	-2.78	121.90	124.45
21	H	201	CLA	O2A-CGA-CBA	2.78	120.62	111.91
21	4	301	CLA	CHD-C1D-ND	-2.77	121.90	124.45
21	A	830	CLA	C1-C2-C3	2.77	130.84	126.04
21	B	840	CLA	CHD-C1D-ND	-2.77	121.91	124.45
21	B	813	CLA	O2A-CGA-CBA	2.77	120.61	111.91
21	2	613	CLA	CHD-C1D-ND	-2.77	121.91	124.45
21	A	830	CLA	CHD-C1D-ND	-2.77	121.91	124.45
21	B	817	CLA	CHD-C1D-ND	-2.77	121.91	124.45
20	Z	307	CHL	C1A-CHA-C4D	2.77	123.61	118.98
21	B	824	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
21	A	839	CLA	CHD-C1D-ND	-2.77	121.91	124.45
20	1	601	CHL	OBD-CAD-CBD	-2.76	121.77	125.82
21	1	609	CLA	CHD-C1D-ND	-2.76	121.92	124.45
21	B	826	CLA	CHD-C1D-ND	-2.76	121.92	124.45
22	5	619	LUT	C8-C9-C10	2.76	123.18	118.94
21	1	610	CLA	CHD-C1D-ND	-2.76	121.92	124.45
21	B	820	CLA	CHD-C1D-ND	-2.76	121.92	124.45
21	B	837	CLA	CHD-C1D-ND	-2.76	121.92	124.45
21	B	825	CLA	CHD-C1D-ND	-2.76	121.92	124.45
21	1	602	CLA	CHD-C1D-ND	-2.76	121.92	124.45
21	2	612	CLA	CHD-C1D-ND	-2.76	121.92	124.45
20	3	608	CHL	OMC-CMC-C2C	-2.75	120.62	125.03
21	B	805	CLA	CHD-C1D-ND	-2.75	121.93	124.45
21	B	805	CLA	O1D-CGD-CBD	-2.75	118.86	124.48
20	Y	608	CHL	C1A-CHA-C4D	2.75	123.57	118.98
20	4	305	CHL	C4C-CHD-C1D	2.75	124.83	115.73
20	2	606	CHL	OMC-CMC-C2C	-2.75	120.63	125.03
21	5	602	CLA	CHD-C1D-ND	-2.75	121.93	124.45
20	Z	307	CHL	O1D-CGD-CBD	-2.75	120.17	124.74
20	2	607	CHL	OBD-CAD-CBD	-2.75	121.80	125.82
20	4	304	CHL	C1A-CHA-C4D	2.74	123.56	118.98
21	B	820	CLA	C1-C2-C3	2.74	130.78	126.04
21	2	604	CLA	CHD-C1D-ND	-2.74	121.94	124.45
21	6	614	CLA	CHD-C1D-ND	-2.73	121.94	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	816	CLA	CHD-C1D-ND	-2.73	121.94	124.45
21	A	843	CLA	O2A-CGA-CBA	2.73	120.49	111.91
20	X	608	CHL	OBD-CAD-CBD	-2.73	121.81	125.82
21	B	806	CLA	CHD-C1D-ND	-2.73	121.94	124.45
20	Y	607	CHL	C1A-CHA-C4D	2.73	123.54	118.98
21	B	827	CLA	C1-C2-C3	2.73	130.76	126.04
21	3	610	CLA	CMA-C3A-C2A	-2.73	109.73	116.10
21	G	202	CLA	CHD-C1D-ND	-2.73	121.95	124.45
21	4	308	CLA	C1-C2-C3	2.73	130.76	126.04
21	A	807	CLA	CHD-C1D-ND	-2.72	121.95	124.45
21	6	612	CLA	C1-C2-C3	2.72	130.75	126.04
21	5	612	CLA	O2A-CGA-CBA	2.72	120.45	111.91
21	B	838	CLA	CHD-C1D-ND	-2.72	121.95	124.45
20	6	605	CHL	C1A-CHA-C4D	2.72	123.52	118.98
21	A	802	CLA	CHB-C1B-NB	2.72	127.14	124.26
20	5	601	CHL	O2A-CGA-CBA	2.72	120.45	111.91
21	A	835	CLA	CHD-C1D-ND	-2.72	121.96	124.45
21	3	614	CLA	CMA-C3A-C2A	-2.72	109.76	116.10
22	1	615	LUT	C32-C33-C34	2.72	123.11	118.94
21	5	604	CLA	CHD-C1D-ND	-2.72	121.96	124.45
20	Z	302	CHL	OBD-CAD-CBD	-2.71	121.84	125.82
20	4	306	CHL	O2A-CGA-CBA	2.71	120.42	111.91
20	Y	601	CHL	OMC-CMC-C2C	-2.71	120.69	125.03
21	6	604	CLA	CHD-C1D-ND	-2.71	121.96	124.45
21	A	832	CLA	O2A-CGA-CBA	2.71	120.41	111.91
21	3	617	CLA	O2A-CGA-CBA	2.71	120.41	111.91
20	6	606	CHL	CHA-C1A-C2A	-2.71	126.94	133.31
21	B	802	CLA	O2A-CGA-CBA	2.71	120.41	111.91
20	2	606	CHL	O1D-CGD-CBD	-2.71	120.23	124.74
21	Z	305	CLA	CHD-C1D-ND	-2.71	121.97	124.45
21	3	605	CLA	O2A-CGA-CBA	2.71	120.40	111.91
21	A	818	CLA	CHD-C1D-ND	-2.71	121.97	124.45
21	5	613	CLA	CHD-C1D-ND	-2.71	121.97	124.45
22	4	315	LUT	C32-C33-C34	2.70	123.09	118.94
21	B	813	CLA	C1-C2-C3	2.70	130.72	126.04
20	5	601	CHL	C1A-CHA-C4D	2.70	123.49	118.98
21	B	808	CLA	C1-C2-C3	2.70	130.71	126.04
20	6	607	CHL	CHA-C1A-C2A	-2.70	126.97	133.31
21	2	618	CLA	O1D-CGD-CBD	-2.70	118.96	124.48
21	6	610	CLA	CHD-C1D-ND	-2.70	121.98	124.45
20	Y	619	CHL	C1A-CHA-C4D	2.69	123.48	118.98
21	A	817	CLA	O2A-CGA-CBA	2.69	120.36	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	K	202	CLA	CHD-C1D-ND	-2.69	121.98	124.45
22	4	315	LUT	C39-C29-C28	2.69	122.31	118.08
21	B	811	CLA	CHD-C1D-ND	-2.69	121.99	124.45
22	X	615	LUT	C12-C13-C14	2.69	123.06	118.94
21	A	808	CLA	O1D-CGD-CBD	-2.68	119.00	124.48
21	Y	613	CLA	CHD-C1D-ND	-2.68	121.99	124.45
20	Y	608	CHL	O1D-CGD-CBD	-2.68	120.27	124.74
20	4	314	CHL	OBD-CAD-CBD	-2.68	121.89	125.82
21	A	809	CLA	CHD-C1D-ND	-2.68	121.99	124.45
21	F	304	CLA	CMA-C3A-C2A	-2.68	109.84	116.10
20	Y	608	CHL	C1C-CHC-C4B	2.68	124.61	115.73
21	A	843	CLA	C1-C2-C3	2.68	130.68	126.04
21	B	807	CLA	CHD-C1D-ND	-2.68	121.99	124.45
21	Y	610	CLA	CHD-C1D-ND	-2.68	121.99	124.45
21	5	612	CLA	CHD-C1D-ND	-2.68	121.99	124.45
21	B	831	CLA	O2A-CGA-O1A	-2.68	116.84	123.59
21	B	824	CLA	O1D-CGD-CBD	-2.67	119.01	124.48
21	B	838	CLA	C1-C2-C3	2.67	130.66	126.04
20	X	605	CHL	CMA-C3A-C2A	-2.67	109.87	116.10
21	5	603	CLA	CHD-C1D-ND	-2.66	122.00	124.45
21	B	824	CLA	C1-C2-C3	2.66	131.06	126.75
21	B	812	CLA	C1-C2-C3	2.66	130.65	126.04
21	6	602	CLA	CHD-C1D-ND	-2.66	122.01	124.45
20	1	606	CHL	C1A-CHA-C4D	2.66	123.41	118.98
21	6	612	CLA	CHD-C1D-ND	-2.66	122.01	124.45
21	A	829	CLA	CHD-C1D-ND	-2.66	122.01	124.45
20	6	615	CHL	CHA-C1A-C2A	-2.65	127.08	133.31
21	3	609	CLA	O1D-CGD-CBD	-2.65	119.06	124.48
21	6	603	CLA	CHD-C1D-ND	-2.65	122.02	124.45
21	A	819	CLA	CHD-C1D-ND	-2.65	122.02	124.45
21	1	608	CLA	C1-C2-C3	2.65	130.63	126.04
21	A	817	CLA	C1-C2-C3	2.65	130.62	126.04
21	O	203	CLA	CHD-C1D-ND	-2.65	122.02	124.45
20	2	605	CHL	O1D-CGD-CBD	-2.65	120.33	124.74
20	X	605	CHL	C1A-CHA-C4D	2.65	123.40	118.98
21	6	601	CLA	CHD-C1D-ND	-2.65	122.02	124.45
21	B	804	CLA	C1-C2-C3	2.65	130.62	126.04
22	Y	616	LUT	C32-C33-C34	2.65	123.00	118.94
20	Y	605	CHL	OBD-CAD-CBD	-2.64	121.94	125.82
20	Z	301	CHL	OMC-CMC-C2C	-2.64	120.79	125.03
21	3	604	CLA	CHD-C1D-ND	-2.64	122.03	124.45
21	X	602	CLA	CHD-C1D-ND	-2.64	122.03	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	Z	309	CHL	OMC-CMC-C2C	-2.64	120.81	125.03
21	A	843	CLA	O1D-CGD-CBD	-2.63	119.10	124.48
21	4	307	CLA	CHD-C1D-ND	-2.63	122.04	124.45
20	3	608	CHL	O1D-CGD-CBD	-2.62	120.37	124.74
21	3	612	CLA	CHD-C1D-ND	-2.62	122.04	124.45
21	B	802	CLA	C1-C2-C3	2.62	130.58	126.04
20	Z	308	CHL	OMC-CMC-C2C	-2.62	120.83	125.03
21	4	302	CLA	CHB-C1B-NB	2.62	127.03	124.26
21	1	612	CLA	CHD-C1D-ND	-2.62	122.05	124.45
21	A	819	CLA	CHB-C1B-NB	2.61	127.03	124.26
21	B	821	CLA	C1-C2-C3	2.61	130.56	126.04
20	Y	619	CHL	OMC-CMC-C2C	-2.61	120.84	125.03
21	4	311	CLA	CHD-C1D-ND	-2.61	122.05	124.45
21	A	833	CLA	CHD-C1D-ND	-2.61	122.05	124.45
21	Z	313	CLA	CHD-C1D-ND	-2.61	122.05	124.45
21	B	819	CLA	CHD-C1D-ND	-2.61	122.05	124.45
21	B	839	CLA	CHD-C1D-ND	-2.61	122.06	124.45
20	2	614	CHL	CHA-C1A-C2A	-2.61	127.18	133.31
20	6	615	CHL	OBD-CAD-CBD	-2.61	122.00	125.82
21	A	841	CLA	CHD-C1D-ND	-2.61	122.06	124.45
22	2	615	LUT	C39-C29-C28	2.60	122.18	118.08
21	4	301	CLA	C1-C2-C3	2.60	130.54	126.04
21	A	841	CLA	C1-C2-C3	2.60	130.54	126.04
21	B	816	CLA	C4-C3-C5	-2.60	110.90	115.27
21	B	809	CLA	CHD-C1D-ND	-2.60	122.07	124.45
21	B	808	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
21	6	602	CLA	C1-C2-C3	2.60	130.53	126.04
20	4	314	CHL	OMC-CMC-C2C	-2.60	120.87	125.03
21	A	820	CLA	CHD-C1D-ND	-2.60	122.07	124.45
20	Z	306	CHL	O1D-CGD-CBD	-2.59	120.42	124.74
21	O	202	CLA	CHD-C1D-ND	-2.59	122.07	124.45
20	Y	605	CHL	C1A-CHA-C4D	2.59	123.30	118.98
21	A	822	CLA	CHD-C1D-ND	-2.59	122.08	124.45
20	2	601	CHL	CHA-C1A-C2A	-2.59	127.23	133.31
20	2	601	CHL	OMC-CMC-C2C	-2.59	120.88	125.03
21	A	802	CLA	CHD-C1D-ND	-2.59	122.08	124.45
21	X	612	CLA	CHB-C1B-NB	2.58	126.99	124.26
22	4	315	LUT	C19-C9-C8	2.58	122.15	118.08
21	2	603	CLA	CHB-C1B-NB	2.58	126.99	124.26
21	A	802	CLA	C12-C11-C10	-2.58	101.38	113.24
23	2	616	XAT	O4-C5-C4	-2.58	111.44	113.38
20	1	606	CHL	OMC-CMC-C2C	-2.58	120.90	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	Z	306	CHL	C1A-CHA-C4D	2.58	123.28	118.98
21	5	605	CLA	O1D-CGD-CBD	-2.58	119.21	124.48
20	6	607	CHL	OMC-CMC-C2C	-2.58	120.90	125.03
20	2	614	CHL	C1A-CHA-C4D	2.58	123.28	118.98
21	A	824	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
23	6	617	XAT	O4-C5-C4	-2.57	111.45	113.38
21	B	820	CLA	C4-C3-C5	-2.57	110.94	115.27
21	A	824	CLA	C1-C2-C3	2.57	130.49	126.04
21	A	828	CLA	O1D-CGD-CBD	-2.57	119.23	124.48
20	Y	607	CHL	O1D-CGD-CBD	-2.57	120.46	124.74
21	4	303	CLA	CHD-C1D-ND	-2.57	122.09	124.45
21	J	102	CLA	CHB-C1B-NB	2.57	126.97	124.26
21	3	602	CLA	O1D-CGD-CBD	-2.57	119.23	124.48
20	X	607	CHL	CHA-C1A-C2A	-2.56	127.29	133.31
21	A	830	CLA	O1D-CGD-CBD	-2.56	119.24	124.48
21	B	821	CLA	CHD-C1D-ND	-2.56	122.10	124.45
21	1	603	CLA	O1D-CGD-CBD	-2.56	119.25	124.48
21	3	613	CLA	CMA-C3A-C2A	-2.56	110.13	116.10
21	A	823	CLA	CHD-C1D-ND	-2.55	122.11	124.45
20	6	605	CHL	OMC-CMC-C2C	-2.55	120.94	125.03
20	X	605	CHL	O1D-CGD-CBD	-2.55	120.49	124.74
22	5	615	LUT	C12-C13-C14	2.55	122.86	118.94
21	A	810	CLA	CHD-C1D-ND	-2.55	122.11	124.45
21	1	603	CLA	CHB-C1B-NB	2.55	126.96	124.26
20	X	607	CHL	O1D-CGD-CBD	-2.55	120.50	124.74
21	A	806	CLA	C1-C2-C3	2.55	130.45	126.04
22	1	615	LUT	C35-C15-C14	2.55	128.69	123.47
20	4	306	CHL	C1A-CHA-C4D	2.54	123.22	118.98
22	Y	615	LUT	C12-C13-C14	2.54	122.84	118.94
22	Z	315	LUT	C12-C13-C14	2.54	122.84	118.94
21	A	803	CLA	CHB-C1B-NB	2.54	126.95	124.26
21	X	603	CLA	C1-C2-C3	2.54	130.44	126.04
21	B	837	CLA	CHB-C1B-NB	2.54	126.94	124.26
21	A	810	CLA	O1D-CGD-CBD	-2.54	119.29	124.48
21	Y	603	CLA	CHD-C1D-ND	-2.54	122.12	124.45
21	3	603	CLA	CHD-C1D-ND	-2.54	122.12	124.45
21	B	802	CLA	CHD-C1D-ND	-2.53	122.12	124.45
21	B	802	CLA	C2C-C1C-NC	-2.53	107.60	109.97
21	A	810	CLA	C1-C2-C3	2.53	130.84	126.75
21	A	837	CLA	O1D-CGD-CBD	-2.53	119.31	124.48
21	5	614	CLA	CHD-C1D-ND	-2.53	122.13	124.45
21	B	839	CLA	C1-C2-C3	2.52	130.41	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	812	CLA	O1D-CGD-CBD	-2.52	119.32	124.48
20	Z	306	CHL	OBD-CAD-CBD	-2.52	122.13	125.82
21	5	612	CLA	C1-C2-C3	2.52	130.40	126.04
20	6	607	CHL	C1A-CHA-C4D	2.52	123.18	118.98
21	B	828	CLA	C1-C2-C3	2.52	130.39	126.04
21	A	841	CLA	O2D-CGD-O1D	-2.51	118.92	123.84
22	Y	616	LUT	C12-C13-C14	2.51	122.80	118.94
21	A	803	CLA	O1D-CGD-CBD	-2.51	119.34	124.48
21	6	601	CLA	O2A-CGA-CBA	2.51	122.15	112.23
21	G	203	CLA	CHB-C1B-NB	2.51	126.91	124.26
21	2	618	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
21	1	604	CLA	CHD-C1D-ND	-2.50	122.15	124.45
21	A	827	CLA	C1-C2-C3	2.50	130.37	126.04
20	Y	609	CHL	CHA-C1A-C2A	-2.50	127.44	133.31
21	B	802	CLA	C4-C3-C5	-2.50	111.07	115.27
21	B	836	CLA	C1-C2-C3	2.50	130.36	126.04
20	Z	306	CHL	CHA-C1A-C2A	-2.50	127.44	133.31
21	A	817	CLA	O1D-CGD-CBD	-2.50	119.37	124.48
21	B	809	CLA	C1-C2-C3	2.50	130.36	126.04
21	B	833	CLA	O1D-CGD-CBD	-2.50	119.38	124.48
20	1	606	CHL	OBD-CAD-CBD	-2.49	122.16	125.82
20	Z	302	CHL	OMC-CMC-C2C	-2.49	121.03	125.03
21	O	203	CLA	O1D-CGD-CBD	-2.49	119.38	124.48
20	Z	302	CHL	CHA-C1A-C2A	-2.49	127.45	133.31
21	A	801	CLA	C12-C11-C10	-2.49	101.80	113.24
21	A	808	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
21	A	830	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
21	5	603	CLA	CHB-C1B-NB	2.49	126.89	124.26
21	B	827	CLA	O1D-CGD-CBD	-2.49	119.40	124.48
20	6	615	CHL	OMC-CMC-C2C	-2.49	121.05	125.03
20	Y	606	CHL	O1D-CGD-CBD	-2.48	120.60	124.74
21	B	810	CLA	O1D-CGD-CBD	-2.48	119.40	124.48
22	2	615	LUT	C32-C33-C34	2.48	122.75	118.94
21	A	837	CLA	CHB-C1B-NB	2.48	126.89	124.26
21	B	802	CLA	C2B-C1B-NB	-2.48	108.57	110.23
21	A	804	CLA	C1-C2-C3	2.48	130.34	126.04
21	2	609	CLA	C1-C2-C3	2.48	130.33	126.04
21	3	603	CLA	CHB-C1B-NB	2.48	126.88	124.26
21	A	833	CLA	C4-C3-C5	-2.48	111.10	115.27
22	2	615	LUT	C12-C13-C14	2.48	122.75	118.94
21	A	818	CLA	O1D-CGD-CBD	-2.48	119.41	124.48
21	G	204	CLA	CHB-C1B-NB	2.48	126.88	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	3	602	CLA	C1-C2-C3	2.48	130.33	126.04
20	X	601	CHL	C1A-CHA-C4D	2.48	123.11	118.98
21	4	309	CLA	C1-C2-C3	2.48	130.33	126.04
22	X	614	LUT	C12-C13-C14	2.48	122.74	118.94
20	Y	606	CHL	CHA-C1A-C2A	-2.47	127.50	133.31
21	H	201	CLA	C12-C11-C10	-2.47	101.88	113.24
21	B	823	CLA	CHB-C1B-NB	2.47	126.87	124.26
21	B	840	CLA	O1D-CGD-CBD	-2.47	119.43	124.48
21	A	830	CLA	C12-C11-C10	-2.47	101.89	113.24
21	Y	604	CLA	CHD-C1D-ND	-2.47	122.19	124.45
20	X	608	CHL	CHA-C1A-C2A	-2.47	127.51	133.31
21	Y	602	CLA	C1-C2-C3	2.47	130.31	126.04
21	A	807	CLA	O1D-CGD-CBD	-2.47	119.43	124.48
21	A	818	CLA	CHB-C1B-NB	2.47	126.87	124.26
21	A	806	CLA	C12-C11-C10	-2.47	101.91	113.24
21	B	817	CLA	CHB-C1B-NB	2.47	126.87	124.26
21	A	826	CLA	C12-C11-C10	-2.46	101.92	113.24
21	B	808	CLA	CHB-C1B-NB	2.46	126.86	124.26
20	Y	605	CHL	OMC-CMC-C2C	-2.46	121.08	125.03
21	B	801	CLA	CHB-C1B-NB	2.46	126.86	124.26
21	X	611	CLA	C2D-C1D-ND	2.46	111.92	110.10
21	A	833	CLA	C12-C11-C10	-2.46	101.94	113.24
20	X	601	CHL	O1D-CGD-CBD	-2.46	120.64	124.74
21	A	816	CLA	CHD-C1D-ND	-2.46	122.19	124.45
20	4	305	CHL	OMC-CMC-C2C	-2.46	121.09	125.03
21	A	839	CLA	CHB-C1B-NB	2.46	126.86	124.26
21	A	819	CLA	C5-C3-C2	2.46	126.09	121.12
21	6	608	CLA	O2A-CGA-CBA	2.46	121.92	114.03
21	A	829	CLA	C12-C11-C10	-2.46	101.96	113.24
21	A	812	CLA	C4-C3-C5	-2.45	111.14	115.27
21	O	202	CLA	C1-C2-C3	2.45	130.72	126.75
22	6	616	LUT	C19-C9-C8	2.45	121.94	118.08
21	4	311	CLA	C1-C2-C3	2.45	130.28	126.04
21	K	201	CLA	OBD-CAD-CBD	-2.45	120.97	125.97
22	Y	615	LUT	C32-C33-C34	2.45	122.70	118.94
21	A	825	CLA	C12-C11-C10	-2.45	102.00	113.24
21	A	841	CLA	O1D-CGD-CBD	-2.45	119.48	124.48
21	B	811	CLA	O2D-CGD-O1D	-2.45	119.06	123.84
21	B	816	CLA	CHB-C1B-NB	2.45	126.85	124.26
21	K	202	CLA	CHB-C1B-NB	2.45	126.85	124.26
22	5	619	LUT	C32-C33-C34	2.45	122.69	118.94
21	3	604	CLA	CHB-C1B-NB	2.44	126.84	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	Y	609	CHL	O1D-CGD-CBD	-2.44	120.67	124.74
21	A	813	CLA	CHB-C1B-NB	2.44	126.84	124.26
21	A	834	CLA	CHB-C1B-NB	2.44	126.84	124.26
21	B	826	CLA	CHB-C1B-NB	2.44	126.84	124.26
21	K	201	CLA	CHD-C1D-ND	-2.44	122.21	124.45
20	Y	619	CHL	CHA-C1A-C2A	-2.44	127.57	133.31
20	Z	301	CHL	C1A-CHA-C4D	2.44	123.06	118.98
20	Y	601	CHL	CHA-C1A-C2A	-2.44	127.58	133.31
20	X	601	CHL	CHA-C1A-C2A	-2.44	127.58	133.31
20	4	314	CHL	CHA-C1A-C2A	-2.44	127.58	133.31
21	B	827	CLA	CHD-C1D-ND	-2.44	122.21	124.45
21	X	609	CLA	O1D-CGD-CBD	-2.44	119.50	124.48
21	B	817	CLA	C4-C3-C5	-2.44	111.17	115.27
21	B	811	CLA	O1D-CGD-CBD	-2.44	119.50	124.48
20	2	607	CHL	OMC-CMC-C2C	-2.44	121.13	125.03
21	Y	611	CLA	O1D-CGD-CBD	-2.43	119.50	124.48
21	A	825	CLA	CHB-C1B-NB	2.43	126.83	124.26
21	4	308	CLA	O1D-CGD-CBD	-2.43	119.51	124.48
21	L	303	CLA	O2A-CGA-CBA	2.43	121.84	114.03
20	1	601	CHL	OMC-CMC-C2C	-2.43	121.13	125.03
20	6	606	CHL	O1D-CGD-CBD	-2.43	120.69	124.74
21	2	613	CLA	CHB-C1B-NB	2.43	126.83	124.26
20	1	601	CHL	CHA-C1A-C2A	-2.43	127.60	133.31
20	2	607	CHL	CHA-C1A-C2A	-2.43	127.61	133.31
21	X	611	CLA	CHB-C1B-NB	2.42	126.82	124.26
22	F	301	LUT	C8-C9-C10	2.42	122.66	118.94
21	A	807	CLA	C12-C11-C10	-2.42	102.11	113.24
21	A	834	CLA	C1-C2-C3	2.42	130.23	126.04
21	B	814	CLA	C1-C2-C3	2.42	130.23	126.04
21	B	802	CLA	C4D-CHA-C1A	2.42	124.19	121.25
21	Y	604	CLA	O2A-CGA-CBA	2.42	121.80	114.03
21	3	613	CLA	CHD-C1D-ND	-2.42	122.23	124.45
20	X	608	CHL	O1D-CGD-CBD	-2.42	120.72	124.74
21	4	312	CLA	CHB-C1B-NB	2.42	126.81	124.26
21	K	201	CLA	CHB-C1B-NB	2.41	126.81	124.26
21	Y	614	CLA	CHD-C1D-ND	-2.41	122.24	124.45
21	Z	305	CLA	C1-C2-C3	2.41	130.66	126.75
21	A	828	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
22	F	301	LUT	C32-C33-C34	2.41	122.64	118.94
21	A	833	CLA	CHB-C1B-NB	2.41	126.81	124.26
21	1	612	CLA	C4-C3-C5	-2.41	111.22	115.27
21	6	603	CLA	O1D-CGD-CBD	-2.41	119.56	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	6	607	CHL	OBD-CAD-CBD	-2.40	122.30	125.82
21	4	303	CLA	O2A-CGA-CBA	2.40	121.75	114.03
20	4	304	CHL	OMC-CMC-C2C	-2.40	121.18	125.03
21	B	818	CLA	CHB-C1B-NB	2.40	126.80	124.26
21	6	614	CLA	CHB-C1B-NB	2.40	126.80	124.26
21	B	827	CLA	CHB-C1B-NB	2.40	126.80	124.26
21	B	820	CLA	O1D-CGD-CBD	-2.40	119.57	124.48
20	2	614	CHL	OMC-CMC-C2C	-2.40	121.19	125.03
21	3	607	CLA	O2A-CGA-CBA	2.40	121.74	114.03
21	B	822	CLA	C1-C2-C3	2.40	130.19	126.04
21	Z	303	CLA	C1-C2-C3	2.40	130.19	126.04
21	5	612	CLA	C12-C11-C10	-2.40	102.22	113.24
21	A	829	CLA	CHB-C1B-NB	2.40	126.80	124.26
20	4	306	CHL	CHA-C1A-C2A	-2.40	127.67	133.31
21	2	608	CLA	O2A-CGA-CBA	2.40	121.73	114.03
21	A	801	CLA	C1-C2-C3	2.40	130.19	126.04
21	Z	311	CLA	O2A-CGA-CBA	2.40	121.73	114.03
21	4	301	CLA	C12-C11-C10	-2.40	102.23	113.24
21	4	309	CLA	O1D-CGD-CBD	-2.39	119.58	124.48
21	5	613	CLA	O2A-CGA-CBA	2.39	121.72	114.03
21	A	841	CLA	C12-C11-C10	-2.39	102.24	113.24
21	B	802	CLA	C3C-C4C-NC	-2.39	107.89	110.57
21	4	307	CLA	CHB-C1B-NB	2.39	126.79	124.26
21	B	816	CLA	C3C-C4C-NC	-2.39	107.89	110.57
21	Z	311	CLA	O1D-CGD-CBD	-2.39	119.59	124.48
21	A	821	CLA	C1-C2-C3	2.39	130.18	126.04
21	5	609	CLA	O2A-CGA-CBA	2.39	121.70	114.03
21	1	614	CLA	CHD-C1D-ND	-2.39	122.26	124.45
20	2	606	CHL	CHA-C1A-C2A	-2.39	127.70	133.31
21	1	611	CLA	O2A-CGA-CBA	2.39	121.70	114.03
20	Y	606	CHL	OMC-CMC-C2C	-2.39	121.21	125.03
21	3	603	CLA	C1-C2-C3	2.39	130.17	126.04
21	B	835	CLA	CHB-C1B-NB	2.39	126.78	124.26
21	A	818	CLA	O2D-CGD-O1D	-2.38	119.17	123.84
21	B	826	CLA	C12-C11-C10	-2.38	102.28	113.24
21	4	312	CLA	O2A-CGA-CBA	2.38	121.69	114.03
21	A	828	CLA	O2A-CGA-O1A	-2.38	117.58	123.59
21	B	804	CLA	C12-C11-C10	-2.38	102.29	113.24
21	5	614	CLA	CHB-C1B-NB	2.38	126.78	124.26
21	B	806	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
21	6	614	CLA	C1-C2-C3	2.38	130.60	126.75
20	4	306	CHL	O1D-CGD-CBD	-2.38	120.77	124.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	6	613	CLA	O2A-CGA-CBA	2.38	121.68	114.03
21	B	807	CLA	C12-C11-C10	-2.38	102.30	113.24
21	B	839	CLA	O1D-CGD-CBD	-2.38	119.62	124.48
21	6	610	CLA	CHB-C1B-NB	2.38	126.77	124.26
21	B	802	CLA	O2A-CGA-O1A	-2.38	117.59	123.59
21	A	805	CLA	O1D-CGD-CBD	-2.38	119.62	124.48
21	5	602	CLA	C12-C11-C10	-2.37	102.33	113.24
21	A	816	CLA	CHB-C1B-NB	2.37	126.77	124.26
21	B	803	CLA	C3C-C4C-NC	-2.37	107.91	110.57
21	A	837	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
21	B	816	CLA	O1D-CGD-CBD	-2.37	119.63	124.48
22	F	301	LUT	C31-C30-C29	2.37	130.69	127.31
21	5	611	CLA	O2A-CGA-CBA	2.37	121.64	114.03
21	5	612	CLA	O1D-CGD-CBD	-2.37	119.64	124.48
20	6	606	CHL	OMC-CMC-C2C	-2.37	121.23	125.03
21	A	803	CLA	C12-C11-C10	-2.37	102.36	113.24
22	4	315	LUT	C7-C8-C9	2.37	129.81	126.23
21	L	305	CLA	CHD-C1D-ND	-2.37	122.28	124.45
20	Y	605	CHL	O1D-CGD-CBD	-2.37	120.80	124.74
21	A	828	CLA	CHB-C1B-NB	2.37	126.76	124.26
21	A	835	CLA	C3C-C4C-NC	-2.37	107.92	110.57
21	A	817	CLA	C12-C11-C10	-2.36	102.38	113.24
21	5	610	CLA	O2A-CGA-CBA	2.36	121.62	114.03
21	H	201	CLA	C3C-C4C-NC	-2.36	107.92	110.57
21	B	840	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
21	A	823	CLA	CHB-C1B-NB	2.36	126.76	124.26
21	H	201	CLA	CMD-C2D-C1D	2.36	128.88	124.71
21	3	610	CLA	CAA-C2A-C3A	-2.36	110.59	116.10
23	2	616	XAT	O24-C25-C24	-2.36	111.61	113.38
21	4	307	CLA	O2A-CGA-CBA	2.36	121.62	114.03
21	2	618	CLA	O2A-CGA-CBA	2.36	121.56	112.23
21	3	602	CLA	C12-C11-C10	-2.36	102.39	113.24
20	Y	608	CHL	CHA-C1A-C2A	-2.36	127.77	133.31
20	3	608	CHL	CHA-C1A-C2A	-2.36	127.77	133.31
21	A	818	CLA	C1-C2-C3	2.36	130.12	126.04
21	4	311	CLA	CHB-C1B-NB	2.36	126.75	124.26
21	A	842	CLA	O2A-CGA-O1A	-2.36	117.65	123.59
21	B	832	CLA	O2A-CGA-CBA	2.36	121.60	114.03
21	X	604	CLA	O2A-CGA-CBA	2.36	121.60	114.03
21	Y	604	CLA	CHB-C1B-NB	2.35	126.75	124.26
21	O	202	CLA	O1D-CGD-CBD	-2.35	119.67	124.48
21	G	204	CLA	O2A-CGA-CBA	2.35	121.59	114.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	K	201	CLA	CMA-C3A-C2A	-2.35	110.61	116.10
20	Y	606	CHL	O2A-CGA-CBA	2.35	121.59	114.03
21	B	806	CLA	C1-C2-C3	2.35	130.11	126.04
21	A	834	CLA	C12-C11-C10	-2.35	102.43	113.24
21	1	613	CLA	O1D-CGD-CBD	-2.35	119.67	124.48
21	B	838	CLA	C12-C11-C10	-2.35	102.44	113.24
21	Y	603	CLA	O2A-CGA-CBA	2.35	121.58	114.03
21	1	605	CLA	O1D-CGD-CBD	-2.35	119.68	124.48
21	1	613	CLA	O2A-CGA-CBA	2.35	121.57	114.03
20	2	601	CHL	O1D-CGD-CBD	-2.35	120.83	124.74
21	4	310	CLA	CHB-C1B-NB	2.35	126.74	124.26
21	A	805	CLA	C3C-C4C-NC	-2.35	107.94	110.57
21	2	604	CLA	CHB-C1B-NB	2.34	126.74	124.26
20	4	304	CHL	CHA-C1A-C2A	-2.34	127.80	133.31
21	O	203	CLA	C12-C11-C10	-2.34	102.47	113.24
20	2	614	CHL	O1D-CGD-CBD	-2.34	120.84	124.74
21	B	802	CLA	C12-C11-C10	-2.34	102.47	113.24
21	K	204	CLA	C3C-C4C-NC	-2.34	107.94	110.57
21	B	806	CLA	CHB-C1B-NB	2.34	126.74	124.26
21	B	805	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
21	B	835	CLA	C1-C2-C3	2.34	130.54	126.75
21	3	609	CLA	O2A-CGA-CBA	2.34	121.54	114.03
21	O	206	CLA	CHB-C1B-NB	2.34	126.73	124.26
20	Z	307	CHL	CHA-C1A-C2A	-2.34	127.82	133.31
20	X	606	CHL	O1D-CGD-CBD	-2.34	120.85	124.74
23	1	616	XAT	O24-C25-C24	-2.34	111.63	113.38
21	A	809	CLA	O1D-CGD-CBD	-2.34	119.70	124.48
21	A	815	CLA	O1D-CGD-CBD	-2.34	119.70	124.48
21	1	608	CLA	CHB-C1B-NB	2.34	126.73	124.26
21	5	613	CLA	CHB-C1B-NB	2.34	126.73	124.26
21	L	301	CLA	C12-C11-C10	-2.34	102.51	113.24
21	A	808	CLA	C1-C2-C3	2.33	130.53	126.75
21	B	813	CLA	C12-C11-C10	-2.33	102.52	113.24
21	2	602	CLA	C12-C11-C10	-2.33	102.52	113.24
21	B	840	CLA	CHB-C1B-NB	2.33	126.73	124.26
21	A	835	CLA	O2A-CGA-CBA	2.33	121.52	114.03
21	B	808	CLA	O1D-CGD-CBD	-2.33	119.71	124.48
21	A	801	CLA	CHB-C1B-NB	2.33	126.72	124.26
21	A	827	CLA	CHB-C1B-NB	2.33	126.72	124.26
21	4	309	CLA	C12-C11-C10	-2.33	102.54	113.24
21	Y	614	CLA	CHB-C1B-NB	2.33	126.72	124.26
21	5	605	CLA	CHB-C1B-NB	2.33	126.72	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	824	CLA	O1D-CGD-CBD	-2.33	119.72	124.48
21	A	836	CLA	O1D-CGD-CBD	-2.33	119.72	124.48
21	A	805	CLA	O2A-CGA-CBA	2.33	121.50	114.03
21	2	611	CLA	O2A-CGA-CBA	2.33	121.50	114.03
21	L	304	CLA	C12-C11-C10	-2.33	102.55	113.24
21	1	603	CLA	C1-C2-C3	2.32	130.06	126.04
22	Y	616	LUT	C39-C29-C28	2.32	121.74	118.08
21	3	613	CLA	CHB-C1B-NB	2.32	126.72	124.26
21	A	838	CLA	CHB-C1B-NB	2.32	126.72	124.26
21	1	610	CLA	O1D-CGD-CBD	-2.32	119.73	124.48
21	B	833	CLA	C3C-C4C-NC	-2.32	107.97	110.57
21	1	614	CLA	CHB-C1B-NB	2.32	126.71	124.26
21	2	612	CLA	C1-C2-C3	2.32	130.06	126.04
21	B	813	CLA	C4-C3-C5	-2.32	111.37	115.27
20	5	601	CHL	OMC-CMC-C2C	-2.32	121.31	125.03
21	6	604	CLA	O2A-CGA-CBA	2.32	121.48	114.03
21	A	828	CLA	C12-C11-C10	-2.32	102.58	113.24
21	B	812	CLA	CHB-C1B-NB	2.32	126.71	124.26
21	B	817	CLA	O1D-CGD-CBD	-2.32	119.74	124.48
21	B	819	CLA	C1-C2-C3	2.32	130.50	126.75
21	B	825	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
21	B	839	CLA	C12-C11-C10	-2.32	102.59	113.24
21	H	201	CLA	CHB-C1B-NB	2.32	126.71	124.26
21	Y	610	CLA	O1D-CGD-CBD	-2.32	119.75	124.48
21	B	805	CLA	C12-C11-C10	-2.32	102.60	113.24
21	A	821	CLA	O2A-CGA-O1A	-2.32	117.75	123.59
21	3	607	CLA	O1D-CGD-CBD	-2.31	119.75	124.48
21	G	202	CLA	O2A-CGA-CBA	2.31	121.46	114.03
21	Y	612	CLA	O2A-CGA-CBA	2.31	121.46	114.03
21	A	811	CLA	C12-C11-C10	-2.31	102.62	113.24
20	X	601	CHL	OMC-CMC-C2C	-2.31	121.33	125.03
21	A	826	CLA	CHB-C1B-NB	2.31	126.70	124.26
21	B	833	CLA	C12-C11-C10	-2.31	102.62	113.24
21	O	207	CLA	C3C-C4C-NC	-2.31	108.05	110.57
21	X	618	CLA	O2A-CGA-CBA	2.31	121.45	114.03
21	Y	611	CLA	O2A-CGA-CBA	2.31	121.45	114.03
21	3	605	CLA	C2D-C1D-ND	2.31	111.81	110.10
21	6	602	CLA	C12-C11-C10	-2.31	102.64	113.24
21	A	838	CLA	O1D-CGD-CBD	-2.31	119.77	124.48
21	A	821	CLA	CHB-C1B-NB	2.31	126.70	124.26
21	3	604	CLA	O1D-CGD-CBD	-2.31	119.77	124.48
21	1	609	CLA	C1-C2-C3	2.30	130.03	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	809	CLA	O1D-CGD-CBD	-2.30	119.77	124.48
21	X	611	CLA	O1D-CGD-CBD	-2.30	119.77	124.48
21	3	603	CLA	O1D-CGD-CBD	-2.30	119.77	124.48
21	L	305	CLA	CHB-C1B-NB	2.30	126.69	124.26
21	A	840	CLA	C12-C11-C10	-2.30	102.67	113.24
21	K	203	CLA	O2A-CGA-CBA	2.30	121.32	112.23
21	A	804	CLA	O2A-CGA-O1A	-2.30	117.79	123.59
21	Z	304	CLA	O2A-CGA-CBA	2.30	121.42	114.03
21	1	611	CLA	CHB-C1B-NB	2.30	126.69	124.26
21	4	301	CLA	O1D-CGD-CBD	-2.30	119.78	124.48
21	4	313	CLA	C1-C2-C3	2.30	130.47	126.75
21	6	609	CLA	C1-C2-C3	2.30	130.02	126.04
21	B	818	CLA	O2A-CGA-O1A	-2.30	117.79	123.59
21	X	602	CLA	O2A-CGA-CBA	2.30	121.41	114.03
20	Y	619	CHL	O2A-CGA-CBA	2.30	121.31	112.23
21	B	813	CLA	C3C-C4C-NC	-2.30	108.00	110.57
21	1	612	CLA	C1-C2-C3	2.29	130.01	126.04
21	A	813	CLA	C12-C11-C10	-2.29	102.69	113.24
21	B	836	CLA	O1D-CGD-CBD	-2.29	119.79	124.48
21	A	804	CLA	CHB-C1B-NB	2.29	126.69	124.26
21	5	605	CLA	O2D-CGD-O1D	-2.29	119.35	123.84
21	5	614	CLA	O2A-CGA-CBA	2.29	121.40	114.03
20	6	605	CHL	CHA-C1A-C2A	-2.29	127.92	133.31
21	A	802	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
21	Z	310	CLA	O2A-CGA-CBA	2.29	121.39	114.03
21	F	304	CLA	CHB-C1B-NB	2.29	126.68	124.26
21	6	610	CLA	O1D-CGD-CBD	-2.29	119.80	124.48
21	6	603	CLA	CHB-C1B-NB	2.29	126.68	124.26
22	6	616	LUT	C39-C29-C28	2.29	121.69	118.08
21	3	614	CLA	CHB-C1B-NB	2.29	126.68	124.26
21	A	802	CLA	C3C-C4C-NC	-2.29	108.00	110.57
21	5	612	CLA	C4-C3-C5	-2.29	111.42	115.27
21	B	829	CLA	C3C-C4C-NC	-2.29	108.00	110.57
21	A	809	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
21	B	823	CLA	C12-C11-C10	-2.29	102.73	113.24
21	K	201	CLA	CAA-C2A-C3A	-2.29	110.76	116.10
21	A	832	CLA	CHB-C1B-NB	2.29	126.68	124.26
20	X	607	CHL	O2A-CGA-CBA	2.29	121.38	114.03
21	4	302	CLA	O2A-CGA-CBA	2.29	121.38	114.03
21	4	312	CLA	O1D-CGD-CBD	-2.29	119.81	124.48
21	1	607	CLA	O2A-CGA-CBA	2.29	121.37	114.03
21	5	608	CLA	C3C-C4C-NC	-2.29	108.01	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	5	607	CLA	O2A-CGA-CBA	2.29	121.37	114.03
21	B	836	CLA	C12-C11-C10	-2.28	102.74	113.24
21	1	604	CLA	CHB-C1B-NB	2.28	126.67	124.26
21	Z	305	CLA	CHB-C1B-NB	2.28	126.67	124.26
21	4	303	CLA	CHB-C1B-NB	2.28	126.67	124.26
21	6	610	CLA	O2A-CGA-CBA	2.28	121.36	114.03
21	A	836	CLA	O2A-CGA-CBA	2.28	121.36	114.03
31	Z	316	NEX	C2-C1-C6	2.28	111.43	109.21
21	B	807	CLA	CHB-C1B-NB	2.28	126.67	124.26
21	A	809	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
21	1	614	CLA	O1D-CGD-CBD	-2.28	119.82	124.48
21	A	821	CLA	O1D-CGD-CBD	-2.28	119.82	124.48
22	3	615	LUT	C30-C31-C32	2.28	130.33	123.22
21	1	612	CLA	C12-C11-C10	-2.28	102.77	113.24
21	Z	304	CLA	CHB-C1B-NB	2.28	126.67	124.26
21	Y	612	CLA	C2D-C1D-ND	2.28	111.78	110.10
21	A	819	CLA	C12-C11-C10	-2.28	102.78	113.24
22	Z	314	LUT	C32-C33-C34	2.28	122.44	118.94
21	Z	303	CLA	C12-C11-C10	-2.28	102.78	113.24
21	1	609	CLA	CHB-C1B-NB	2.28	126.67	124.26
21	B	839	CLA	O2D-CGD-O1D	-2.28	119.39	123.84
21	B	833	CLA	CMD-C2D-C1D	2.28	128.72	124.71
21	B	817	CLA	O2D-CGD-O1D	-2.28	119.39	123.84
21	1	614	CLA	O2A-CGA-CBA	2.28	121.34	114.03
21	A	816	CLA	O2A-CGA-CBA	2.27	121.34	114.03
21	1	612	CLA	CHB-C1B-NB	2.27	126.67	124.26
21	2	612	CLA	O1D-CGD-CBD	-2.27	119.83	124.48
21	X	612	CLA	CMD-C2D-C1D	2.27	128.72	124.71
21	A	807	CLA	CHB-C1B-NB	2.27	126.66	124.26
21	A	842	CLA	C4-C3-C5	-2.27	111.45	115.27
20	X	605	CHL	OMC-CMC-C2C	-2.27	121.39	125.03
21	Y	610	CLA	O2A-CGA-CBA	2.27	121.33	114.03
21	B	822	CLA	C12-C11-C10	-2.27	102.80	113.24
21	A	842	CLA	CHB-C1B-NB	2.27	126.66	124.26
21	1	602	CLA	C12-C11-C10	-2.27	102.81	113.24
21	A	832	CLA	C3C-C4C-NC	-2.27	108.03	110.57
21	Z	312	CLA	C3C-C4C-NC	-2.27	108.03	110.57
21	X	618	CLA	CHB-C1B-NB	2.27	126.66	124.26
21	6	612	CLA	O2D-CGD-O1D	-2.27	119.40	123.84
22	1	615	LUT	C19-C9-C8	2.27	121.65	118.08
21	1	609	CLA	C12-C11-C10	-2.27	102.82	113.24
21	B	833	CLA	O2A-CGA-O1A	-2.27	117.87	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	Y	616	LUT	C19-C9-C8	2.27	121.65	118.08
21	2	604	CLA	C12-C11-C10	-2.27	102.83	113.24
21	H	201	CLA	C4-C3-C5	-2.27	111.46	115.27
21	B	817	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
21	O	206	CLA	C3C-C4C-NC	-2.26	108.03	110.57
21	A	814	CLA	O1D-CGD-CBD	-2.26	119.85	124.48
21	B	809	CLA	C3C-C4C-NC	-2.26	108.03	110.57
21	6	612	CLA	C4-C3-C5	-2.26	111.47	115.27
21	1	609	CLA	O1D-CGD-CBD	-2.26	119.86	124.48
21	2	603	CLA	O2A-CGA-CBA	2.26	121.28	114.03
21	B	801	CLA	O1D-CGD-CBD	-2.26	119.86	124.48
20	Z	308	CHL	O1D-CGD-CBD	-2.26	120.98	124.74
21	A	804	CLA	O1D-CGD-CBD	-2.26	119.87	124.48
21	G	204	CLA	C2D-C1D-ND	2.26	111.77	110.10
21	B	831	CLA	C12-C11-C10	-2.26	102.87	113.24
21	B	832	CLA	C3C-C4C-NC	-2.26	108.04	110.57
21	3	613	CLA	CAA-C2A-C3A	-2.26	110.83	116.10
21	B	801	CLA	C12-C11-C10	-2.25	102.88	113.24
20	Y	608	CHL	O2A-CGA-CBA	2.25	121.27	114.03
21	X	603	CLA	O1D-CGD-CBD	-2.25	119.87	124.48
21	5	603	CLA	C3C-C4C-NC	-2.25	108.04	110.57
21	X	612	CLA	O2A-CGA-CBA	2.25	121.27	114.03
21	B	830	CLA	CHB-C1B-NB	2.25	126.64	124.26
22	Y	615	LUT	C39-C29-C28	2.25	121.63	118.08
21	A	839	CLA	C1-C2-C3	2.25	130.40	126.75
21	A	810	CLA	C3C-C4C-NC	-2.25	108.05	110.57
21	B	838	CLA	O1D-CGD-CBD	-2.25	119.88	124.48
21	6	602	CLA	CHB-C1B-NB	2.25	126.64	124.26
21	B	824	CLA	C3C-C4C-NC	-2.25	108.05	110.57
21	6	608	CLA	C3C-C4C-NC	-2.25	108.05	110.57
21	A	817	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
21	A	834	CLA	C4-C3-C5	-2.25	111.49	115.27
21	2	602	CLA	C3C-C4C-NC	-2.25	108.05	110.57
20	Y	601	CHL	O1D-CGD-CBD	-2.25	120.99	124.74
21	5	603	CLA	O2A-CGA-CBA	2.25	121.25	114.03
21	B	840	CLA	C12-C11-C10	-2.25	102.91	113.24
21	X	603	CLA	CHB-C1B-NB	2.25	126.64	124.26
21	B	828	CLA	C3C-C4C-NC	-2.25	108.05	110.57
21	B	836	CLA	C3C-C4C-NC	-2.25	108.05	110.57
21	A	815	CLA	CHB-C1B-NB	2.25	126.63	124.26
21	O	206	CLA	O1D-CGD-CBD	-2.25	119.89	124.48
21	Y	604	CLA	O1D-CGD-CBD	-2.25	119.89	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	2	618	CLA	CHB-C1B-NB	2.24	126.63	124.26
21	6	613	CLA	CHB-C1B-NB	2.24	126.63	124.26
21	A	824	CLA	C3C-C4C-NC	-2.24	108.05	110.57
21	B	817	CLA	C3C-C4C-NC	-2.24	108.05	110.57
22	6	616	LUT	C12-C13-C14	2.24	122.38	118.94
21	A	820	CLA	O2A-CGA-CBA	2.24	121.23	114.03
21	3	609	CLA	C3C-C4C-NC	-2.24	108.06	110.57
21	A	808	CLA	C3C-C4C-NC	-2.24	108.06	110.57
21	X	613	CLA	O1D-CGD-CBD	-2.24	119.90	124.48
21	B	803	CLA	O1D-CGD-CBD	-2.24	119.90	124.48
21	B	825	CLA	CHB-C1B-NB	2.24	126.63	124.26
21	1	609	CLA	C3C-C4C-NC	-2.24	108.13	110.57
21	A	809	CLA	C1-C2-C3	2.24	129.92	126.04
21	L	301	CLA	CHB-C1B-NB	2.24	126.63	124.26
22	2	615	LUT	C19-C9-C8	2.24	121.60	118.08
21	A	839	CLA	O1D-CGD-CBD	-2.24	119.91	124.48
21	5	608	CLA	O2A-CGA-CBA	2.24	121.22	114.03
20	2	601	CHL	O2A-CGA-CBA	2.24	121.07	112.23
21	B	816	CLA	O2D-CGD-O1D	-2.24	119.47	123.84
21	Z	311	CLA	CHB-C1B-NB	2.24	126.62	124.26
21	A	814	CLA	O2D-CGD-O1D	-2.24	119.47	123.84
21	A	808	CLA	CHB-C1B-NB	2.23	126.62	124.26
21	A	843	CLA	CHB-C1B-NB	2.23	126.62	124.26
21	B	839	CLA	CHB-C1B-NB	2.23	126.62	124.26
21	Y	602	CLA	C4-C3-C5	-2.23	111.51	115.27
20	4	305	CHL	O1D-CGD-CBD	-2.23	121.02	124.74
21	K	202	CLA	O2A-CGA-CBA	2.23	121.20	114.03
21	A	812	CLA	C1-C2-C3	2.23	129.90	126.04
20	2	607	CHL	O1D-CGD-CBD	-2.23	121.02	124.74
20	Y	609	CHL	OMC-CMC-C2C	-2.23	121.45	125.03
21	5	604	CLA	CHB-C1B-NB	2.23	126.62	124.26
21	K	202	CLA	O1D-CGD-CBD	-2.23	119.92	124.48
21	3	602	CLA	C3C-C4C-NC	-2.23	108.07	110.57
21	B	812	CLA	C3C-C4C-NC	-2.23	108.07	110.57
21	X	610	CLA	O2A-CGA-CBA	2.23	121.19	114.03
21	B	826	CLA	C1-C2-C3	2.23	129.90	126.04
21	A	821	CLA	C12-C11-C10	-2.23	103.00	113.24
21	2	611	CLA	O1D-CGD-CBD	-2.23	119.92	124.48
21	B	805	CLA	CHB-C1B-NB	2.23	126.61	124.26
21	2	612	CLA	C4-C3-C5	-2.23	111.53	115.27
21	A	820	CLA	O2D-CGD-O1D	-2.23	119.49	123.84
21	B	821	CLA	CHB-C1B-NB	2.23	126.61	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	2	619	BCR	C10-C11-C12	2.23	130.16	123.22
21	B	817	CLA	C12-C11-C10	-2.23	103.01	113.24
21	3	606	CLA	CHB-C1B-NB	2.22	126.61	124.26
21	F	304	CLA	C2D-C1D-ND	2.22	111.74	110.10
21	Z	312	CLA	CHB-C1B-NB	2.22	126.61	124.26
20	Z	309	CHL	C1A-CHA-C4D	2.22	122.69	118.98
21	1	607	CLA	CHB-C1B-NB	2.22	126.61	124.26
21	B	819	CLA	CHB-C1B-NB	2.22	126.61	124.26
21	A	813	CLA	C1-C2-C3	2.22	129.89	126.04
22	3	615	LUT	C1-C6-C7	2.22	122.06	115.78
20	Z	301	CHL	O2A-CGA-CBA	2.22	121.17	114.03
21	A	822	CLA	C3C-C4C-NC	-2.22	108.08	110.57
21	A	836	CLA	C3C-C4C-NC	-2.22	108.08	110.57
21	B	836	CLA	CHB-C1B-NB	2.22	126.61	124.26
21	J	102	CLA	C2D-C1D-ND	2.22	111.74	110.10
21	2	602	CLA	CHB-C1B-NB	2.22	126.61	124.26
21	6	608	CLA	O1D-CGD-CBD	-2.22	119.94	124.48
21	A	807	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
21	X	612	CLA	O1D-CGD-CBD	-2.22	119.94	124.48
21	A	801	CLA	O1D-CGD-CBD	-2.22	119.95	124.48
21	A	823	CLA	CAA-C2A-C3A	-2.22	110.92	116.10
21	5	614	CLA	C3C-C4C-NC	-2.22	108.08	110.57
21	A	840	CLA	O2A-CGA-O1A	-2.22	118.00	123.59
21	A	832	CLA	O1D-CGD-CBD	-2.22	119.95	124.48
21	2	609	CLA	C3C-C4C-NC	-2.22	108.09	110.57
21	Y	613	CLA	C3C-C4C-NC	-2.22	108.09	110.57
21	A	827	CLA	C12-C11-C10	-2.22	103.06	113.24
21	J	101	CLA	CHB-C1B-NB	2.22	126.60	124.26
21	4	311	CLA	C12-C11-C10	-2.21	102.60	113.29
21	F	304	CLA	CAA-C2A-C3A	-2.21	110.93	116.10
20	6	606	CHL	O2A-CGA-CBA	2.21	121.14	114.03
21	X	609	CLA	O2A-CGA-CBA	2.21	121.14	114.03
20	5	601	CHL	CHA-C1A-C2A	-2.21	128.11	133.31
21	3	610	CLA	O1D-CGD-CBD	-2.21	119.96	124.48
21	A	816	CLA	O1D-CGD-CBD	-2.21	119.96	124.48
21	A	839	CLA	C3C-C4C-NC	-2.21	108.09	110.57
21	B	818	CLA	C3C-C4C-NC	-2.21	108.09	110.57
21	K	202	CLA	O2D-CGD-O1D	-2.21	119.52	123.84
21	A	838	CLA	C1-C2-C3	2.21	129.87	126.04
21	B	827	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
21	3	612	CLA	CHB-C1B-NB	2.21	126.59	124.26
21	Z	313	CLA	CHB-C1B-NB	2.21	126.59	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	Z	309	CHL	CHA-C1A-C2A	-2.21	128.12	133.31
21	A	832	CLA	C1-C2-C3	2.21	129.86	126.04
21	1	602	CLA	O1D-CGD-CBD	-2.21	119.97	124.48
21	1	603	CLA	C3C-C4C-NC	-2.21	108.10	110.57
21	B	805	CLA	C3C-C4C-NC	-2.21	108.10	110.57
21	3	614	CLA	CAA-C2A-C3A	-2.21	110.95	116.10
21	A	831	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
21	2	610	CLA	CHB-C1B-NB	2.21	126.59	124.26
21	A	840	CLA	C3C-C4C-NC	-2.21	108.10	110.57
21	A	843	CLA	C12-C11-C10	-2.21	102.64	113.29
21	5	612	CLA	CHB-C1B-NB	2.21	126.59	124.26
21	1	608	CLA	C12-C11-C10	-2.21	103.11	113.24
21	B	835	CLA	O1D-CGD-CBD	-2.21	119.97	124.48
20	X	607	CHL	OMC-CMC-C2C	-2.20	121.50	125.03
21	2	612	CLA	CHB-C1B-NB	2.20	126.59	124.26
22	6	616	LUT	C7-C8-C9	2.20	129.57	126.23
21	B	812	CLA	C12-C11-C10	-2.20	103.11	113.24
21	X	611	CLA	O2A-CGA-CBA	2.20	121.11	114.03
21	2	612	CLA	O2D-CGD-O1D	-2.20	119.53	123.84
21	B	834	CLA	CHB-C1B-NB	2.20	126.59	124.26
21	L	305	CLA	O2A-CGA-CBA	2.20	121.11	114.03
21	5	610	CLA	O1D-CGD-CBD	-2.20	119.97	124.48
21	3	604	CLA	O2A-CGA-CBA	2.20	121.11	114.03
20	X	606	CHL	O2A-CGA-CBA	2.20	121.10	114.03
21	3	610	CLA	CHB-C1B-NB	2.20	126.59	124.26
21	B	840	CLA	C4-C3-C5	-2.20	111.57	115.27
21	A	811	CLA	C3C-C4C-NC	-2.20	108.10	110.57
21	A	843	CLA	O2D-CGD-O1D	-2.20	119.54	123.84
21	A	830	CLA	C3C-C4C-NC	-2.20	108.11	110.57
21	J	101	CLA	C3C-C4C-NC	-2.20	108.11	110.57
21	B	831	CLA	C5-C3-C2	2.20	125.57	121.12
21	A	829	CLA	C4-C3-C5	-2.20	111.57	115.27
20	Z	301	CHL	O2D-CGD-O1D	-2.20	119.54	123.84
21	A	802	CLA	O1D-CGD-CBD	-2.20	119.99	124.48
21	1	613	CLA	CHB-C1B-NB	2.20	126.58	124.26
21	G	203	CLA	C3C-C4C-NC	-2.20	108.11	110.57
20	5	606	CHL	OMC-CMC-C2C	-2.20	121.51	125.03
21	A	812	CLA	O2D-CGD-O1D	-2.20	119.54	123.84
23	5	616	XAT	C7-C8-C9	2.19	128.94	125.53
21	A	838	CLA	C3C-C4C-NC	-2.19	108.11	110.57
21	A	818	CLA	C3C-C4C-NC	-2.19	108.11	110.57
20	5	601	CHL	O2A-CGA-O1A	-2.19	118.06	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	831	CLA	O1D-CGD-CBD	-2.19	120.00	124.48
21	3	617	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
24	A	846	BCR	C21-C20-C19	2.19	130.05	123.22
21	X	604	CLA	CMD-C2D-C1D	2.19	128.57	124.71
22	3	615	LUT	C19-C9-C8	2.19	121.53	118.08
21	Y	610	CLA	CHB-C1B-NB	2.19	126.58	124.26
21	O	203	CLA	C1-C2-C3	2.19	129.83	126.04
21	1	602	CLA	CHB-C1B-NB	2.19	126.57	124.26
21	3	607	CLA	CHB-C1B-NB	2.19	126.57	124.26
21	X	611	CLA	CMD-C2D-C1D	2.19	128.57	124.71
21	B	837	CLA	O1D-CGD-CBD	-2.19	120.01	124.48
21	Y	612	CLA	CHB-C1B-NB	2.19	126.57	124.26
21	Y	613	CLA	CHB-C1B-NB	2.19	126.57	124.26
20	X	608	CHL	OMC-CMC-C2C	-2.19	121.53	125.03
21	B	819	CLA	O2D-CGD-O1D	-2.19	119.56	123.84
21	1	613	CLA	O2D-CGD-O1D	-2.18	119.57	123.84
20	Z	302	CHL	O2A-CGA-O1A	-2.18	117.85	123.30
22	4	315	LUT	C11-C10-C9	2.18	130.43	127.31
20	Z	302	CHL	O2D-CGD-O1D	-2.18	119.57	123.84
20	3	608	CHL	O2A-CGA-CBA	2.18	120.86	112.23
21	K	202	CLA	C3C-C4C-NC	-2.18	108.12	110.57
21	L	304	CLA	C3C-C4C-NC	-2.18	108.12	110.57
21	Z	304	CLA	C3C-C4C-NC	-2.18	108.12	110.57
21	B	825	CLA	O1D-CGD-CBD	-2.18	120.02	124.48
21	4	302	CLA	O1D-CGD-CBD	-2.18	120.02	124.48
21	A	842	CLA	C12-C11-C10	-2.18	103.21	113.24
21	A	817	CLA	C3C-C4C-NC	-2.18	108.12	110.57
21	X	604	CLA	C3C-C4C-NC	-2.18	108.12	110.57
20	Y	619	CHL	O2D-CGD-O1D	-2.18	119.58	123.84
21	A	806	CLA	C3C-C4C-NC	-2.18	108.13	110.57
21	2	611	CLA	C2D-C1D-ND	2.18	111.71	110.10
20	Z	309	CHL	O2A-CGA-CBA	2.18	121.03	114.03
21	A	820	CLA	C3C-C4C-NC	-2.18	108.13	110.57
21	B	815	CLA	C3C-C4C-NC	-2.18	108.13	110.57
21	3	605	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
21	B	830	CLA	C3C-C4C-NC	-2.18	108.13	110.57
21	Z	303	CLA	O1D-CGD-CBD	-2.18	120.03	124.48
20	4	306	CHL	O2A-CGA-O1A	-2.18	118.10	123.59
21	A	823	CLA	C3C-C4C-NC	-2.18	108.13	110.57
21	B	828	CLA	O1D-CGD-CBD	-2.18	120.03	124.48
21	K	203	CLA	CHB-C1B-NB	2.18	126.56	124.26
21	O	202	CLA	CHB-C1B-NB	2.18	126.56	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	2	609	CLA	O1D-CGD-CBD	-2.18	120.03	124.48
24	O	201	BCR	C8-C7-C6	2.18	133.31	127.20
21	2	611	CLA	CHB-C1B-NB	2.17	126.56	124.26
21	3	617	CLA	C4-C3-C5	-2.17	111.61	115.27
21	A	827	CLA	C4-C3-C5	-2.17	111.62	115.27
21	A	805	CLA	CHB-C1B-NB	2.17	126.56	124.26
21	A	806	CLA	O1D-CGD-CBD	-2.17	120.04	124.48
21	Y	603	CLA	CHB-C1B-NB	2.17	126.56	124.26
21	Y	603	CLA	C3C-C4C-NC	-2.17	108.14	110.57
21	A	843	CLA	C3C-C4C-NC	-2.17	108.14	110.57
21	2	602	CLA	C4-C3-C5	-2.17	111.62	115.27
21	5	608	CLA	C2C-C1C-NC	-2.17	107.94	109.97
21	Z	313	CLA	O2A-CGA-CBA	2.17	120.80	112.23
21	A	832	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
21	B	826	CLA	C3C-C4C-NC	-2.17	108.14	110.57
21	B	830	CLA	O1D-CGD-CBD	-2.17	120.05	124.48
21	4	309	CLA	CHB-C1B-NB	2.17	126.55	124.26
21	3	605	CLA	O1D-CGD-CBD	-2.17	120.05	124.48
21	3	606	CLA	CMD-C2D-C1D	2.17	128.53	124.71
21	A	807	CLA	C3C-C4C-NC	-2.17	108.14	110.57
21	G	202	CLA	C2D-C1D-ND	2.17	111.70	110.10
21	A	810	CLA	O2D-CGD-O1D	-2.17	119.61	123.84
21	B	801	CLA	O2D-CGD-O1D	-2.17	119.61	123.84
20	Y	609	CHL	O2A-CGA-CBA	2.16	120.98	114.03
21	Y	613	CLA	O1D-CGD-CBD	-2.16	120.06	124.48
21	A	819	CLA	O2A-CGA-O1A	-2.16	118.13	123.59
20	Y	607	CHL	OMC-CMC-C2C	-2.16	121.56	125.03
21	5	602	CLA	C3C-C4C-NC	-2.16	108.15	110.57
21	6	612	CLA	O1D-CGD-CBD	-2.16	120.06	124.48
20	Y	601	CHL	O2A-CGA-O1A	-2.16	117.91	123.30
21	2	604	CLA	C4-C3-C5	-2.16	111.64	115.27
21	A	812	CLA	C3C-C4C-NC	-2.16	108.15	110.57
21	A	811	CLA	CHB-C1B-NB	2.16	126.55	124.26
21	2	604	CLA	O1D-CGD-CBD	-2.16	120.06	124.48
21	X	603	CLA	C3C-C4C-NC	-2.16	108.15	110.57
21	Z	310	CLA	C3C-C4C-NC	-2.16	108.15	110.57
21	3	607	CLA	C3C-C4C-NC	-2.16	108.15	110.57
21	K	203	CLA	C3C-C4C-NC	-2.16	108.15	110.57
21	A	827	CLA	C3C-C4C-NC	-2.16	108.15	110.57
21	Z	303	CLA	C3C-C4C-NC	-2.16	108.15	110.57
21	5	610	CLA	CHB-C1B-NB	2.16	126.54	124.26
21	B	831	CLA	O1D-CGD-CBD	-2.16	120.07	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	837	CLA	C3C-C4C-NC	-2.16	108.15	110.57
21	B	811	CLA	C3C-C4C-NC	-2.16	108.15	110.57
21	B	809	CLA	CHB-C1B-NB	2.16	126.54	124.26
21	H	201	CLA	C1-C2-C3	2.16	129.77	126.04
21	L	304	CLA	CHB-C1B-NB	2.16	126.54	124.26
21	1	604	CLA	C3C-C4C-NC	-2.15	108.16	110.57
21	1	607	CLA	C3C-C4C-NC	-2.15	108.16	110.57
21	6	604	CLA	C3C-C4C-NC	-2.15	108.16	110.57
21	B	834	CLA	O1D-CGD-CBD	-2.15	120.08	124.48
21	5	609	CLA	CHB-C1B-NB	2.15	126.54	124.26
21	K	201	CLA	C3C-C4C-NC	-2.15	108.16	110.57
21	6	612	CLA	C12-C11-C10	-2.15	102.90	113.29
21	B	807	CLA	O2D-CGD-O1D	-2.15	119.63	123.84
21	A	839	CLA	CMD-C2D-C1D	2.15	128.51	124.71
20	6	607	CHL	O1D-CGD-CBD	-2.15	121.16	124.74
21	B	806	CLA	CMD-C2D-C1D	2.15	128.50	124.71
21	A	836	CLA	O2D-CGD-O1D	-2.15	119.63	123.84
21	A	812	CLA	CHB-C1B-NB	2.15	126.53	124.26
21	6	614	CLA	O2D-CGD-O1D	-2.15	119.64	123.84
21	4	313	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
21	H	201	CLA	O1D-CGD-CBD	-2.15	120.09	124.48
21	B	821	CLA	O1D-CGD-CBD	-2.15	120.09	124.48
21	3	602	CLA	CHB-C1B-NB	2.15	126.53	124.26
22	X	615	LUT	C28-C29-C30	2.15	122.23	118.94
21	A	813	CLA	C3C-C4C-NC	-2.15	108.17	110.57
21	6	603	CLA	C2D-C1D-ND	2.15	111.69	110.10
21	2	613	CLA	O1D-CGD-CBD	-2.15	120.09	124.48
21	B	819	CLA	O1D-CGD-CBD	-2.15	120.09	124.48
21	L	304	CLA	C4-C3-C5	-2.14	111.67	115.27
21	6	614	CLA	C3C-C4C-NC	-2.14	108.17	110.57
21	A	819	CLA	C3C-C4C-NC	-2.14	108.17	110.57
21	Z	310	CLA	CHB-C1B-NB	2.14	126.53	124.26
21	B	801	CLA	C2D-C1D-ND	2.14	111.68	110.10
20	2	601	CHL	O2D-CGD-O1D	-2.14	119.65	123.84
21	6	613	CLA	CMD-C2D-C1D	2.14	128.49	124.71
21	5	605	CLA	C2A-C1A-CHA	2.14	126.03	122.71
20	4	304	CHL	O2D-CGD-O1D	-2.14	119.65	123.84
21	X	613	CLA	O2A-CGA-CBA	2.14	120.91	114.03
21	5	614	CLA	O1D-CGD-CBD	-2.14	120.10	124.48
21	3	609	CLA	O2D-CGD-O1D	-2.14	119.65	123.84
21	B	803	CLA	O2D-CGD-O1D	-2.14	119.65	123.84
21	Z	304	CLA	O1D-CGD-CBD	-2.14	120.11	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	Y	616	LUT	C1-C6-C7	2.14	121.83	115.78
21	B	839	CLA	C3C-C4C-NC	-2.14	108.17	110.57
22	3	615	LUT	C35-C15-C14	2.14	127.86	123.47
21	X	610	CLA	C2D-C1D-ND	2.14	111.68	110.10
21	B	827	CLA	C12-C11-C10	-2.14	103.41	113.24
21	4	309	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
21	A	804	CLA	C3C-C4C-NC	-2.14	108.17	110.57
21	1	614	CLA	C2D-C1D-ND	2.14	111.68	110.10
21	Z	312	CLA	O2A-CGA-CBA	2.14	120.90	114.03
21	1	610	CLA	C4-C3-C5	-2.14	111.68	115.27
21	2	602	CLA	O1D-CGD-CBD	-2.14	120.11	124.48
21	3	611	CLA	C2D-C1D-ND	2.14	111.68	110.10
21	4	303	CLA	C3C-C4C-NC	-2.14	108.18	110.57
21	B	820	CLA	C3C-C4C-NC	-2.13	108.18	110.57
21	B	831	CLA	C3C-C4C-NC	-2.13	108.18	110.57
21	3	603	CLA	C2D-C1D-ND	2.13	111.68	110.10
21	B	815	CLA	C1-C2-C3	2.13	129.73	126.04
21	B	824	CLA	CHB-C1B-NB	2.13	126.52	124.26
21	A	805	CLA	O2D-CGD-O1D	-2.13	119.67	123.84
21	6	604	CLA	O1D-CGD-CBD	-2.13	120.12	124.48
21	X	618	CLA	CMD-C2D-C1D	2.13	128.47	124.71
22	4	315	LUT	C12-C13-C14	2.13	122.21	118.94
21	5	604	CLA	O1D-CGD-CBD	-2.13	120.12	124.48
21	A	833	CLA	O1D-CGD-CBD	-2.13	120.12	124.48
21	B	833	CLA	O2D-CGD-O1D	-2.13	119.67	123.84
21	B	837	CLA	CMD-C2D-C1D	2.13	128.47	124.71
21	B	803	CLA	CHB-C1B-NB	2.13	126.51	124.26
21	B	835	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
22	1	615	LUT	C31-C30-C29	2.13	130.35	127.31
21	A	814	CLA	CHB-C1B-NB	2.13	126.51	124.26
21	X	610	CLA	CHB-C1B-NB	2.13	126.51	124.26
21	Y	614	CLA	O2A-CGA-CBA	2.13	120.87	114.03
21	A	810	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
21	A	831	CLA	C3C-C4C-NC	-2.13	108.18	110.57
21	A	841	CLA	C3C-C4C-NC	-2.13	108.19	110.57
21	2	603	CLA	C3C-C4C-NC	-2.13	108.19	110.57
21	B	833	CLA	C5-C3-C2	2.13	125.42	121.12
21	6	612	CLA	C3C-C4C-NC	-2.13	108.19	110.57
21	A	823	CLA	O1D-CGD-CBD	-2.13	120.14	124.48
21	6	604	CLA	CHB-C1B-NB	2.13	126.51	124.26
21	4	302	CLA	C2D-C1D-ND	2.13	111.67	110.10
21	X	603	CLA	O2A-CGA-O1A	-2.12	118.23	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	809	CLA	CHB-C1B-NB	2.12	126.50	124.26
21	A	819	CLA	O1D-CGD-CBD	-2.12	120.14	124.48
21	A	811	CLA	CMD-C2D-C1D	2.12	128.45	124.71
21	B	805	CLA	CMD-C2D-C1D	2.12	128.45	124.71
21	B	823	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
21	3	617	CLA	C3C-C4C-NC	-2.12	108.19	110.57
21	B	810	CLA	C3C-C4C-NC	-2.12	108.19	110.57
21	A	830	CLA	CHB-C1B-NB	2.12	126.50	124.26
21	3	612	CLA	O2A-CGA-CBA	2.12	120.84	114.03
21	L	303	CLA	C3C-C4C-NC	-2.12	108.19	110.57
21	Z	303	CLA	C2C-C1C-NC	-2.12	107.99	109.97
21	A	810	CLA	CHB-C1B-NB	2.12	126.50	124.26
21	B	806	CLA	C3C-C4C-NC	-2.12	108.19	110.57
21	5	604	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
21	A	828	CLA	C1-C2-C3	2.12	129.71	126.04
21	B	838	CLA	CHB-C1B-NB	2.12	126.50	124.26
21	K	204	CLA	CHB-C1B-NB	2.12	126.50	124.26
21	B	804	CLA	CHB-C1B-NB	2.12	126.50	124.26
21	Y	602	CLA	O1D-CGD-CBD	-2.12	120.15	124.48
21	3	605	CLA	CMD-C2D-C1D	2.12	128.44	124.71
20	X	608	CHL	O2A-CGA-CBA	2.12	120.83	114.03
21	X	609	CLA	C3C-C4C-NC	-2.12	108.20	110.57
20	X	601	CHL	O2A-CGA-CBA	2.12	120.83	114.03
21	B	808	CLA	C3C-C4C-NC	-2.12	108.20	110.57
21	4	313	CLA	CMD-C2D-C1D	2.11	128.44	124.71
21	A	803	CLA	O2D-CGD-O1D	-2.11	119.70	123.84
21	4	313	CLA	C3C-C4C-NC	-2.11	108.20	110.57
21	Y	610	CLA	C3C-C4C-NC	-2.11	108.20	110.57
21	B	827	CLA	C4-C3-C5	-2.11	111.72	115.27
21	B	808	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
21	B	835	CLA	C2D-C1D-ND	2.11	111.66	110.10
21	B	804	CLA	C3C-C4C-NC	-2.11	108.20	110.57
21	A	839	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
21	A	835	CLA	CHB-C1B-NB	2.11	126.49	124.26
21	5	602	CLA	C1-C2-C3	2.11	129.69	126.04
21	A	828	CLA	C3C-C4C-NC	-2.11	108.20	110.57
20	X	607	CHL	O2D-CGD-O1D	-2.11	119.71	123.84
21	6	614	CLA	O1D-CGD-CBD	-2.11	120.17	124.48
21	X	609	CLA	C2C-C1C-NC	-2.11	108.00	109.97
21	B	822	CLA	C3C-C4C-NC	-2.11	108.21	110.57
21	B	825	CLA	C3C-C4C-NC	-2.11	108.21	110.57
20	5	601	CHL	O2D-CGD-O1D	-2.11	119.30	124.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	3	604	CLA	C3C-C4C-NC	-2.11	108.21	110.57
21	A	826	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
21	A	815	CLA	C3C-C4C-NC	-2.11	108.21	110.57
20	Z	306	CHL	O2A-CGA-CBA	2.11	120.80	114.03
21	A	843	CLA	C4-C3-C5	-2.10	111.73	115.27
21	A	806	CLA	O2D-CGD-O1D	-2.10	119.72	123.84
21	4	308	CLA	C3C-C4C-NC	-2.10	108.21	110.57
21	X	613	CLA	C3C-C4C-NC	-2.10	108.21	110.57
21	B	809	CLA	O2D-CGD-O1D	-2.10	119.72	123.84
21	B	811	CLA	CHB-C1B-NB	2.10	126.48	124.26
21	4	301	CLA	C3C-C4C-NC	-2.10	108.21	110.57
21	B	807	CLA	O1D-CGD-CBD	-2.10	120.18	124.48
21	A	816	CLA	O2D-CGD-O1D	-2.10	119.73	123.84
21	A	802	CLA	C2A-C1A-CHA	2.10	127.53	123.86
21	B	825	CLA	C1-C2-C3	2.10	129.68	126.04
21	2	608	CLA	C3C-C4C-NC	-2.10	108.22	110.57
21	1	608	CLA	C4-C3-C5	-2.10	111.74	115.27
21	A	801	CLA	C3C-C4C-NC	-2.10	108.22	110.57
21	A	820	CLA	CHB-C1B-NB	2.10	126.48	124.26
21	X	613	CLA	CHB-C1B-NB	2.10	126.48	124.26
21	2	610	CLA	CAA-C2A-C3A	-2.10	111.20	116.10
21	X	604	CLA	CHB-C1B-NB	2.10	126.48	124.26
21	2	612	CLA	C3C-C4C-NC	-2.10	108.22	110.57
21	B	814	CLA	C3C-C4C-NC	-2.10	108.22	110.57
21	B	818	CLA	O1D-CGD-CBD	-2.10	120.19	124.48
21	1	603	CLA	CMD-C2D-C1D	2.10	128.41	124.71
21	B	823	CLA	C3C-C4C-NC	-2.10	108.22	110.57
21	6	613	CLA	O1D-CGD-CBD	-2.10	120.20	124.48
21	B	806	CLA	O1D-CGD-CBD	-2.10	120.20	124.48
21	Z	310	CLA	O1D-CGD-CBD	-2.10	120.20	124.48
21	1	613	CLA	CMD-C2D-C1D	2.09	128.41	124.71
21	B	815	CLA	O1D-CGD-CBD	-2.09	120.20	124.48
21	6	601	CLA	C3C-C4C-NC	-2.09	108.22	110.57
21	2	609	CLA	CHB-C1B-NB	2.09	126.47	124.26
21	L	303	CLA	CHB-C1B-NB	2.09	126.47	124.26
21	B	809	CLA	C12-C11-C10	-2.09	103.62	113.24
21	1	608	CLA	C2D-C1D-ND	2.09	111.65	110.10
21	B	822	CLA	C4D-CHA-C1A	2.09	123.80	121.25
21	B	820	CLA	O2D-CGD-O1D	-2.09	119.75	123.84
21	A	826	CLA	O1D-CGD-CBD	-2.09	120.20	124.48
21	B	814	CLA	CED-O2D-CGD	2.09	120.67	115.94
21	6	610	CLA	C3C-C4C-NC	-2.09	108.22	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	Y	611	CLA	CMD-C2D-C1D	2.09	128.40	124.71
20	Y	601	CHL	O2A-CGA-CBA	2.09	120.75	114.03
21	B	813	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
21	3	602	CLA	CMD-C2D-C1D	2.09	128.40	124.71
20	4	304	CHL	O2A-CGA-O1A	-2.09	118.32	123.59
21	B	825	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
21	Y	611	CLA	CHB-C1B-NB	2.09	126.47	124.26
22	X	614	LUT	C35-C15-C14	2.09	127.75	123.47
21	Y	603	CLA	O1D-CGD-CBD	-2.09	120.21	124.48
21	6	611	CLA	CHB-C1B-NB	2.09	126.47	124.26
21	6	602	CLA	O1D-CGD-CBD	-2.09	120.21	124.48
20	3	608	CHL	O2D-CGD-O1D	-2.09	119.75	123.84
20	Y	607	CHL	O2A-CGA-O1A	-2.09	118.10	123.30
21	Y	613	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
21	A	838	CLA	O2D-CGD-O1D	-2.09	119.76	123.84
21	1	605	CLA	CHB-C1B-NB	2.09	126.47	124.26
21	2	608	CLA	CHB-C1B-NB	2.09	126.47	124.26
21	A	801	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
21	1	608	CLA	O1D-CGD-CBD	-2.09	120.22	124.48
20	2	605	CHL	OMC-CMC-C2C	-2.09	121.69	125.03
20	Z	307	CHL	O2A-CGA-O1A	-2.08	118.10	123.30
21	X	602	CLA	CHB-C1B-NB	2.08	126.46	124.26
21	3	606	CLA	C3C-C4C-NC	-2.08	108.23	110.57
21	A	801	CLA	C2D-C1D-ND	2.08	111.64	110.10
20	4	306	CHL	O2D-CGD-O1D	-2.08	119.77	123.84
21	B	829	CLA	CMD-C2D-C1D	2.08	128.38	124.71
21	Y	614	CLA	O1D-CGD-CBD	-2.08	120.22	124.48
21	2	613	CLA	CMD-C2D-C1D	2.08	128.38	124.71
21	B	823	CLA	C4-C3-C5	-2.08	111.77	115.27
21	B	821	CLA	O2D-CGD-O1D	-2.08	119.77	123.84
21	6	601	CLA	CHB-C1B-NB	2.08	126.46	124.26
21	B	822	CLA	CHB-C1B-NB	2.08	126.46	124.26
21	4	301	CLA	C4-C3-C5	-2.08	111.77	115.27
21	J	101	CLA	O1D-CGD-CBD	-2.08	120.23	124.48
21	B	831	CLA	CMD-C2D-C1D	2.08	128.38	124.71
21	B	801	CLA	C1-C2-C3	2.08	129.64	126.04
21	4	308	CLA	C4-C3-C5	-2.08	111.77	115.27
21	5	605	CLA	C3C-C4C-NC	-2.08	108.24	110.57
21	A	826	CLA	C1-C2-C3	2.08	129.64	126.04
22	4	315	LUT	C31-C30-C29	2.08	130.28	127.31
21	B	820	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
21	G	202	CLA	O1D-CGD-CBD	-2.08	120.23	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	814	CLA	C3C-C4C-NC	-2.08	108.24	110.57
21	A	807	CLA	CMD-C2D-C1D	2.08	128.38	124.71
21	3	602	CLA	O2D-CGD-O1D	-2.08	119.78	123.84
21	B	829	CLA	O1D-CGD-CBD	-2.08	120.23	124.48
21	A	843	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
21	2	618	CLA	C3C-C4C-NC	-2.08	108.24	110.57
21	B	837	CLA	C3C-C4C-NC	-2.08	108.24	110.57
21	6	609	CLA	CHB-C1B-NB	2.08	126.46	124.26
21	X	604	CLA	O1D-CGD-CBD	-2.08	120.23	124.48
21	6	613	CLA	C3C-C4C-NC	-2.08	108.24	110.57
21	6	603	CLA	O2D-CGD-O1D	-2.08	119.78	123.84
21	3	606	CLA	C2D-C1D-ND	2.08	111.63	110.10
21	A	842	CLA	C2D-C1D-ND	2.08	111.63	110.10
22	5	619	LUT	C31-C30-C29	2.08	130.27	127.31
21	X	618	CLA	O1D-CGD-CBD	-2.08	120.24	124.48
21	1	612	CLA	C3C-C4C-NC	-2.08	108.24	110.57
21	A	809	CLA	C3C-C4C-NC	-2.08	108.24	110.57
21	A	829	CLA	C3C-C4C-NC	-2.08	108.24	110.57
21	A	822	CLA	O1D-CGD-CBD	-2.08	120.24	124.48
21	3	610	CLA	C3C-C4C-NC	-2.07	108.24	110.57
21	4	311	CLA	C3C-C4C-NC	-2.07	108.24	110.57
21	X	612	CLA	C3C-C4C-NC	-2.07	108.24	110.57
21	A	841	CLA	CHB-C1B-NB	2.07	126.45	124.26
21	4	308	CLA	CHB-C1B-NB	2.07	126.45	124.26
21	B	821	CLA	C3C-C4C-NC	-2.07	108.25	110.57
21	3	603	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
21	A	837	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
21	A	818	CLA	C5-C3-C2	2.07	125.31	121.12
20	Z	309	CHL	O2D-CGD-O1D	-2.07	119.78	123.84
21	O	202	CLA	O2D-CGD-O1D	-2.07	119.78	123.84
21	Z	312	CLA	O1D-CGD-CBD	-2.07	120.24	124.48
21	1	602	CLA	C3C-C4C-NC	-2.07	108.25	110.57
21	O	207	CLA	C2A-C1A-CHA	2.07	125.92	122.71
21	5	602	CLA	O1D-CGD-CBD	-2.07	120.25	124.48
20	1	601	CHL	O2A-CGA-O1A	-2.07	118.37	123.59
21	A	833	CLA	C3C-C4C-NC	-2.07	108.25	110.57
21	B	815	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
21	A	804	CLA	O2D-CGD-O1D	-2.07	119.79	123.84
21	5	607	CLA	CHB-C1B-NB	2.07	126.45	124.26
21	B	838	CLA	C3C-C4C-NC	-2.07	108.25	110.57
21	5	608	CLA	CHD-C4C-C3C	2.07	127.88	124.84
23	3	616	XAT	C27-C28-C29	2.07	128.74	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	5	612	CLA	C3C-C4C-NC	-2.07	108.25	110.57
21	5	610	CLA	C3C-C4C-NC	-2.07	108.25	110.57
21	X	612	CLA	C2A-C1A-CHA	2.07	127.47	123.86
21	6	608	CLA	CHB-C1B-NB	2.07	126.44	124.26
21	4	302	CLA	O2A-CGA-O1A	-2.07	118.15	123.30
21	A	832	CLA	C5-C3-C2	2.07	125.30	121.12
21	A	843	CLA	CMD-C2D-C1D	2.07	128.35	124.71
21	A	813	CLA	C4-C3-C5	-2.07	111.80	115.27
21	3	611	CLA	CMD-C2D-C1D	2.07	128.35	124.71
21	5	609	CLA	CMD-C2D-C1D	2.07	128.35	124.71
21	A	813	CLA	CMD-C2D-C1D	2.07	128.35	124.71
21	B	840	CLA	C3C-C4C-NC	-2.07	108.25	110.57
22	Z	314	LUT	C31-C30-C29	2.06	130.26	127.31
21	A	820	CLA	O1D-CGD-CBD	-2.06	120.26	124.48
21	5	613	CLA	CMD-C2D-C1D	2.06	128.35	124.71
21	A	817	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
22	X	615	LUT	C8-C9-C10	2.06	122.11	118.94
21	3	612	CLA	C3C-C4C-NC	-2.06	108.26	110.57
21	A	826	CLA	C3C-C4C-NC	-2.06	108.26	110.57
21	A	812	CLA	C4D-CHA-C1A	2.06	123.76	121.25
21	1	610	CLA	C3C-C4C-NC	-2.06	108.26	110.57
21	B	835	CLA	C3C-C4C-NC	-2.06	108.26	110.57
21	O	202	CLA	CMD-C2D-C1D	2.06	128.34	124.71
21	4	302	CLA	CMD-C2D-C1D	2.06	128.34	124.71
20	X	606	CHL	OMC-CMC-C2C	-2.06	121.73	125.03
22	2	615	LUT	C31-C30-C29	2.06	130.25	127.31
21	6	612	CLA	CHB-C1B-NB	2.06	126.44	124.26
21	5	611	CLA	CHB-C1B-NB	2.06	126.44	124.26
21	3	614	CLA	C3C-C4C-NC	-2.06	108.26	110.57
21	B	807	CLA	C4-C3-C5	-2.06	111.81	115.27
21	4	311	CLA	O1D-CGD-CBD	-2.06	120.28	124.48
21	O	203	CLA	CHB-C1B-NB	2.06	126.43	124.26
21	1	613	CLA	C3C-C4C-NC	-2.06	108.27	110.57
21	B	828	CLA	CHB-C1B-NB	2.06	126.43	124.26
21	5	609	CLA	O1D-CGD-CBD	-2.06	120.28	124.48
21	B	822	CLA	C2C-C1C-NC	-2.05	108.05	109.97
22	1	615	LUT	C12-C13-C14	2.05	122.09	118.94
21	O	203	CLA	C3C-C4C-NC	-2.05	108.27	110.57
21	J	102	CLA	C2A-C1A-CHA	2.05	127.45	123.86
21	5	612	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
21	A	802	CLA	C1-C2-C3	2.05	129.59	126.04
21	1	611	CLA	CMD-C2D-C1D	2.05	128.33	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	L	301	CLA	C2D-C1D-ND	2.05	111.62	110.10
21	Z	313	CLA	C3C-C4C-NC	-2.05	108.27	110.57
21	A	801	CLA	CMD-C2D-C1D	2.05	128.33	124.71
21	B	801	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
21	A	831	CLA	C1-C2-C3	2.05	130.07	126.75
21	X	610	CLA	O1D-CGD-CBD	-2.05	120.29	124.48
21	A	840	CLA	CHB-C1B-NB	2.05	126.43	124.26
21	A	816	CLA	CMD-C2D-C1D	2.05	128.32	124.71
21	5	612	CLA	C2D-C1D-ND	2.05	111.61	110.10
21	L	305	CLA	CMD-C2D-C1D	2.05	128.32	124.71
21	2	604	CLA	C3C-C4C-NC	-2.05	108.27	110.57
20	6	605	CHL	O2A-CGA-O1A	-2.05	118.42	123.59
21	1	614	CLA	C3C-C4C-NC	-2.05	108.28	110.57
21	A	806	CLA	CMD-C2D-C1D	2.05	128.32	124.71
21	B	812	CLA	C4-C3-C5	-2.05	111.83	115.27
21	Y	614	CLA	C3C-C4C-NC	-2.05	108.28	110.57
21	Z	313	CLA	O1D-CGD-CBD	-2.05	120.30	124.48
23	4	316	XAT	C27-C28-C29	2.05	128.71	125.53
21	Y	614	CLA	O2A-CGA-O1A	-2.05	118.20	123.30
21	2	612	CLA	CMD-C2D-C1D	2.05	128.32	124.71
21	3	605	CLA	CHB-C1B-NB	2.05	126.42	124.26
21	B	837	CLA	O2D-CGD-O1D	-2.05	119.84	123.84
21	Y	613	CLA	C4-C3-C5	-2.05	111.83	115.27
21	A	815	CLA	O2D-CGD-O1D	-2.05	119.84	123.84
21	B	802	CLA	O1D-CGD-CBD	-2.04	120.30	124.48
21	Y	611	CLA	C3C-C4C-NC	-2.04	108.28	110.57
21	G	204	CLA	CMD-C2D-C1D	2.04	128.32	124.71
21	B	826	CLA	O1D-CGD-CBD	-2.04	120.30	124.48
21	A	804	CLA	CMD-C2D-C1D	2.04	128.31	124.71
20	2	607	CHL	O2A-CGA-O1A	-2.04	118.44	123.59
20	Y	607	CHL	O2A-CGA-CBA	2.04	120.59	114.03
21	4	308	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
21	3	604	CLA	O2D-CGD-O1D	-2.04	119.85	123.84
21	A	833	CLA	CMD-C2D-C1D	2.04	128.31	124.71
21	G	203	CLA	CMD-C2D-C1D	2.04	128.31	124.71
21	B	810	CLA	C4-C3-C5	-2.04	111.84	115.27
21	5	604	CLA	C3C-C4C-NC	-2.04	108.29	110.57
22	X	615	LUT	C1-C6-C7	2.04	121.54	115.78
21	Z	311	CLA	C3C-C4C-NC	-2.03	108.29	110.57
21	A	825	CLA	C3C-C4C-NC	-2.03	108.29	110.57
21	J	102	CLA	CMD-C2D-C1D	2.03	128.30	124.71
21	5	611	CLA	CMD-C2D-C1D	2.03	128.30	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	817	CLA	CMD-C2D-C1D	2.03	128.30	124.71
20	4	305	CHL	O2A-CGA-CBA	2.03	120.56	114.03
21	A	815	CLA	CMD-C2D-C1D	2.03	128.29	124.71
21	Y	613	CLA	CMD-C2D-C1D	2.03	128.29	124.71
21	A	834	CLA	C3C-C4C-NC	-2.03	108.29	110.57
21	1	603	CLA	C4-C3-C5	-2.03	111.85	115.27
21	3	609	CLA	CHB-C1B-NB	2.03	126.41	124.26
21	5	607	CLA	C3C-C4C-NC	-2.03	108.29	110.57
21	6	609	CLA	C3C-C4C-NC	-2.03	108.29	110.57
21	B	807	CLA	C3C-C4C-NC	-2.03	108.29	110.57
21	A	827	CLA	O1D-CGD-CBD	-2.03	120.33	124.48
20	Y	607	CHL	O2D-CGD-O1D	-2.03	119.87	123.84
22	X	614	LUT	C1-C6-C7	2.03	121.52	115.78
21	X	603	CLA	CMD-C2D-C1D	2.03	128.29	124.71
21	A	829	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
21	3	605	CLA	C3C-C4C-NC	-2.03	108.30	110.57
21	4	307	CLA	C3C-C4C-NC	-2.03	108.30	110.57
21	B	821	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
21	3	612	CLA	O2A-CGA-O1A	-2.03	118.24	123.30
21	B	817	CLA	C1-C2-C3	2.03	129.55	126.04
21	3	611	CLA	O1D-CGD-CBD	-2.03	120.33	124.48
21	A	826	CLA	CMD-C2D-C1D	2.03	128.29	124.71
21	4	303	CLA	O1D-CGD-CBD	-2.03	120.34	124.48
21	4	303	CLA	CMD-C2D-C1D	2.03	128.28	124.71
21	A	813	CLA	C2D-C1D-ND	2.03	111.60	110.10
21	B	814	CLA	CHB-C1B-NB	2.03	126.40	124.26
21	O	203	CLA	CMD-C2D-C1D	2.02	128.28	124.71
23	O	208	XAT	C18-C5-C4	-2.02	112.00	114.28
21	5	605	CLA	CBD-CHA-C1A	2.02	130.88	128.50
21	B	807	CLA	C2D-C1D-ND	2.02	111.59	110.10
21	3	617	CLA	C4D-CHA-C1A	2.02	123.71	121.25
21	A	840	CLA	O1D-CGD-CBD	-2.02	120.34	124.48
21	Y	602	CLA	C12-C11-C10	-2.02	103.94	113.24
21	5	613	CLA	C2D-C1D-ND	2.02	111.59	110.10
24	A	849	BCR	C7-C8-C9	-2.02	123.18	126.23
21	4	312	CLA	C3C-C4C-NC	-2.02	108.30	110.57
21	B	826	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
21	1	602	CLA	O2D-CGD-O1D	-2.02	119.89	123.84
21	O	207	CLA	CMD-C2D-C1D	2.02	128.27	124.71
21	1	611	CLA	C3C-C4C-NC	-2.02	108.31	110.57
21	5	611	CLA	C3C-C4C-NC	-2.02	108.31	110.57
21	B	819	CLA	C3C-C4C-NC	-2.02	108.31	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	X	602	CLA	C3C-C4C-NC	-2.02	108.31	110.57
21	X	618	CLA	CED-O2D-CGD	2.02	120.50	115.94
21	2	604	CLA	C2D-C1D-ND	2.02	111.59	110.10
21	L	305	CLA	C2D-C1D-ND	2.02	111.59	110.10
21	X	609	CLA	C2D-C1D-ND	2.02	111.59	110.10
20	6	605	CHL	O2D-CGD-O1D	-2.02	119.89	123.84
21	1	612	CLA	O1D-CGD-CBD	-2.02	120.36	124.48
21	4	309	CLA	C3C-C4C-NC	-2.02	108.31	110.57
21	A	803	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
21	X	613	CLA	CMD-C2D-C1D	2.02	128.26	124.71
21	B	834	CLA	C3C-C4C-NC	-2.02	108.31	110.57
21	G	202	CLA	C3C-C4C-NC	-2.02	108.31	110.57
21	G	204	CLA	C3C-C4C-NC	-2.02	108.31	110.57
21	5	609	CLA	C2D-C1D-ND	2.02	111.59	110.10
21	1	609	CLA	C4-C3-C5	-2.01	111.88	115.27
21	3	611	CLA	CHB-C1B-NB	2.01	126.39	124.26
21	1	612	CLA	CMD-C2D-C1D	2.01	128.26	124.71
21	B	840	CLA	CMD-C2D-C1D	2.01	128.26	124.71
21	2	603	CLA	CMD-C2D-C1D	2.01	128.26	124.71
21	2	608	CLA	O1D-CGD-CBD	-2.01	120.36	124.48
21	4	303	CLA	C2D-C1D-ND	2.01	111.59	110.10
21	4	313	CLA	CHB-C1B-NB	2.01	126.39	124.26
21	G	203	CLA	O1D-CGD-CBD	-2.01	120.37	124.48
21	2	604	CLA	CMD-C2D-C1D	2.01	128.25	124.71
21	X	610	CLA	CMD-C2D-C1D	2.01	128.25	124.71
21	A	804	CLA	C2D-C1D-ND	2.01	111.58	110.10
21	O	206	CLA	C2D-C1D-ND	2.01	111.58	110.10
21	Z	310	CLA	CMD-C2D-C1D	2.01	128.25	124.71
21	6	603	CLA	O2A-CGA-CBA	2.01	120.48	114.03
21	3	611	CLA	CED-O2D-CGD	2.01	120.48	115.94
21	B	805	CLA	C4-C3-C5	-2.01	111.89	115.27
21	1	603	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
21	A	824	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
21	1	611	CLA	O1D-CGD-CBD	-2.01	120.38	124.48
21	6	609	CLA	O1D-CGD-CBD	-2.01	120.38	124.48
21	X	602	CLA	C2D-C1D-ND	2.01	111.58	110.10
21	6	611	CLA	C3C-C4C-NC	-2.01	108.32	110.57
21	A	803	CLA	C2A-C1A-CHA	2.00	127.36	123.86
21	K	204	CLA	CMD-C2D-C1D	2.00	128.25	124.71
21	5	609	CLA	C3C-C4C-NC	-2.00	108.32	110.57
21	B	825	CLA	C4D-CHA-C1A	2.00	123.69	121.25
21	X	618	CLA	C2D-C1D-ND	2.00	111.58	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	810	CLA	CHB-C1B-NB	2.00	126.38	124.26
21	L	301	CLA	C1-C2-C3	2.00	129.51	126.04
21	B	803	CLA	CAA-C2A-C3A	-2.00	111.43	116.10
20	6	607	CHL	O2D-CGD-O1D	-2.00	119.92	123.84
21	A	817	CLA	CHB-C1B-NB	2.00	126.38	124.26
21	2	609	CLA	C4-C3-C5	-2.00	111.90	115.27
21	6	602	CLA	C2D-C1D-ND	2.00	111.58	110.10
21	A	821	CLA	O2D-CGD-O1D	-2.00	119.92	123.84
21	L	304	CLA	O1D-CGD-CBD	-2.00	120.39	124.48
21	K	201	CLA	CMD-C2D-C1D	2.00	128.24	124.71
21	B	823	CLA	O2D-CGD-O1D	-2.00	119.93	123.84
21	B	810	CLA	O2D-CGD-O1D	-2.00	119.93	123.84
21	A	803	CLA	C3C-C4C-NC	-2.00	108.33	110.57

There are no chirality outliers.

All (2265) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	1	606	CHL	C4C-C3C-CAC-CBC
20	2	605	CHL	C1A-C2A-CAA-CBA
20	2	605	CHL	C3A-C2A-CAA-CBA
20	2	606	CHL	C1A-C2A-CAA-CBA
20	2	606	CHL	C3A-C2A-CAA-CBA
20	2	606	CHL	C1C-C2C-CMC-OMC
20	2	606	CHL	C3C-C2C-CMC-OMC
20	2	606	CHL	C4C-C3C-CAC-CBC
20	2	614	CHL	CBD-CGD-O2D-CED
20	3	608	CHL	C3A-C2A-CAA-CBA
20	4	304	CHL	C3C-C2C-CMC-OMC
20	4	305	CHL	C1A-C2A-CAA-CBA
20	4	305	CHL	C4C-C3C-CAC-CBC
20	4	306	CHL	C3A-C2A-CAA-CBA
20	4	306	CHL	O2A-C1-C2-C3
20	4	314	CHL	C1A-C2A-CAA-CBA
20	4	314	CHL	C3A-C2A-CAA-CBA
20	5	601	CHL	C1A-C2A-CAA-CBA
20	5	601	CHL	C3A-C2A-CAA-CBA
20	6	605	CHL	C1C-C2C-CMC-OMC
20	6	606	CHL	C3C-C2C-CMC-OMC
20	6	606	CHL	CHA-CBD-CGD-O1D
20	6	606	CHL	CBD-CGD-O2D-CED
20	6	607	CHL	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
20	X	601	CHL	C3A-C2A-CAA-CBA
20	X	601	CHL	C2A-CAA-CBA-CGA
20	X	601	CHL	C3C-C2C-CMC-OMC
20	X	606	CHL	CBD-CGD-O2D-CED
20	X	608	CHL	C1C-C2C-CMC-OMC
20	X	608	CHL	C3C-C2C-CMC-OMC
20	Y	601	CHL	C1C-C2C-CMC-OMC
20	Y	601	CHL	C3C-C2C-CMC-OMC
20	Y	605	CHL	C1C-C2C-CMC-OMC
20	Y	605	CHL	CBD-CGD-O2D-CED
20	Y	607	CHL	C1A-C2A-CAA-CBA
20	Y	608	CHL	C1C-C2C-CMC-OMC
20	Y	608	CHL	C3C-C2C-CMC-OMC
20	Y	608	CHL	CBD-CGD-O2D-CED
20	Y	619	CHL	CBD-CGD-O2D-CED
20	Z	301	CHL	C1A-C2A-CAA-CBA
20	Z	301	CHL	C3A-C2A-CAA-CBA
20	Z	301	CHL	C1C-C2C-CMC-OMC
20	Z	302	CHL	CBD-CGD-O2D-CED
20	Z	302	CHL	O1D-CGD-O2D-CED
20	Z	306	CHL	C1C-C2C-CMC-OMC
20	Z	306	CHL	C3C-C2C-CMC-OMC
20	Z	306	CHL	CBD-CGD-O2D-CED
20	Z	307	CHL	C1C-C2C-CMC-OMC
20	Z	307	CHL	C3C-C2C-CMC-OMC
20	Z	307	CHL	CBD-CGD-O2D-CED
20	Z	308	CHL	CBD-CGD-O2D-CED
20	Z	309	CHL	C4C-C3C-CAC-CBC
21	1	602	CLA	CBD-CGD-O2D-CED
21	1	602	CLA	C4-C3-C5-C6
21	1	605	CLA	CBD-CGD-O2D-CED
21	1	608	CLA	CBD-CGD-O2D-CED
21	1	609	CLA	C2-C3-C5-C6
21	1	611	CLA	CBD-CGD-O2D-CED
21	1	611	CLA	O1D-CGD-O2D-CED
21	1	612	CLA	C1-C2-C3-C4
21	2	602	CLA	CBD-CGD-O2D-CED
21	2	604	CLA	CHA-CBD-CGD-O1D
21	2	604	CLA	C1-C2-C3-C4
21	2	608	CLA	C3A-C2A-CAA-CBA
21	2	610	CLA	CHA-CBD-CGD-O1D
21	2	611	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	2	612	CLA	C1-C2-C3-C5
21	2	618	CLA	CHA-CBD-CGD-O1D
21	2	618	CLA	CAD-CBD-CGD-O1D
21	3	602	CLA	CBD-CGD-O2D-CED
21	3	604	CLA	C1A-C2A-CAA-CBA
21	3	604	CLA	C3A-C2A-CAA-CBA
21	3	604	CLA	CHA-CBD-CGD-O1D
21	3	605	CLA	CBA-CGA-O2A-C1
21	3	605	CLA	O1A-CGA-O2A-C1
21	3	606	CLA	C1A-C2A-CAA-CBA
21	3	607	CLA	C1A-C2A-CAA-CBA
21	3	607	CLA	C3A-C2A-CAA-CBA
21	3	609	CLA	C1A-C2A-CAA-CBA
21	3	611	CLA	C2A-CAA-CBA-CGA
21	3	611	CLA	CBD-CGD-O2D-CED
21	3	613	CLA	C2B-C3B-CAB-CBB
21	3	613	CLA	C4B-C3B-CAB-CBB
21	3	617	CLA	C1-C2-C3-C5
21	3	617	CLA	C4-C3-C5-C6
21	4	301	CLA	CHA-CBD-CGD-O1D
21	4	302	CLA	CBD-CGD-O2D-CED
21	4	303	CLA	C1A-C2A-CAA-CBA
21	4	303	CLA	C3A-C2A-CAA-CBA
21	4	307	CLA	C1A-C2A-CAA-CBA
21	4	307	CLA	C3A-C2A-CAA-CBA
21	4	309	CLA	C1A-C2A-CAA-CBA
21	4	311	CLA	CHA-CBD-CGD-O1D
21	4	312	CLA	C2A-CAA-CBA-CGA
21	5	602	CLA	CBD-CGD-O2D-CED
21	5	602	CLA	C4-C3-C5-C6
21	5	603	CLA	CBD-CGD-O2D-CED
21	5	608	CLA	C1A-C2A-CAA-CBA
21	5	608	CLA	C3A-C2A-CAA-CBA
21	5	608	CLA	CBD-CGD-O2D-CED
21	5	609	CLA	C2B-C3B-CAB-CBB
21	5	609	CLA	C4B-C3B-CAB-CBB
21	5	610	CLA	C2A-CAA-CBA-CGA
21	5	610	CLA	CBD-CGD-O2D-CED
21	5	611	CLA	C1A-C2A-CAA-CBA
21	5	611	CLA	C3A-C2A-CAA-CBA
21	5	611	CLA	CBD-CGD-O2D-CED
21	5	611	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	5	612	CLA	C1-C2-C3-C4
21	5	612	CLA	C1-C2-C3-C5
21	5	613	CLA	CBD-CGD-O2D-CED
21	5	614	CLA	C1A-C2A-CAA-CBA
21	5	614	CLA	C2B-C3B-CAB-CBB
21	5	614	CLA	C4B-C3B-CAB-CBB
21	6	601	CLA	CHA-CBD-CGD-O1D
21	6	601	CLA	CAD-CBD-CGD-O1D
21	6	602	CLA	C2-C3-C5-C6
21	6	603	CLA	C1A-C2A-CAA-CBA
21	6	608	CLA	C1A-C2A-CAA-CBA
21	6	608	CLA	C3A-C2A-CAA-CBA
21	6	610	CLA	C1A-C2A-CAA-CBA
21	6	612	CLA	C1-C2-C3-C5
21	6	614	CLA	CHA-CBD-CGD-O1D
21	6	614	CLA	CBD-CGD-O2D-CED
21	A	801	CLA	C1A-C2A-CAA-CBA
21	A	801	CLA	C3A-C2A-CAA-CBA
21	A	801	CLA	CBD-CGD-O2D-CED
21	A	801	CLA	O1D-CGD-O2D-CED
21	A	801	CLA	C1-C2-C3-C5
21	A	801	CLA	C4-C3-C5-C6
21	A	802	CLA	C2B-C3B-CAB-CBB
21	A	802	CLA	C4B-C3B-CAB-CBB
21	A	804	CLA	CHA-CBD-CGD-O1D
21	A	804	CLA	C2-C3-C5-C6
21	A	805	CLA	C1A-C2A-CAA-CBA
21	A	805	CLA	C3A-C2A-CAA-CBA
21	A	806	CLA	C1A-C2A-CAA-CBA
21	A	806	CLA	C3A-C2A-CAA-CBA
21	A	806	CLA	CBA-CGA-O2A-C1
21	A	806	CLA	O1A-CGA-O2A-C1
21	A	806	CLA	C1-C2-C3-C5
21	A	807	CLA	C2B-C3B-CAB-CBB
21	A	807	CLA	C4B-C3B-CAB-CBB
21	A	809	CLA	CHA-CBD-CGD-O1D
21	A	810	CLA	C3A-C2A-CAA-CBA
21	A	812	CLA	C1-C2-C3-C5
21	A	813	CLA	C2B-C3B-CAB-CBB
21	A	813	CLA	C4B-C3B-CAB-CBB
21	A	814	CLA	CHA-CBD-CGD-O1D
21	A	814	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	A	815	CLA	C1A-C2A-CAA-CBA
21	A	815	CLA	C3A-C2A-CAA-CBA
21	A	817	CLA	C1-C2-C3-C4
21	A	817	CLA	C1-C2-C3-C5
21	A	818	CLA	C1A-C2A-CAA-CBA
21	A	818	CLA	C3A-C2A-CAA-CBA
21	A	818	CLA	CHA-CBD-CGD-O1D
21	A	819	CLA	C3A-C2A-CAA-CBA
21	A	820	CLA	C1A-C2A-CAA-CBA
21	A	820	CLA	C3A-C2A-CAA-CBA
21	A	820	CLA	C2B-C3B-CAB-CBB
21	A	820	CLA	C4B-C3B-CAB-CBB
21	A	821	CLA	CBD-CGD-O2D-CED
21	A	822	CLA	C1A-C2A-CAA-CBA
21	A	822	CLA	C3A-C2A-CAA-CBA
21	A	824	CLA	C3A-C2A-CAA-CBA
21	A	825	CLA	O1A-CGA-O2A-C1
21	A	825	CLA	C2B-C3B-CAB-CBB
21	A	825	CLA	C4B-C3B-CAB-CBB
21	A	828	CLA	C1-C2-C3-C5
21	A	828	CLA	C4-C3-C5-C6
21	A	829	CLA	CHA-CBD-CGD-O1D
21	A	829	CLA	CHA-CBD-CGD-O2D
21	A	829	CLA	C11-C12-C13-C14
21	A	831	CLA	C1A-C2A-CAA-CBA
21	A	831	CLA	C3A-C2A-CAA-CBA
21	A	837	CLA	C2B-C3B-CAB-CBB
21	A	837	CLA	C4B-C3B-CAB-CBB
21	A	837	CLA	C2-C3-C5-C6
21	A	840	CLA	C2B-C3B-CAB-CBB
21	A	840	CLA	C4B-C3B-CAB-CBB
21	A	840	CLA	CHA-CBD-CGD-O2D
21	A	840	CLA	C1-C2-C3-C4
21	A	841	CLA	C4-C3-C5-C6
21	A	842	CLA	C2B-C3B-CAB-CBB
21	A	842	CLA	C4B-C3B-CAB-CBB
21	A	843	CLA	CBA-CGA-O2A-C1
21	A	843	CLA	C1-C2-C3-C5
21	B	802	CLA	C1A-C2A-CAA-CBA
21	B	802	CLA	C3A-C2A-CAA-CBA
21	B	802	CLA	C2B-C3B-CAB-CBB
21	B	802	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
21	B	802	CLA	C1-C2-C3-C5
21	B	804	CLA	C3A-C2A-CAA-CBA
21	B	804	CLA	CHA-CBD-CGD-O1D
21	B	804	CLA	CHA-CBD-CGD-O2D
21	B	804	CLA	CAD-CBD-CGD-O1D
21	B	804	CLA	CAD-CBD-CGD-O2D
21	B	806	CLA	CHA-CBD-CGD-O1D
21	B	806	CLA	CHA-CBD-CGD-O2D
21	B	807	CLA	C11-C12-C13-C14
21	B	808	CLA	CHA-CBD-CGD-O1D
21	B	809	CLA	C1A-C2A-CAA-CBA
21	B	810	CLA	C1A-C2A-CAA-CBA
21	B	810	CLA	C3A-C2A-CAA-CBA
21	B	812	CLA	C3A-C2A-CAA-CBA
21	B	812	CLA	C2B-C3B-CAB-CBB
21	B	812	CLA	C4B-C3B-CAB-CBB
21	B	812	CLA	C1-C2-C3-C5
21	B	813	CLA	C2B-C3B-CAB-CBB
21	B	813	CLA	C4B-C3B-CAB-CBB
21	B	813	CLA	CHA-CBD-CGD-O1D
21	B	813	CLA	CHA-CBD-CGD-O2D
21	B	813	CLA	CBD-CGD-O2D-CED
21	B	813	CLA	C1-C2-C3-C5
21	B	814	CLA	C1A-C2A-CAA-CBA
21	B	814	CLA	C3A-C2A-CAA-CBA
21	B	814	CLA	CHA-CBD-CGD-O1D
21	B	816	CLA	O2A-C1-C2-C3
21	B	816	CLA	C1-C2-C3-C4
21	B	816	CLA	C1-C2-C3-C5
21	B	816	CLA	C11-C10-C8-C9
21	B	817	CLA	C3A-C2A-CAA-CBA
21	B	817	CLA	C1-C2-C3-C5
21	B	817	CLA	C6-C7-C8-C9
21	B	818	CLA	C1A-C2A-CAA-CBA
21	B	818	CLA	CHA-CBD-CGD-O1D
21	B	818	CLA	CHA-CBD-CGD-O2D
21	B	819	CLA	C1A-C2A-CAA-CBA
21	B	820	CLA	CBA-CGA-O2A-C1
21	B	820	CLA	O1A-CGA-O2A-C1
21	B	820	CLA	C1-C2-C3-C4
21	B	821	CLA	C1A-C2A-CAA-CBA
21	B	821	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
21	B	822	CLA	CBD-CGD-O2D-CED
21	B	823	CLA	C2B-C3B-CAB-CBB
21	B	823	CLA	C4B-C3B-CAB-CBB
21	B	823	CLA	CHA-CBD-CGD-O1D
21	B	823	CLA	CAD-CBD-CGD-O1D
21	B	824	CLA	C2B-C3B-CAB-CBB
21	B	824	CLA	C4B-C3B-CAB-CBB
21	B	826	CLA	C3A-C2A-CAA-CBA
21	B	826	CLA	C2B-C3B-CAB-CBB
21	B	826	CLA	C4B-C3B-CAB-CBB
21	B	827	CLA	C1A-C2A-CAA-CBA
21	B	827	CLA	C3A-C2A-CAA-CBA
21	B	827	CLA	C2A-CAA-CBA-CGA
21	B	827	CLA	CHA-CBD-CGD-O1D
21	B	827	CLA	CHA-CBD-CGD-O2D
21	B	828	CLA	C11-C10-C8-C7
21	B	829	CLA	C1A-C2A-CAA-CBA
21	B	829	CLA	C3A-C2A-CAA-CBA
21	B	831	CLA	C1A-C2A-CAA-CBA
21	B	834	CLA	C3A-C2A-CAA-CBA
21	B	837	CLA	C1A-C2A-CAA-CBA
21	B	837	CLA	CHA-CBD-CGD-O1D
21	B	839	CLA	C1A-C2A-CAA-CBA
21	B	839	CLA	C3A-C2A-CAA-CBA
21	B	839	CLA	CHA-CBD-CGD-O1D
21	B	839	CLA	CHA-CBD-CGD-O2D
21	B	840	CLA	C1A-C2A-CAA-CBA
21	B	840	CLA	C3A-C2A-CAA-CBA
21	B	840	CLA	C14-C13-C15-C16
21	F	304	CLA	CBD-CGD-O2D-CED
21	G	202	CLA	CBD-CGD-O2D-CED
21	G	203	CLA	C1A-C2A-CAA-CBA
21	G	203	CLA	C3A-C2A-CAA-CBA
21	G	204	CLA	CBD-CGD-O2D-CED
21	H	201	CLA	C1A-C2A-CAA-CBA
21	H	201	CLA	C1-C2-C3-C4
21	J	102	CLA	C1A-C2A-CAA-CBA
21	J	102	CLA	C3A-C2A-CAA-CBA
21	J	102	CLA	CAD-CBD-CGD-O1D
21	K	203	CLA	C3A-C2A-CAA-CBA
21	L	303	CLA	C1A-C2A-CAA-CBA
21	L	303	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
21	L	304	CLA	C2-C3-C5-C6
21	L	305	CLA	CHA-CBD-CGD-O1D
21	L	305	CLA	CHA-CBD-CGD-O2D
21	O	202	CLA	C1A-C2A-CAA-CBA
21	O	202	CLA	C3A-C2A-CAA-CBA
21	O	202	CLA	C2B-C3B-CAB-CBB
21	O	202	CLA	C4B-C3B-CAB-CBB
21	O	203	CLA	O2A-C1-C2-C3
21	X	602	CLA	C1A-C2A-CAA-CBA
21	X	602	CLA	C3A-C2A-CAA-CBA
21	X	602	CLA	C2B-C3B-CAB-CBB
21	X	602	CLA	C4B-C3B-CAB-CBB
21	X	603	CLA	C1A-C2A-CAA-CBA
21	X	603	CLA	C3A-C2A-CAA-CBA
21	X	603	CLA	CHA-CBD-CGD-O1D
21	X	609	CLA	C1A-C2A-CAA-CBA
21	X	609	CLA	C3A-C2A-CAA-CBA
21	X	609	CLA	C2B-C3B-CAB-CBB
21	X	609	CLA	C4B-C3B-CAB-CBB
21	X	609	CLA	CBD-CGD-O2D-CED
21	X	610	CLA	C1A-C2A-CAA-CBA
21	X	610	CLA	C3A-C2A-CAA-CBA
21	X	610	CLA	CHA-CBD-CGD-O1D
21	X	610	CLA	CHA-CBD-CGD-O2D
21	X	612	CLA	CBD-CGD-O2D-CED
21	X	613	CLA	C2B-C3B-CAB-CBB
21	X	613	CLA	C4B-C3B-CAB-CBB
21	X	613	CLA	CBD-CGD-O2D-CED
21	X	618	CLA	C1A-C2A-CAA-CBA
21	X	618	CLA	C3A-C2A-CAA-CBA
21	Y	602	CLA	C2B-C3B-CAB-CBB
21	Y	602	CLA	C4B-C3B-CAB-CBB
21	Y	602	CLA	CHA-CBD-CGD-O2D
21	Y	602	CLA	C1-C2-C3-C5
21	Y	602	CLA	C12-C13-C15-C16
21	Y	603	CLA	C1A-C2A-CAA-CBA
21	Y	603	CLA	C3A-C2A-CAA-CBA
21	Y	604	CLA	C1A-C2A-CAA-CBA
21	Y	604	CLA	C3A-C2A-CAA-CBA
21	Y	604	CLA	CHA-CBD-CGD-O1D
21	Y	604	CLA	CAD-CBD-CGD-O1D
21	Y	610	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
21	Y	610	CLA	C4B-C3B-CAB-CBB
21	Y	611	CLA	CHA-CBD-CGD-O2D
21	Y	612	CLA	CBD-CGD-O2D-CED
21	Y	613	CLA	CBD-CGD-O2D-CED
21	Z	303	CLA	C1A-C2A-CAA-CBA
21	Z	303	CLA	C3A-C2A-CAA-CBA
21	Z	303	CLA	C2B-C3B-CAB-CBB
21	Z	303	CLA	C4B-C3B-CAB-CBB
21	Z	304	CLA	C1A-C2A-CAA-CBA
21	Z	304	CLA	C3A-C2A-CAA-CBA
21	Z	304	CLA	CHA-CBD-CGD-O2D
21	Z	304	CLA	CAD-CBD-CGD-O1D
21	Z	305	CLA	C1A-C2A-CAA-CBA
21	Z	305	CLA	C3A-C2A-CAA-CBA
21	Z	305	CLA	C2B-C3B-CAB-CBB
21	Z	305	CLA	C4B-C3B-CAB-CBB
21	Z	305	CLA	C1-C2-C3-C5
21	Z	310	CLA	C3A-C2A-CAA-CBA
21	Z	310	CLA	C2B-C3B-CAB-CBB
21	Z	310	CLA	C4B-C3B-CAB-CBB
21	Z	310	CLA	CBD-CGD-O2D-CED
21	Z	311	CLA	CHA-CBD-CGD-O2D
21	Z	311	CLA	CBD-CGD-O2D-CED
21	Z	312	CLA	C1A-C2A-CAA-CBA
21	Z	312	CLA	C3A-C2A-CAA-CBA
21	Z	313	CLA	C2B-C3B-CAB-CBB
21	Z	313	CLA	C4B-C3B-CAB-CBB
21	Z	313	CLA	CBD-CGD-O2D-CED
22	3	615	LUT	C27-C28-C29-C30
22	3	615	LUT	C27-C28-C29-C39
22	X	615	LUT	C27-C28-C29-C30
22	X	615	LUT	C27-C28-C29-C39
22	Z	315	LUT	C27-C28-C29-C30
22	Z	315	LUT	C27-C28-C29-C39
24	2	619	BCR	C7-C8-C9-C10
24	2	619	BCR	C11-C12-C13-C14
24	2	619	BCR	C11-C12-C13-C35
24	2	619	BCR	C17-C18-C19-C20
24	2	619	BCR	C36-C18-C19-C20
24	6	620	BCR	C7-C8-C9-C10
24	6	620	BCR	C7-C8-C9-C34
24	6	620	BCR	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
24	6	620	BCR	C11-C12-C13-C35
24	6	620	BCR	C17-C18-C19-C20
24	6	620	BCR	C36-C18-C19-C20
24	A	845	BCR	C23-C24-C25-C26
24	A	845	BCR	C23-C24-C25-C30
24	A	846	BCR	C36-C18-C19-C20
24	A	847	BCR	C21-C22-C23-C24
24	A	847	BCR	C37-C22-C23-C24
24	A	849	BCR	C1-C6-C7-C8
24	A	849	BCR	C11-C12-C13-C14
24	A	849	BCR	C11-C12-C13-C35
24	A	854	BCR	C23-C24-C25-C26
24	A	854	BCR	C23-C24-C25-C30
24	B	843	BCR	C7-C8-C9-C10
24	B	843	BCR	C7-C8-C9-C34
24	B	848	BCR	C22-C23-C24-C25
24	J	103	BCR	C23-C24-C25-C30
24	K	205	BCR	C1-C6-C7-C8
24	K	205	BCR	C23-C24-C25-C26
24	L	302	BCR	C21-C22-C23-C24
24	L	302	BCR	C37-C22-C23-C24
24	L	306	BCR	C21-C22-C23-C24
24	L	306	BCR	C23-C24-C25-C26
24	L	306	BCR	C23-C24-C25-C30
24	L	307	BCR	C23-C24-C25-C26
24	L	307	BCR	C23-C24-C25-C30
24	L	308	BCR	C1-C6-C7-C8
24	O	205	BCR	C1-C6-C7-C8
25	1	620	LHG	C3-O3-P-O5
25	1	620	LHG	C4-O6-P-O4
25	1	620	LHG	C4-O6-P-O5
25	1	620	LHG	O9-C7-O7-C5
25	1	620	LHG	C8-C7-O7-C5
25	1	620	LHG	O10-C23-O8-C6
25	1	620	LHG	C24-C23-O8-C6
25	2	617	LHG	C4-O6-P-O4
25	5	618	LHG	C4-O6-P-O3
25	5	618	LHG	C4-O6-P-O5
25	A	851	LHG	C3-O3-P-O4
25	A	851	LHG	C3-O3-P-O5
25	A	851	LHG	C3-O3-P-O6
25	A	853	LHG	O10-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
25	A	853	LHG	C24-C23-O8-C6
25	X	617	LHG	C3-O3-P-O4
25	X	617	LHG	C3-O3-P-O5
25	Y	618	LHG	O10-C23-O8-C6
25	Y	618	LHG	C24-C23-O8-C6
25	Z	317	LHG	C3-O3-P-O5
26	4	318	LMG	C2-C1-O1-C7
26	4	318	LMG	O6-C1-O1-C7
26	6	619	LMG	O6-C1-O1-C7
26	B	850	LMG	C2-C1-O1-C7
26	B	850	LMG	O6-C1-O1-C7
26	B	850	LMG	O1-C7-C8-O7
26	B	850	LMG	O9-C10-O7-C8
26	B	850	LMG	C11-C10-O7-C8
26	B	850	LMG	O10-C28-O8-C9
26	B	850	LMG	C29-C28-O8-C9
26	F	306	LMG	C2-C1-O1-C7
26	F	306	LMG	O6-C1-O1-C7
26	F	306	LMG	O1-C7-C8-O7
26	F	306	LMG	O9-C10-O7-C8
26	F	306	LMG	C11-C10-O7-C8
26	F	306	LMG	O10-C28-O8-C9
26	F	306	LMG	C29-C28-O8-C9
26	G	206	LMG	O6-C1-O1-C7
26	G	206	LMG	O10-C28-O8-C9
26	G	206	LMG	C29-C28-O8-C9
27	A	852	LMT	C2'-C1'-O1'-C1
27	A	852	LMT	O5'-C1'-O1'-C1
27	A	852	LMT	C2-C1-O1'-C1'
27	F	303	LMT	O5'-C1'-O1'-C1
27	G	201	LMT	O5'-C1'-O1'-C1
28	B	841	PQN	C19-C18-C20-C21
30	B	849	DGD	C2B-C1B-O2G-C2G
30	B	849	DGD	O1B-C1B-O2G-C2G
30	B	849	DGD	O2G-C2G-C3G-O3G
31	Y	617	NEX	C26-C27-C28-C29
31	Z	316	NEX	O24-C26-C27-C28
31	Z	316	NEX	C26-C27-C28-C29
20	2	614	CHL	O1D-CGD-O2D-CED
20	X	606	CHL	O1D-CGD-O2D-CED
20	Y	609	CHL	O1D-CGD-O2D-CED
20	Z	306	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	3	611	CLA	O1D-CGD-O2D-CED
21	4	303	CLA	O1D-CGD-O2D-CED
21	5	610	CLA	O1D-CGD-O2D-CED
21	X	609	CLA	O1D-CGD-O2D-CED
21	X	610	CLA	O1D-CGD-O2D-CED
21	X	618	CLA	O1D-CGD-O2D-CED
21	Y	612	CLA	O1D-CGD-O2D-CED
21	Y	613	CLA	O1D-CGD-O2D-CED
20	Y	605	CHL	O1D-CGD-O2D-CED
20	Z	307	CHL	O1D-CGD-O2D-CED
20	Z	308	CHL	O1D-CGD-O2D-CED
21	1	605	CLA	O1D-CGD-O2D-CED
21	1	608	CLA	O1D-CGD-O2D-CED
21	2	611	CLA	O1D-CGD-O2D-CED
21	5	603	CLA	O1D-CGD-O2D-CED
21	5	608	CLA	O1D-CGD-O2D-CED
21	B	813	CLA	O1D-CGD-O2D-CED
21	F	304	CLA	O1D-CGD-O2D-CED
21	J	102	CLA	O1D-CGD-O2D-CED
21	X	612	CLA	O1D-CGD-O2D-CED
21	Z	311	CLA	O1D-CGD-O2D-CED
20	4	304	CHL	CBD-CGD-O2D-CED
20	Y	609	CHL	CBD-CGD-O2D-CED
20	Z	309	CHL	CBD-CGD-O2D-CED
21	1	610	CLA	CBD-CGD-O2D-CED
21	3	603	CLA	CBD-CGD-O2D-CED
21	3	605	CLA	CBD-CGD-O2D-CED
21	3	610	CLA	CBD-CGD-O2D-CED
21	4	303	CLA	CBD-CGD-O2D-CED
21	4	309	CLA	CBD-CGD-O2D-CED
21	4	311	CLA	CBD-CGD-O2D-CED
21	4	312	CLA	CBD-CGD-O2D-CED
21	5	605	CLA	CBD-CGD-O2D-CED
21	5	612	CLA	CBD-CGD-O2D-CED
21	6	601	CLA	CBD-CGD-O2D-CED
21	6	604	CLA	CBD-CGD-O2D-CED
21	6	610	CLA	CBD-CGD-O2D-CED
21	6	613	CLA	CBD-CGD-O2D-CED
21	A	811	CLA	CBD-CGD-O2D-CED
21	B	803	CLA	CBD-CGD-O2D-CED
21	B	805	CLA	CBD-CGD-O2D-CED
21	H	201	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	J	102	CLA	CBD-CGD-O2D-CED
21	X	602	CLA	CBD-CGD-O2D-CED
21	X	603	CLA	CBD-CGD-O2D-CED
21	X	604	CLA	CBD-CGD-O2D-CED
21	X	610	CLA	CBD-CGD-O2D-CED
21	X	611	CLA	CBD-CGD-O2D-CED
21	X	618	CLA	CBD-CGD-O2D-CED
21	Y	602	CLA	CBD-CGD-O2D-CED
21	Y	610	CLA	CBD-CGD-O2D-CED
21	Z	303	CLA	CBD-CGD-O2D-CED
21	Z	304	CLA	CBD-CGD-O2D-CED
21	Z	312	CLA	CBD-CGD-O2D-CED
21	6	612	CLA	O1A-CGA-O2A-C1
21	A	804	CLA	O1A-CGA-O2A-C1
21	A	843	CLA	O1A-CGA-O2A-C1
20	3	608	CHL	O1A-CGA-O2A-C1
20	Y	608	CHL	O1D-CGD-O2D-CED
21	5	614	CLA	O1D-CGD-O2D-CED
21	G	202	CLA	O1D-CGD-O2D-CED
21	X	613	CLA	O1D-CGD-O2D-CED
21	Z	313	CLA	O1D-CGD-O2D-CED
27	6	621	LMT	O5B-C1B-O1B-C4'
20	Y	607	CHL	O1D-CGD-O2D-CED
21	6	601	CLA	O1D-CGD-O2D-CED
21	6	613	CLA	O1D-CGD-O2D-CED
21	G	204	CLA	O1D-CGD-O2D-CED
21	H	201	CLA	O1D-CGD-O2D-CED
21	X	602	CLA	O1D-CGD-O2D-CED
21	Y	602	CLA	O1D-CGD-O2D-CED
21	Z	303	CLA	O1D-CGD-O2D-CED
21	Z	304	CLA	O1D-CGD-O2D-CED
21	5	612	CLA	CBA-CGA-O2A-C1
21	6	612	CLA	CBA-CGA-O2A-C1
21	A	825	CLA	CBA-CGA-O2A-C1
20	Y	607	CHL	CBD-CGD-O2D-CED
21	5	609	CLA	CBD-CGD-O2D-CED
21	5	614	CLA	CBD-CGD-O2D-CED
21	A	805	CLA	CBD-CGD-O2D-CED
21	A	812	CLA	CBD-CGD-O2D-CED
21	B	823	CLA	CBD-CGD-O2D-CED
21	B	824	CLA	CBD-CGD-O2D-CED
21	B	829	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	K	202	CLA	CBD-CGD-O2D-CED
21	Y	604	CLA	CBD-CGD-O2D-CED
21	3	617	CLA	O1A-CGA-O2A-C1
21	4	311	CLA	O1A-CGA-O2A-C1
21	5	612	CLA	O1A-CGA-O2A-C1
21	A	801	CLA	O1A-CGA-O2A-C1
21	A	817	CLA	O1A-CGA-O2A-C1
21	B	805	CLA	O1A-CGA-O2A-C1
21	B	812	CLA	O1A-CGA-O2A-C1
21	B	817	CLA	O1A-CGA-O2A-C1
21	B	840	CLA	O1A-CGA-O2A-C1
21	O	203	CLA	O1A-CGA-O2A-C1
21	Z	303	CLA	O1A-CGA-O2A-C1
21	5	612	CLA	O1D-CGD-O2D-CED
21	X	604	CLA	O1D-CGD-O2D-CED
21	Y	610	CLA	O1D-CGD-O2D-CED
21	Z	312	CLA	O1D-CGD-O2D-CED
21	Y	602	CLA	C10-C11-C12-C13
21	B	822	CLA	O1D-CGD-O2D-CED
27	F	303	LMT	C3'-C4'-O1B-C1B
21	2	612	CLA	CBD-CGD-O2D-CED
21	A	813	CLA	CBD-CGD-O2D-CED
21	A	822	CLA	CBD-CGD-O2D-CED
21	A	832	CLA	CBD-CGD-O2D-CED
21	B	803	CLA	O1D-CGD-O2D-CED
20	3	608	CHL	CBA-CGA-O2A-C1
20	6	606	CHL	O1D-CGD-O2D-CED
20	1	601	CHL	C3-C5-C6-C7
21	A	829	CLA	C3-C5-C6-C7
21	A	833	CLA	C3-C5-C6-C7
21	B	833	CLA	C3-C5-C6-C7
21	B	840	CLA	C3-C5-C6-C7
21	Z	303	CLA	C3-C5-C6-C7
21	3	617	CLA	CBA-CGA-O2A-C1
21	4	311	CLA	CBA-CGA-O2A-C1
21	A	817	CLA	CBA-CGA-O2A-C1
21	B	809	CLA	CBA-CGA-O2A-C1
21	B	812	CLA	CBA-CGA-O2A-C1
21	B	817	CLA	CBA-CGA-O2A-C1
21	B	840	CLA	CBA-CGA-O2A-C1
21	L	304	CLA	CBA-CGA-O2A-C1
21	O	203	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
21	Z	303	CLA	CBA-CGA-O2A-C1
21	5	613	CLA	O1D-CGD-O2D-CED
21	Z	310	CLA	O1D-CGD-O2D-CED
21	1	612	CLA	CBD-CGD-O2D-CED
21	Z	313	CLA	O1A-CGA-O2A-C1
27	A	852	LMT	O5B-C1B-O1B-C4'
20	6	605	CHL	C4-C3-C5-C6
21	6	602	CLA	C4-C3-C5-C6
21	A	824	CLA	C4-C3-C5-C6
21	A	832	CLA	C4-C3-C5-C6
21	A	830	CLA	C2-C3-C5-C6
20	2	605	CHL	CBD-CGD-O2D-CED
21	A	818	CLA	CBD-CGD-O2D-CED
21	A	824	CLA	CBD-CGD-O2D-CED
20	4	306	CHL	C2A-CAA-CBA-CGA
20	Y	607	CHL	C2A-CAA-CBA-CGA
20	Z	301	CHL	C2A-CAA-CBA-CGA
21	1	612	CLA	C2A-CAA-CBA-CGA
21	6	604	CLA	C2A-CAA-CBA-CGA
21	6	612	CLA	C2A-CAA-CBA-CGA
21	A	803	CLA	C2A-CAA-CBA-CGA
21	A	809	CLA	C2A-CAA-CBA-CGA
21	A	813	CLA	C2A-CAA-CBA-CGA
21	A	833	CLA	C2A-CAA-CBA-CGA
21	A	842	CLA	C2A-CAA-CBA-CGA
21	B	838	CLA	C2A-CAA-CBA-CGA
21	L	301	CLA	C2A-CAA-CBA-CGA
21	O	202	CLA	C2A-CAA-CBA-CGA
21	O	206	CLA	C2A-CAA-CBA-CGA
21	Z	303	CLA	C2A-CAA-CBA-CGA
21	Z	304	CLA	C2A-CAA-CBA-CGA
21	Z	311	CLA	C2A-CAA-CBA-CGA
21	X	611	CLA	O1D-CGD-O2D-CED
21	A	843	CLA	C3-C5-C6-C7
21	B	805	CLA	C3-C5-C6-C7
21	B	807	CLA	C3-C5-C6-C7
21	B	814	CLA	C3-C5-C6-C7
21	B	839	CLA	C3-C5-C6-C7
21	1	612	CLA	CBA-CGA-O2A-C1
21	A	801	CLA	CBA-CGA-O2A-C1
21	O	206	CLA	CBA-CGA-O2A-C1
21	1	612	CLA	C1-C2-C3-C5

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Mol	Chain	Res	Type	Atoms
21	2	604	CLA	C1-C2-C3-C5
21	B	820	CLA	C1-C2-C3-C5
21	B	822	CLA	C1-C2-C3-C5
21	H	201	CLA	C1-C2-C3-C5
21	2	604	CLA	CBD-CGD-O2D-CED
21	3	617	CLA	CBD-CGD-O2D-CED
21	2	604	CLA	O1D-CGD-O2D-CED
21	3	607	CLA	O1D-CGD-O2D-CED
21	5	609	CLA	O1D-CGD-O2D-CED
21	B	810	CLA	O1D-CGD-O2D-CED
21	1	612	CLA	O1A-CGA-O2A-C1
21	A	819	CLA	O1A-CGA-O2A-C1
21	H	201	CLA	O1A-CGA-O2A-C1
20	Y	619	CHL	O1A-CGA-O2A-C1
20	Z	309	CHL	O1D-CGD-O2D-CED
24	2	619	BCR	C9-C10-C11-C12
24	6	620	BCR	C9-C10-C11-C12
21	6	602	CLA	CBD-CGD-O2D-CED
21	B	811	CLA	CBD-CGD-O2D-CED
21	A	804	CLA	CBA-CGA-O2A-C1
21	B	805	CLA	CBA-CGA-O2A-C1
21	L	301	CLA	CBA-CGA-O2A-C1
21	Z	305	CLA	CBA-CGA-O2A-C1
20	6	607	CHL	O1A-CGA-O2A-C1
21	A	813	CLA	O1A-CGA-O2A-C1
21	A	832	CLA	O1A-CGA-O2A-C1
21	O	206	CLA	O1A-CGA-O2A-C1
21	5	602	CLA	O1D-CGD-O2D-CED
21	A	843	CLA	O1D-CGD-O2D-CED
20	Y	619	CHL	CBA-CGA-O2A-C1
21	1	603	CLA	CBD-CGD-O2D-CED
21	3	607	CLA	CBD-CGD-O2D-CED
21	B	801	CLA	CBD-CGD-O2D-CED
21	O	203	CLA	CBD-CGD-O2D-CED
20	2	606	CHL	O1D-CGD-O2D-CED
21	O	206	CLA	O1D-CGD-O2D-CED
20	X	601	CHL	CBD-CGD-O2D-CED
20	X	608	CHL	CBD-CGD-O2D-CED
21	B	810	CLA	CBD-CGD-O2D-CED
20	6	607	CHL	CBA-CGA-O2A-C1
21	L	301	CLA	O1A-CGA-O2A-C1
21	A	817	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
21	A	830	CLA	C4-C3-C5-C6
21	B	838	CLA	C4-C3-C5-C6
21	A	817	CLA	C2-C3-C5-C6
21	A	841	CLA	C2-C3-C5-C6
21	B	838	CLA	C2-C3-C5-C6
20	2	606	CHL	CBD-CGD-O2D-CED
20	Z	309	CHL	C2A-CAA-CBA-CGA
21	A	817	CLA	C2A-CAA-CBA-CGA
21	G	204	CLA	C2A-CAA-CBA-CGA
21	Z	310	CLA	C2A-CAA-CBA-CGA
21	B	809	CLA	O1A-CGA-O2A-C1
21	B	819	CLA	O1A-CGA-O2A-C1
21	L	304	CLA	O1A-CGA-O2A-C1
21	X	603	CLA	O1A-CGA-O2A-C1
26	1	621	LMG	O6-C1-O1-C7
26	F	307	LMG	O6-C1-O1-C7
21	A	819	CLA	CBA-CGA-O2A-C1
21	H	201	CLA	CBA-CGA-O2A-C1
21	Z	313	CLA	CBA-CGA-O2A-C1
21	4	302	CLA	O1D-CGD-O2D-CED
21	6	614	CLA	O1D-CGD-O2D-CED
21	A	826	CLA	C1-C2-C3-C5
21	A	827	CLA	C1-C2-C3-C5
21	B	810	CLA	C1-C2-C3-C5
21	B	816	CLA	C10-C11-C12-C13
21	B	804	CLA	O1A-CGA-O2A-C1
21	2	618	CLA	CBA-CGA-O2A-C1
21	1	602	CLA	O1D-CGD-O2D-CED
21	A	821	CLA	O1D-CGD-O2D-CED
21	3	602	CLA	CBA-CGA-O2A-C1
21	6	614	CLA	CBA-CGA-O2A-C1
21	A	803	CLA	CBA-CGA-O2A-C1
21	A	813	CLA	CBA-CGA-O2A-C1
21	A	821	CLA	CBA-CGA-O2A-C1
21	A	829	CLA	CBA-CGA-O2A-C1
21	A	832	CLA	CBA-CGA-O2A-C1
21	B	828	CLA	CBA-CGA-O2A-C1
21	Y	602	CLA	CBA-CGA-O2A-C1
21	O	206	CLA	CBD-CGD-O2D-CED
21	A	832	CLA	C5-C6-C7-C8
21	1	614	CLA	O1D-CGD-O2D-CED
21	A	811	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
21	A	842	CLA	C15-C16-C17-C18
21	B	807	CLA	C15-C16-C17-C18
21	B	826	CLA	C3-C5-C6-C7
26	1	621	LMG	C2-C1-O1-C7
27	F	303	LMT	C2'-C1'-O1'-C1
27	G	201	LMT	C2'-C1'-O1'-C1
26	6	619	LMG	O7-C8-C9-O8
21	L	305	CLA	C2C-C3C-CAC-CBC
21	6	614	CLA	O1A-CGA-O2A-C1
21	B	828	CLA	O1A-CGA-O2A-C1
21	1	609	CLA	C4-C3-C5-C6
21	A	843	CLA	C2-C3-C5-C6
21	1	608	CLA	C11-C12-C13-C14
21	1	608	CLA	C14-C13-C15-C16
21	1	612	CLA	C11-C10-C8-C9
21	5	612	CLA	C11-C10-C8-C9
21	A	803	CLA	C11-C10-C8-C9
21	A	813	CLA	C11-C12-C13-C14
21	A	825	CLA	C11-C12-C13-C14
21	A	826	CLA	C14-C13-C15-C16
21	A	827	CLA	C14-C13-C15-C16
21	A	828	CLA	C11-C10-C8-C9
21	A	833	CLA	C11-C10-C8-C9
21	A	834	CLA	C11-C10-C8-C9
21	A	841	CLA	C11-C12-C13-C14
21	A	842	CLA	C11-C10-C8-C9
21	B	801	CLA	C11-C12-C13-C14
21	B	807	CLA	C11-C10-C8-C9
21	B	822	CLA	C6-C7-C8-C9
21	B	825	CLA	C11-C12-C13-C14
21	B	827	CLA	C14-C13-C15-C16
21	B	836	CLA	C14-C13-C15-C16
21	B	840	CLA	C6-C7-C8-C9
21	L	301	CLA	C11-C12-C13-C14
21	O	203	CLA	C11-C12-C13-C14
21	O	203	CLA	C14-C13-C15-C16
21	Z	303	CLA	C11-C10-C8-C9
28	A	844	PQN	C24-C23-C25-C26
20	Y	619	CHL	O1D-CGD-O2D-CED
21	B	818	CLA	O1D-CGD-O2D-CED
21	B	834	CLA	O1D-CGD-O2D-CED
21	6	603	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	6	612	CLA	CBD-CGD-O2D-CED
21	B	818	CLA	CBD-CGD-O2D-CED
21	B	839	CLA	C10-C11-C12-C13
21	L	301	CLA	C5-C6-C7-C8
21	A	837	CLA	C2A-CAA-CBA-CGA
24	2	619	BCR	C7-C8-C9-C34
24	L	306	BCR	C37-C22-C23-C24
21	2	602	CLA	O1D-CGD-O2D-CED
21	A	840	CLA	O1A-CGA-O2A-C1
21	B	813	CLA	O1A-CGA-O2A-C1
21	1	612	CLA	C13-C15-C16-C17
21	A	807	CLA	C13-C15-C16-C17
21	A	811	CLA	C13-C15-C16-C17
21	B	801	CLA	C5-C6-C7-C8
21	B	815	CLA	C5-C6-C7-C8
21	A	814	CLA	O1D-CGD-O2D-CED
21	6	612	CLA	C8-C10-C11-C12
21	A	830	CLA	CBA-CGA-O2A-C1
21	B	821	CLA	CBA-CGA-O2A-C1
21	B	827	CLA	CBA-CGA-O2A-C1
21	5	612	CLA	C5-C6-C7-C8
21	5	612	CLA	C8-C10-C11-C12
21	A	804	CLA	C5-C6-C7-C8
21	A	806	CLA	C5-C6-C7-C8
21	A	811	CLA	C10-C11-C12-C13
21	A	819	CLA	C10-C11-C12-C13
21	A	828	CLA	C10-C11-C12-C13
21	B	802	CLA	C10-C11-C12-C13
21	B	805	CLA	C10-C11-C12-C13
21	B	822	CLA	C5-C6-C7-C8
21	L	301	CLA	C10-C11-C12-C13
21	L	301	CLA	C15-C16-C17-C18
21	L	304	CLA	C10-C11-C12-C13
26	1	619	LMG	C28-C29-C30-C31
21	A	811	CLA	O1D-CGD-O2D-CED
21	1	608	CLA	C10-C11-C12-C13
21	1	612	CLA	C8-C10-C11-C12
21	4	311	CLA	C5-C6-C7-C8
21	A	803	CLA	C10-C11-C12-C13
21	A	806	CLA	C13-C15-C16-C17
21	A	807	CLA	C10-C11-C12-C13
21	A	813	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
21	A	817	CLA	C10-C11-C12-C13
21	A	825	CLA	C5-C6-C7-C8
21	A	826	CLA	C15-C16-C17-C18
21	A	828	CLA	C15-C16-C17-C18
21	B	801	CLA	C10-C11-C12-C13
21	B	804	CLA	C10-C11-C12-C13
21	B	814	CLA	C5-C6-C7-C8
21	B	840	CLA	C8-C10-C11-C12
21	H	201	CLA	C8-C10-C11-C12
21	O	203	CLA	C5-C6-C7-C8
21	Y	602	CLA	C8-C10-C11-C12
28	B	841	PQN	C15-C16-C17-C18
21	4	308	CLA	O1D-CGD-O2D-CED
21	4	311	CLA	O1D-CGD-O2D-CED
21	Z	305	CLA	O1A-CGA-O2A-C1
21	3	604	CLA	CBD-CGD-O2D-CED
21	B	828	CLA	CBD-CGD-O2D-CED
21	2	602	CLA	C10-C11-C12-C13
21	A	802	CLA	C5-C6-C7-C8
21	A	806	CLA	C15-C16-C17-C18
21	A	830	CLA	C15-C16-C17-C18
21	B	817	CLA	C10-C11-C12-C13
21	B	827	CLA	C10-C11-C12-C13
21	6	602	CLA	CBA-CGA-O2A-C1
21	A	807	CLA	CBA-CGA-O2A-C1
21	B	819	CLA	CBA-CGA-O2A-C1
21	5	602	CLA	C8-C10-C11-C12
21	A	830	CLA	C10-C11-C12-C13
21	A	833	CLA	C5-C6-C7-C8
21	B	838	CLA	C10-C11-C12-C13
21	6	608	CLA	CBD-CGD-O2D-CED
21	A	808	CLA	CBD-CGD-O2D-CED
21	4	311	CLA	C8-C10-C11-C12
21	1	602	CLA	C5-C6-C7-C8
21	2	612	CLA	C5-C6-C7-C8
21	B	802	CLA	C13-C15-C16-C17
21	A	801	CLA	C11-C12-C13-C15
21	A	807	CLA	C11-C12-C13-C15
21	B	804	CLA	C11-C12-C13-C15
21	B	822	CLA	C6-C7-C8-C10
21	B	823	CLA	C11-C10-C8-C7
21	B	823	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
21	B	831	CLA	C11-C12-C13-C15
21	L	301	CLA	C12-C13-C15-C16
28	B	841	PQN	C21-C22-C23-C25
21	A	826	CLA	O1A-CGA-O2A-C1
21	Y	613	CLA	O1A-CGA-O2A-C1
21	A	838	CLA	CBD-CGD-O2D-CED
20	6	607	CHL	C2A-CAA-CBA-CGA
21	5	614	CLA	C2A-CAA-CBA-CGA
21	A	801	CLA	C2A-CAA-CBA-CGA
21	B	812	CLA	C2A-CAA-CBA-CGA
21	K	203	CLA	C2A-CAA-CBA-CGA
21	X	603	CLA	C2A-CAA-CBA-CGA
21	3	605	CLA	O1D-CGD-O2D-CED
21	X	603	CLA	O1D-CGD-O2D-CED
21	5	602	CLA	C10-C11-C12-C13
21	A	839	CLA	CBD-CGD-O2D-CED
21	A	842	CLA	C13-C15-C16-C17
21	B	836	CLA	C10-C11-C12-C13
21	2	609	CLA	O1D-CGD-O2D-CED
21	4	312	CLA	O1D-CGD-O2D-CED
21	A	801	CLA	C15-C16-C17-C18
21	A	840	CLA	C15-C16-C17-C18
21	B	825	CLA	C10-C11-C12-C13
21	H	201	CLA	C5-C6-C7-C8
21	O	202	CLA	CBA-CGA-O2A-C1
21	1	610	CLA	O1A-CGA-O2A-C1
21	A	807	CLA	O1A-CGA-O2A-C1
21	A	834	CLA	O1A-CGA-O2A-C1
21	B	836	CLA	O1A-CGA-O2A-C1
21	Y	602	CLA	O1A-CGA-O2A-C1
20	1	601	CHL	C5-C6-C7-C8
21	3	617	CLA	C5-C6-C7-C8
21	A	811	CLA	C15-C16-C17-C18
21	A	825	CLA	C15-C16-C17-C18
21	A	830	CLA	C5-C6-C7-C8
21	B	802	CLA	C8-C10-C11-C12
21	B	805	CLA	C5-C6-C7-C8
21	B	813	CLA	C8-C10-C11-C12
21	B	840	CLA	C5-C6-C7-C8
21	1	612	CLA	C15-C16-C17-C18
21	5	602	CLA	C5-C6-C7-C8
21	A	827	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
21	A	833	CLA	C15-C16-C17-C18
21	A	841	CLA	C15-C16-C17-C18
21	B	813	CLA	C13-C15-C16-C17
21	B	839	CLA	C15-C16-C17-C18
25	1	620	LHG	C4-O6-P-O3
25	1	622	LHG	C3-O3-P-O6
25	2	617	LHG	C4-O6-P-O3
25	X	617	LHG	C3-O3-P-O6
25	Y	618	LHG	C3-O3-P-O6
25	Z	317	LHG	C3-O3-P-O6
21	A	808	CLA	CBA-CGA-O2A-C1
21	1	602	CLA	C8-C10-C11-C12
21	1	608	CLA	C5-C6-C7-C8
21	A	834	CLA	C10-C11-C12-C13
21	4	309	CLA	O1D-CGD-O2D-CED
21	B	821	CLA	O1D-CGD-O2D-CED
21	B	832	CLA	O1D-CGD-O2D-CED
21	A	813	CLA	C4-C3-C5-C6
21	B	801	CLA	C4-C3-C5-C6
21	4	309	CLA	C10-C11-C12-C13
21	A	833	CLA	C10-C11-C12-C13
20	Z	306	CHL	C2A-CAA-CBA-CGA
20	Z	307	CHL	C2A-CAA-CBA-CGA
21	2	604	CLA	C2A-CAA-CBA-CGA
21	5	612	CLA	C2A-CAA-CBA-CGA
21	A	807	CLA	C2A-CAA-CBA-CGA
21	A	818	CLA	C2A-CAA-CBA-CGA
21	B	805	CLA	C2A-CAA-CBA-CGA
21	B	806	CLA	C2A-CAA-CBA-CGA
21	B	826	CLA	C2A-CAA-CBA-CGA
21	X	604	CLA	C2A-CAA-CBA-CGA
20	4	304	CHL	C6-C7-C8-C10
26	1	621	LMG	O6-C5-C6-O5
21	B	812	CLA	C3-C5-C6-C7
21	2	602	CLA	CBA-CGA-O2A-C1
21	4	313	CLA	CBA-CGA-O2A-C1
21	B	804	CLA	CBA-CGA-O2A-C1
21	B	816	CLA	CBA-CGA-O2A-C1
21	X	603	CLA	CBA-CGA-O2A-C1
21	1	609	CLA	C10-C11-C12-C13
21	2	609	CLA	C5-C6-C7-C8
20	4	305	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	3	609	CLA	CBD-CGD-O2D-CED
21	B	807	CLA	CBD-CGD-O2D-CED
21	3	603	CLA	O1D-CGD-O2D-CED
21	Y	614	CLA	O1D-CGD-O2D-CED
21	3	603	CLA	C6-C7-C8-C10
21	A	803	CLA	C16-C17-C18-C20
21	L	304	CLA	C11-C12-C13-C15
21	3	602	CLA	O1D-CGD-O2D-CED
21	A	835	CLA	O1D-CGD-O2D-CED
20	4	306	CHL	C1-C2-C3-C5
21	6	614	CLA	C1-C2-C3-C5
21	A	808	CLA	C1-C2-C3-C5
21	A	831	CLA	C1-C2-C3-C5
21	A	839	CLA	C1-C2-C3-C5
21	B	835	CLA	C1-C2-C3-C5
21	O	202	CLA	C1-C2-C3-C5
21	1	613	CLA	CBD-CGD-O2D-CED
26	5	620	LMG	C35-C36-C37-C38
21	Y	611	CLA	O1D-CGD-O2D-CED
21	A	828	CLA	C8-C10-C11-C12
21	A	824	CLA	C3-C5-C6-C7
26	1	619	LMG	C2-C1-O1-C7
26	5	620	LMG	C2-C1-O1-C7
21	A	813	CLA	C8-C10-C11-C12
21	A	824	CLA	C6-C7-C8-C9
21	A	833	CLA	C16-C17-C18-C20
21	B	807	CLA	C16-C17-C18-C20
21	B	818	CLA	C6-C7-C8-C10
21	A	807	CLA	C4-C3-C5-C6
21	1	602	CLA	C2-C3-C5-C6
21	A	806	CLA	C11-C12-C13-C14
21	A	840	CLA	C11-C12-C13-C14
21	B	802	CLA	C6-C7-C8-C9
21	B	805	CLA	C14-C13-C15-C16
21	B	839	CLA	C11-C10-C8-C9
21	B	817	CLA	CBD-CGD-O2D-CED
21	B	809	CLA	C15-C16-C17-C18
21	3	605	CLA	C2A-CAA-CBA-CGA
21	3	607	CLA	C2A-CAA-CBA-CGA
21	A	804	CLA	C2A-CAA-CBA-CGA
21	A	820	CLA	C2A-CAA-CBA-CGA
21	A	836	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
21	1	610	CLA	O1D-CGD-O2D-CED
21	3	602	CLA	O1A-CGA-O2A-C1
20	6	607	CHL	O1D-CGD-O2D-CED
21	A	814	CLA	C4B-C3B-CAB-CBB
21	3	603	CLA	C6-C7-C8-C9
21	A	824	CLA	C6-C7-C8-C10
21	B	820	CLA	C6-C7-C8-C9
21	B	820	CLA	C6-C7-C8-C10
21	L	304	CLA	C11-C12-C13-C14
21	Z	303	CLA	C11-C12-C13-C14
26	1	619	LMG	O6-C1-O1-C7
21	A	806	CLA	C10-C11-C12-C13
21	B	801	CLA	C15-C16-C17-C18
21	Z	303	CLA	C5-C6-C7-C8
21	A	813	CLA	O1D-CGD-O2D-CED
21	A	820	CLA	O1D-CGD-O2D-CED
25	A	851	LHG	C24-C25-C26-C27
21	B	807	CLA	C13-C15-C16-C17
26	B	850	LMG	C14-C15-C16-C17
21	B	822	CLA	CBA-CGA-O2A-C1
20	4	305	CHL	C3A-C2A-CAA-CBA
20	6	605	CHL	C3A-C2A-CAA-CBA
20	X	607	CHL	C3A-C2A-CAA-CBA
20	Y	607	CHL	C3A-C2A-CAA-CBA
21	3	603	CLA	C3A-C2A-CAA-CBA
21	4	302	CLA	C3A-C2A-CAA-CBA
21	4	309	CLA	C3A-C2A-CAA-CBA
21	6	603	CLA	C3A-C2A-CAA-CBA
21	6	610	CLA	C3A-C2A-CAA-CBA
21	A	804	CLA	C3A-C2A-CAA-CBA
21	A	843	CLA	C3A-C2A-CAA-CBA
21	B	822	CLA	C3A-C2A-CAA-CBA
21	O	203	CLA	C3A-C2A-CAA-CBA
21	X	611	CLA	C3A-C2A-CAA-CBA
21	X	612	CLA	C3A-C2A-CAA-CBA
21	5	612	CLA	C15-C16-C17-C18
21	A	802	CLA	C8-C10-C11-C12
27	4	319	LMT	C2-C1-O1'-C1'
26	6	619	LMG	C31-C32-C33-C34
20	4	304	CHL	C6-C7-C8-C9
21	A	803	CLA	C16-C17-C18-C19
21	A	833	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
21	Z	303	CLA	C11-C12-C13-C15
26	4	318	LMG	O1-C7-C8-C9
21	B	827	CLA	CBD-CGD-O2D-CED
21	B	838	CLA	CBD-CGD-O2D-CED
20	6	607	CHL	O2A-C1-C2-C3
21	A	804	CLA	O2A-C1-C2-C3
21	L	304	CLA	C3-C5-C6-C7
27	6	621	LMT	C2B-C1B-O1B-C4'
21	A	813	CLA	C10-C11-C12-C13
21	A	806	CLA	C4-C3-C5-C6
21	B	828	CLA	C4-C3-C5-C6
21	B	813	CLA	CBA-CGA-O2A-C1
21	B	828	CLA	C2-C3-C5-C6
21	B	833	CLA	C2-C3-C5-C6
21	3	610	CLA	O1D-CGD-O2D-CED
21	A	806	CLA	C16-C17-C18-C19
21	B	817	CLA	C11-C12-C13-C14
30	B	849	DGD	C4A-C5A-C6A-C7A
21	A	814	CLA	C2B-C3B-CAB-CBB
21	B	817	CLA	C3-C5-C6-C7
21	Y	604	CLA	C2C-C3C-CAC-CBC
26	B	850	LMG	C16-C17-C18-C19
27	4	319	LMT	C5'-C4'-O1B-C1B
21	A	833	CLA	O1A-CGA-O2A-C1
21	B	806	CLA	O1A-CGA-O2A-C1
21	L	305	CLA	C4C-C3C-CAC-CBC
21	A	819	CLA	C15-C16-C17-C18
21	A	827	CLA	O1A-CGA-O2A-C1
21	B	807	CLA	C16-C17-C18-C19
22	5	615	LUT	C1-C6-C7-C8
22	5	615	LUT	C5-C6-C7-C8
22	5	619	LUT	C1-C6-C7-C8
22	5	619	LUT	C5-C6-C7-C8
22	F	301	LUT	C1-C6-C7-C8
22	F	301	LUT	C5-C6-C7-C8
22	Y	615	LUT	C1-C6-C7-C8
22	Z	314	LUT	C1-C6-C7-C8
22	Z	314	LUT	C5-C6-C7-C8
22	Z	315	LUT	C1-C6-C7-C8
22	Z	315	LUT	C5-C6-C7-C8
24	2	619	BCR	C1-C6-C7-C8
24	2	619	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	2	619	BCR	C23-C24-C25-C26
24	A	845	BCR	C1-C6-C7-C8
24	A	845	BCR	C5-C6-C7-C8
24	A	849	BCR	C5-C6-C7-C8
24	B	848	BCR	C23-C24-C25-C26
24	B	848	BCR	C23-C24-C25-C30
24	J	103	BCR	C23-C24-C25-C26
24	K	205	BCR	C5-C6-C7-C8
24	K	205	BCR	C23-C24-C25-C30
24	L	302	BCR	C1-C6-C7-C8
24	L	302	BCR	C5-C6-C7-C8
24	L	308	BCR	C5-C6-C7-C8
24	O	204	BCR	C1-C6-C7-C8
24	O	204	BCR	C5-C6-C7-C8
24	O	204	BCR	C23-C24-C25-C26
24	O	204	BCR	C23-C24-C25-C30
24	O	205	BCR	C5-C6-C7-C8
21	6	610	CLA	O1D-CGD-O2D-CED
21	1	610	CLA	CBA-CGA-O2A-C1
21	A	840	CLA	CBA-CGA-O2A-C1
21	A	802	CLA	C10-C11-C12-C13
21	A	842	CLA	C5-C6-C7-C8
21	B	825	CLA	C5-C6-C7-C8
21	B	808	CLA	CBD-CGD-O2D-CED
21	B	828	CLA	C11-C10-C8-C9
21	H	201	CLA	C10-C11-C12-C13
21	A	818	CLA	C10-C11-C12-C13
21	B	833	CLA	C4-C3-C5-C6
21	1	612	CLA	C12-C13-C15-C16
21	2	604	CLA	C11-C10-C8-C7
21	4	311	CLA	C2-C3-C5-C6
21	5	612	CLA	C11-C10-C8-C7
21	5	612	CLA	C11-C12-C13-C15
21	A	806	CLA	C12-C13-C15-C16
21	A	807	CLA	C2-C3-C5-C6
21	A	811	CLA	C11-C12-C13-C15
21	A	821	CLA	C2-C3-C5-C6
21	A	825	CLA	C2-C3-C5-C6
21	A	842	CLA	C6-C7-C8-C10
21	B	802	CLA	C11-C10-C8-C7
21	B	805	CLA	C11-C10-C8-C7
21	B	807	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
21	B	825	CLA	C11-C12-C13-C15
21	B	831	CLA	C2-C3-C5-C6
21	B	838	CLA	C11-C10-C8-C7
21	L	301	CLA	C11-C10-C8-C7
21	O	203	CLA	C11-C12-C13-C15
21	A	801	CLA	C8-C10-C11-C12
21	Y	602	CLA	C15-C16-C17-C18
21	G	203	CLA	O1D-CGD-O2D-CED
20	4	304	CHL	CBA-CGA-O2A-C1
21	2	604	CLA	CBA-CGA-O2A-C1
21	A	812	CLA	CBA-CGA-O2A-C1
21	A	834	CLA	CBA-CGA-O2A-C1
21	3	612	CLA	C2A-CAA-CBA-CGA
21	A	812	CLA	C2A-CAA-CBA-CGA
21	A	841	CLA	C2A-CAA-CBA-CGA
21	B	819	CLA	C2A-CAA-CBA-CGA
21	X	610	CLA	C2A-CAA-CBA-CGA
21	X	611	CLA	C2A-CAA-CBA-CGA
21	1	608	CLA	C8-C10-C11-C12
20	1	601	CHL	C1-C2-C3-C5
21	B	813	CLA	C15-C16-C17-C18
21	B	806	CLA	CBA-CGA-O2A-C1
21	B	818	CLA	CBA-CGA-O2A-C1
21	B	836	CLA	CBA-CGA-O2A-C1
21	Y	613	CLA	CBA-CGA-O2A-C1
21	A	838	CLA	C6-C7-C8-C10
21	A	841	CLA	C16-C17-C18-C20
26	5	620	LMG	O6-C1-O1-C7
21	A	821	CLA	C13-C15-C16-C17
21	A	812	CLA	C5-C6-C7-C8
26	G	206	LMG	C36-C37-C38-C39
21	A	829	CLA	C15-C16-C17-C18
21	A	838	CLA	C5-C6-C7-C8
21	B	802	CLA	C15-C16-C17-C18
21	2	609	CLA	CBD-CGD-O2D-CED
21	B	834	CLA	CBD-CGD-O2D-CED
26	5	621	LMG	C2-C1-O1-C7
21	B	822	CLA	C8-C10-C11-C12
26	4	318	LMG	O7-C8-C9-O8
26	B	850	LMG	O6-C5-C6-O5
21	B	823	CLA	C10-C11-C12-C13
21	B	838	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
21	A	816	CLA	O1D-CGD-O2D-CED
21	B	807	CLA	C4-C3-C5-C6
21	L	301	CLA	C4-C3-C5-C6
20	6	605	CHL	C2-C3-C5-C6
21	A	812	CLA	C2-C3-C5-C6
21	A	832	CLA	C2-C3-C5-C6
21	B	805	CLA	C2-C3-C5-C6
21	1	612	CLA	C14-C13-C15-C16
21	2	604	CLA	C11-C10-C8-C9
21	4	309	CLA	C6-C7-C8-C9
21	5	612	CLA	C11-C12-C13-C14
21	A	801	CLA	C11-C12-C13-C14
21	A	842	CLA	C6-C7-C8-C9
21	B	801	CLA	C11-C10-C8-C9
21	B	802	CLA	C11-C10-C8-C9
21	B	804	CLA	C11-C12-C13-C14
21	B	823	CLA	C11-C10-C8-C9
21	L	301	CLA	C11-C10-C8-C9
21	Y	602	CLA	C11-C12-C13-C14
27	4	319	LMT	C3'-C4'-O1B-C1B
21	B	836	CLA	C2A-CAA-CBA-CGA
21	O	203	CLA	C2A-CAA-CBA-CGA
21	Y	602	CLA	C2A-CAA-CBA-CGA
24	O	201	BCR	C7-C8-C9-C34
21	3	602	CLA	C5-C6-C7-C8
21	6	602	CLA	C5-C6-C7-C8
21	B	826	CLA	C8-C10-C11-C12
21	A	821	CLA	O1A-CGA-O2A-C1
21	A	830	CLA	O1A-CGA-O2A-C1
21	B	816	CLA	O1A-CGA-O2A-C1
21	B	822	CLA	O1A-CGA-O2A-C1
21	B	823	CLA	O1A-CGA-O2A-C1
21	2	608	CLA	C1A-C2A-CAA-CBA
21	2	609	CLA	C1A-C2A-CAA-CBA
21	2	613	CLA	C1A-C2A-CAA-CBA
21	3	603	CLA	C1A-C2A-CAA-CBA
21	3	617	CLA	C1A-C2A-CAA-CBA
21	4	302	CLA	C1A-C2A-CAA-CBA
21	5	604	CLA	C1A-C2A-CAA-CBA
21	6	613	CLA	C1A-C2A-CAA-CBA
21	A	804	CLA	C1A-C2A-CAA-CBA
21	A	810	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
21	A	816	CLA	C1A-C2A-CAA-CBA
21	A	819	CLA	C1A-C2A-CAA-CBA
21	A	824	CLA	C1A-C2A-CAA-CBA
21	A	841	CLA	C1A-C2A-CAA-CBA
21	A	843	CLA	C1A-C2A-CAA-CBA
21	B	804	CLA	C1A-C2A-CAA-CBA
21	B	811	CLA	C1A-C2A-CAA-CBA
21	B	812	CLA	C1A-C2A-CAA-CBA
21	B	817	CLA	C1A-C2A-CAA-CBA
21	B	826	CLA	C1A-C2A-CAA-CBA
21	G	202	CLA	C1A-C2A-CAA-CBA
21	K	203	CLA	C1A-C2A-CAA-CBA
21	O	203	CLA	C1A-C2A-CAA-CBA
21	X	604	CLA	C1A-C2A-CAA-CBA
21	X	611	CLA	C1A-C2A-CAA-CBA
21	X	612	CLA	C1A-C2A-CAA-CBA
21	X	613	CLA	C1A-C2A-CAA-CBA
21	Y	602	CLA	C1A-C2A-CAA-CBA
21	Y	614	CLA	C1A-C2A-CAA-CBA
21	Z	310	CLA	C1A-C2A-CAA-CBA
21	Z	311	CLA	C1A-C2A-CAA-CBA
27	F	303	LMT	O5'-C5'-C6'-O6'
21	A	806	CLA	C16-C17-C18-C20
21	A	838	CLA	C6-C7-C8-C9
21	B	818	CLA	C6-C7-C8-C9
31	Z	316	NEX	C29-C30-C31-C32
21	A	819	CLA	C5-C6-C7-C8
21	A	825	CLA	C10-C11-C12-C13
21	B	804	CLA	C15-C16-C17-C18
21	B	817	CLA	C5-C6-C7-C8
21	Z	303	CLA	C8-C10-C11-C12
30	B	849	DGD	C1B-C2B-C3B-C4B
25	Y	618	LHG	C2-C3-O3-P
20	2	607	CHL	O1A-CGA-O2A-C1
21	3	617	CLA	O1D-CGD-O2D-CED
21	A	825	CLA	C16-C17-C18-C20
21	A	841	CLA	C16-C17-C18-C19
21	B	833	CLA	CBD-CGD-O2D-CED
21	A	826	CLA	CBA-CGA-O2A-C1
21	A	825	CLA	C4-C3-C5-C6
21	B	818	CLA	C4-C3-C5-C6
21	B	831	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
21	L	304	CLA	C4-C3-C5-C6
21	3	606	CLA	C3A-C2A-CAA-CBA
21	4	310	CLA	C3A-C2A-CAA-CBA
21	B	818	CLA	C2-C3-C5-C6
21	2	602	CLA	C15-C16-C17-C18
21	4	301	CLA	C10-C11-C12-C13
21	B	836	CLA	C5-C6-C7-C8
21	A	807	CLA	C16-C17-C18-C19
21	B	810	CLA	C6-C7-C8-C9
21	6	604	CLA	O1D-CGD-O2D-CED
21	B	830	CLA	O1D-CGD-O2D-CED
26	5	620	LMG	O1-C7-C8-C9
26	6	619	LMG	C7-C8-C9-O8
26	B	850	LMG	O1-C7-C8-C9
26	F	306	LMG	O1-C7-C8-C9
30	B	849	DGD	C1G-C2G-C3G-O3G
26	1	619	LMG	C8-C7-O1-C1
26	5	620	LMG	C8-C7-O1-C1
21	B	811	CLA	C2A-CAA-CBA-CGA
21	4	313	CLA	O1D-CGD-O2D-CED
21	5	605	CLA	O1D-CGD-O2D-CED
21	B	820	CLA	CBD-CGD-O2D-CED
21	A	826	CLA	C5-C6-C7-C8
25	1	620	LHG	C26-C27-C28-C29
21	H	201	CLA	CAA-CBA-CGA-O2A
21	A	829	CLA	O1A-CGA-O2A-C1
27	6	621	LMT	O1'-C1-C2-C3
21	1	608	CLA	C15-C16-C17-C18
21	B	827	CLA	C15-C16-C17-C18
27	F	303	LMT	O5B-C5B-C6B-O6B
20	2	601	CHL	O1A-CGA-O2A-C1
21	B	805	CLA	C4-C3-C5-C6
21	B	820	CLA	C4-C3-C5-C6
21	5	602	CLA	C2-C3-C5-C6
21	B	810	CLA	C6-C7-C8-C10
21	A	833	CLA	CBA-CGA-O2A-C1
21	A	826	CLA	C10-C11-C12-C13
26	G	206	LMG	O6-C5-C6-O5
21	3	602	CLA	C10-C11-C12-C13
21	B	823	CLA	C13-C15-C16-C17
20	4	306	CHL	C1-C2-C3-C4
21	A	810	CLA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
21	X	603	CLA	C5-C6-C7-C8
21	4	308	CLA	C6-C7-C8-C9
21	A	807	CLA	C16-C17-C18-C20
21	B	823	CLA	O1D-CGD-O2D-CED
21	B	804	CLA	C13-C15-C16-C17
26	6	619	LMG	C2-C1-O1-C7
26	4	318	LMG	C31-C32-C33-C34
25	5	618	LHG	O7-C5-C6-O8
21	B	809	CLA	C5-C6-C7-C8
21	6	602	CLA	O1A-CGA-O2A-C1
20	Y	608	CHL	CHA-CBD-CGD-O2D
20	Y	619	CHL	CHA-CBD-CGD-O2D
20	Z	301	CHL	CHA-CBD-CGD-O1D
20	Z	309	CHL	CHA-CBD-CGD-O1D
21	B	826	CLA	C4-C3-C5-C6
21	B	840	CLA	C13-C15-C16-C17
21	1	612	CLA	C6-C7-C8-C10
21	1	612	CLA	C11-C10-C8-C7
21	4	309	CLA	C6-C7-C8-C10
21	5	612	CLA	C6-C7-C8-C10
21	A	801	CLA	C12-C13-C15-C16
21	A	811	CLA	C11-C10-C8-C7
21	A	817	CLA	C6-C7-C8-C10
21	A	818	CLA	C11-C10-C8-C7
21	A	819	CLA	C11-C12-C13-C15
21	A	828	CLA	C11-C10-C8-C7
21	A	829	CLA	C11-C12-C13-C15
21	A	829	CLA	C12-C13-C15-C16
21	B	801	CLA	C11-C10-C8-C7
21	B	809	CLA	C11-C12-C13-C15
21	B	812	CLA	C6-C7-C8-C10
21	B	812	CLA	C11-C12-C13-C15
21	B	813	CLA	C11-C10-C8-C7
21	B	827	CLA	C6-C7-C8-C10
21	B	828	CLA	C6-C7-C8-C10
21	B	836	CLA	C12-C13-C15-C16
21	B	840	CLA	C12-C13-C15-C16
21	L	301	CLA	C11-C12-C13-C15
21	Y	602	CLA	C11-C12-C13-C15
28	A	844	PQN	C22-C23-C25-C26
28	B	841	PQN	C17-C18-C20-C21
21	A	803	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
21	2	604	CLA	C11-C12-C13-C14
21	3	602	CLA	C6-C7-C8-C9
21	5	612	CLA	C6-C7-C8-C9
21	A	802	CLA	C14-C13-C15-C16
21	A	803	CLA	C6-C7-C8-C9
21	A	817	CLA	C6-C7-C8-C9
21	A	818	CLA	C11-C10-C8-C9
21	A	819	CLA	C6-C7-C8-C9
21	A	821	CLA	C11-C10-C8-C9
21	A	828	CLA	C11-C12-C13-C14
21	A	828	CLA	C14-C13-C15-C16
21	B	812	CLA	C6-C7-C8-C9
21	B	812	CLA	C11-C12-C13-C14
21	B	822	CLA	C11-C10-C8-C9
21	B	823	CLA	C6-C7-C8-C9
21	B	825	CLA	C6-C7-C8-C9
21	B	825	CLA	C14-C13-C15-C16
21	B	828	CLA	C6-C7-C8-C9
21	Y	602	CLA	C6-C7-C8-C9
21	Y	602	CLA	C11-C10-C8-C9
28	A	844	PQN	C19-C18-C20-C21
21	1	604	CLA	CBA-CGA-O2A-C1
21	B	801	CLA	CBA-CGA-O2A-C1
21	B	831	CLA	CBA-CGA-O2A-C1
21	B	839	CLA	C5-C6-C7-C8
21	5	607	CLA	C2A-CAA-CBA-CGA
21	Y	613	CLA	C2A-CAA-CBA-CGA
24	A	846	BCR	C17-C18-C19-C20
21	A	824	CLA	C5-C6-C7-C8
21	B	822	CLA	C10-C11-C12-C13
21	B	816	CLA	C5-C6-C7-C8
21	1	603	CLA	CBA-CGA-O2A-C1
21	A	827	CLA	CBA-CGA-O2A-C1
21	Y	613	CLA	C4-C3-C5-C6
21	B	826	CLA	C2-C3-C5-C6
21	B	840	CLA	C2-C3-C5-C6
26	1	619	LMG	C22-C23-C24-C25
21	1	609	CLA	C5-C6-C7-C8
21	6	613	CLA	C2A-CAA-CBA-CGA
21	B	813	CLA	C2A-CAA-CBA-CGA
21	B	814	CLA	O1A-CGA-O2A-C1
20	6	607	CHL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	Y	601	CHL	C3A-C2A-CAA-CBA
20	Y	608	CHL	C3A-C2A-CAA-CBA
21	3	609	CLA	C3A-C2A-CAA-CBA
21	5	604	CLA	C3A-C2A-CAA-CBA
21	5	612	CLA	C3A-C2A-CAA-CBA
21	A	836	CLA	C3A-C2A-CAA-CBA
21	A	841	CLA	C3A-C2A-CAA-CBA
21	B	837	CLA	C3A-C2A-CAA-CBA
21	Y	604	CLA	C4C-C3C-CAC-CBC
27	6	621	LMT	C2-C1-O1'-C1'
21	5	604	CLA	O1A-CGA-O2A-C1
20	4	305	CHL	O1D-CGD-O2D-CED
21	A	840	CLA	C5-C6-C7-C8
25	5	618	LHG	C4-C5-C6-O8
25	Y	618	LHG	C4-C5-C6-O8
26	1	621	LMG	C7-C8-C9-O8
26	4	318	LMG	C7-C8-C9-O8
26	G	206	LMG	C7-C8-C9-O8
21	A	806	CLA	O2A-C1-C2-C3
20	4	304	CHL	O1D-CGD-O2D-CED
21	A	812	CLA	O1A-CGA-O2A-C1
21	A	833	CLA	C8-C10-C11-C12
20	4	304	CHL	C4-C3-C5-C6
21	A	804	CLA	C4-C3-C5-C6
20	6	605	CHL	CBA-CGA-O2A-C1
21	A	824	CLA	C2-C3-C5-C6
20	6	605	CHL	C3C-C2C-CMC-OMC
20	Y	605	CHL	C3C-C2C-CMC-OMC
20	Z	301	CHL	C3C-C2C-CMC-OMC
20	Z	302	CHL	C3C-C2C-CMC-OMC
20	Z	308	CHL	C3C-C2C-CMC-OMC
21	2	602	CLA	C2A-CAA-CBA-CGA
21	3	602	CLA	C2A-CAA-CBA-CGA
21	X	618	CLA	C2A-CAA-CBA-CGA
21	B	827	CLA	O1A-CGA-O2A-C1
21	A	819	CLA	C16-C17-C18-C19
21	A	825	CLA	C16-C17-C18-C19
21	B	817	CLA	C11-C12-C13-C15
21	2	602	CLA	O1A-CGA-O2A-C1
26	4	318	LMG	O1-C7-C8-O7
26	6	619	LMG	O1-C7-C8-O7
26	F	307	LMG	O1-C7-C8-O7

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Mol	Chain	Res	Type	Atoms
21	4	309	CLA	CAA-CBA-CGA-O2A
24	2	619	BCR	C19-C20-C21-C22
24	6	620	BCR	C19-C20-C21-C22
21	A	817	CLA	C11-C12-C13-C15
21	A	819	CLA	C16-C17-C18-C20
21	A	840	CLA	C16-C17-C18-C19
21	5	604	CLA	CBD-CGD-O2D-CED
21	A	809	CLA	C2-C1-O2A-CGA
21	B	801	CLA	C2-C3-C5-C6
21	1	610	CLA	C5-C6-C7-C8
21	1	612	CLA	C6-C7-C8-C9
21	2	604	CLA	C14-C13-C15-C16
21	A	803	CLA	C14-C13-C15-C16
21	A	833	CLA	C11-C12-C13-C14
21	A	840	CLA	C14-C13-C15-C16
21	B	805	CLA	C6-C7-C8-C9
21	B	838	CLA	C6-C7-C8-C9
21	Z	303	CLA	C6-C7-C8-C9
21	B	826	CLA	C10-C11-C12-C13
21	B	840	CLA	C10-C11-C12-C13
20	6	605	CHL	C1A-C2A-CAA-CBA
20	Y	601	CHL	C1A-C2A-CAA-CBA
21	A	824	CLA	O1A-CGA-O2A-C1
21	A	831	CLA	O1A-CGA-O2A-C1
21	O	202	CLA	O1A-CGA-O2A-C1
21	2	609	CLA	C2A-CAA-CBA-CGA
21	4	311	CLA	C2A-CAA-CBA-CGA
21	5	611	CLA	C2A-CAA-CBA-CGA
20	6	605	CHL	C6-C7-C8-C10
21	A	834	CLA	C1-C2-C3-C5
21	O	203	CLA	C1-C2-C3-C5
22	4	315	LUT	C1-C6-C7-C8
22	6	616	LUT	C1-C6-C7-C8
22	Y	615	LUT	C5-C6-C7-C8
24	5	617	BCR	C23-C24-C25-C26
24	5	617	BCR	C23-C24-C25-C30
24	6	618	BCR	C23-C24-C25-C26
24	6	618	BCR	C23-C24-C25-C30
24	6	620	BCR	C1-C6-C7-C8
24	6	620	BCR	C5-C6-C7-C8
24	B	846	BCR	C23-C24-C25-C26
24	L	308	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
24	L	308	BCR	C23-C24-C25-C30
24	A	854	BCR	C21-C22-C23-C24
21	1	602	CLA	C10-C11-C12-C13
21	1	609	CLA	C11-C12-C13-C15
21	2	612	CLA	C6-C7-C8-C9
21	1	608	CLA	C6-C7-C8-C10
21	1	608	CLA	C11-C12-C13-C15
21	2	604	CLA	C11-C12-C13-C15
21	3	602	CLA	C6-C7-C8-C10
21	A	803	CLA	C6-C7-C8-C10
21	A	803	CLA	C11-C12-C13-C15
21	A	813	CLA	C11-C10-C8-C7
21	A	819	CLA	C6-C7-C8-C10
21	A	826	CLA	C11-C12-C13-C15
21	A	827	CLA	C12-C13-C15-C16
21	A	829	CLA	C11-C10-C8-C7
21	A	840	CLA	C6-C7-C8-C10
21	A	843	CLA	C6-C7-C8-C10
21	B	801	CLA	C11-C12-C13-C15
21	B	805	CLA	C11-C12-C13-C15
21	B	805	CLA	C12-C13-C15-C16
21	B	807	CLA	C11-C12-C13-C15
21	B	816	CLA	C6-C7-C8-C10
21	B	817	CLA	C11-C10-C8-C7
21	B	822	CLA	C11-C10-C8-C7
21	B	823	CLA	C6-C7-C8-C10
21	B	838	CLA	C6-C7-C8-C10
21	B	840	CLA	C6-C7-C8-C10
21	B	840	CLA	C11-C12-C13-C15
21	Z	303	CLA	C6-C7-C8-C10
20	4	304	CHL	C1C-C2C-CMC-OMC
20	6	606	CHL	C1C-C2C-CMC-OMC
20	X	601	CHL	C1C-C2C-CMC-OMC
20	X	606	CHL	C1C-C2C-CMC-OMC
20	Z	308	CHL	C1C-C2C-CMC-OMC
21	A	806	CLA	C1-C2-C3-C4
21	2	612	CLA	C6-C7-C8-C10
21	A	834	CLA	C8-C10-C11-C12
21	2	612	CLA	C3-C5-C6-C7
21	6	609	CLA	C3-C5-C6-C7
21	A	808	CLA	O1A-CGA-O2A-C1
20	2	607	CHL	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
21	5	602	CLA	C12-C13-C15-C16
21	B	812	CLA	C8-C10-C11-C12
20	X	606	CHL	CAD-CBD-CGD-O2D
20	Y	605	CHL	CAD-CBD-CGD-O2D
20	Y	607	CHL	CAD-CBD-CGD-O2D
21	1	603	CLA	CAD-CBD-CGD-O2D
21	1	605	CLA	CAD-CBD-CGD-O2D
21	2	608	CLA	CAD-CBD-CGD-O2D
21	3	603	CLA	CAD-CBD-CGD-O2D
21	3	610	CLA	CAD-CBD-CGD-O2D
21	4	308	CLA	CAD-CBD-CGD-O2D
21	5	603	CLA	CAD-CBD-CGD-O2D
21	6	608	CLA	CAD-CBD-CGD-O2D
21	6	612	CLA	CAD-CBD-CGD-O2D
21	A	805	CLA	CAD-CBD-CGD-O2D
21	A	808	CLA	CAD-CBD-CGD-O2D
21	A	811	CLA	CAD-CBD-CGD-O2D
21	A	812	CLA	CAD-CBD-CGD-O2D
21	A	836	CLA	CAD-CBD-CGD-O2D
21	B	803	CLA	CAD-CBD-CGD-O2D
21	B	811	CLA	CAD-CBD-CGD-O2D
21	B	817	CLA	CAD-CBD-CGD-O2D
21	B	824	CLA	CAD-CBD-CGD-O2D
21	B	830	CLA	CAD-CBD-CGD-O2D
21	B	831	CLA	CAD-CBD-CGD-O2D
21	B	838	CLA	CAD-CBD-CGD-O2D
21	J	102	CLA	CAD-CBD-CGD-O2D
21	K	202	CLA	CAD-CBD-CGD-O2D
21	L	304	CLA	CAD-CBD-CGD-O2D
21	O	206	CLA	CAD-CBD-CGD-O2D
21	X	602	CLA	CAD-CBD-CGD-O2D
21	Y	610	CLA	CAD-CBD-CGD-O2D
21	Y	613	CLA	CAD-CBD-CGD-O2D
21	Z	304	CLA	CAD-CBD-CGD-O2D
26	5	620	LMG	C21-C22-C23-C24
20	1	601	CHL	CBA-CGA-O2A-C1
21	A	834	CLA	C16-C17-C18-C19
25	1	618	LHG	C4-C5-C6-O8
25	X	617	LHG	C2-C3-O3-P
26	1	619	LMG	C7-C8-C9-O8
26	1	621	LMG	O1-C7-C8-C9
26	5	621	LMG	C7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
21	A	828	CLA	C13-C15-C16-C17
21	B	813	CLA	C10-C11-C12-C13
21	1	604	CLA	O2A-C1-C2-C3
21	B	809	CLA	C2A-CAA-CBA-CGA
21	B	817	CLA	C2A-CAA-CBA-CGA
21	Z	305	CLA	C2A-CAA-CBA-CGA
21	1	603	CLA	CHA-CBD-CGD-O1D
21	1	613	CLA	CHA-CBD-CGD-O1D
21	2	604	CLA	CHA-CBD-CGD-O2D
21	2	612	CLA	CHA-CBD-CGD-O2D
21	3	604	CLA	CHA-CBD-CGD-O2D
21	4	301	CLA	CHA-CBD-CGD-O2D
21	4	302	CLA	CHA-CBD-CGD-O1D
21	5	609	CLA	CHA-CBD-CGD-O2D
21	6	601	CLA	CHA-CBD-CGD-O2D
21	6	604	CLA	CHA-CBD-CGD-O1D
21	A	806	CLA	CHA-CBD-CGD-O2D
21	A	809	CLA	CHA-CBD-CGD-O2D
21	A	813	CLA	CHA-CBD-CGD-O1D
21	A	813	CLA	CHA-CBD-CGD-O2D
21	A	815	CLA	CHA-CBD-CGD-O1D
21	A	824	CLA	CHA-CBD-CGD-O1D
21	A	825	CLA	CHA-CBD-CGD-O2D
21	A	837	CLA	CHA-CBD-CGD-O1D
21	A	840	CLA	CHA-CBD-CGD-O1D
21	B	807	CLA	CHA-CBD-CGD-O2D
21	B	809	CLA	CHA-CBD-CGD-O1D
21	B	809	CLA	CHA-CBD-CGD-O2D
21	B	814	CLA	CHA-CBD-CGD-O2D
21	B	822	CLA	CHA-CBD-CGD-O1D
21	B	822	CLA	CHA-CBD-CGD-O2D
21	B	823	CLA	CHA-CBD-CGD-O2D
21	B	825	CLA	CHA-CBD-CGD-O2D
21	B	840	CLA	CHA-CBD-CGD-O1D
21	L	303	CLA	CHA-CBD-CGD-O1D
21	L	303	CLA	CHA-CBD-CGD-O2D
21	L	304	CLA	CHA-CBD-CGD-O1D
21	X	603	CLA	CHA-CBD-CGD-O2D
21	X	604	CLA	CHA-CBD-CGD-O2D
21	Y	602	CLA	CHA-CBD-CGD-O1D
21	Y	604	CLA	CHA-CBD-CGD-O2D
21	Y	612	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
21	Z	304	CLA	CHA-CBD-CGD-O1D
21	Z	312	CLA	CHA-CBD-CGD-O1D
21	2	602	CLA	C3-C5-C6-C7
21	B	821	CLA	O1A-CGA-O2A-C1
25	1	618	LHG	O7-C5-C6-O8
25	A	853	LHG	O7-C5-C6-O8
25	Y	618	LHG	O7-C5-C6-O8
26	G	206	LMG	O1-C7-C8-O7
26	G	206	LMG	O7-C8-C9-O8
21	4	313	CLA	O1A-CGA-O2A-C1
21	B	837	CLA	O1A-CGA-O2A-C1
21	A	826	CLA	C3-C5-C6-C7
21	1	614	CLA	CBD-CGD-O2D-CED
21	A	813	CLA	C11-C10-C8-C9
21	A	843	CLA	C6-C7-C8-C9
21	Y	602	CLA	C14-C13-C15-C16
21	B	812	CLA	O1D-CGD-O2D-CED
21	B	815	CLA	O1D-CGD-O2D-CED
21	B	827	CLA	C13-C15-C16-C17
20	Y	608	CHL	C2A-CAA-CBA-CGA
21	1	613	CLA	C2A-CAA-CBA-CGA
21	3	609	CLA	C2A-CAA-CBA-CGA
21	H	201	CLA	C2A-CAA-CBA-CGA
21	Z	305	CLA	CBD-CGD-O2D-CED
21	B	833	CLA	C10-C11-C12-C13
21	B	819	CLA	O1D-CGD-O2D-CED
21	1	607	CLA	C1A-C2A-CAA-CBA
21	2	603	CLA	CHA-CBD-CGD-O2D
21	3	606	CLA	CHA-CBD-CGD-O2D
21	4	312	CLA	C1A-C2A-CAA-CBA
21	A	839	CLA	C1A-C2A-CAA-CBA
21	B	822	CLA	C1A-C2A-CAA-CBA
21	B	825	CLA	C1A-C2A-CAA-CBA
21	Y	610	CLA	C1A-C2A-CAA-CBA
21	B	802	CLA	C16-C17-C18-C19
21	B	815	CLA	C6-C7-C8-C9
21	A	817	CLA	O1D-CGD-O2D-CED
25	A	851	LHG	C4-O6-P-O3
21	B	829	CLA	O1D-CGD-O2D-CED
25	1	618	LHG	C33-C34-C35-C36
21	B	825	CLA	C3-C5-C6-C7
25	5	618	LHG	C5-C4-O6-P

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Mol	Chain	Res	Type	Atoms
21	Y	604	CLA	O1D-CGD-O2D-CED
20	4	304	CHL	C2-C3-C5-C6
21	A	803	CLA	C4B-C3B-CAB-CBB
21	A	808	CLA	C4B-C3B-CAB-CBB
21	A	827	CLA	C4B-C3B-CAB-CBB
21	B	828	CLA	C4B-C3B-CAB-CBB
25	1	622	LHG	C3-O3-P-O5
25	A	853	LHG	C3-O3-P-O5
25	Y	618	LHG	C3-O3-P-O5
25	Z	317	LHG	C3-O3-P-O4
21	5	604	CLA	O2A-C1-C2-C3
21	B	809	CLA	C13-C15-C16-C17
21	A	827	CLA	C3-C5-C6-C7
21	B	816	CLA	C3-C5-C6-C7
21	B	821	CLA	C3-C5-C6-C7
21	B	805	CLA	O1D-CGD-O2D-CED
20	2	601	CHL	CAD-CBD-CGD-O1D
20	Z	306	CHL	CAD-CBD-CGD-O1D
21	4	312	CLA	CAD-CBD-CGD-O1D
21	5	602	CLA	CAD-CBD-CGD-O1D
21	5	604	CLA	CAD-CBD-CGD-O1D
21	6	613	CLA	CAD-CBD-CGD-O1D
21	A	813	CLA	CAD-CBD-CGD-O1D
21	A	824	CLA	CAD-CBD-CGD-O1D
21	A	825	CLA	CAD-CBD-CGD-O1D
21	A	830	CLA	CAD-CBD-CGD-O1D
21	A	841	CLA	CAD-CBD-CGD-O1D
21	B	828	CLA	CAD-CBD-CGD-O1D
21	X	612	CLA	CAD-CBD-CGD-O1D
21	Z	312	CLA	CAD-CBD-CGD-O1D
21	A	840	CLA	C16-C17-C18-C20
21	A	826	CLA	C4-C3-C5-C6
21	1	608	CLA	C12-C13-C15-C16
21	A	807	CLA	C11-C10-C8-C7
21	A	825	CLA	C11-C12-C13-C15
21	A	833	CLA	C11-C10-C8-C7
21	A	840	CLA	C11-C10-C8-C7
21	B	809	CLA	C12-C13-C15-C16
21	B	825	CLA	C3A-C2A-CAA-CBA
21	B	827	CLA	C12-C13-C15-C16
21	B	831	CLA	C3A-C2A-CAA-CBA
21	B	839	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
21	B	840	CLA	C11-C10-C8-C7
21	L	301	CLA	C3A-C2A-CAA-CBA
21	Y	602	CLA	C6-C7-C8-C10
21	Z	303	CLA	C11-C10-C8-C7
21	1	602	CLA	C2A-CAA-CBA-CGA
21	2	611	CLA	C2A-CAA-CBA-CGA
21	6	602	CLA	C2A-CAA-CBA-CGA
21	B	809	CLA	C16-C17-C18-C19
21	B	801	CLA	CAA-CBA-CGA-O2A
21	2	604	CLA	C10-C11-C12-C13
21	B	831	CLA	C5-C6-C7-C8
26	6	619	LMG	O1-C7-C8-C9
26	G	206	LMG	O1-C7-C8-C9
26	1	621	LMG	O1-C7-C8-O7
26	1	621	LMG	O7-C8-C9-O8
26	5	620	LMG	O1-C7-C8-O7
26	5	621	LMG	O7-C8-C9-O8
26	1	619	LMG	C17-C18-C19-C20
21	B	831	CLA	O2A-C1-C2-C3
21	A	829	CLA	O1D-CGD-O2D-CED
21	1	608	CLA	C4-C3-C5-C6
21	B	809	CLA	C2-C3-C5-C6
21	L	301	CLA	C13-C15-C16-C17
21	1	608	CLA	C6-C7-C8-C9
21	1	608	CLA	C11-C10-C8-C9
21	4	311	CLA	C6-C7-C8-C9
21	A	803	CLA	C11-C12-C13-C14
21	A	807	CLA	C11-C12-C13-C14
21	A	826	CLA	C11-C12-C13-C14
21	A	840	CLA	C6-C7-C8-C9
21	B	805	CLA	C11-C12-C13-C14
21	B	809	CLA	C6-C7-C8-C9
21	B	812	CLA	C14-C13-C15-C16
21	B	813	CLA	C11-C10-C8-C9
21	B	816	CLA	C6-C7-C8-C9
21	B	817	CLA	C11-C10-C8-C9
21	B	836	CLA	C11-C10-C8-C9
21	B	840	CLA	C11-C12-C13-C14
24	O	201	BCR	C6-C7-C8-C9
21	B	816	CLA	C2A-CAA-CBA-CGA
24	2	619	BCR	C10-C11-C12-C13
24	6	620	BCR	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
24	A	846	BCR	C18-C19-C20-C21
24	A	849	BCR	C10-C11-C12-C13
21	1	608	CLA	C16-C17-C18-C20
21	B	810	CLA	C5-C6-C7-C8
21	B	828	CLA	C2B-C3B-CAB-CBB
21	A	833	CLA	C4-C3-C5-C6
21	3	617	CLA	C2-C3-C5-C6
21	A	842	CLA	C8-C10-C11-C12
21	A	834	CLA	C16-C17-C18-C20
21	B	840	CLA	C16-C17-C18-C19
21	Y	602	CLA	C16-C17-C18-C20
20	1	601	CHL	CAA-CBA-CGA-O2A
21	A	841	CLA	C8-C10-C11-C12
21	B	823	CLA	C5-C6-C7-C8
20	X	607	CHL	C2A-CAA-CBA-CGA
21	6	612	CLA	C2-C1-O2A-CGA
21	A	813	CLA	C2-C1-O2A-CGA
21	A	818	CLA	C2-C1-O2A-CGA
21	A	840	CLA	C2-C1-O2A-CGA
21	3	603	CLA	C3-C5-C6-C7
21	4	309	CLA	C3-C5-C6-C7
21	A	818	CLA	CAA-CBA-CGA-O2A
21	A	829	CLA	C16-C17-C18-C20
21	B	836	CLA	C16-C17-C18-C19
24	B	846	BCR	C23-C24-C25-C30
24	B	848	BCR	C5-C6-C7-C8
21	B	836	CLA	C8-C10-C11-C12
26	1	619	LMG	O7-C8-C9-O8
21	A	813	CLA	C1-C2-C3-C5
25	1	618	LHG	C4-O6-P-O3
25	1	620	LHG	C3-O3-P-O6
25	2	617	LHG	C3-O3-P-O6
21	B	825	CLA	CBD-CGD-O2D-CED
20	3	608	CHL	CHA-CBD-CGD-O2D
20	6	606	CHL	CHA-CBD-CGD-O2D
20	Z	302	CHL	CHA-CBD-CGD-O1D
21	A	838	CLA	C4-C3-C5-C6
21	B	828	CLA	C5-C6-C7-C8
21	A	828	CLA	C12-C13-C15-C16
21	B	802	CLA	C6-C7-C8-C10
21	B	839	CLA	C11-C10-C8-C7
21	A	807	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
21	A	811	CLA	C11-C12-C13-C14
21	A	819	CLA	C11-C12-C13-C14
21	A	840	CLA	C11-C10-C8-C9
21	B	827	CLA	C6-C7-C8-C9
20	6	605	CHL	C6-C7-C8-C9
21	A	827	CLA	C16-C17-C18-C20
21	2	608	CLA	C2A-CAA-CBA-CGA
25	2	617	LHG	C2-C3-O3-P
21	A	802	CLA	C15-C16-C17-C18
24	B	848	BCR	C17-C18-C19-C20
21	A	826	CLA	C2C-C3C-CAC-CBC
21	A	835	CLA	CBD-CGD-O2D-CED
25	X	617	LHG	C26-C27-C28-C29
26	5	621	LMG	C20-C21-C22-C23
21	3	603	CLA	C4-C3-C5-C6
21	B	836	CLA	C2-C3-C5-C6
21	3	617	CLA	C6-C7-C8-C10
21	A	817	CLA	C11-C12-C13-C14
21	B	805	CLA	C16-C17-C18-C19
28	A	844	PQN	C26-C27-C28-C30
21	B	807	CLA	C5-C6-C7-C8
20	Y	601	CHL	CAA-CBA-CGA-O1A
20	2	601	CHL	CBA-CGA-O2A-C1
21	2	604	CLA	O1A-CGA-O2A-C1
21	A	837	CLA	CBD-CGD-O2D-CED
27	4	319	LMT	C11-C10-C9-C8
21	A	843	CLA	C5-C6-C7-C8
21	A	826	CLA	C16-C17-C18-C20
21	A	829	CLA	C1-C2-C3-C5
21	Y	610	CLA	CAA-CBA-CGA-O2A
21	4	309	CLA	C5-C6-C7-C8
21	B	817	CLA	C8-C10-C11-C12
27	F	303	LMT	C5'-C4'-O1B-C1B
21	5	602	CLA	C14-C13-C15-C16
20	1	601	CHL	C2-C1-O2A-CGA
20	6	605	CHL	C2-C1-O2A-CGA
21	3	603	CLA	C2-C1-O2A-CGA
21	6	602	CLA	C2-C1-O2A-CGA
21	A	807	CLA	C2-C1-O2A-CGA
21	A	817	CLA	C2-C1-O2A-CGA
21	Y	602	CLA	C2-C1-O2A-CGA
21	2	618	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
21	A	825	CLA	C8-C10-C11-C12
21	3	603	CLA	C2A-CAA-CBA-CGA
21	A	828	CLA	C2A-CAA-CBA-CGA
21	A	840	CLA	C2A-CAA-CBA-CGA
21	B	804	CLA	C2A-CAA-CBA-CGA
21	Y	612	CLA	C2A-CAA-CBA-CGA
25	A	851	LHG	C31-C32-C33-C34
26	G	206	LMG	C11-C12-C13-C14
21	1	604	CLA	C3A-C2A-CAA-CBA
21	1	614	CLA	C3A-C2A-CAA-CBA
21	2	603	CLA	C3A-C2A-CAA-CBA
21	2	618	CLA	C3A-C2A-CAA-CBA
21	A	833	CLA	C3A-C2A-CAA-CBA
21	B	809	CLA	C3A-C2A-CAA-CBA
21	B	821	CLA	C3A-C2A-CAA-CBA
21	B	835	CLA	C3A-C2A-CAA-CBA
21	H	201	CLA	C3A-C2A-CAA-CBA
21	Y	610	CLA	CAA-CBA-CGA-O1A
26	5	620	LMG	C11-C12-C13-C14
21	B	809	CLA	C4-C3-C5-C6
21	A	806	CLA	C11-C10-C8-C9
21	A	819	CLA	C11-C10-C8-C9
21	A	827	CLA	C6-C7-C8-C9
21	A	830	CLA	C11-C10-C8-C9
21	A	834	CLA	C11-C12-C13-C14
21	B	804	CLA	C14-C13-C15-C16
21	B	823	CLA	C11-C12-C13-C14
21	3	617	CLA	C6-C7-C8-C9
21	B	815	CLA	C6-C7-C8-C10
21	B	821	CLA	C6-C7-C8-C10
24	A	848	BCR	C11-C10-C9-C34
24	A	848	BCR	C16-C17-C18-C36
24	A	849	BCR	C16-C17-C18-C36
24	B	844	BCR	C11-C10-C9-C34
24	B	844	BCR	C20-C21-C22-C37
24	F	305	BCR	C35-C13-C14-C15
24	L	308	BCR	C11-C10-C9-C34
31	X	616	NEX	C39-C29-C30-C31
31	Y	617	NEX	C39-C29-C30-C31
31	Z	316	NEX	C11-C10-C9-C19
20	Y	607	CHL	CAA-CBA-CGA-O2A
20	Z	307	CHL	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
21	B	831	CLA	C2A-CAA-CBA-CGA
21	A	812	CLA	O2A-C1-C2-C3
26	1	619	LMG	C11-C12-C13-C14
20	Y	601	CHL	CAA-CBA-CGA-O2A
21	G	202	CLA	CAA-CBA-CGA-O1A
21	Z	312	CLA	CAA-CBA-CGA-O1A
21	Z	304	CLA	CAA-CBA-CGA-O1A
21	B	840	CLA	C4-C3-C5-C6
21	1	614	CLA	C1A-C2A-CAA-CBA
21	2	603	CLA	C1A-C2A-CAA-CBA
21	2	618	CLA	C1A-C2A-CAA-CBA
21	5	612	CLA	C1A-C2A-CAA-CBA
21	A	836	CLA	C1A-C2A-CAA-CBA
21	L	301	CLA	C1A-C2A-CAA-CBA
21	6	601	CLA	CAA-CBA-CGA-O2A
21	2	604	CLA	C12-C13-C15-C16
21	A	803	CLA	C11-C10-C8-C7
21	A	813	CLA	C11-C12-C13-C15
21	A	828	CLA	C11-C12-C13-C15
21	B	807	CLA	C11-C10-C8-C7
21	B	816	CLA	C11-C10-C8-C7
21	B	817	CLA	C6-C7-C8-C10
21	B	823	CLA	C12-C13-C15-C16
21	B	827	CLA	C11-C10-C8-C7
28	A	844	PQN	C17-C18-C20-C21
21	3	607	CLA	CAA-CBA-CGA-O1A
21	L	305	CLA	CAA-CBA-CGA-O1A
21	X	610	CLA	CAA-CBA-CGA-O2A
21	A	825	CLA	O1D-CGD-O2D-CED
21	A	829	CLA	C5-C6-C7-C8
20	X	606	CHL	C3C-C2C-CMC-OMC
20	Y	619	CHL	C3C-C2C-CMC-OMC
25	2	617	LHG	C5-C4-O6-P
21	A	829	CLA	C2A-CAA-CBA-CGA
21	B	825	CLA	C2A-CAA-CBA-CGA
21	5	603	CLA	CAA-CBA-CGA-O1A
21	1	612	CLA	C16-C17-C18-C19
21	A	813	CLA	C16-C17-C18-C19
21	A	826	CLA	C16-C17-C18-C19
20	X	608	CHL	CAA-CBA-CGA-O1A
20	Z	307	CHL	CAA-CBA-CGA-O2A
21	A	816	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
21	2	604	CLA	C4-C3-C5-C6
21	Y	602	CLA	C4-C3-C5-C6
21	Z	303	CLA	C10-C11-C12-C13
21	A	803	CLA	C2B-C3B-CAB-CBB
21	A	808	CLA	C2B-C3B-CAB-CBB
21	A	827	CLA	C2B-C3B-CAB-CBB
21	1	611	CLA	CAA-CBA-CGA-O1A
21	G	204	CLA	CAA-CBA-CGA-O2A
21	Z	312	CLA	CAA-CBA-CGA-O2A
20	X	607	CHL	CBD-CGD-O2D-CED
24	A	848	BCR	C11-C10-C9-C8
24	A	848	BCR	C16-C17-C18-C19
24	A	849	BCR	C16-C17-C18-C19
24	B	844	BCR	C11-C10-C9-C8
24	B	844	BCR	C20-C21-C22-C23
24	F	305	BCR	C12-C13-C14-C15
24	L	308	BCR	C11-C10-C9-C8
31	X	616	NEX	C28-C29-C30-C31
31	Y	617	NEX	C28-C29-C30-C31
31	Z	316	NEX	C11-C10-C9-C8
21	5	603	CLA	CAA-CBA-CGA-O2A
21	5	611	CLA	CAA-CBA-CGA-O2A
21	4	308	CLA	CBA-CGA-O2A-C1
21	1	609	CLA	O1D-CGD-O2D-CED
20	X	601	CHL	CAA-CBA-CGA-O2A
21	Y	603	CLA	CAA-CBA-CGA-O2A
20	4	306	CHL	O1D-CGD-O2D-CED
21	A	841	CLA	CAA-CBA-CGA-O2A
21	X	618	CLA	CAA-CBA-CGA-O2A
21	B	821	CLA	C4-C3-C5-C6
20	4	304	CHL	C2-C1-O2A-CGA
20	6	607	CHL	C2-C1-O2A-CGA
21	A	839	CLA	C2-C1-O2A-CGA
21	B	820	CLA	C5-C6-C7-C8
21	2	611	CLA	CAA-CBA-CGA-O1A
21	A	821	CLA	C11-C12-C13-C14
21	B	809	CLA	C14-C13-C15-C16
21	B	831	CLA	C11-C12-C13-C14
28	B	841	PQN	C16-C17-C18-C19
21	3	607	CLA	CAA-CBA-CGA-O2A
20	3	608	CHL	C1A-C2A-CAA-CBA
20	6	606	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	X	601	CHL	C1A-C2A-CAA-CBA
20	Y	619	CHL	C1A-C2A-CAA-CBA
21	A	821	CLA	C15-C16-C17-C18
21	X	613	CLA	CAA-CBA-CGA-O2A
21	6	609	CLA	CBD-CGD-O2D-CED
22	1	615	LUT	C1-C6-C7-C8
22	2	615	LUT	C1-C6-C7-C8
24	2	619	BCR	C23-C24-C25-C30
24	B	848	BCR	C1-C6-C7-C8
21	A	801	CLA	C5-C6-C7-C8
21	L	303	CLA	CAA-CBA-CGA-O2A
21	Z	310	CLA	CAA-CBA-CGA-O2A
21	B	815	CLA	C4-C3-C5-C6
28	B	841	PQN	C14-C13-C15-C16
21	4	310	CLA	C1A-C2A-CAA-CBA
21	B	834	CLA	C1A-C2A-CAA-CBA
21	B	818	CLA	C5-C6-C7-C8
21	2	608	CLA	CAA-CBA-CGA-O2A
21	A	820	CLA	CAA-CBA-CGA-O2A
21	X	611	CLA	CAA-CBA-CGA-O2A
21	Z	310	CLA	CAA-CBA-CGA-O1A
21	A	818	CLA	C5-C6-C7-C8
25	A	851	LHG	C32-C33-C34-C35
21	2	602	CLA	C16-C17-C18-C20
28	A	844	PQN	C26-C27-C28-C29
20	X	608	CHL	CAA-CBA-CGA-O2A
21	2	611	CLA	CAA-CBA-CGA-O2A
21	X	609	CLA	CAA-CBA-CGA-O2A
21	1	604	CLA	C2A-CAA-CBA-CGA
21	A	821	CLA	C2A-CAA-CBA-CGA
21	L	305	CLA	CAA-CBA-CGA-O2A
20	1	601	CHL	C4-C3-C5-C6
21	X	603	CLA	C4-C3-C5-C6
21	2	602	CLA	C6-C7-C8-C10
21	A	826	CLA	C12-C13-C15-C16
21	A	841	CLA	C12-C13-C15-C16
21	Y	613	CLA	C2-C3-C5-C6
21	5	611	CLA	CAA-CBA-CGA-O1A
21	G	204	CLA	CAA-CBA-CGA-O1A
21	Y	603	CLA	CAA-CBA-CGA-O1A
20	4	305	CHL	C1C-C2C-CMC-OMC
20	Y	607	CHL	C1C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
20	Z	302	CHL	C1C-C2C-CMC-OMC
21	3	617	CLA	C1-C2-C3-C4
21	6	612	CLA	C1-C2-C3-C4
21	A	801	CLA	C1-C2-C3-C4
21	A	812	CLA	C1-C2-C3-C4
21	B	808	CLA	C1-C2-C3-C4
21	B	813	CLA	C1-C2-C3-C4
21	B	817	CLA	C1-C2-C3-C4
21	Y	602	CLA	C1-C2-C3-C4
21	X	618	CLA	CAA-CBA-CGA-O1A
21	B	816	CLA	CAA-CBA-CGA-O2A
21	Y	602	CLA	CAA-CBA-CGA-O2A
21	B	810	CLA	O1A-CGA-O2A-C1
20	4	304	CHL	C2A-CAA-CBA-CGA
21	B	835	CLA	C2A-CAA-CBA-CGA
21	B	840	CLA	C2A-CAA-CBA-CGA
21	1	612	CLA	C16-C17-C18-C20
21	A	813	CLA	C16-C17-C18-C20
21	3	612	CLA	CAA-CBA-CGA-O2A
21	5	609	CLA	CAA-CBA-CGA-O2A
21	Y	614	CLA	CAA-CBA-CGA-O1A
21	A	833	CLA	CAA-CBA-CGA-O2A
21	2	612	CLA	C4-C3-C5-C6
21	2	608	CLA	CAA-CBA-CGA-O1A
25	X	617	LHG	C4-O6-P-O3
21	A	806	CLA	C2-C3-C5-C6
21	B	816	CLA	C2-C3-C5-C6
25	1	622	LHG	O7-C7-C8-C9
21	A	841	CLA	C11-C10-C8-C9
21	B	831	CLA	C14-C13-C15-C16
21	B	838	CLA	C11-C10-C8-C9
21	B	839	CLA	C11-C12-C13-C14
21	B	840	CLA	C11-C10-C8-C9
21	Z	304	CLA	CAA-CBA-CGA-O2A
20	2	607	CHL	C3A-C2A-CAA-CBA
20	Z	307	CHL	C3A-C2A-CAA-CBA
21	4	313	CLA	C3A-C2A-CAA-CBA
21	A	811	CLA	C3A-C2A-CAA-CBA
21	A	837	CLA	C3A-C2A-CAA-CBA
21	B	833	CLA	C3A-C2A-CAA-CBA
21	B	838	CLA	C3A-C2A-CAA-CBA
20	Y	607	CHL	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
21	1	611	CLA	CAA-CBA-CGA-O2A
21	1	613	CLA	CAA-CBA-CGA-O2A
21	G	202	CLA	CAA-CBA-CGA-O2A
20	2	605	CHL	CAD-CBD-CGD-O2D
20	Z	308	CHL	CAD-CBD-CGD-O2D
21	1	608	CLA	CAD-CBD-CGD-O2D
21	1	612	CLA	CAD-CBD-CGD-O2D
21	3	602	CLA	CAD-CBD-CGD-O2D
21	4	307	CLA	CAD-CBD-CGD-O2D
21	5	602	CLA	CAD-CBD-CGD-O2D
21	5	614	CLA	CAD-CBD-CGD-O2D
21	6	603	CLA	CAD-CBD-CGD-O2D
21	6	609	CLA	CAD-CBD-CGD-O2D
21	A	810	CLA	CAD-CBD-CGD-O2D
21	A	815	CLA	CAD-CBD-CGD-O2D
21	A	819	CLA	CAD-CBD-CGD-O2D
21	A	823	CLA	CAD-CBD-CGD-O2D
21	A	824	CLA	CAD-CBD-CGD-O2D
21	A	826	CLA	CAD-CBD-CGD-O2D
21	A	827	CLA	CAD-CBD-CGD-O2D
21	A	831	CLA	CAD-CBD-CGD-O2D
21	A	833	CLA	CAD-CBD-CGD-O2D
21	A	843	CLA	CAD-CBD-CGD-O2D
21	B	819	CLA	CAD-CBD-CGD-O2D
21	B	821	CLA	CAD-CBD-CGD-O2D
21	B	826	CLA	CAD-CBD-CGD-O2D
21	B	829	CLA	CAD-CBD-CGD-O2D
21	B	840	CLA	CAD-CBD-CGD-O2D
21	G	203	CLA	CAD-CBD-CGD-O2D
21	G	204	CLA	CAD-CBD-CGD-O2D
21	K	203	CLA	CAD-CBD-CGD-O2D
21	O	202	CLA	CAD-CBD-CGD-O2D
21	X	612	CLA	CAD-CBD-CGD-O2D
21	Y	603	CLA	CAD-CBD-CGD-O2D
21	Y	614	CLA	CAD-CBD-CGD-O2D
21	Z	310	CLA	CAD-CBD-CGD-O2D
21	4	303	CLA	C2A-CAA-CBA-CGA
21	Y	603	CLA	C2A-CAA-CBA-CGA
21	X	603	CLA	C3-C5-C6-C7
20	2	607	CHL	C1-C2-C3-C5
21	A	816	CLA	CAA-CBA-CGA-O2A
21	5	612	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
21	B	813	CLA	C4-C3-C5-C6
21	X	610	CLA	CAA-CBA-CGA-O1A
21	B	820	CLA	C2-C3-C5-C6
20	4	304	CHL	CAA-CBA-CGA-O2A
21	A	804	CLA	CAA-CBA-CGA-O2A
24	2	619	BCR	C21-C22-C23-C24
24	O	201	BCR	C7-C8-C9-C10
23	O	208	XAT	O24-C26-C27-C28
21	4	301	CLA	CAA-CBA-CGA-O2A
21	5	602	CLA	CAA-CBA-CGA-O2A
21	B	840	CLA	CAA-CBA-CGA-O2A
21	5	609	CLA	CAA-CBA-CGA-O1A
21	4	311	CLA	O2A-C1-C2-C3
21	4	313	CLA	O2A-C1-C2-C3
21	6	612	CLA	O2A-C1-C2-C3
21	6	614	CLA	O2A-C1-C2-C3
21	A	818	CLA	O2A-C1-C2-C3
21	B	802	CLA	O2A-C1-C2-C3
21	B	820	CLA	O2A-C1-C2-C3
21	B	821	CLA	O2A-C1-C2-C3
21	Y	602	CLA	O2A-C1-C2-C3
21	A	809	CLA	CBA-CGA-O2A-C1
21	1	614	CLA	C2A-CAA-CBA-CGA
21	A	834	CLA	C2A-CAA-CBA-CGA
21	1	602	CLA	CAA-CBA-CGA-O2A
26	5	620	LMG	C19-C20-C21-C22
21	1	612	CLA	O1D-CGD-O2D-CED
21	1	602	CLA	CHA-CBD-CGD-O2D
21	2	610	CLA	CHA-CBD-CGD-O2D
21	3	617	CLA	CHA-CBD-CGD-O1D
21	3	617	CLA	CHA-CBD-CGD-O2D
21	4	311	CLA	CHA-CBD-CGD-O2D
21	4	313	CLA	CHA-CBD-CGD-O2D
21	5	602	CLA	CHA-CBD-CGD-O1D
21	5	609	CLA	CHA-CBD-CGD-O1D
21	6	614	CLA	CHA-CBD-CGD-O2D
21	A	804	CLA	CHA-CBD-CGD-O2D
21	A	807	CLA	CHA-CBD-CGD-O1D
21	A	818	CLA	CHA-CBD-CGD-O2D
21	A	819	CLA	CHA-CBD-CGD-O2D
21	A	822	CLA	CHA-CBD-CGD-O2D
21	A	825	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
21	B	808	CLA	CHA-CBD-CGD-O2D
21	B	812	CLA	CHA-CBD-CGD-O2D
21	B	816	CLA	CHA-CBD-CGD-O1D
21	B	837	CLA	CHA-CBD-CGD-O2D
21	H	201	CLA	CHA-CBD-CGD-O1D
21	O	202	CLA	CHA-CBD-CGD-O2D
21	Y	612	CLA	CHA-CBD-CGD-O2D
21	Y	614	CLA	CHA-CBD-CGD-O1D
21	Z	305	CLA	CHA-CBD-CGD-O1D
21	Z	305	CLA	CHA-CBD-CGD-O2D
21	Z	313	CLA	CHA-CBD-CGD-O2D
20	Z	302	CHL	CAA-CBA-CGA-O1A
21	Y	614	CLA	CAA-CBA-CGA-O2A
26	5	621	LMG	O7-C10-C11-C12
26	6	619	LMG	O8-C28-C29-C30
28	B	841	PQN	C12-C13-C15-C16
25	A	851	LHG	C28-C29-C30-C31
26	5	620	LMG	C33-C34-C35-C36
21	K	202	CLA	CAA-CBA-CGA-O2A
30	B	849	DGD	CBB-CCB-CDB-CEB
21	1	609	CLA	C11-C12-C13-C14
21	3	603	CLA	O1A-CGA-O2A-C1
21	B	801	CLA	C8-C10-C11-C12
21	2	609	CLA	C3-C5-C6-C7
21	A	807	CLA	C15-C16-C17-C18
25	5	618	LHG	O8-C23-C24-C25
25	X	617	LHG	O7-C7-C8-C9
26	4	318	LMG	O8-C28-C29-C30
26	G	206	LMG	O7-C10-C11-C12
20	2	601	CHL	C2A-CAA-CBA-CGA
21	B	812	CLA	C16-C17-C18-C19
21	B	838	CLA	C16-C17-C18-C19
21	3	609	CLA	CAA-CBA-CGA-O2A
20	2	606	CHL	CHA-CBD-CGD-O1D
20	X	601	CHL	CHA-CBD-CGD-O1D
20	X	606	CHL	CHA-CBD-CGD-O1D
20	Y	608	CHL	CHA-CBD-CGD-O1D
20	Y	609	CHL	CHA-CBD-CGD-O1D
21	B	804	CLA	C5-C6-C7-C8
21	2	602	CLA	CAA-CBA-CGA-O2A
21	2	609	CLA	CAA-CBA-CGA-O2A
21	A	807	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
21	B	822	CLA	CAA-CBA-CGA-O2A
21	B	812	CLA	C10-C11-C12-C13
21	A	834	CLA	C11-C10-C8-C7
21	B	826	CLA	C11-C10-C8-C7
21	O	203	CLA	C12-C13-C15-C16
25	2	617	LHG	O8-C23-C24-C25
21	6	609	CLA	C6-C7-C8-C9
26	B	850	LMG	C21-C22-C23-C24
21	2	602	CLA	C6-C7-C8-C9
21	6	612	CLA	C11-C10-C8-C9
21	A	801	CLA	C14-C13-C15-C16
21	A	841	CLA	C14-C13-C15-C16
21	B	823	CLA	C14-C13-C15-C16
21	B	826	CLA	C11-C10-C8-C9
21	B	827	CLA	C11-C10-C8-C9
21	L	301	CLA	C14-C13-C15-C16
20	4	304	CHL	O1A-CGA-O2A-C1
21	X	604	CLA	CAA-CBA-CGA-O2A
21	A	802	CLA	O1A-CGA-O2A-C1
21	2	612	CLA	C2A-CAA-CBA-CGA
21	2	618	CLA	C2A-CAA-CBA-CGA
21	6	608	CLA	C2A-CAA-CBA-CGA
21	A	838	CLA	C2A-CAA-CBA-CGA
21	A	810	CLA	CAA-CBA-CGA-O2A
21	A	821	CLA	CAA-CBA-CGA-O1A
21	A	819	CLA	C2-C3-C5-C6
21	A	817	CLA	CAA-CBA-CGA-O2A
25	X	617	LHG	O8-C23-C24-C25
21	L	303	CLA	CAA-CBA-CGA-O1A
21	2	609	CLA	CAA-CBA-CGA-O1A
24	B	846	BCR	C21-C22-C23-C24
21	A	832	CLA	O1D-CGD-O2D-CED
20	5	601	CHL	CHA-CBD-CGD-O1D
20	5	601	CHL	CHA-CBD-CGD-O2D
20	5	606	CHL	CHA-CBD-CGD-O1D
21	1	604	CLA	C1A-C2A-CAA-CBA
21	3	611	CLA	C1A-C2A-CAA-CBA
21	4	313	CLA	C1A-C2A-CAA-CBA
21	5	607	CLA	CHA-CBD-CGD-O2D
21	A	811	CLA	C1A-C2A-CAA-CBA
21	A	833	CLA	C1A-C2A-CAA-CBA
21	A	837	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
21	B	816	CLA	C1A-C2A-CAA-CBA
21	B	832	CLA	C1A-C2A-CAA-CBA
21	B	835	CLA	C1A-C2A-CAA-CBA
21	B	838	CLA	C1A-C2A-CAA-CBA
21	G	204	CLA	C1A-C2A-CAA-CBA
21	K	204	CLA	CHA-CBD-CGD-O2D
21	A	827	CLA	C16-C17-C18-C19
21	B	821	CLA	CAA-CBA-CGA-O1A
21	B	840	CLA	CAA-CBA-CGA-O1A
25	2	617	LHG	O10-C23-C24-C25
21	A	835	CLA	CAA-CBA-CGA-O1A
20	1	606	CHL	C2C-C3C-CAC-CBC
21	6	614	CLA	C2-C1-O2A-CGA
21	B	814	CLA	CBA-CGA-O2A-C1
21	B	823	CLA	CBA-CGA-O2A-C1
21	A	825	CLA	CAA-CBA-CGA-O1A
21	Y	602	CLA	CAA-CBA-CGA-O1A
26	6	619	LMG	O10-C28-C29-C30
21	6	603	CLA	CAA-CBA-CGA-O1A
21	X	602	CLA	CAA-CBA-CGA-O2A
21	X	613	CLA	CAA-CBA-CGA-O1A
25	A	853	LHG	C4-C5-C6-O8
26	F	307	LMG	O1-C7-C8-C9
20	3	608	CHL	C2A-CAA-CBA-CGA
21	4	301	CLA	C2A-CAA-CBA-CGA
21	A	819	CLA	C2A-CAA-CBA-CGA
21	G	202	CLA	C2A-CAA-CBA-CGA
21	Y	610	CLA	C2A-CAA-CBA-CGA
21	B	805	CLA	CAA-CBA-CGA-O1A
25	X	617	LHG	O9-C7-C8-C9
20	Z	302	CHL	CAA-CBA-CGA-O2A
21	A	806	CLA	CAA-CBA-CGA-O2A
21	B	808	CLA	C5-C6-C7-C8
20	4	304	CHL	CAA-CBA-CGA-O1A
21	2	602	CLA	CAA-CBA-CGA-O1A
21	A	817	CLA	CAA-CBA-CGA-O1A
25	1	622	LHG	O9-C7-C8-C9
25	5	618	LHG	O10-C23-C24-C25
26	G	206	LMG	O9-C10-C11-C12
21	1	610	CLA	C4B-C3B-CAB-CBB
21	B	808	CLA	C4B-C3B-CAB-CBB
21	X	604	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	1	618	LHG	C4-O6-P-O5
25	X	617	LHG	C4-O6-P-O5
21	A	801	CLA	CAA-CBA-CGA-O1A
21	A	806	CLA	CAA-CBA-CGA-O1A
21	A	833	CLA	CAA-CBA-CGA-O1A
26	5	621	LMG	O9-C10-C11-C12
24	B	843	BCR	C1-C6-C7-C8
21	B	814	CLA	CAA-CBA-CGA-O2A
21	4	307	CLA	CAA-CBA-CGA-O1A
21	1	603	CLA	CAA-CBA-CGA-O1A
21	4	301	CLA	CAA-CBA-CGA-O1A
21	B	822	CLA	CAA-CBA-CGA-O1A
21	A	818	CLA	O1A-CGA-O2A-C1
21	A	818	CLA	CAA-CBA-CGA-O1A
21	4	309	CLA	C4-C3-C5-C6
21	1	608	CLA	C2-C3-C5-C6
21	5	614	CLA	CAA-CBA-CGA-O1A
20	2	605	CHL	CAD-CBD-CGD-O1D
21	1	614	CLA	CAD-CBD-CGD-O1D
21	2	602	CLA	CAD-CBD-CGD-O1D
21	2	612	CLA	CAD-CBD-CGD-O1D
21	2	613	CLA	CAD-CBD-CGD-O1D
21	A	801	CLA	CAD-CBD-CGD-O1D
21	A	806	CLA	CAD-CBD-CGD-O1D
21	A	808	CLA	CAD-CBD-CGD-O1D
21	A	810	CLA	CAD-CBD-CGD-O1D
21	A	827	CLA	CAD-CBD-CGD-O1D
21	B	803	CLA	CAD-CBD-CGD-O1D
21	B	811	CLA	CAD-CBD-CGD-O1D
21	B	817	CLA	CAD-CBD-CGD-O1D
21	B	825	CLA	CAD-CBD-CGD-O1D
21	B	838	CLA	CAD-CBD-CGD-O1D
21	G	202	CLA	CAD-CBD-CGD-O1D
21	X	611	CLA	CAD-CBD-CGD-O1D
21	Y	610	CLA	CAD-CBD-CGD-O1D
21	Z	311	CLA	CAD-CBD-CGD-O1D
21	5	602	CLA	CAA-CBA-CGA-O1A
21	A	807	CLA	CAA-CBA-CGA-O1A
26	F	306	LMG	C32-C33-C34-C35
21	A	825	CLA	C6-C7-C8-C9
28	B	841	PQN	C21-C22-C23-C24
25	2	617	LHG	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
21	A	821	CLA	CAA-CBA-CGA-O2A
25	2	617	LHG	O7-C7-C8-C9
25	A	853	LHG	O7-C7-C8-C9
21	L	304	CLA	C5-C6-C7-C8
21	5	608	CLA	CAA-CBA-CGA-O1A
26	1	621	LMG	C20-C21-C22-C23
21	Z	313	CLA	C2A-CAA-CBA-CGA
21	A	834	CLA	CAA-CBA-CGA-O2A
21	O	203	CLA	CAA-CBA-CGA-O2A
21	1	614	CLA	CAA-CBA-CGA-O2A
26	4	318	LMG	O10-C28-C29-C30
21	A	815	CLA	CBD-CGD-O2D-CED
26	5	621	LMG	C24-C25-C26-C27
20	6	606	CHL	C3A-C2A-CAA-CBA
20	Z	309	CHL	C3A-C2A-CAA-CBA
21	3	606	CLA	CHA-CBD-CGD-O1D
21	5	607	CLA	CAD-CBD-CGD-O2D
21	5	614	CLA	C3A-C2A-CAA-CBA
21	6	612	CLA	C11-C10-C8-C7
21	A	807	CLA	C12-C13-C15-C16
21	A	821	CLA	C11-C12-C13-C15
21	B	832	CLA	C3A-C2A-CAA-CBA
21	H	201	CLA	C6-C7-C8-C10
21	K	204	CLA	CAD-CBD-CGD-O2D
21	O	207	CLA	CAD-CBD-CGD-O2D
22	X	615	LUT	C25-C26-C27-C28
26	6	619	LMG	C28-C29-C30-C31
20	Z	301	CHL	CAA-CBA-CGA-O1A
21	6	610	CLA	CAA-CBA-CGA-O1A
20	3	608	CHL	CAA-CBA-CGA-O2A
21	3	605	CLA	CAA-CBA-CGA-O2A
21	B	819	CLA	CAA-CBA-CGA-O2A
21	O	206	CLA	CAA-CBA-CGA-O2A
25	Y	618	LHG	O8-C23-C24-C25
26	1	619	LMG	O7-C10-C11-C12
20	2	606	CHL	C2C-C3C-CAC-CBC
20	2	607	CHL	CAA-CBA-CGA-O1A
21	B	823	CLA	CAA-CBA-CGA-O1A
26	1	619	LMG	O9-C10-C11-C12
20	X	601	CHL	CAA-CBA-CGA-O1A
20	Y	609	CHL	CAA-CBA-CGA-O1A
21	A	802	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
21	B	808	CLA	CAA-CBA-CGA-O2A
21	B	818	CLA	CAA-CBA-CGA-O1A
21	O	203	CLA	CAA-CBA-CGA-O1A
25	X	617	LHG	O10-C23-C24-C25
21	6	602	CLA	O1D-CGD-O2D-CED
21	Z	313	CLA	CAA-CBA-CGA-O2A
25	1	620	LHG	O8-C23-C24-C25
25	Y	618	LHG	O7-C7-C8-C9
21	A	829	CLA	C13-C15-C16-C17
21	A	841	CLA	C5-C6-C7-C8
21	B	827	CLA	CAA-CBA-CGA-O1A
25	2	617	LHG	O9-C7-C8-C9
20	5	601	CHL	C2A-CAA-CBA-CGA
21	1	614	CLA	CAA-CBA-CGA-O1A
21	1	603	CLA	C5-C6-C7-C8

There are no ring outliers.

239 monomers are involved in 453 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	B	822	CLA	2	0
21	2	612	CLA	2	0
21	B	821	CLA	1	0
21	B	809	CLA	6	0
21	A	824	CLA	3	0
21	A	803	CLA	3	0
21	X	609	CLA	4	0
21	L	304	CLA	4	0
26	5	620	LMG	1	0
24	4	317	BCR	2	0
21	A	832	CLA	2	0
24	B	846	BCR	2	0
21	A	838	CLA	1	0
20	X	605	CHL	1	0
21	B	838	CLA	6	0
31	Y	617	NEX	2	0
24	I	101	BCR	1	0
21	B	811	CLA	1	0
20	4	306	CHL	2	0
20	2	605	CHL	2	0
21	A	807	CLA	1	0
24	F	302	BCR	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	L	308	BCR	5	0
20	2	606	CHL	1	0
24	2	619	BCR	2	0
24	B	843	BCR	1	0
26	F	306	LMG	1	0
21	A	816	CLA	1	0
21	Z	305	CLA	3	0
24	B	848	BCR	8	0
21	A	825	CLA	1	0
25	A	853	LHG	2	0
21	O	202	CLA	2	0
26	1	619	LMG	1	0
21	A	830	CLA	2	0
24	A	849	BCR	4	0
21	2	611	CLA	3	0
23	O	208	XAT	4	0
21	B	804	CLA	2	0
21	B	825	CLA	2	0
21	3	610	CLA	2	0
21	B	813	CLA	2	0
21	4	313	CLA	2	0
21	1	612	CLA	3	0
24	A	854	BCR	4	0
20	Z	309	CHL	3	0
21	A	805	CLA	1	0
29	A	850	SF4	1	0
21	A	821	CLA	1	0
21	Y	610	CLA	1	0
20	X	608	CHL	2	0
20	Y	606	CHL	2	0
24	L	302	BCR	5	0
21	4	308	CLA	1	0
21	J	102	CLA	2	0
21	B	839	CLA	3	0
21	X	611	CLA	4	0
21	Z	313	CLA	3	0
21	A	842	CLA	3	0
20	X	606	CHL	1	0
21	A	810	CLA	3	0
21	Z	310	CLA	4	0
24	L	307	BCR	2	0
23	5	616	XAT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	4	314	CHL	1	0
24	5	617	BCR	1	0
21	K	203	CLA	1	0
22	1	615	LUT	4	0
21	A	840	CLA	1	0
21	B	805	CLA	1	0
22	5	619	LUT	3	0
27	4	319	LMT	1	0
21	2	602	CLA	1	0
21	B	824	CLA	1	0
24	A	846	BCR	4	0
25	5	618	LHG	2	0
21	B	820	CLA	1	0
21	6	609	CLA	1	0
24	O	201	BCR	2	0
21	A	808	CLA	1	0
21	5	608	CLA	1	0
24	6	618	BCR	1	0
24	F	305	BCR	1	0
25	A	851	LHG	1	0
23	3	616	XAT	2	0
21	A	820	CLA	1	0
25	1	620	LHG	2	0
22	2	615	LUT	4	0
20	4	305	CHL	1	0
20	Z	301	CHL	2	0
22	F	301	LUT	3	0
21	3	609	CLA	1	0
21	B	802	CLA	5	0
21	6	610	CLA	3	0
21	5	605	CLA	2	0
21	1	614	CLA	1	0
31	X	616	NEX	1	0
21	4	311	CLA	1	0
21	X	610	CLA	3	0
21	3	607	CLA	1	0
21	5	611	CLA	1	0
21	5	612	CLA	4	0
20	2	607	CHL	2	0
21	L	301	CLA	4	0
21	1	613	CLA	1	0
20	Y	601	CHL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	B	837	CLA	1	0
21	X	618	CLA	2	0
24	A	848	BCR	2	0
25	2	617	LHG	2	0
22	5	615	LUT	6	0
30	B	849	DGD	2	0
21	1	603	CLA	2	0
25	1	618	LHG	5	0
26	G	206	LMG	1	0
21	A	834	CLA	2	0
20	Y	608	CHL	3	0
21	B	840	CLA	2	0
20	X	607	CHL	2	0
22	Y	615	LUT	8	0
31	Z	316	NEX	3	0
21	3	612	CLA	3	0
21	5	609	CLA	1	0
21	B	808	CLA	2	0
26	6	619	LMG	1	0
21	2	610	CLA	1	0
21	A	841	CLA	2	0
21	L	305	CLA	2	0
20	2	614	CHL	1	0
21	B	826	CLA	4	0
25	X	617	LHG	3	0
24	A	847	BCR	1	0
20	Y	605	CHL	1	0
22	6	616	LUT	3	0
22	Z	315	LUT	6	0
20	Y	607	CHL	2	0
21	A	809	CLA	2	0
24	O	204	BCR	1	0
21	O	203	CLA	3	0
21	B	817	CLA	1	0
20	Y	609	CHL	1	0
24	L	306	BCR	3	0
20	Y	619	CHL	2	0
22	Z	314	LUT	7	0
21	Y	603	CLA	1	0
25	Y	618	LHG	3	0
21	A	828	CLA	3	0
24	J	103	BCR	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	801	CLA	1	0
21	3	617	CLA	1	0
21	B	831	CLA	1	0
24	G	205	BCR	2	0
21	Z	303	CLA	5	0
20	1	601	CHL	2	0
21	B	801	CLA	1	0
21	J	101	CLA	2	0
25	1	622	LHG	1	0
28	B	841	PQN	4	0
21	A	819	CLA	2	0
21	B	810	CLA	1	0
21	Y	604	CLA	2	0
21	1	604	CLA	1	0
21	A	827	CLA	2	0
21	H	201	CLA	2	0
22	Y	616	LUT	8	0
25	Z	317	LHG	2	0
22	4	315	LUT	4	0
21	Y	602	CLA	6	0
20	5	601	CHL	3	0
26	B	850	LMG	3	0
21	2	604	CLA	1	0
21	2	608	CLA	1	0
21	A	837	CLA	2	0
21	B	827	CLA	1	0
23	4	316	XAT	1	0
21	Z	312	CLA	4	0
24	A	845	BCR	2	0
20	Z	308	CHL	1	0
24	O	205	BCR	3	0
21	5	613	CLA	1	0
21	4	303	CLA	1	0
21	X	603	CLA	3	0
24	B	847	BCR	3	0
21	X	604	CLA	1	0
20	Z	307	CHL	3	0
21	2	613	CLA	1	0
21	6	602	CLA	3	0
21	A	826	CLA	2	0
21	Y	613	CLA	1	0
23	6	617	XAT	2	0

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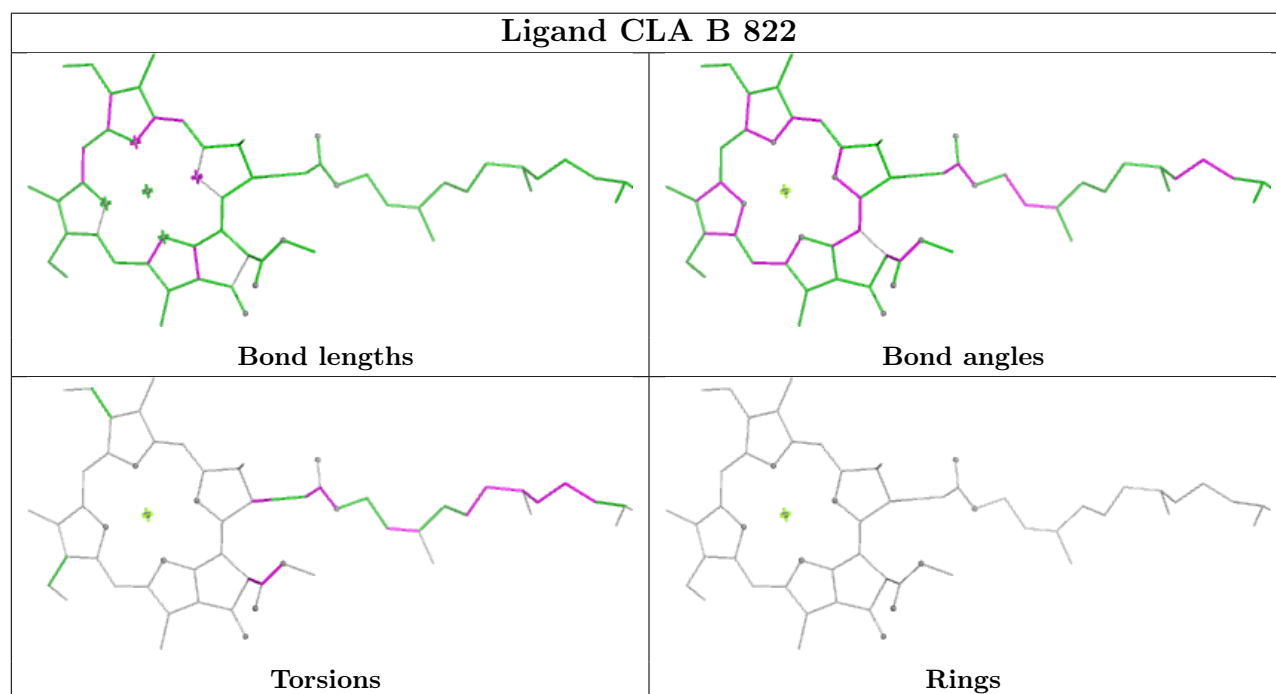
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	845	BCR	1	0
21	A	839	CLA	1	0
20	6	606	CHL	2	0
24	6	620	BCR	4	0
21	B	828	CLA	2	0
21	A	829	CLA	3	0
21	A	813	CLA	5	0
21	K	202	CLA	1	0
21	1	605	CLA	1	0
21	2	609	CLA	2	0
20	4	304	CHL	2	0
21	O	206	CLA	4	0
22	3	615	LUT	6	0
21	A	804	CLA	3	0
21	B	812	CLA	3	0
21	A	817	CLA	2	0
21	A	802	CLA	7	0
20	Z	302	CHL	4	0
21	X	602	CLA	2	0
21	X	613	CLA	1	0
21	B	807	CLA	1	0
20	1	606	CHL	1	0
24	3	601	BCR	2	0
20	6	607	CHL	1	0
20	2	601	CHL	3	0
21	B	816	CLA	2	0
20	3	608	CHL	1	0
23	1	616	XAT	1	0
21	G	203	CLA	2	0
24	B	842	BCR	2	0
21	K	204	CLA	1	0
21	3	605	CLA	1	0
21	B	823	CLA	1	0
21	6	601	CLA	1	0
21	4	301	CLA	1	0
26	5	621	LMG	1	0
21	6	612	CLA	2	0
21	5	604	CLA	3	0
21	A	812	CLA	1	0
21	3	603	CLA	1	0
21	5	602	CLA	1	0
21	A	811	CLA	2	0

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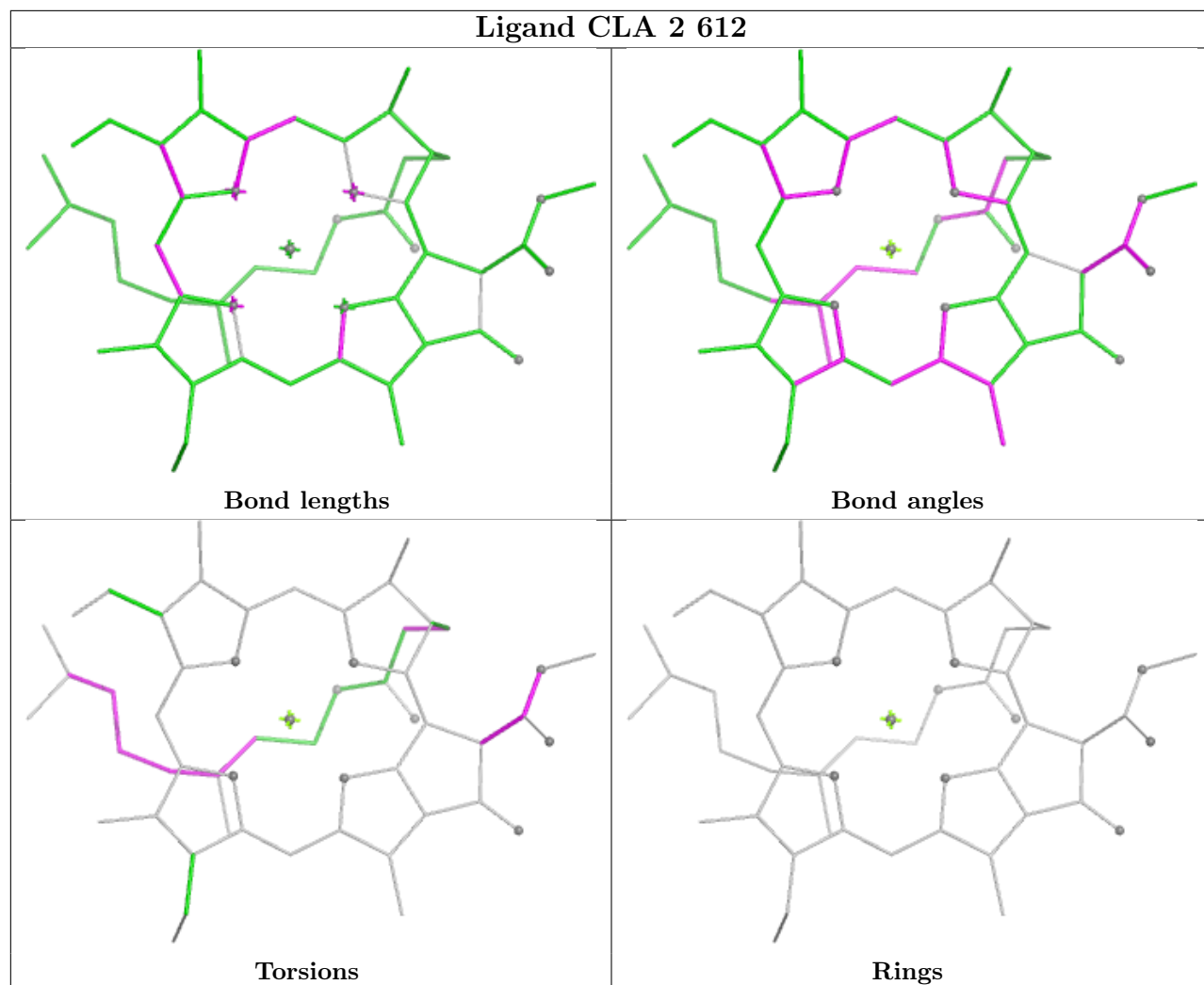
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	X	614	LUT	8	0
22	X	615	LUT	8	0
21	1	609	CLA	3	0
21	A	818	CLA	3	0
20	6	605	CHL	4	0
20	X	601	CHL	3	0
21	A	806	CLA	1	0

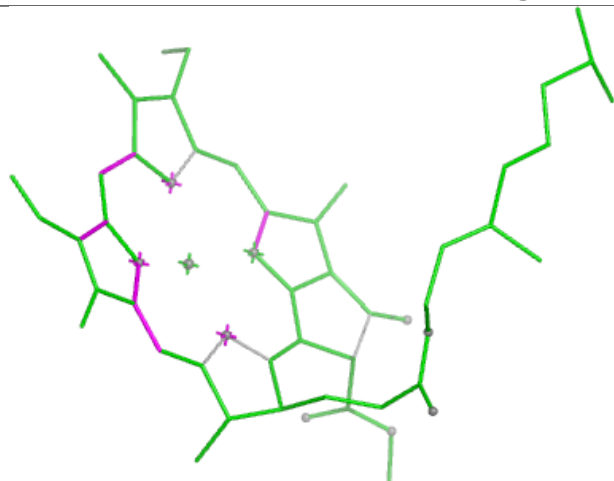
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



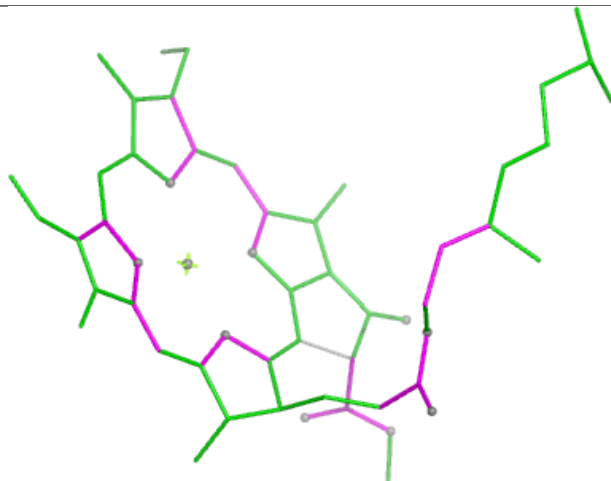
Ligand CLA 2 612



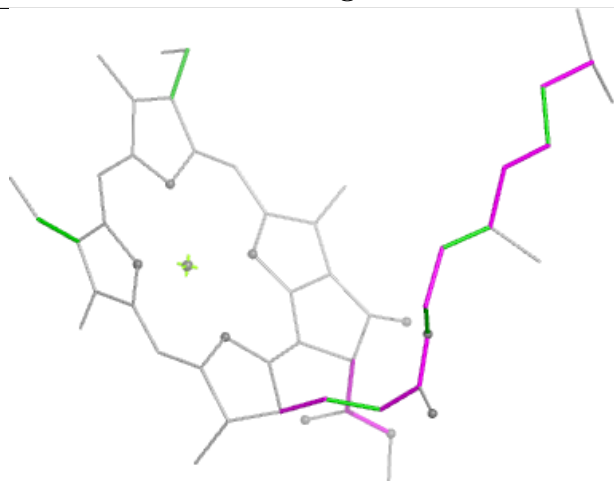
Ligand CLA B 821



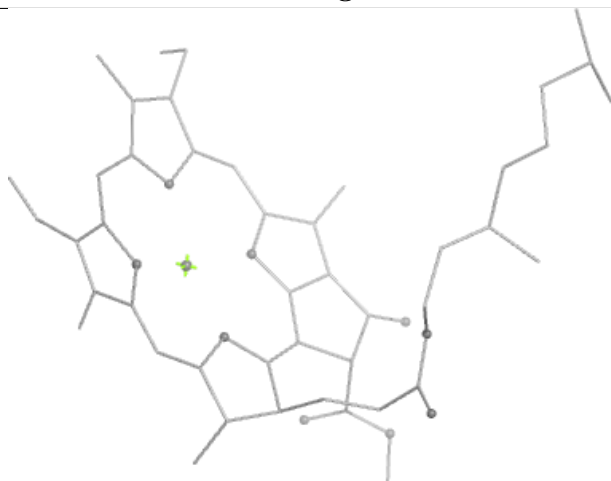
Bond lengths



Bond angles

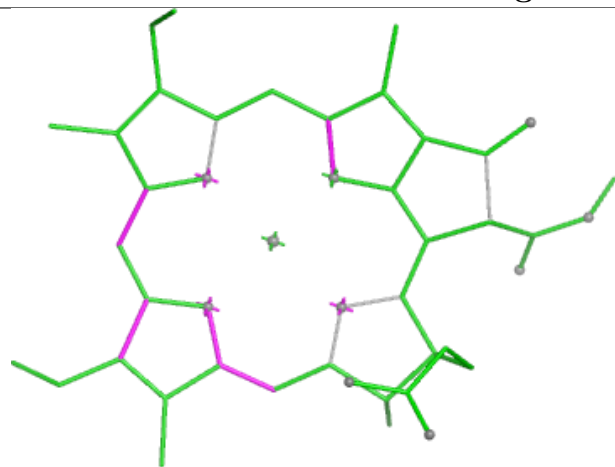


Torsions

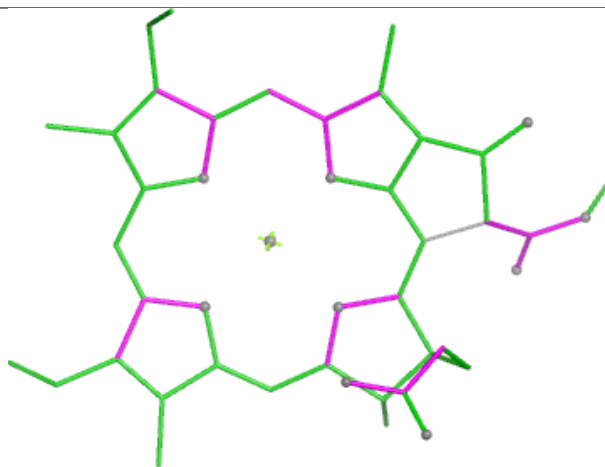


Rings

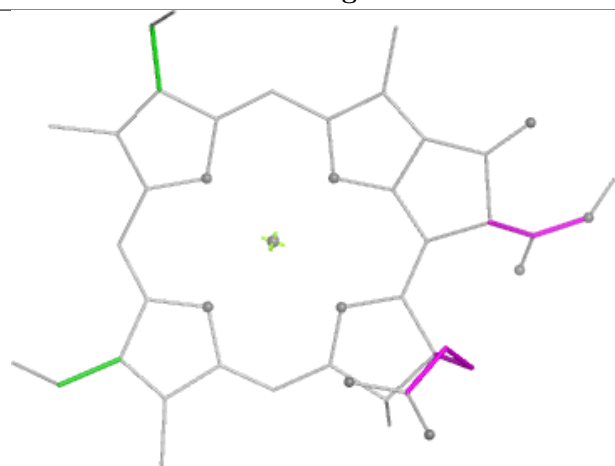
Ligand CLA G 202



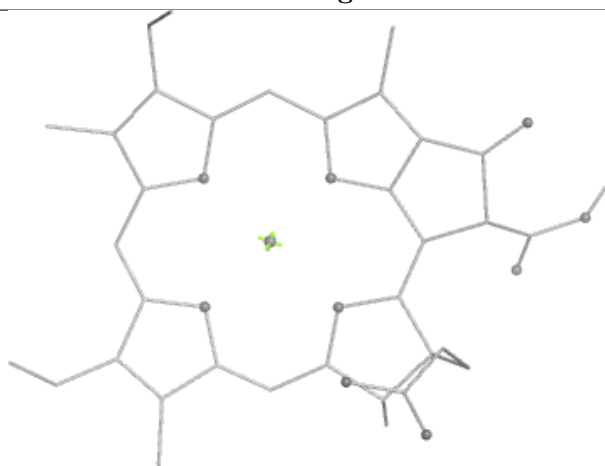
Bond lengths



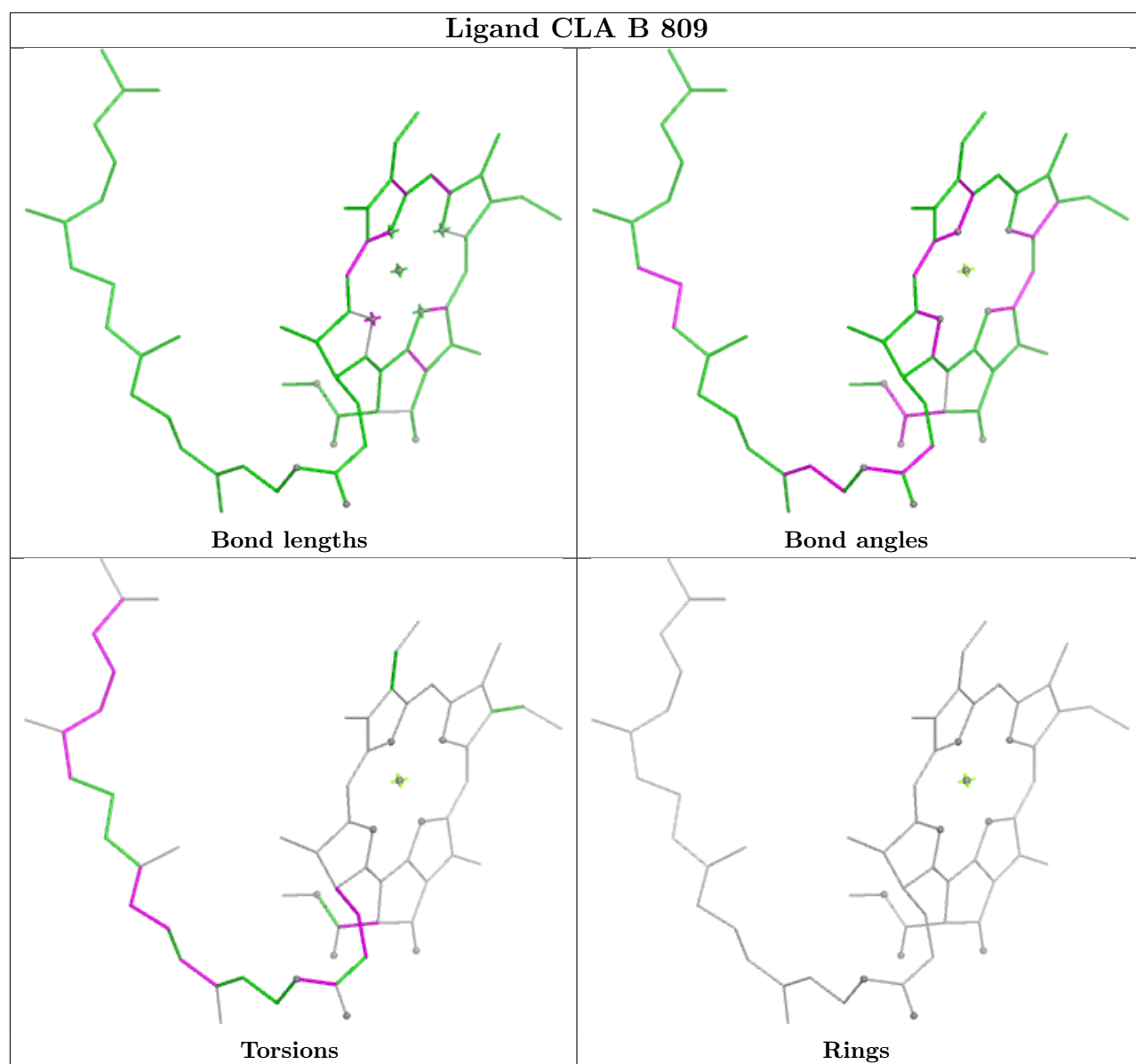
Bond angles

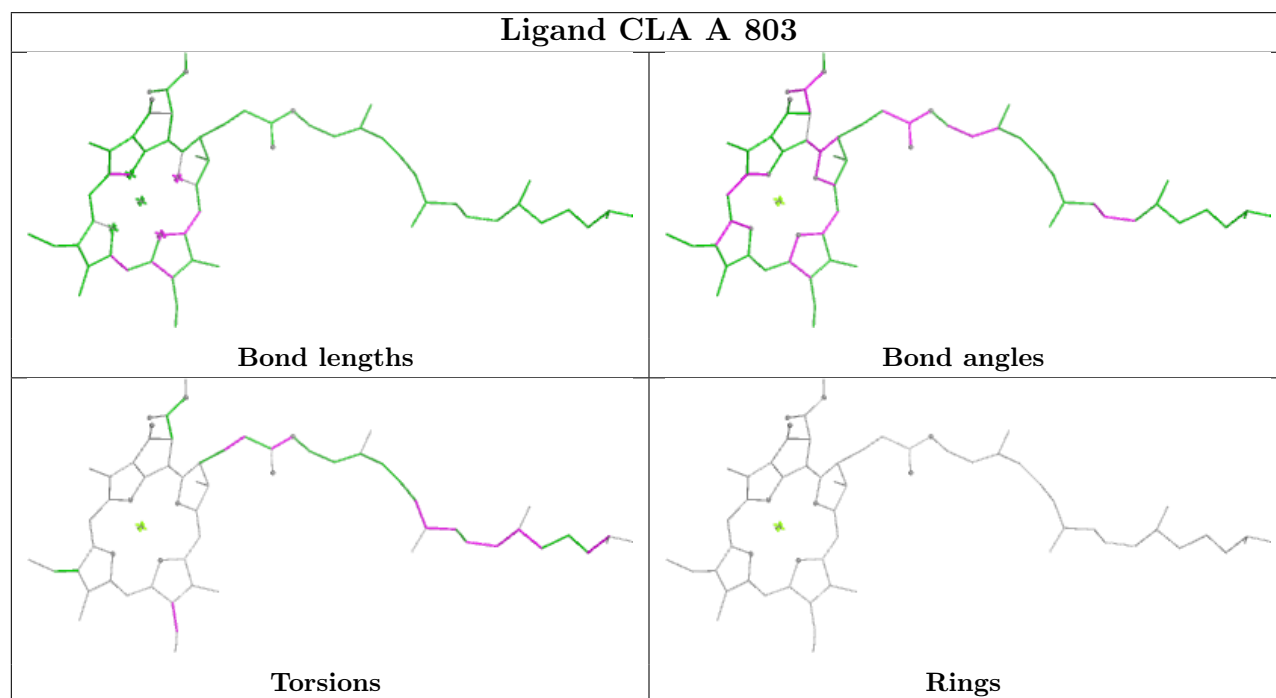
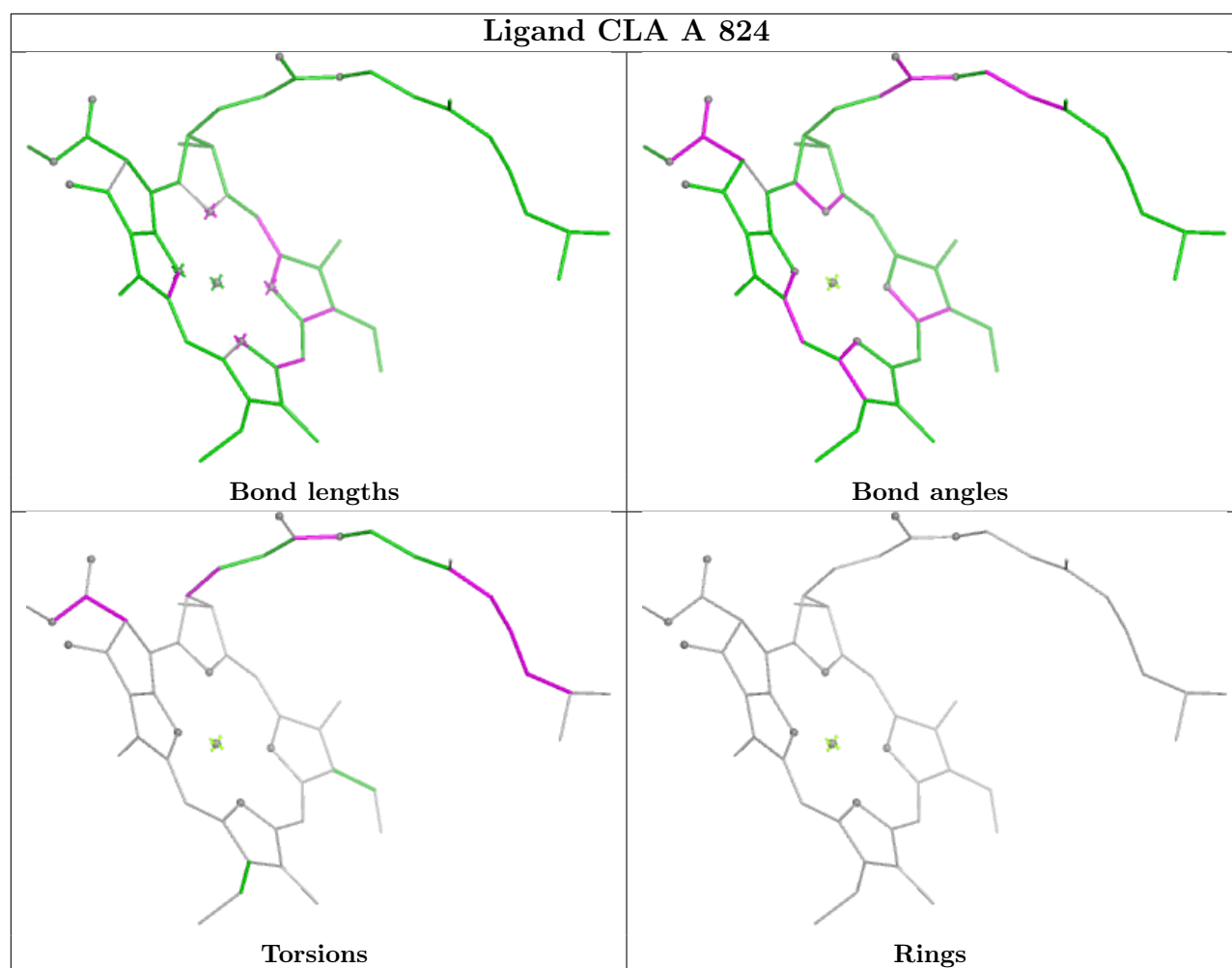


Torsions

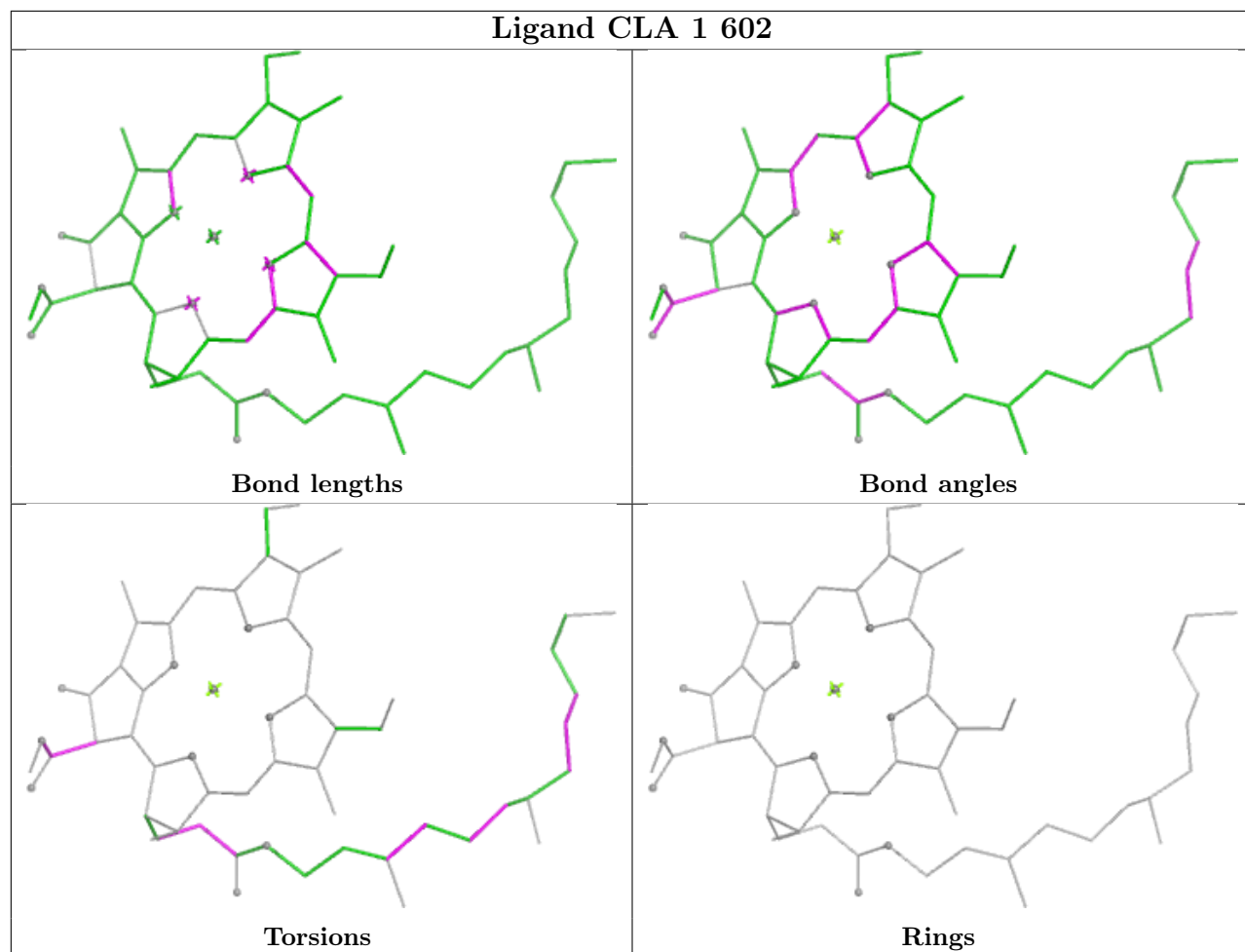


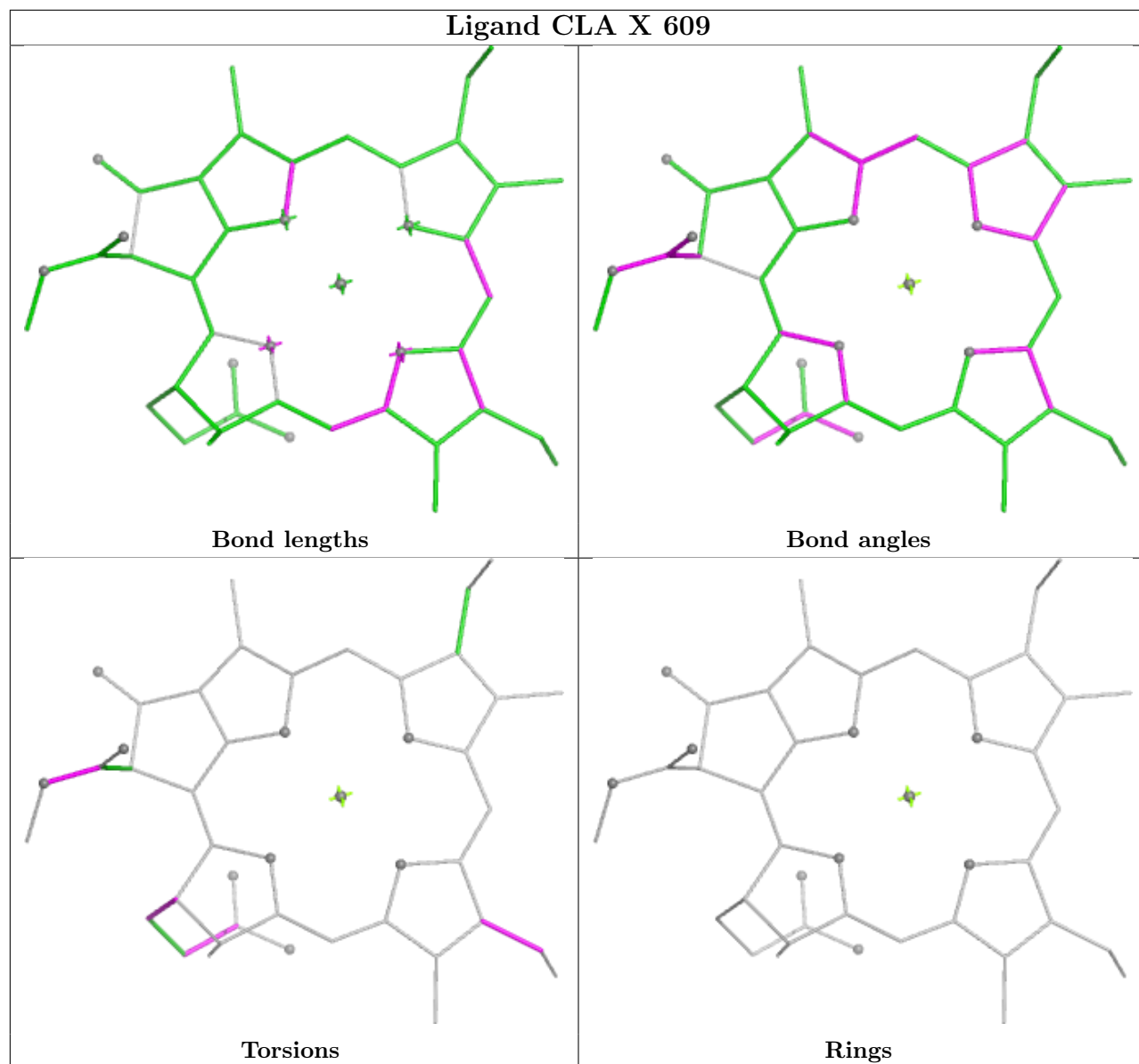
Rings

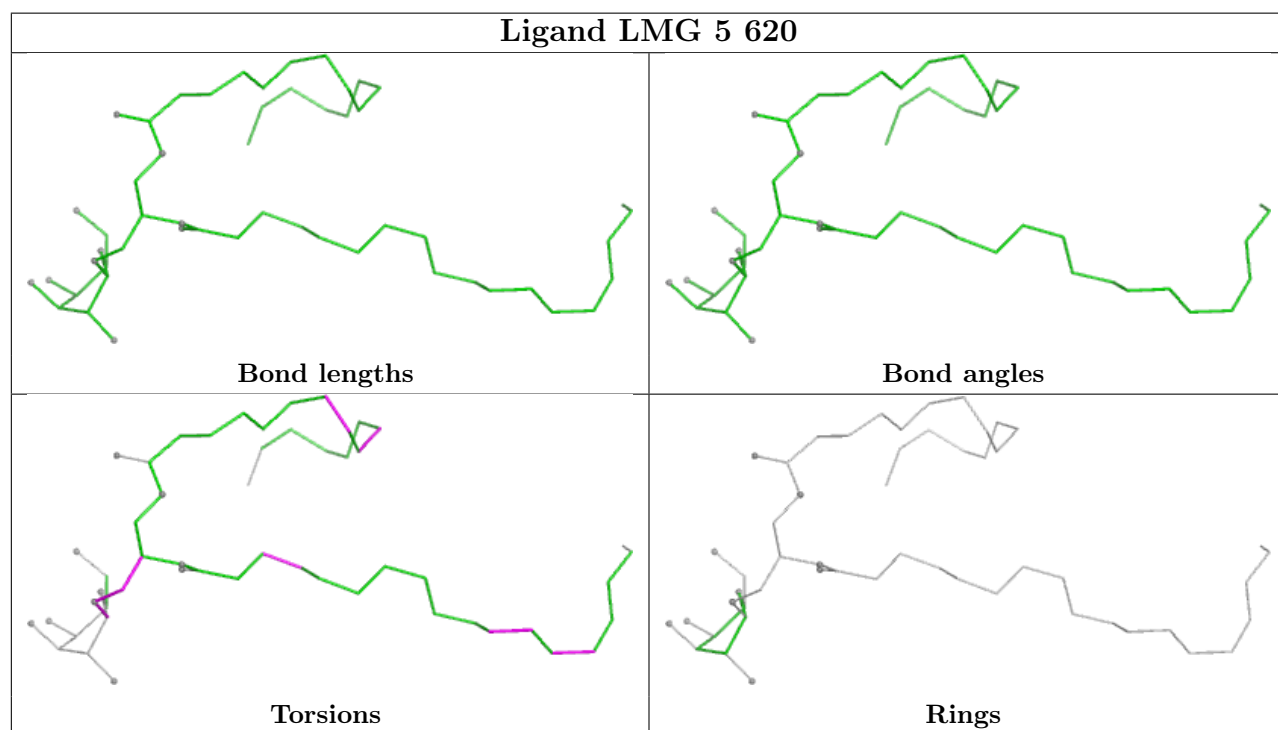
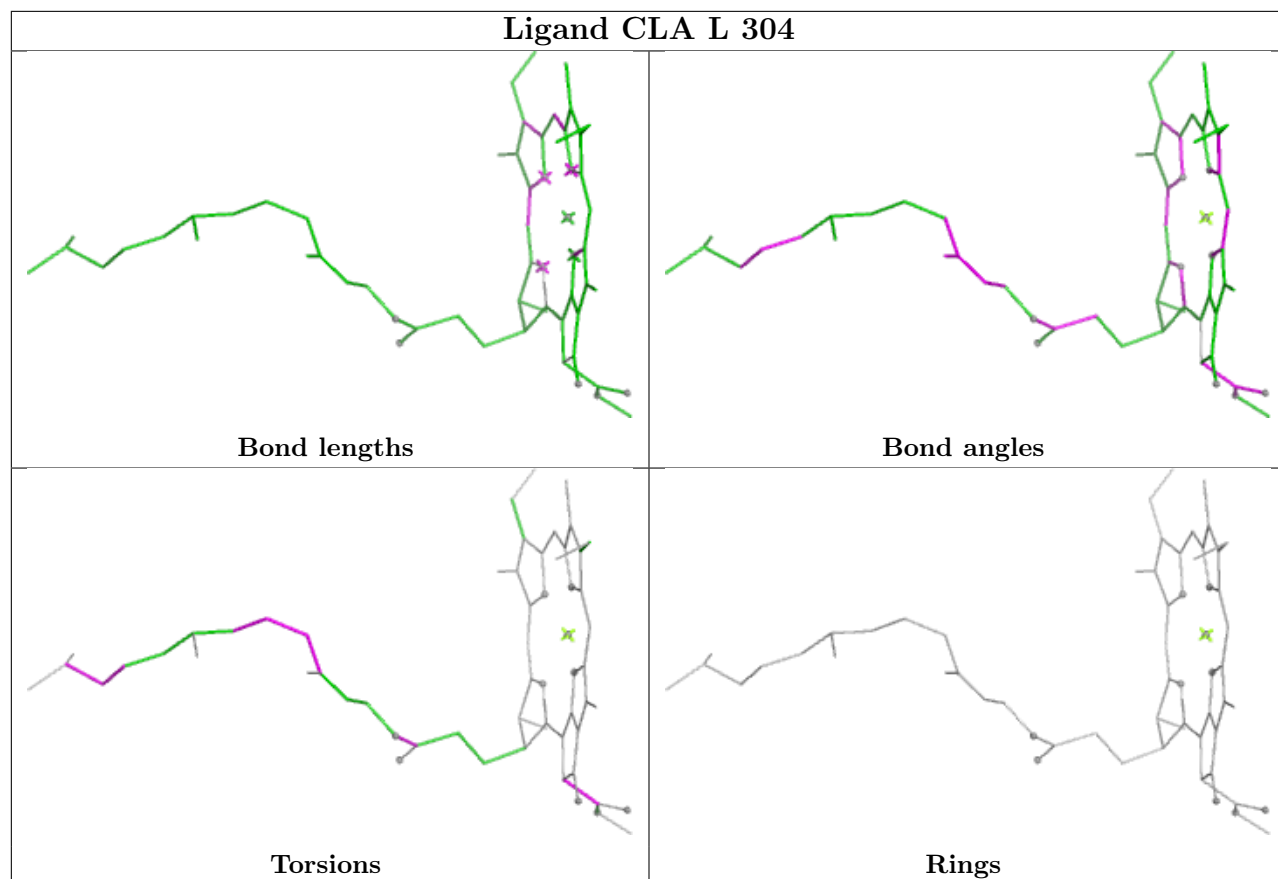


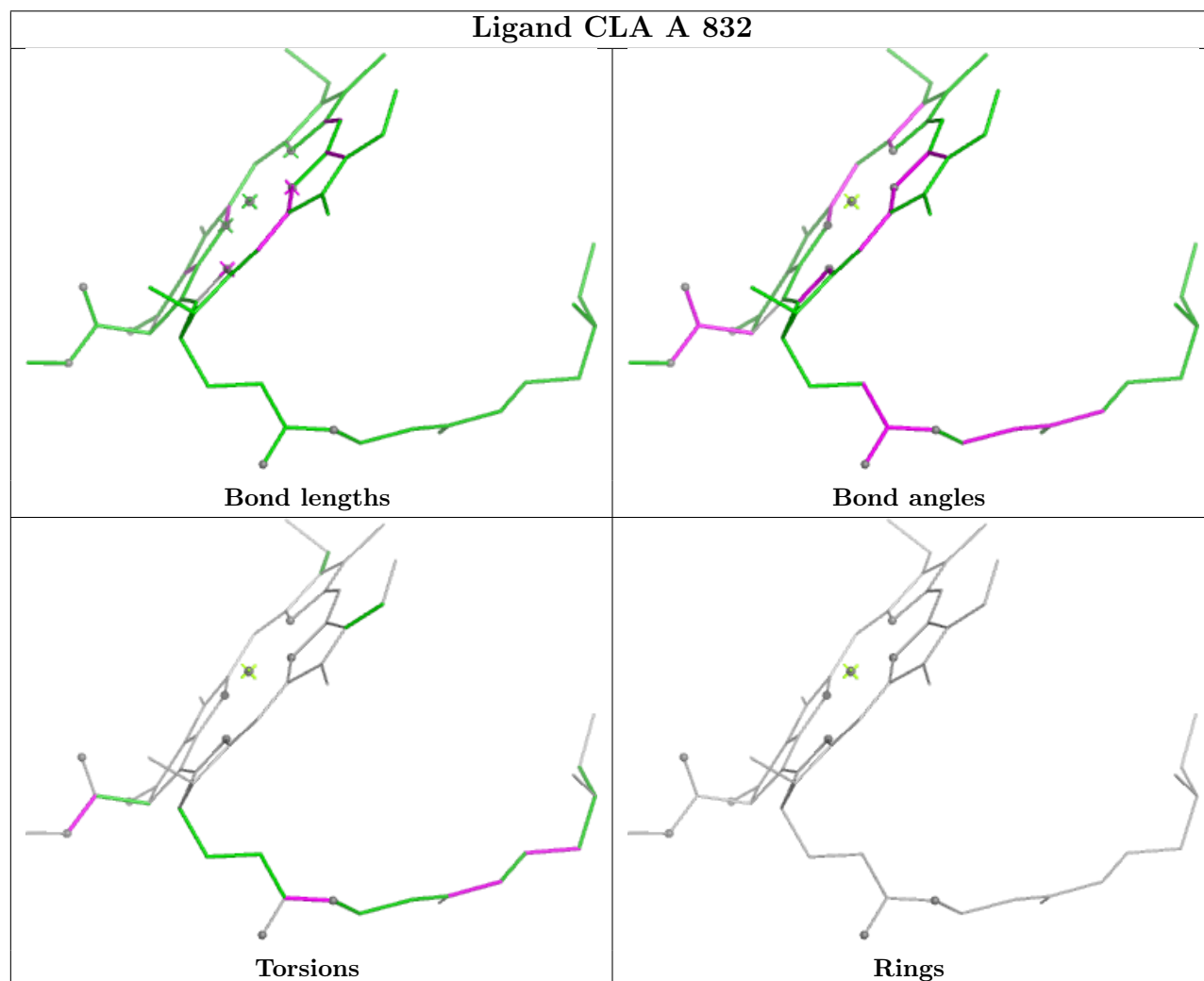
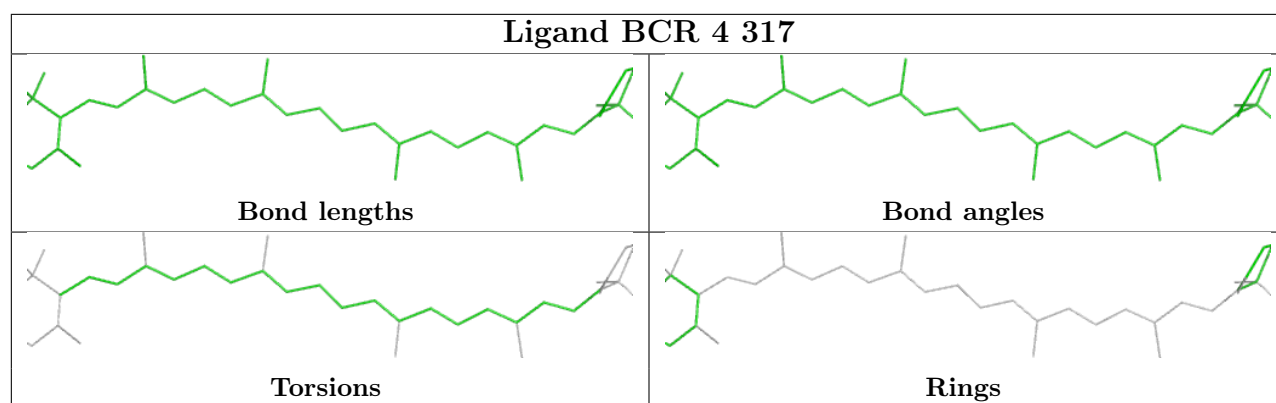


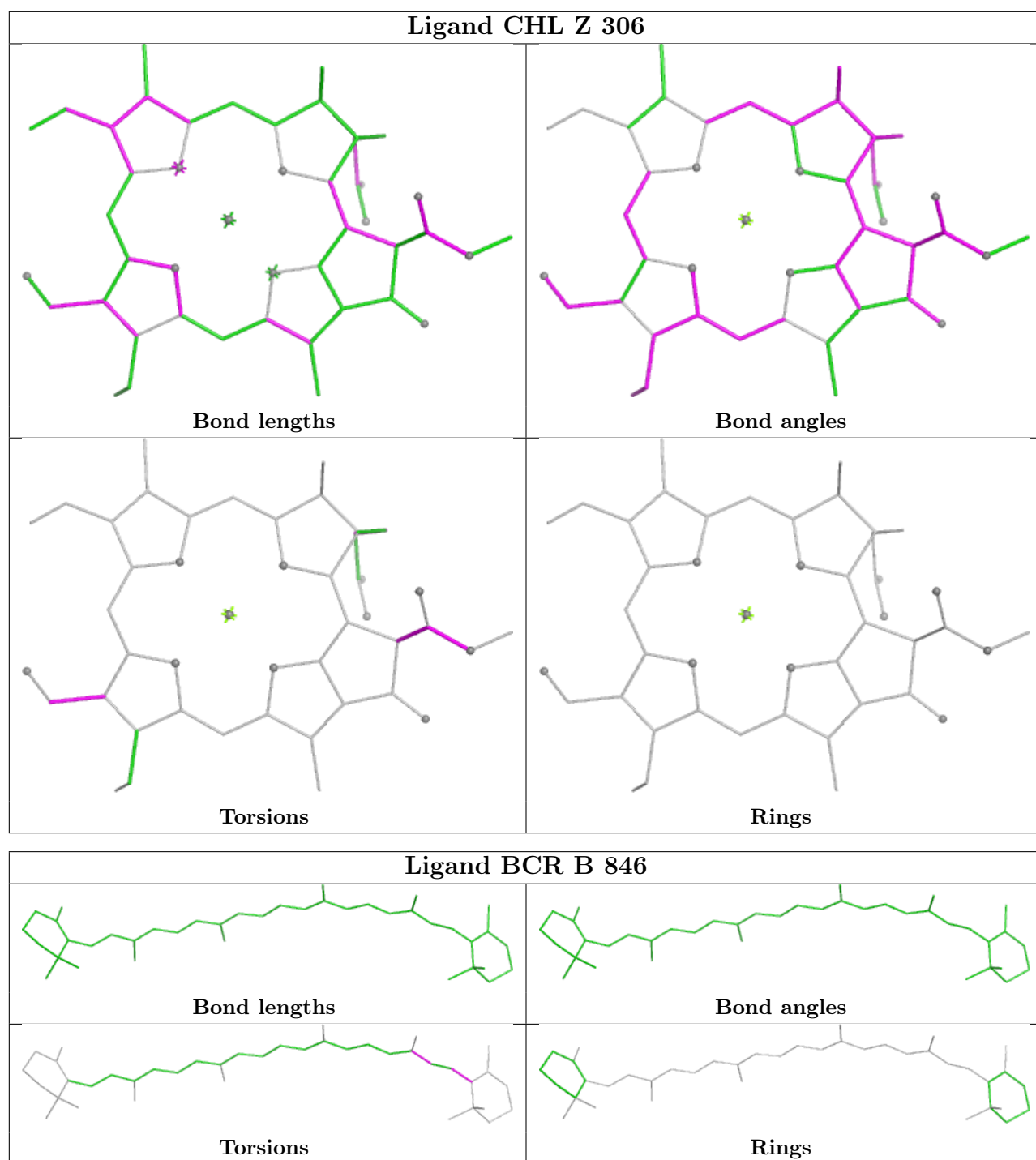
Ligand CLA 1 602

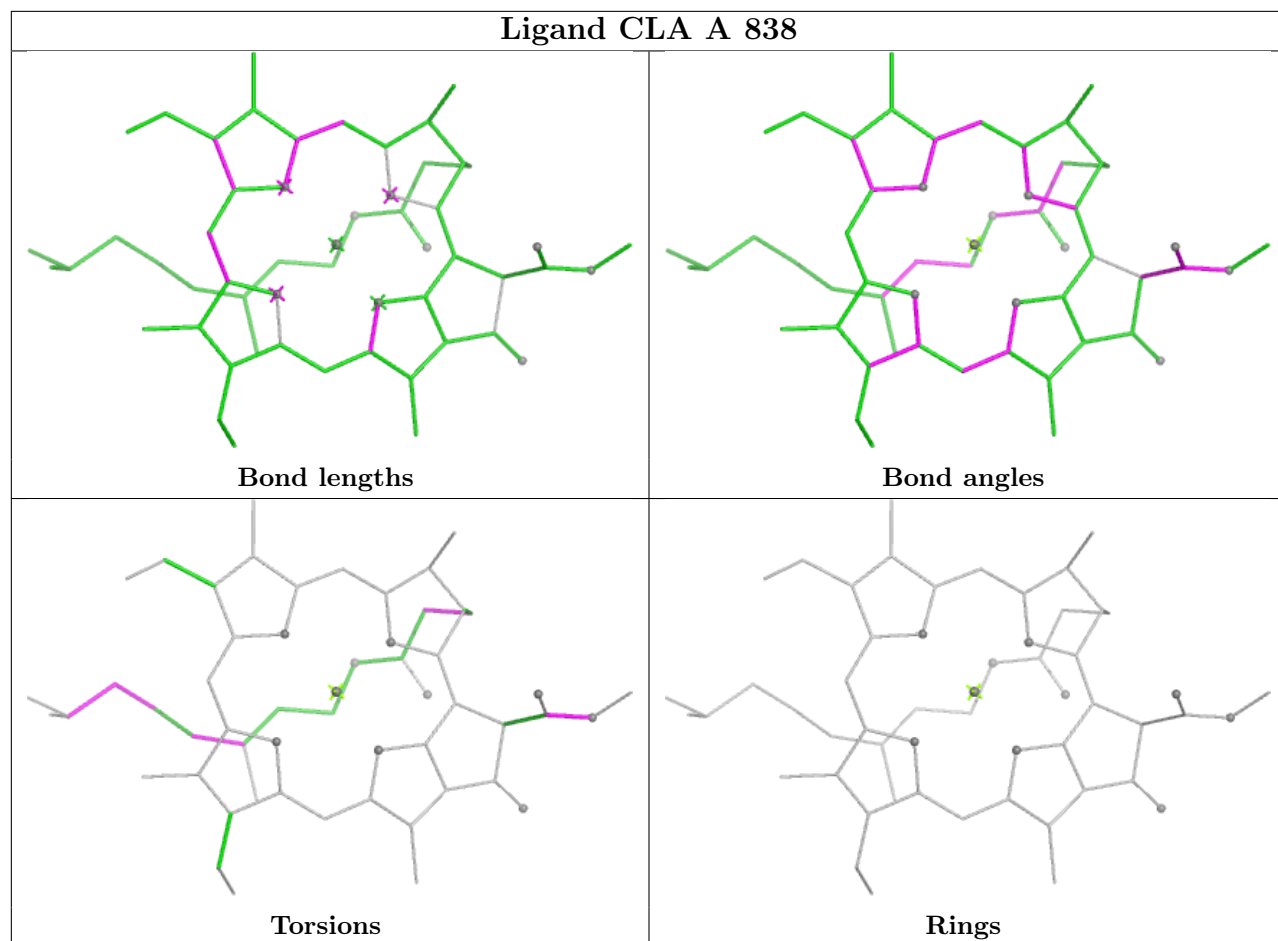


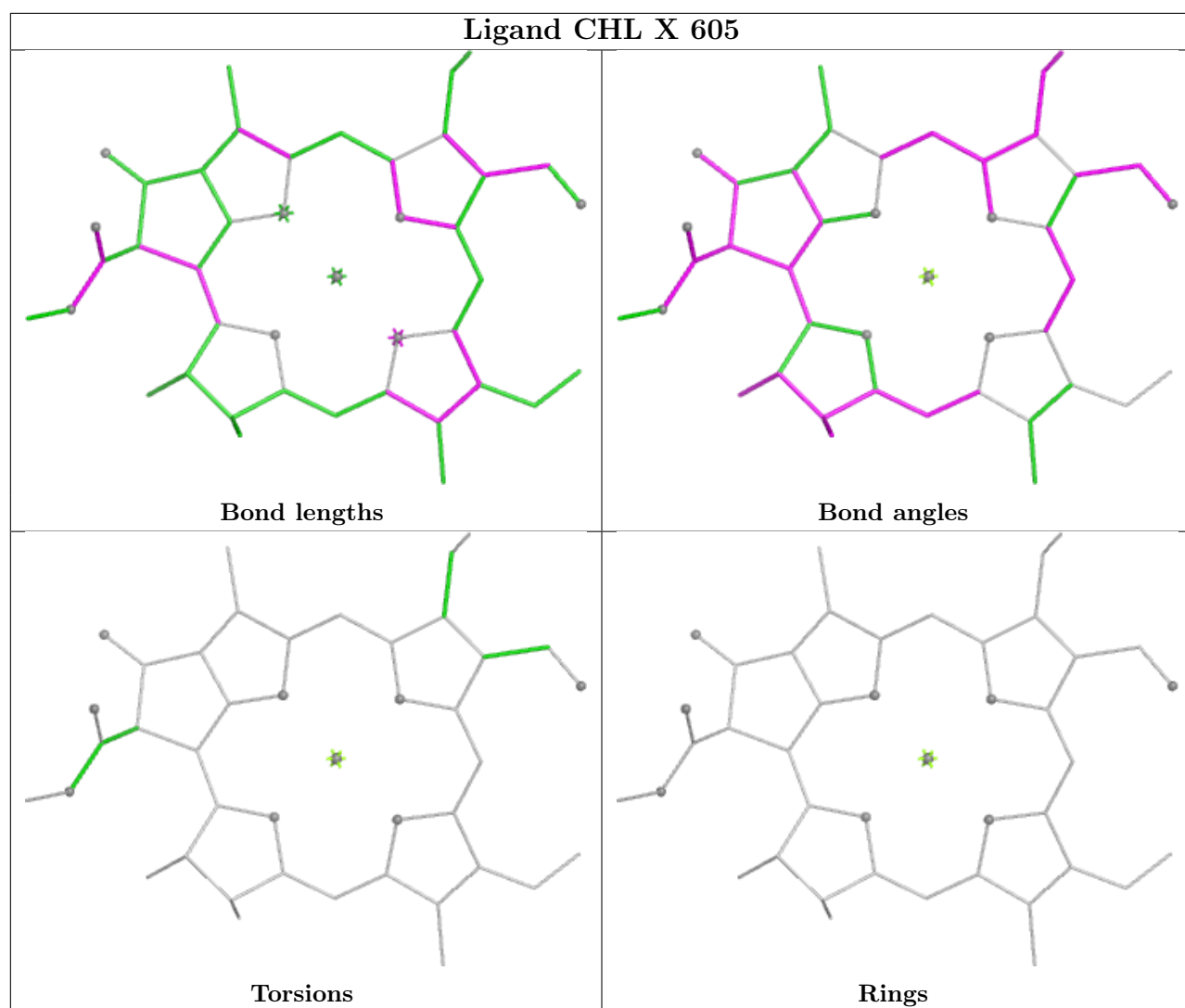


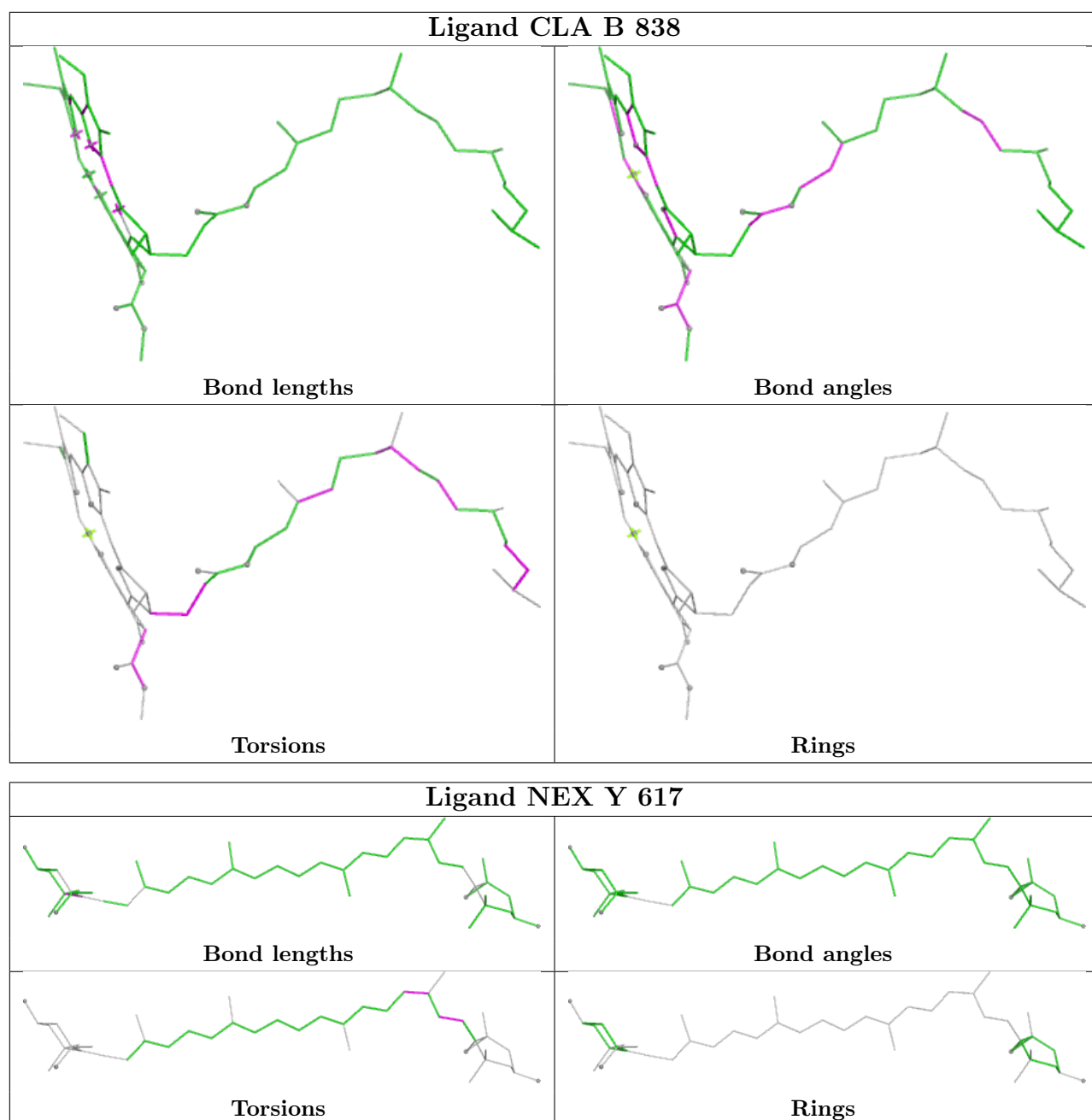




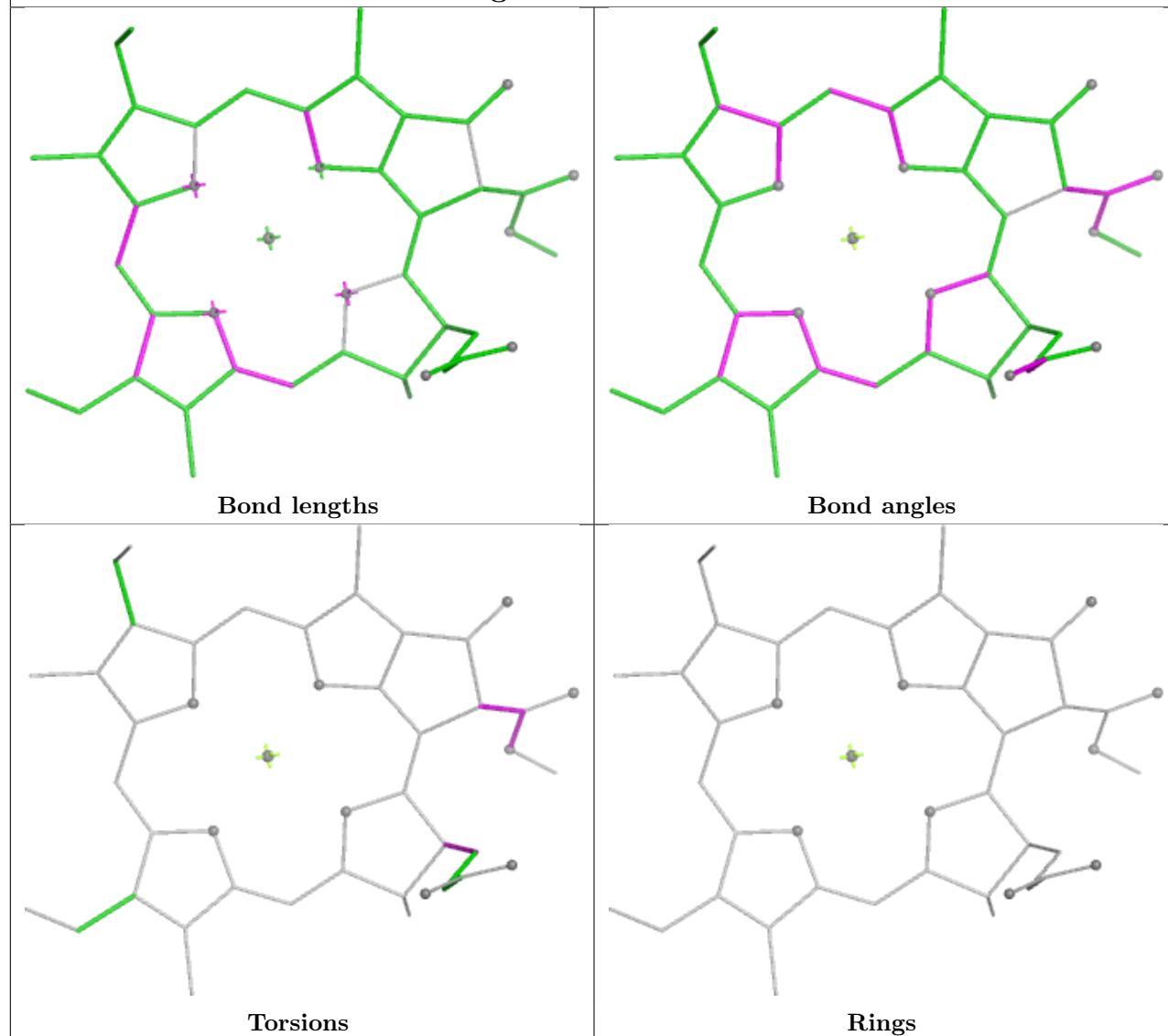




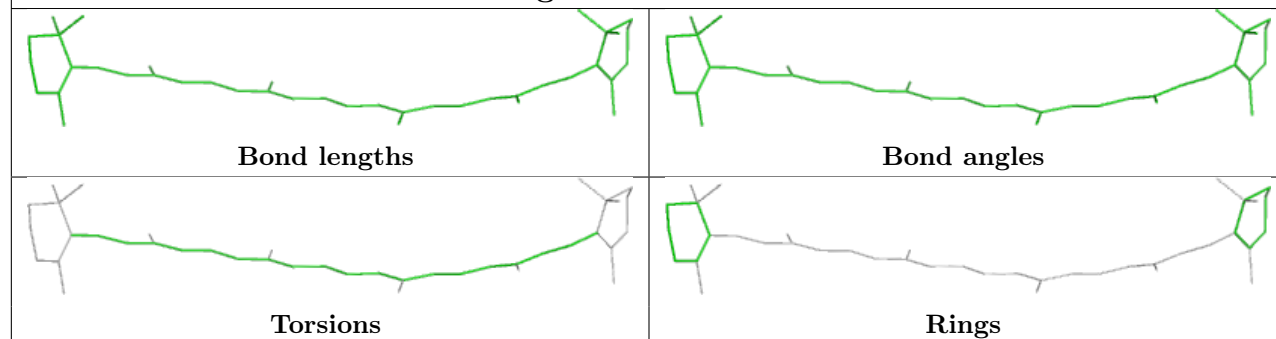




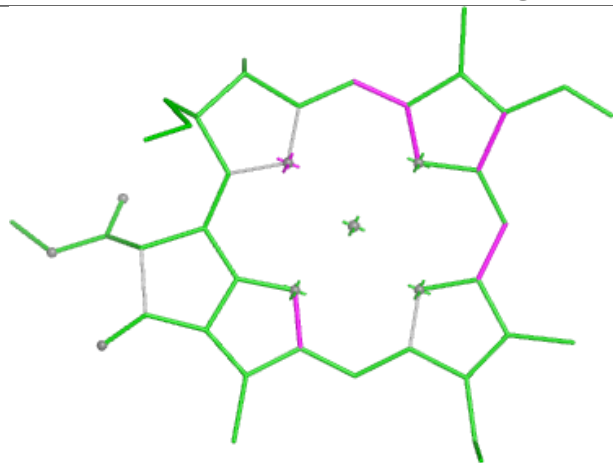
Ligand CLA 3 604



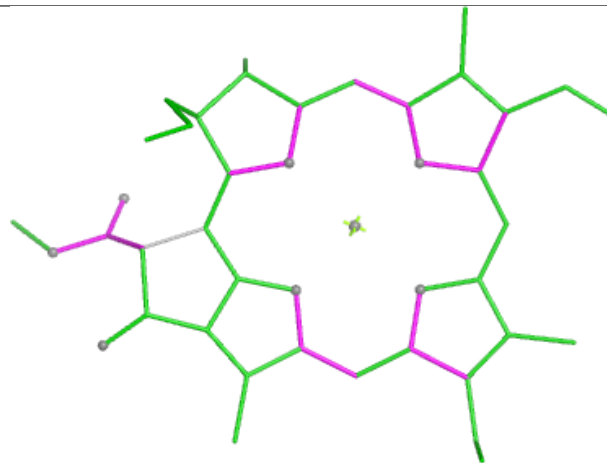
Ligand BCR I 101



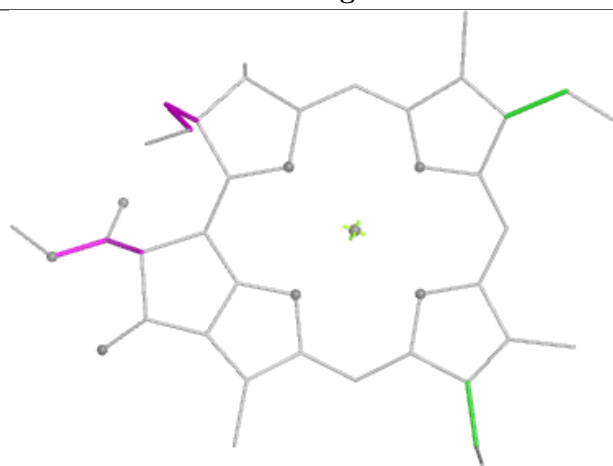
Ligand CLA B 811



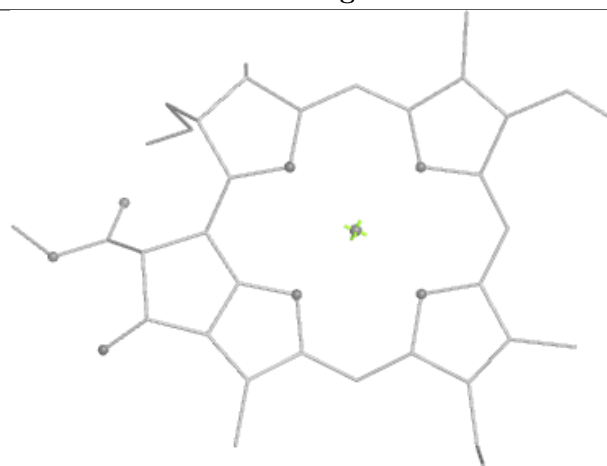
Bond lengths



Bond angles

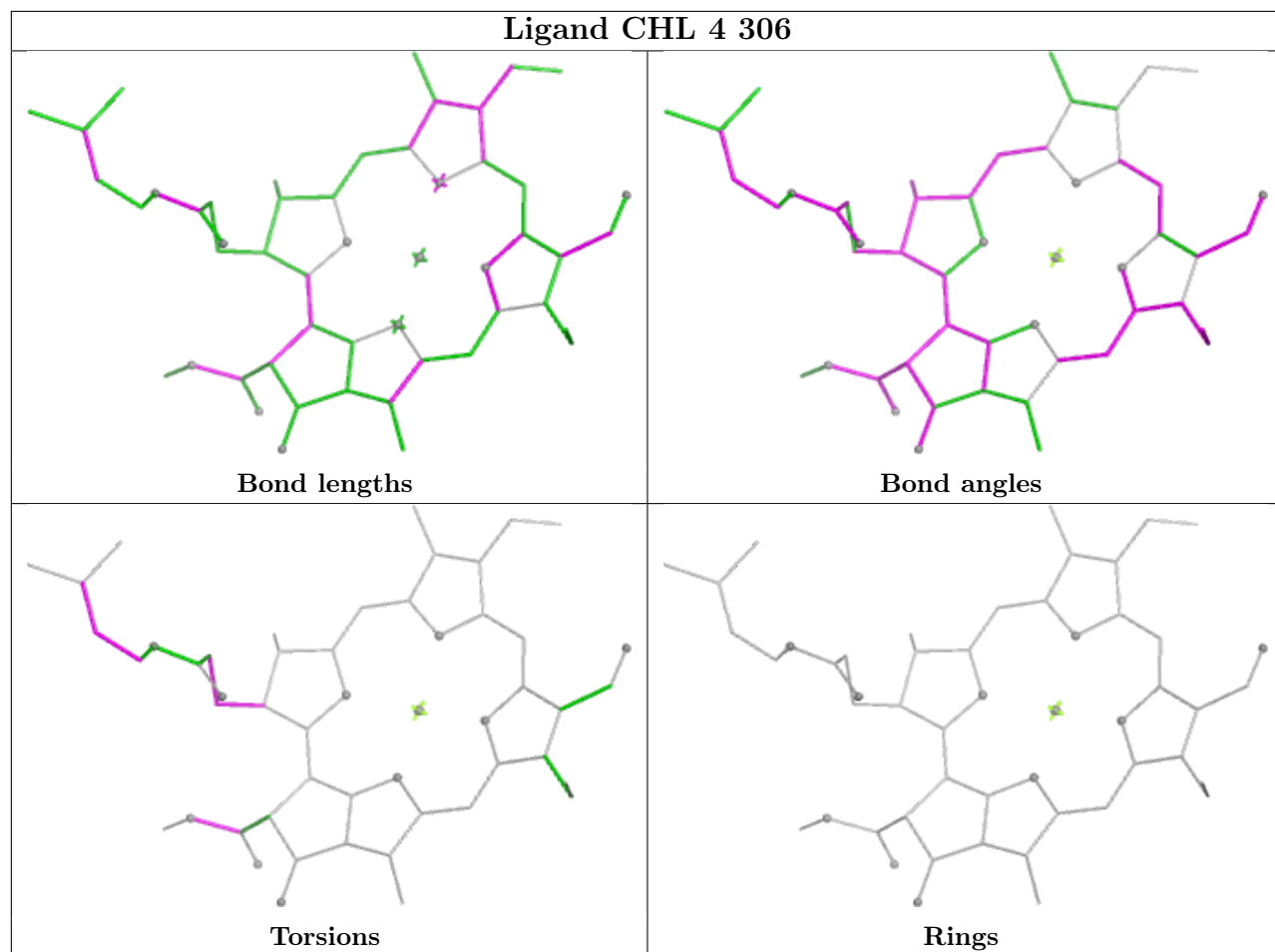


Torsions

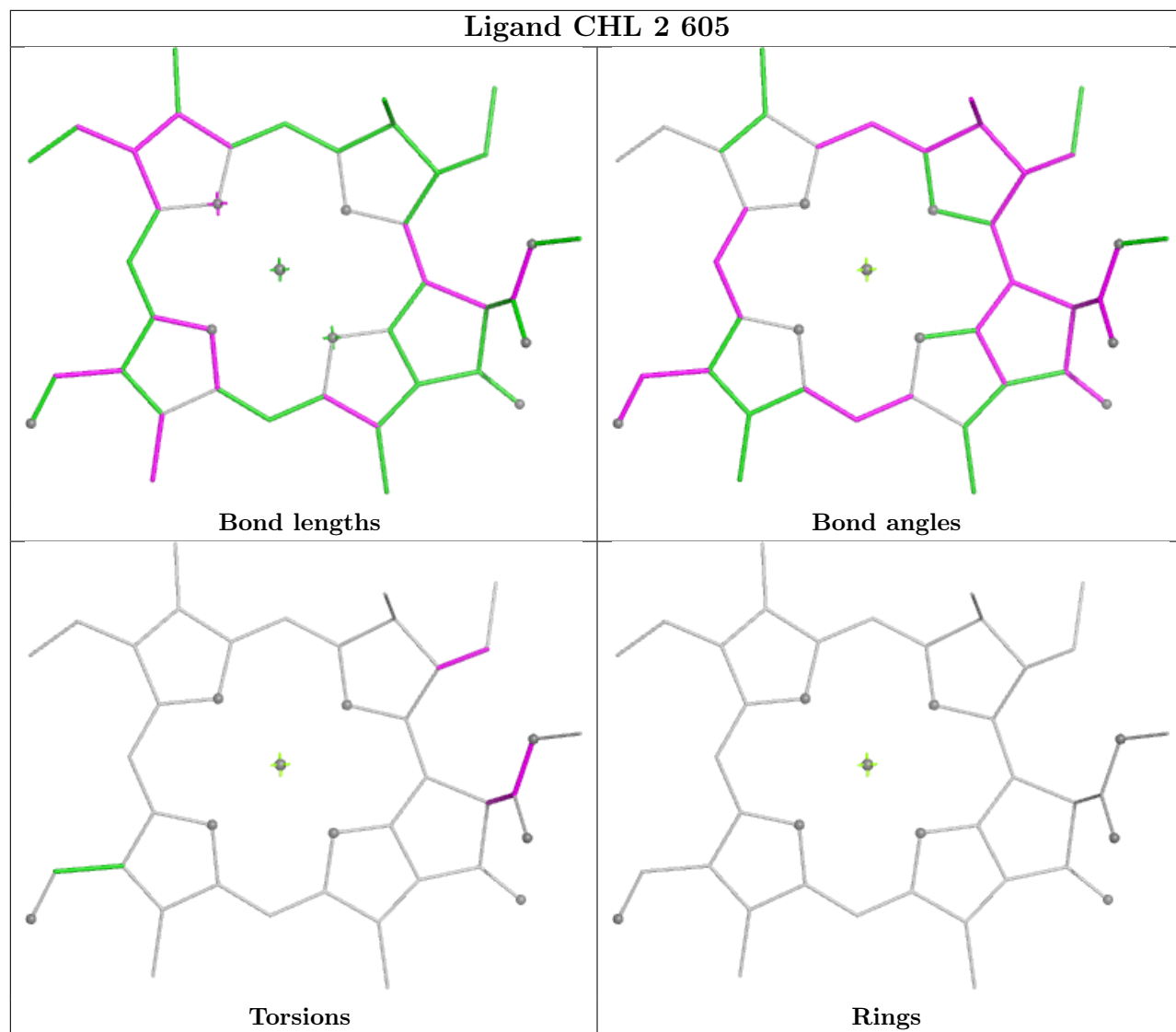


Rings

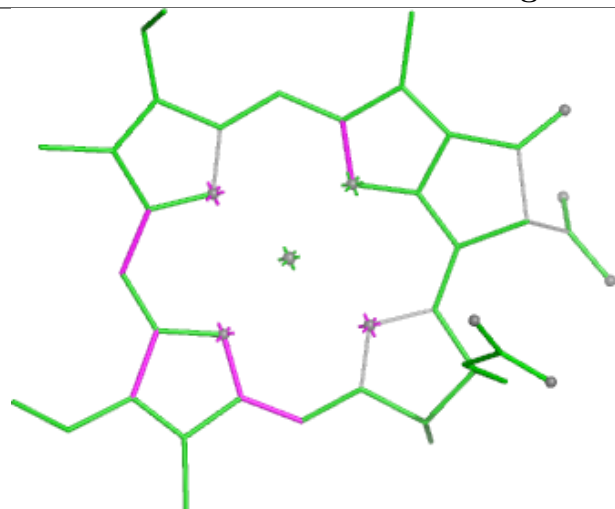
Ligand CHL 4 306



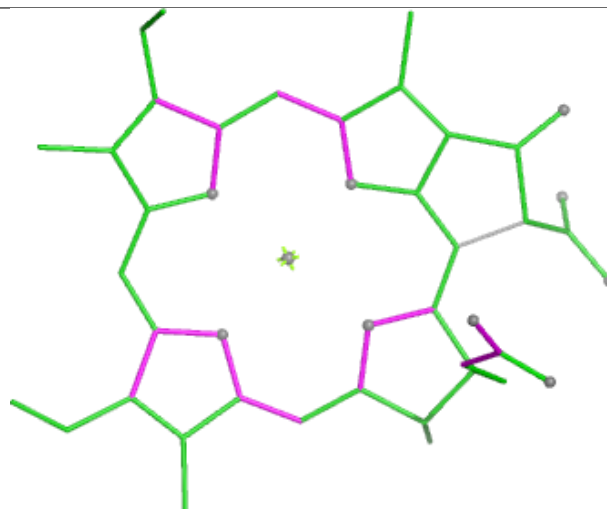
Ligand CHL 2 605



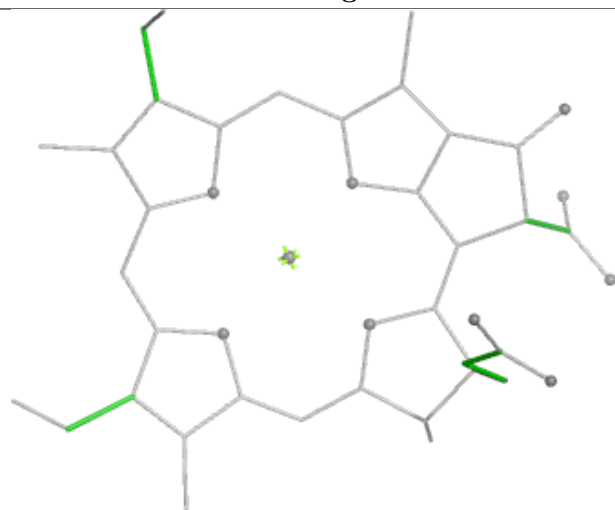
Ligand CLA 1 607



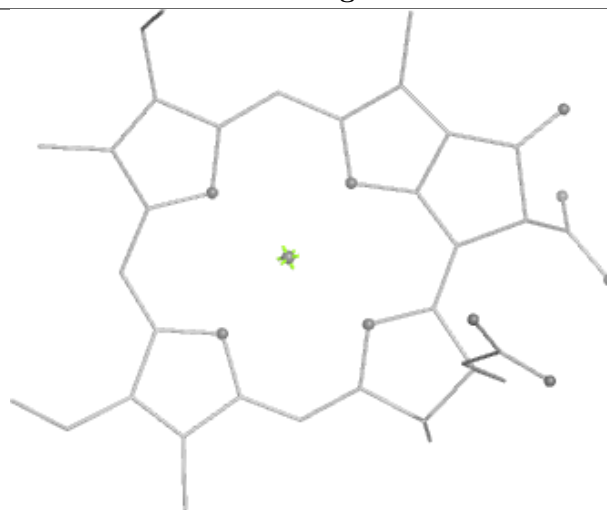
Bond lengths



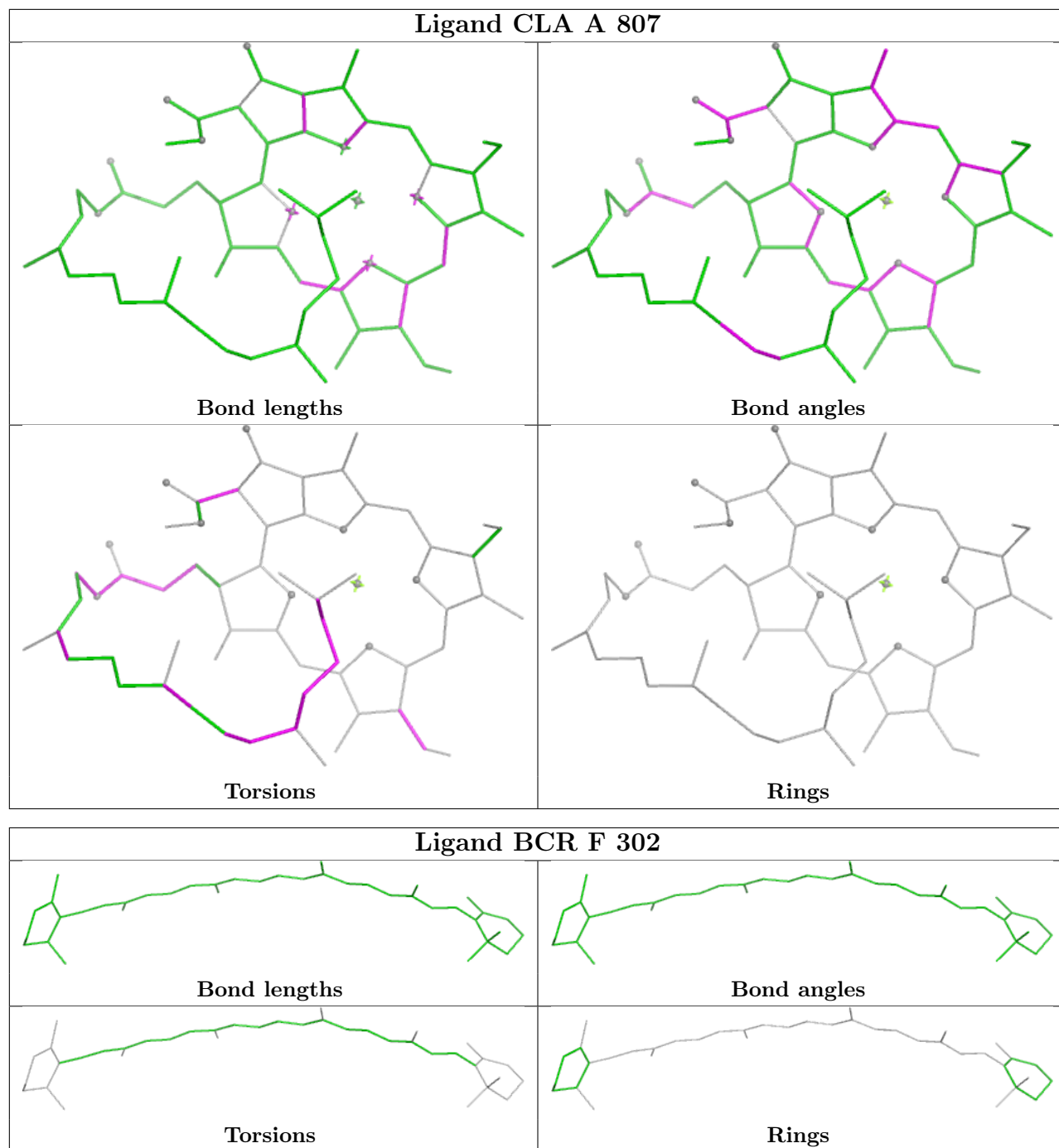
Bond angles



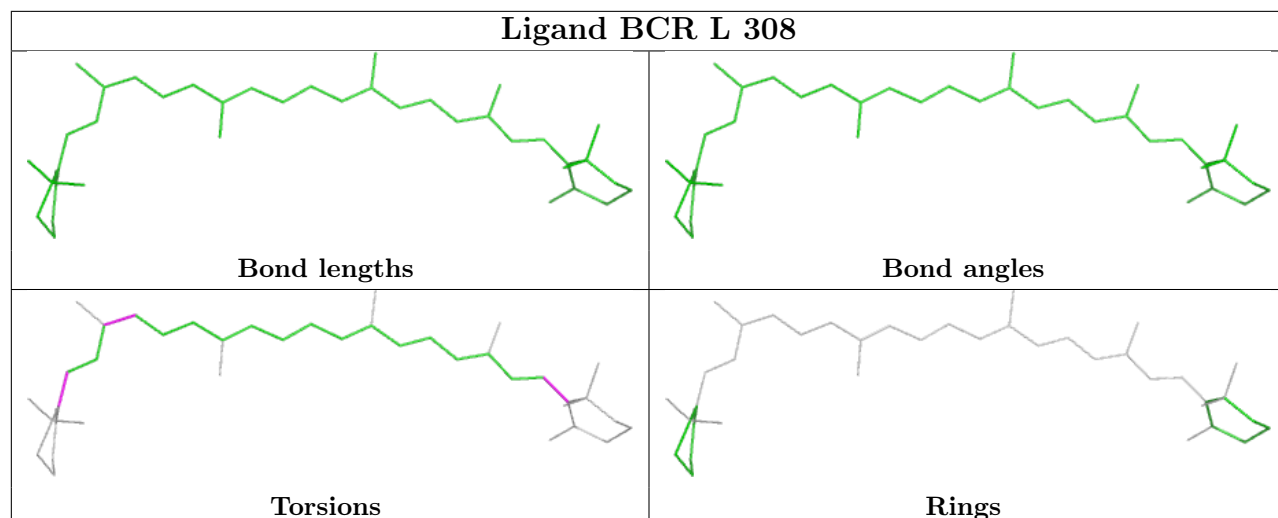
Torsions



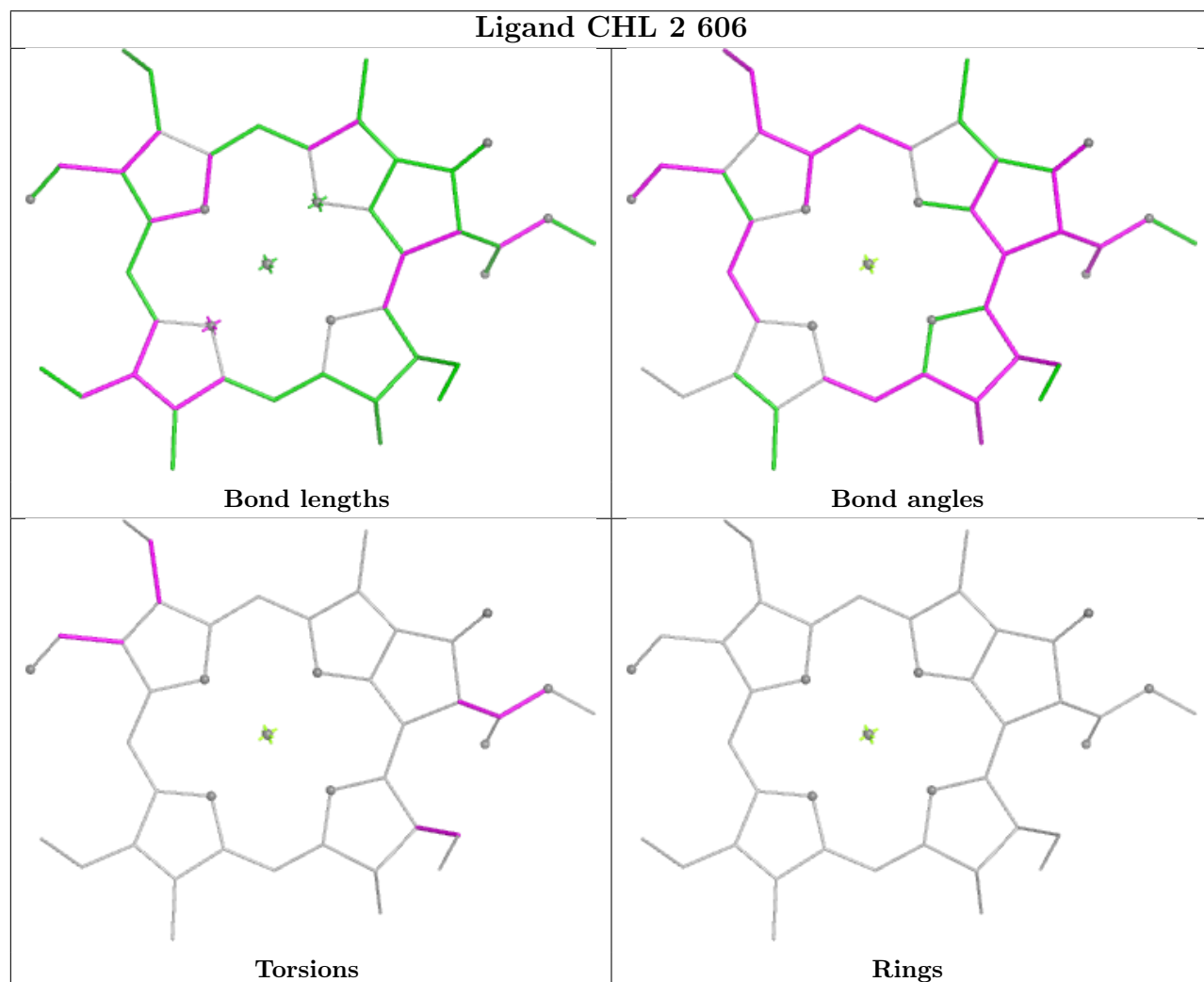
Rings



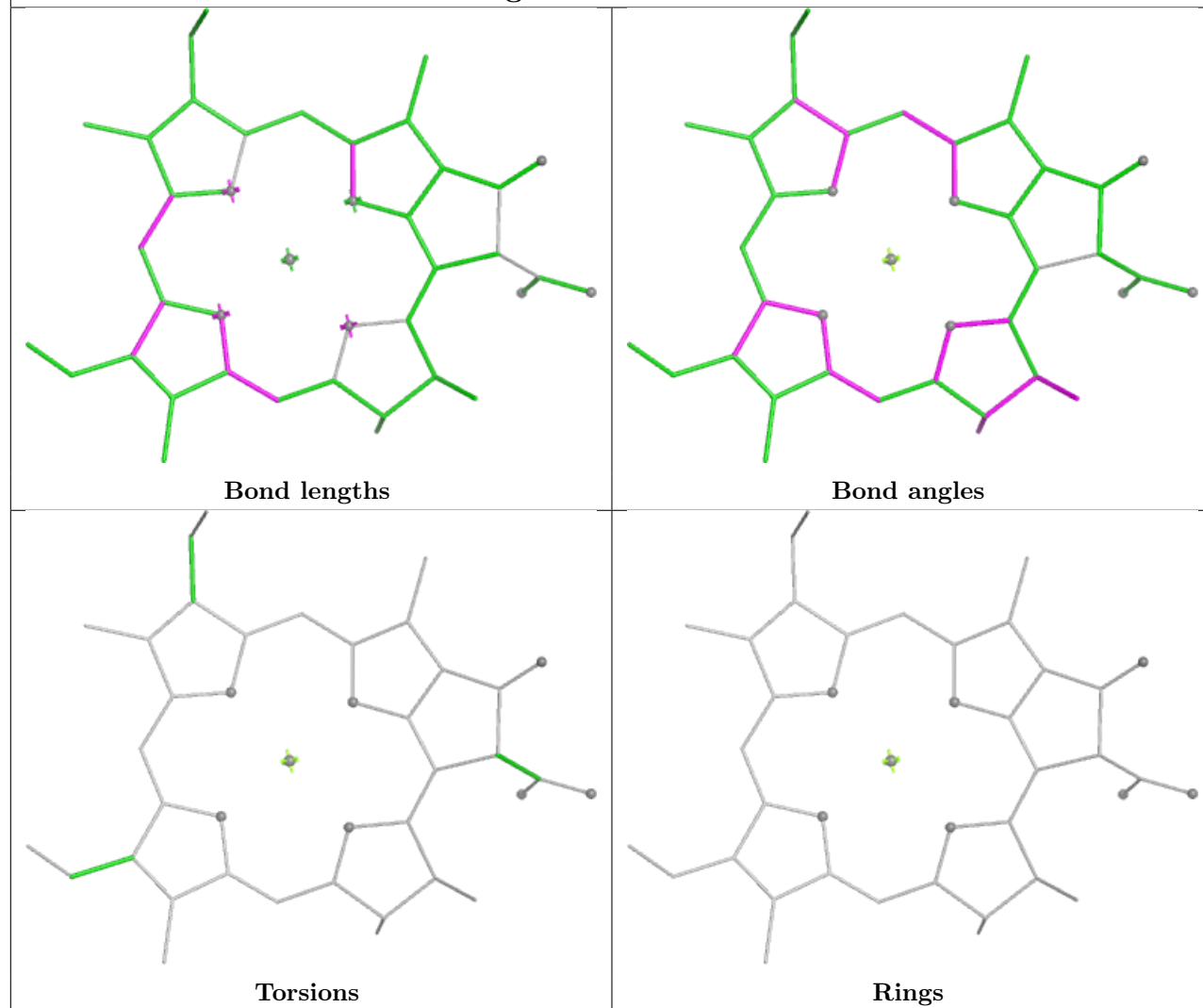
Ligand BCR L 308



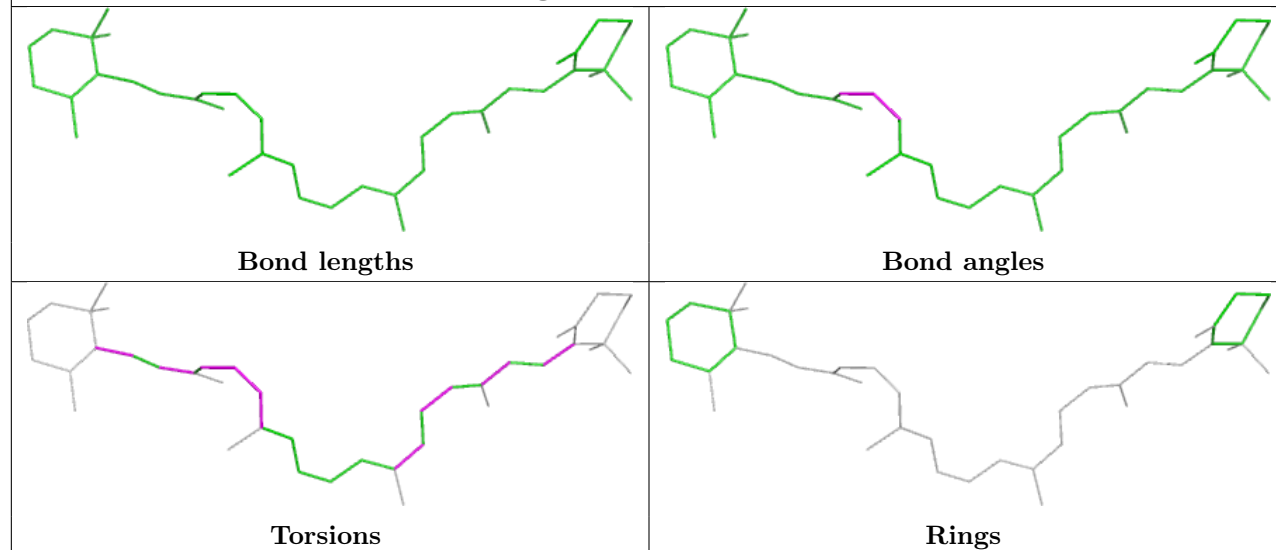
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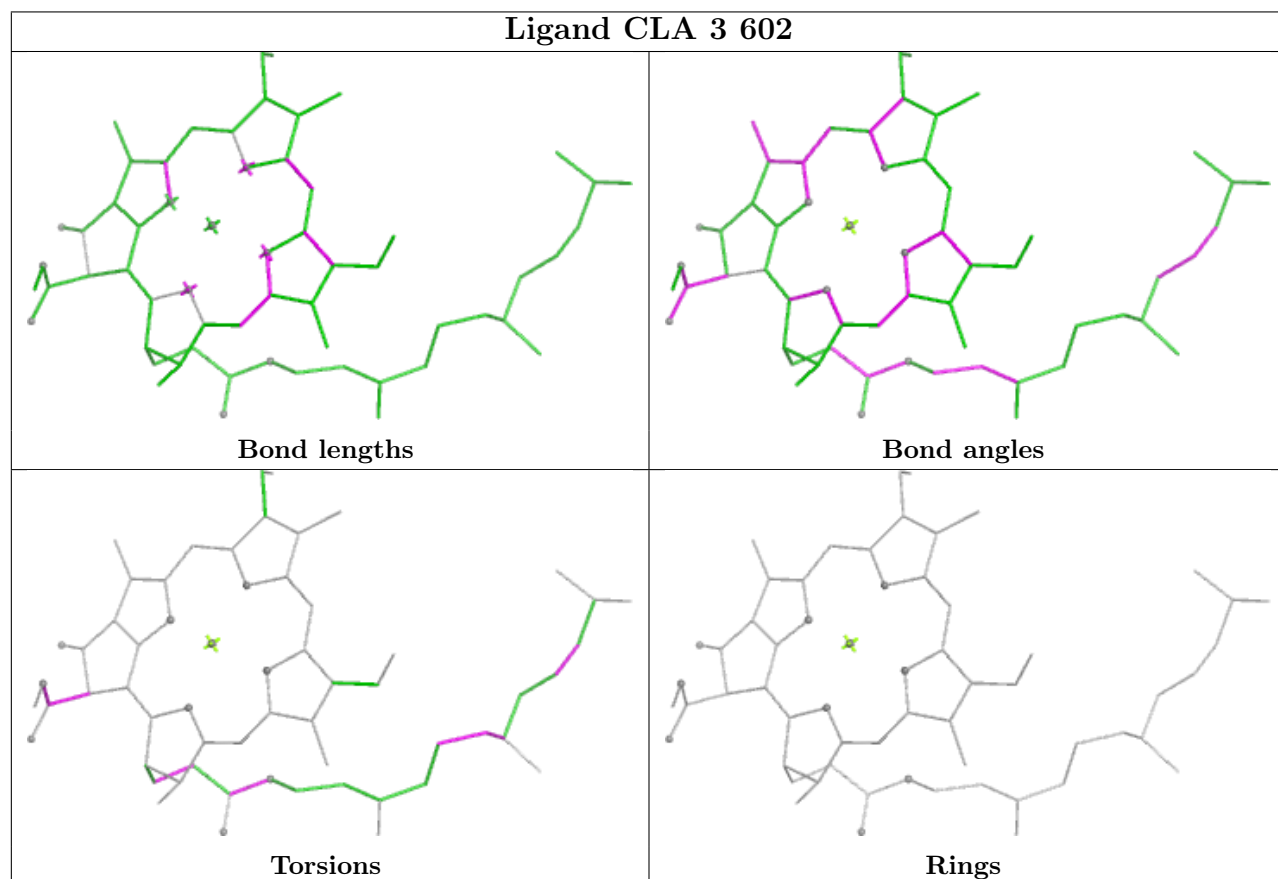
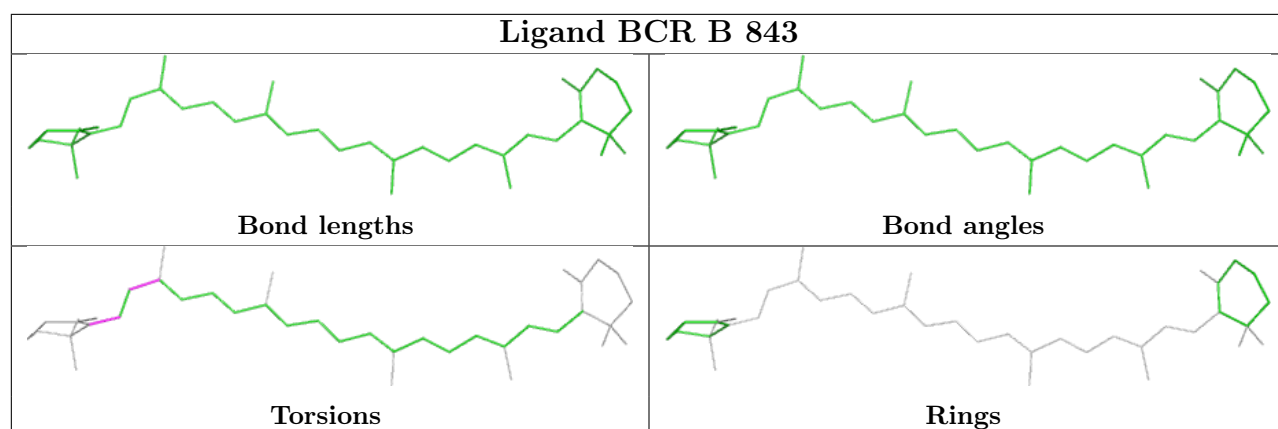


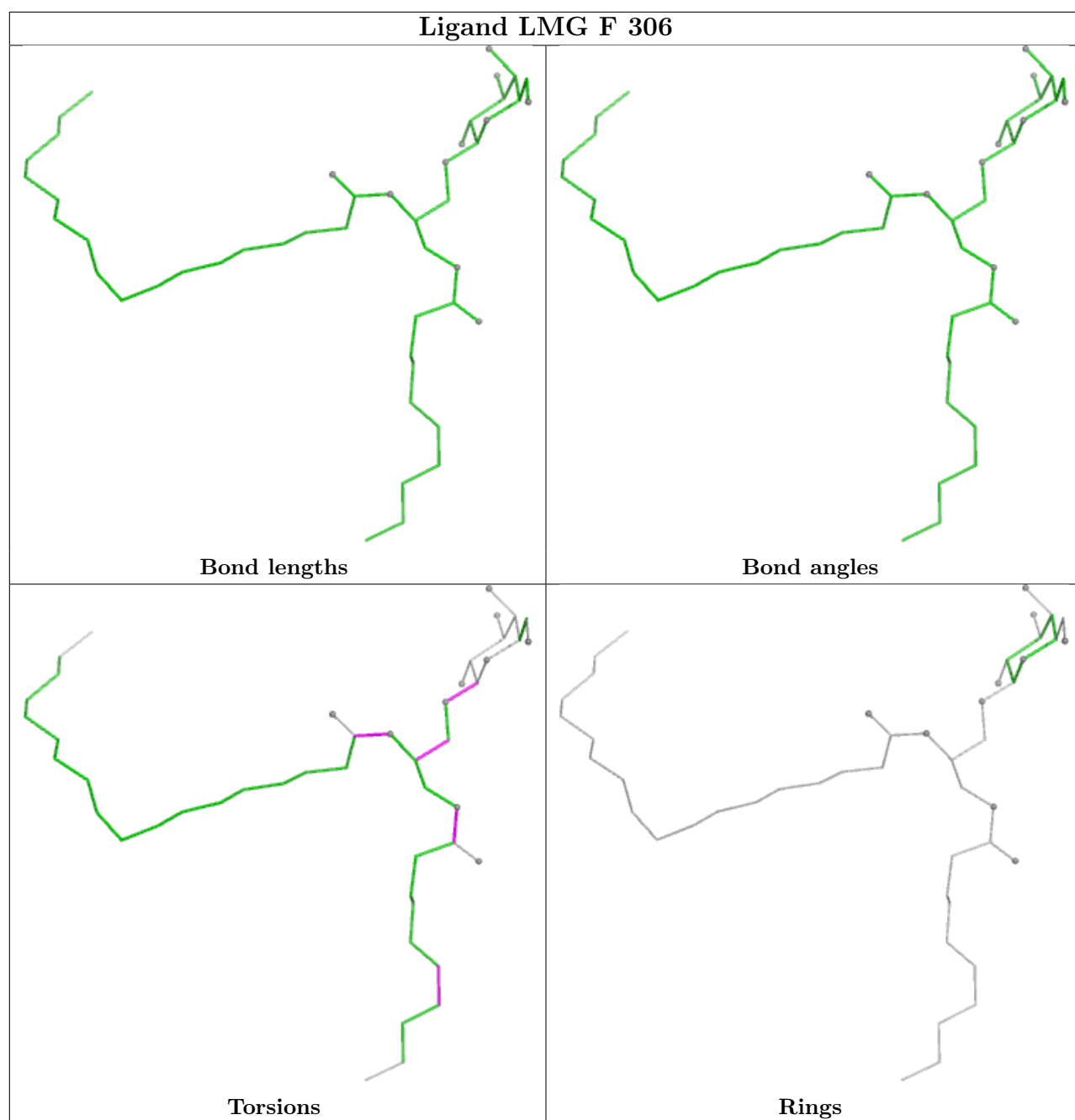
Ligand CLA 3 614



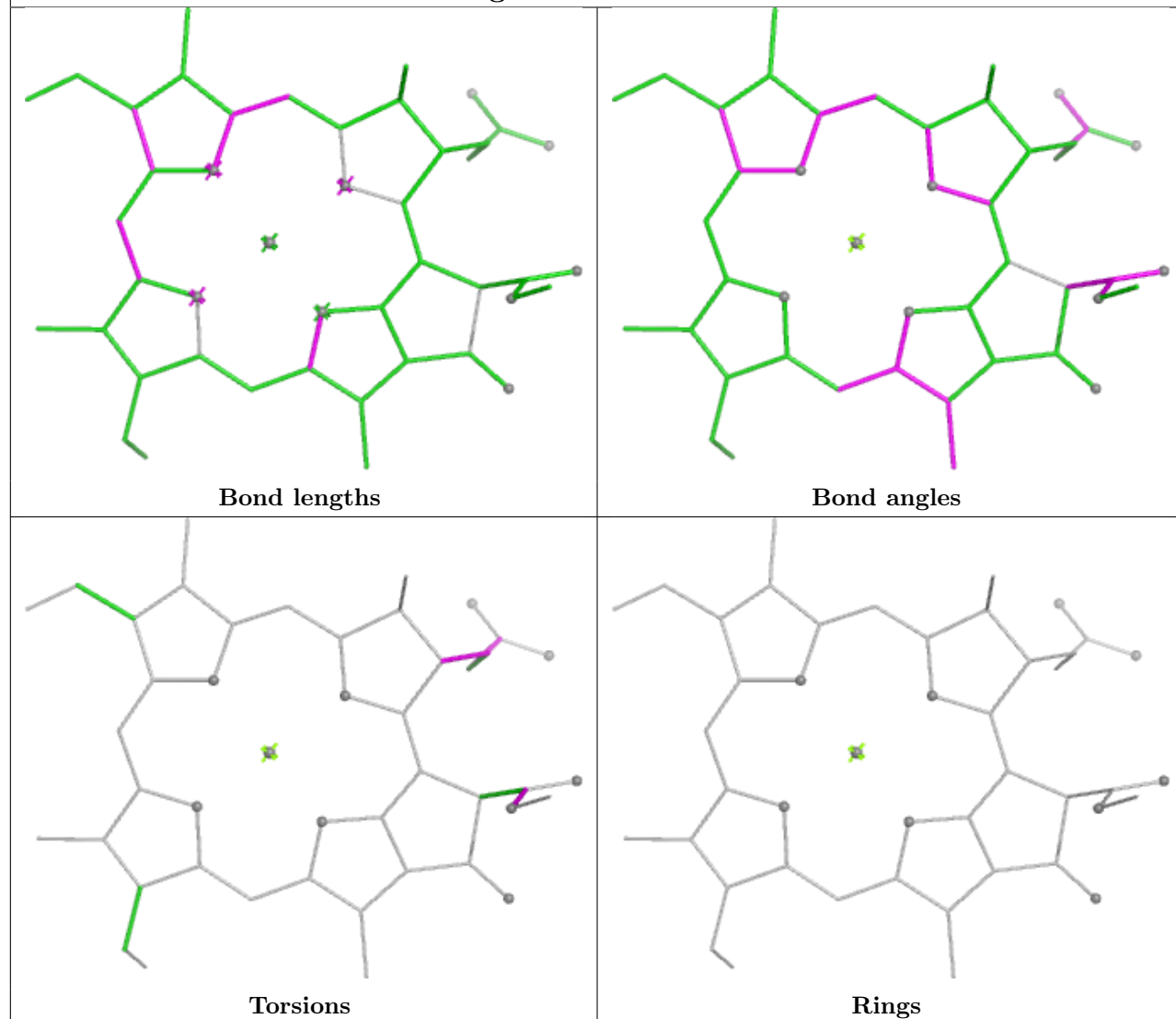
Ligand BCR 2 619



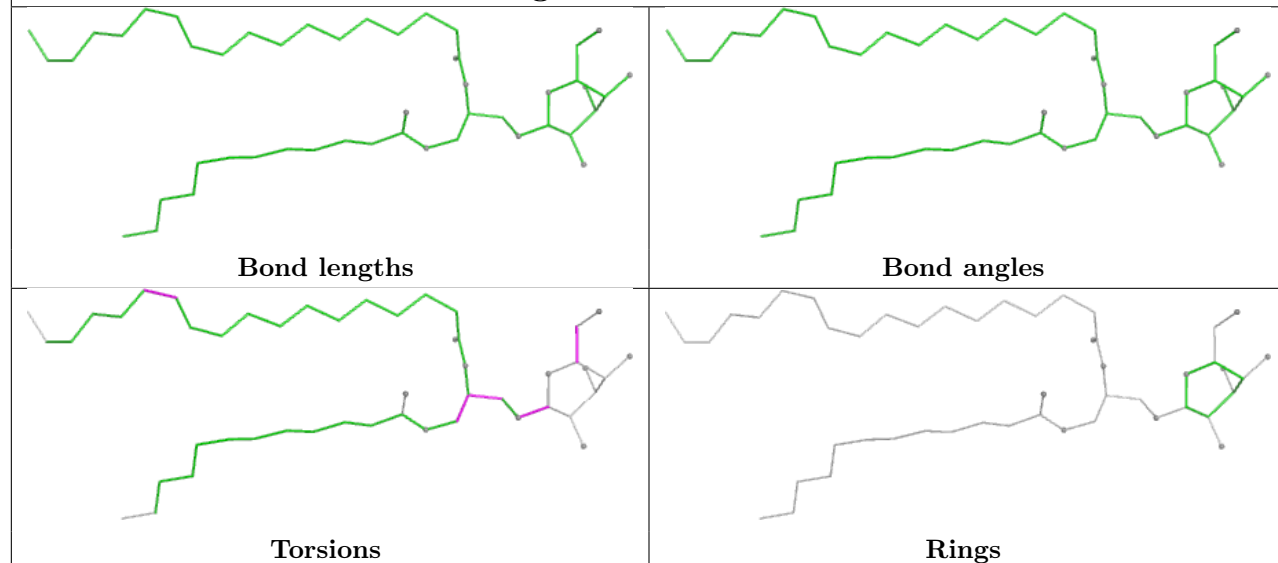




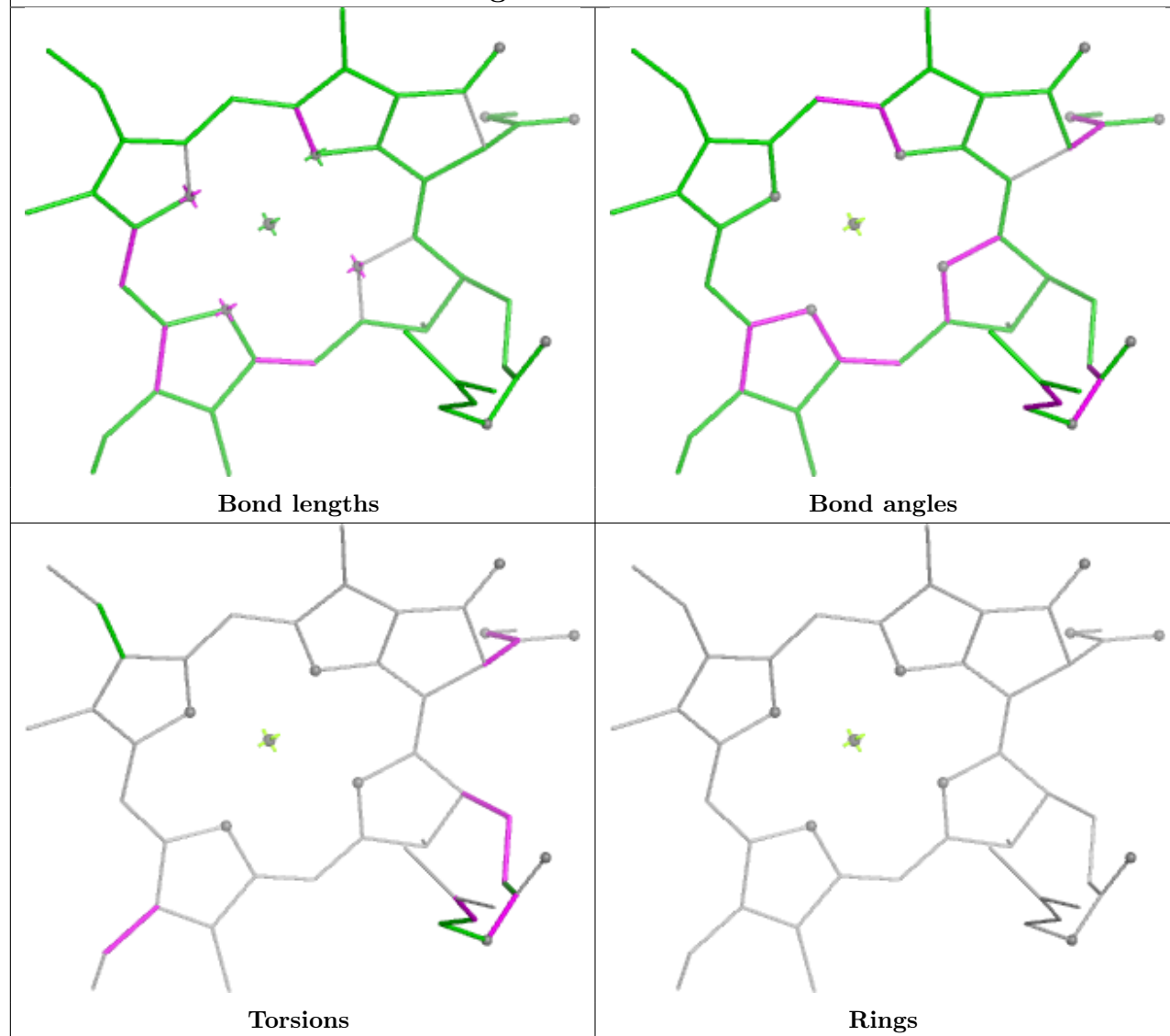
Ligand CLA A 816



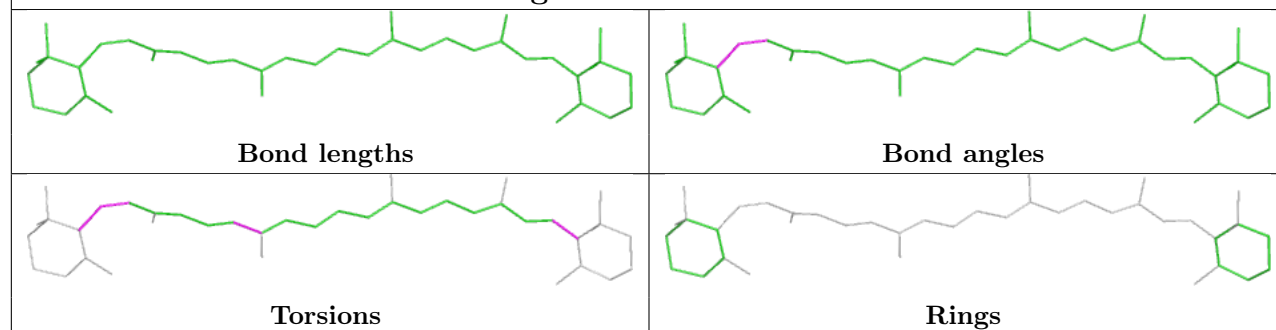
Ligand LMG 1 621

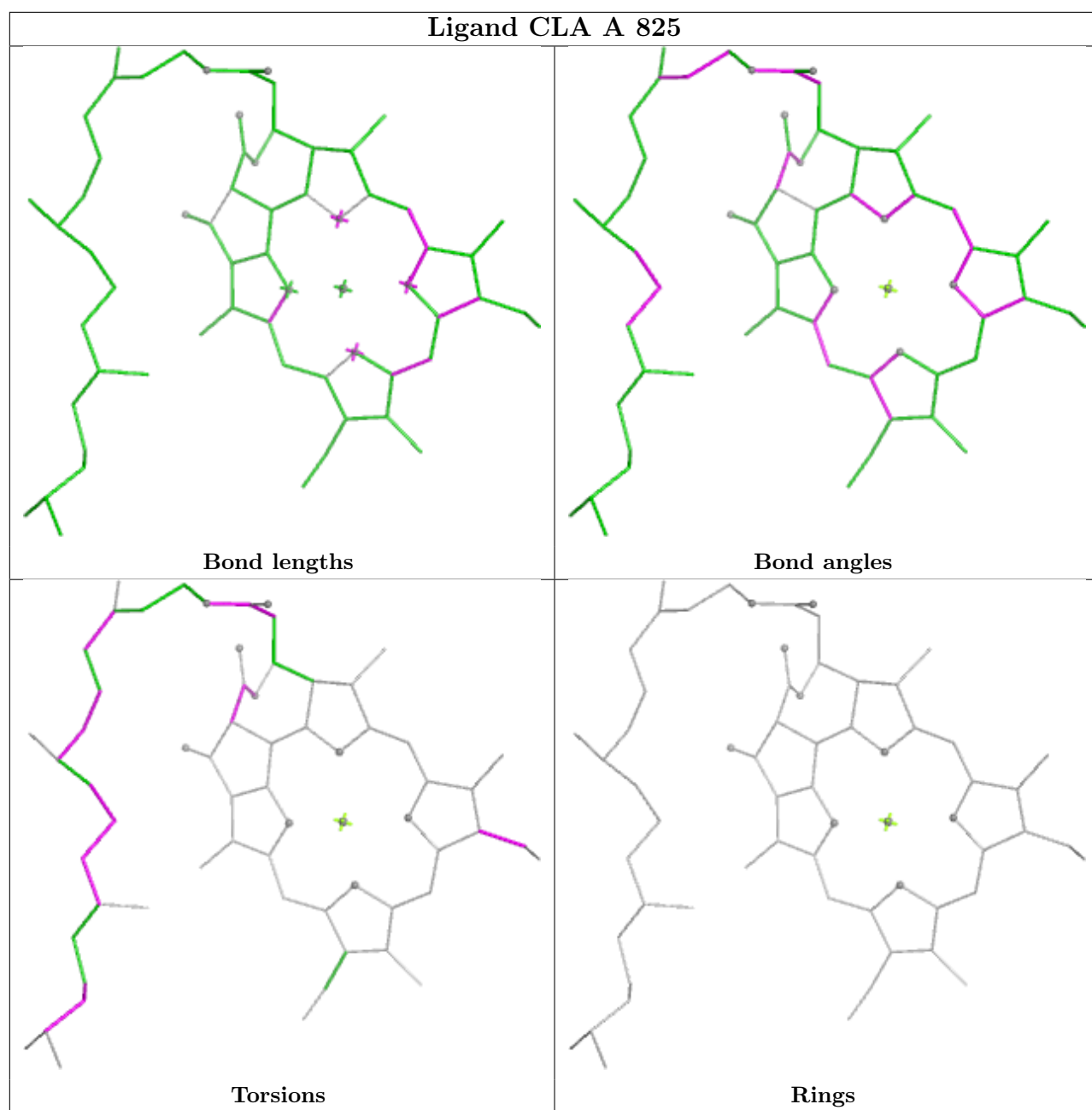


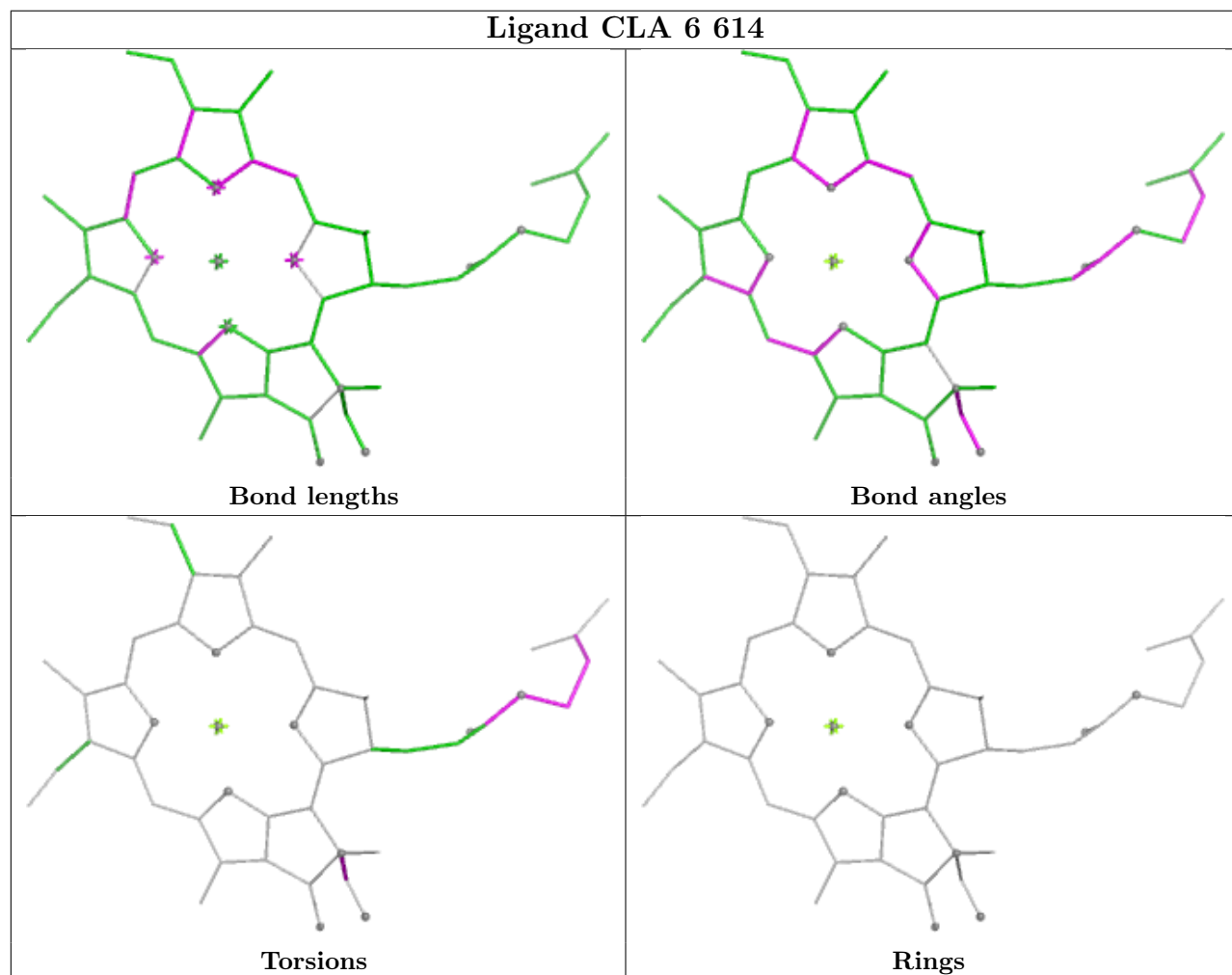
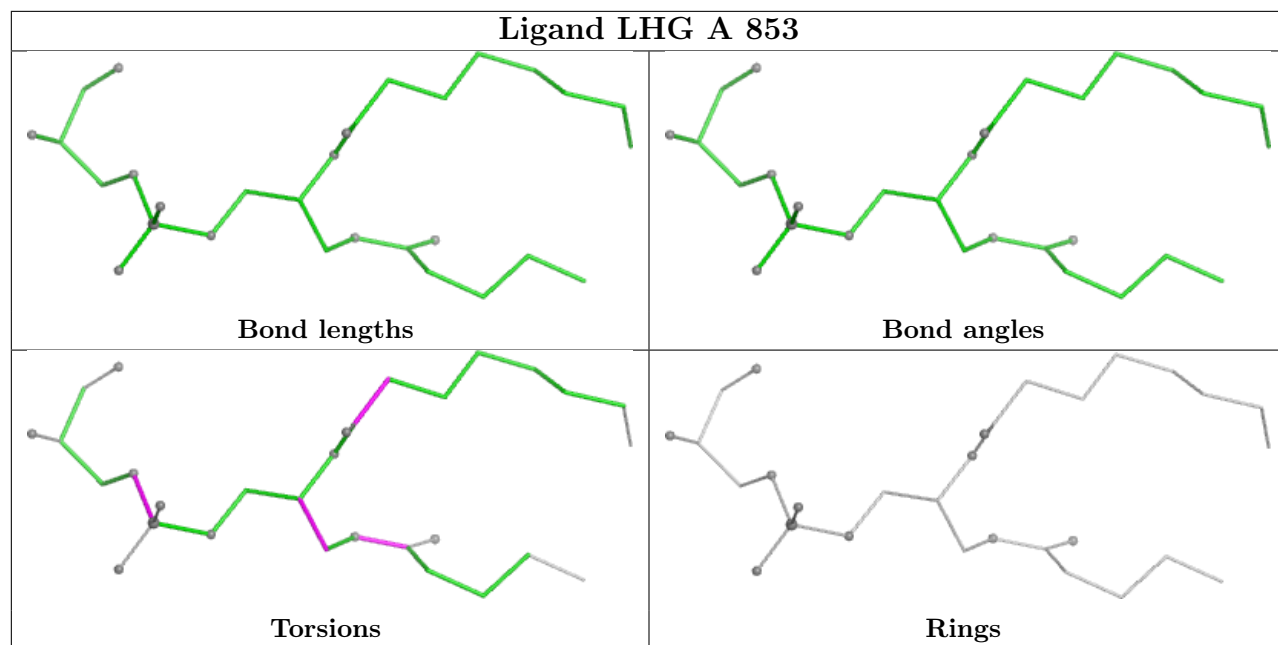
Ligand CLA Z 305

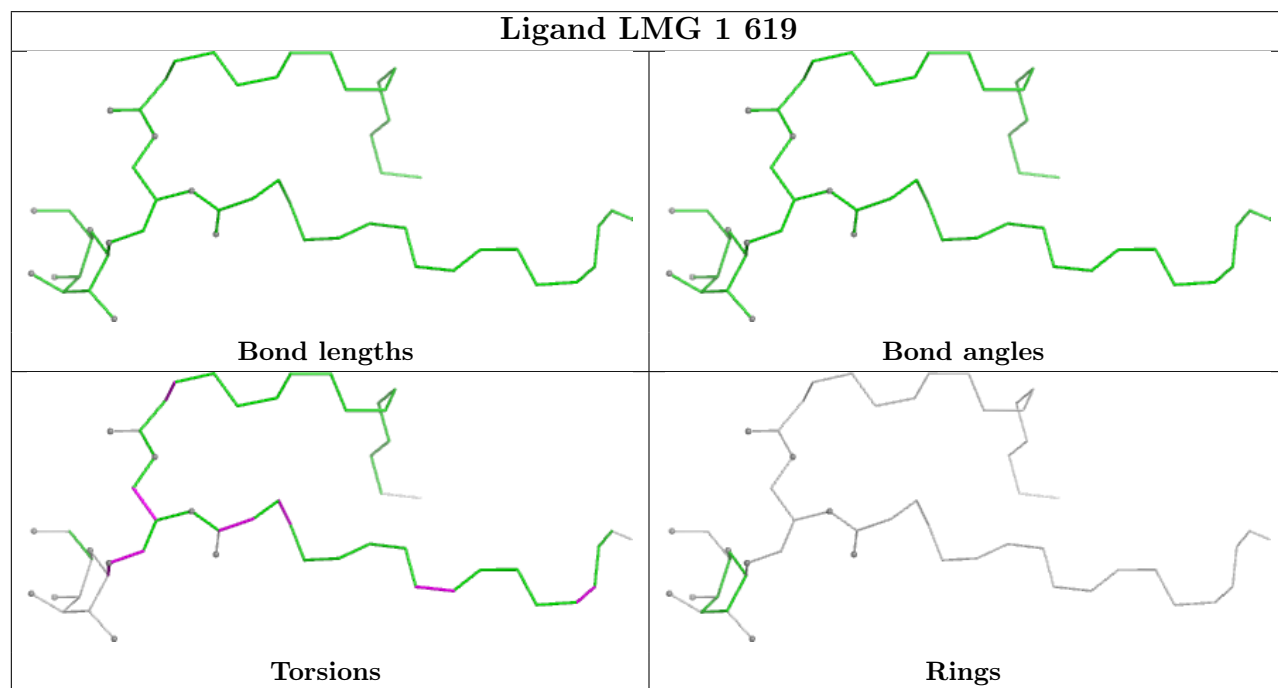
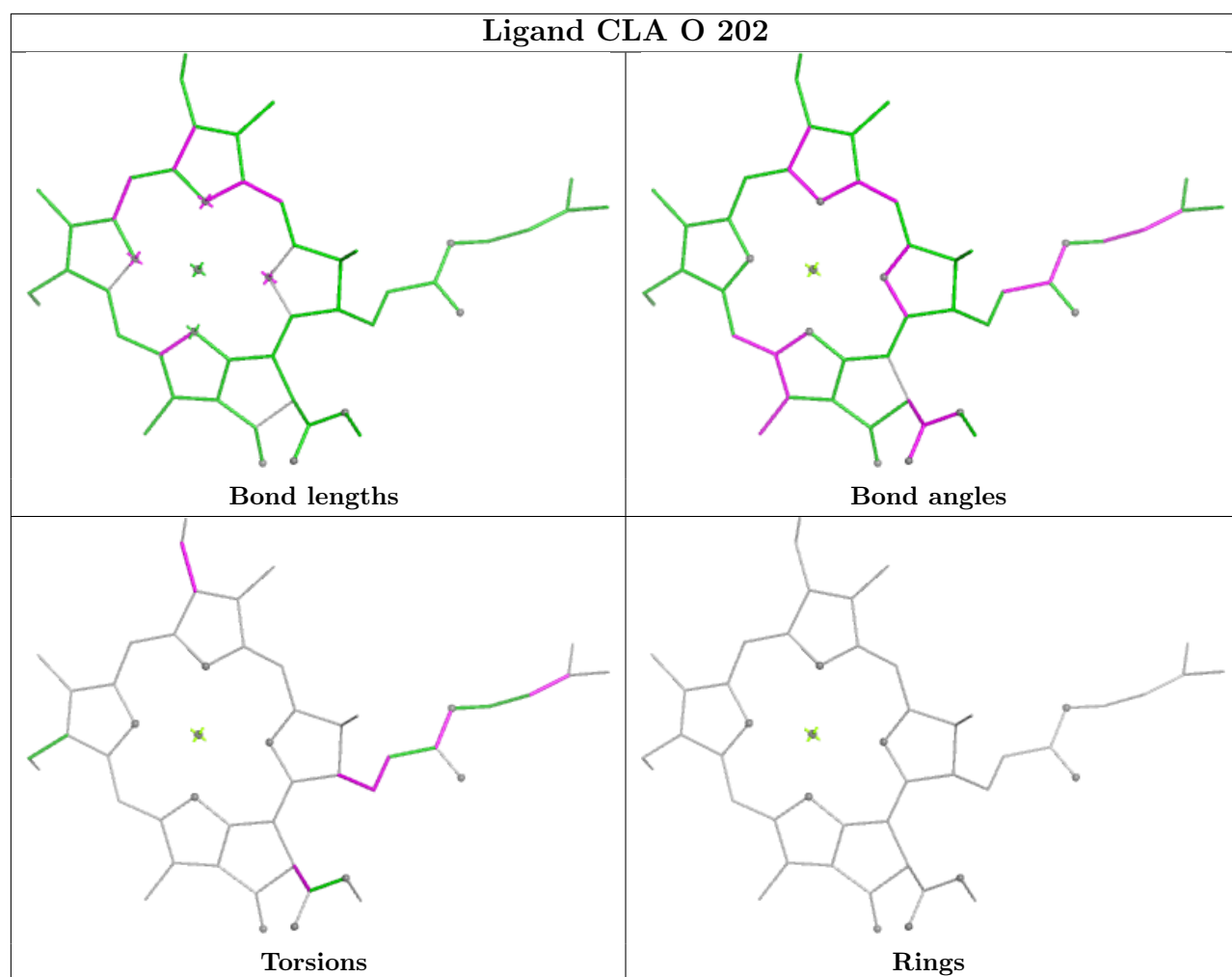


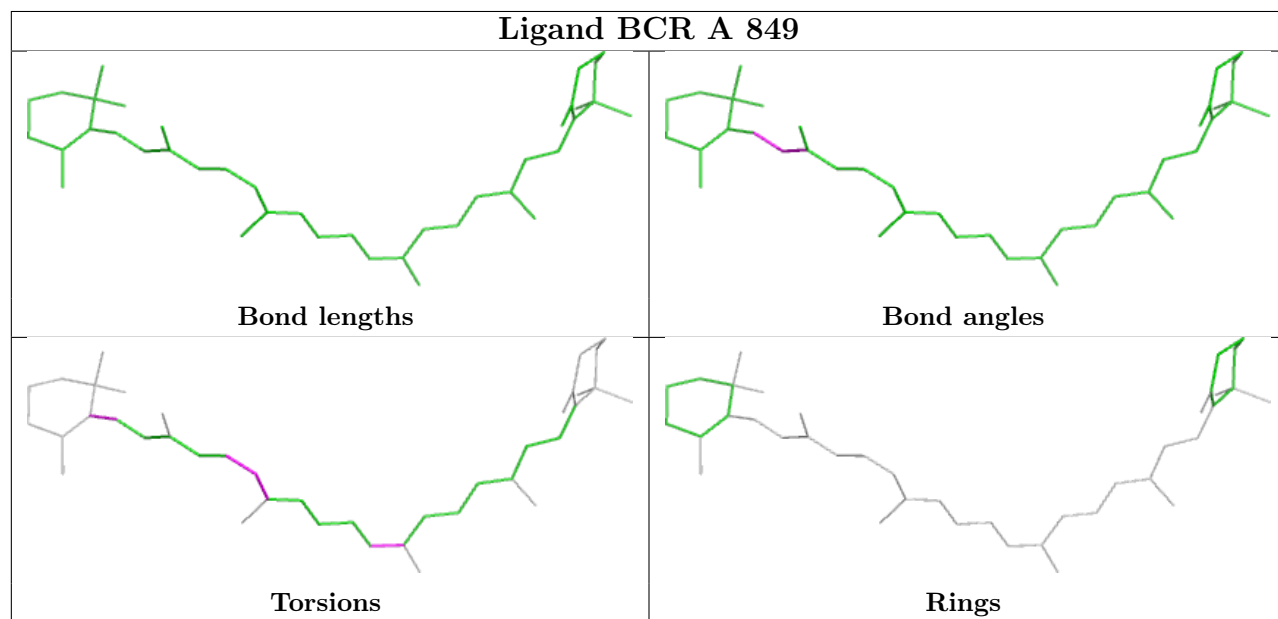
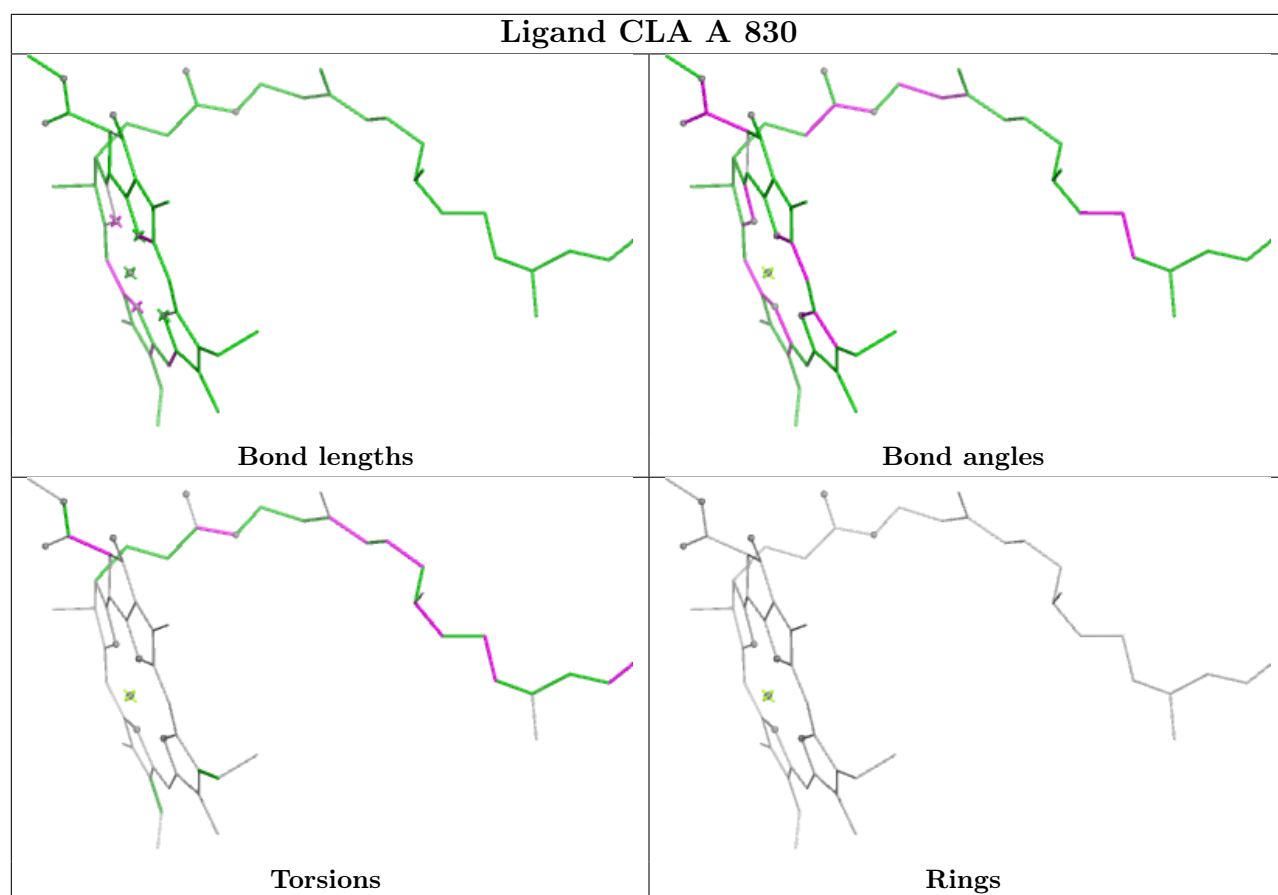
Ligand BCR B 848



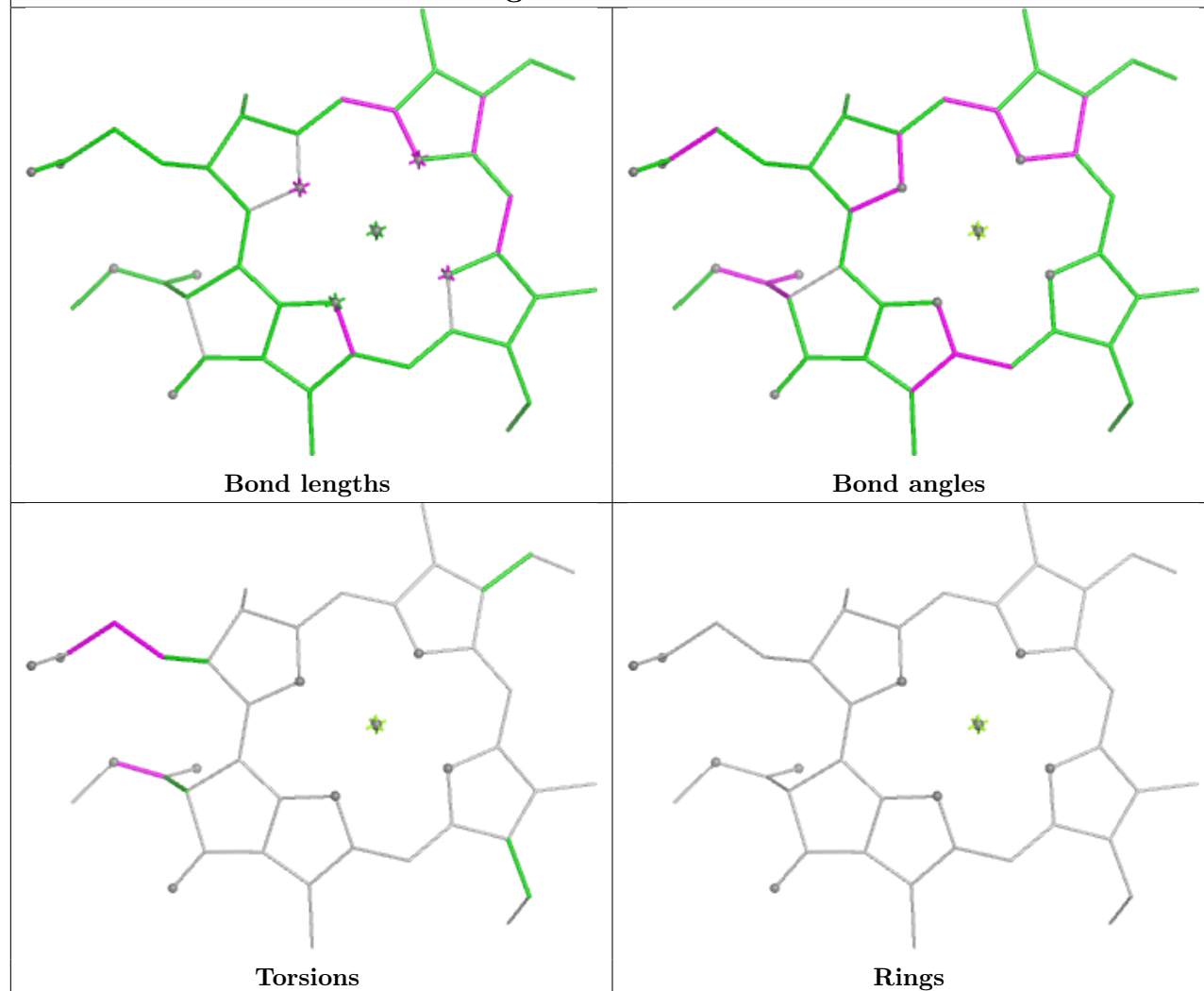




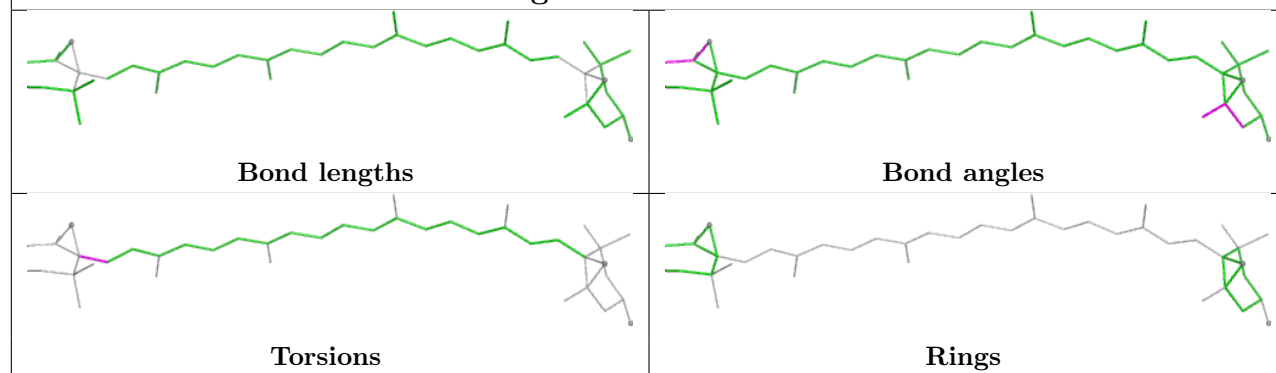




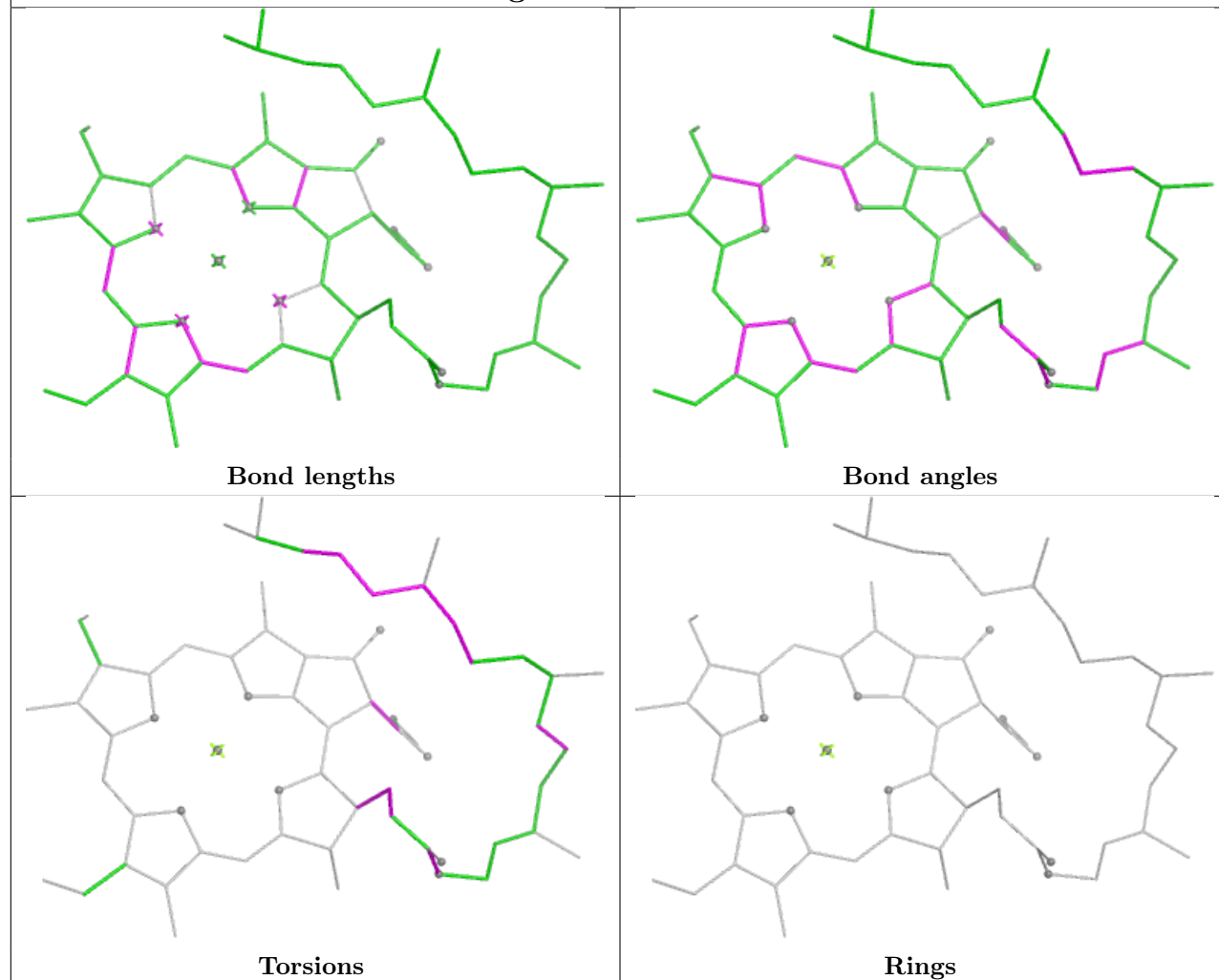
Ligand CLA 2 611



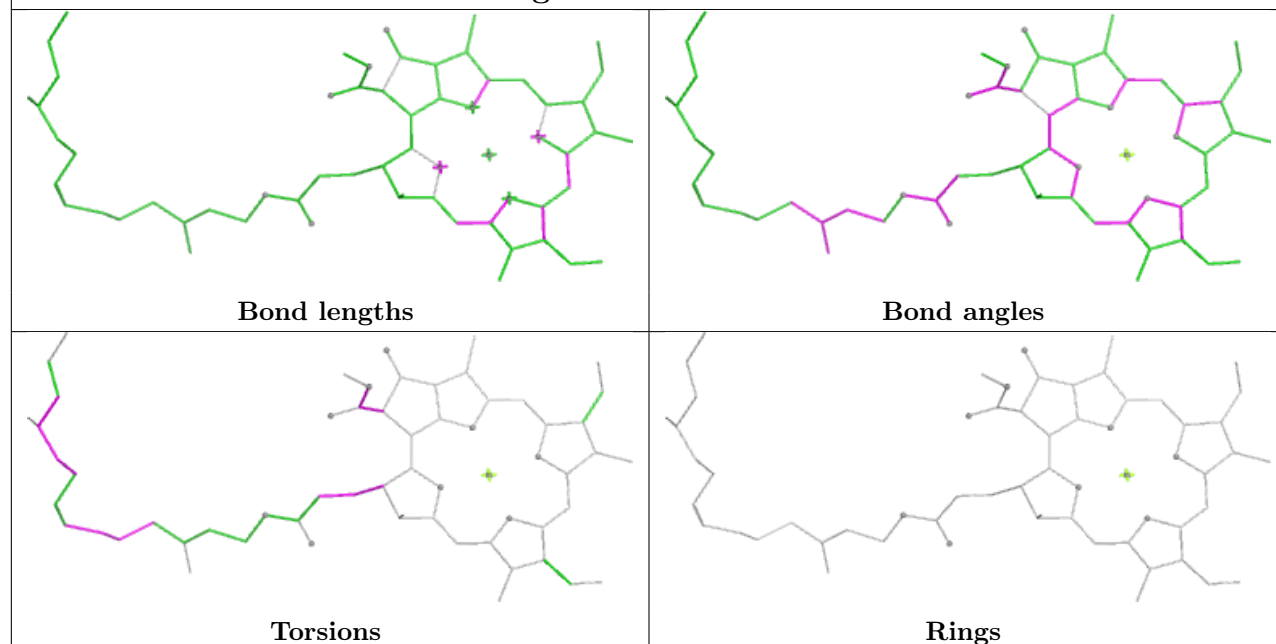
Ligand XAT O 208

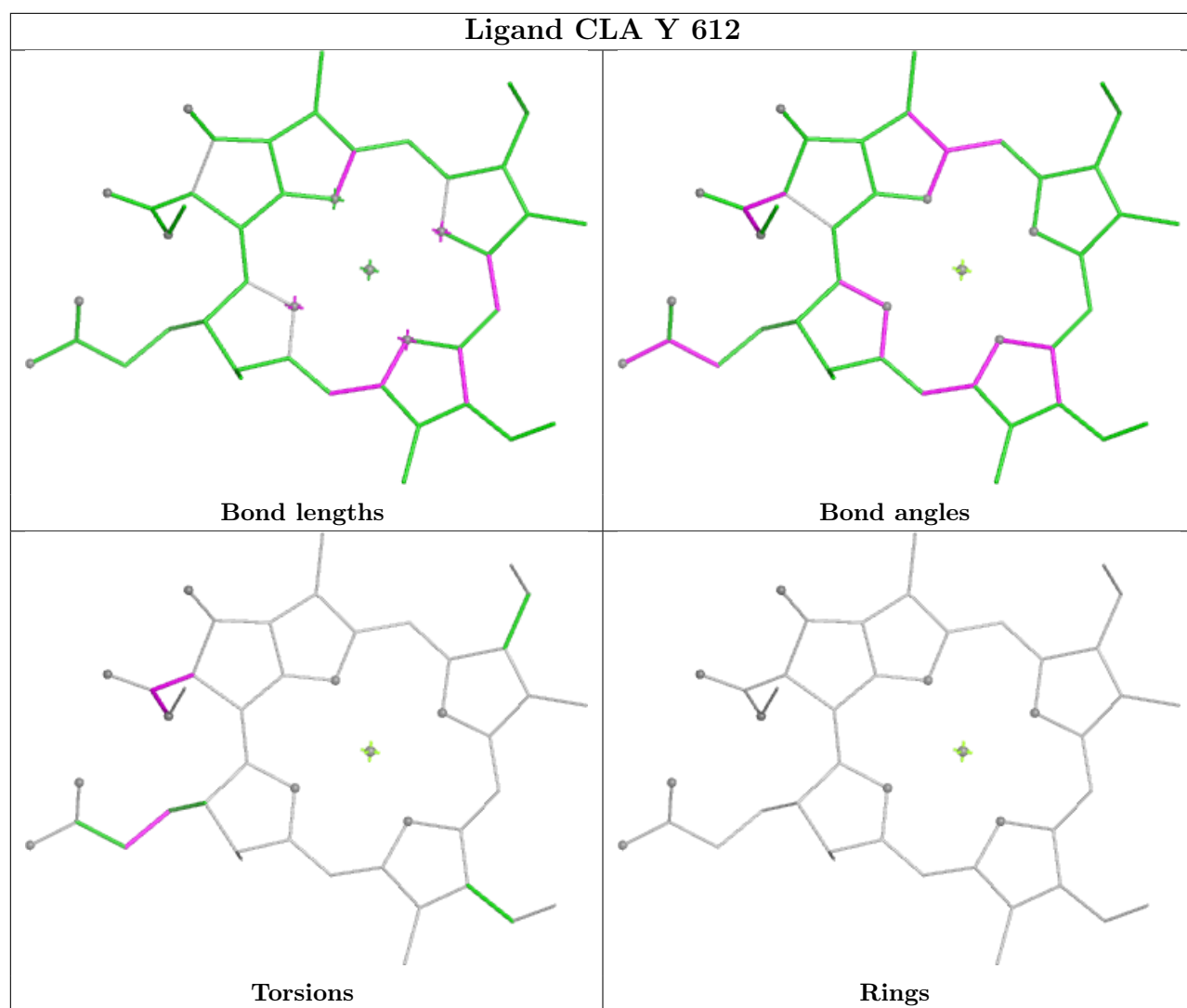


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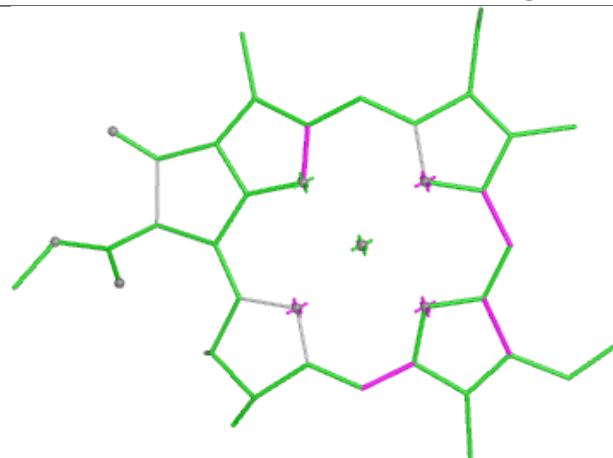


Ligand CLA B 825

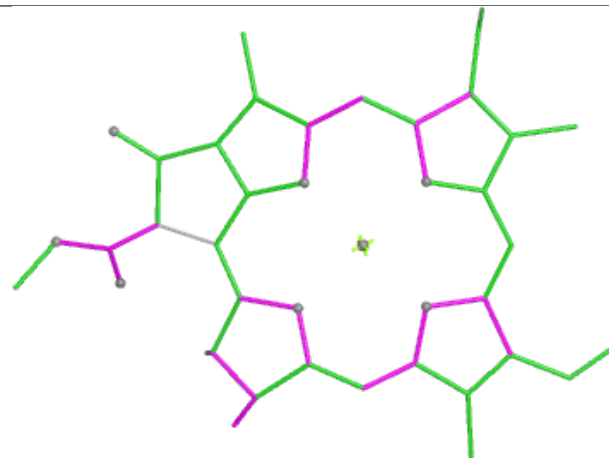




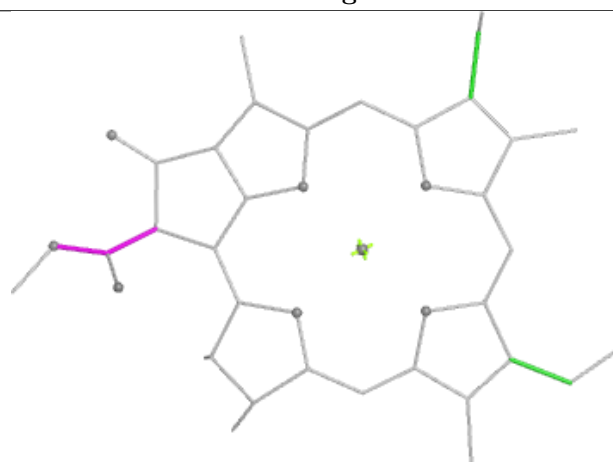
Ligand CLA 3 610



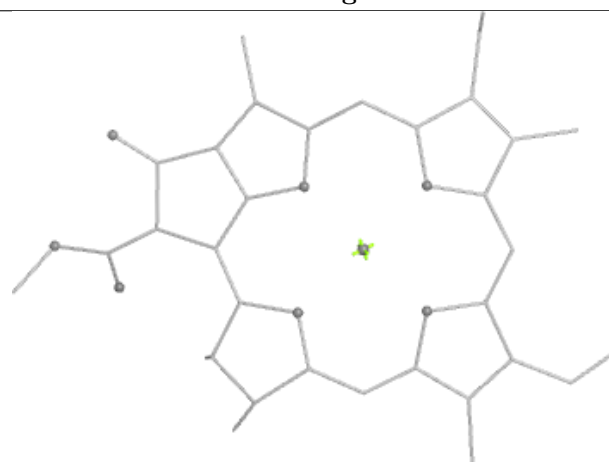
Bond lengths



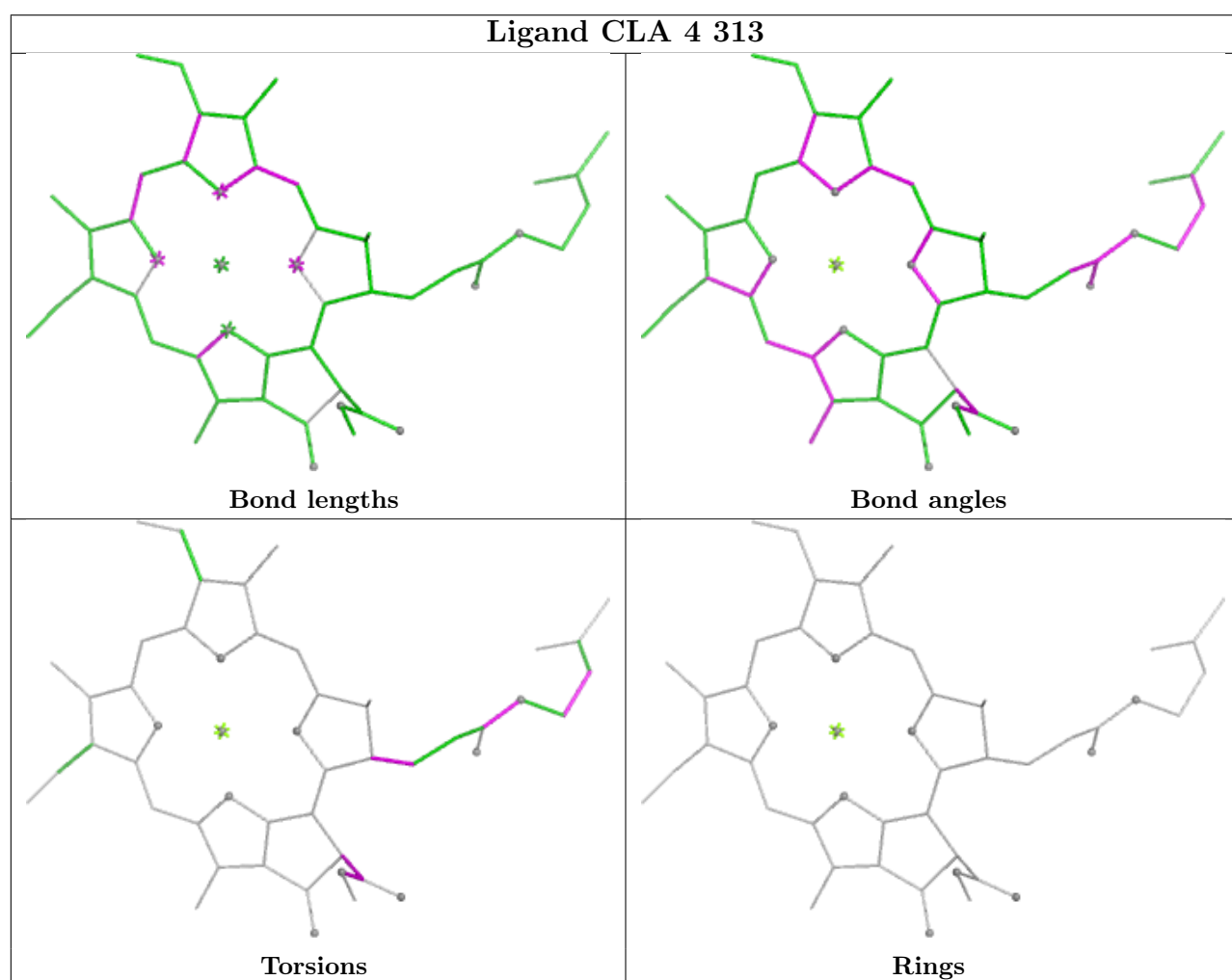
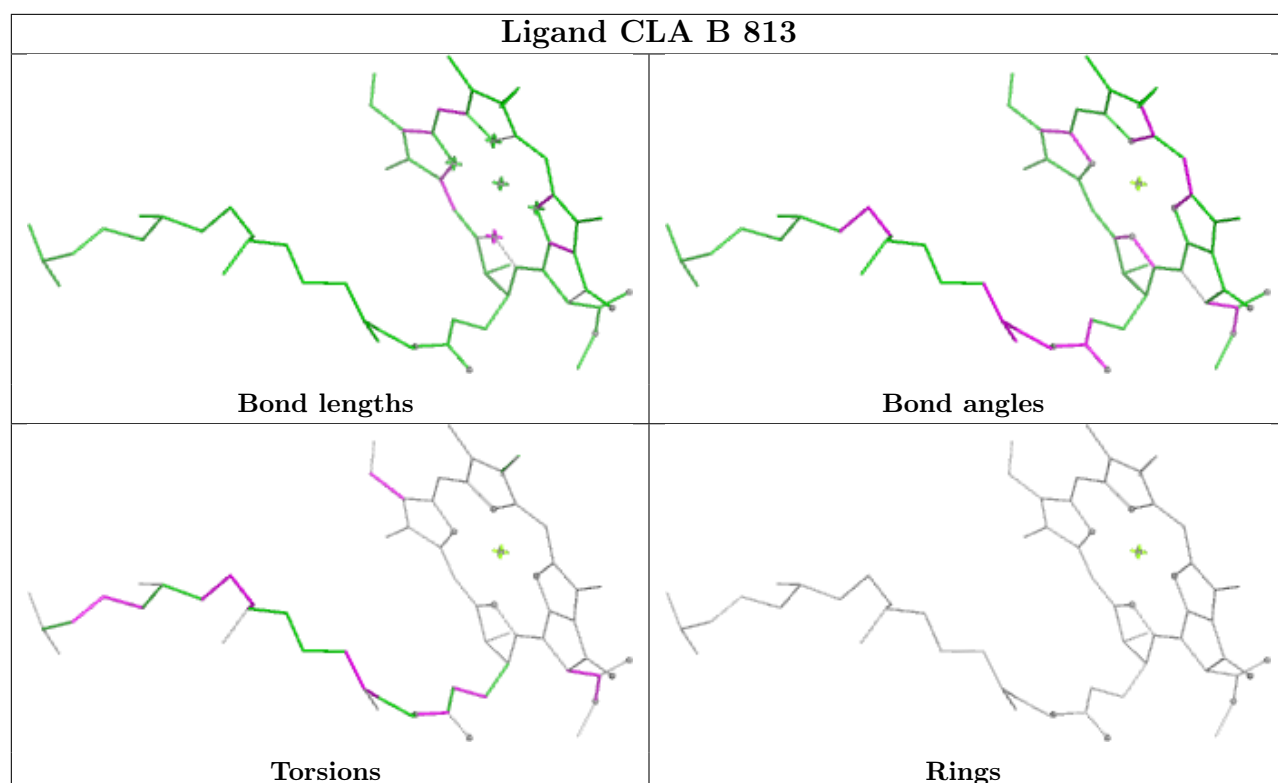
Bond angles



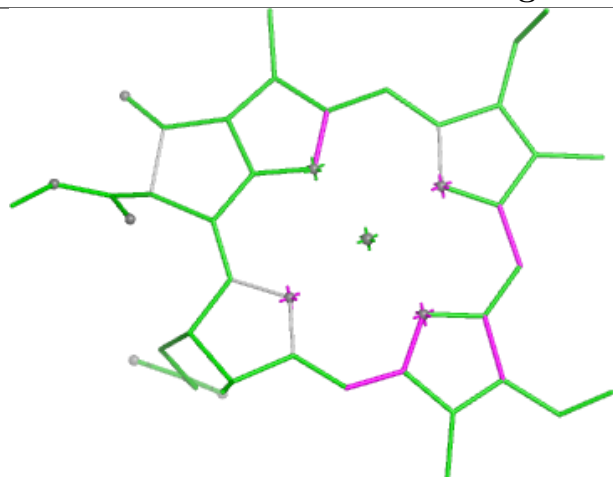
Torsions



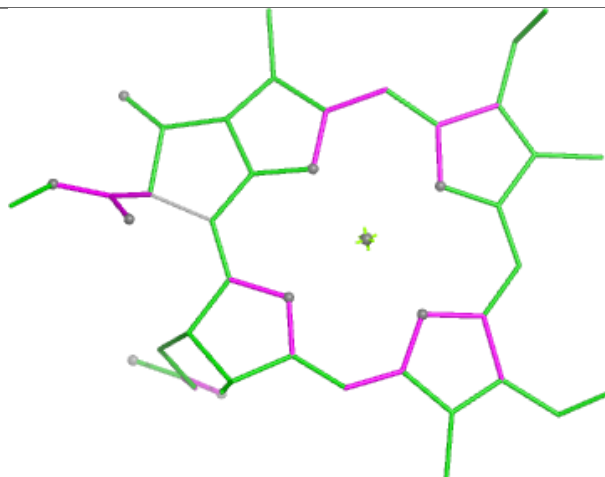
Rings



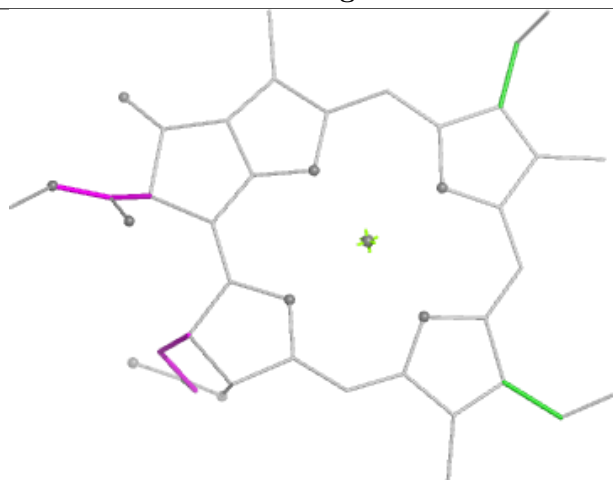
Ligand CLA 6 608



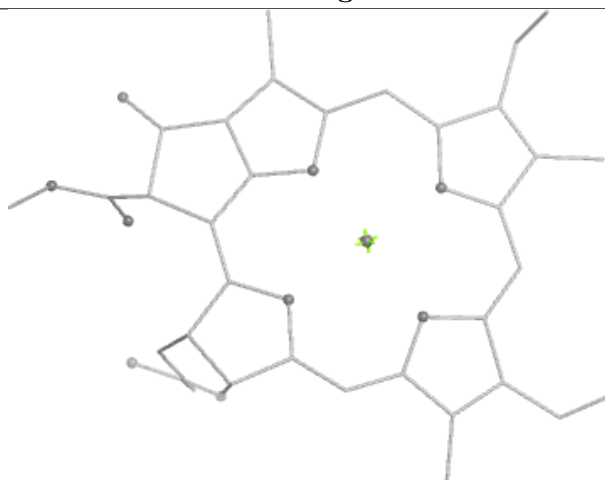
Bond lengths



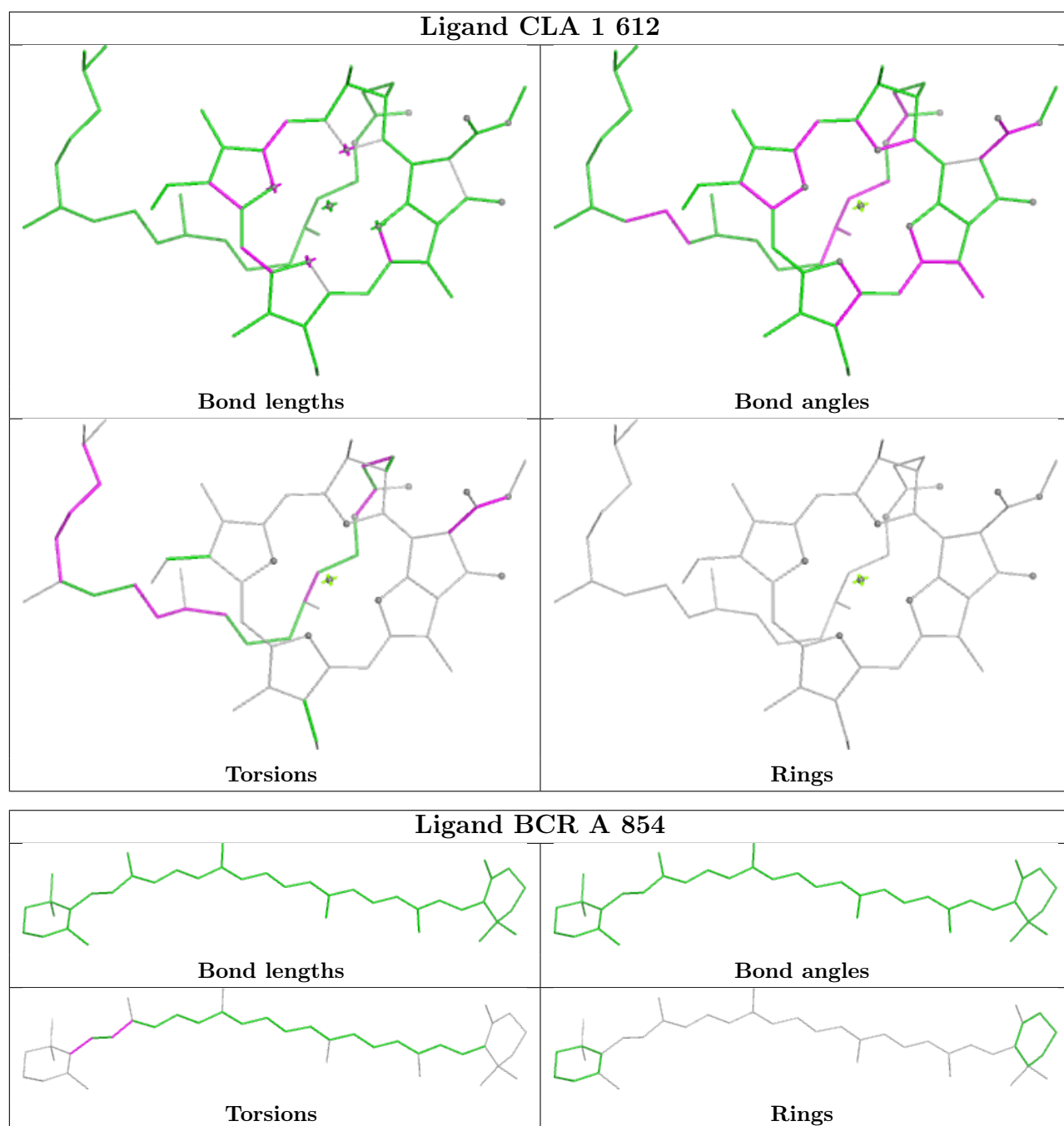
Bond angles



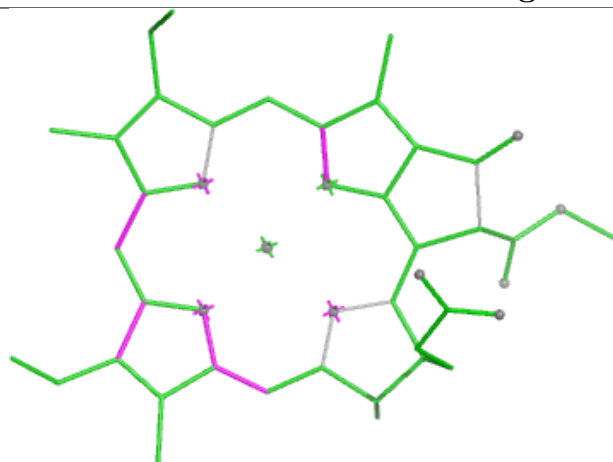
Torsions



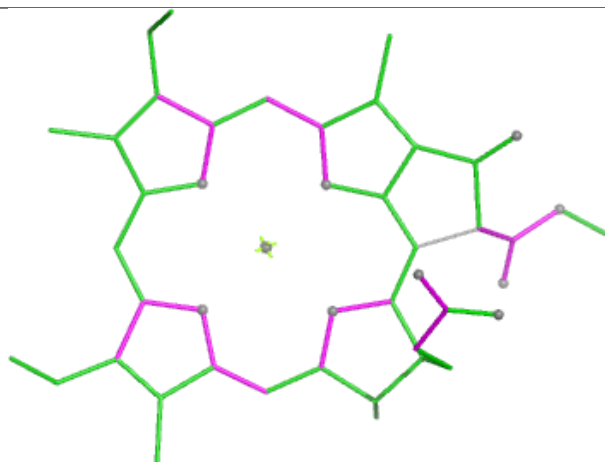
Rings



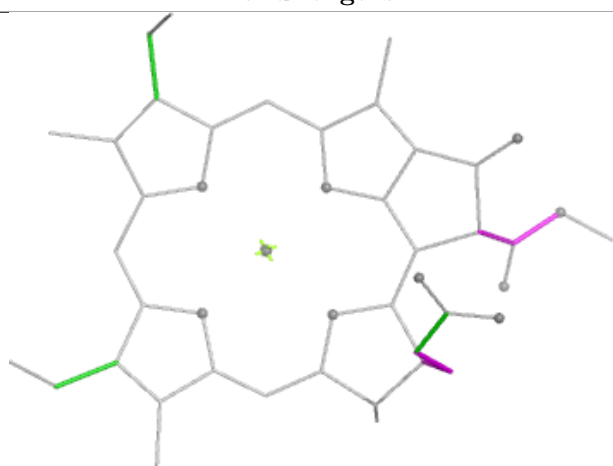
Ligand CLA 4 312



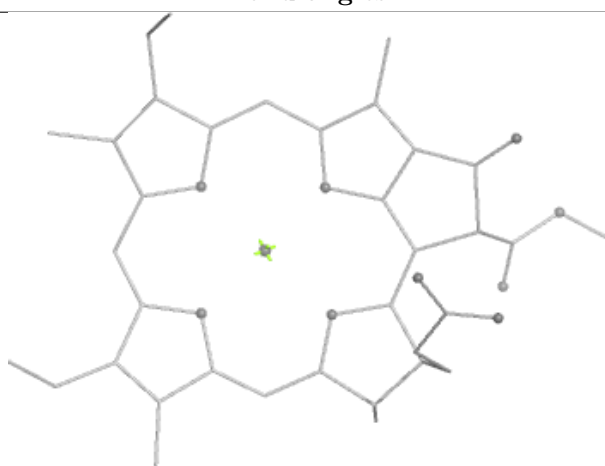
Bond lengths



Bond angles

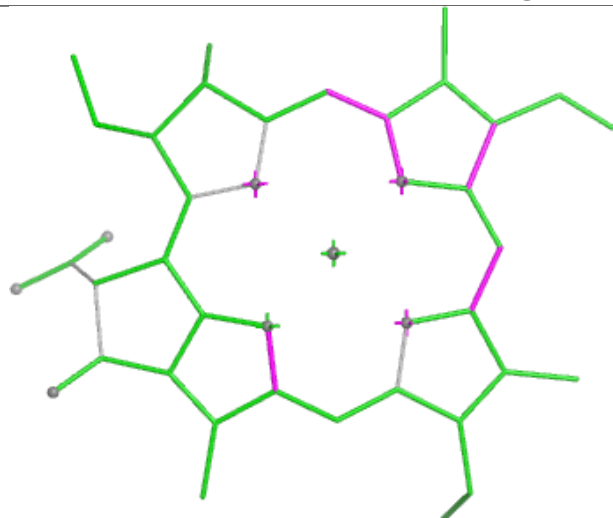


Torsions

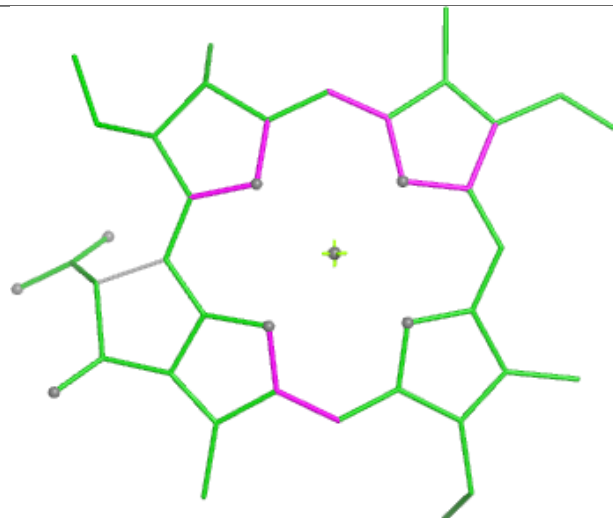


Rings

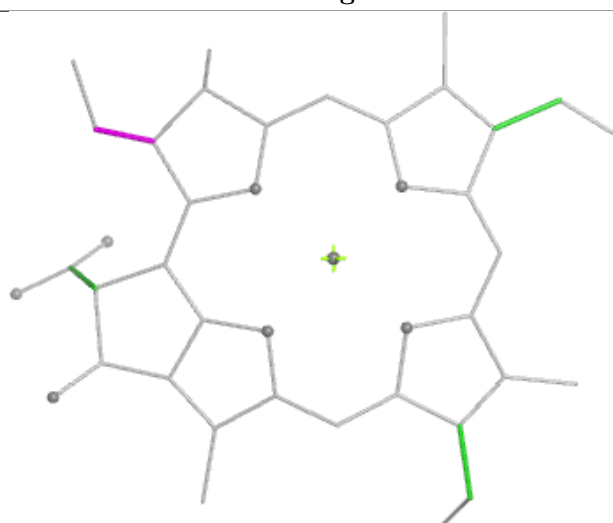
Ligand CLA 4 310



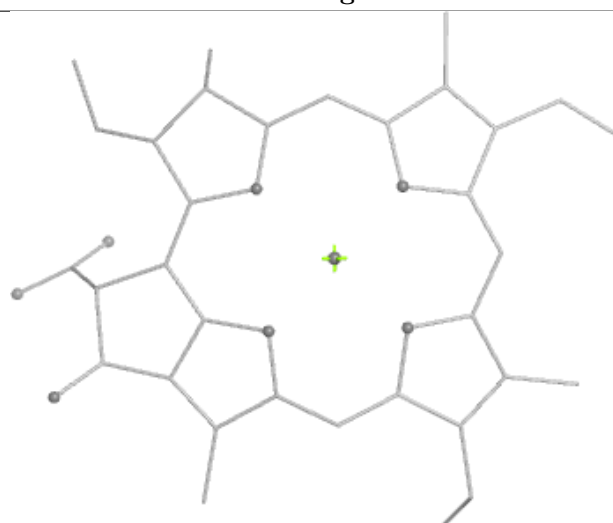
Bond lengths



Bond angles

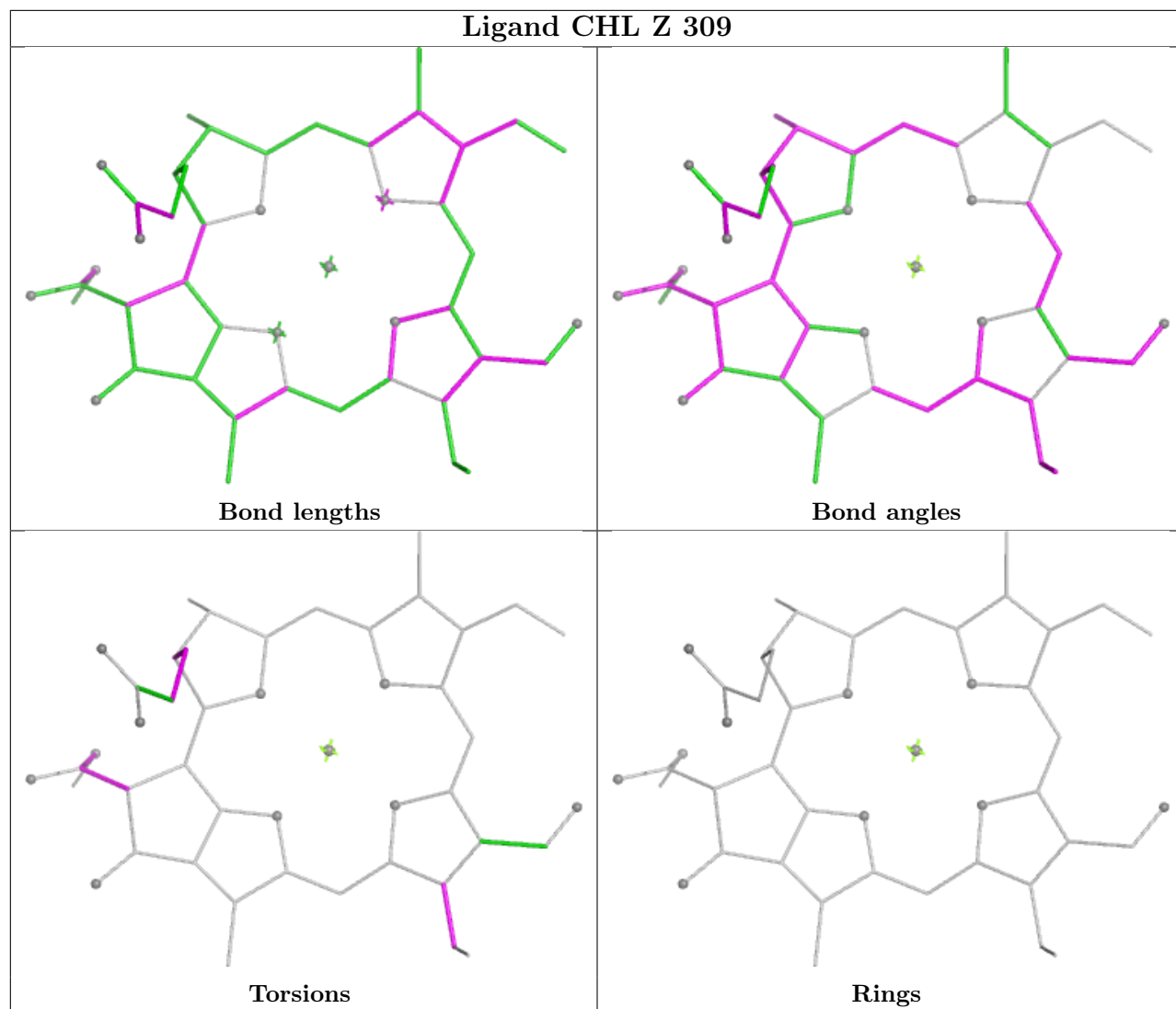


Torsions

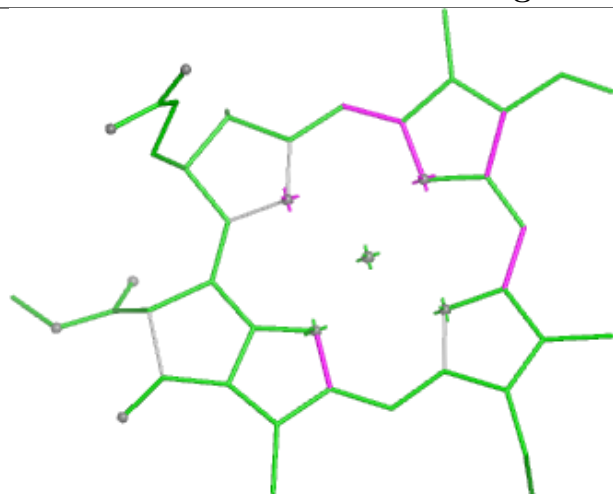


Rings

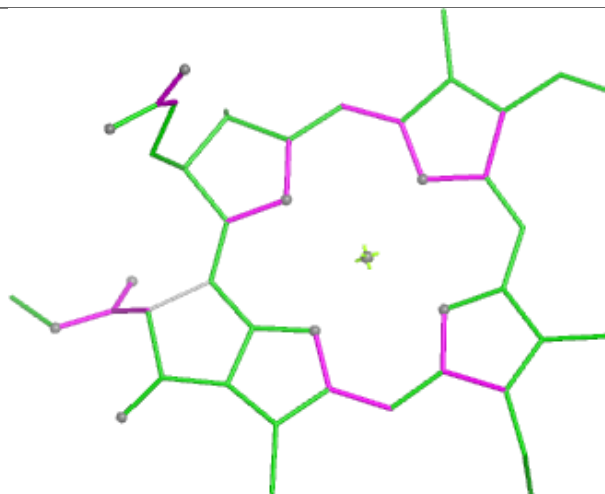
Ligand CHL Z 309



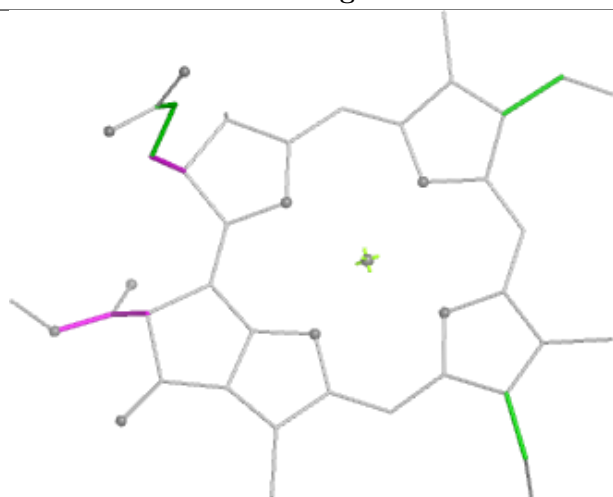
Ligand CLA A 805



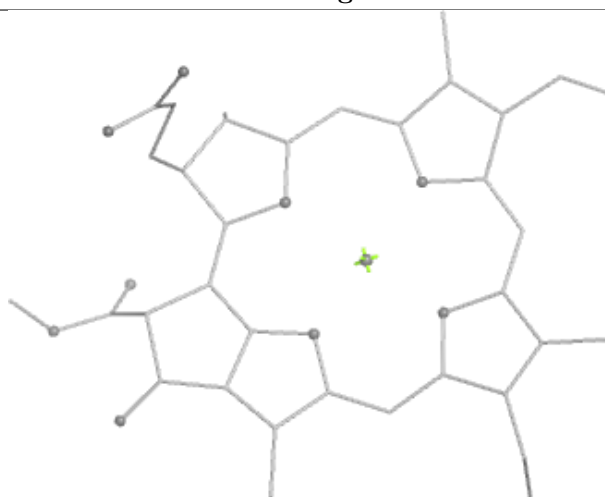
Bond lengths



Bond angles

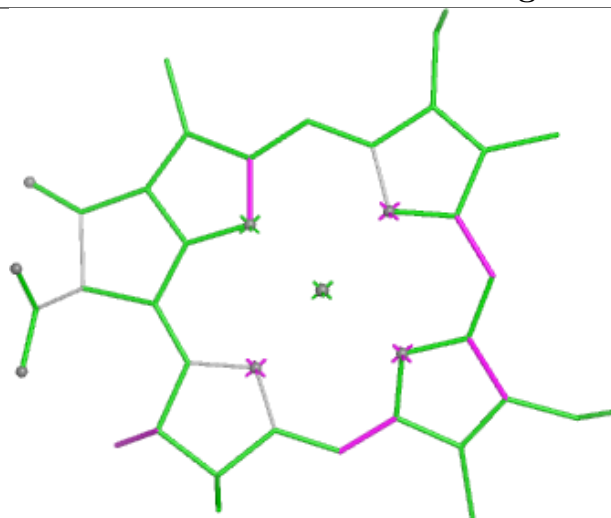


Torsions

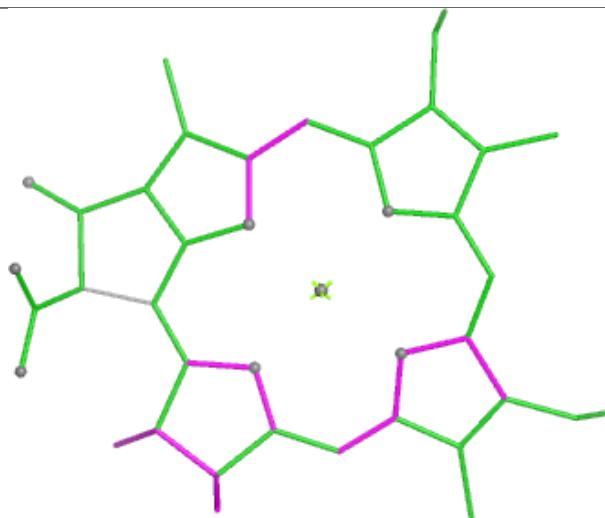


Rings

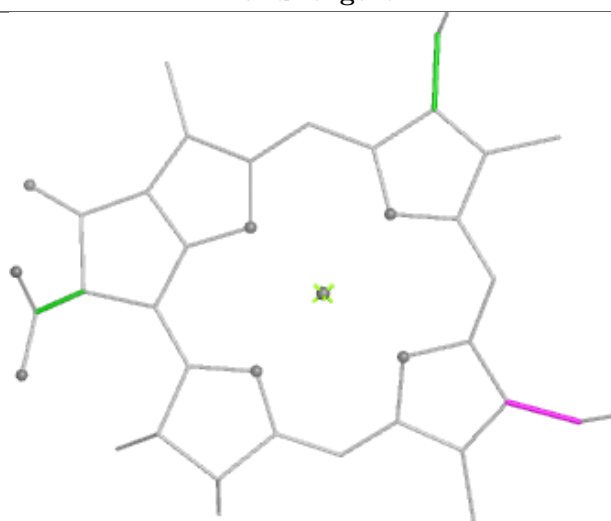
Ligand CLA 3 613



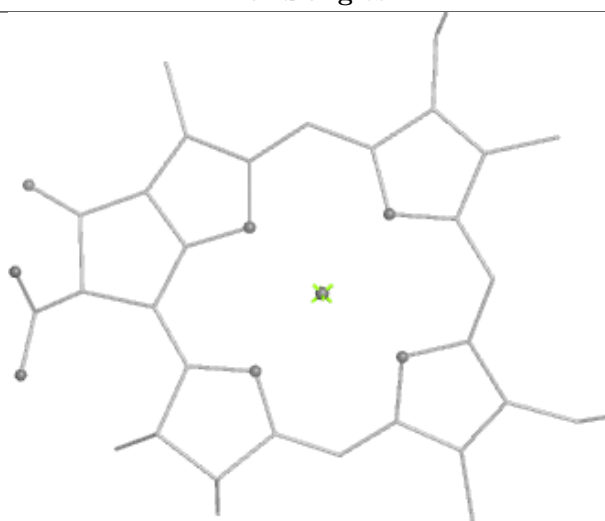
Bond lengths



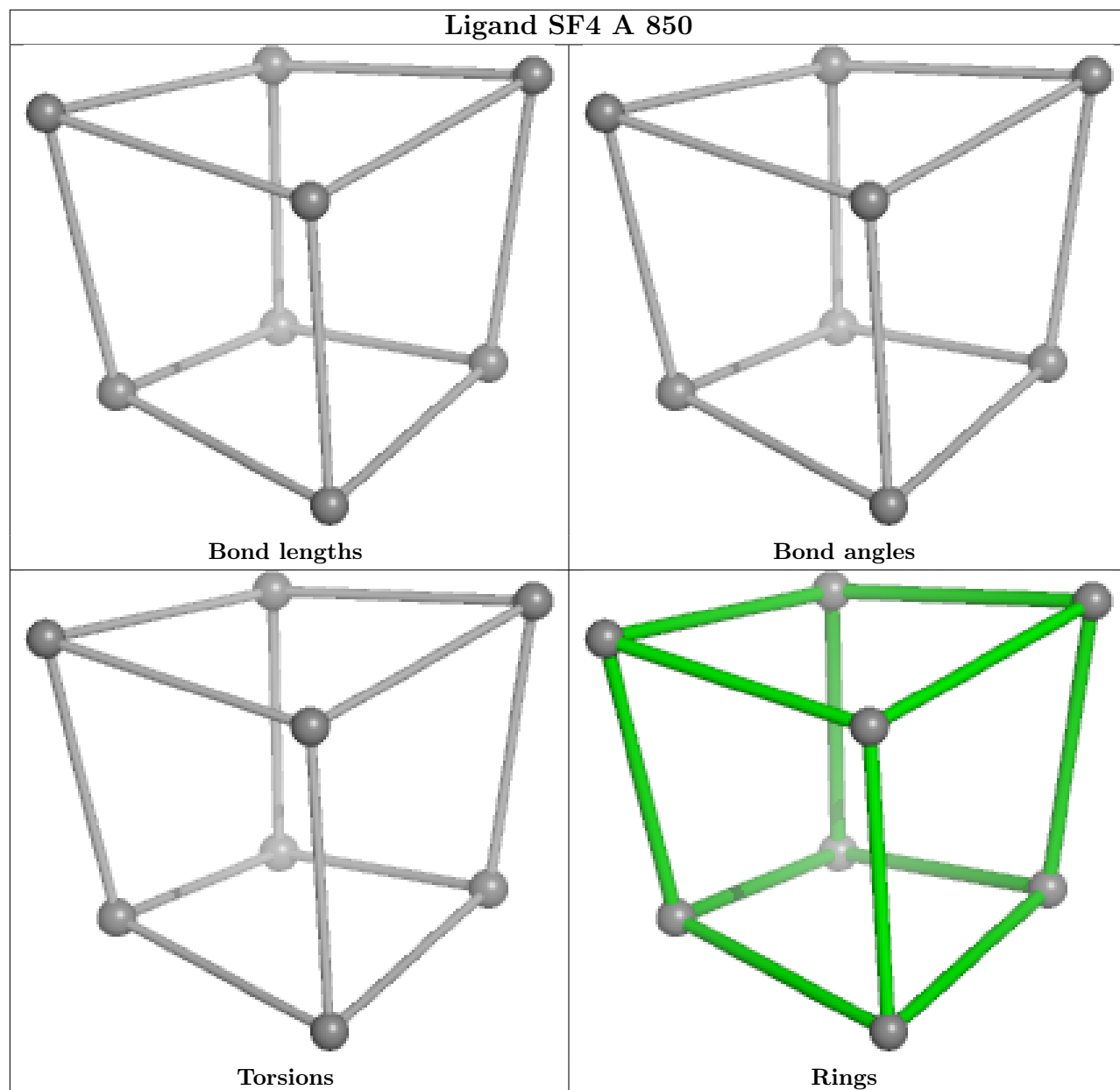
Bond angles

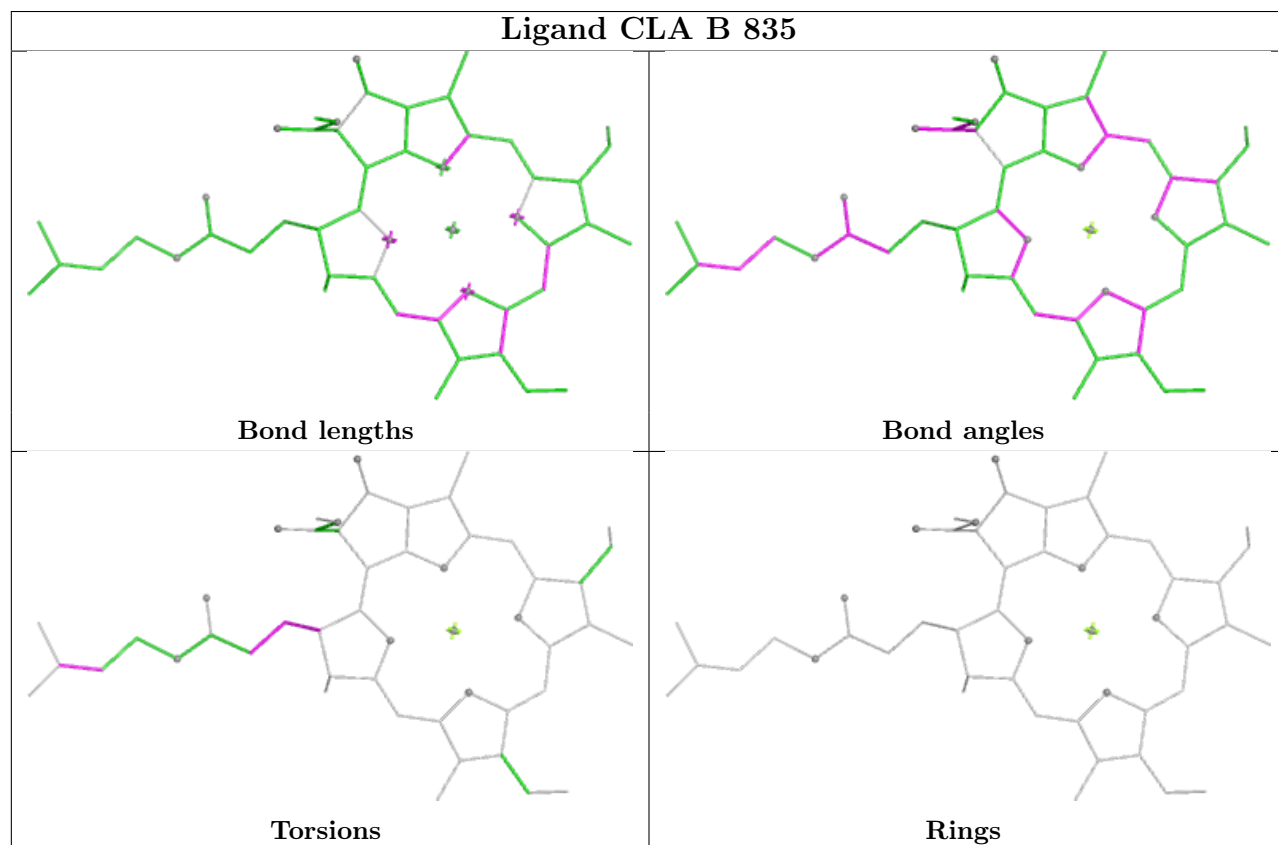
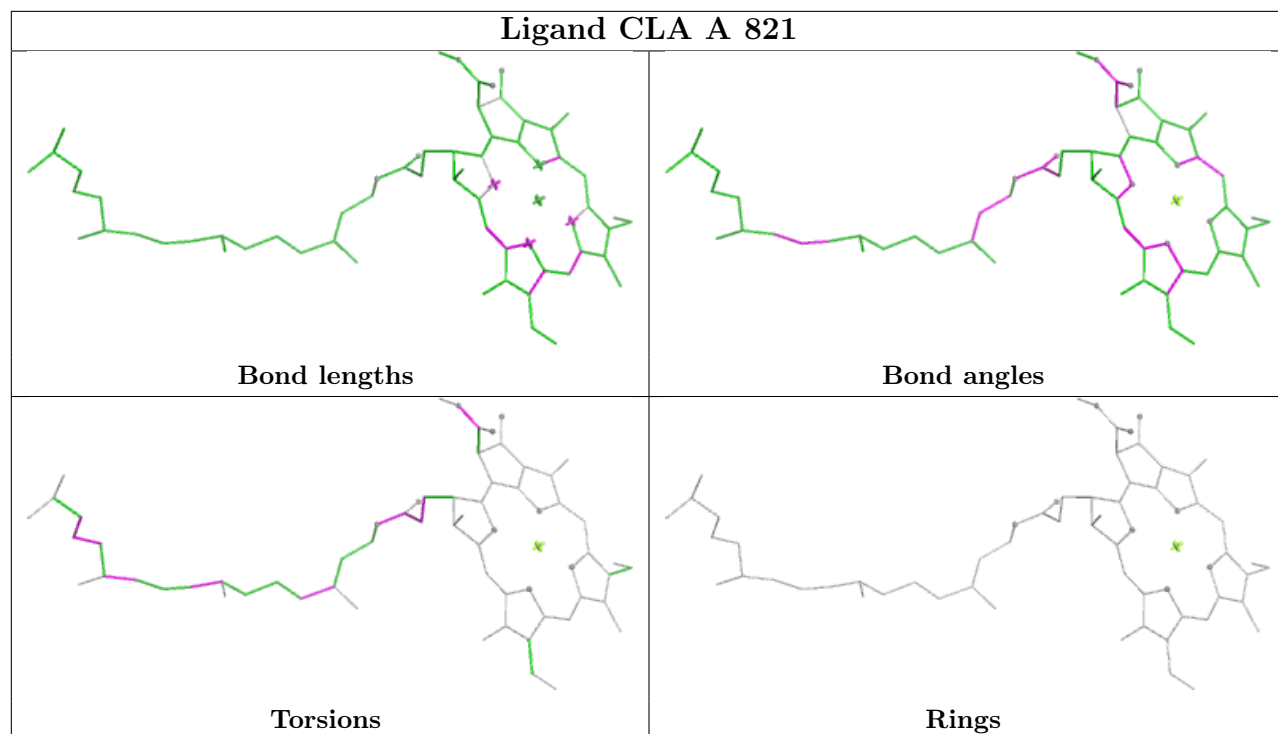


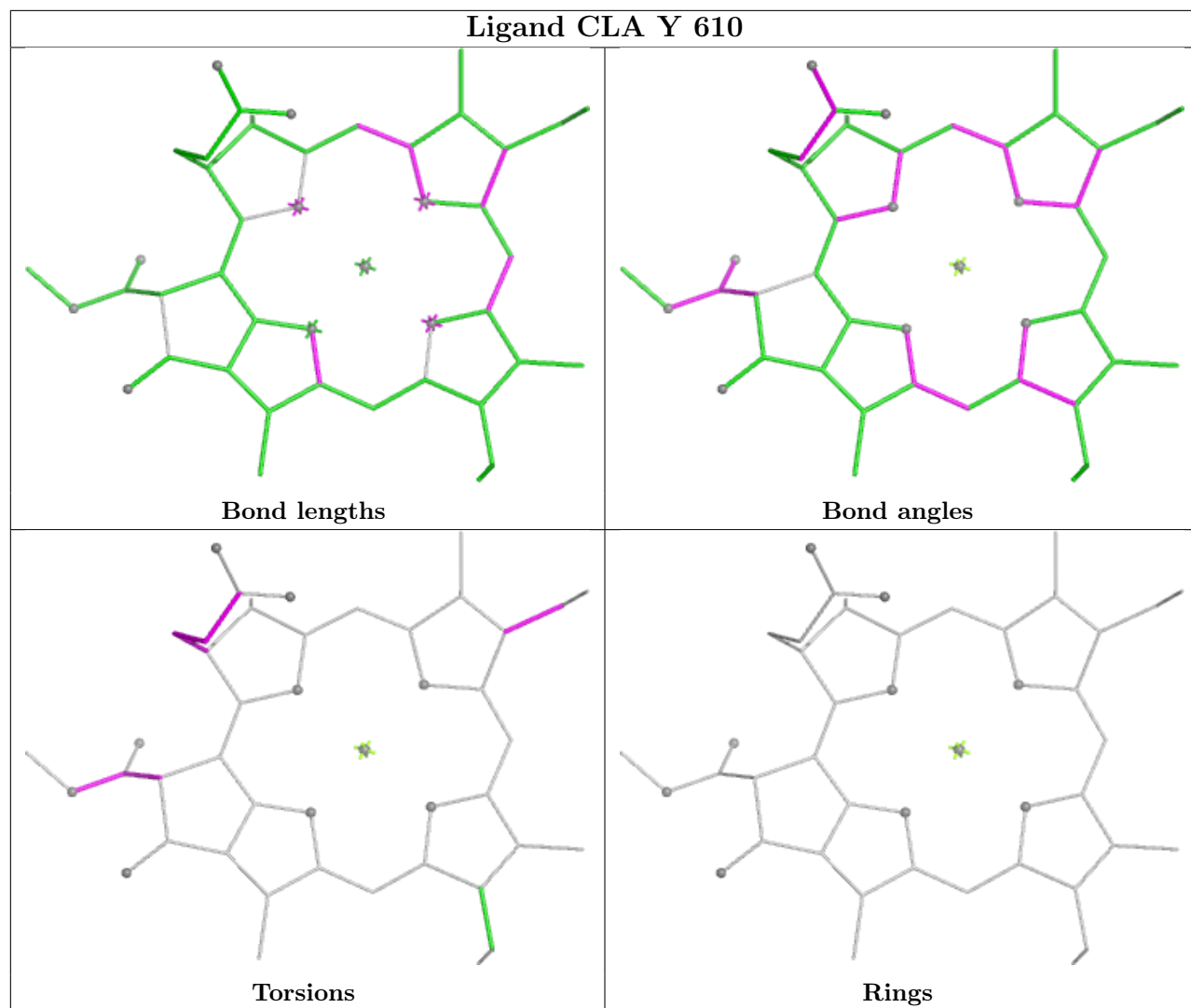
Torsions

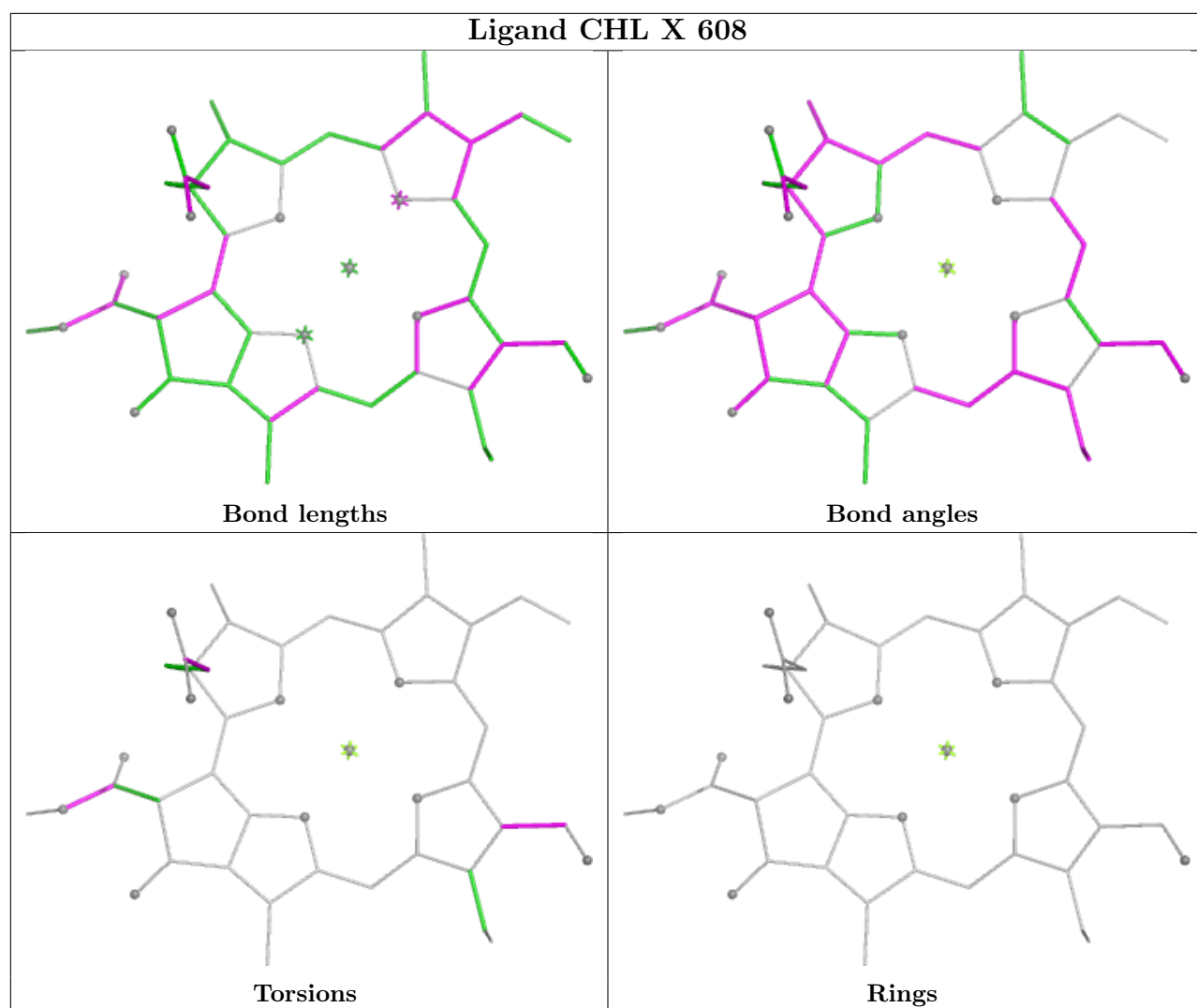


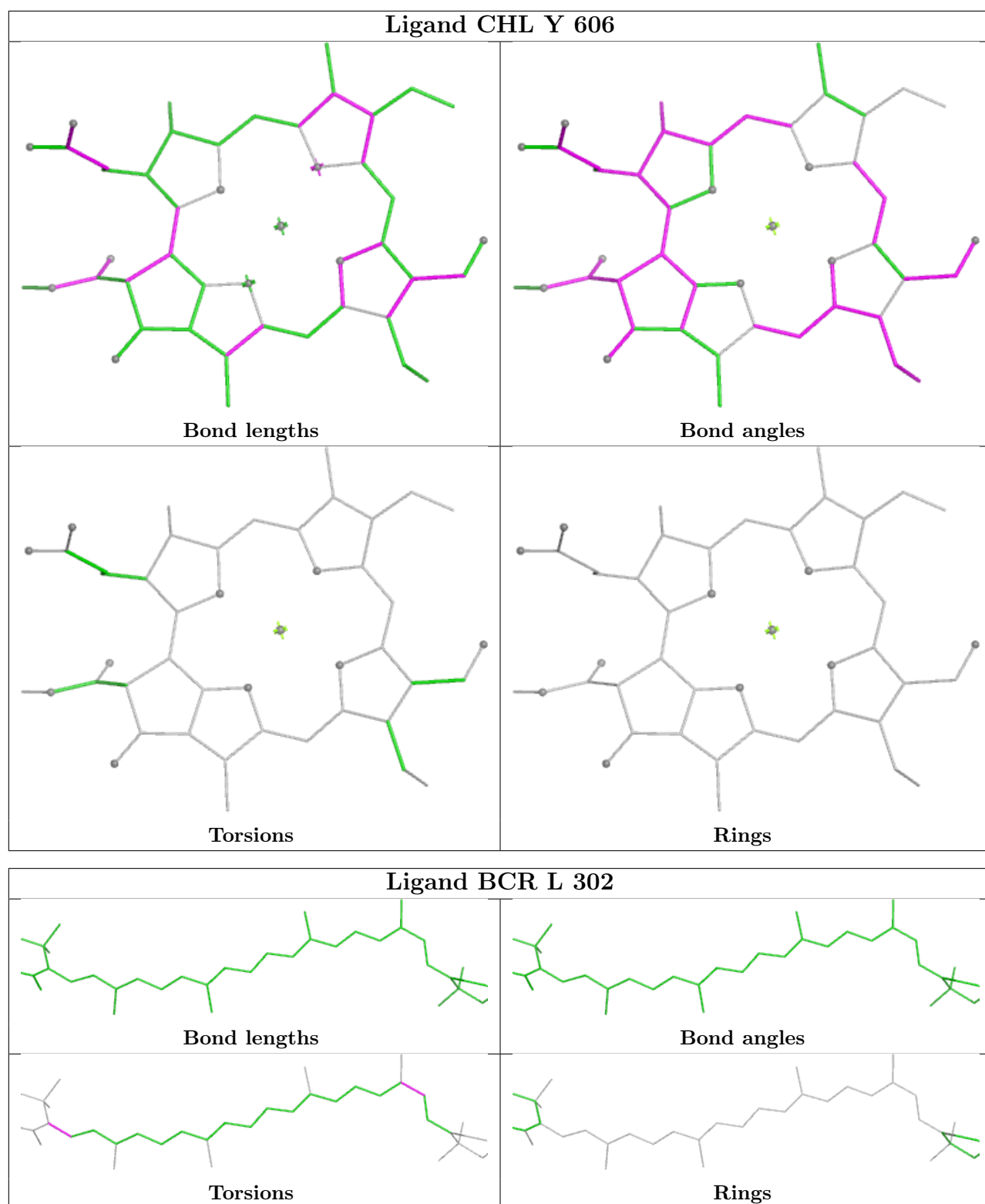
Rings



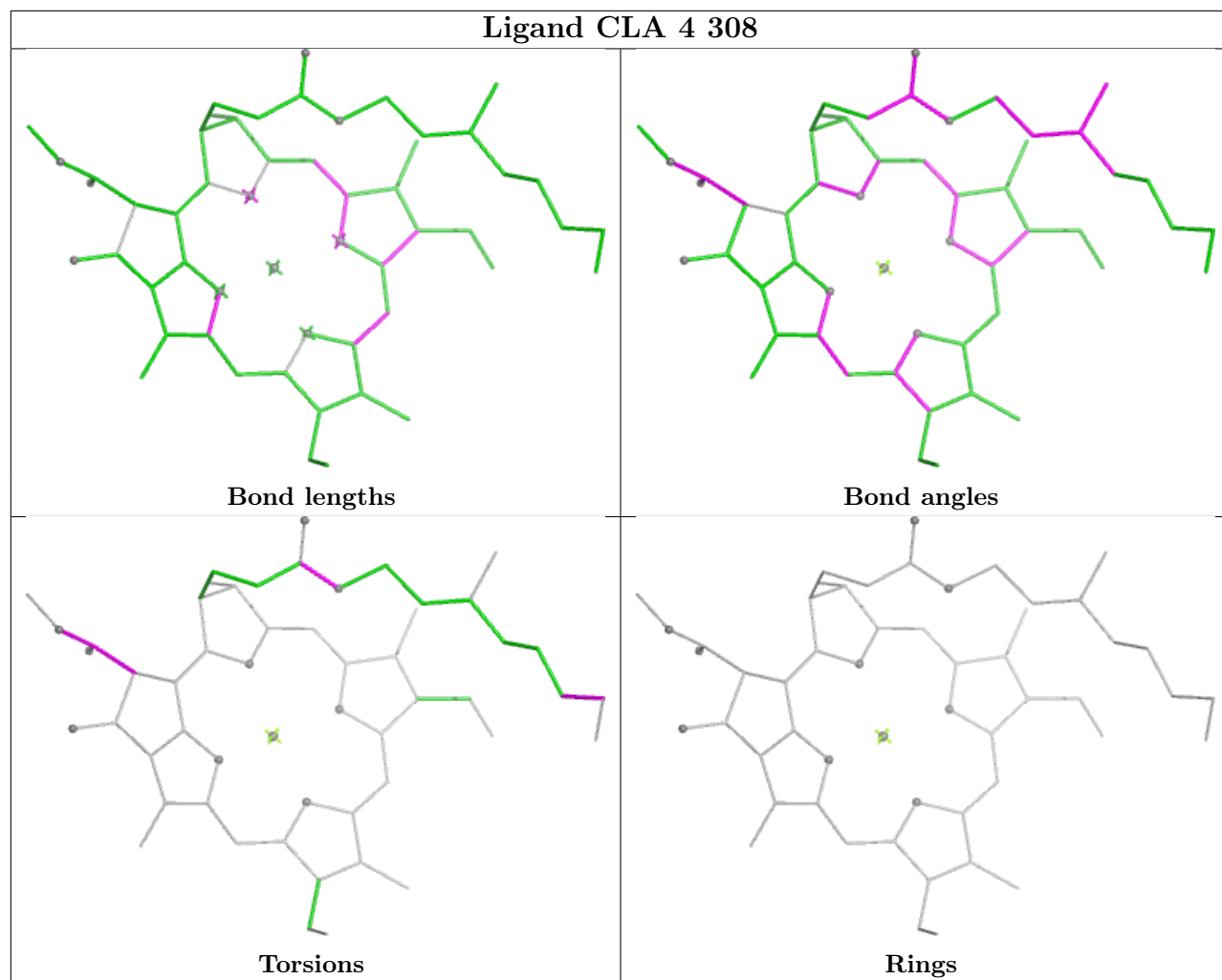




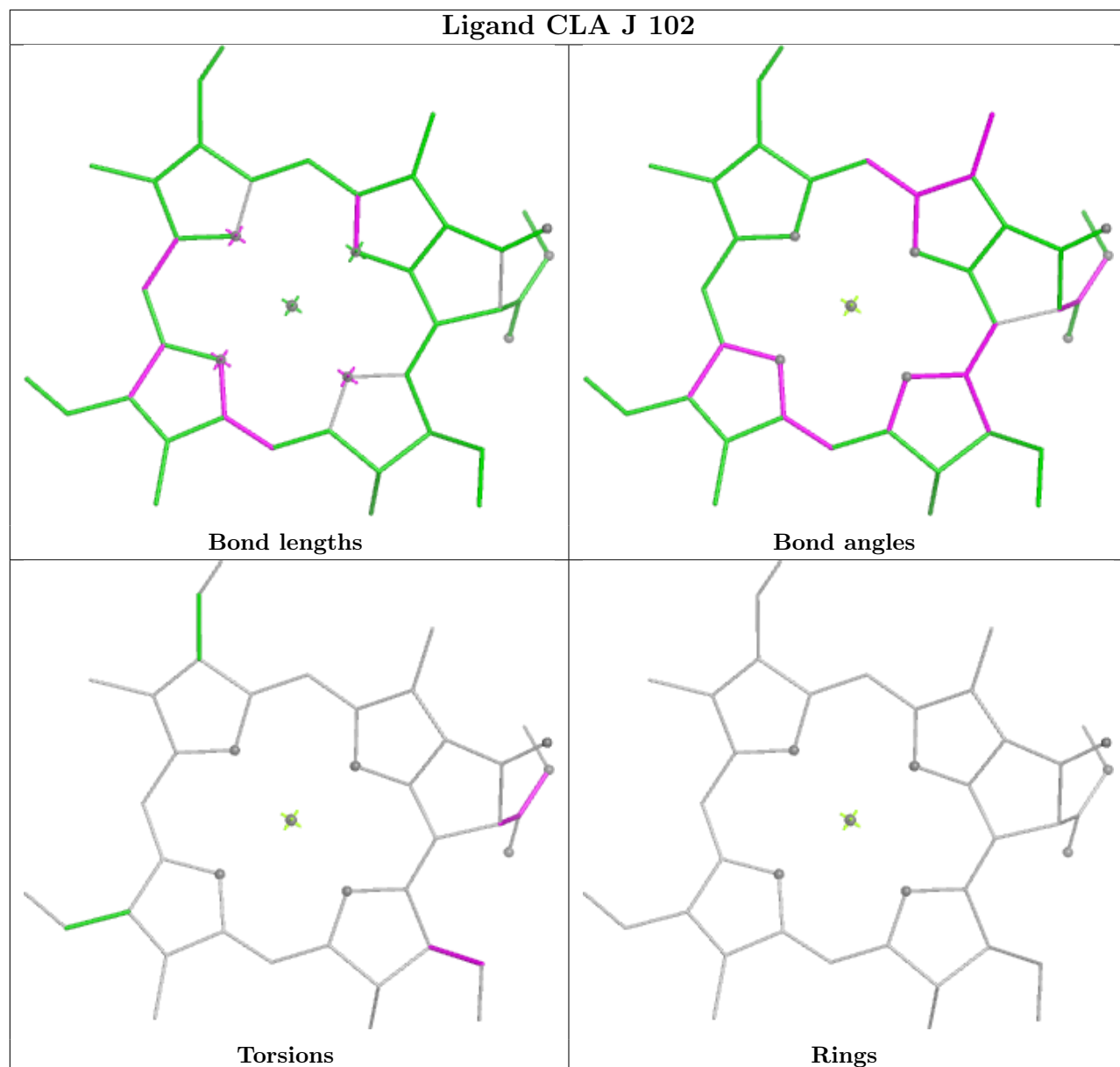


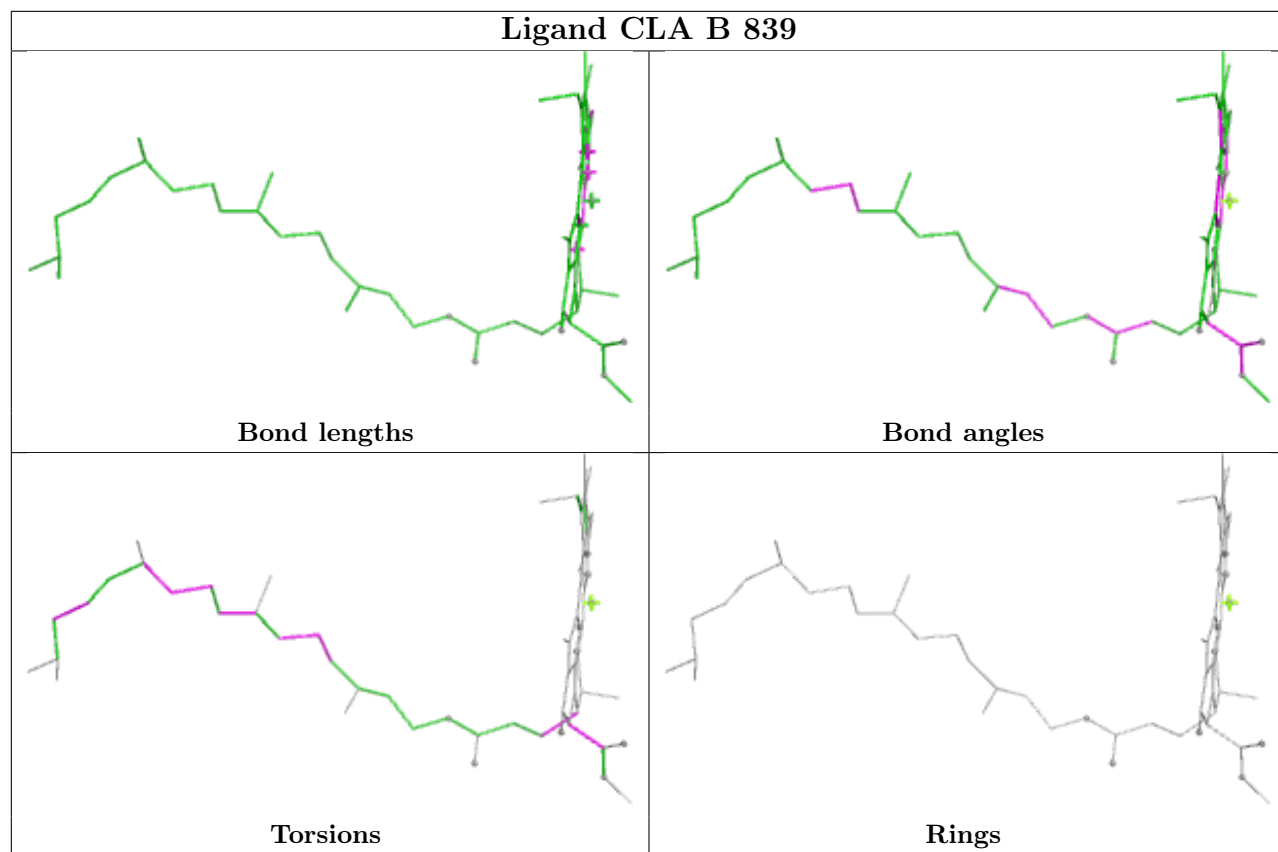


Ligand CLA 4 308

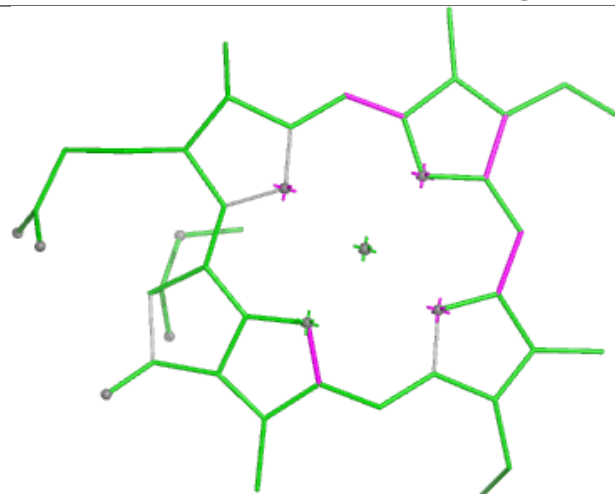


Ligand CLA J 102

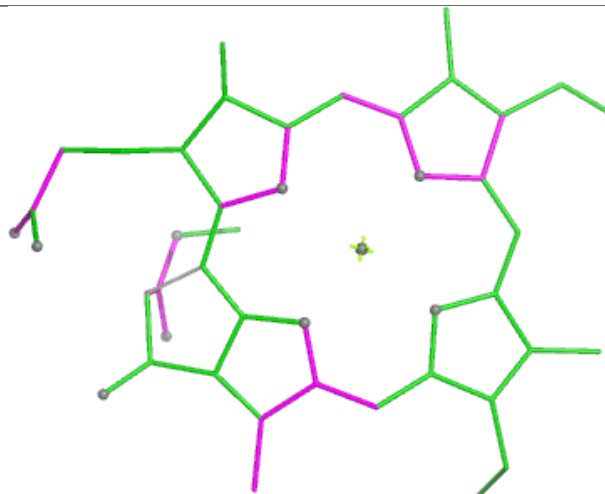




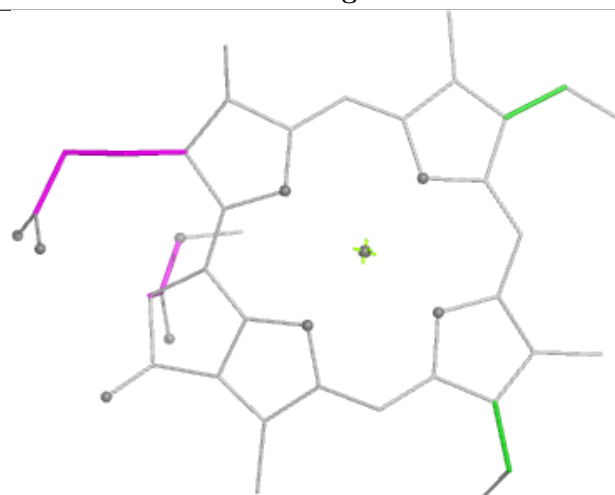
Ligand CLA X 611



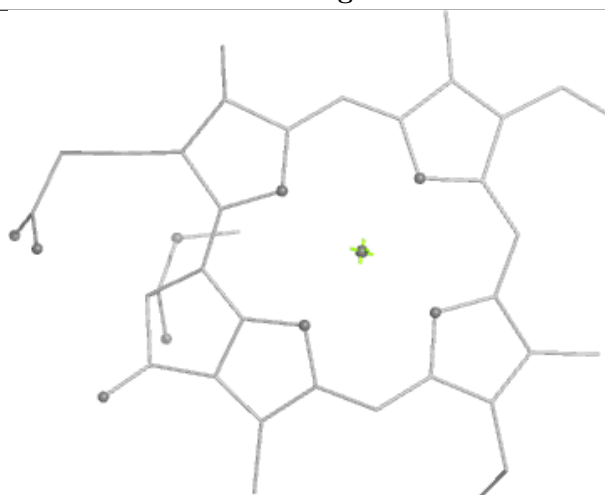
Bond lengths



Bond angles

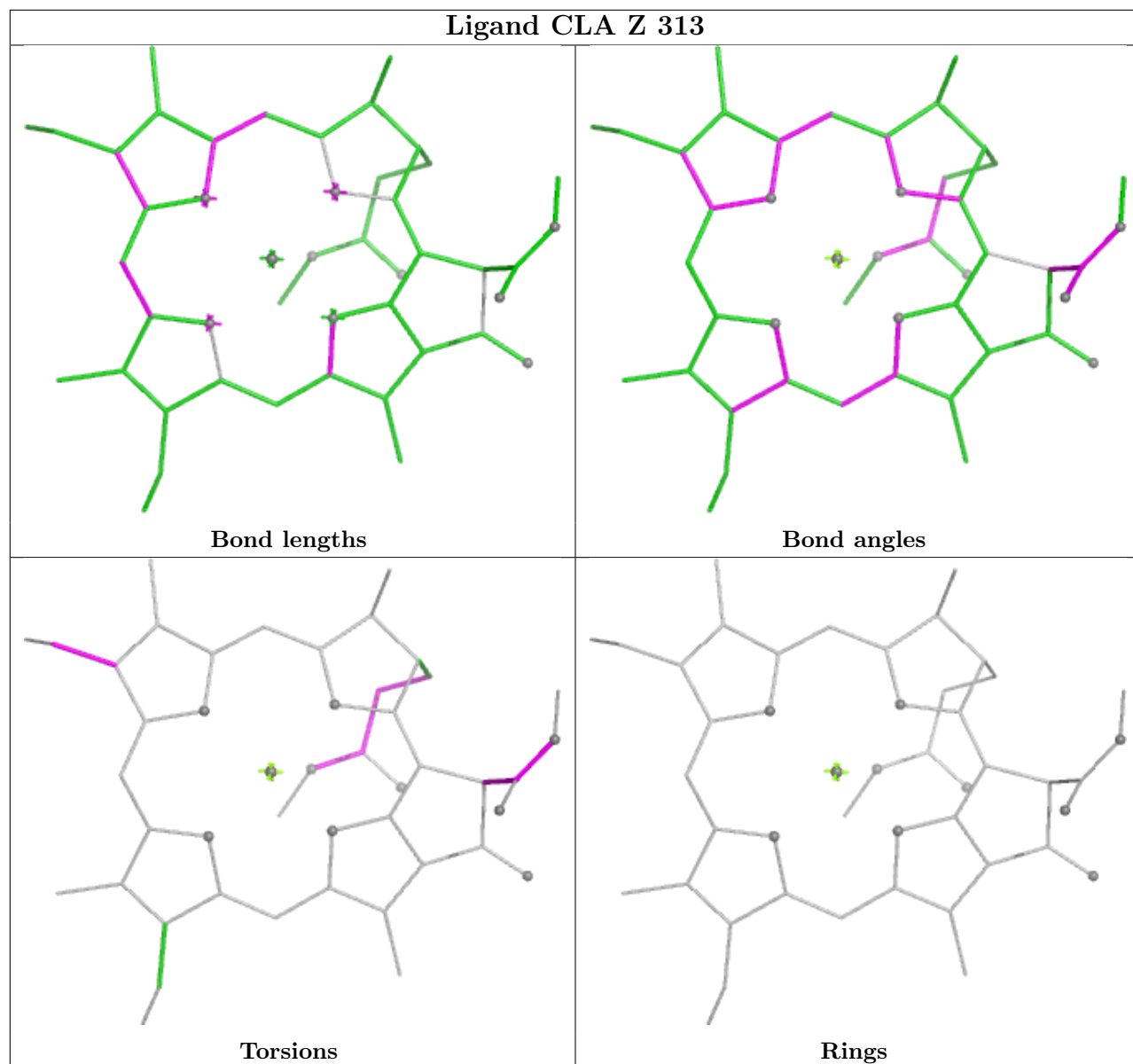


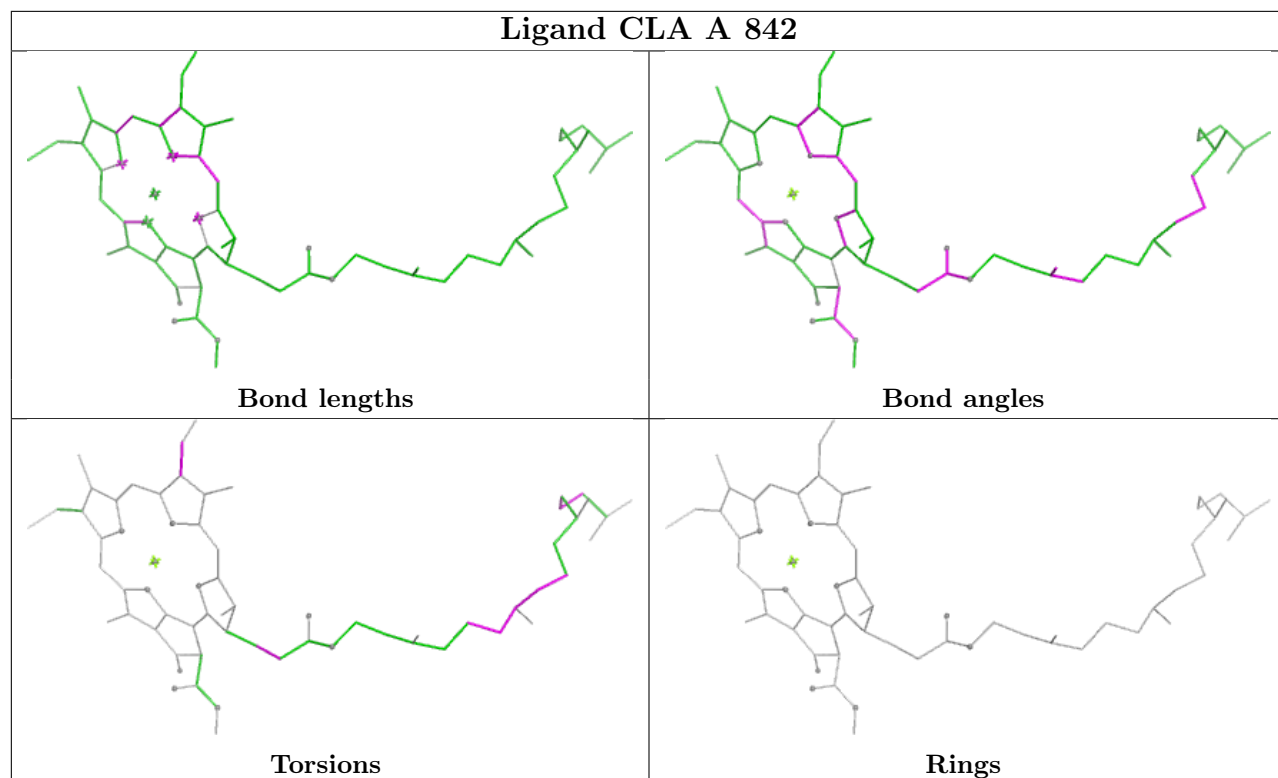
Torsions

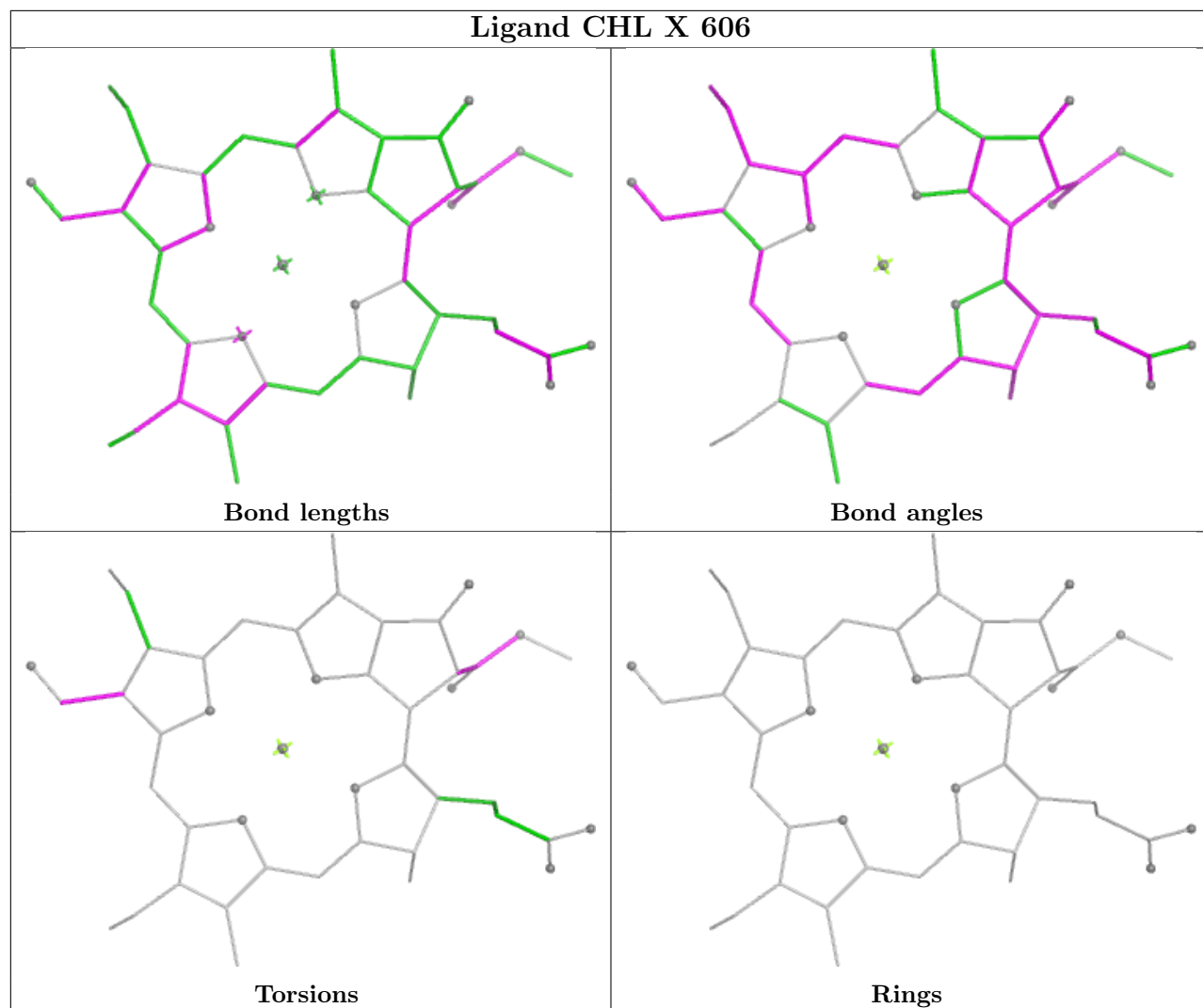


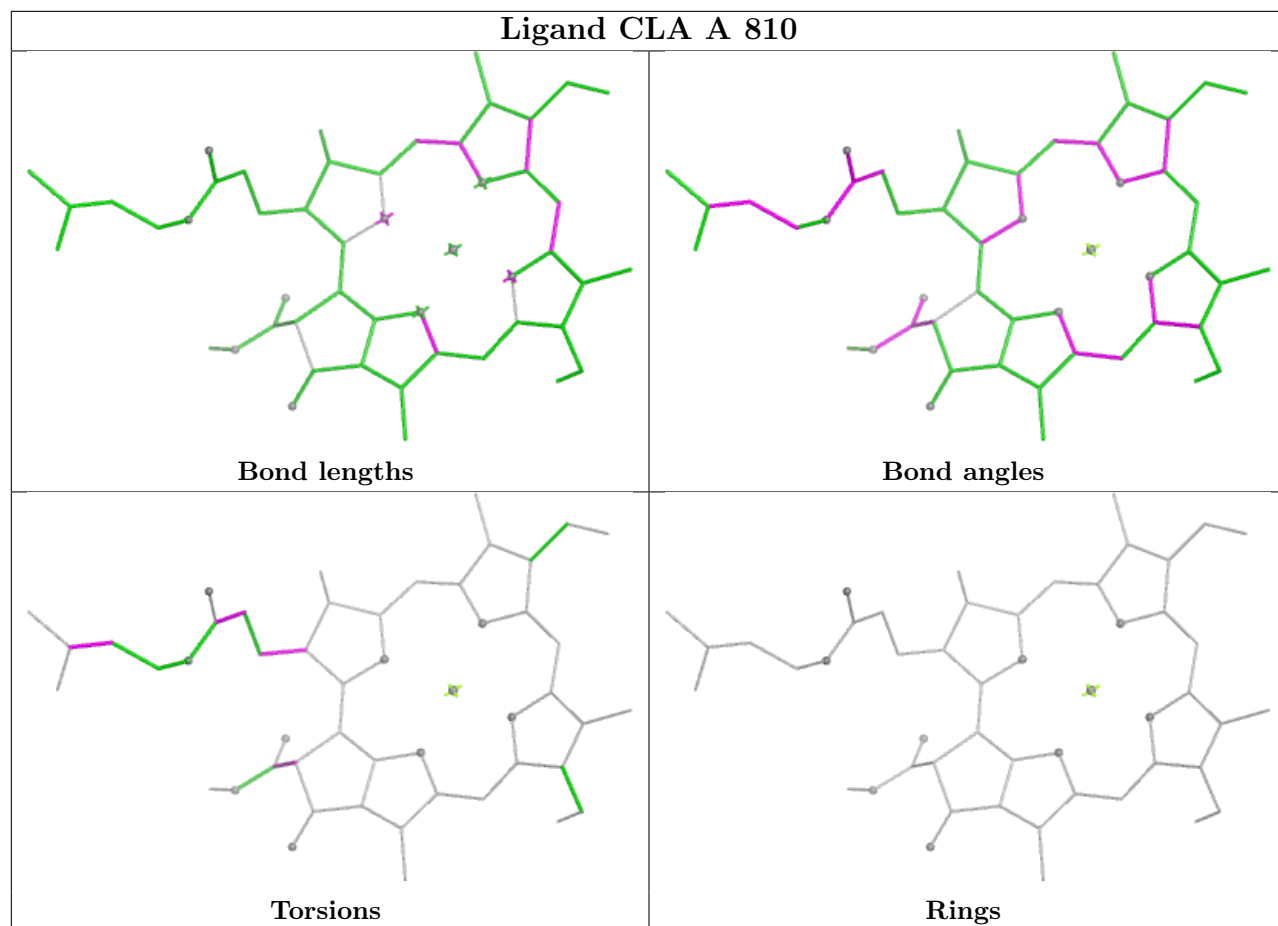
Rings

Ligand CLA Z 313

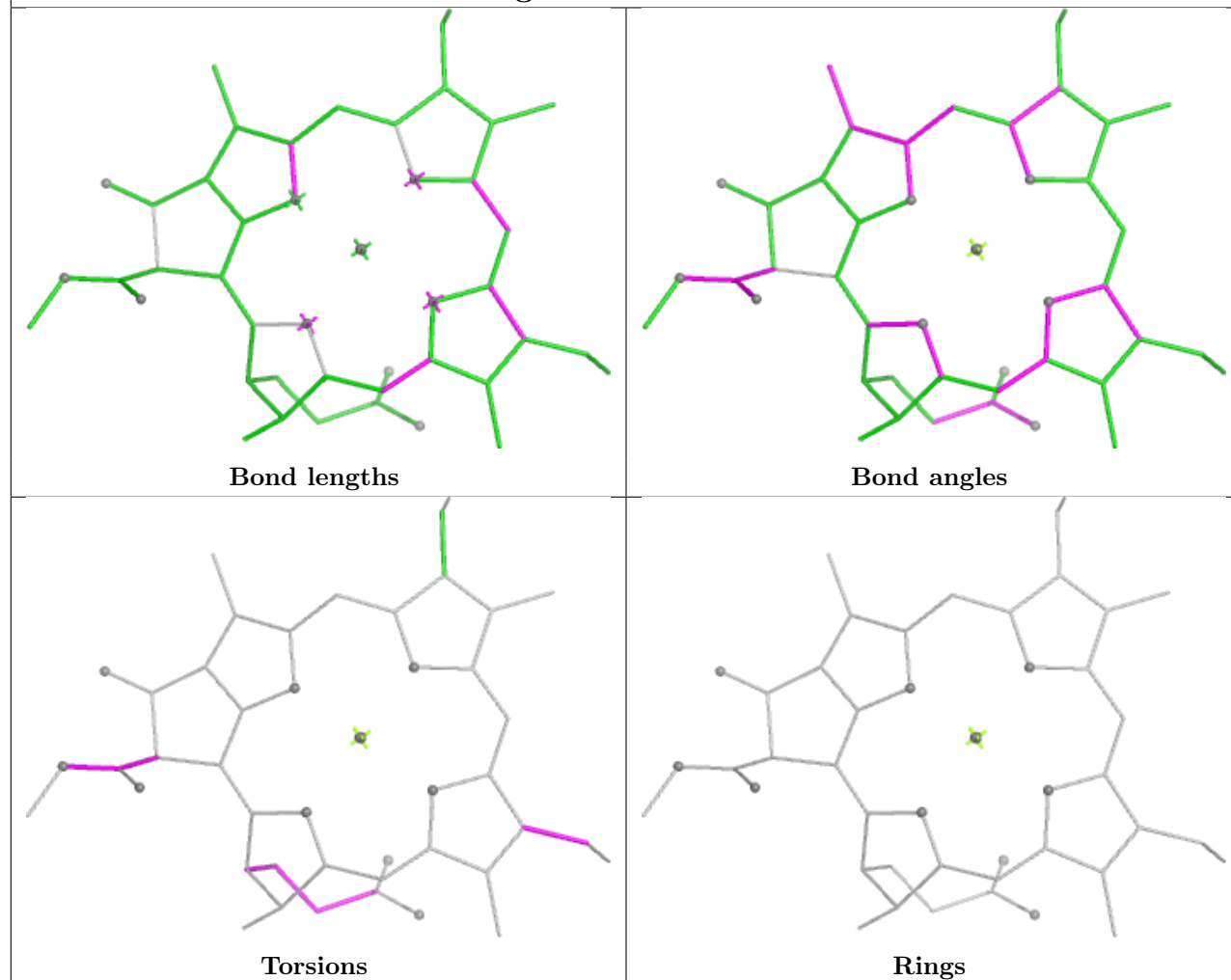




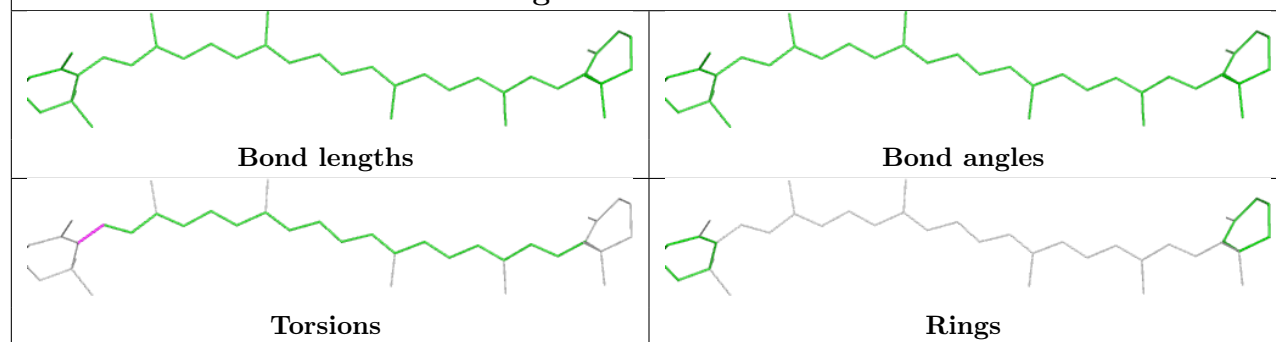




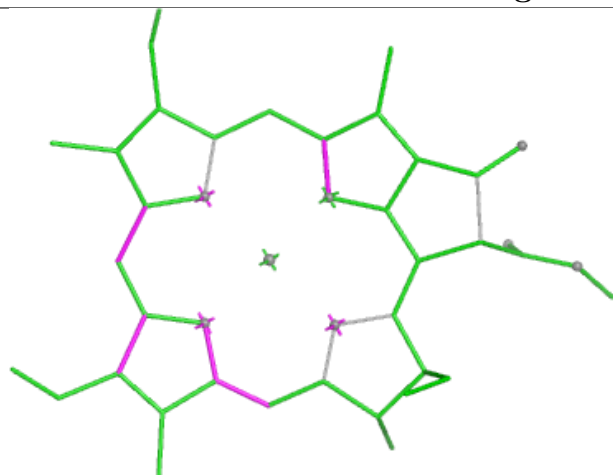
Ligand CLA Z 310



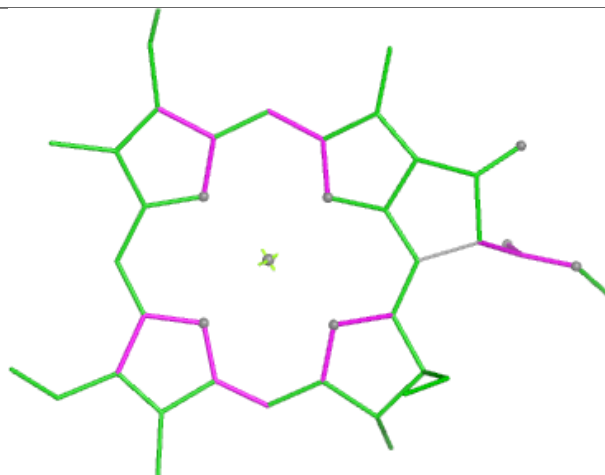
Ligand BCR L 307



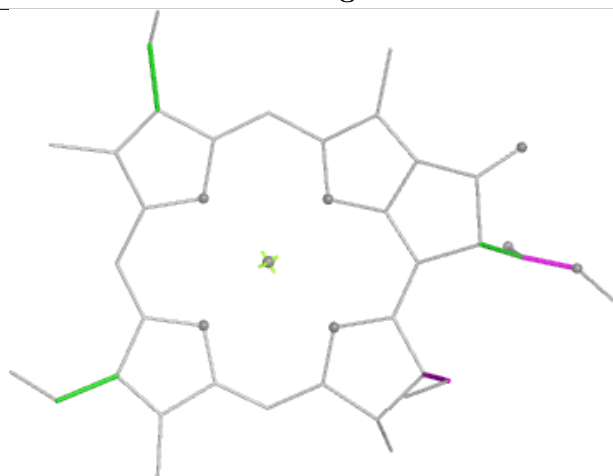
Ligand CLA B 834



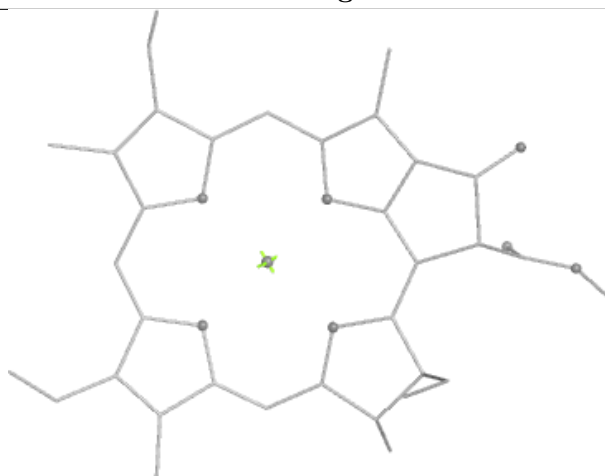
Bond lengths



Bond angles

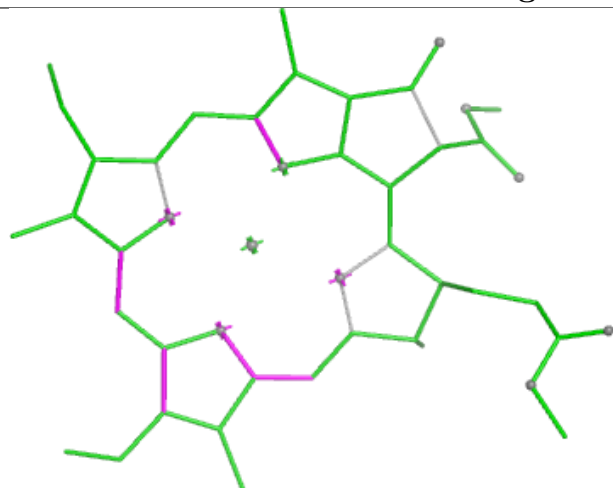


Torsions

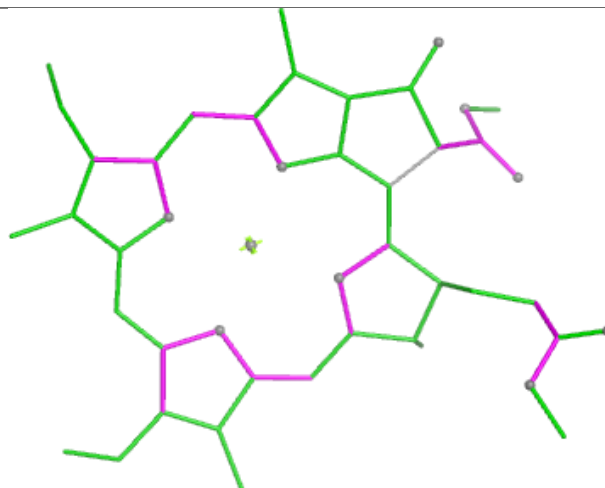


Rings

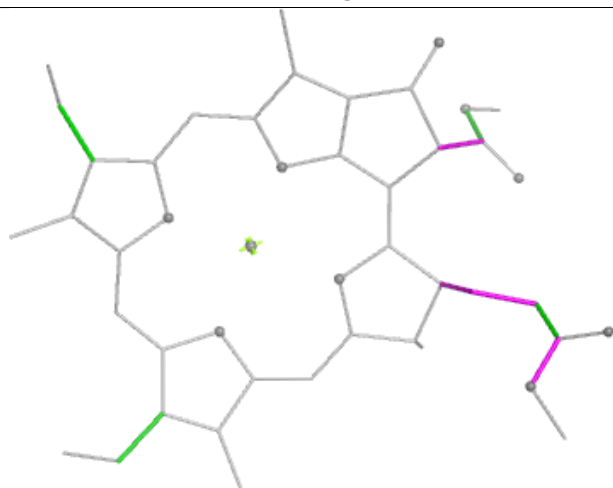
Ligand CLA 2 618



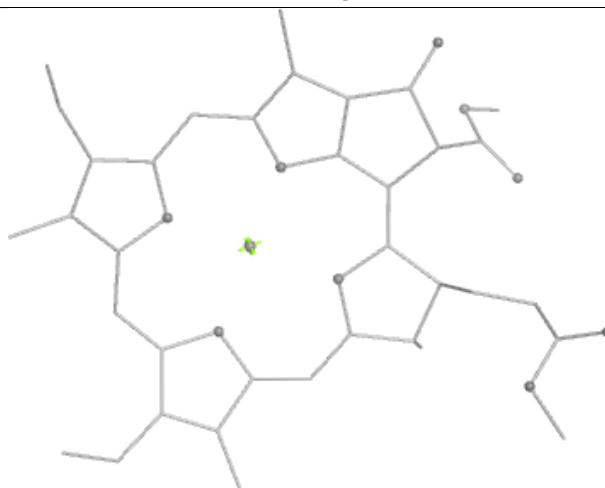
Bond lengths



Bond angles

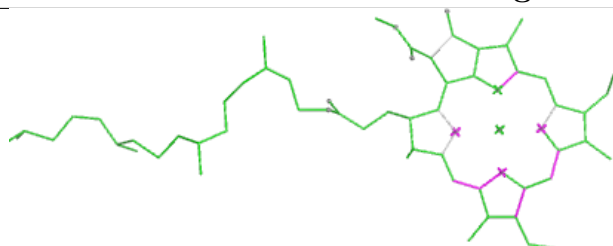


Torsions

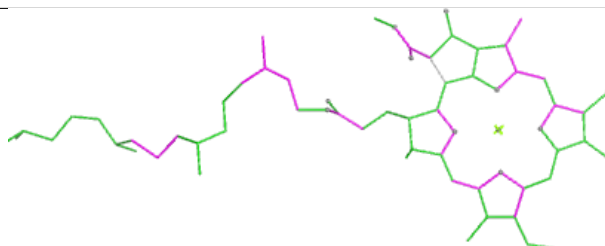


Rings

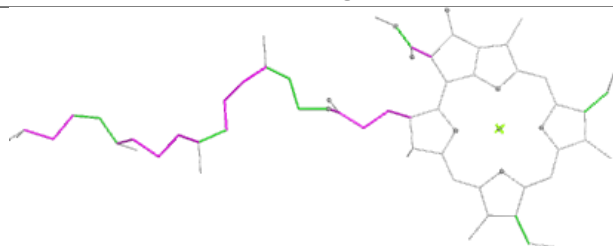
Ligand CLA A 833



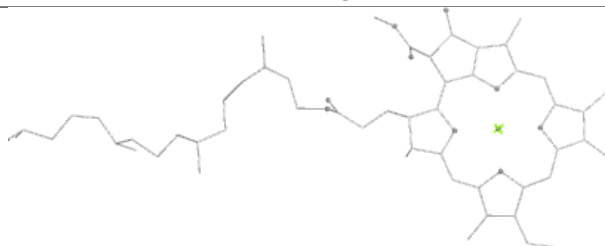
Bond lengths



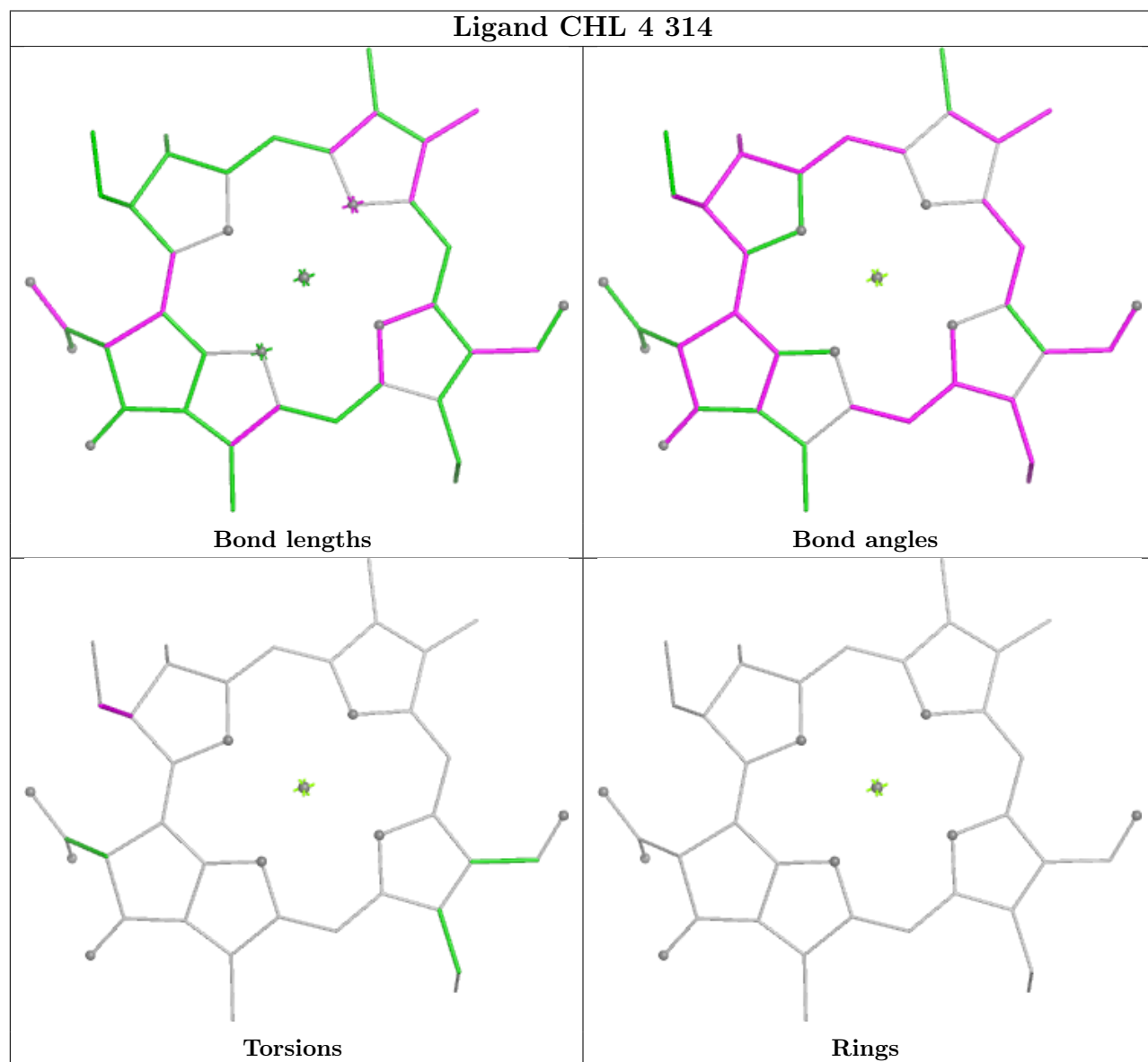
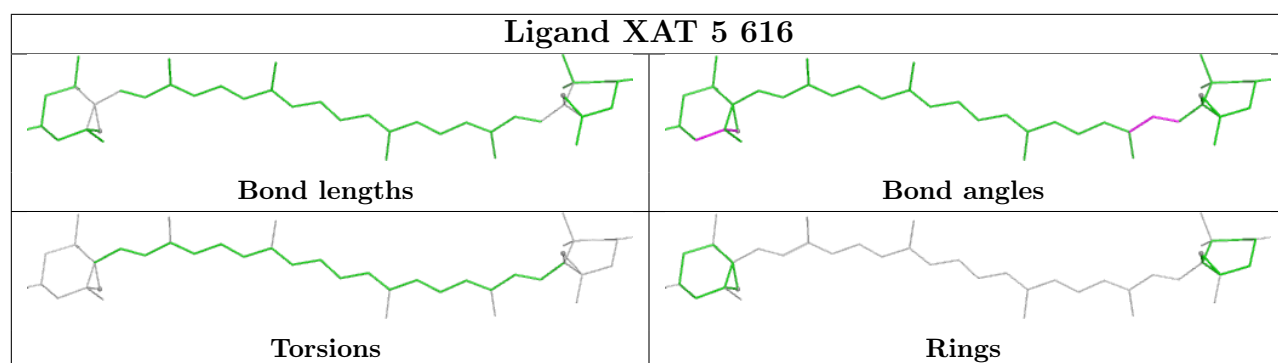
Bond angles

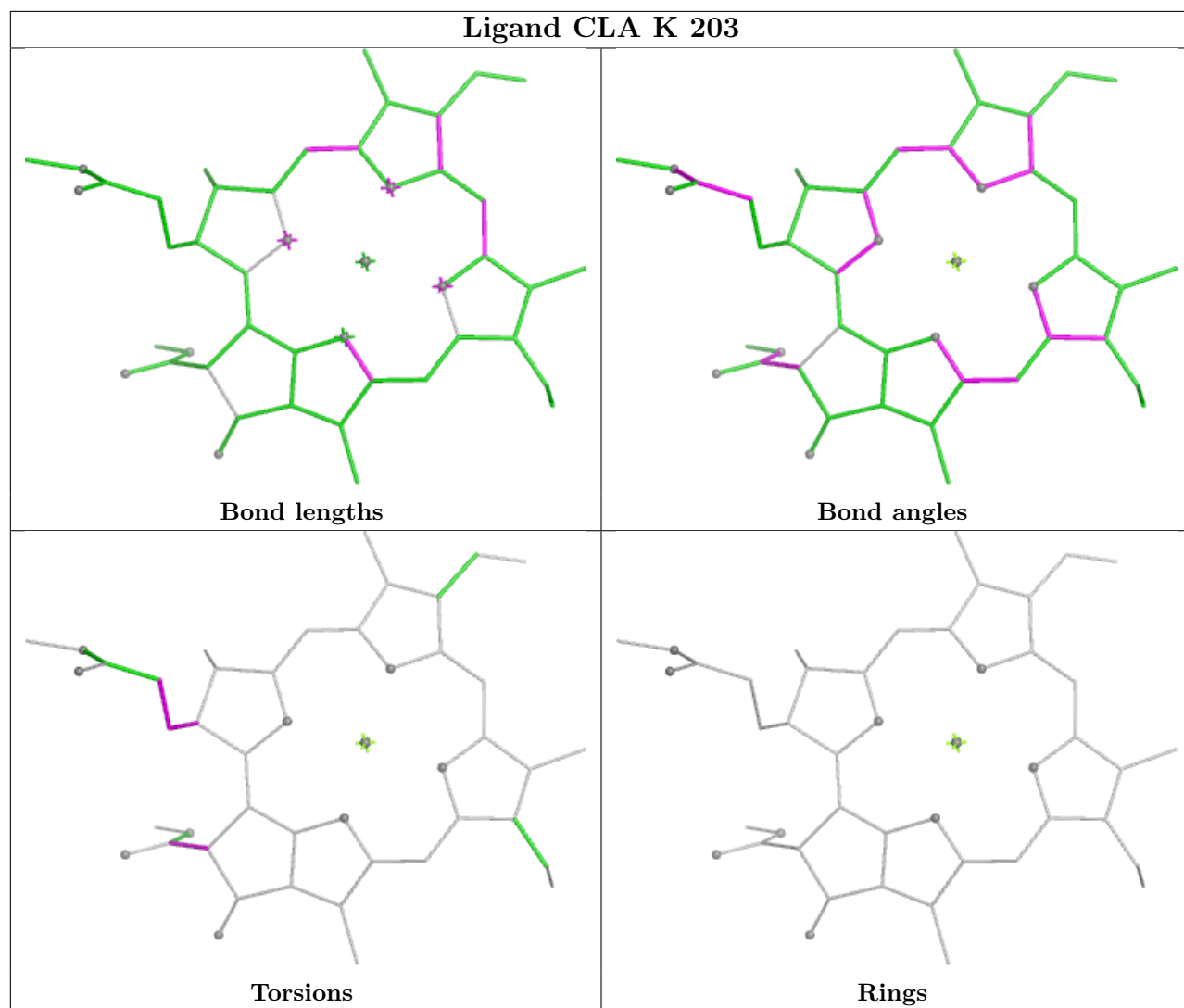
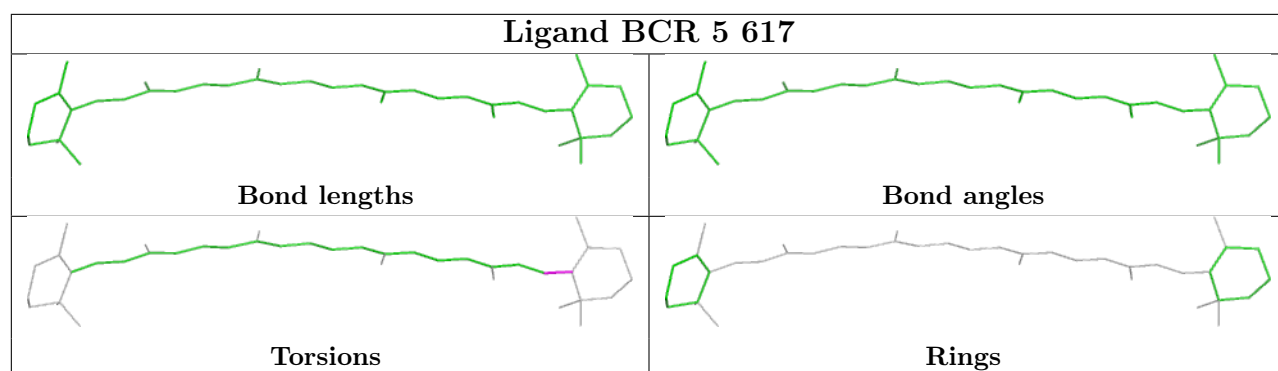


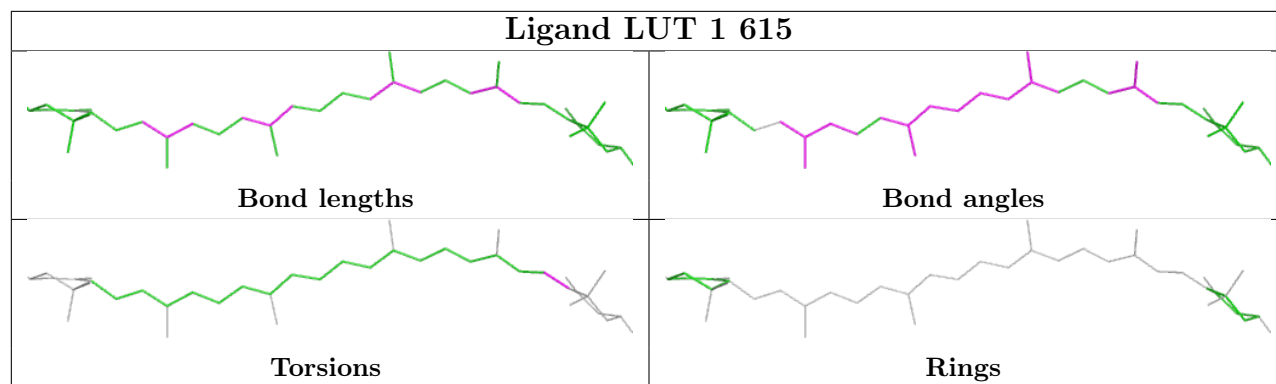
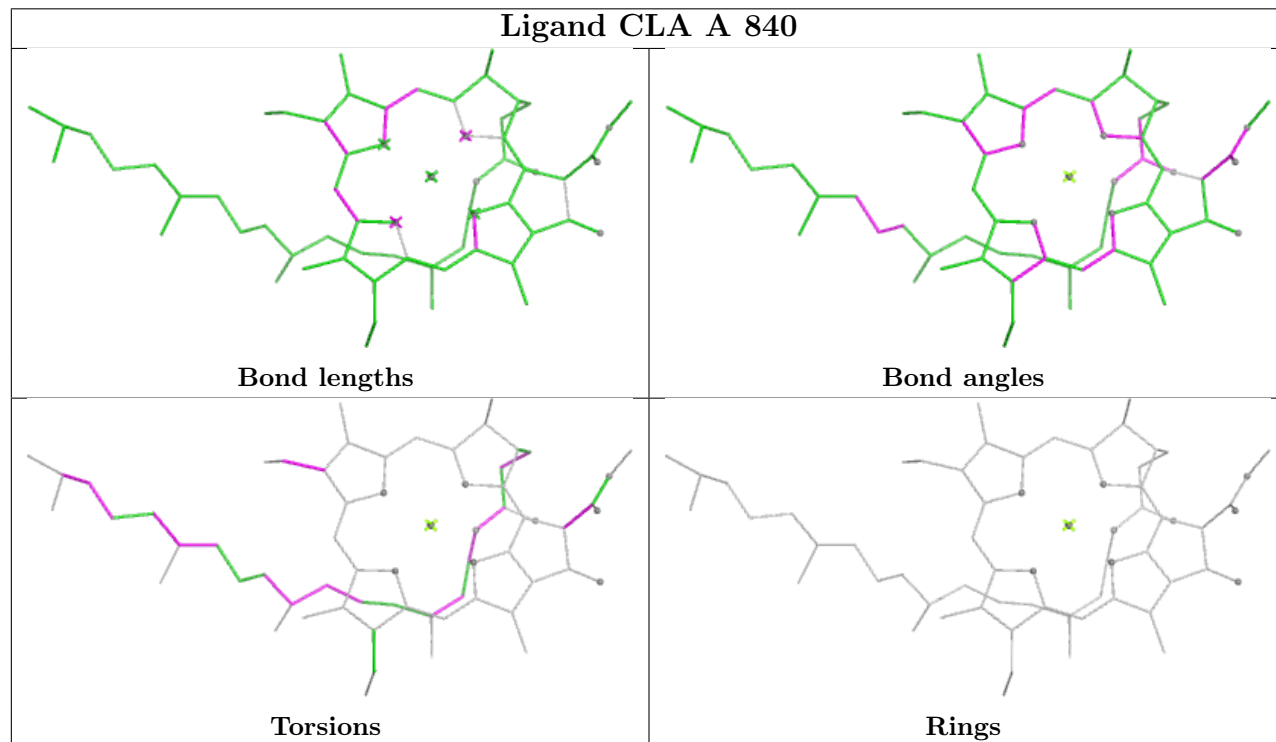
Torsions

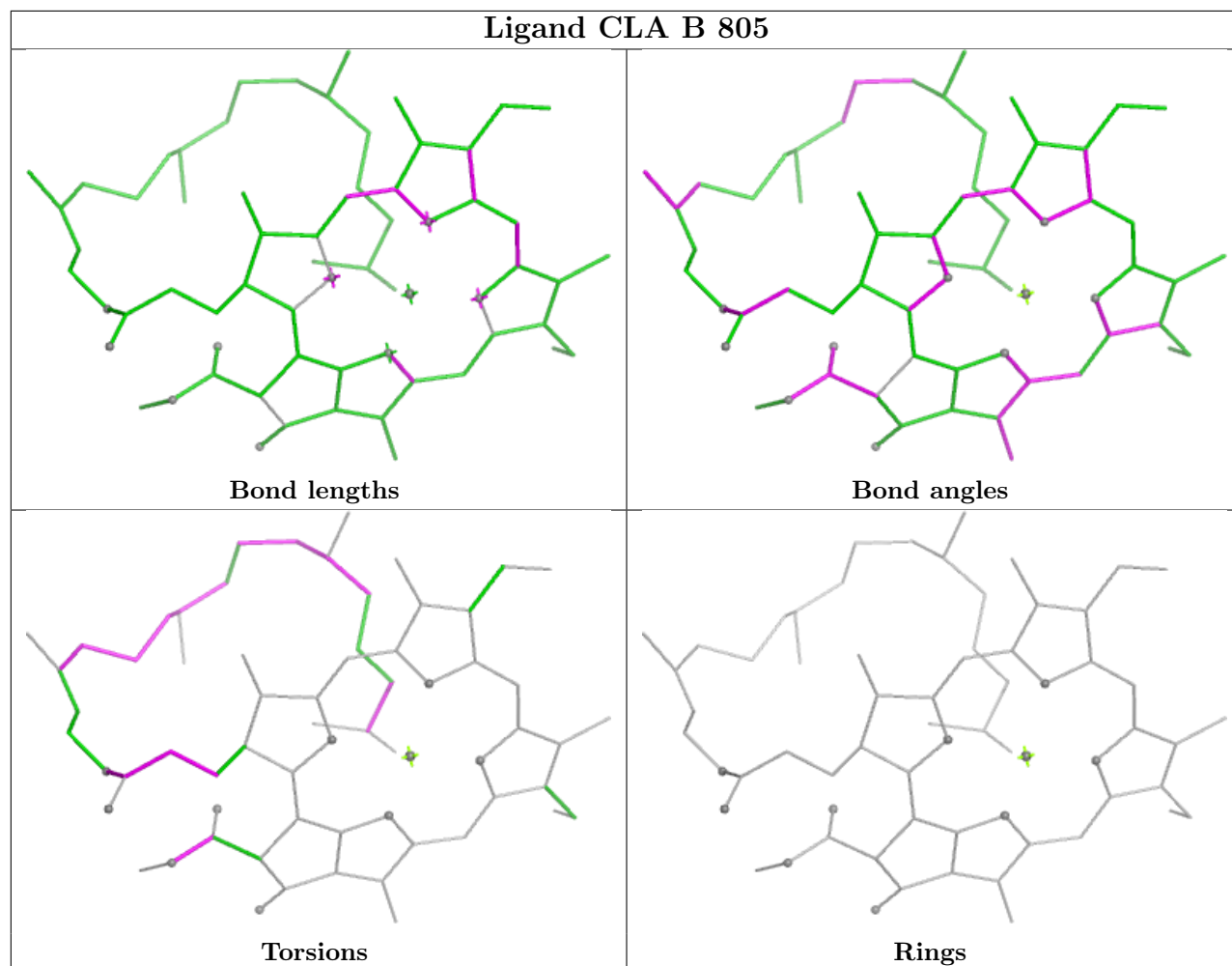
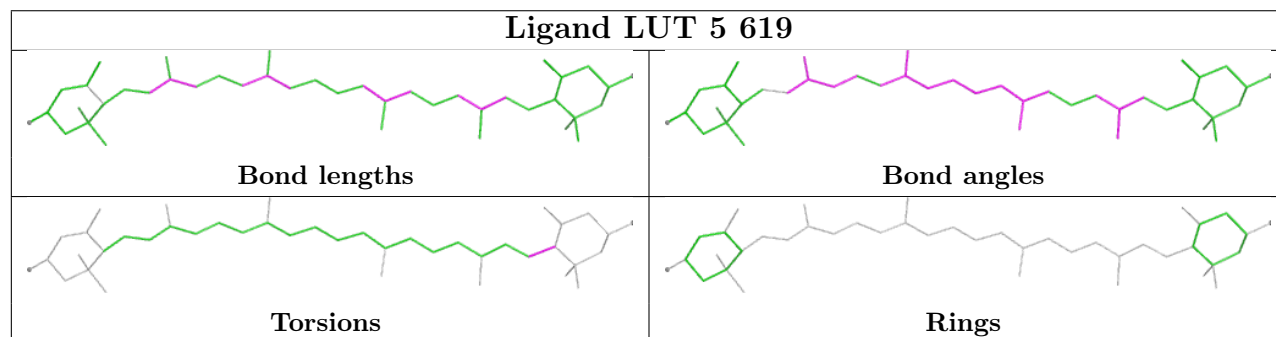


Rings

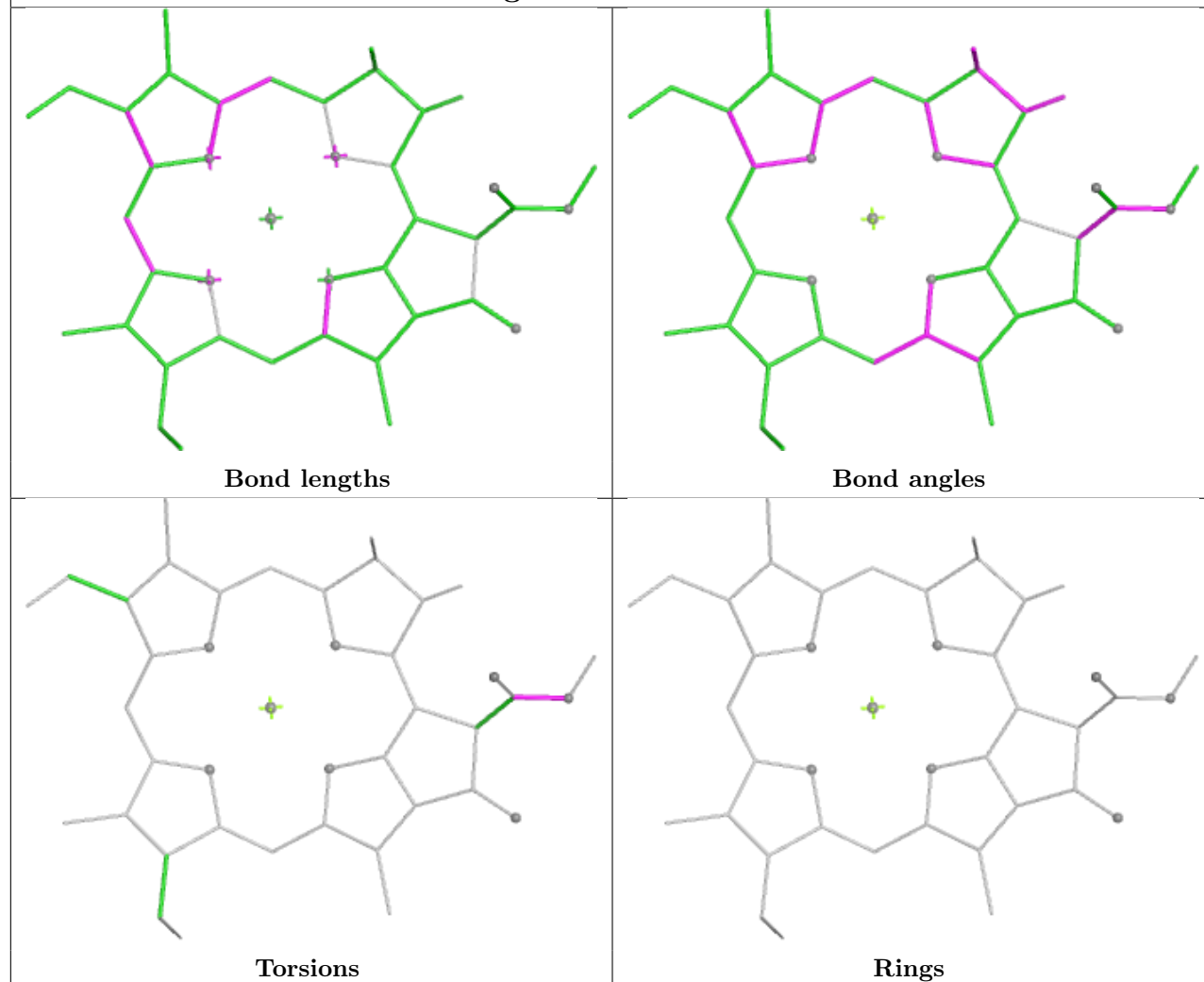




Ligand LUT 1 615**Ligand CLA A 840**

Ligand CLA B 805**Ligand LUT 5 619**

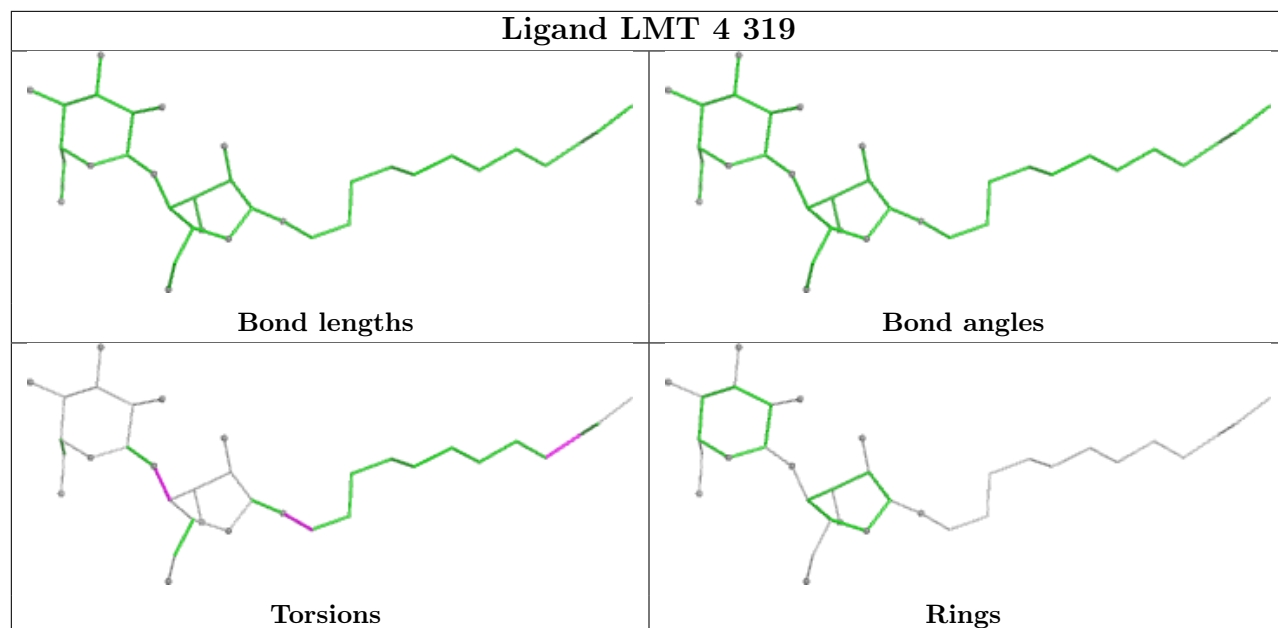
Ligand CLA F 304



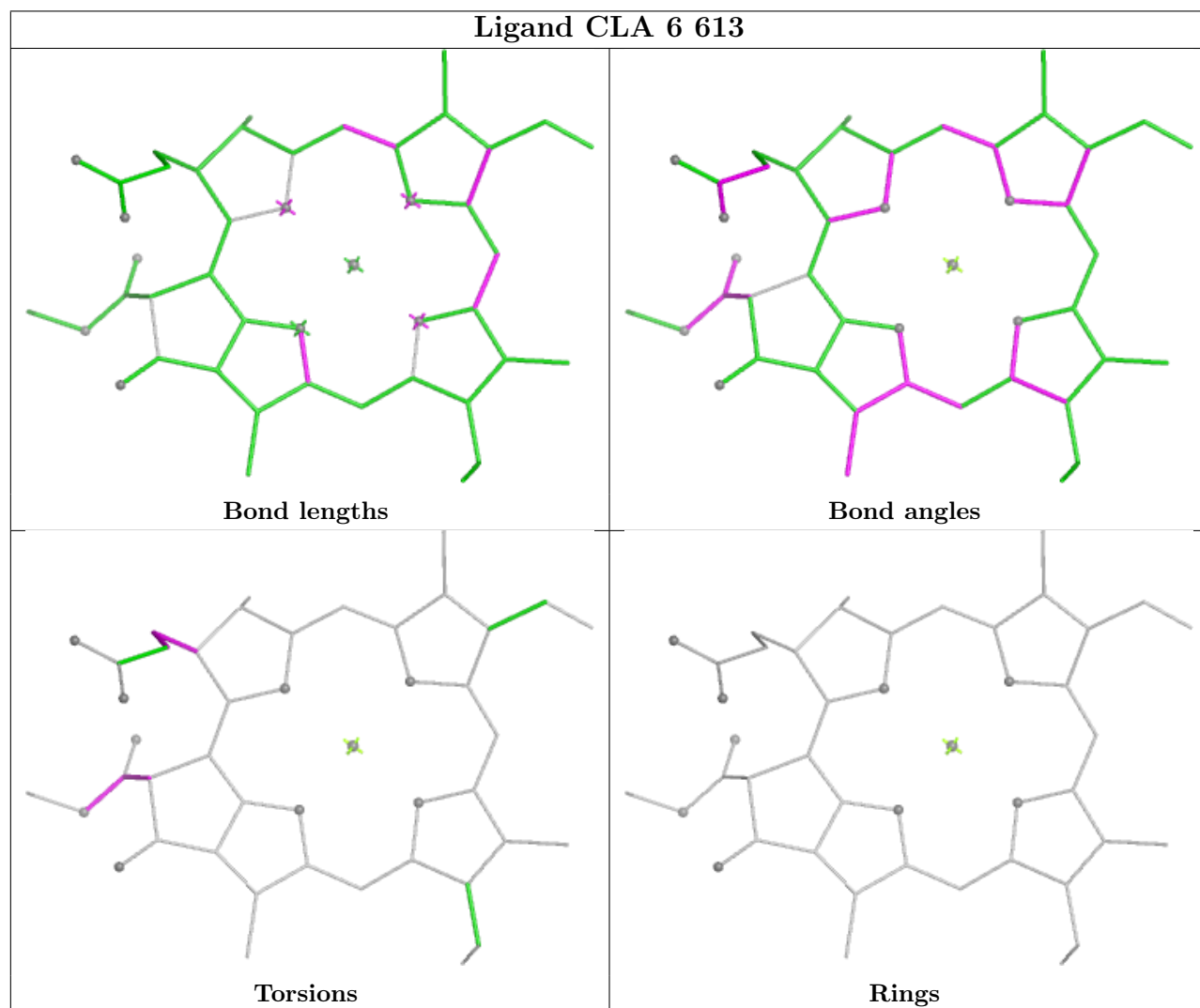
Ligand BCR B 844

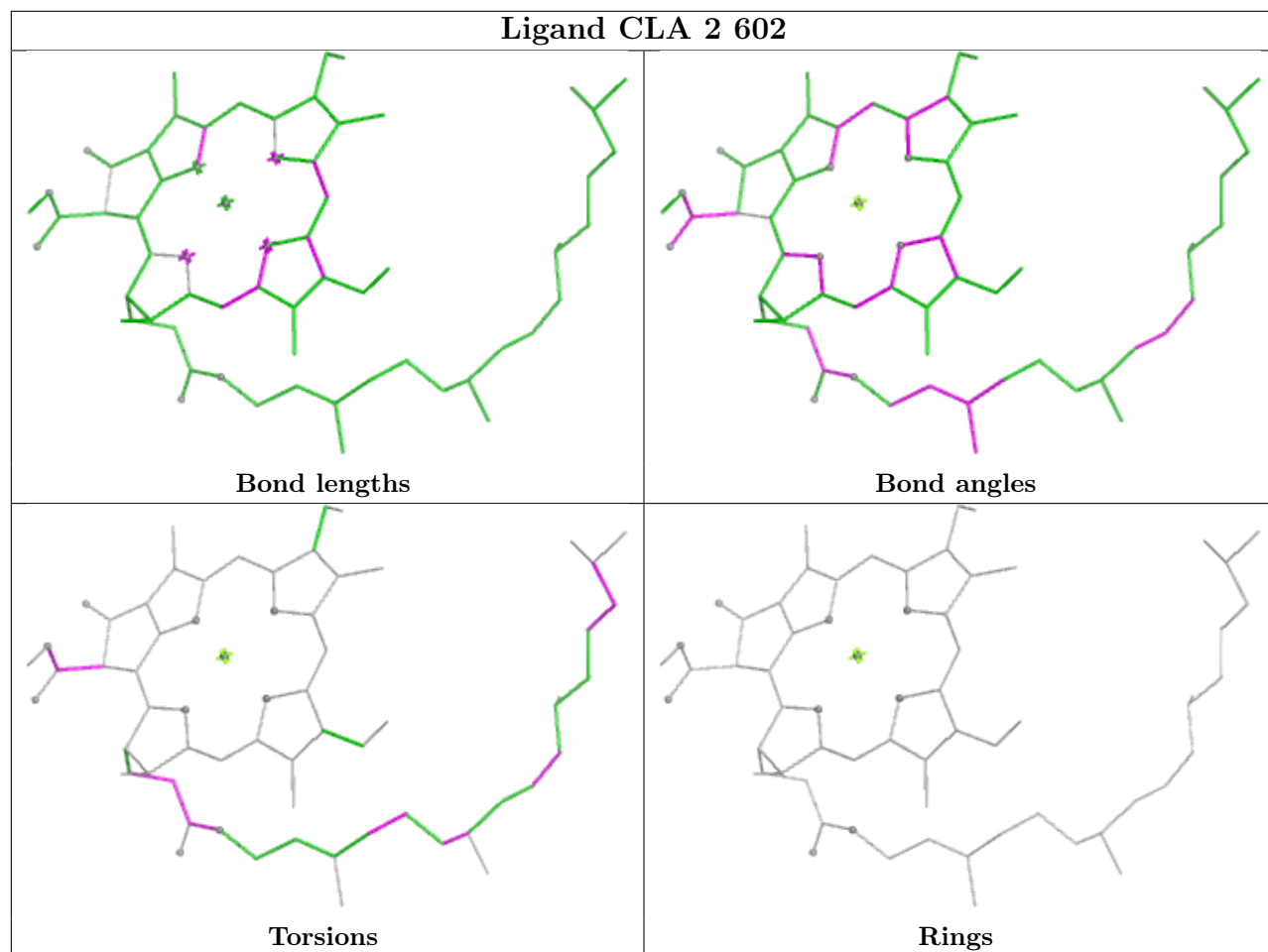


Ligand LMT 4 319

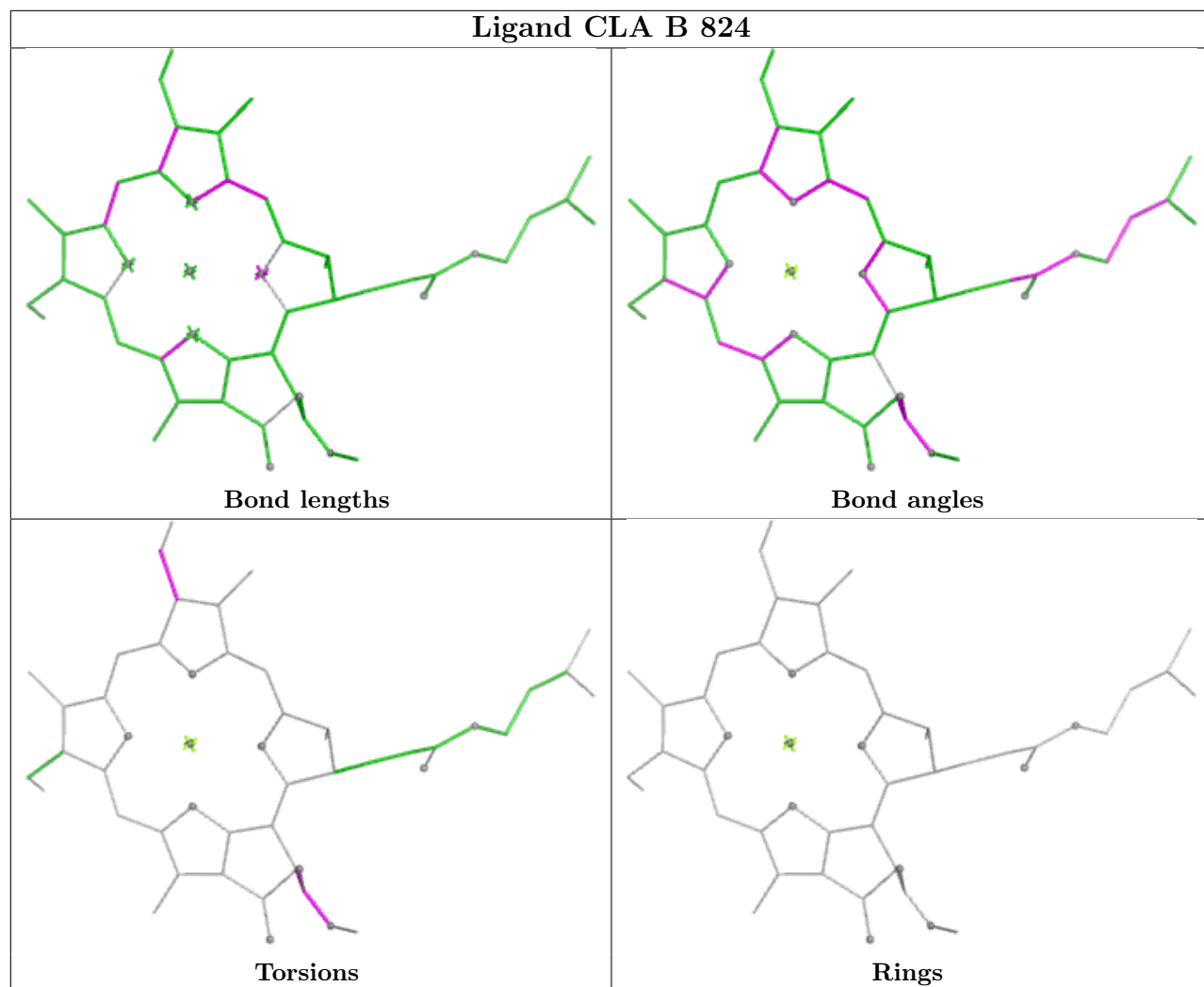


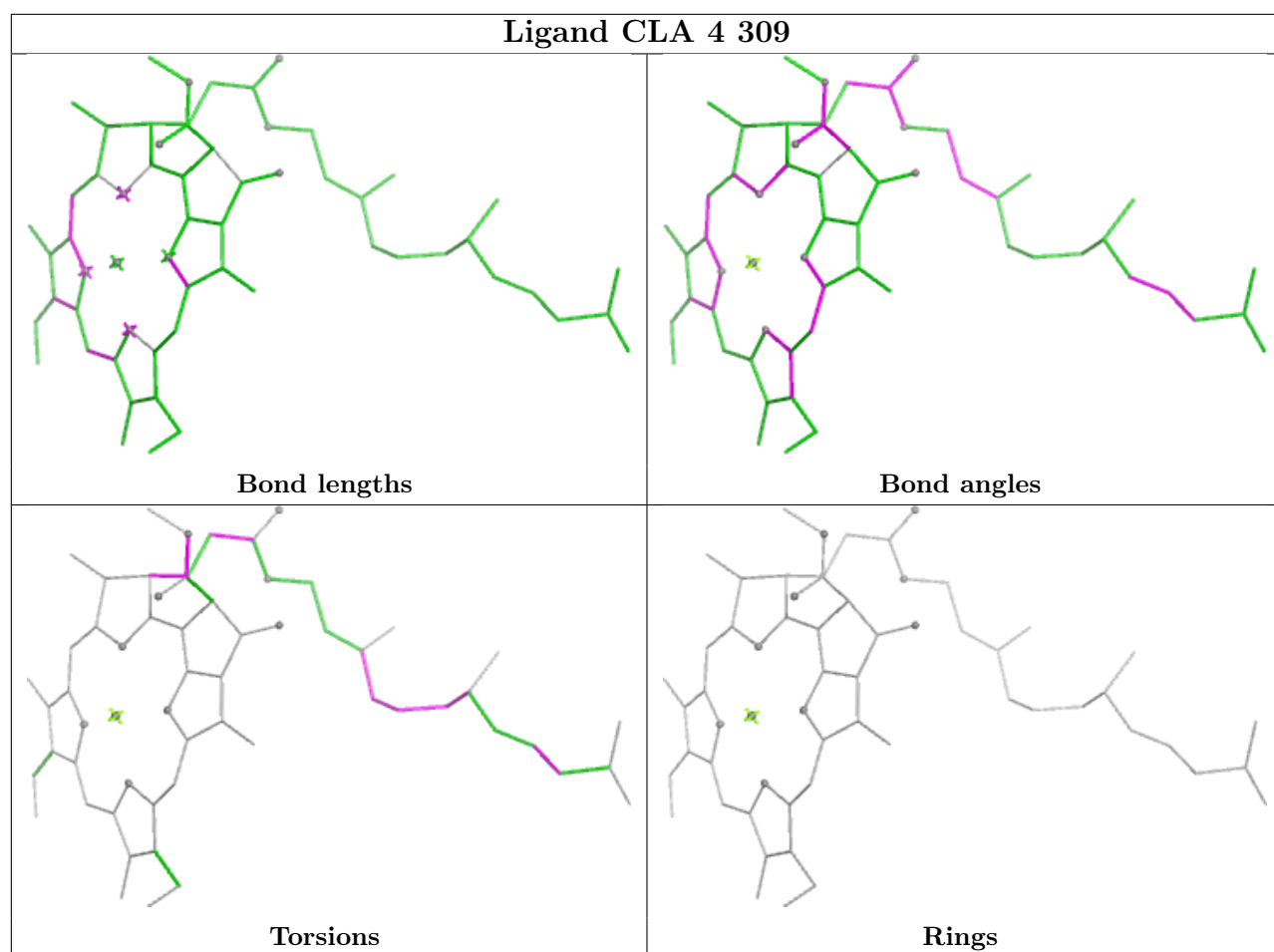
Ligand CLA 6 613



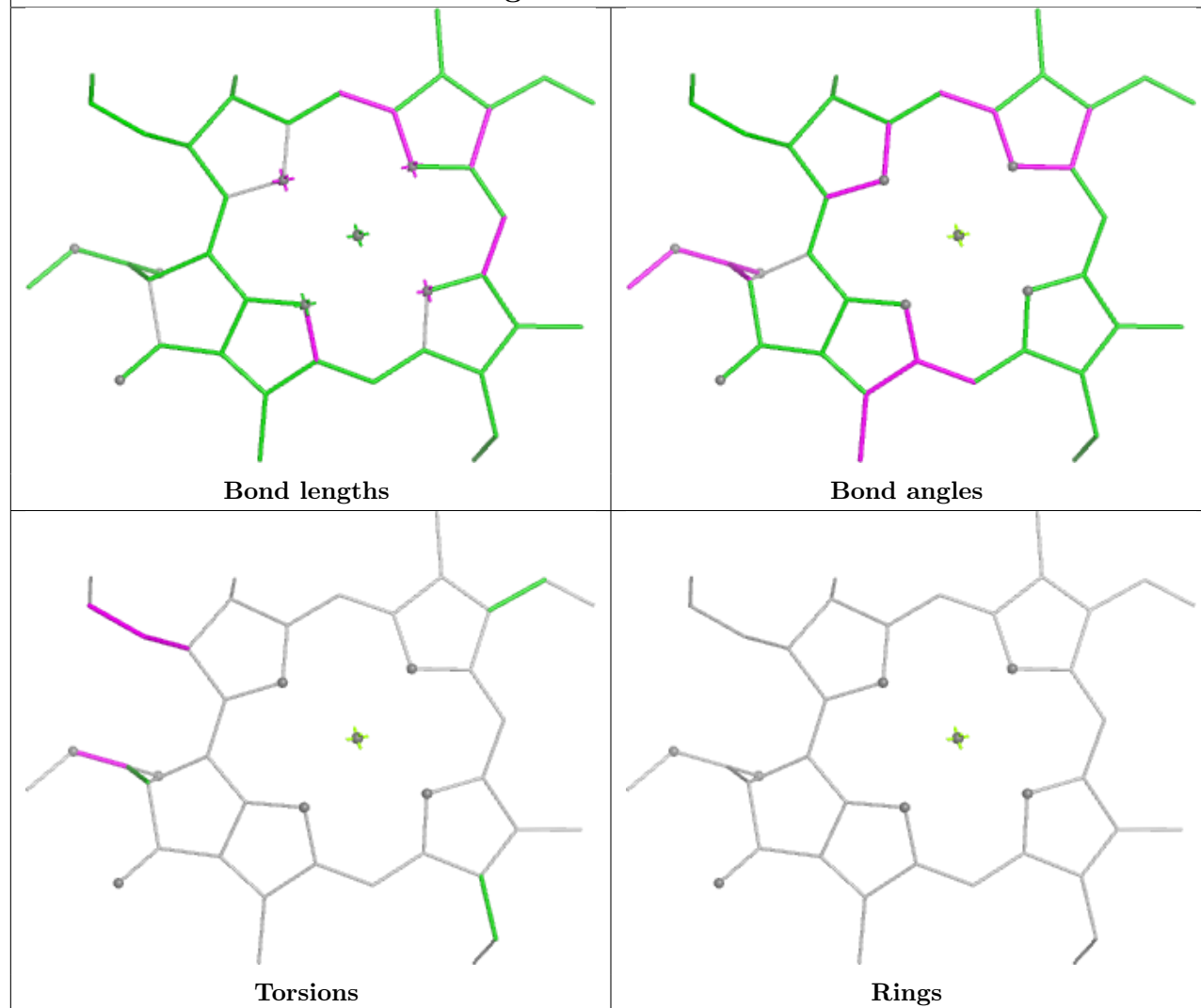


Ligand CLA B 824

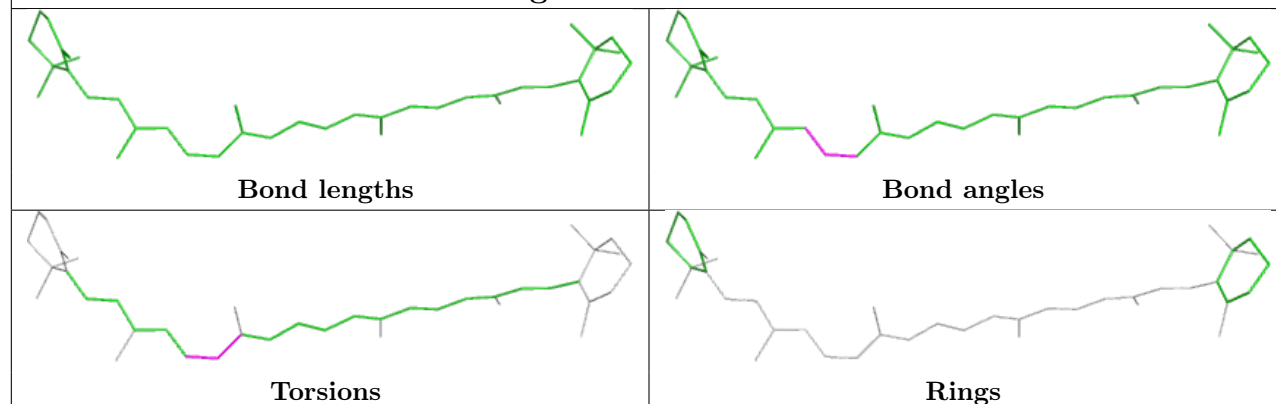




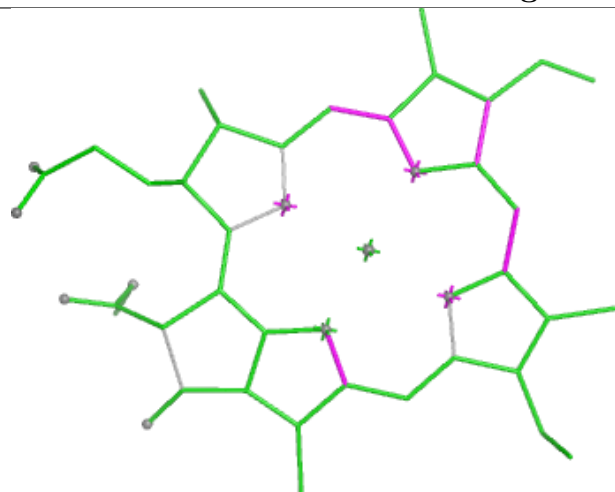
Ligand CLA 3 611



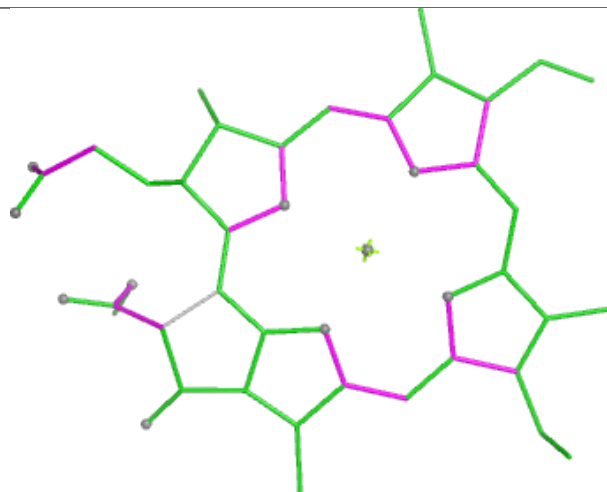
Ligand BCR A 846



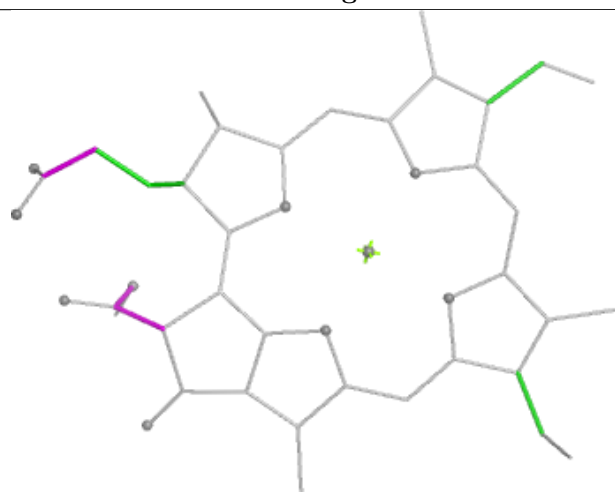
Ligand CLA 5 603



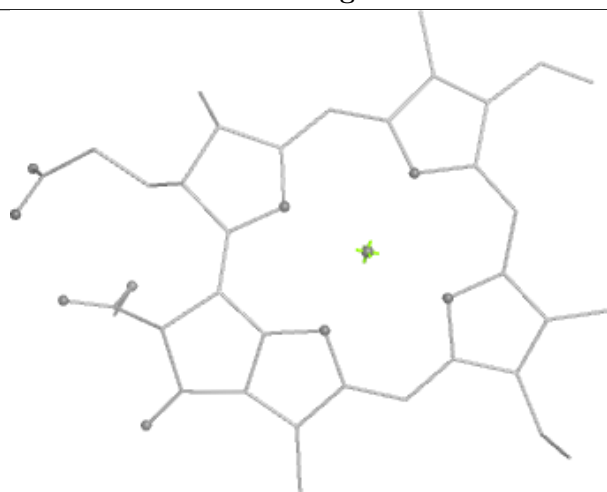
Bond lengths



Bond angles

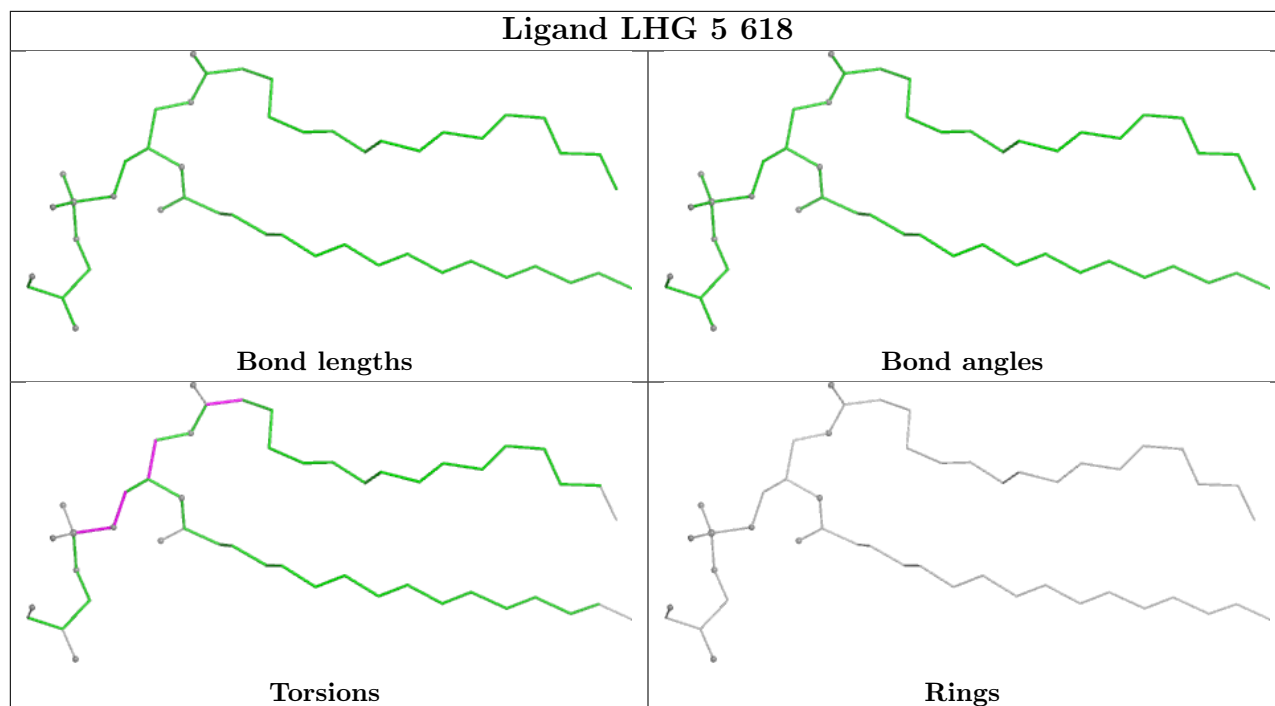


Torsions

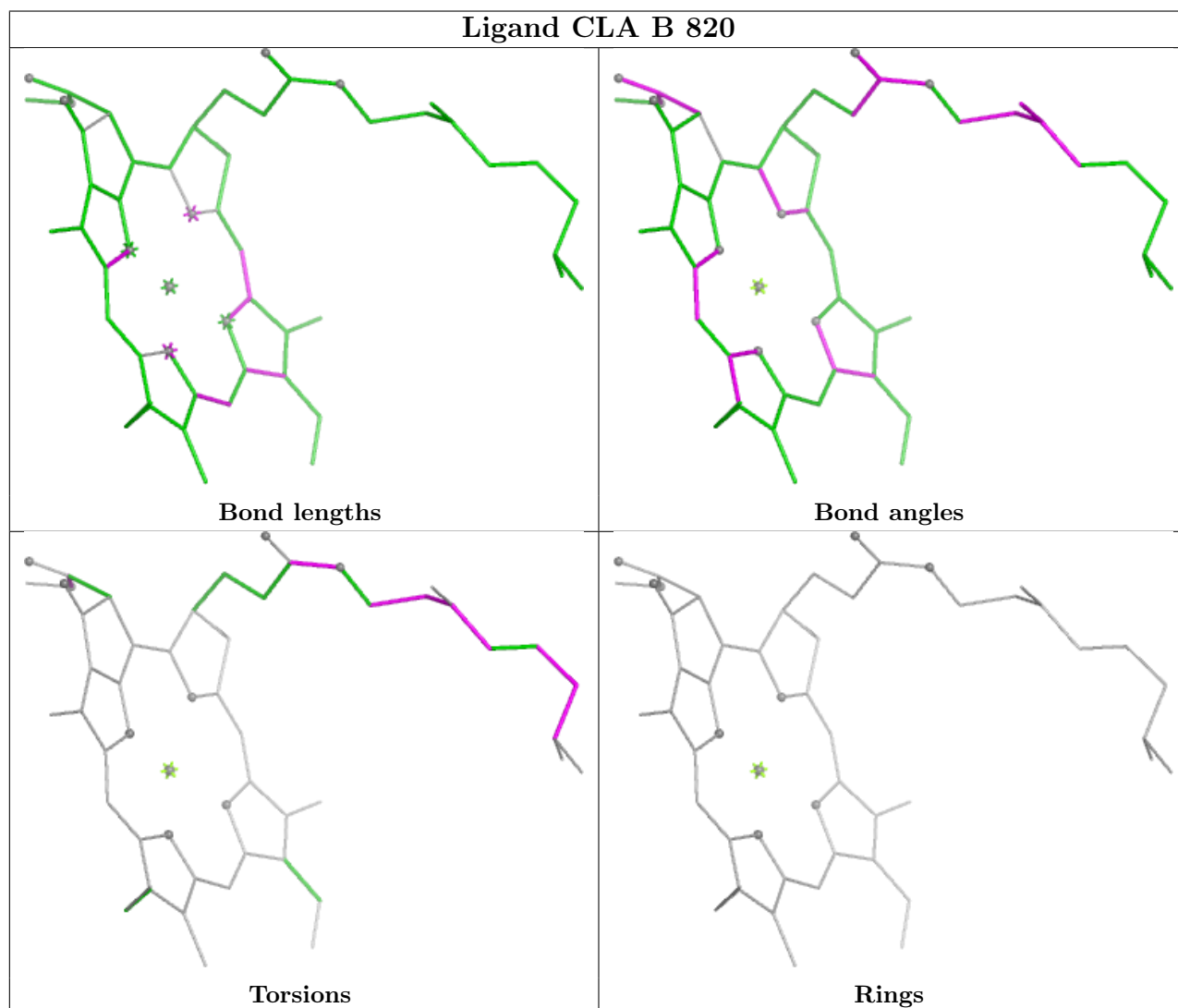


Rings

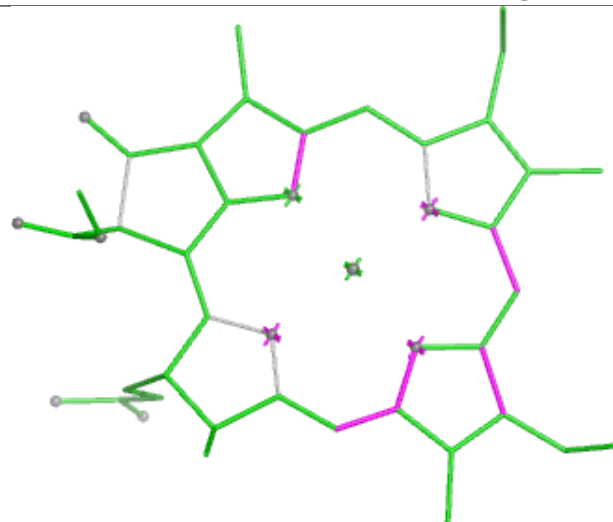
Ligand LHG 5 618



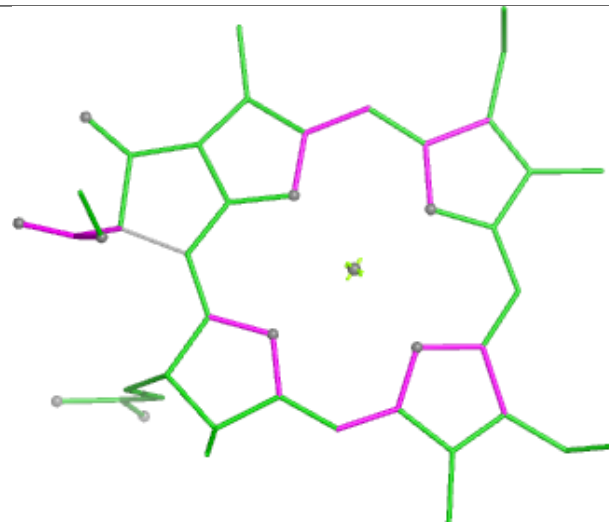
Ligand CLA B 820



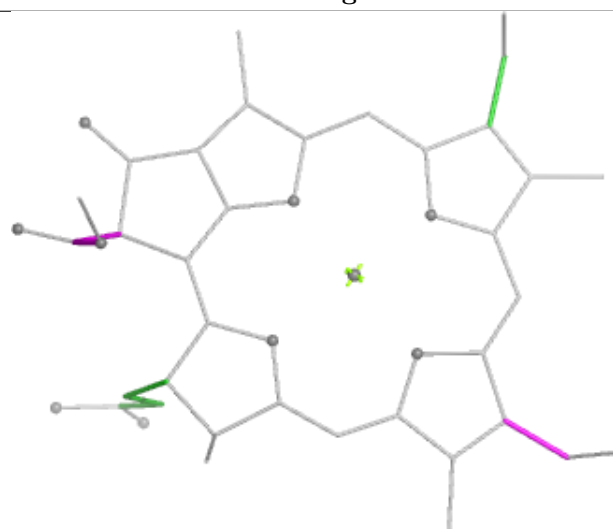
Ligand CLA A 814



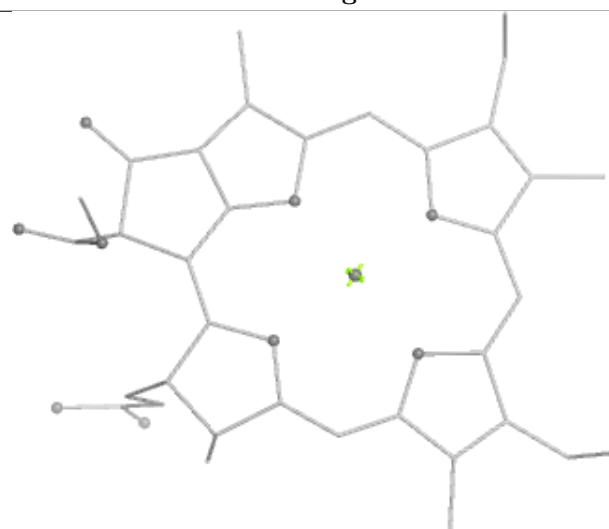
Bond lengths



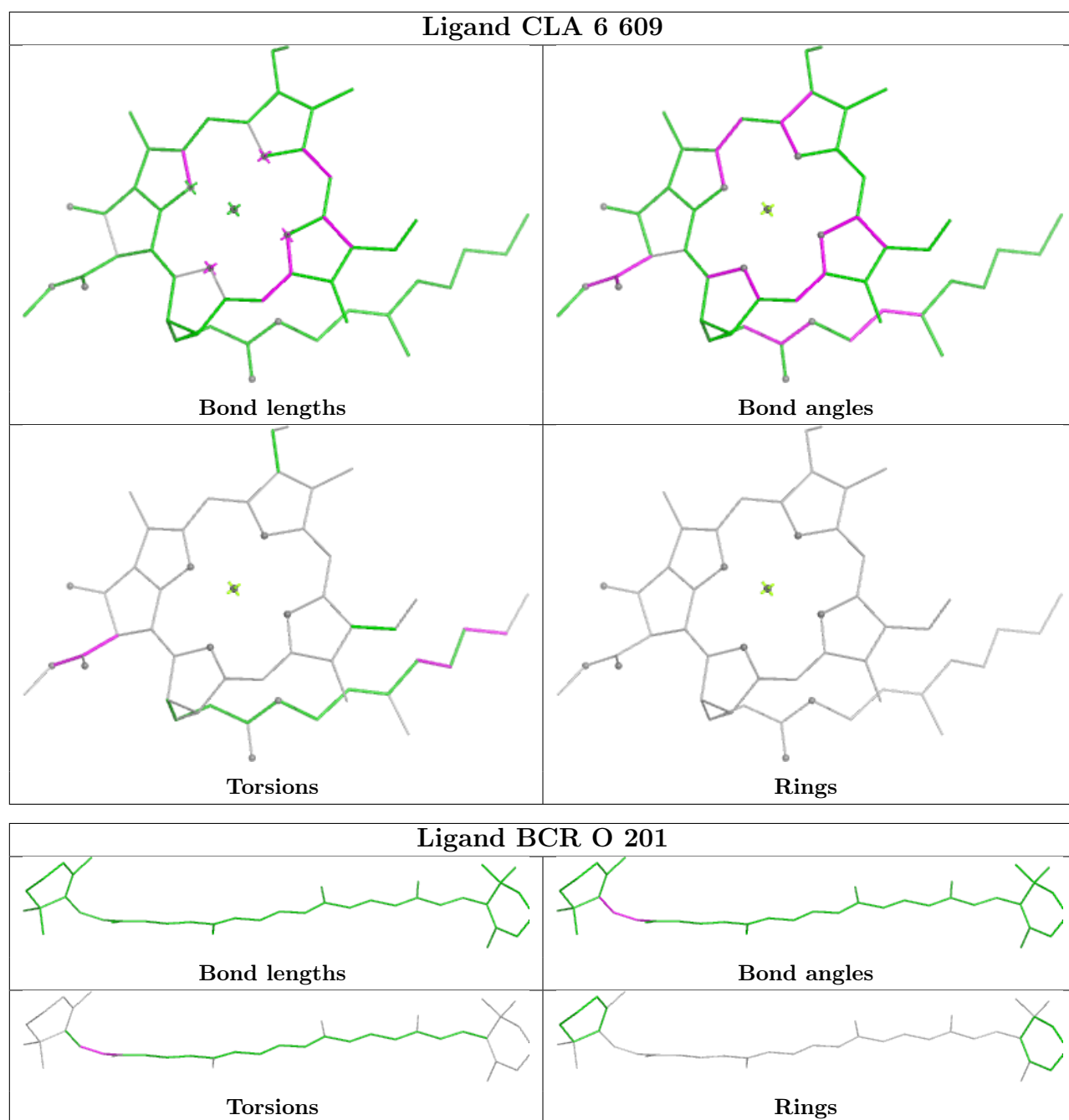
Bond angles

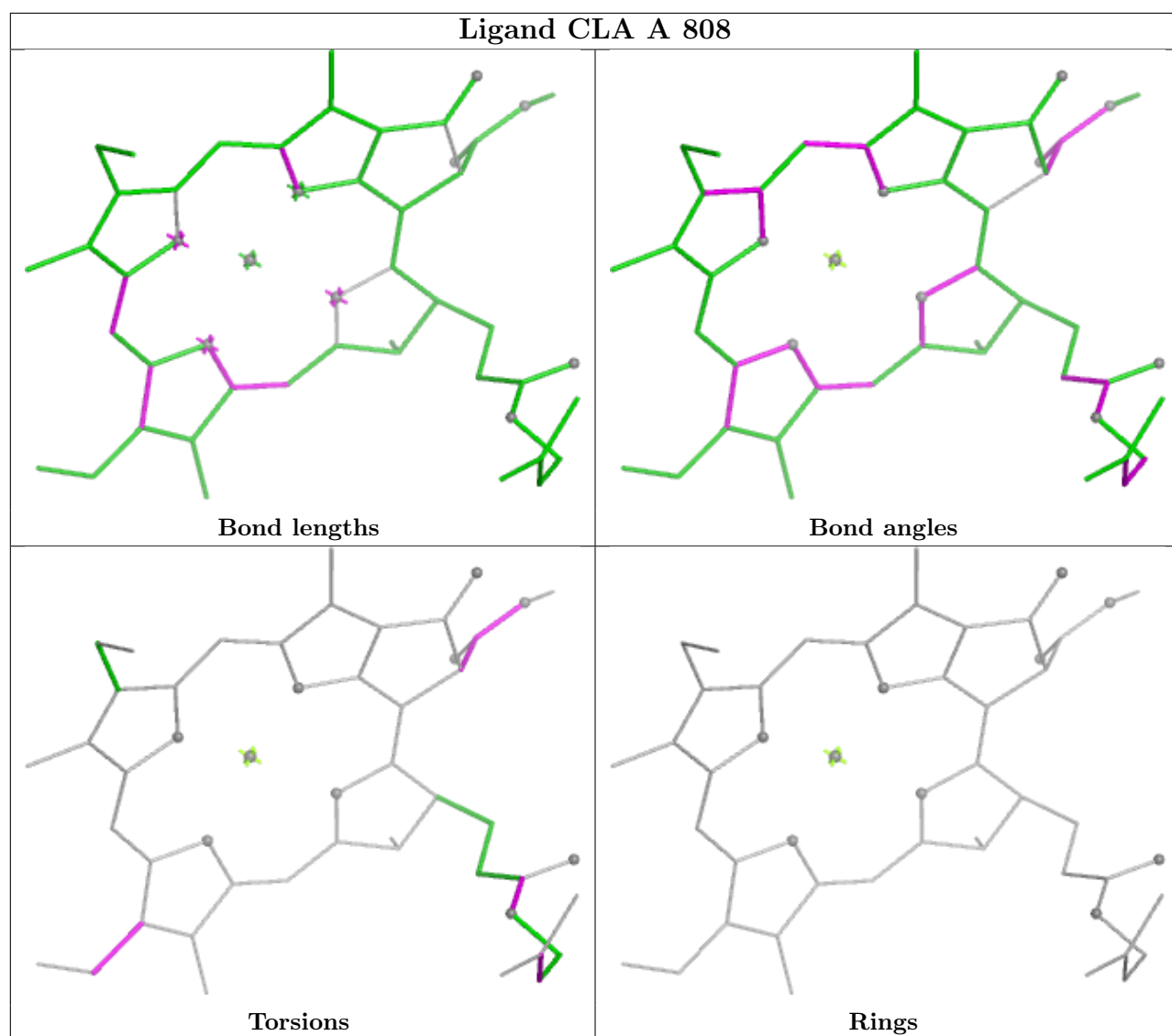


Torsions

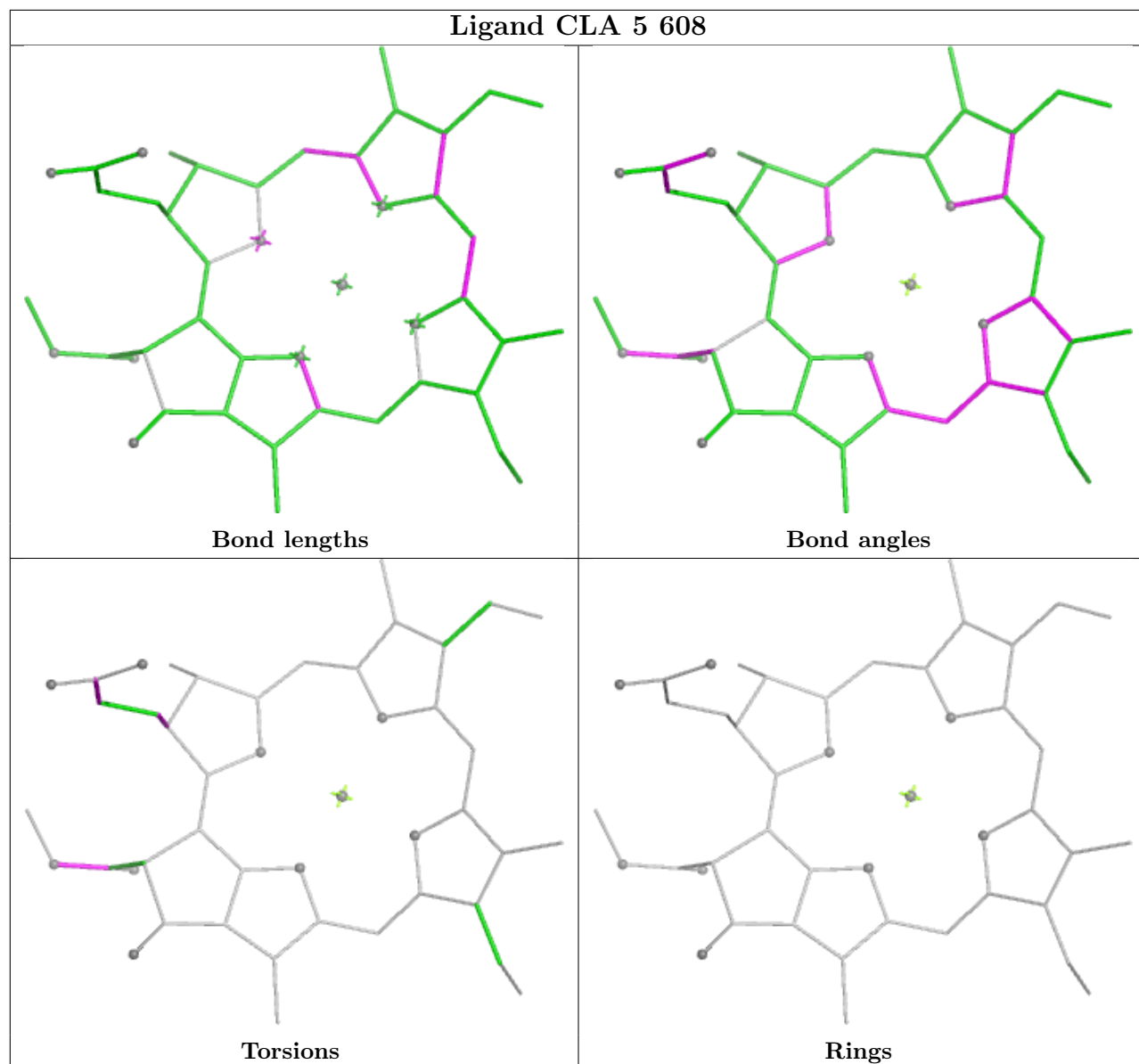


Rings

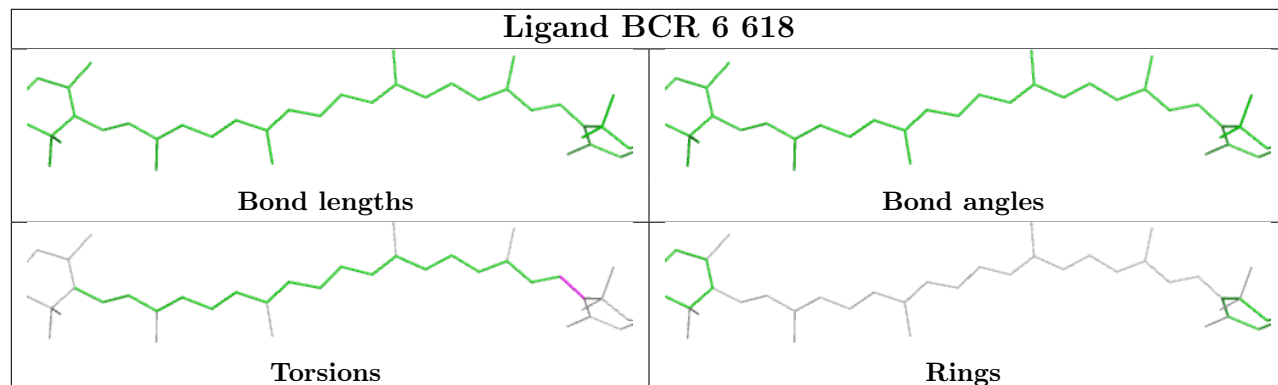


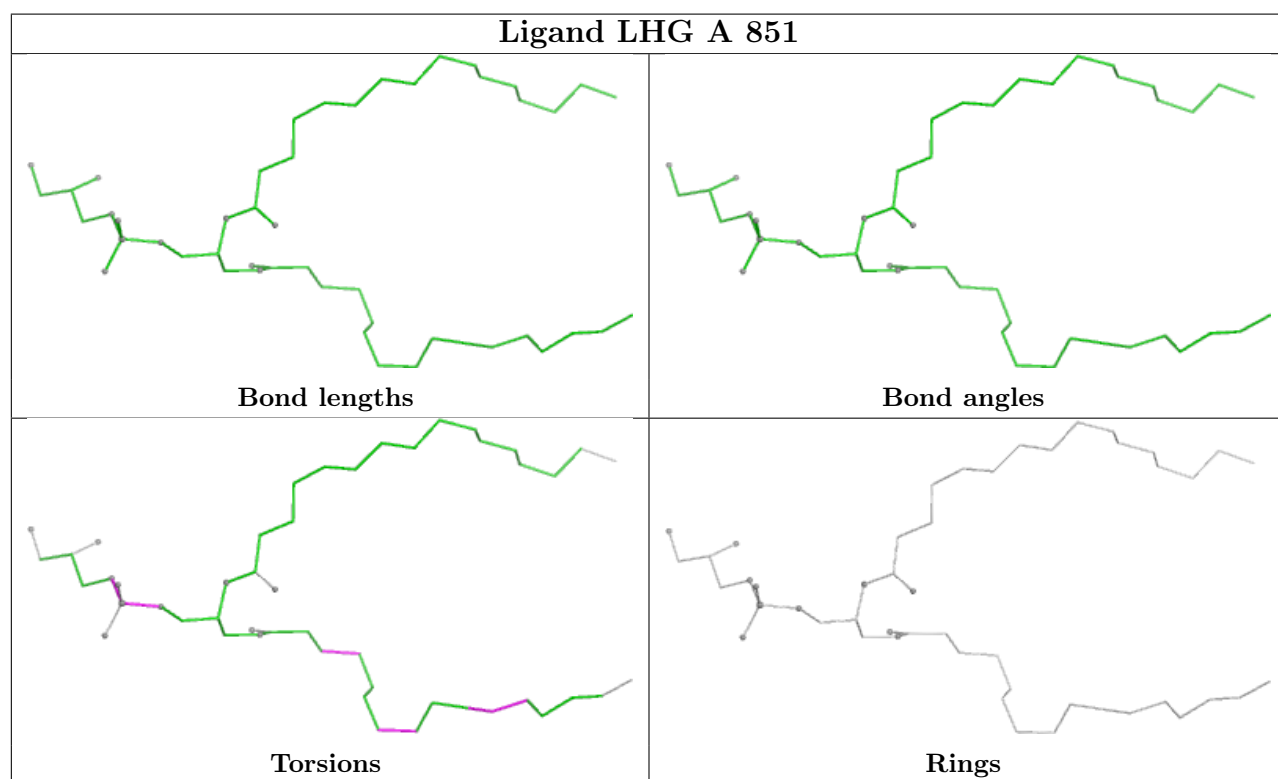
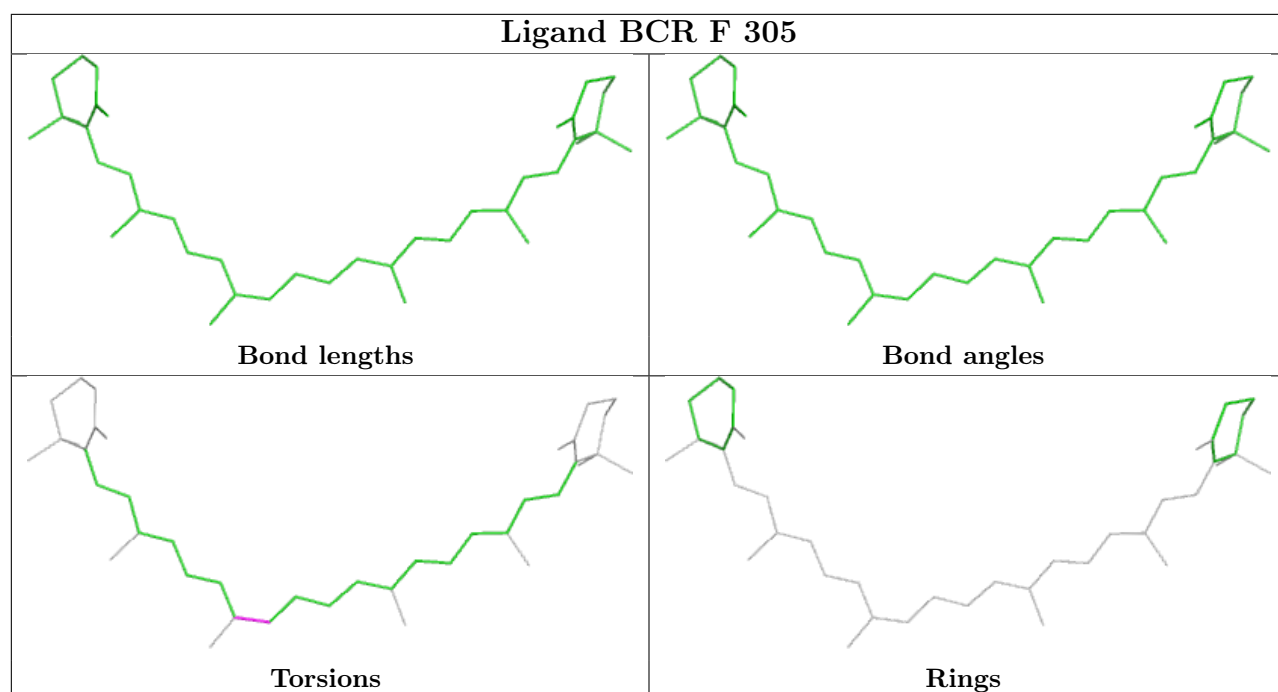


Ligand CLA 5 608

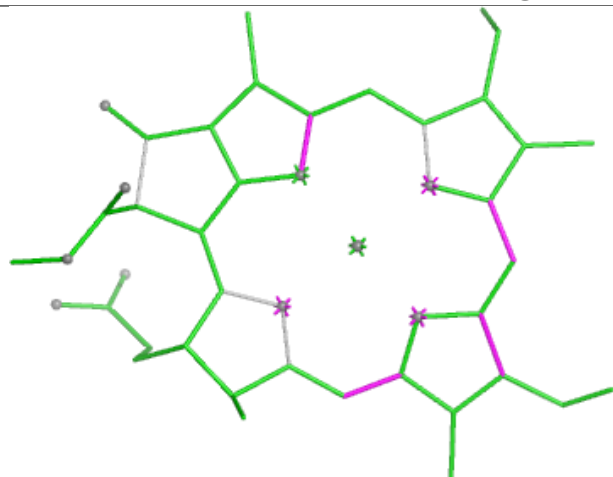


Ligand BCR 6 618

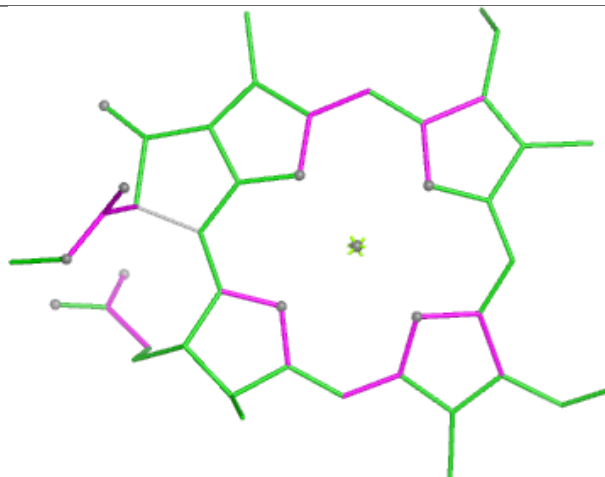




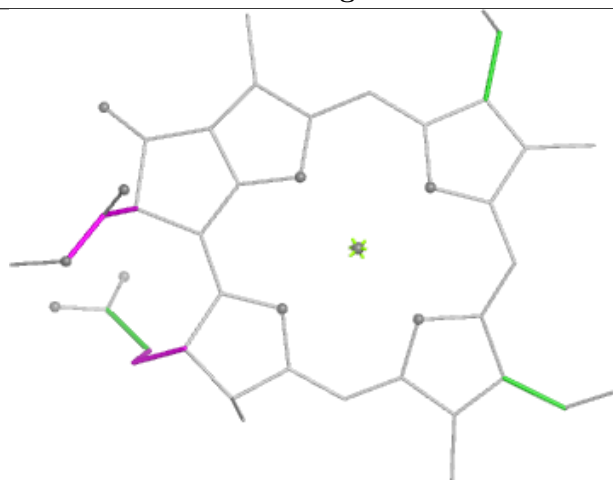
Ligand CLA Z 311



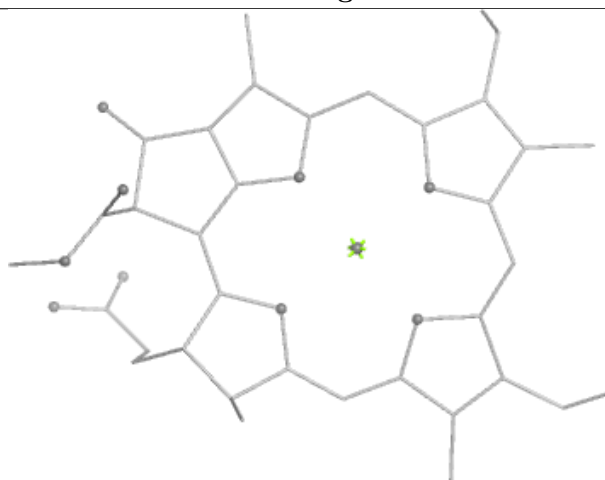
Bond lengths



Bond angles



Torsions



Rings

Ligand XAT 3 616



Bond lengths



Bond angles

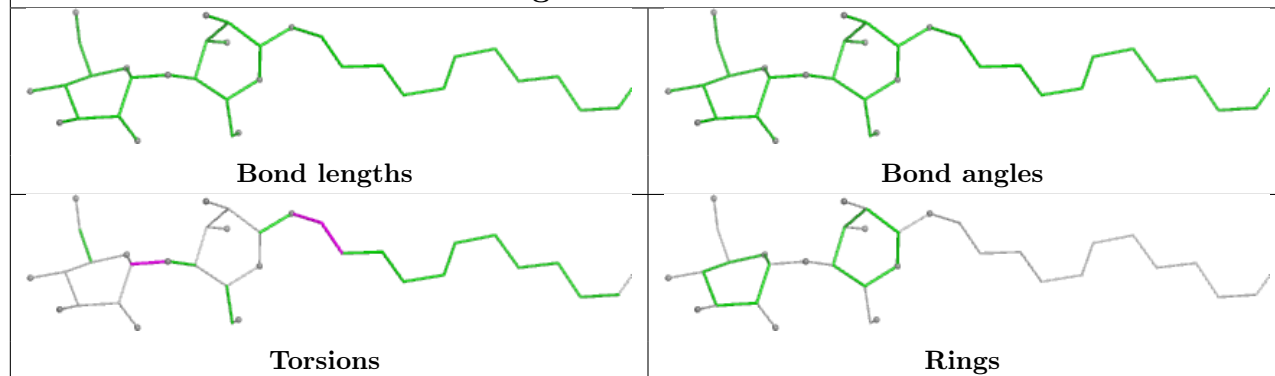


Torsions

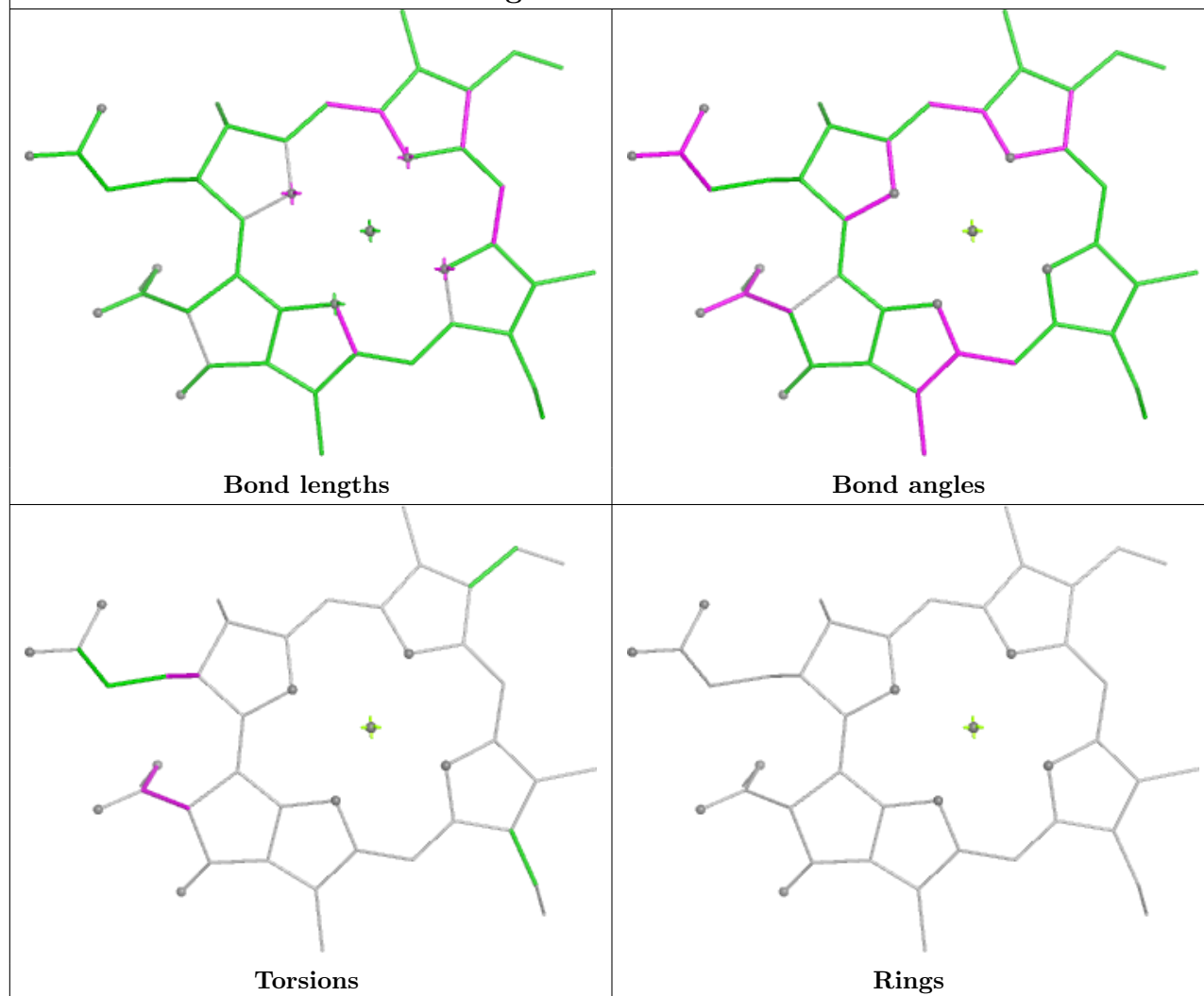


Rings

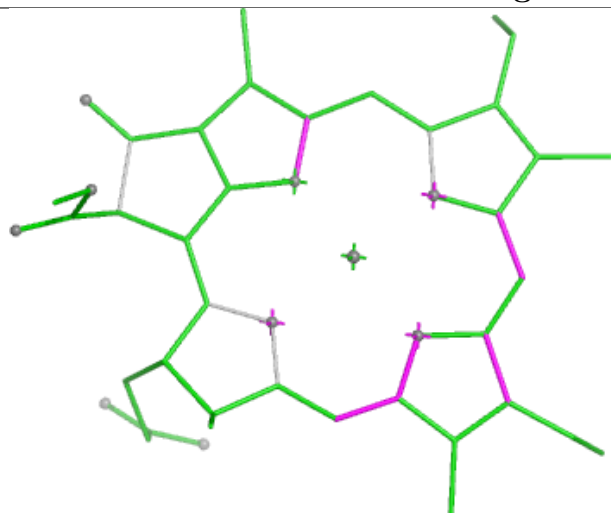
Ligand LMT 6 621



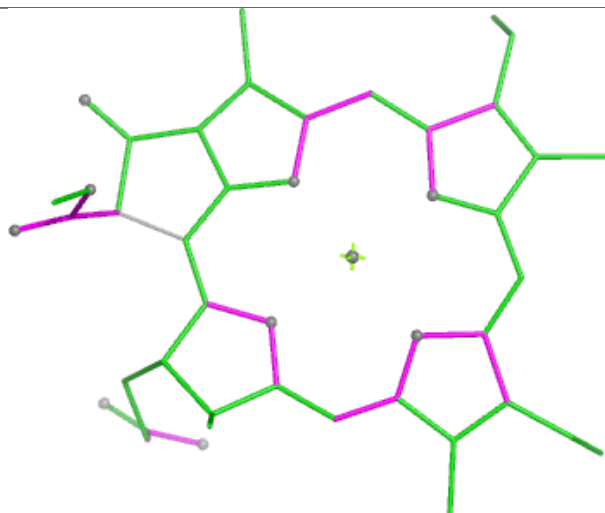
Ligand CLA 4 302



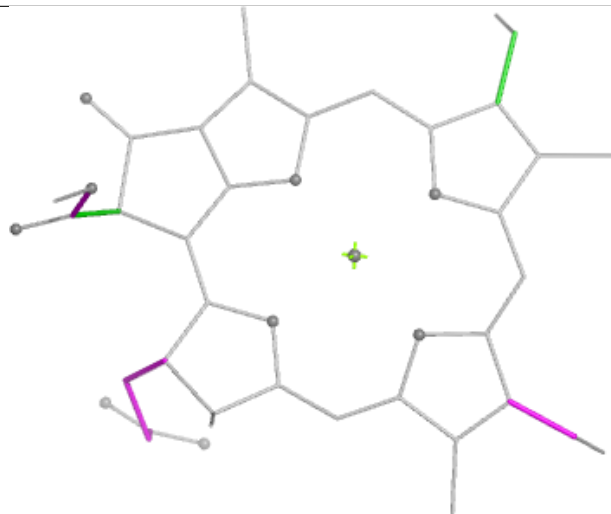
Ligand CLA A 820



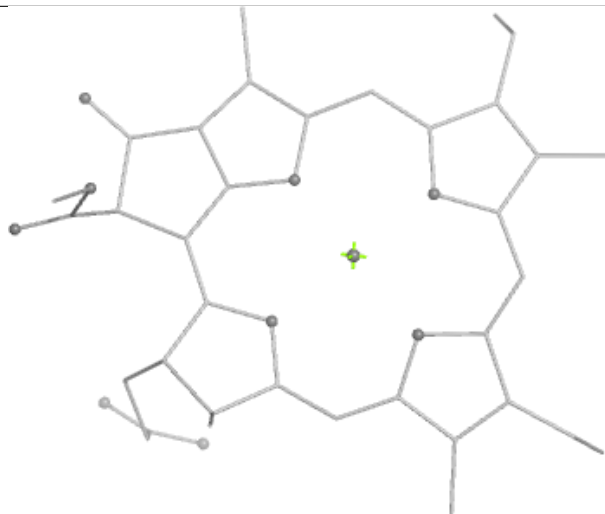
Bond lengths



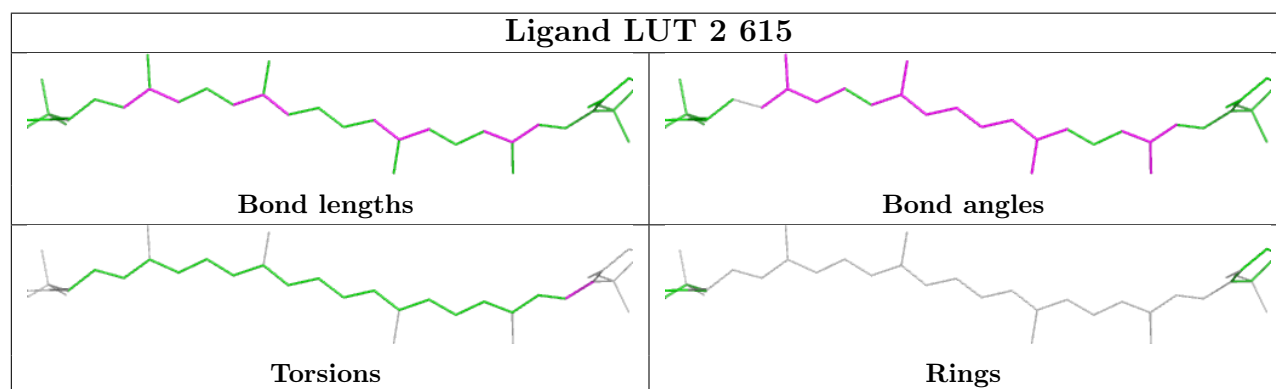
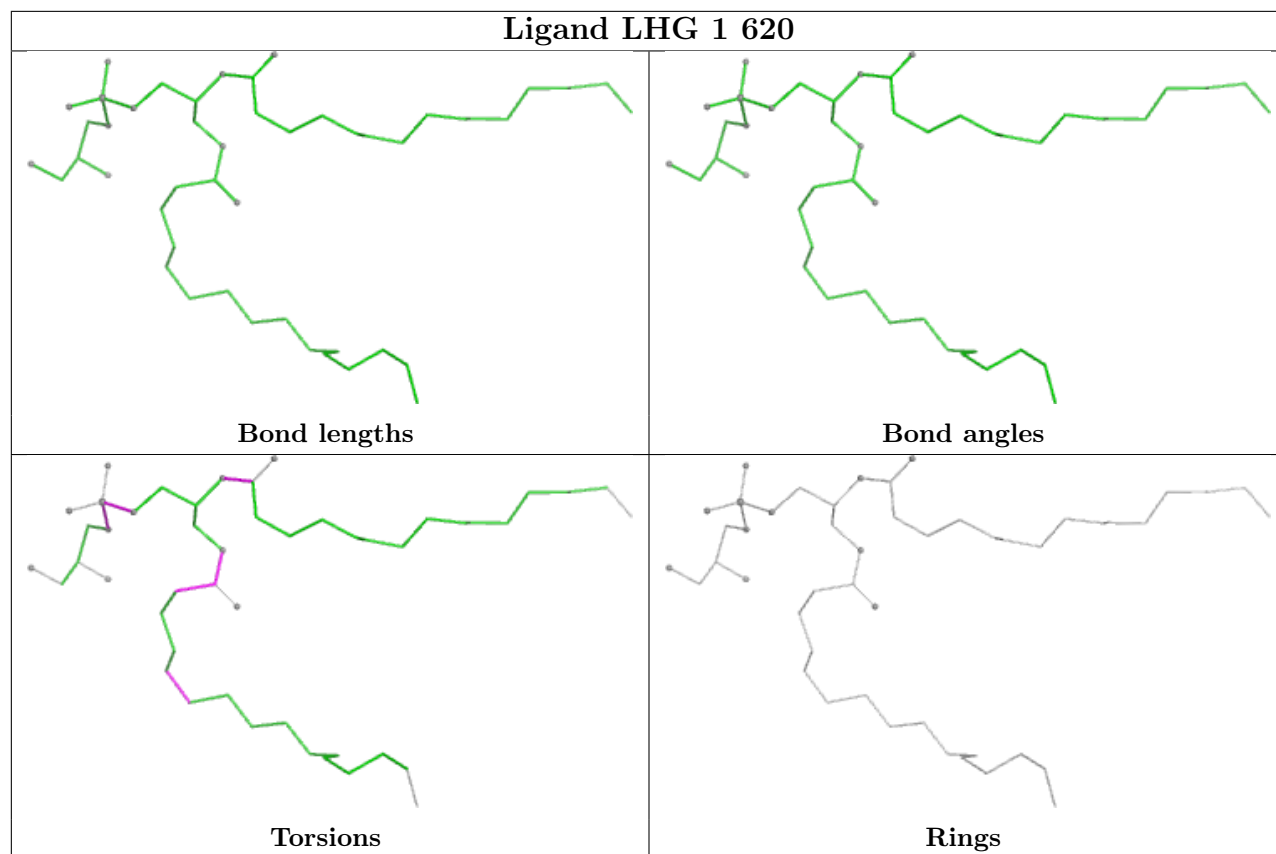
Bond angles



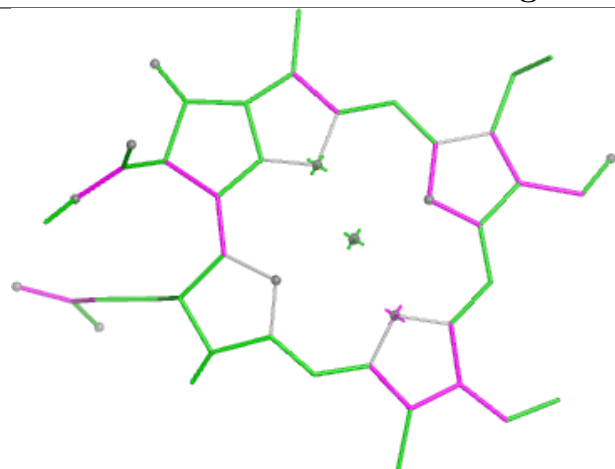
Torsions



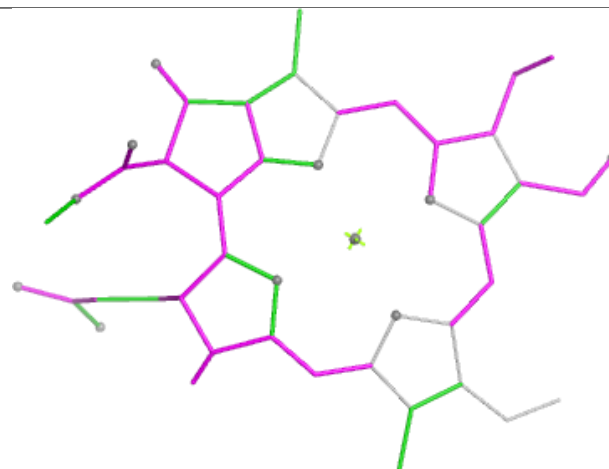
Rings



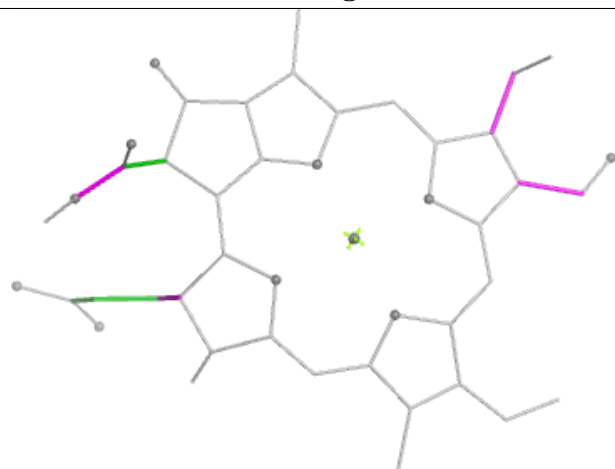
Ligand CHL 4 305



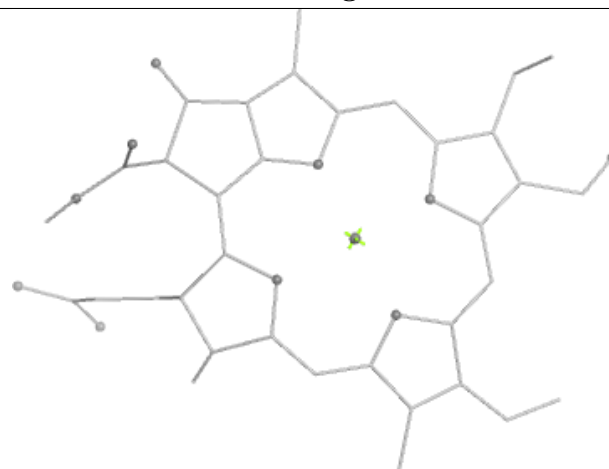
Bond lengths



Bond angles

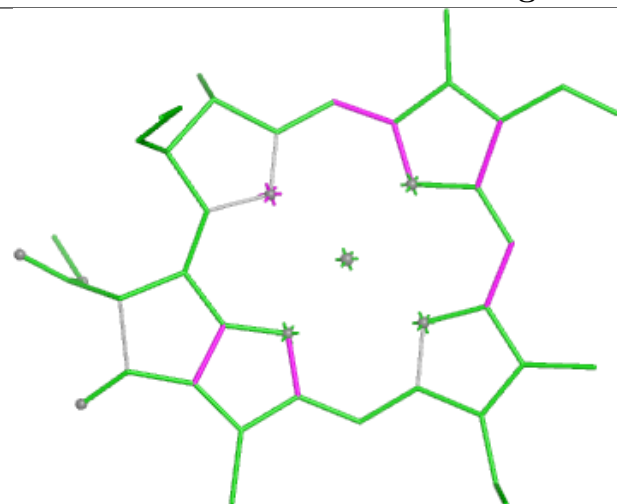


Torsions

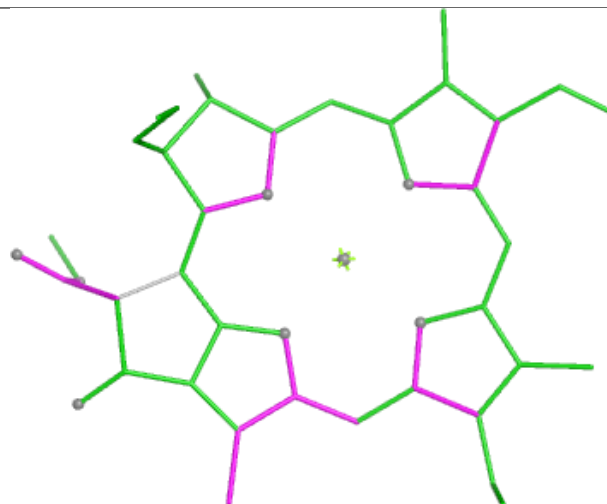


Rings

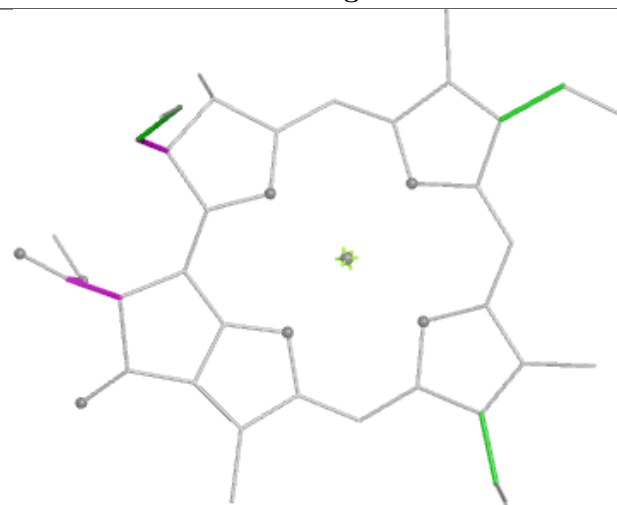
Ligand CLA B 829



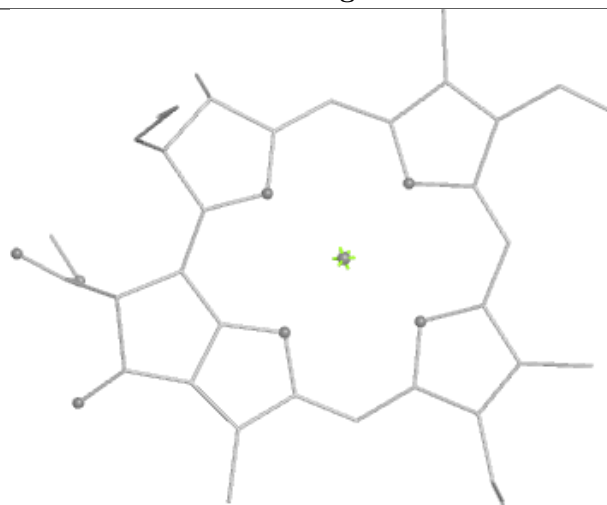
Bond lengths



Bond angles

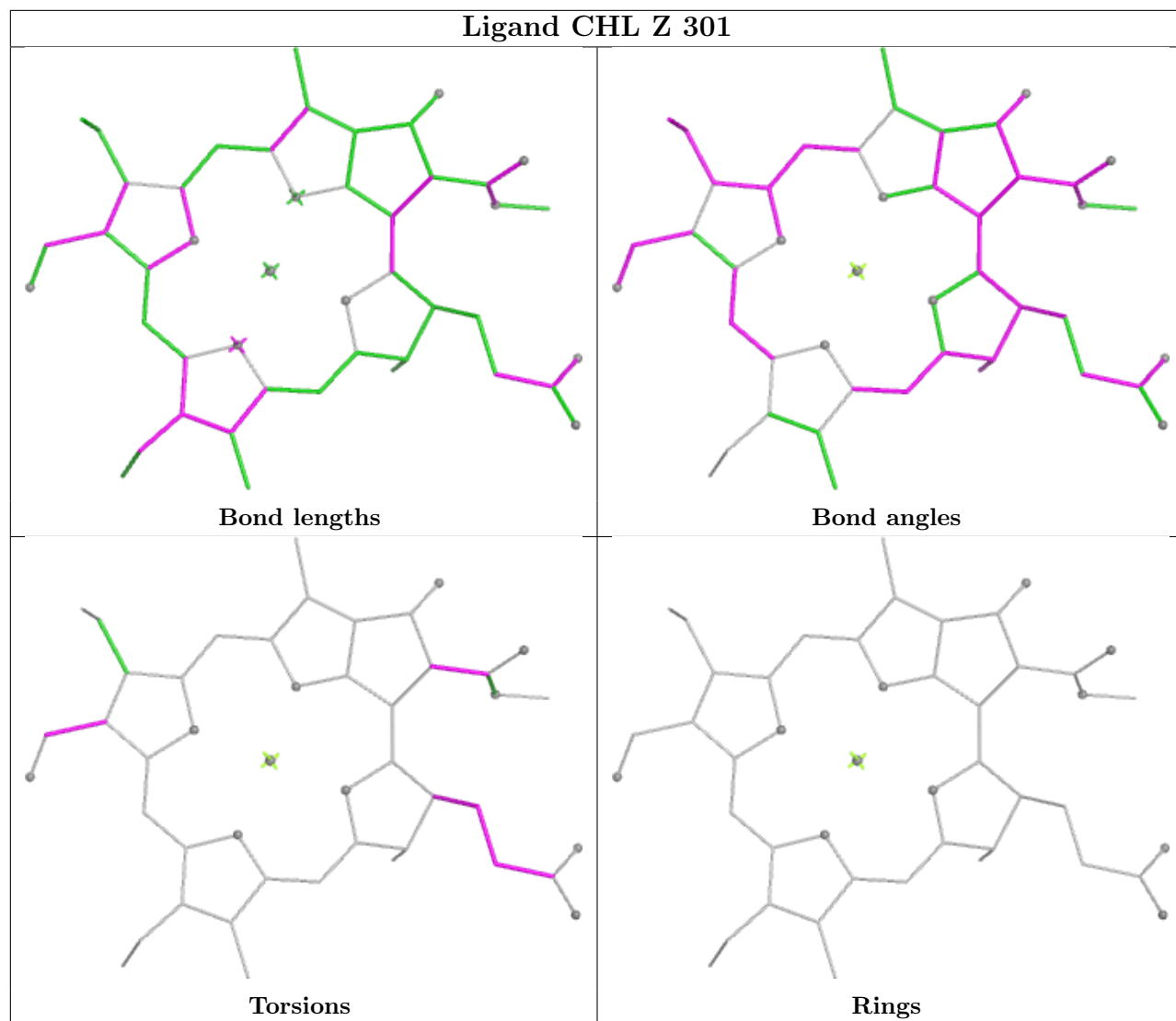


Torsions

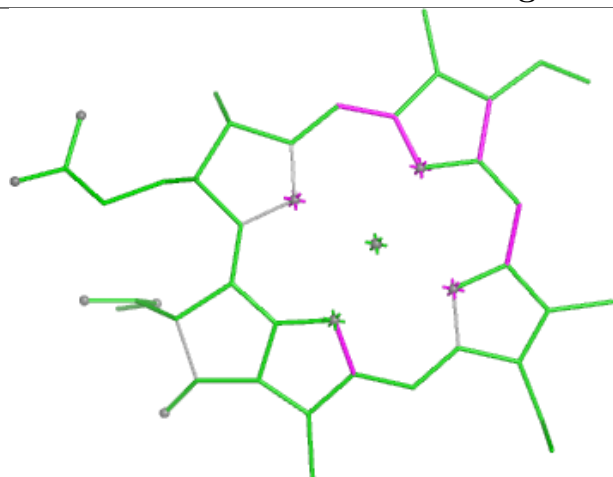


Rings

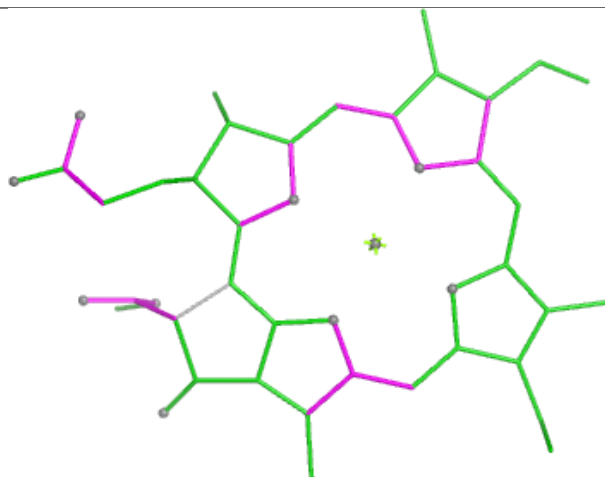
Ligand CHL Z 301



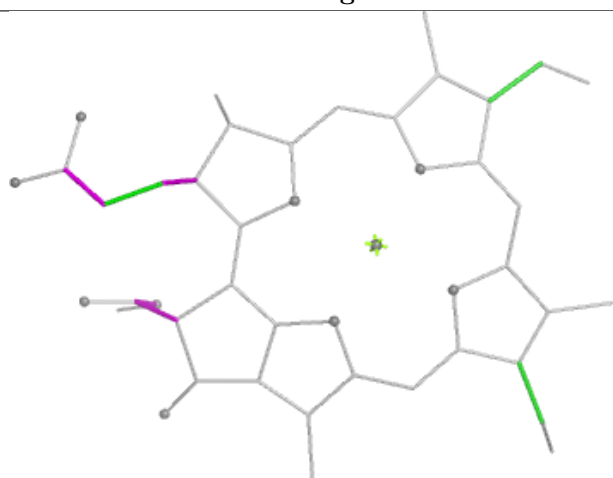
Ligand CLA 6 603



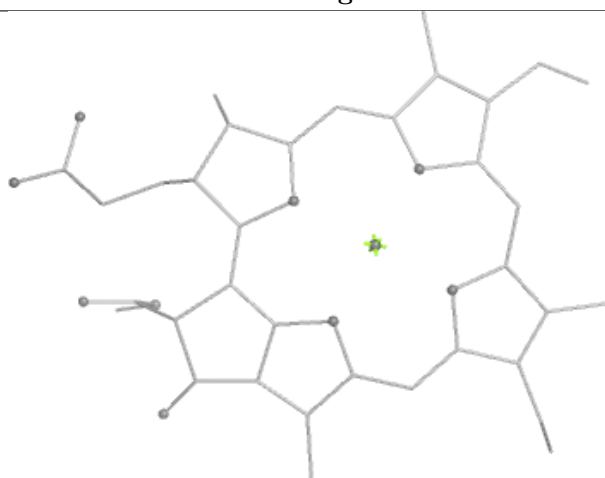
Bond lengths



Bond angles

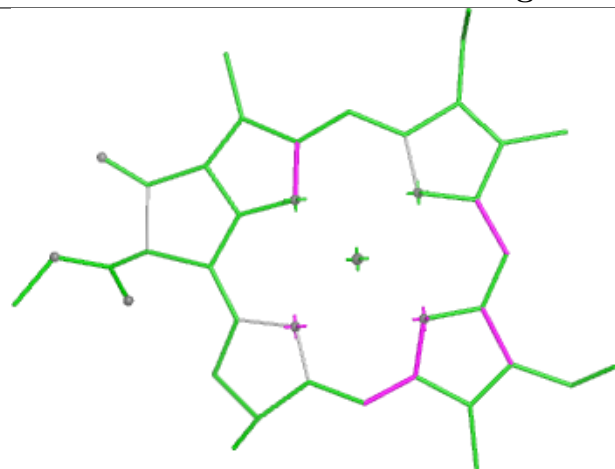


Torsions

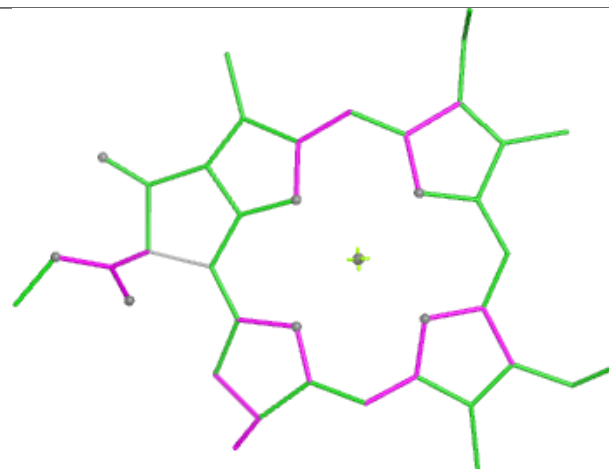


Rings

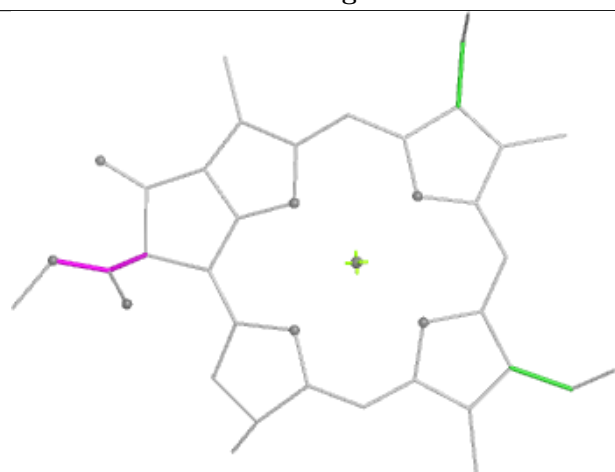
Ligand CLA B 803



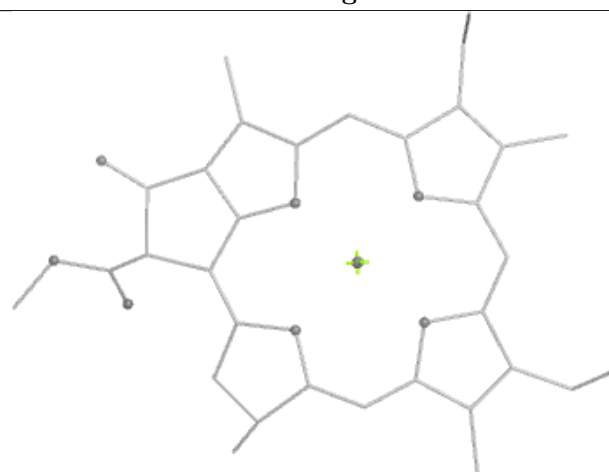
Bond lengths



Bond angles

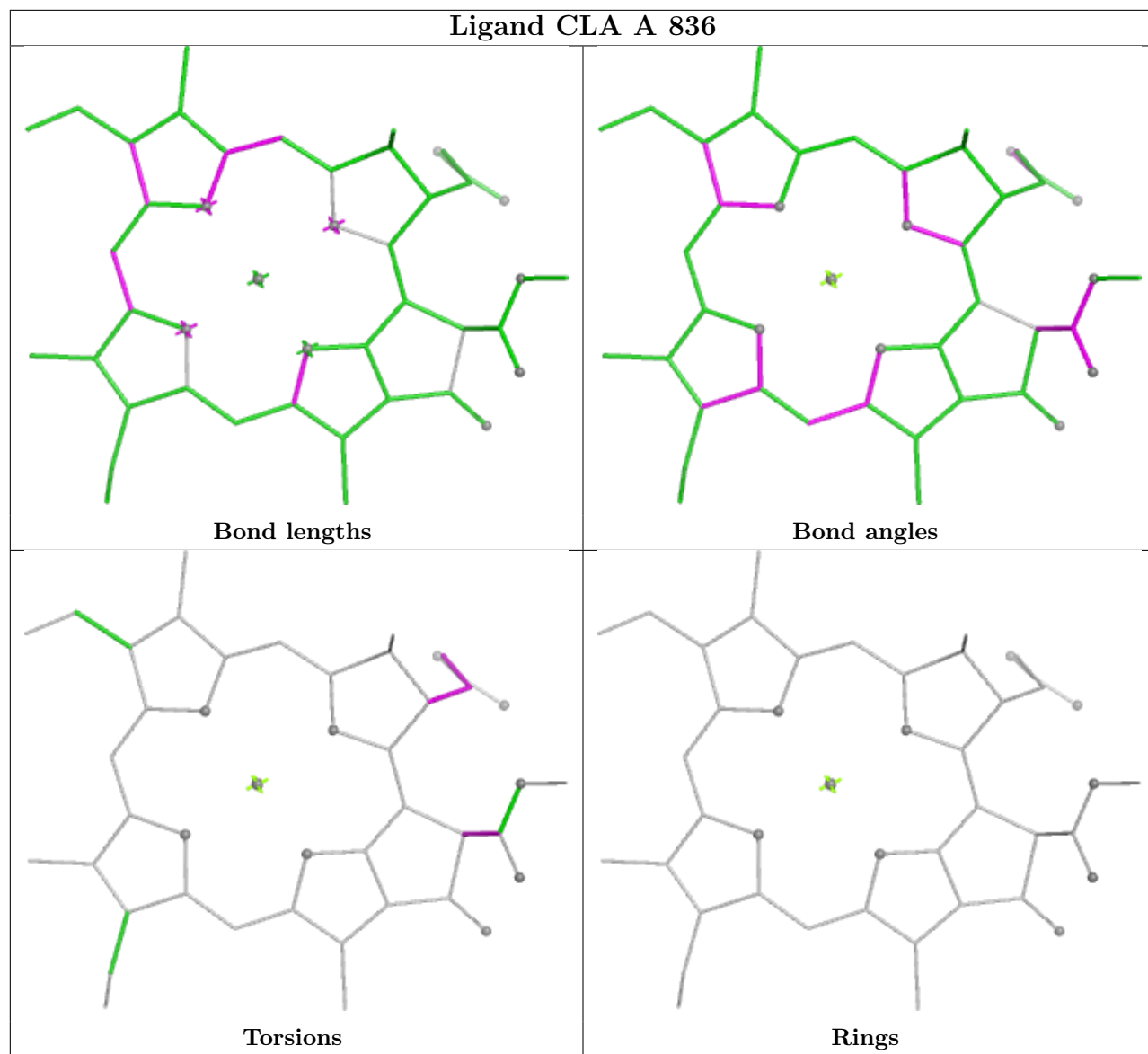


Torsions

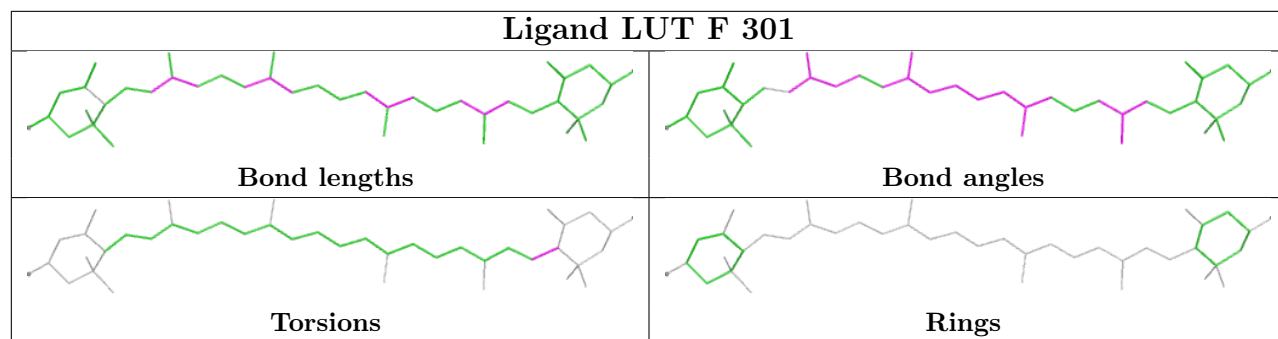


Rings

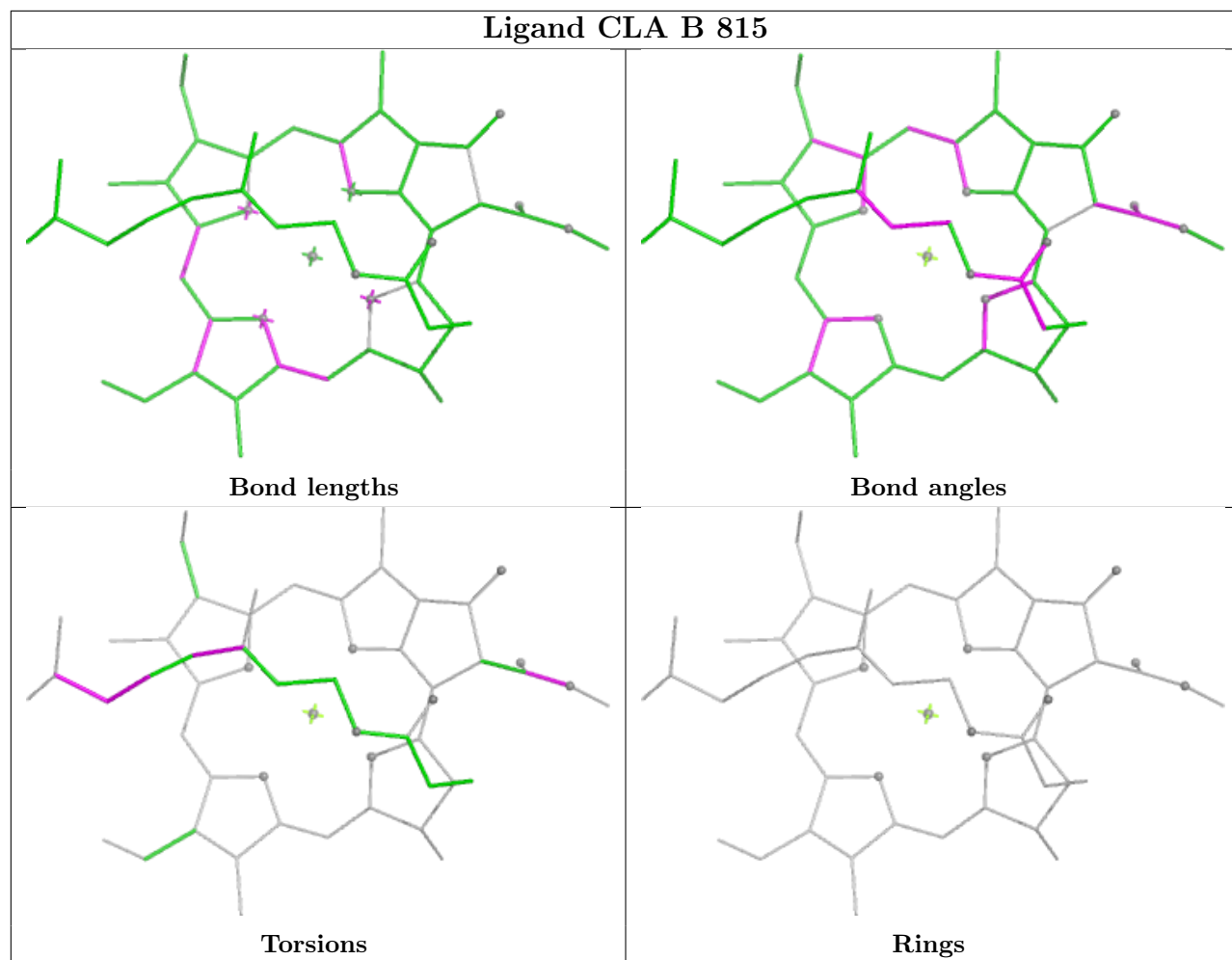
Ligand CLA A 836



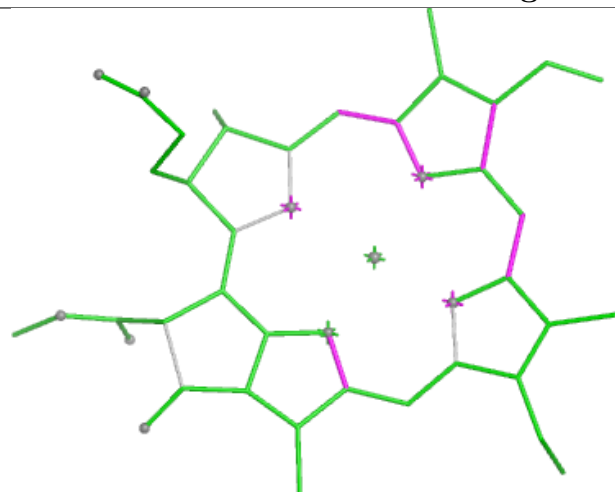
Ligand LUT F 301



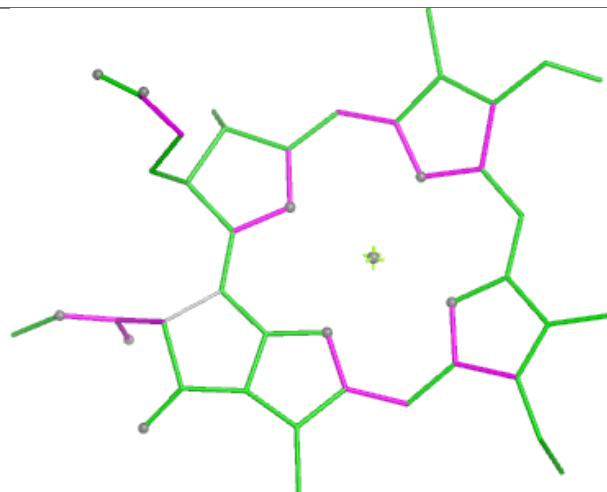
Ligand CLA B 815



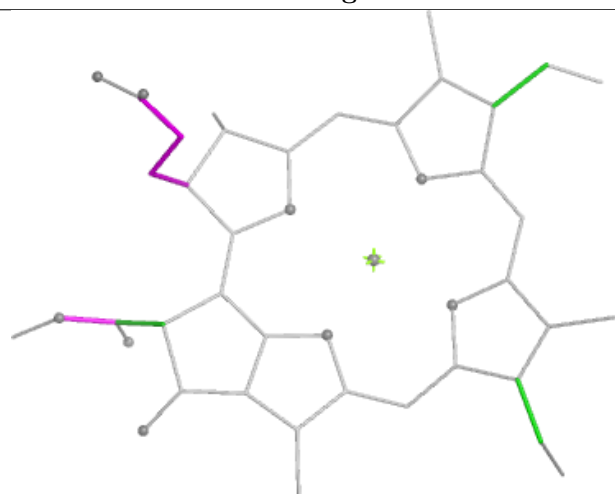
Ligand CLA 3 609



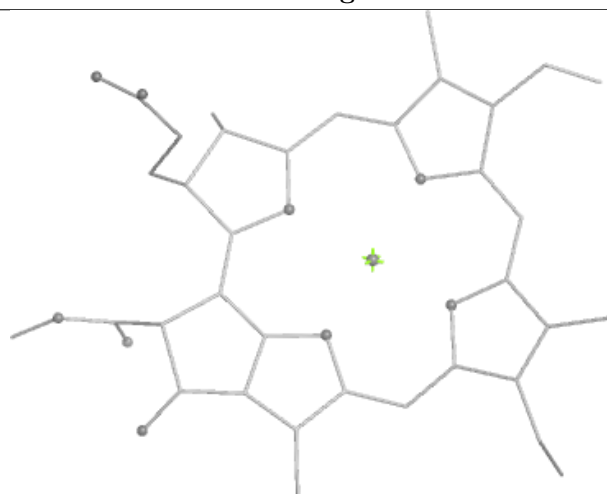
Bond lengths



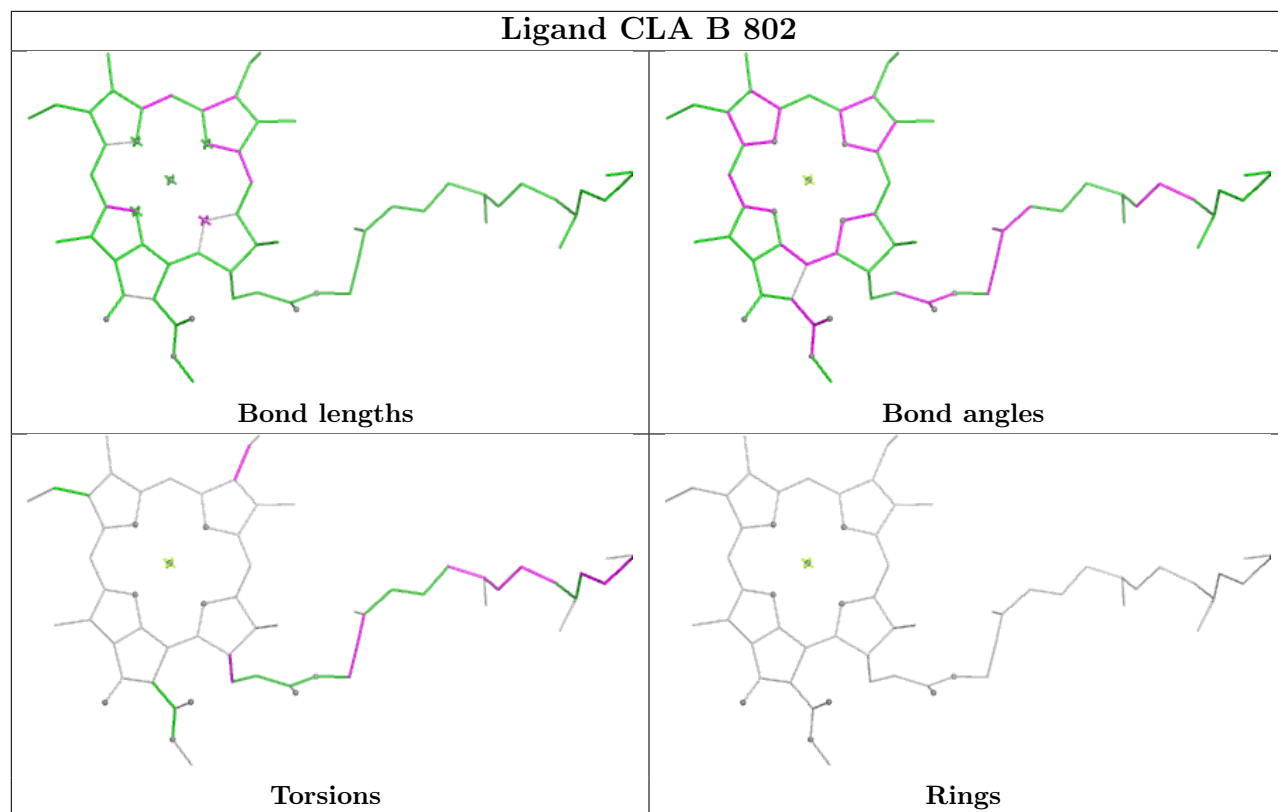
Bond angles



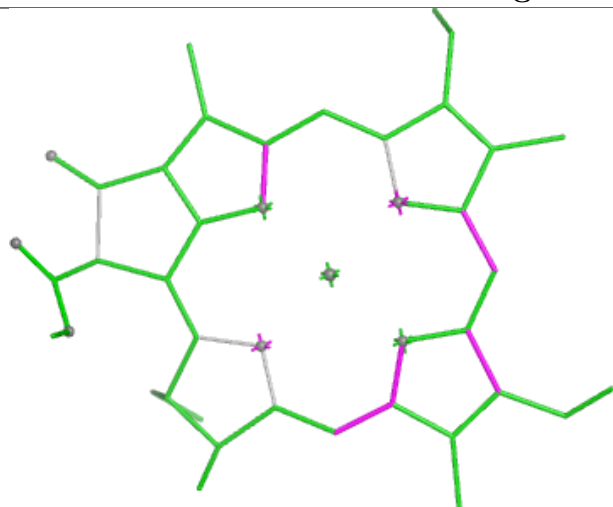
Torsions



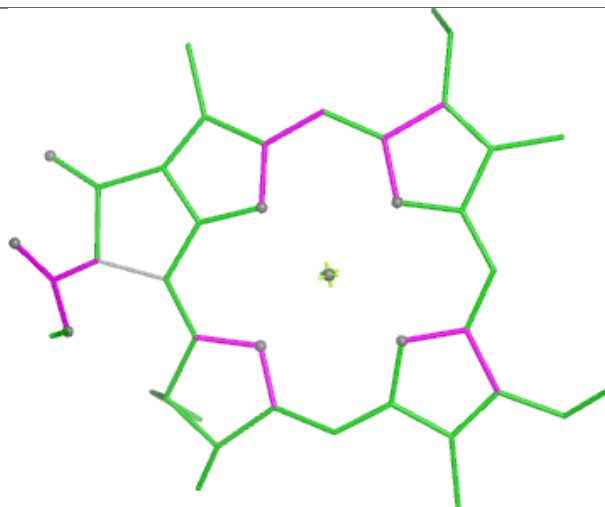
Rings



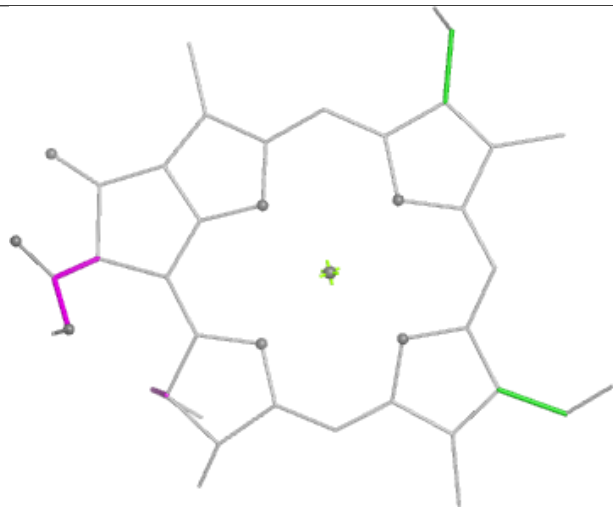
Ligand CLA A 822



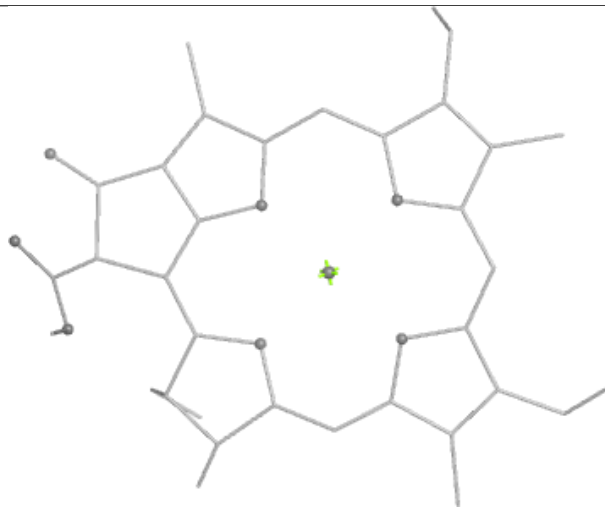
Bond lengths



Bond angles

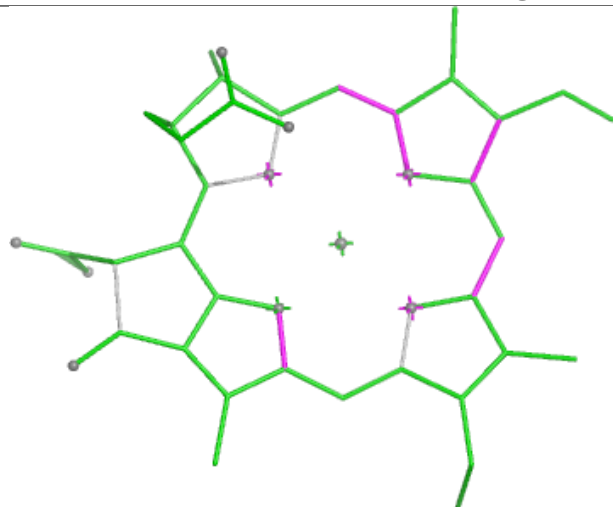


Torsions

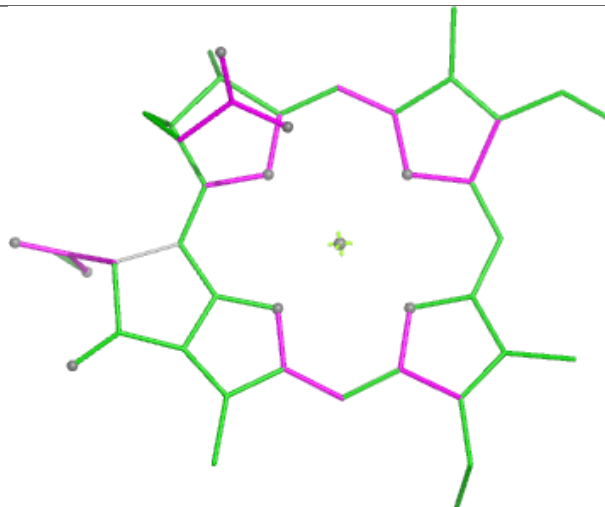


Rings

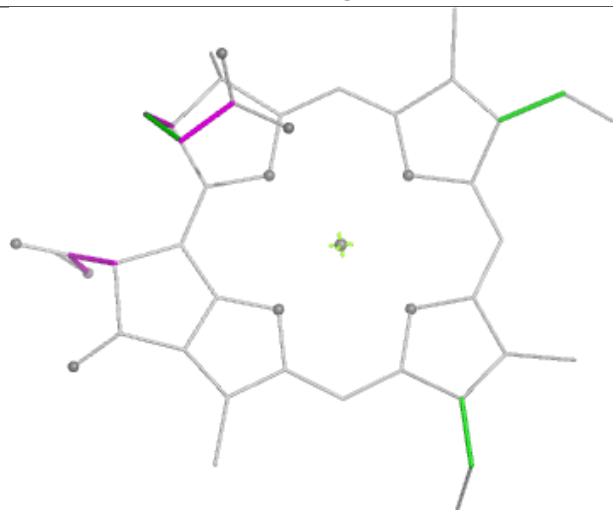
Ligand CLA Y 614



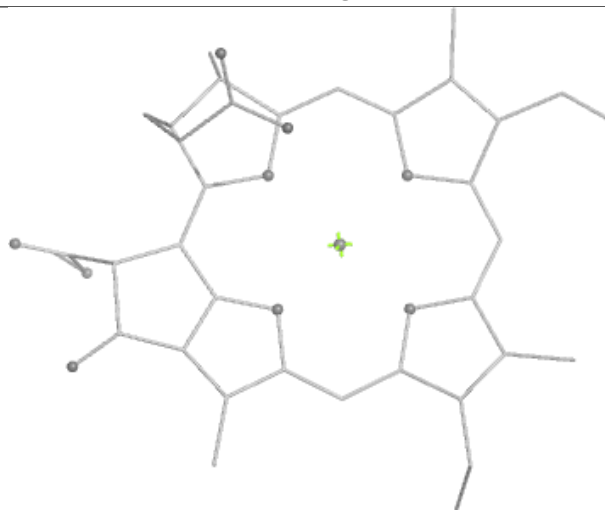
Bond lengths



Bond angles

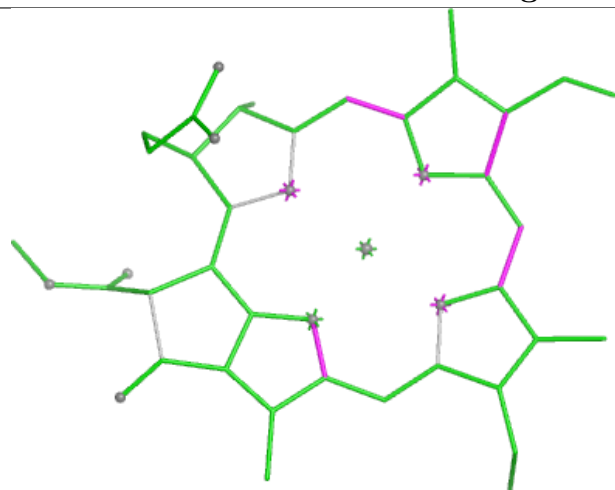


Torsions

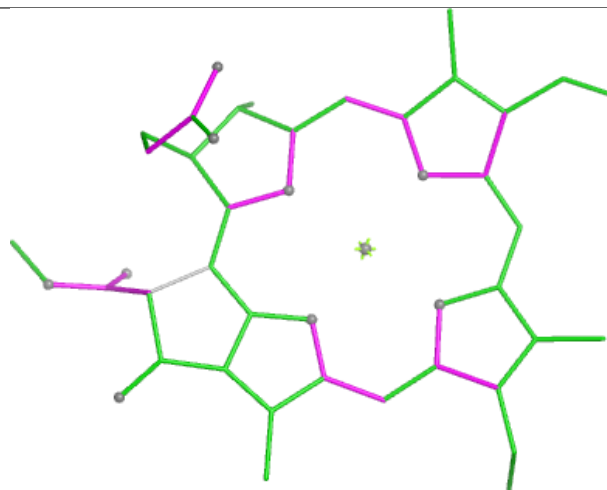


Rings

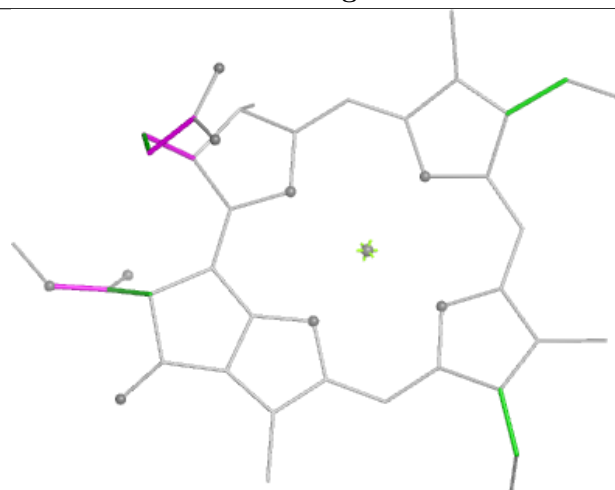
Ligand CLA 6 610



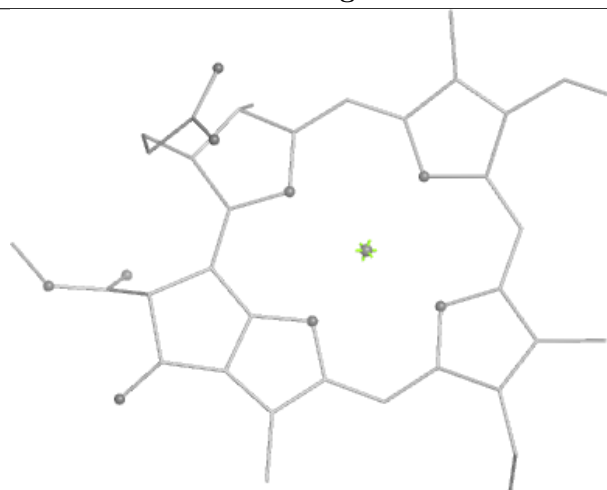
Bond lengths



Bond angles

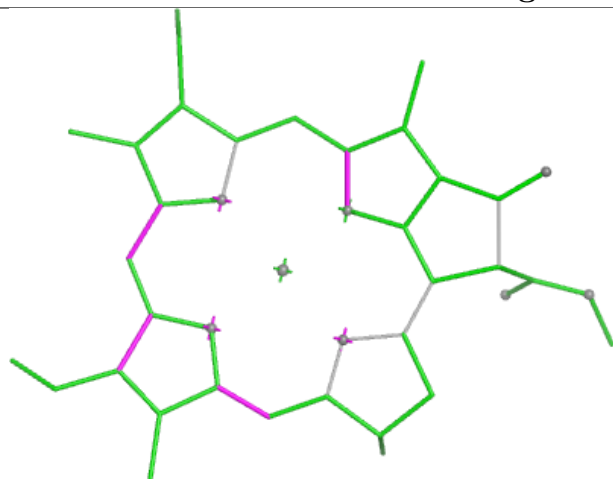


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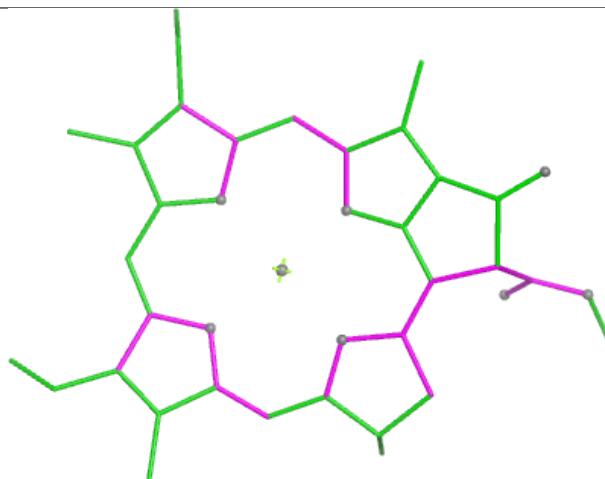


Rings

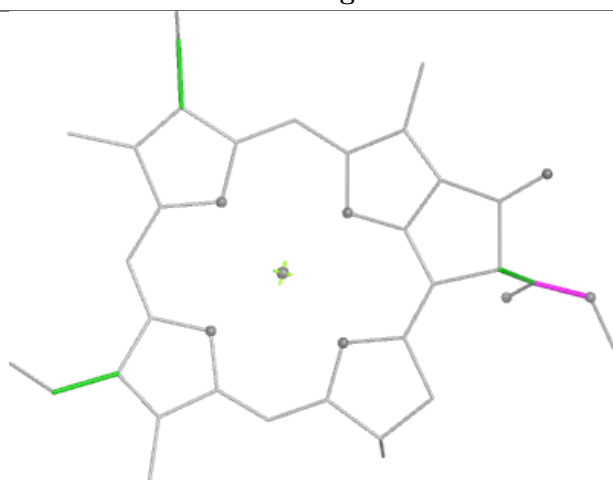
Ligand CLA 5 605



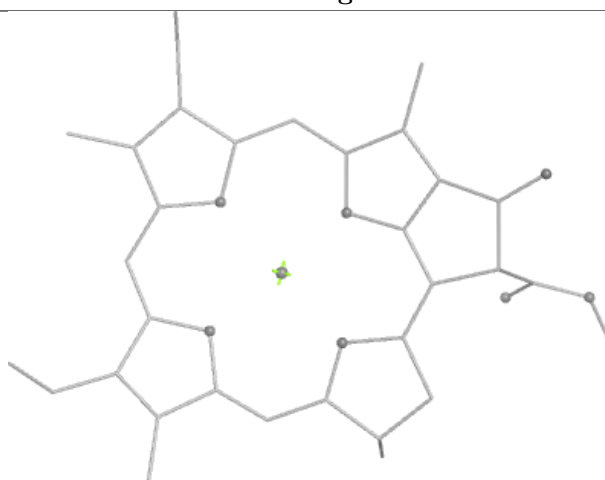
Bond lengths



Bond angles

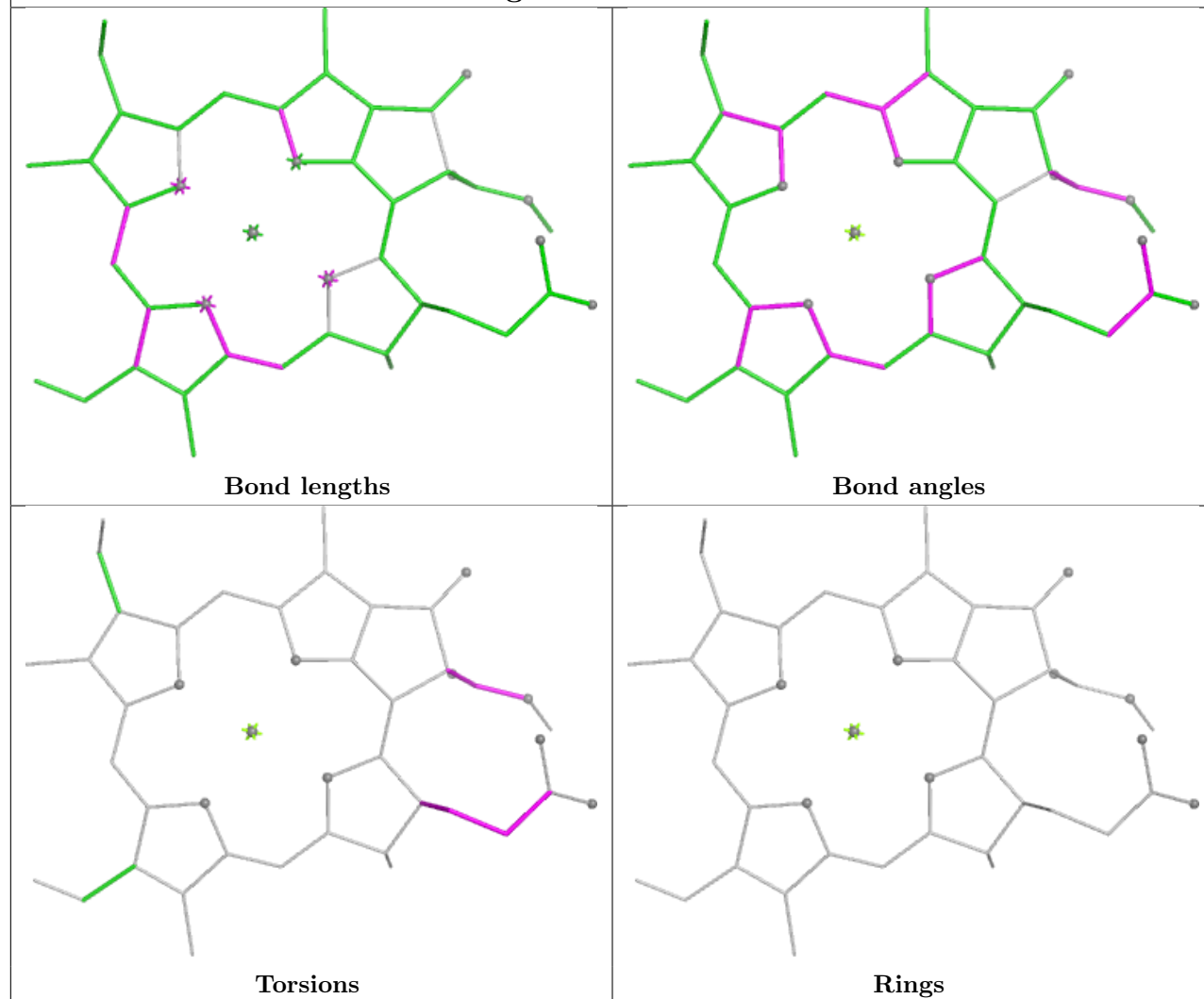


Torsions

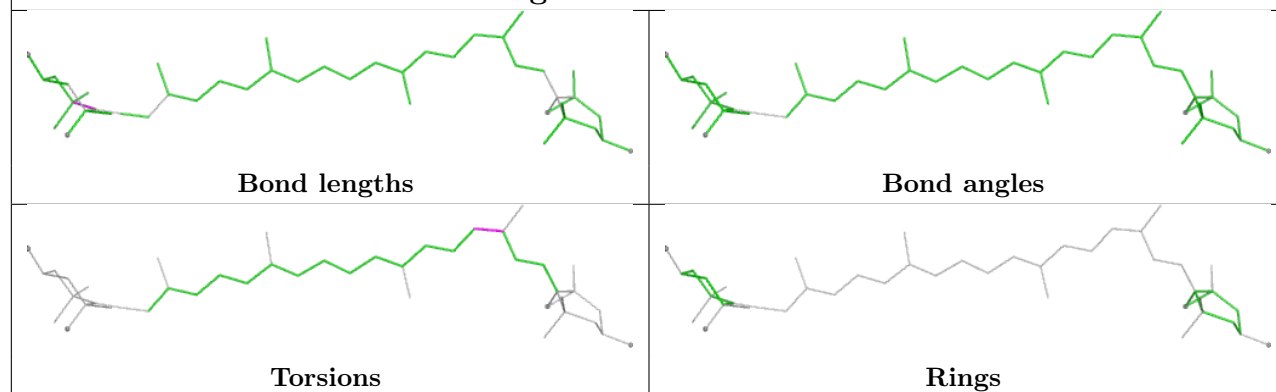


Rings

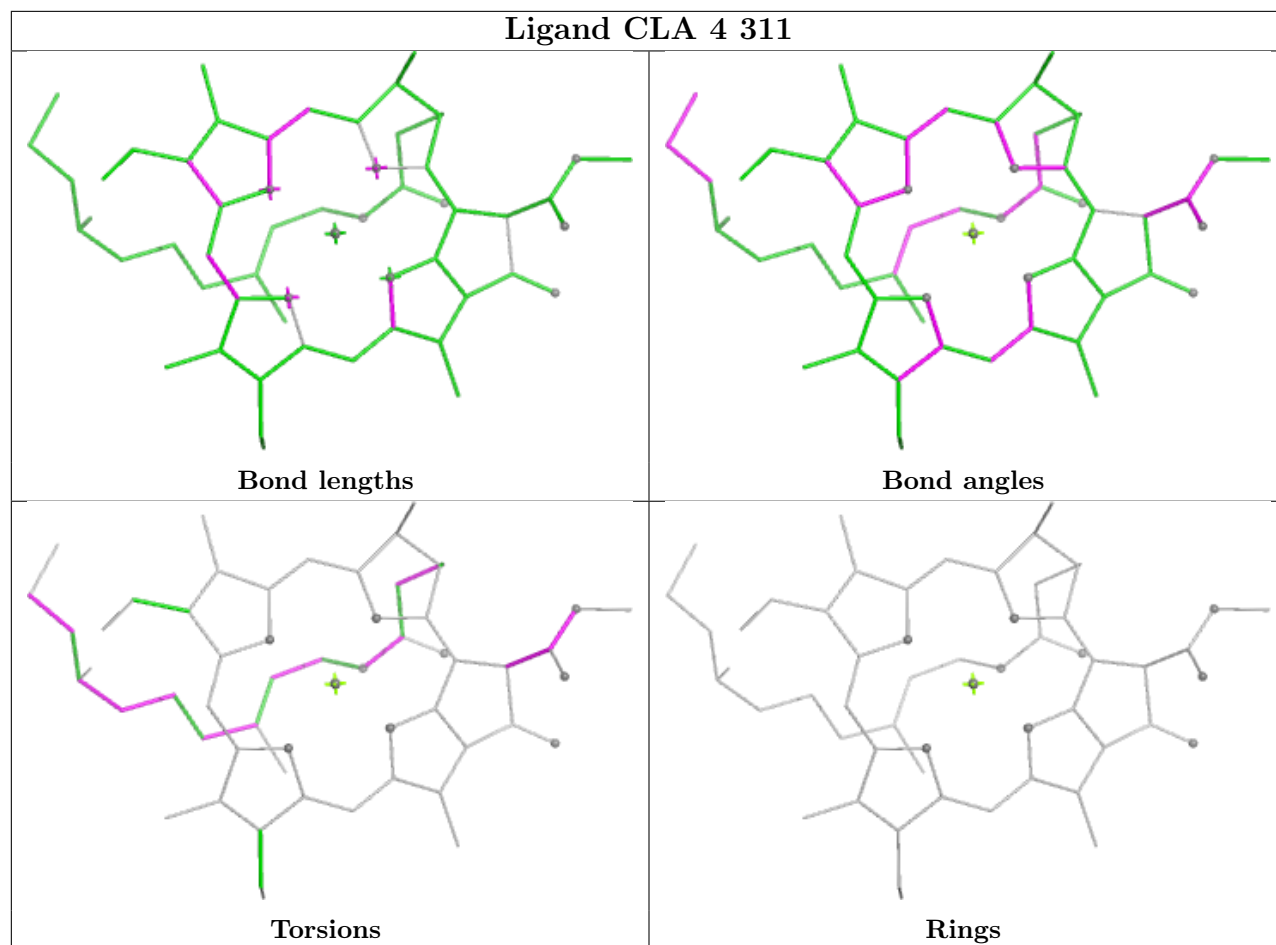
Ligand CLA 1 614



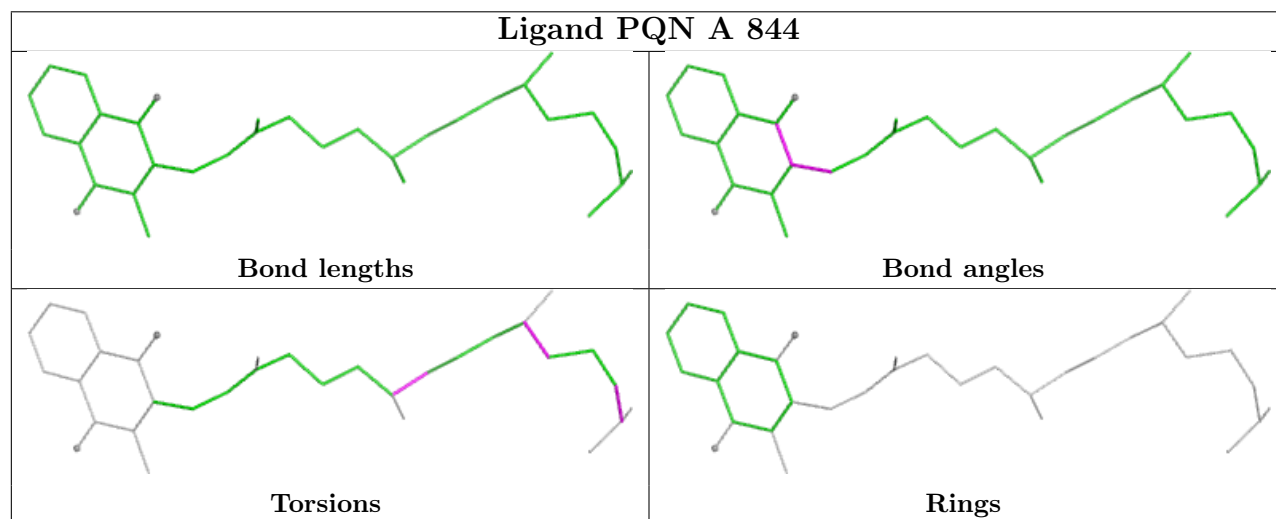
Ligand NEX X 616

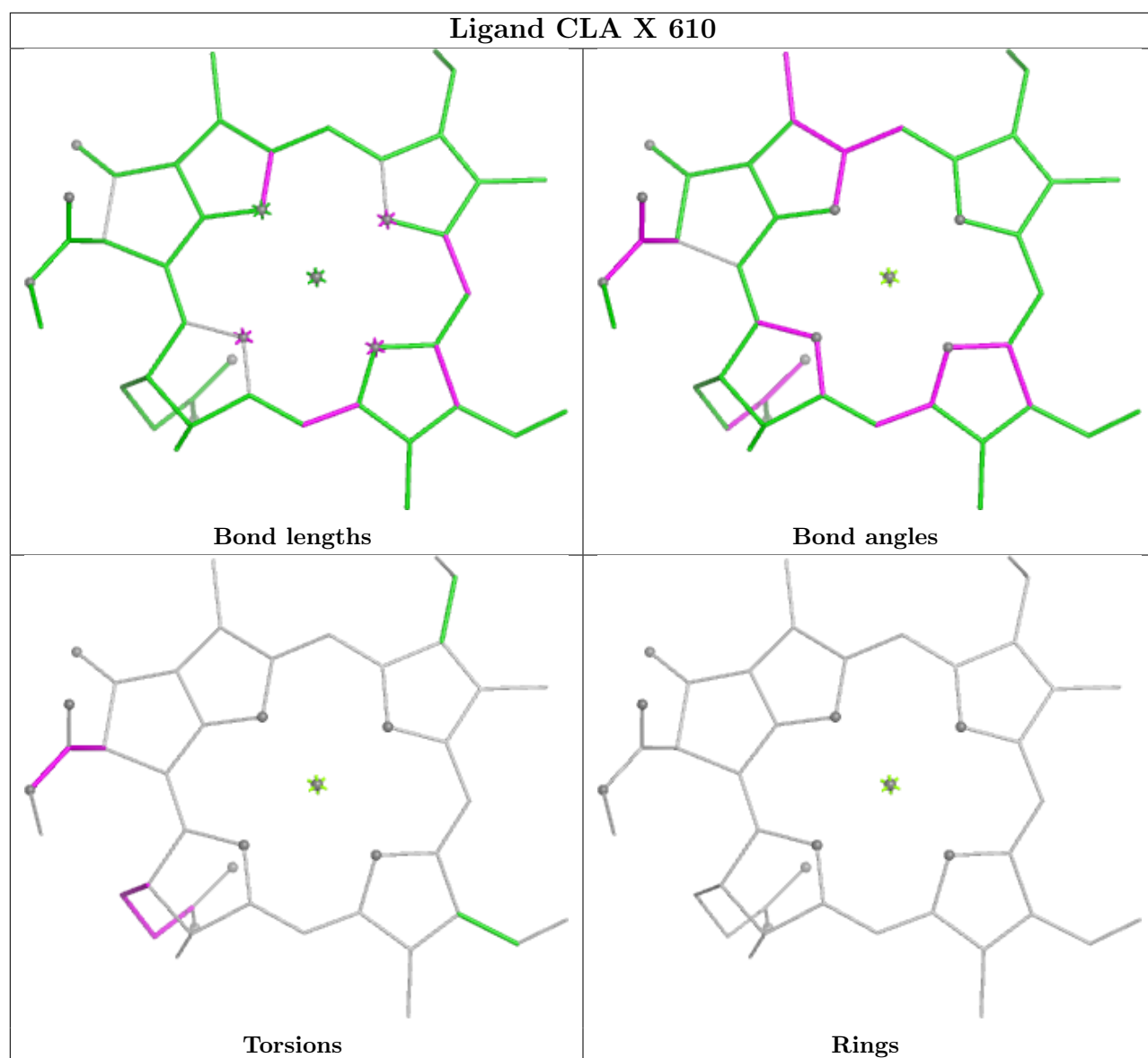


Ligand CLA 4 311

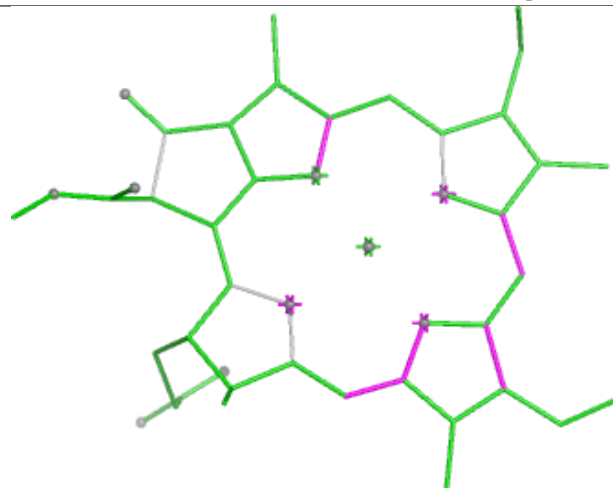


Ligand PQN A 844

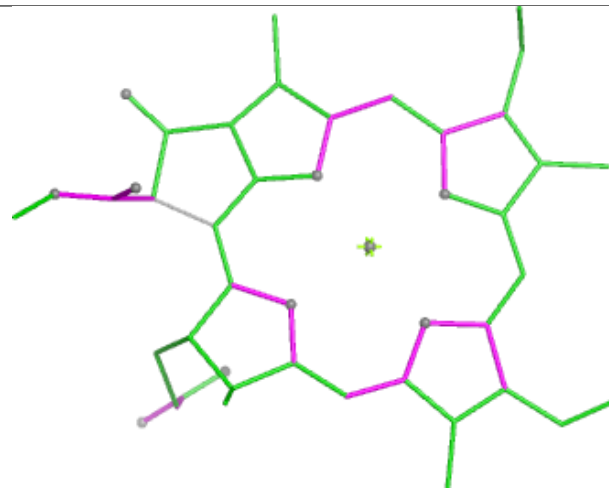




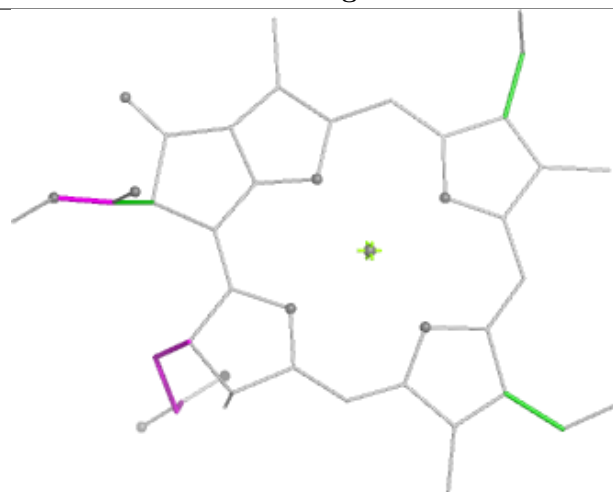
Ligand CLA 3 607



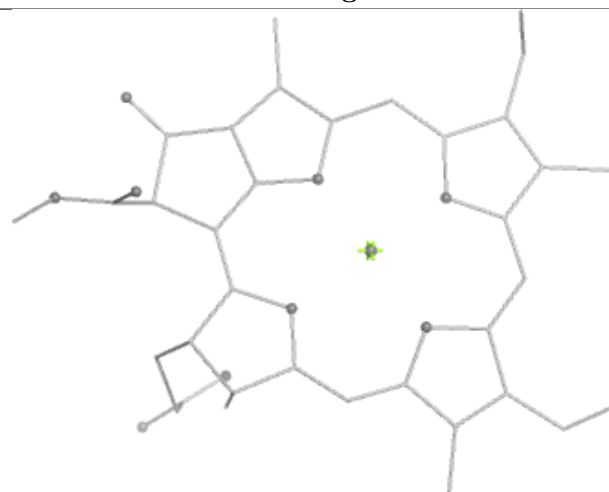
Bond lengths



Bond angles

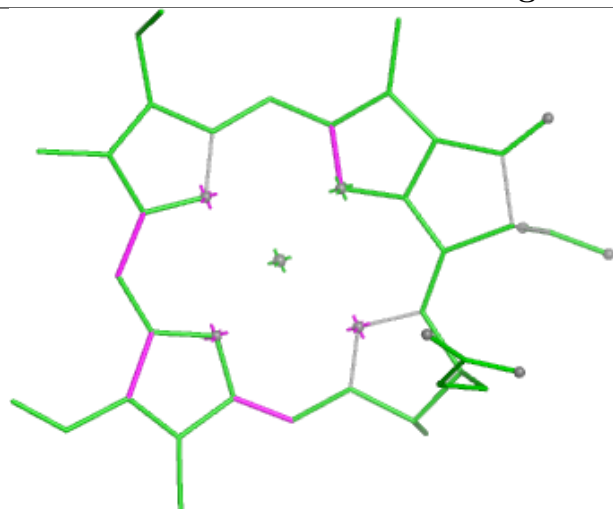


Torsions

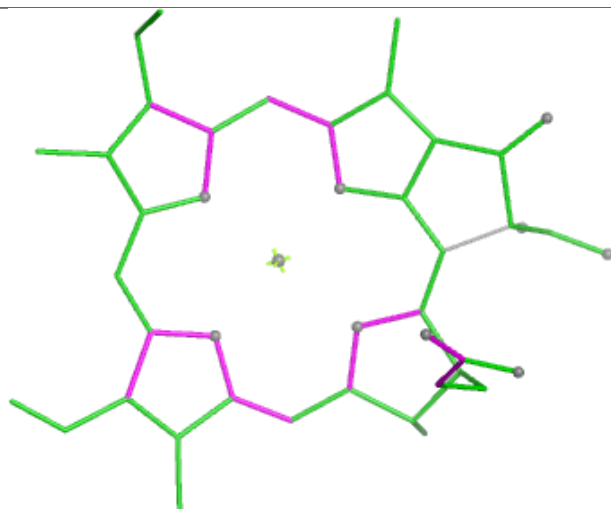


Rings

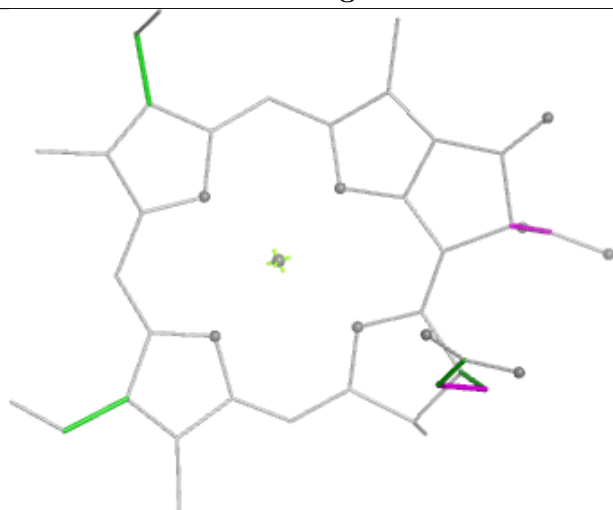
Ligand CLA 5 607



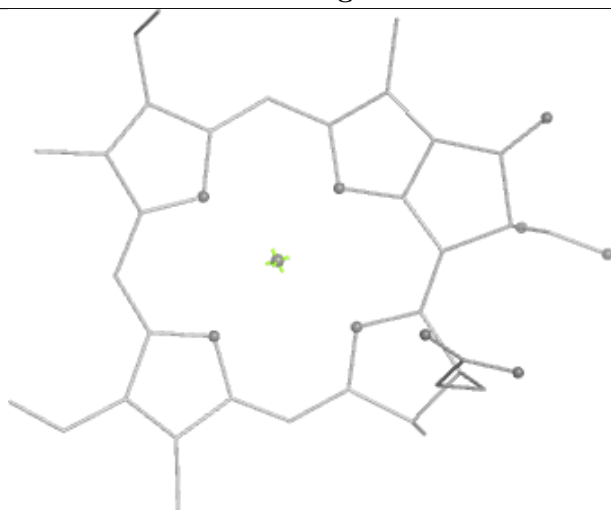
Bond lengths



Bond angles

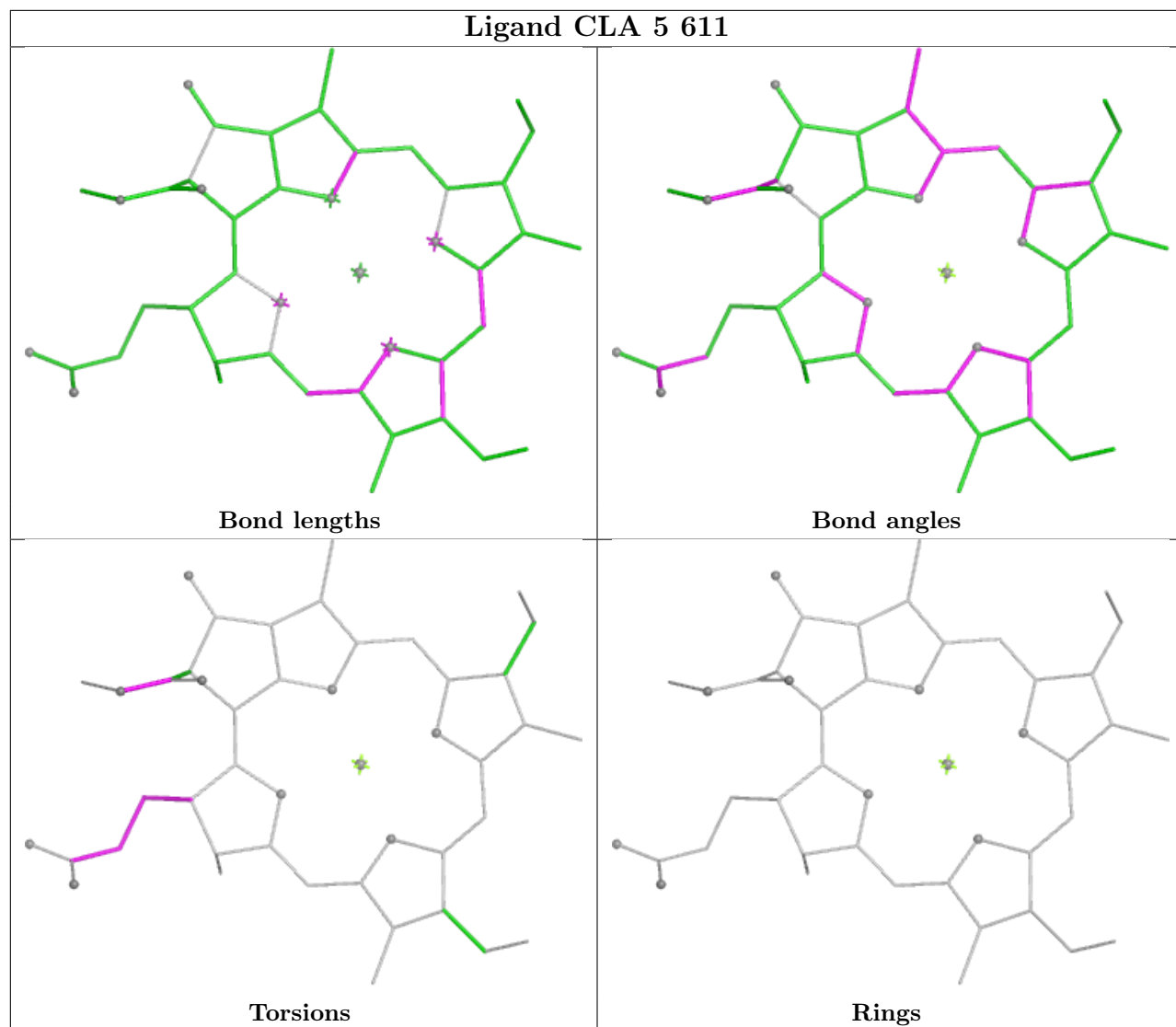


Torsions

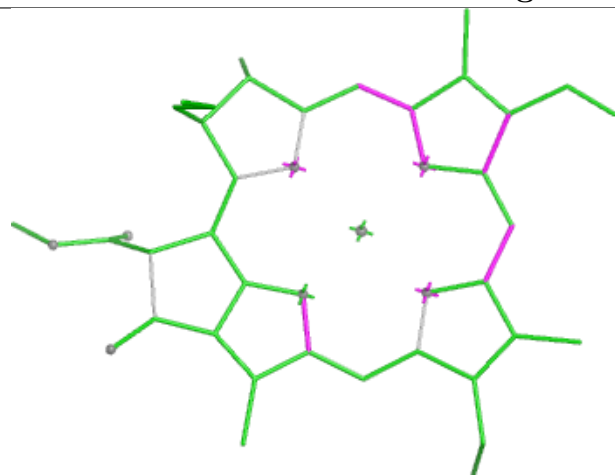


Rings

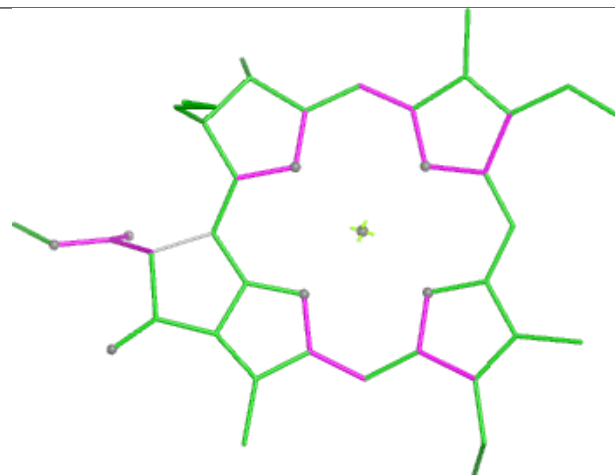
Ligand CLA 5 611



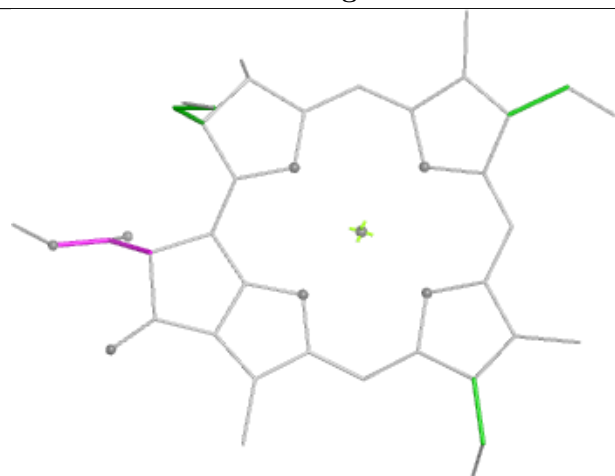
Ligand CLA B 830



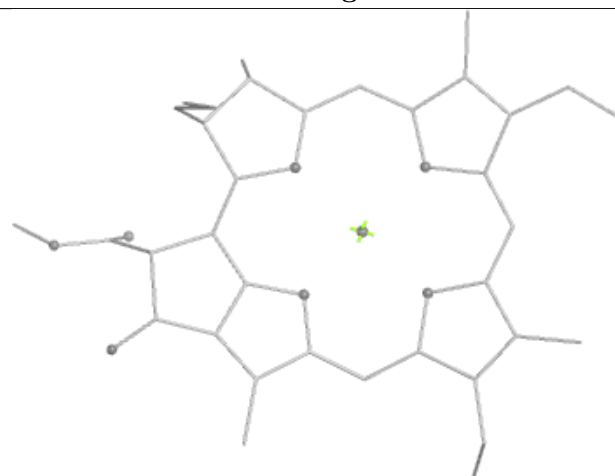
Bond lengths



Bond angles

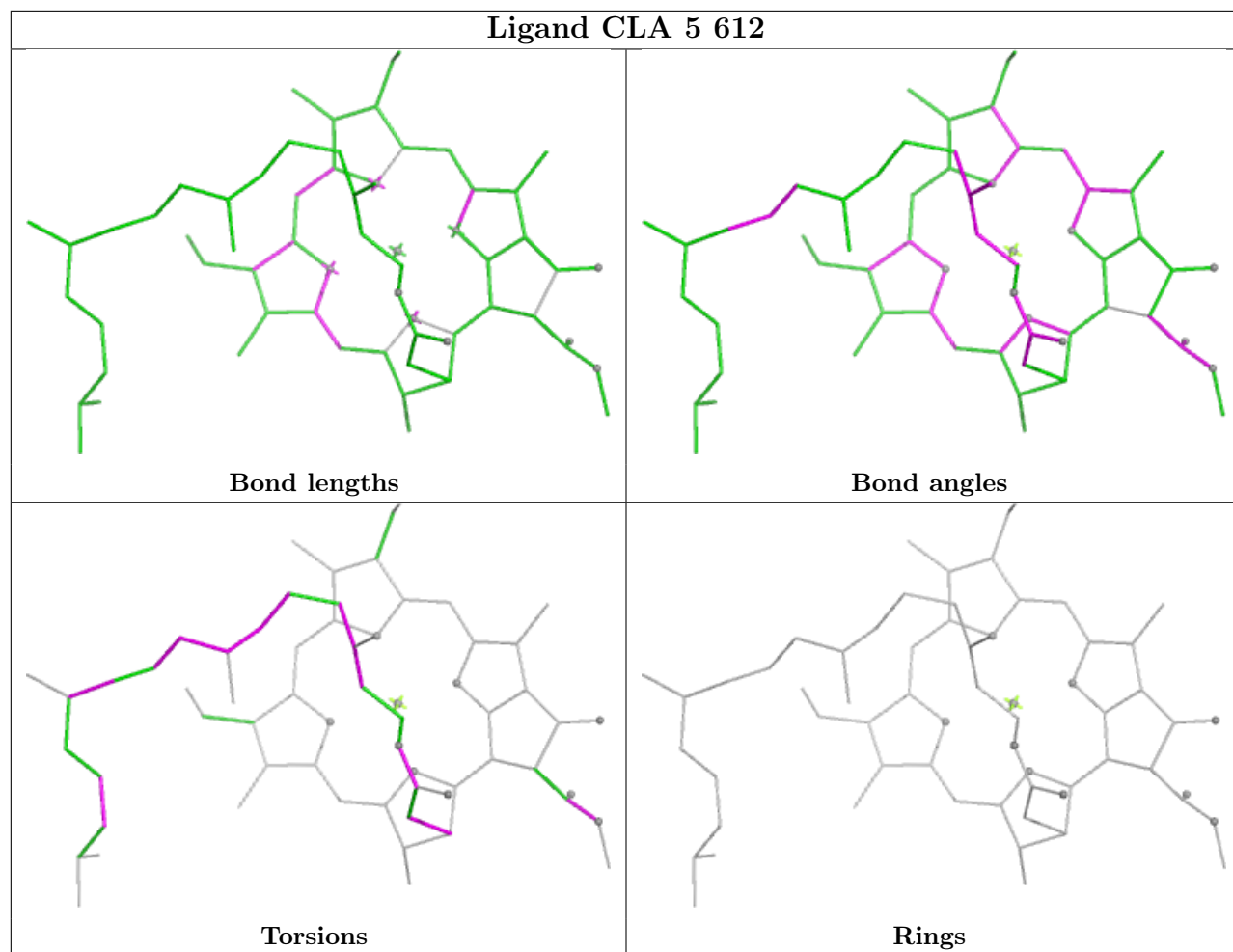


Torsions

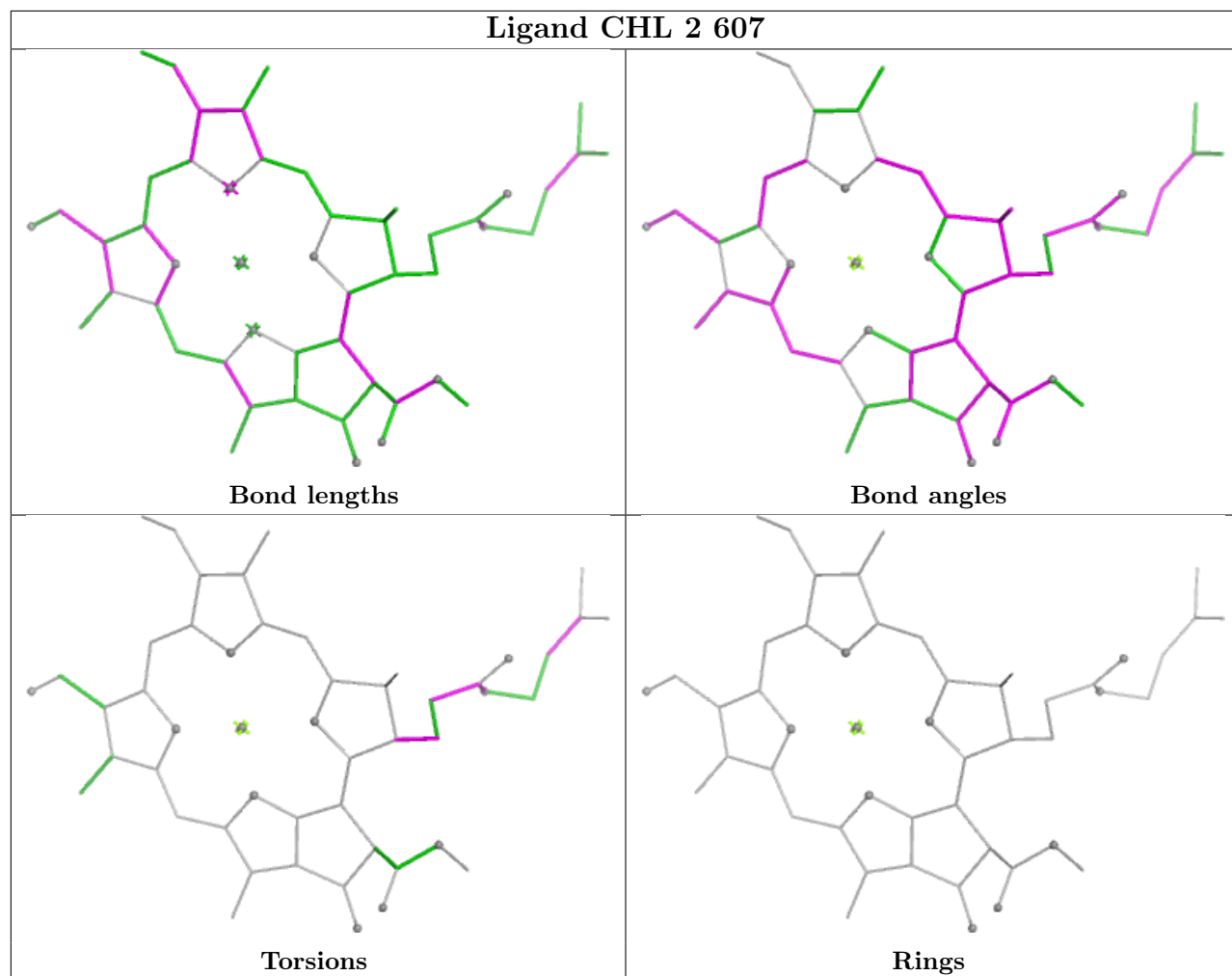


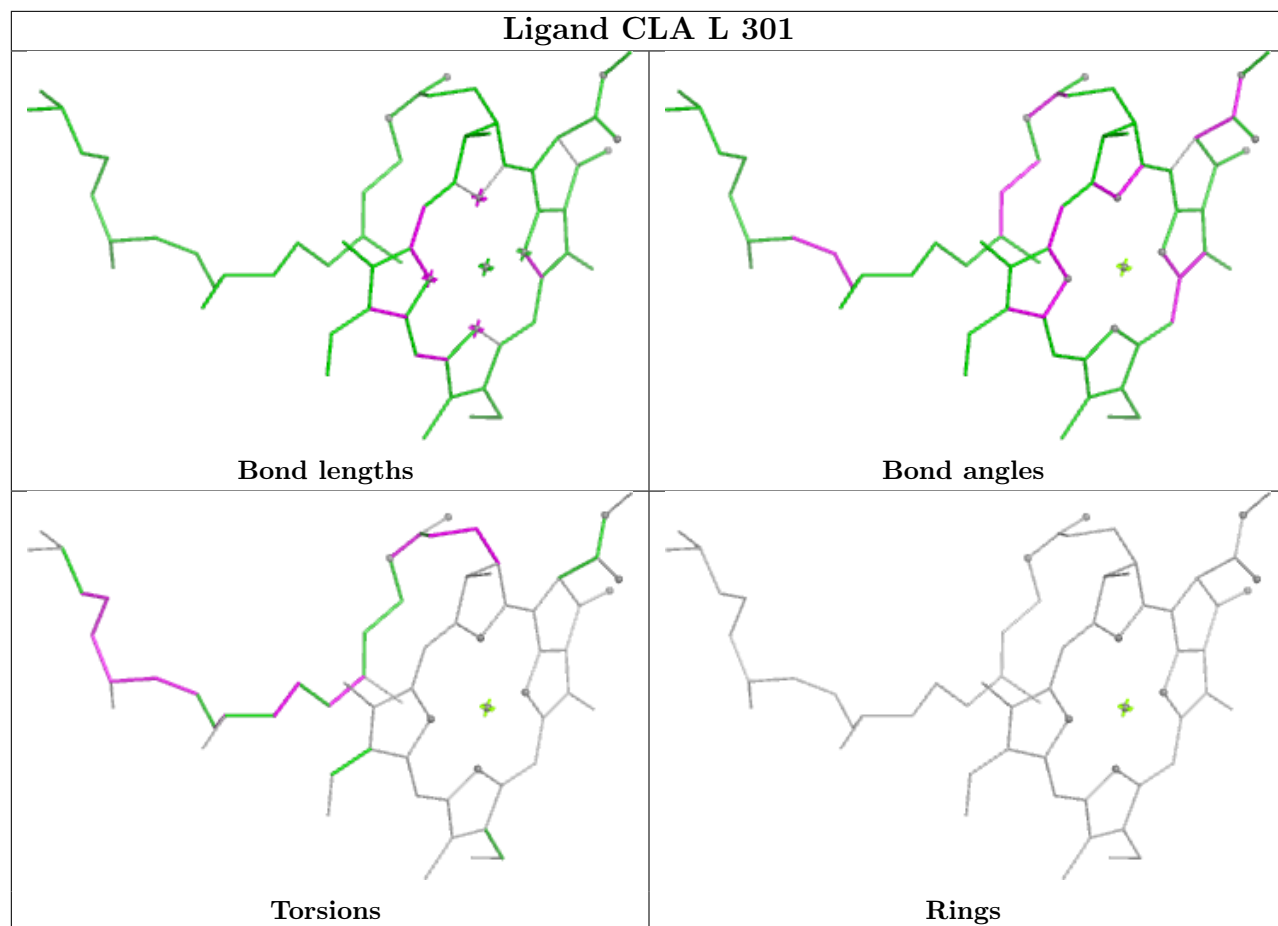
Rings

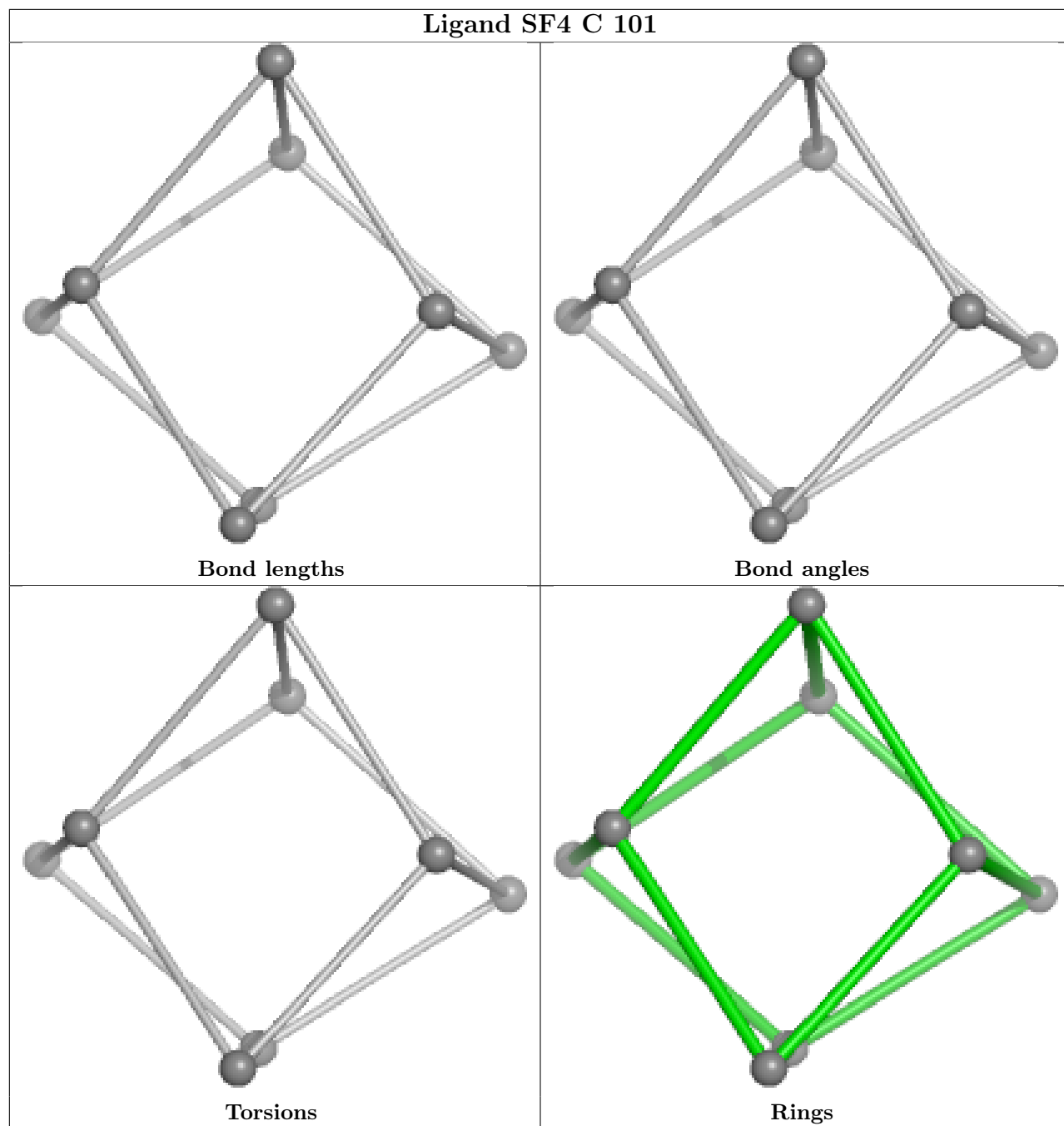
Ligand CLA 5 612



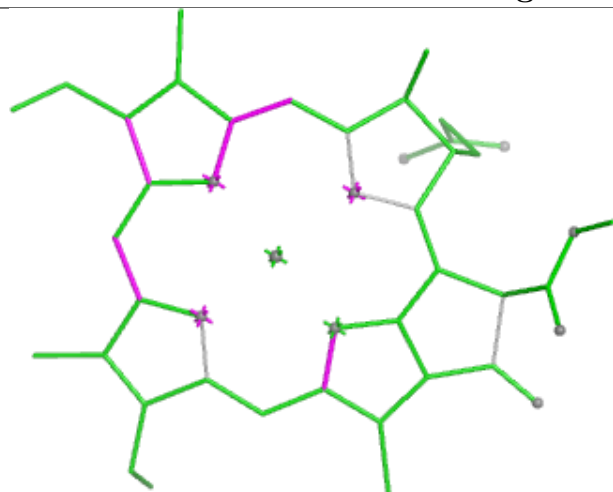
Ligand CHL 2 607



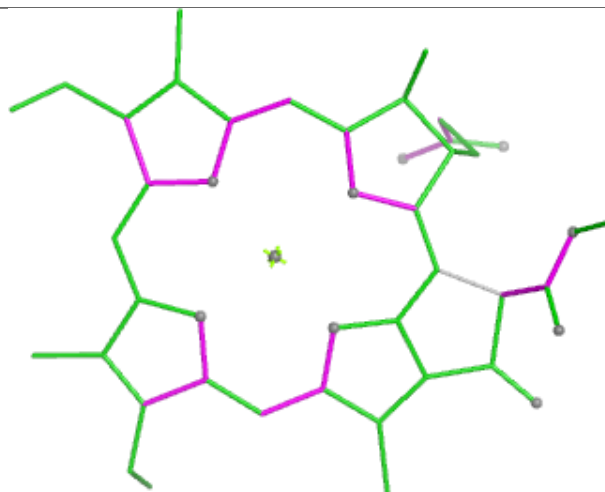




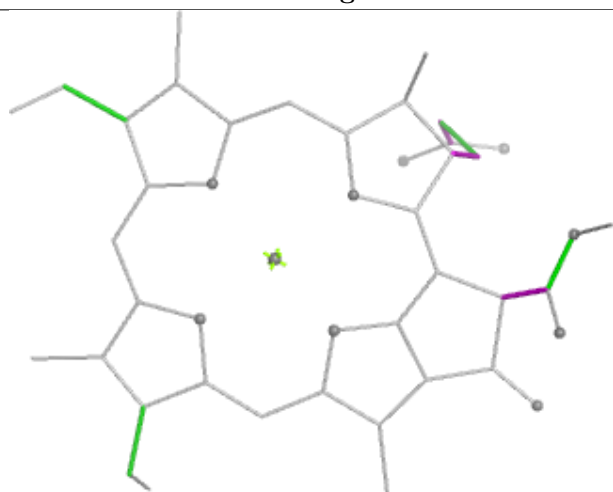
Ligand CLA L 303



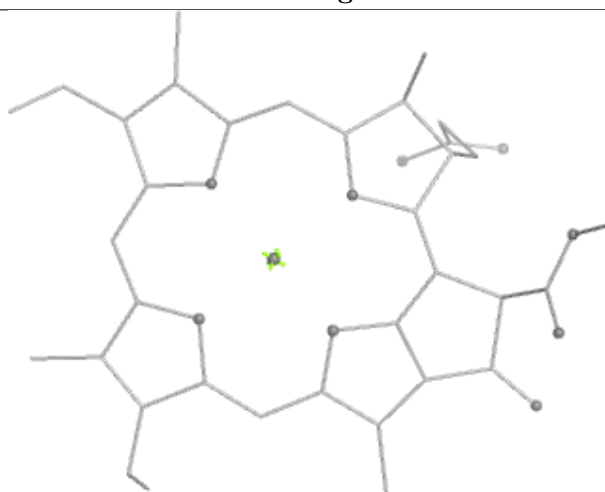
Bond lengths



Bond angles

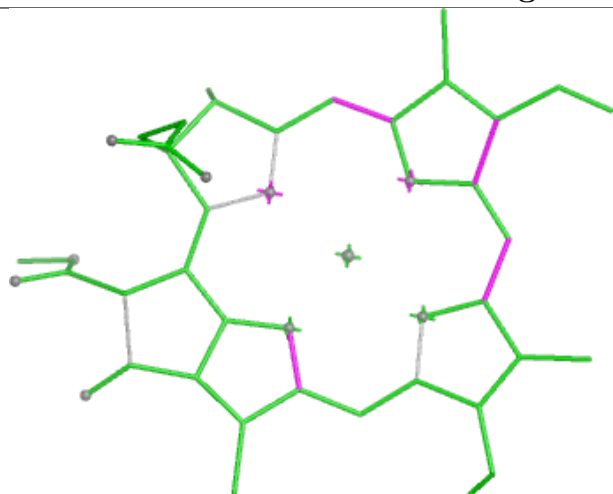


Torsions

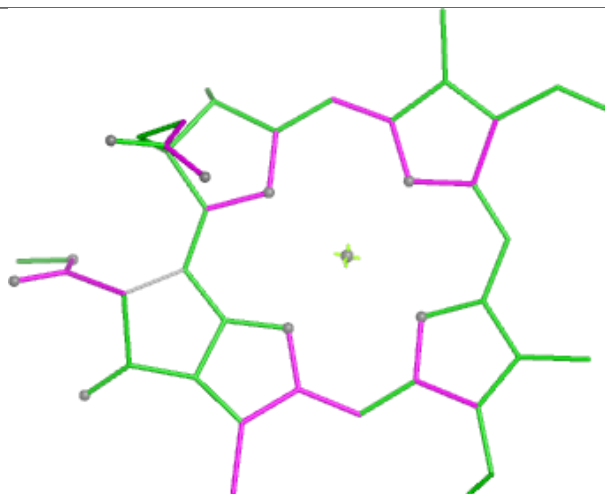


Rings

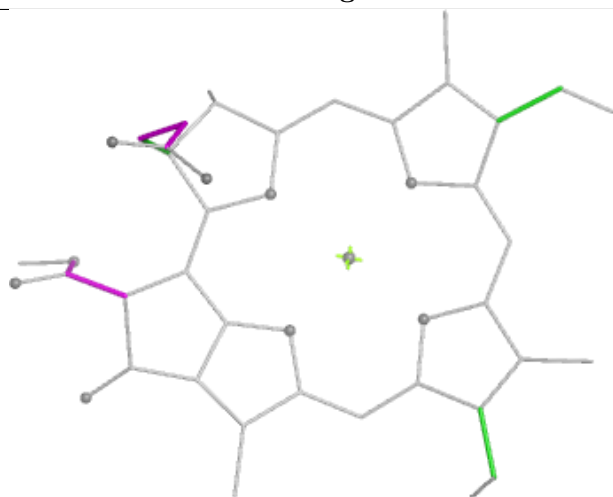
Ligand CLA 1 613



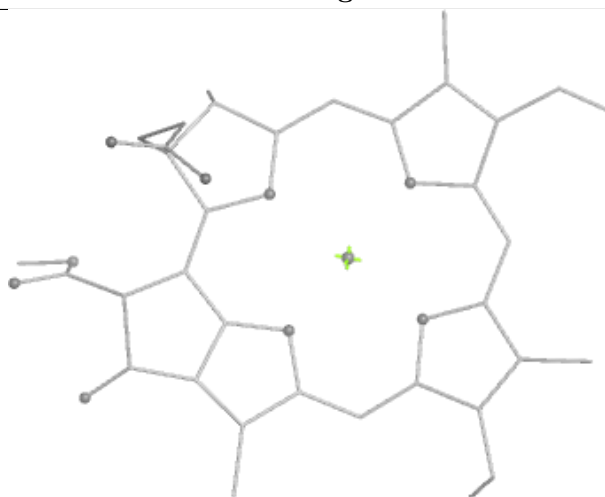
Bond lengths



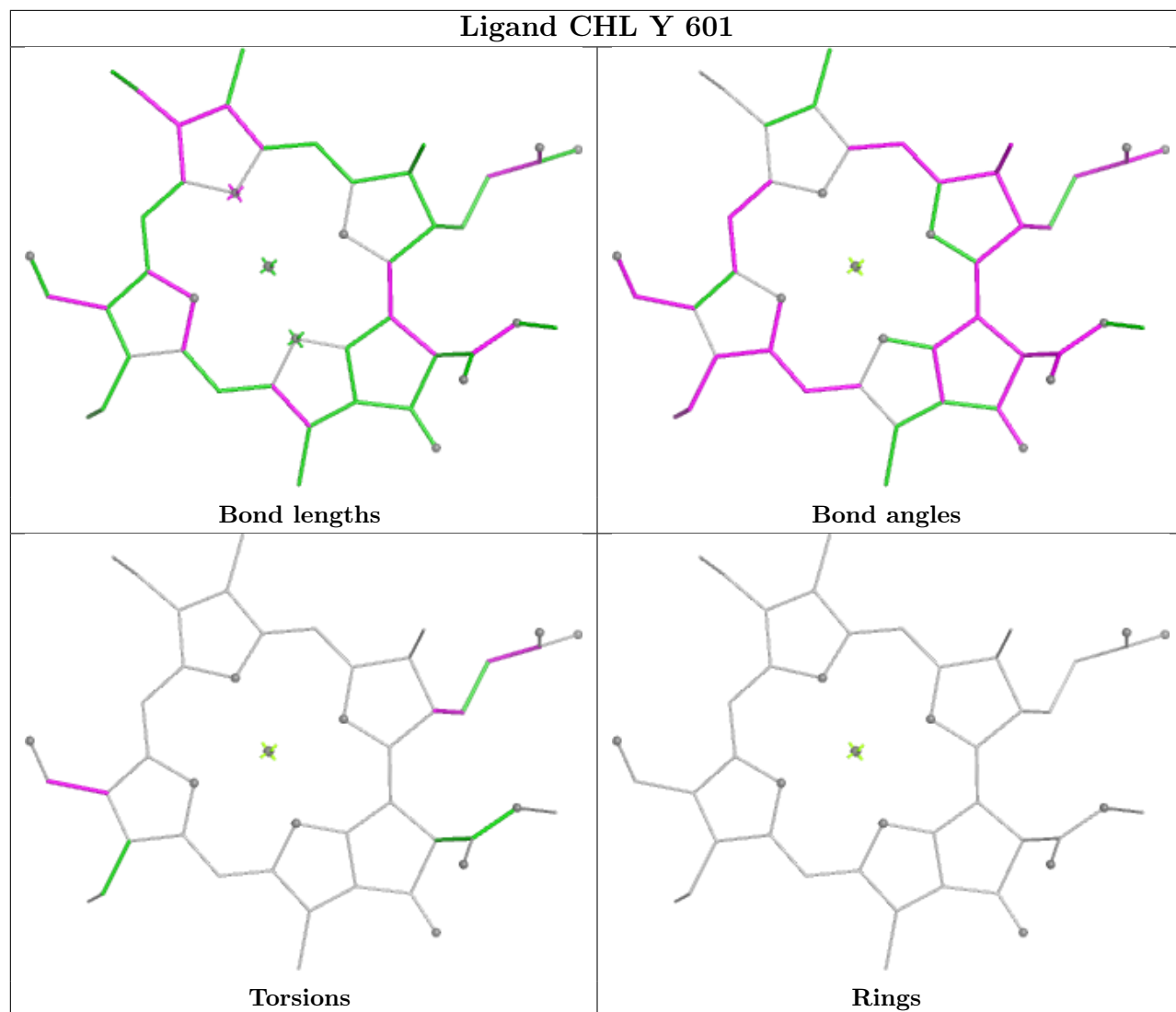
Bond angles



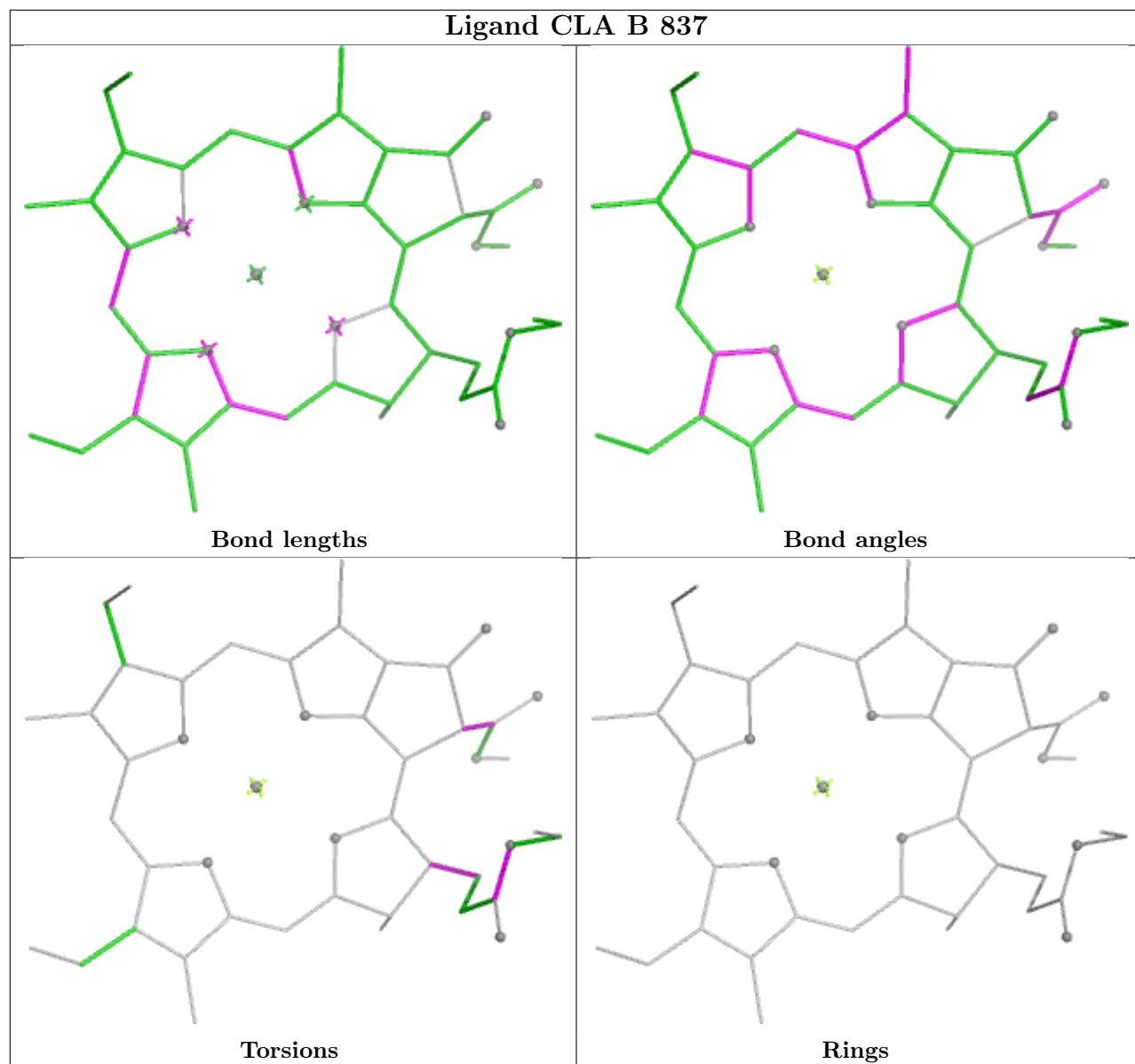
Torsions



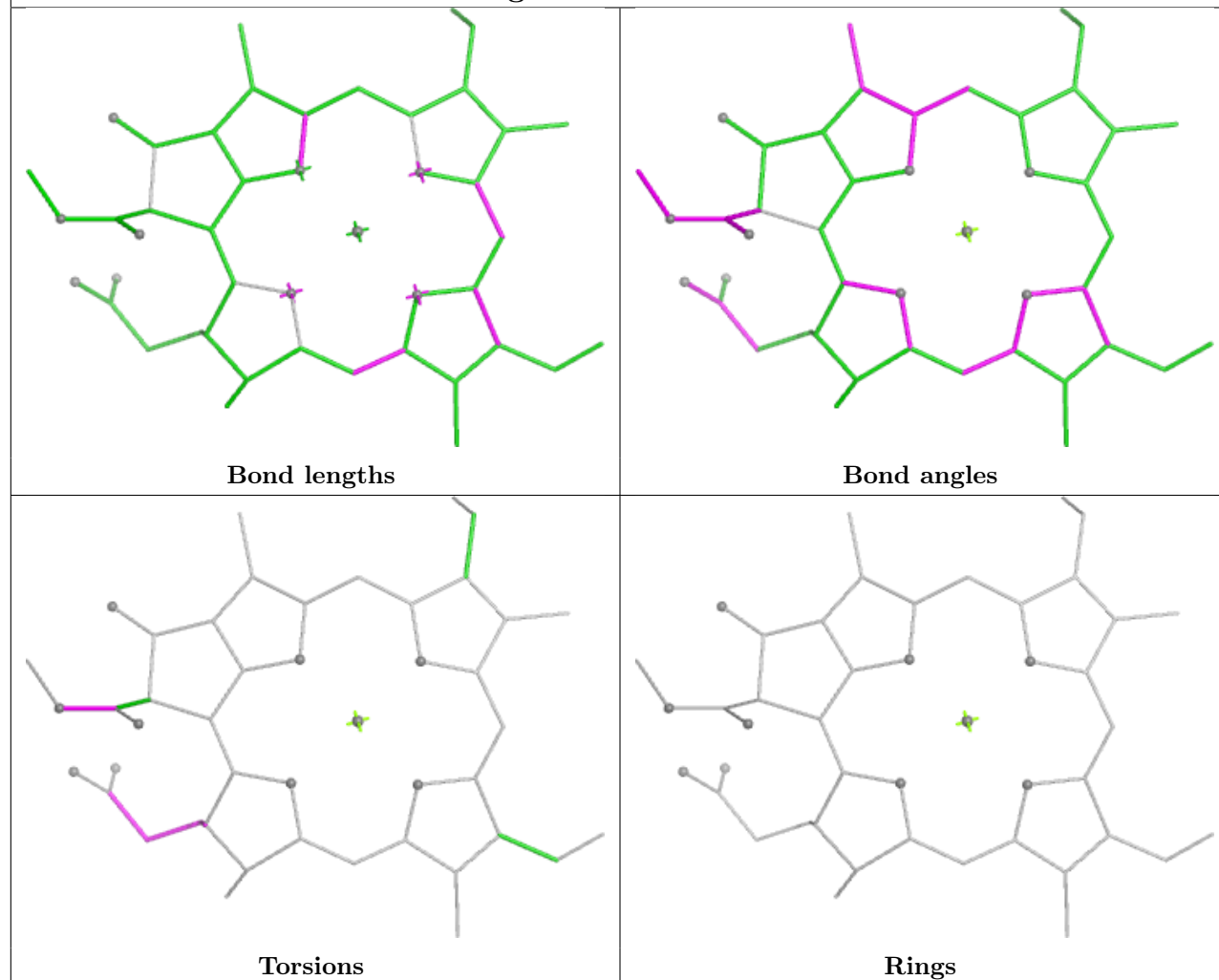
Rings



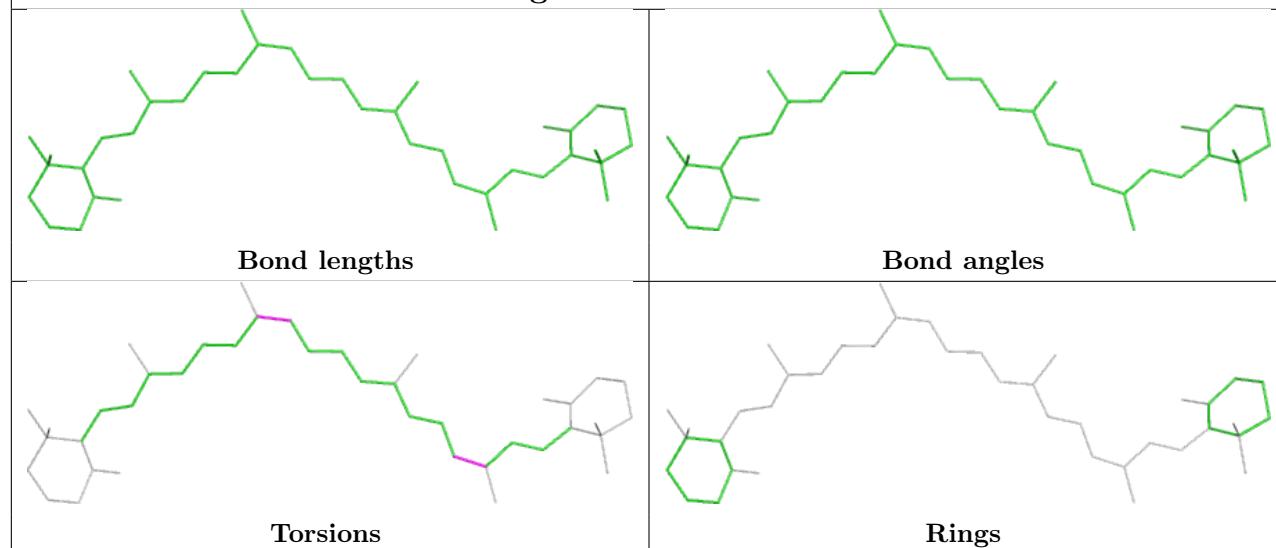
Ligand CLA B 837

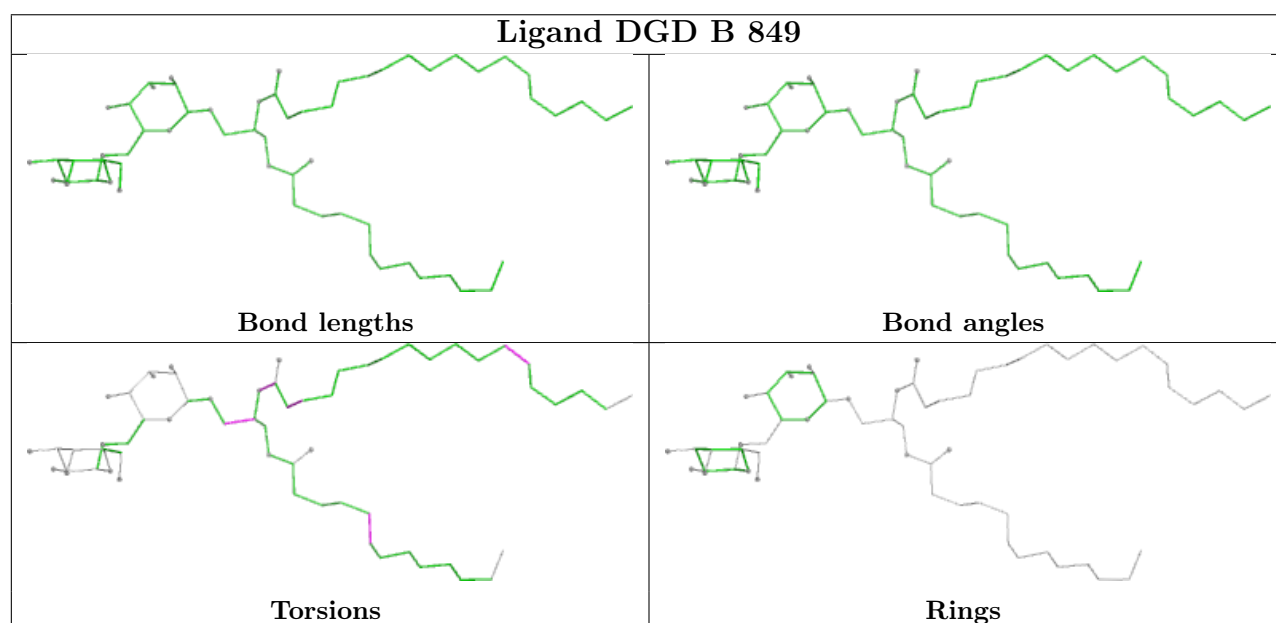
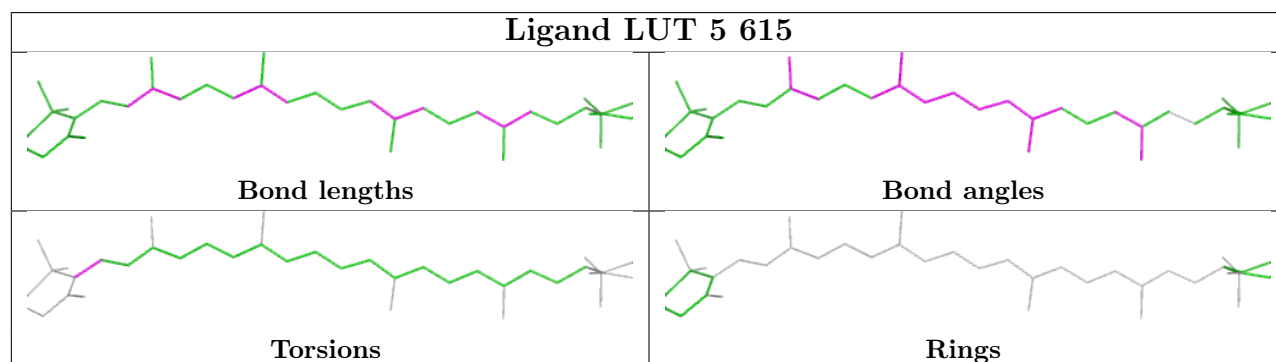
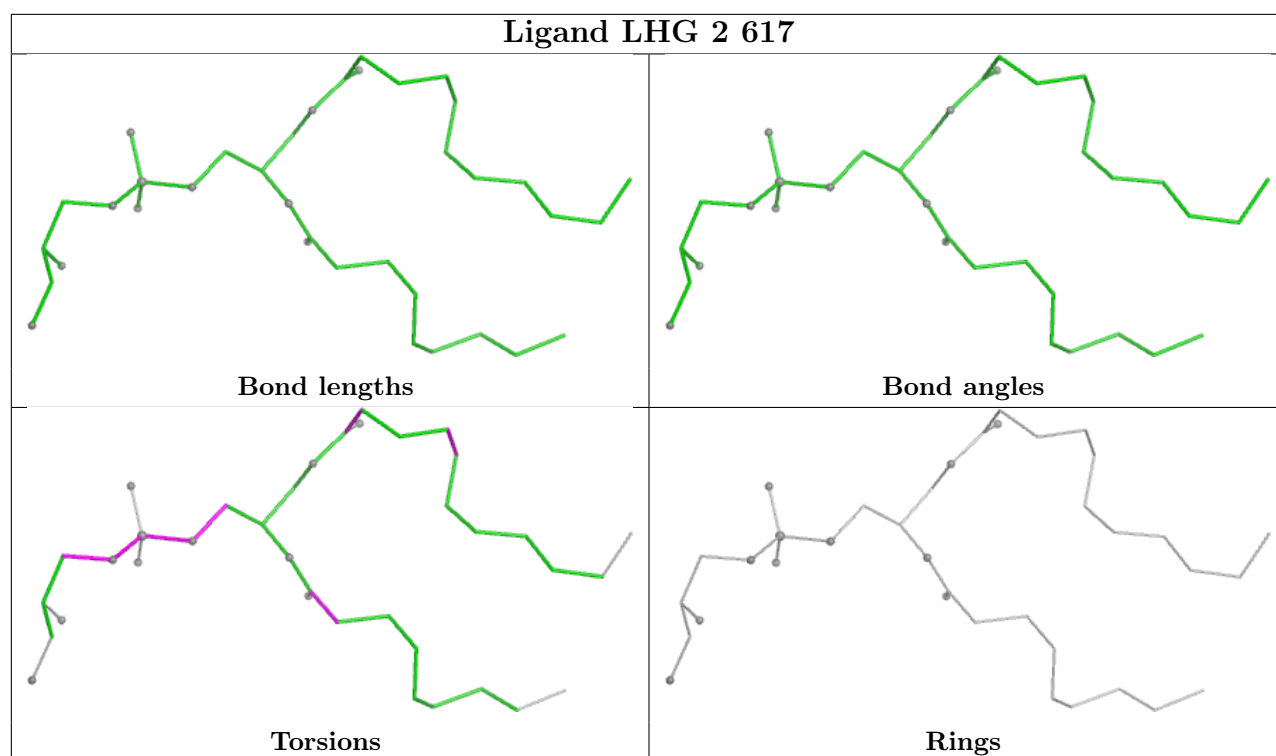


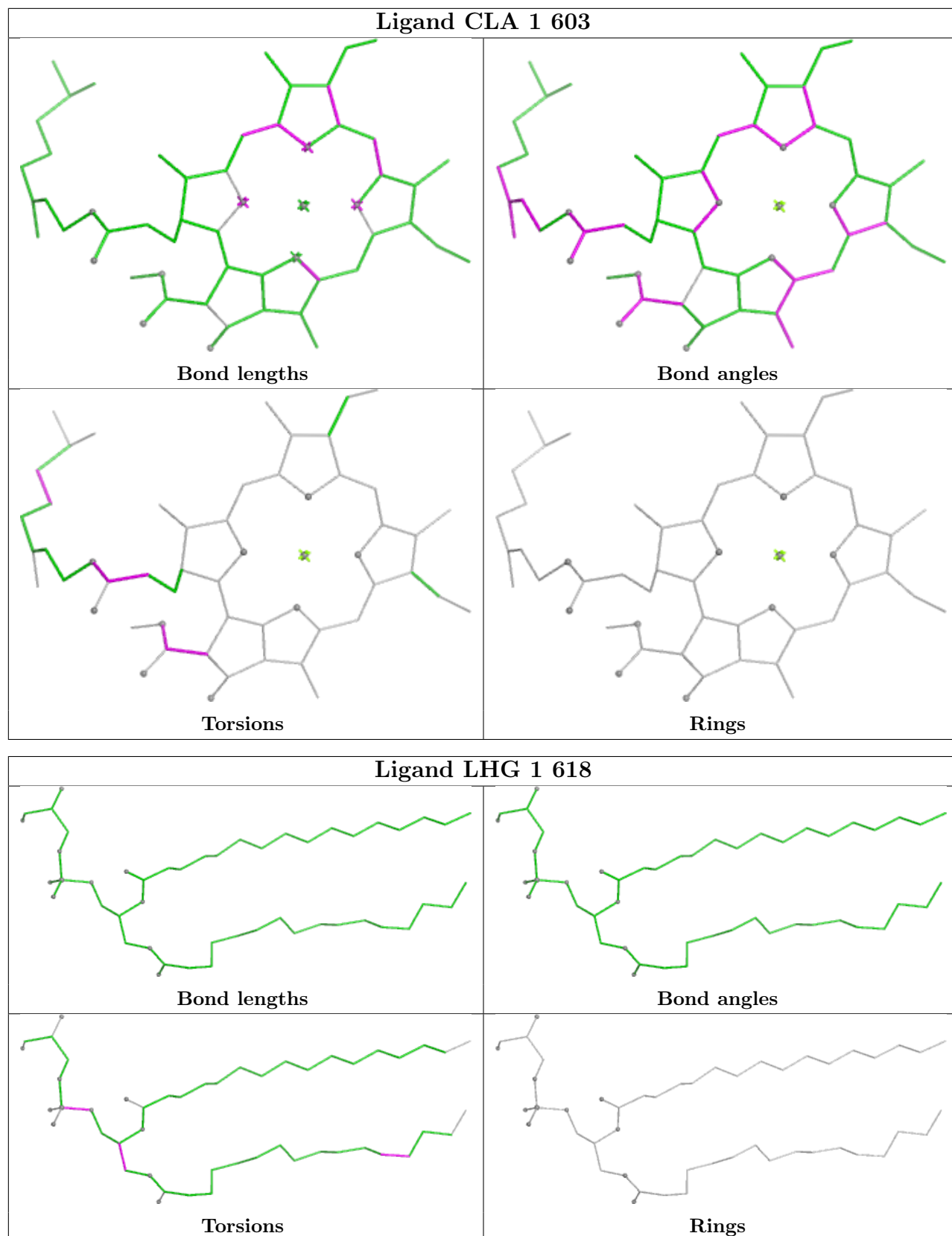
Ligand CLA X 618

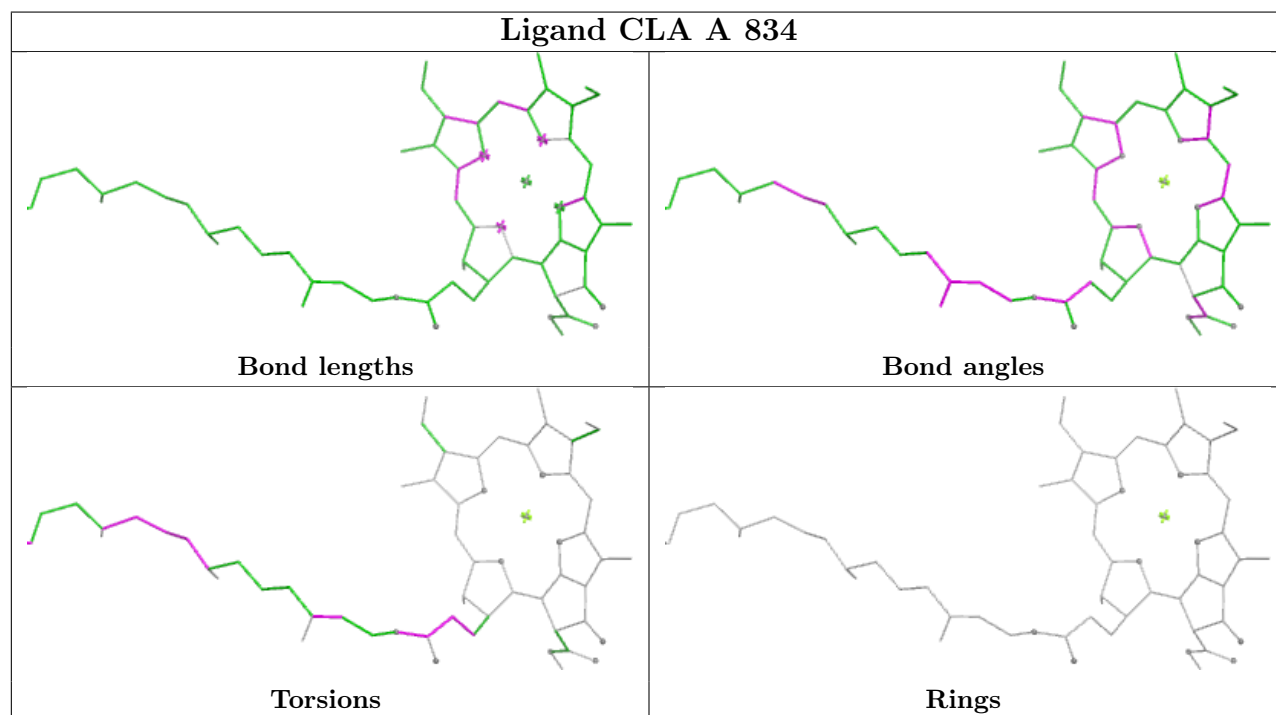
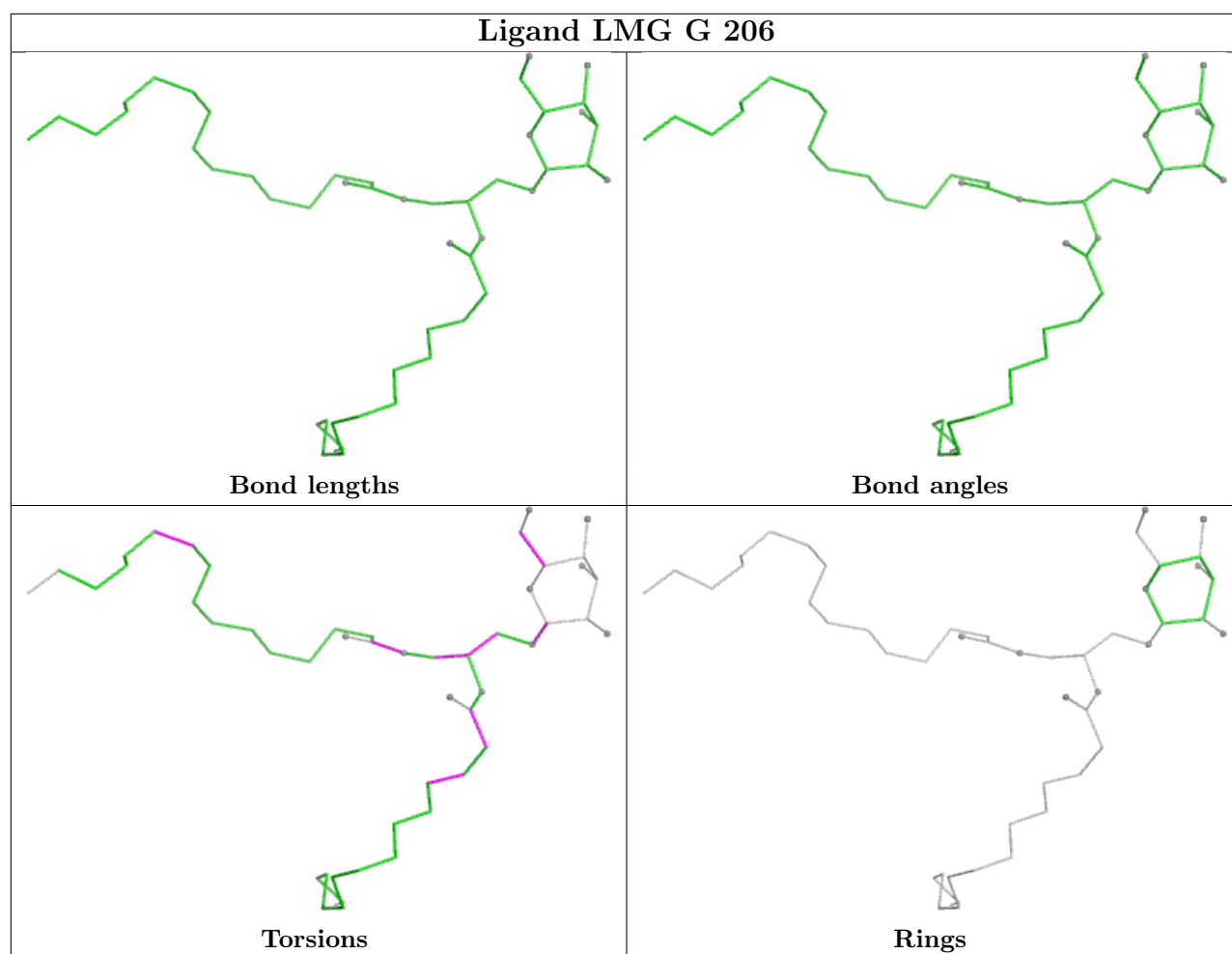


Ligand BCR A 848

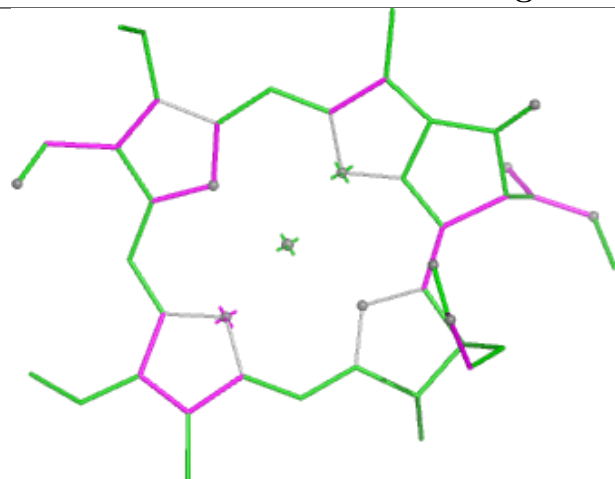




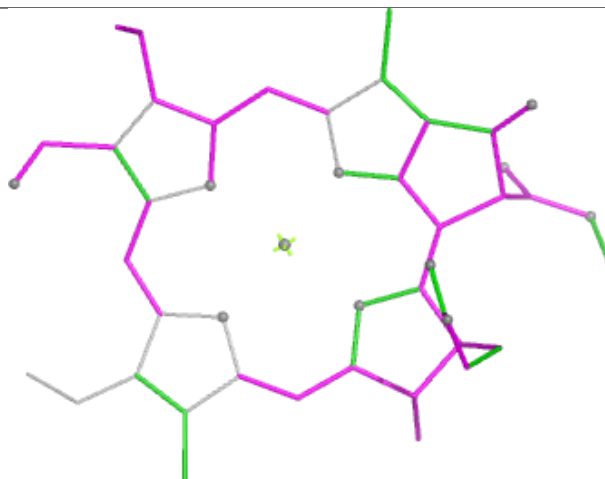




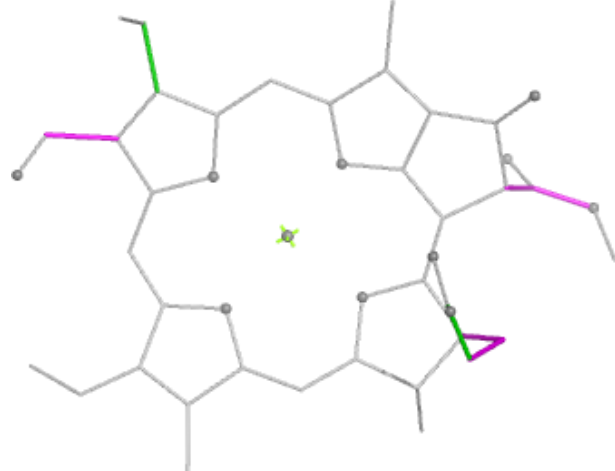
Ligand CHL Y 608



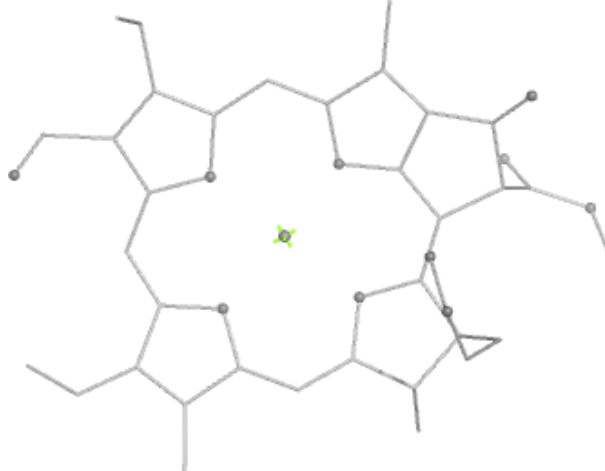
Bond lengths



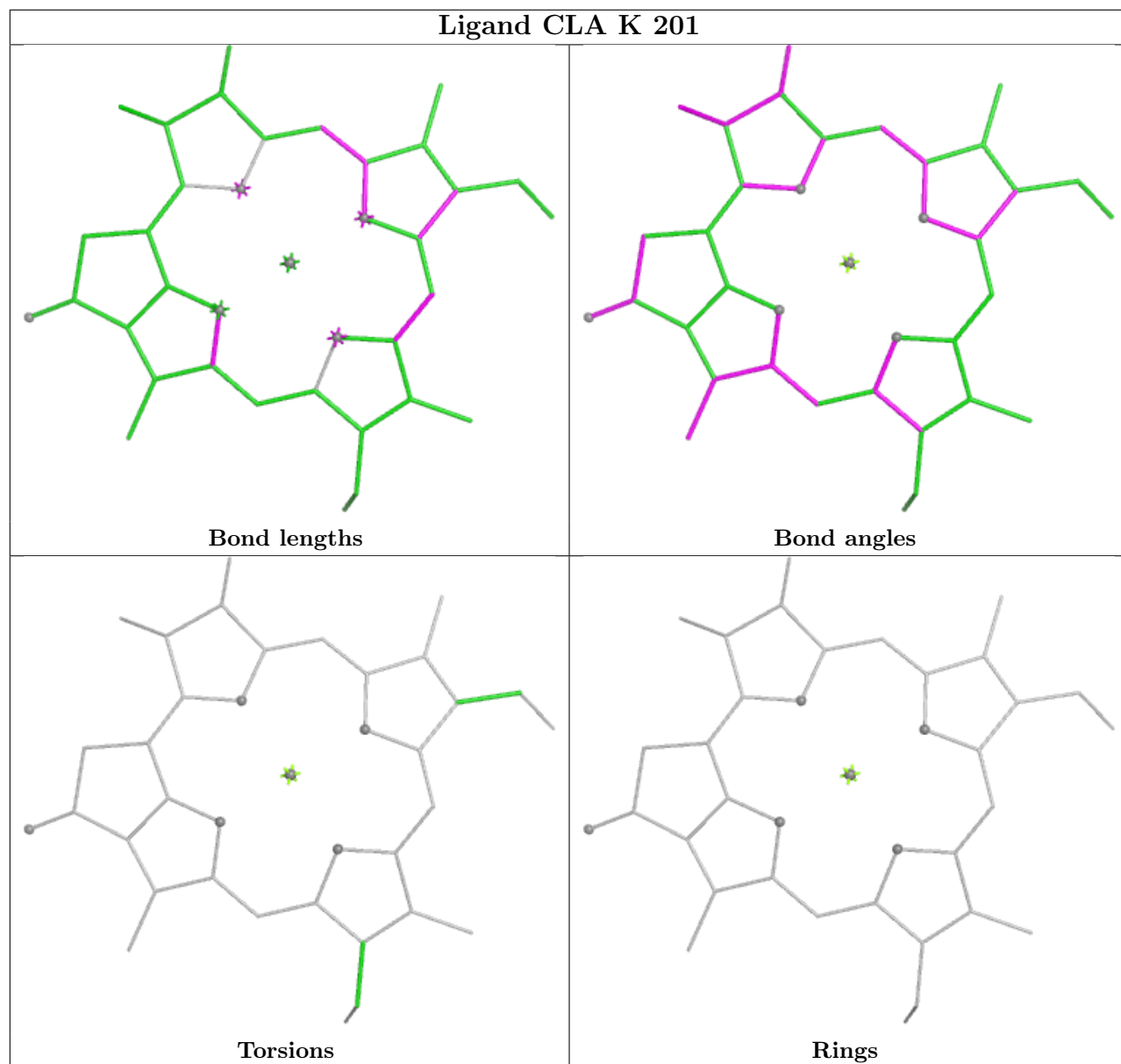
Bond angles



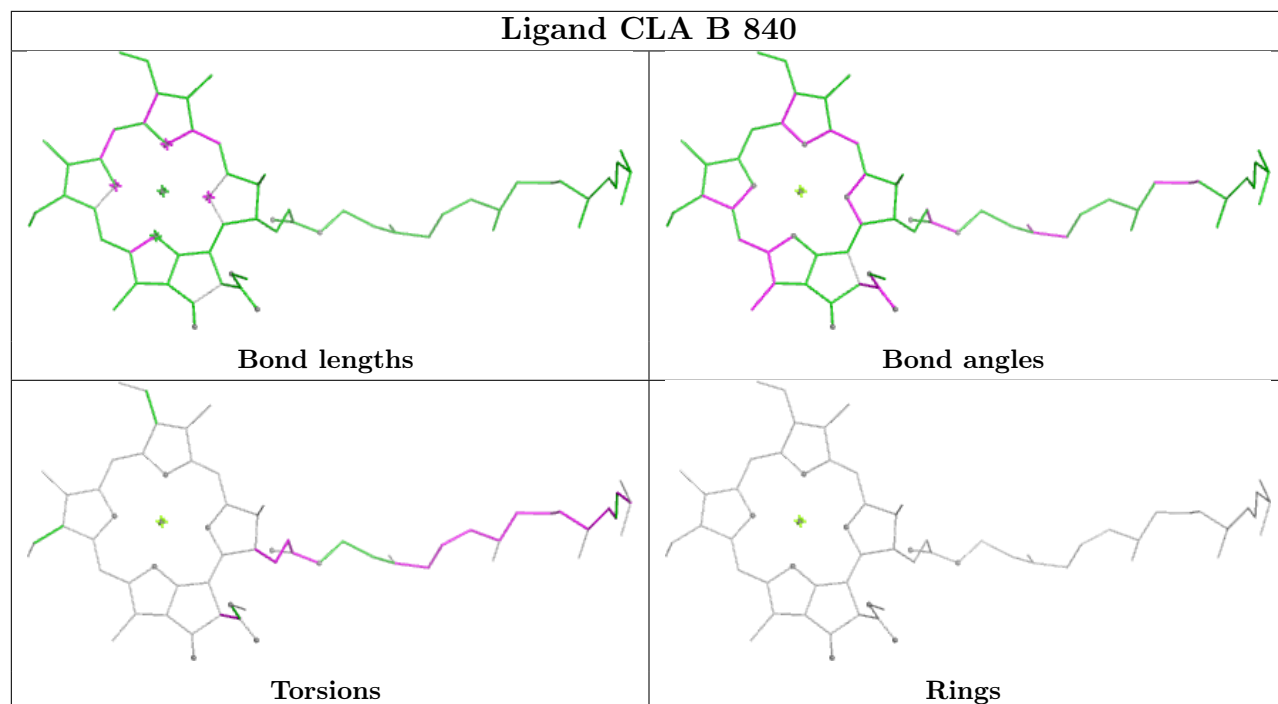
Torsions



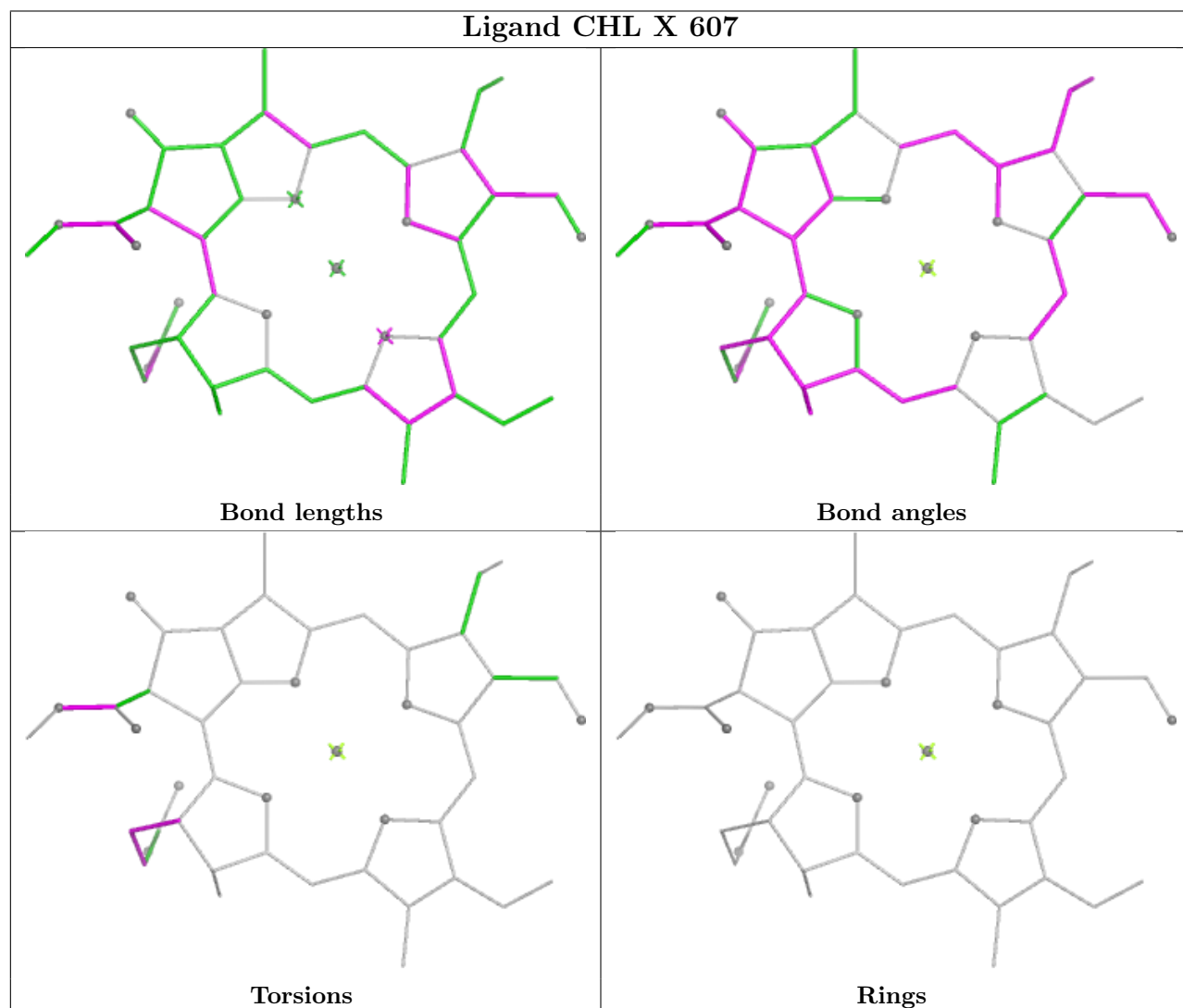
Rings



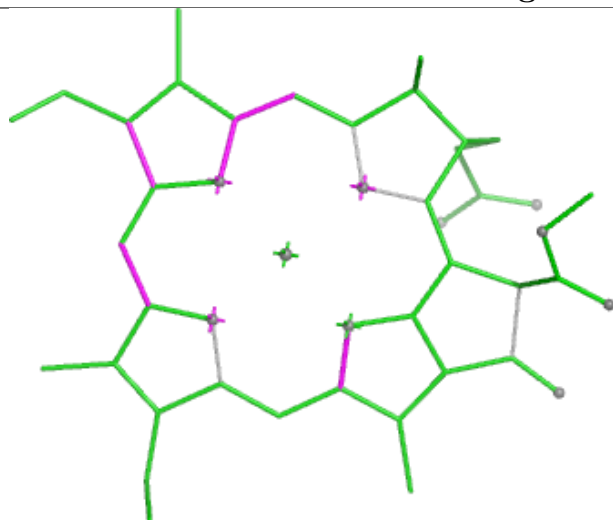
Ligand CLA B 840



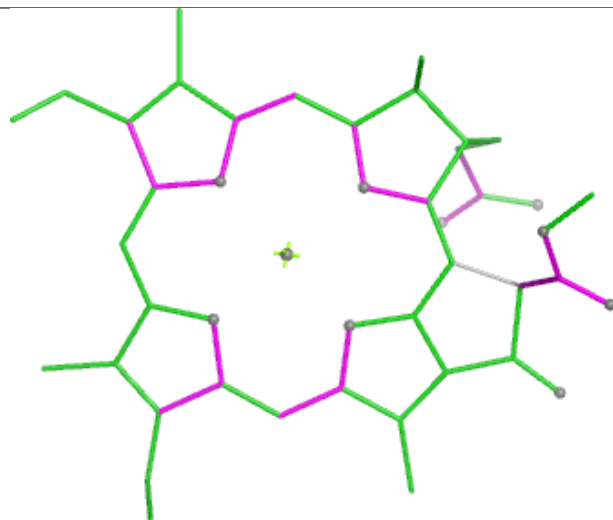
Ligand CHL X 607



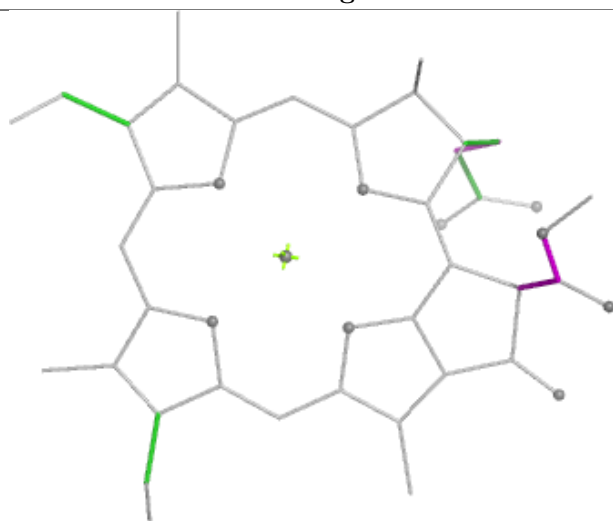
Ligand CLA 6 604



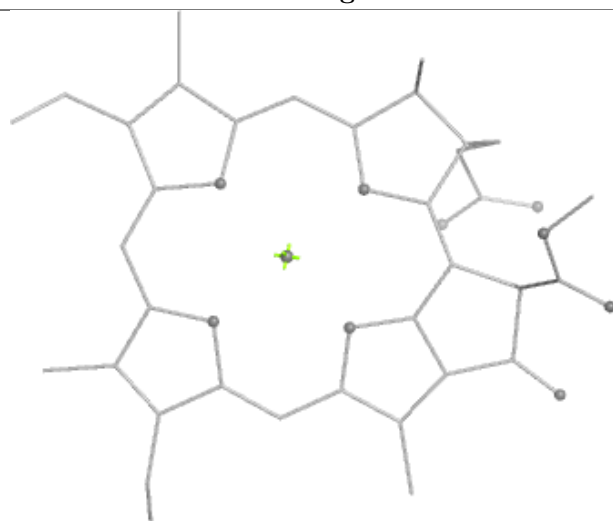
Bond lengths



Bond angles

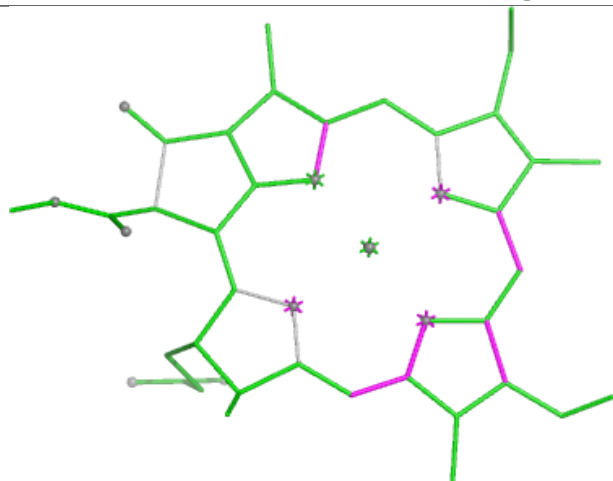


Torsions

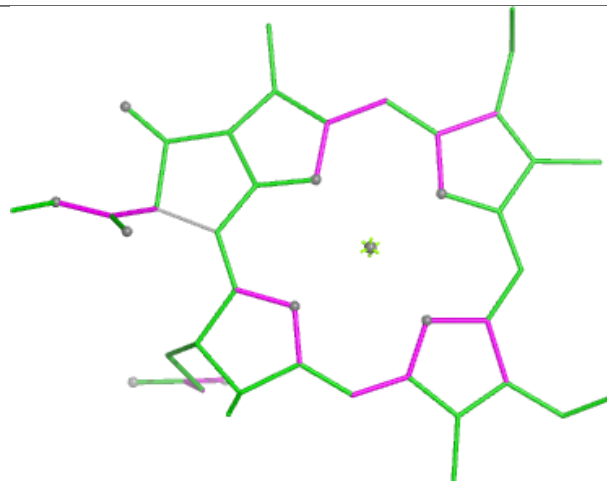


Rings

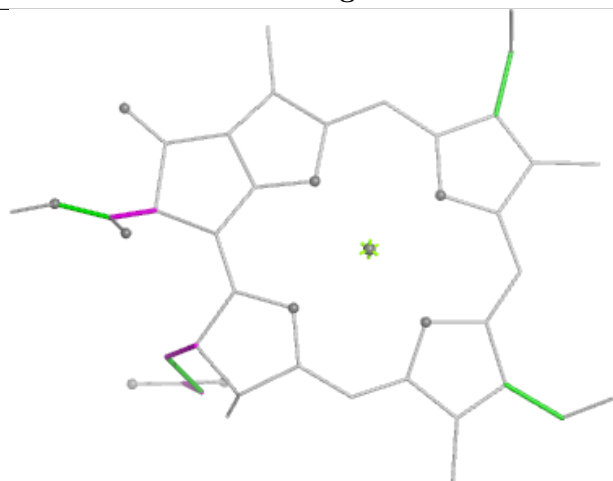
Ligand CLA 4 307



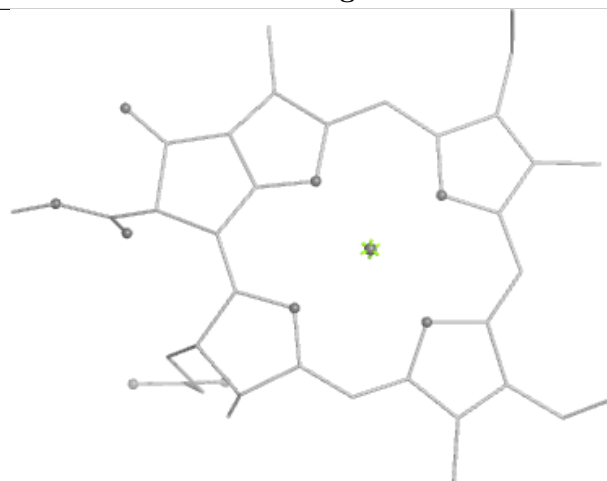
Bond lengths



Bond angles

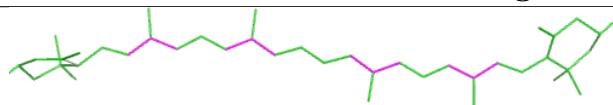


Torsions

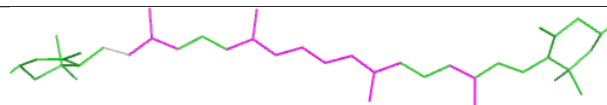


Rings

Ligand LUT Y 615



Bond lengths



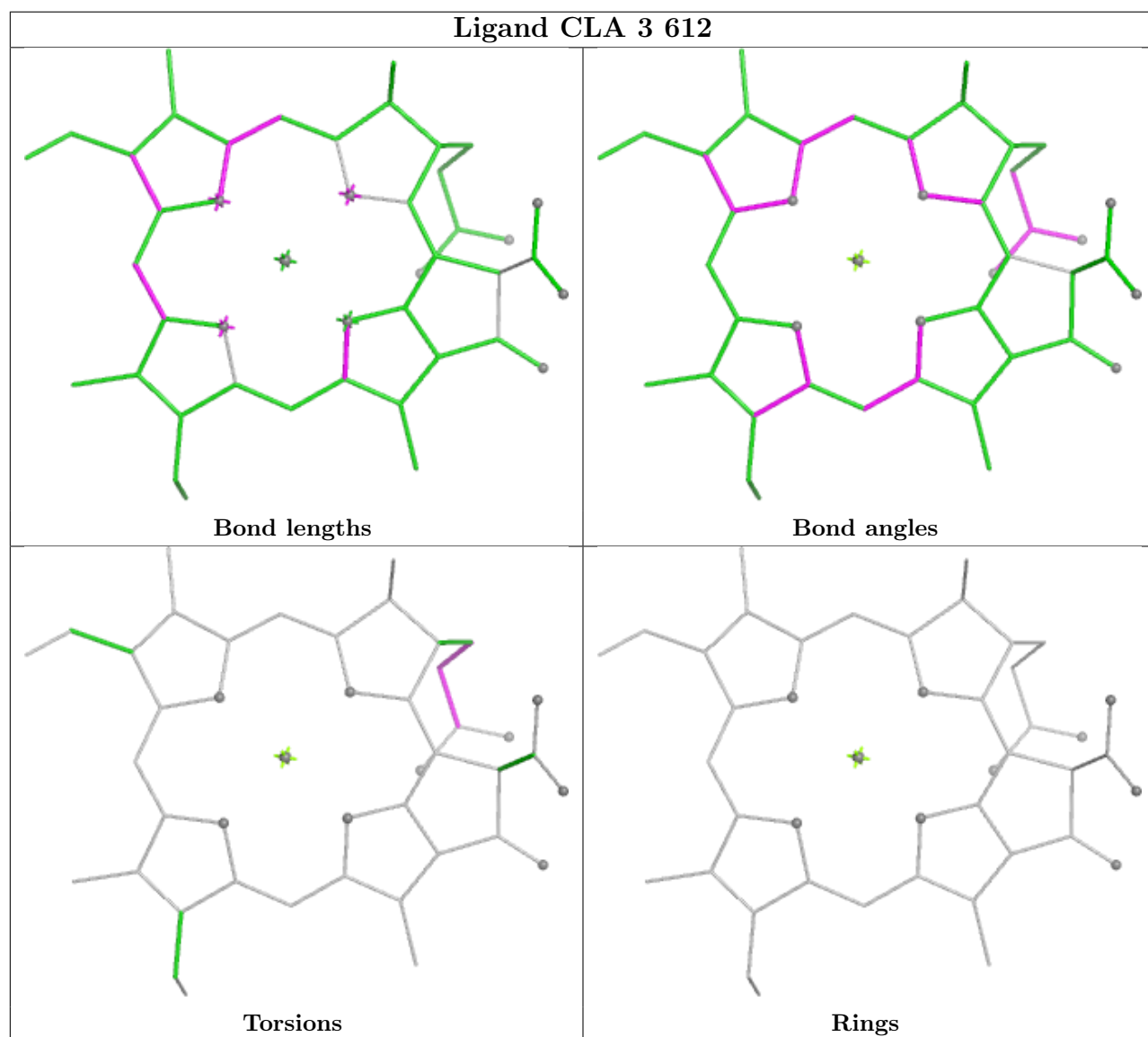
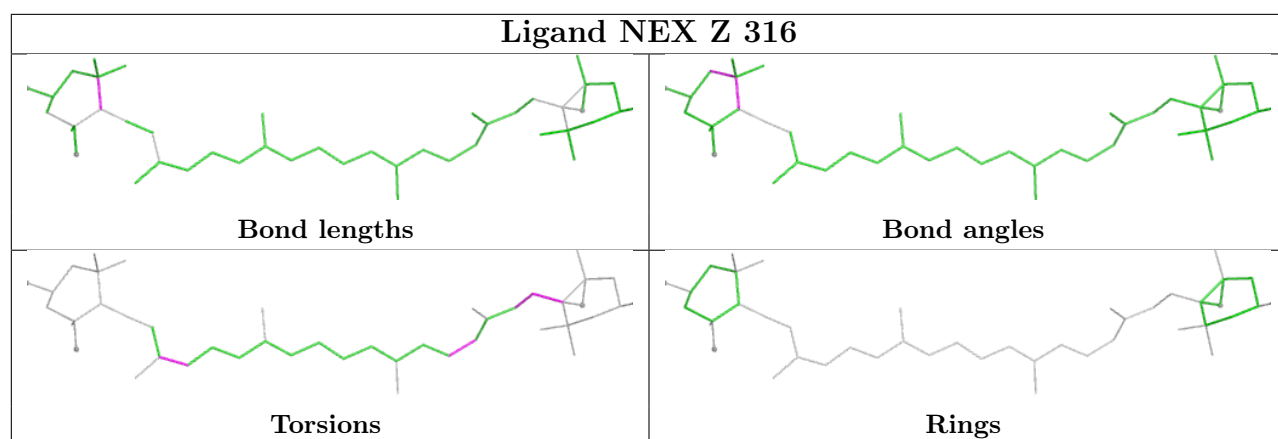
Bond angles

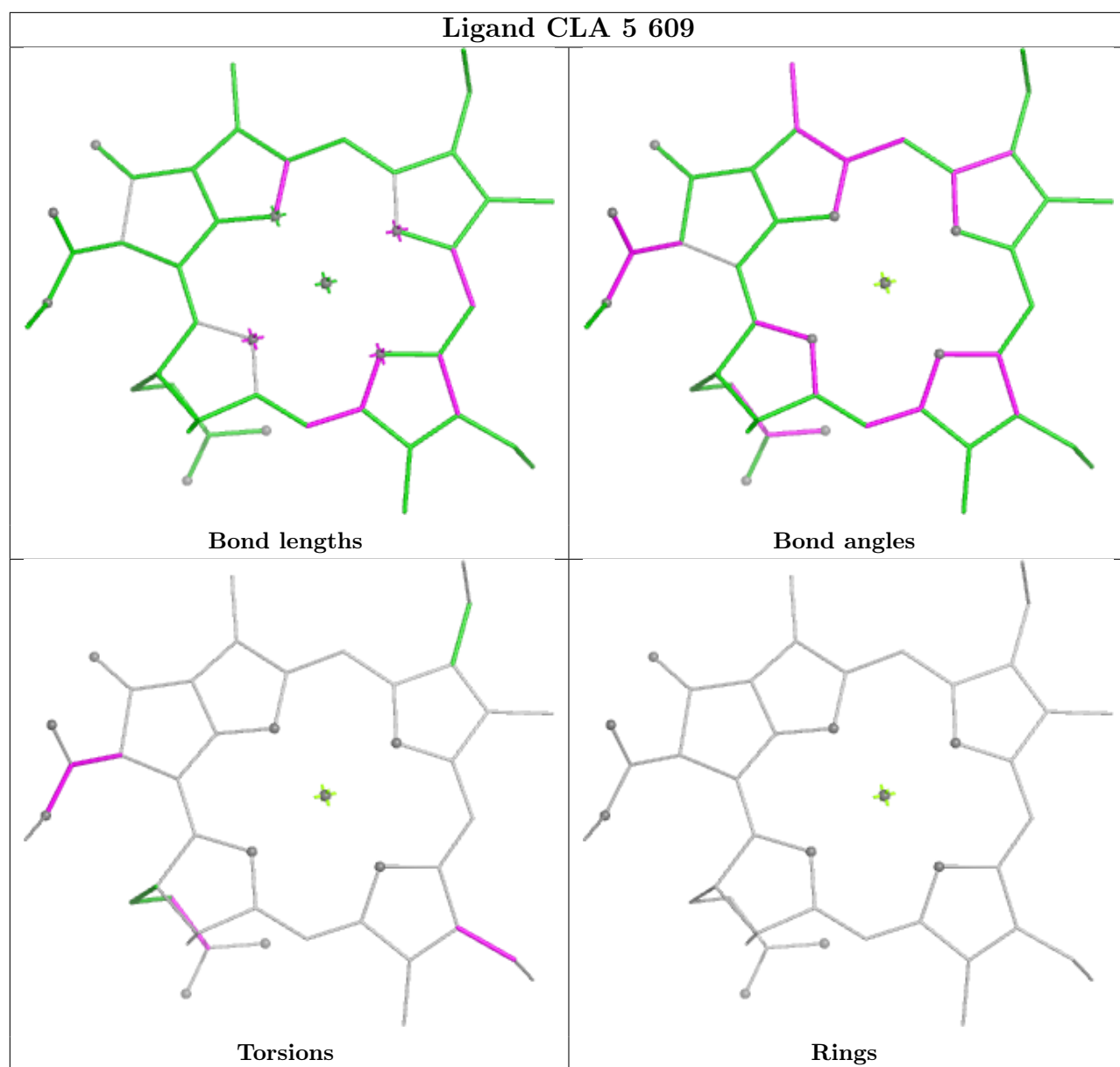


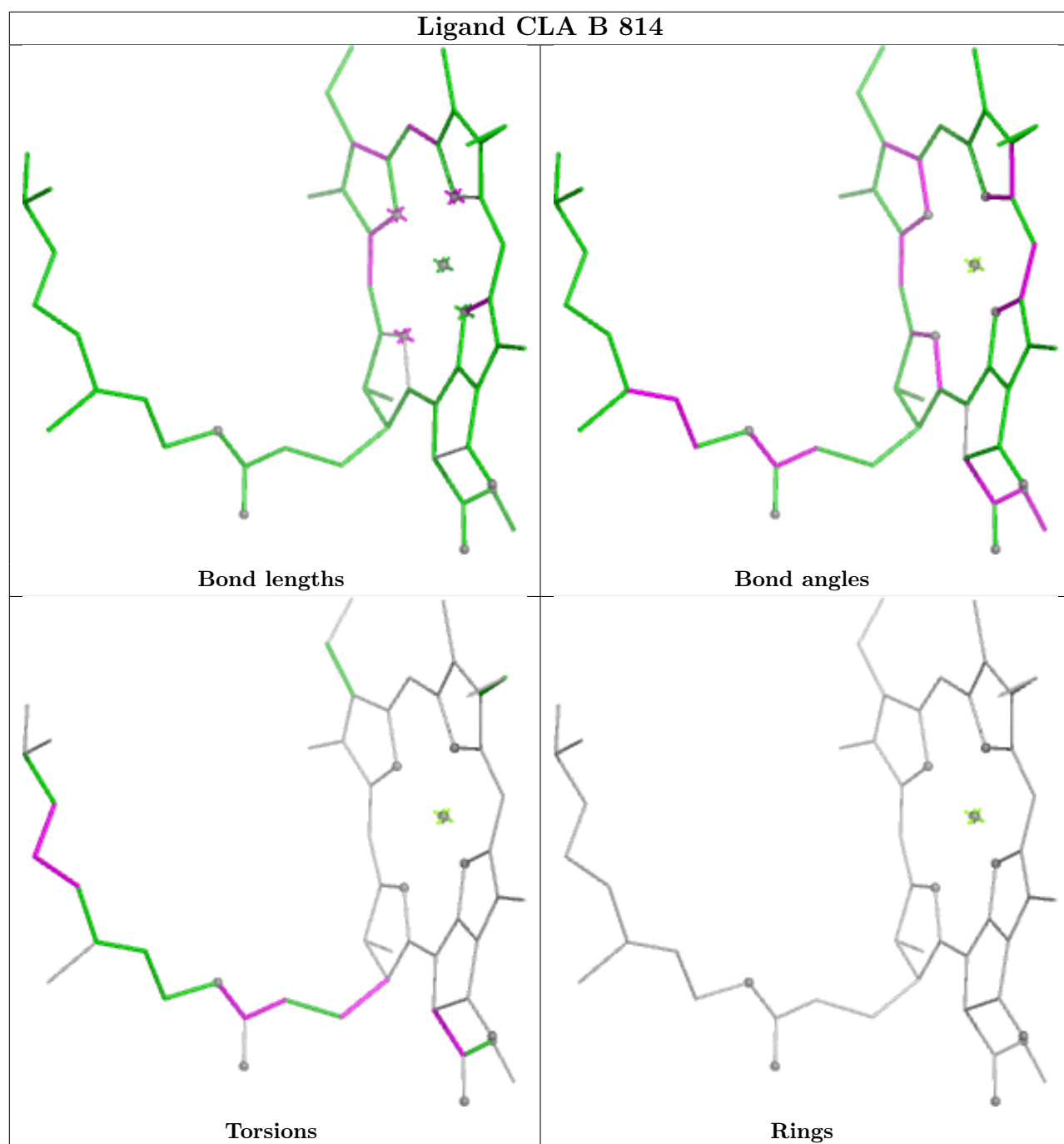
Torsions

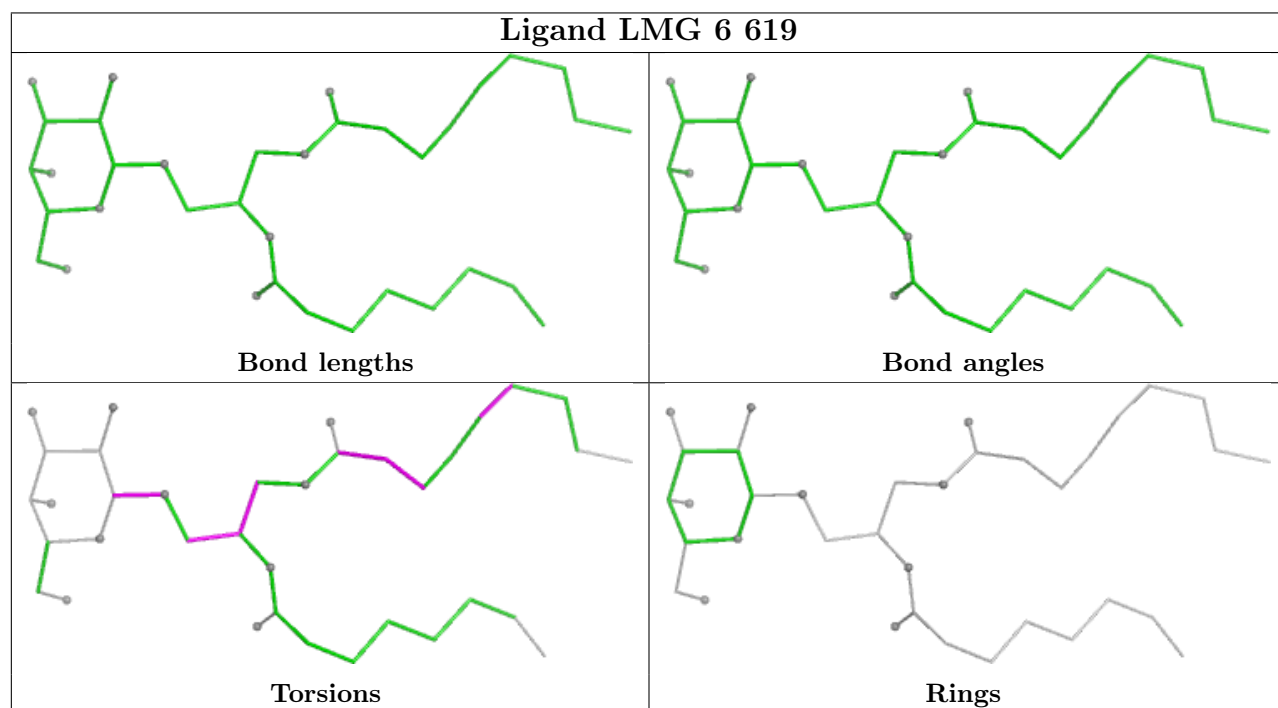
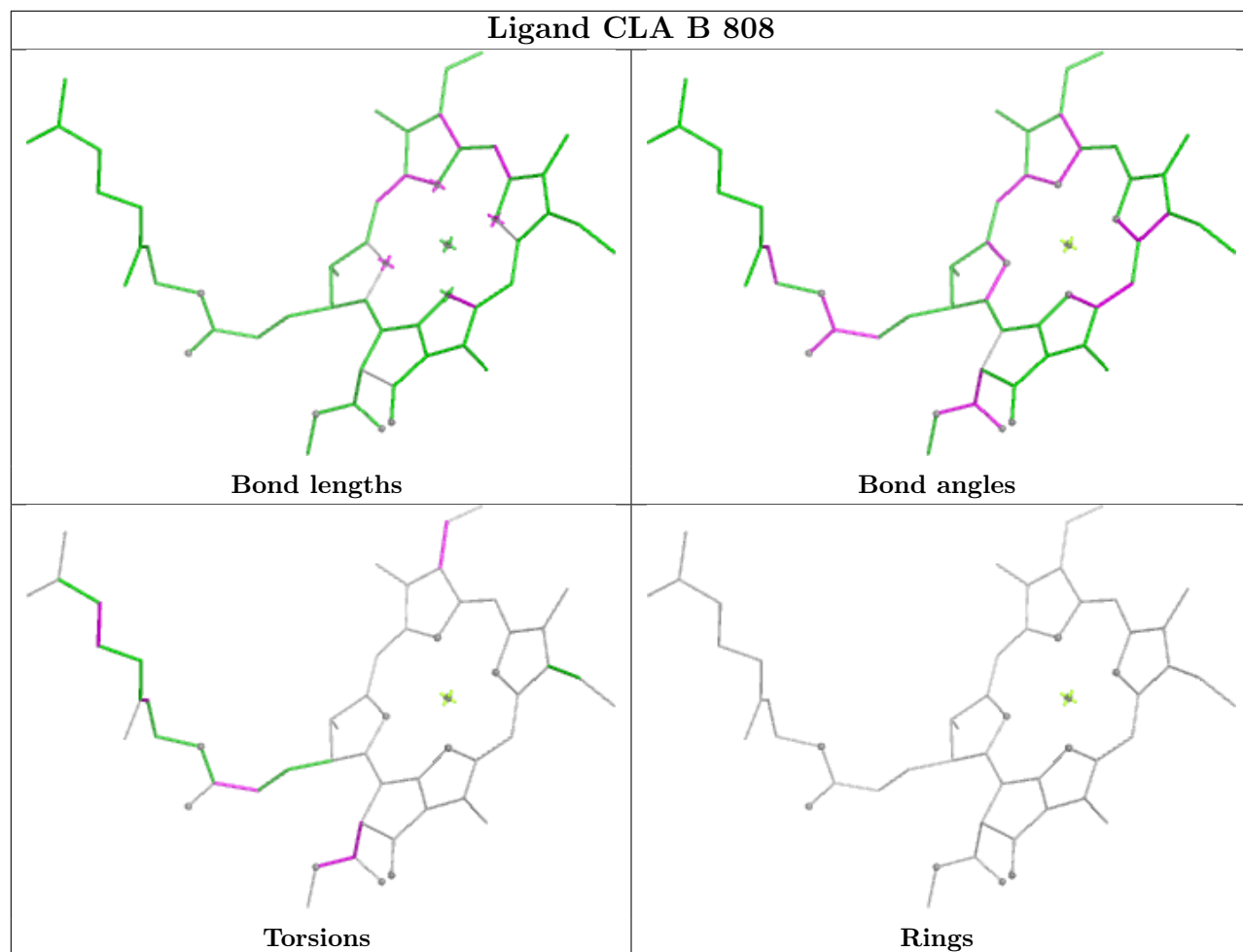


Rings

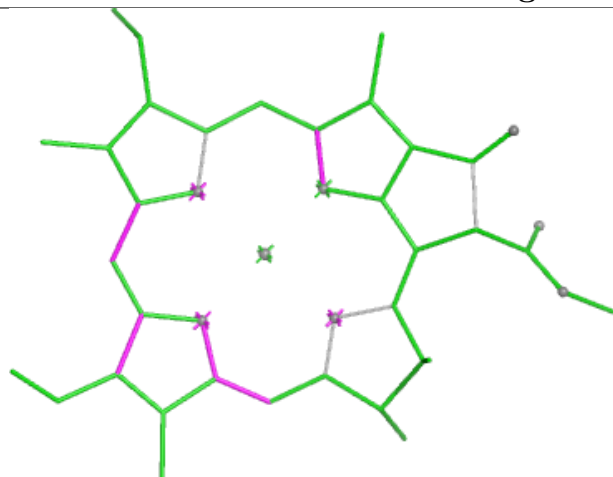




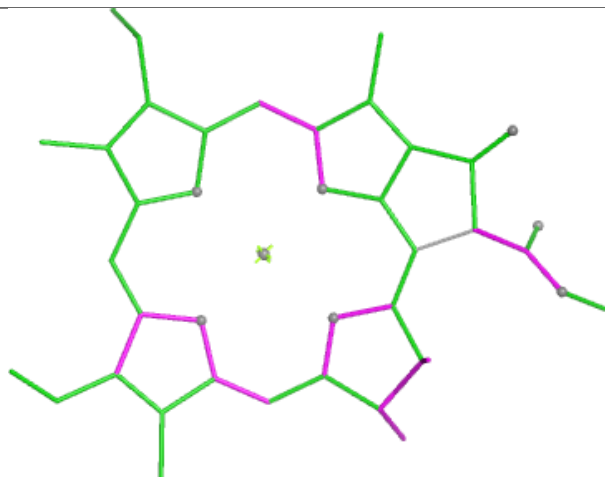




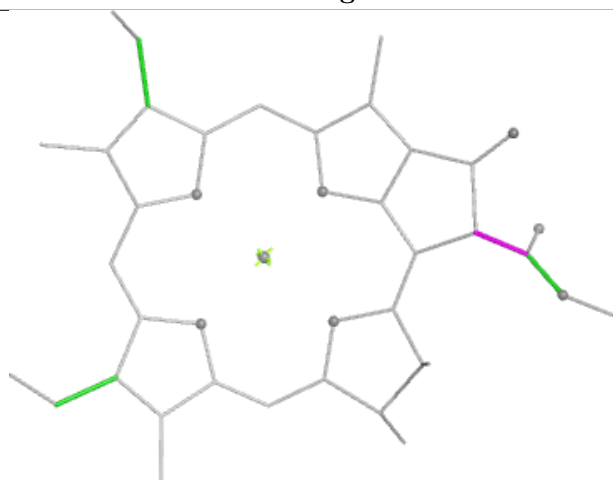
Ligand CLA 2 610



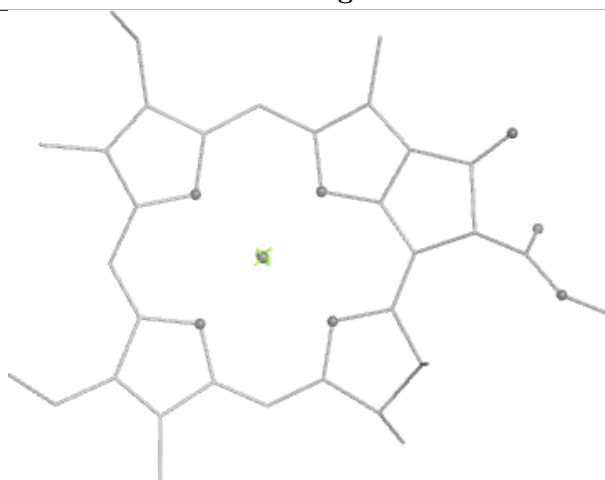
Bond lengths



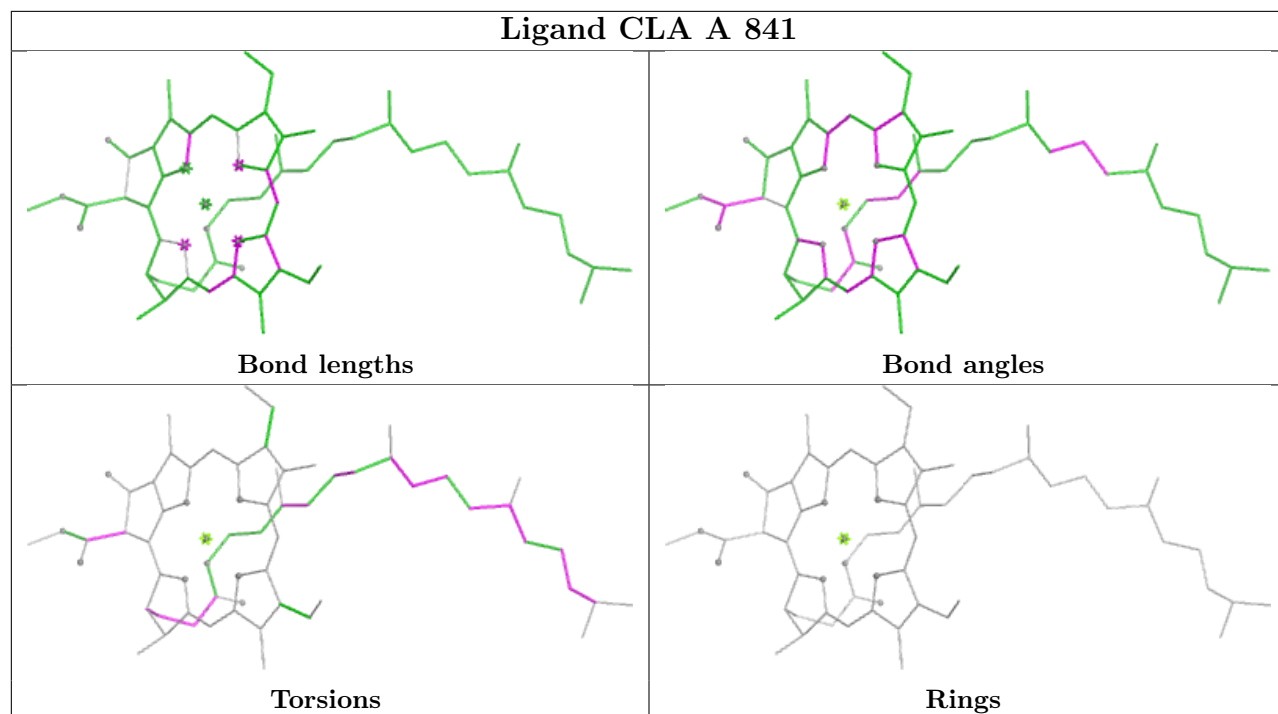
Bond angles



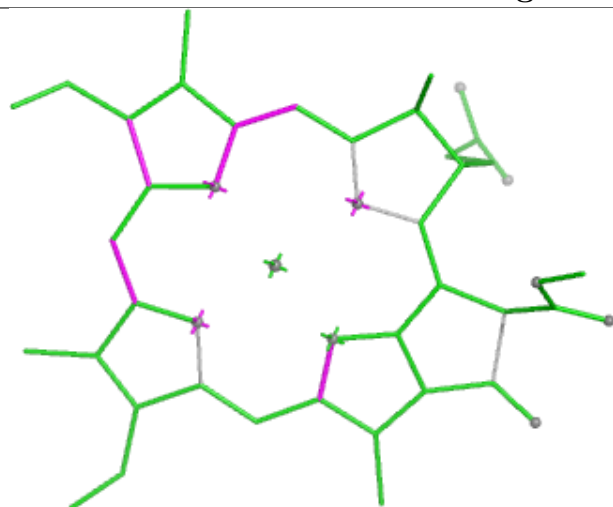
Torsions



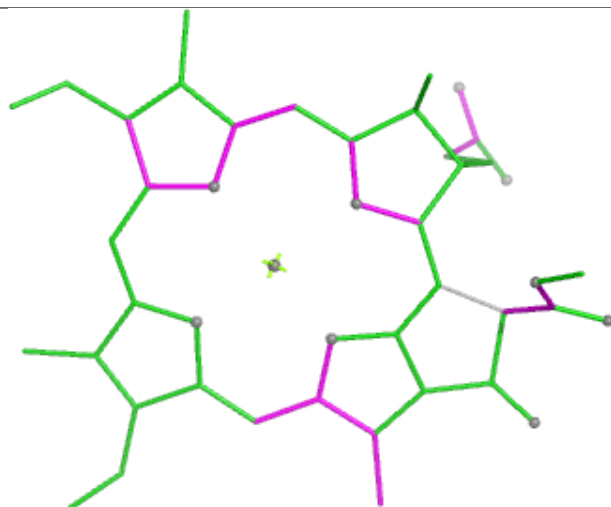
Rings



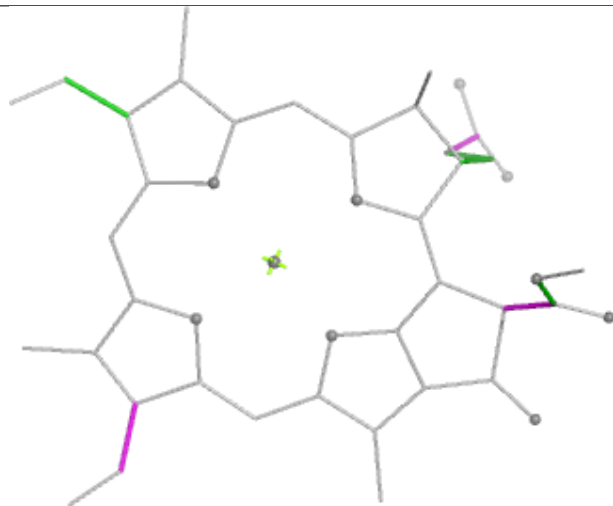
Ligand CLA L 305



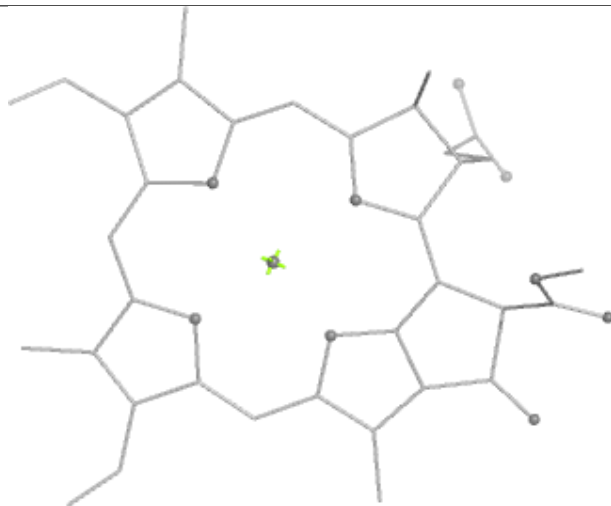
Bond lengths



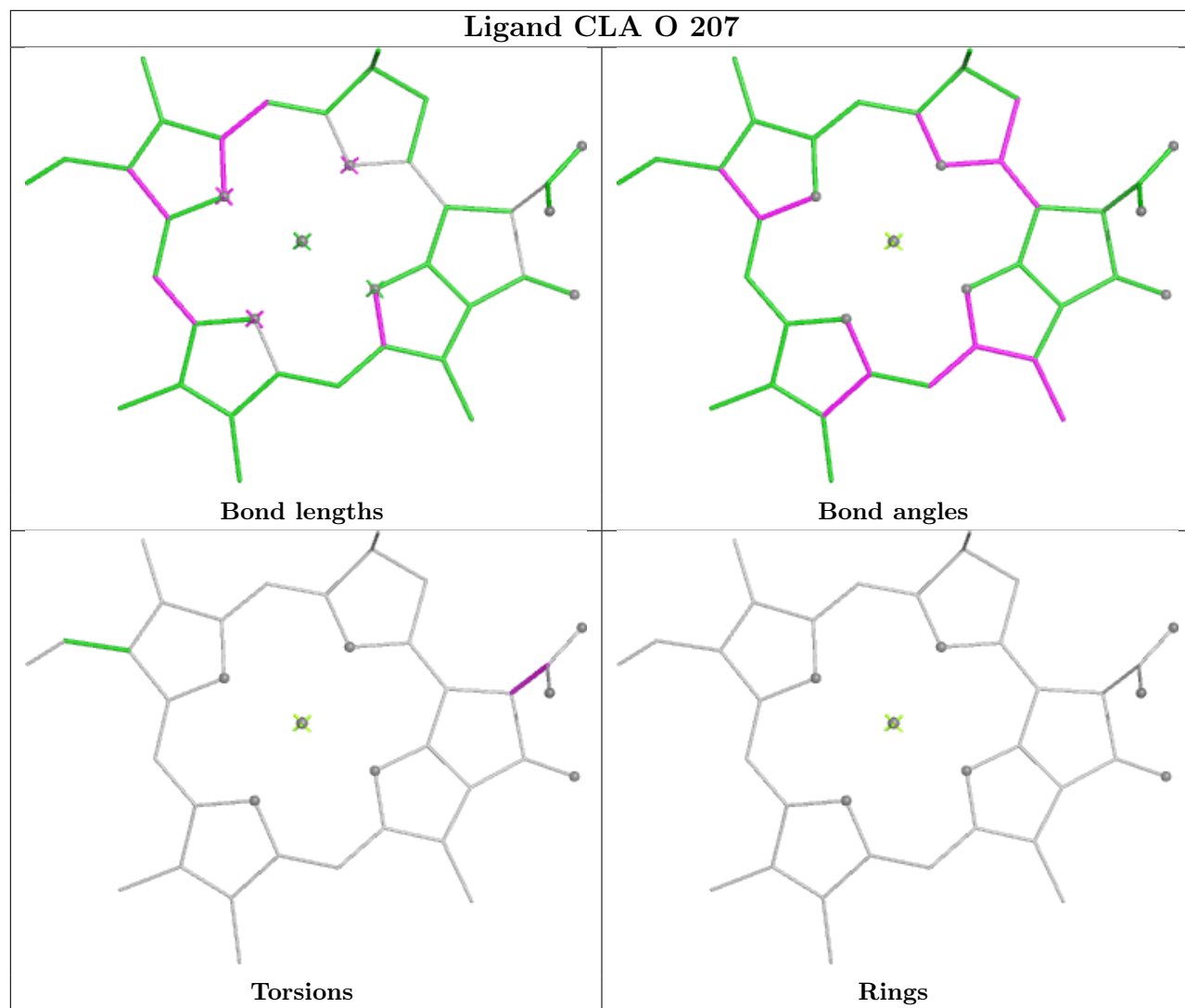
Bond angles

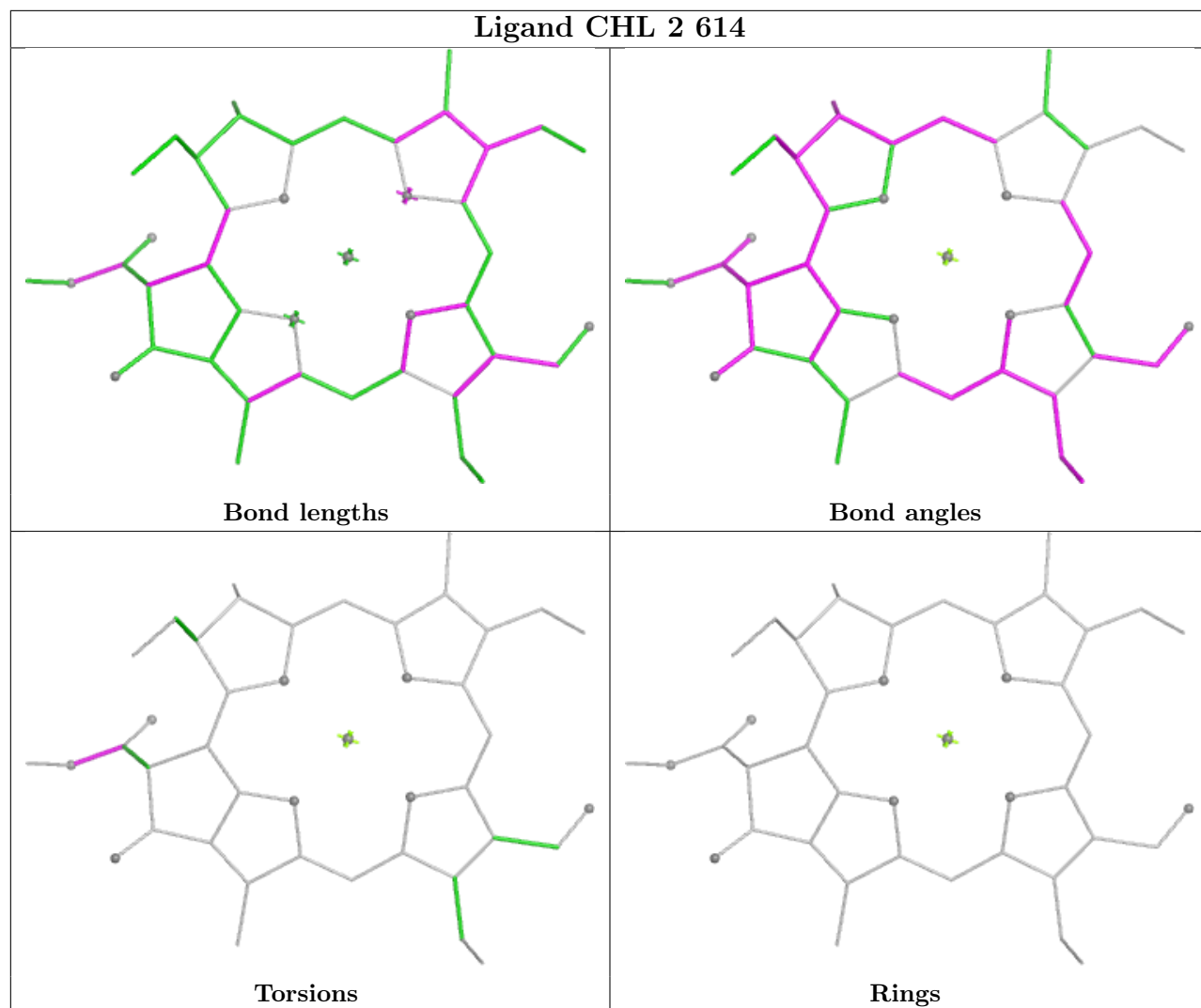


Torsions

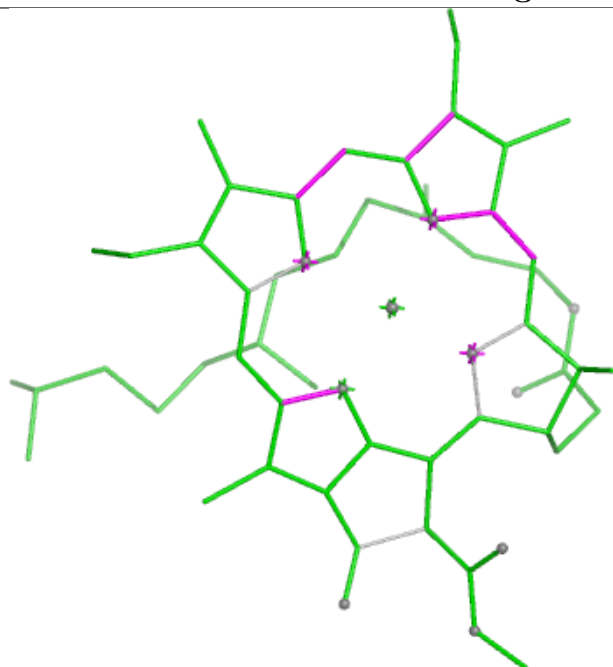


Rings

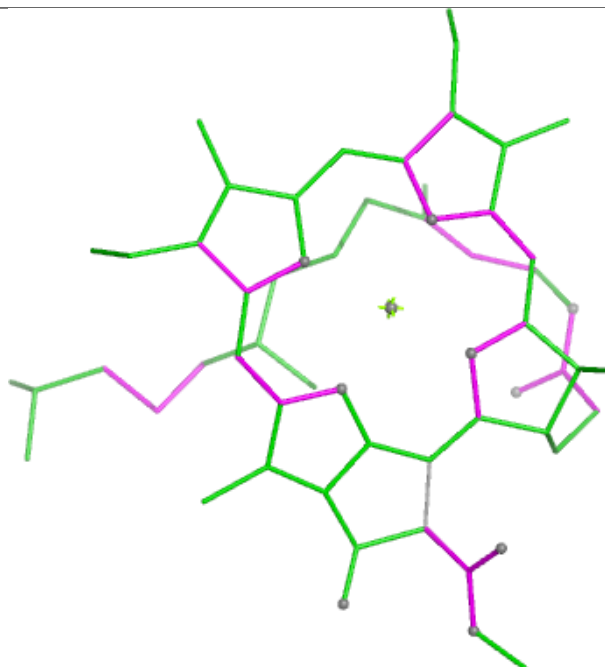




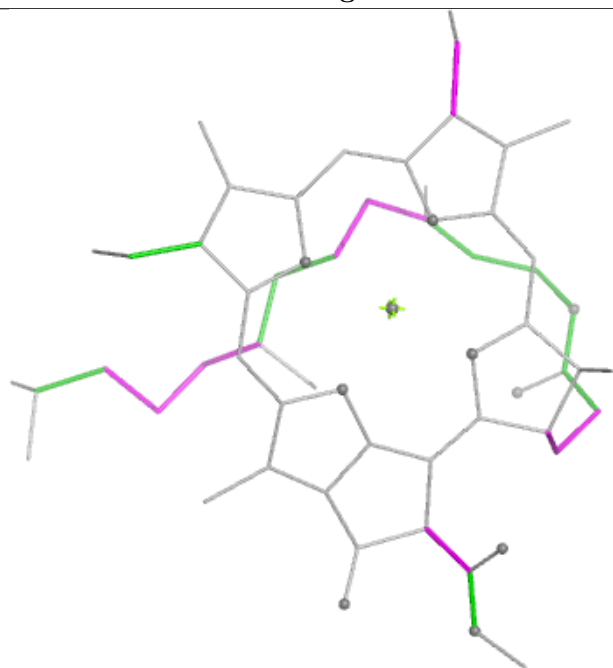
Ligand CLA B 826



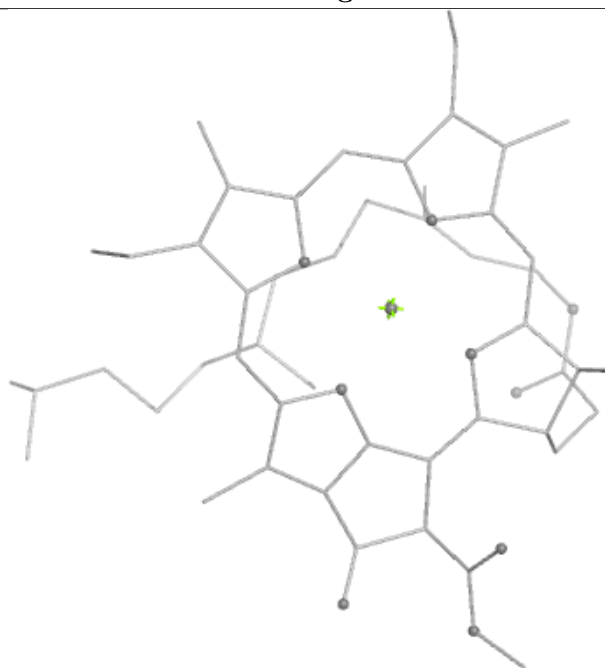
Bond lengths



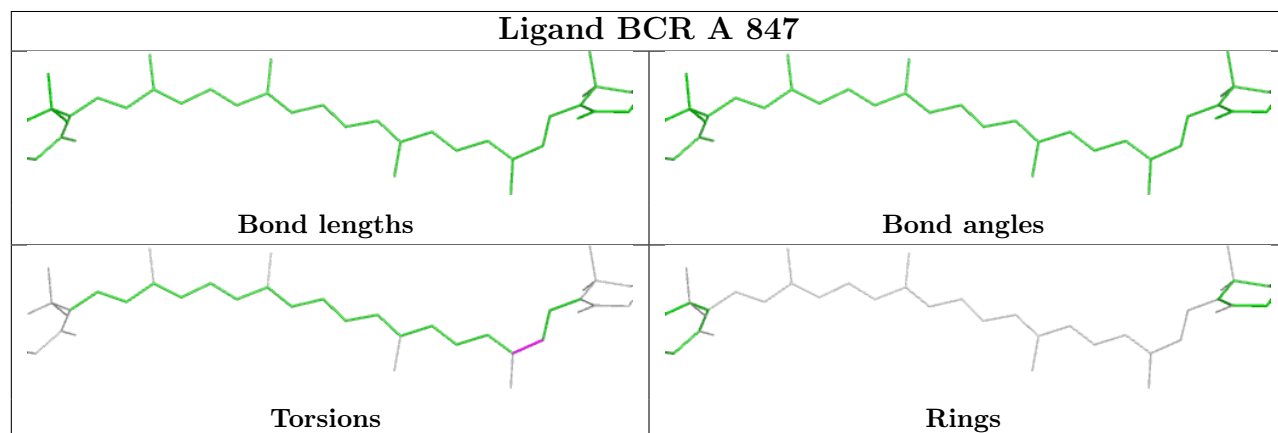
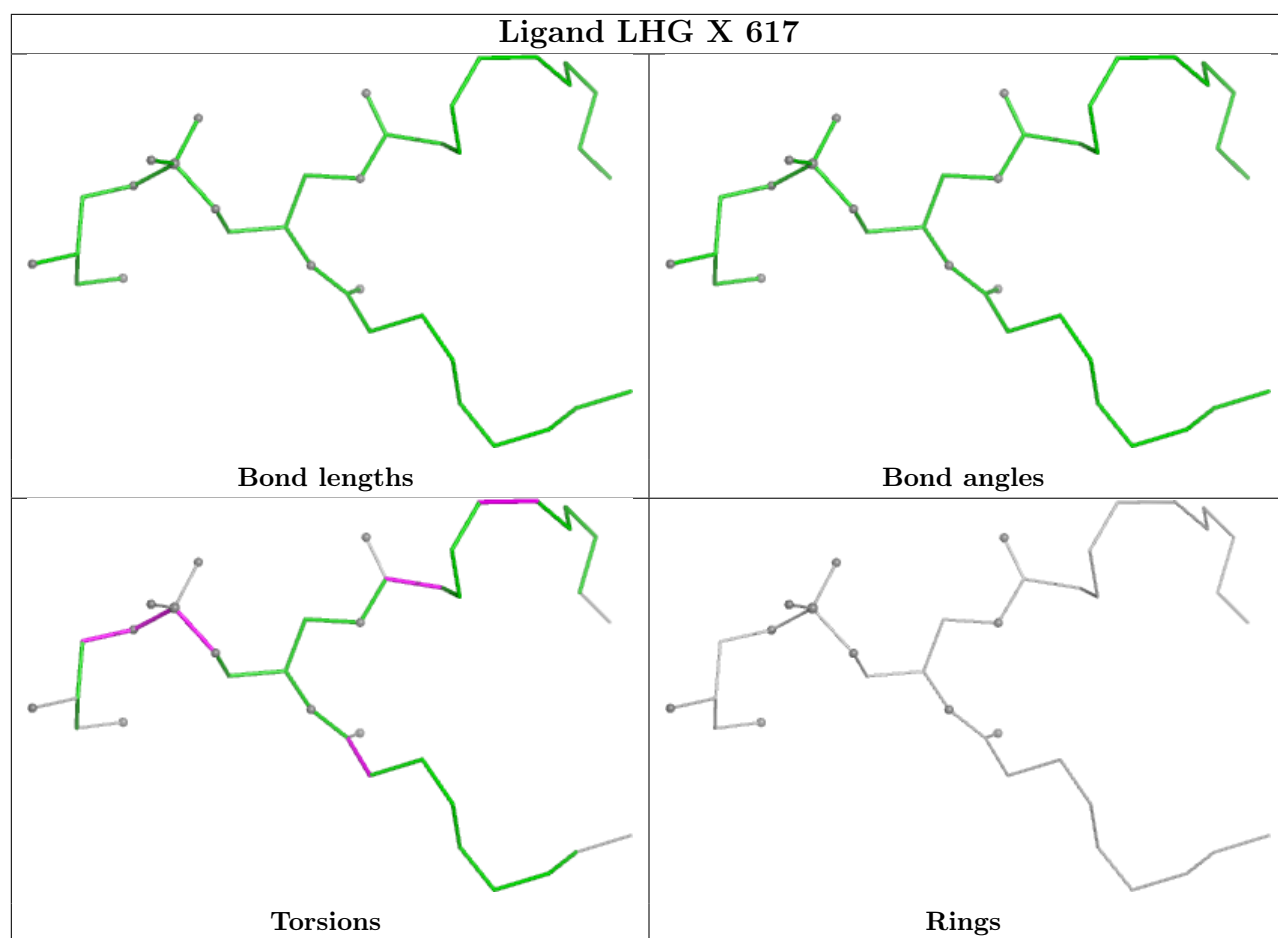
Bond angles



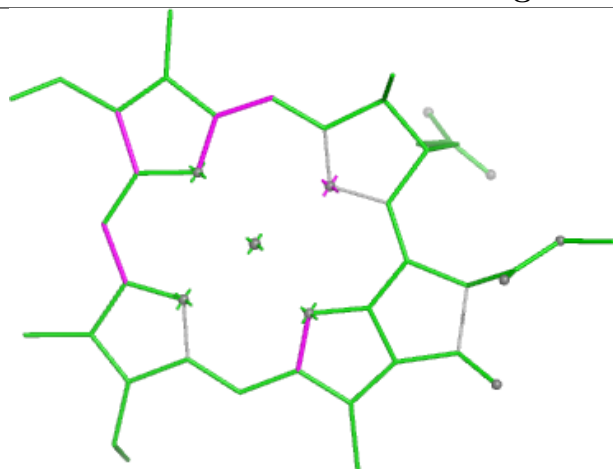
Torsions



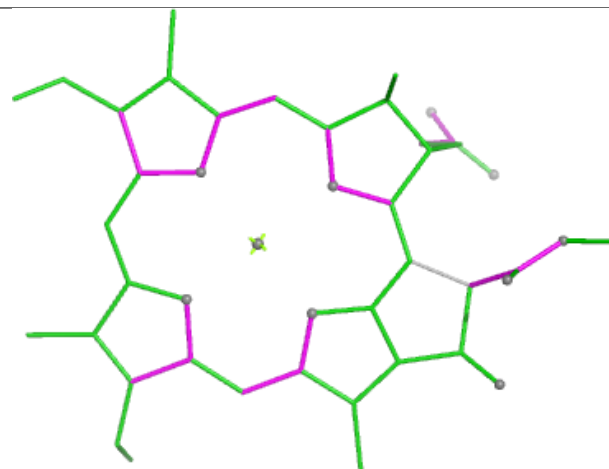
Rings



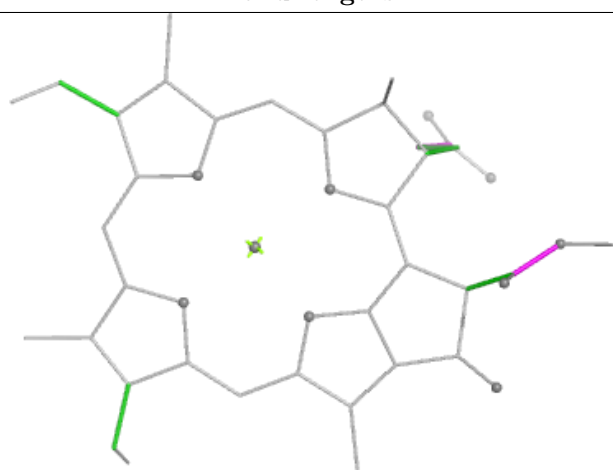
Ligand CLA A 835



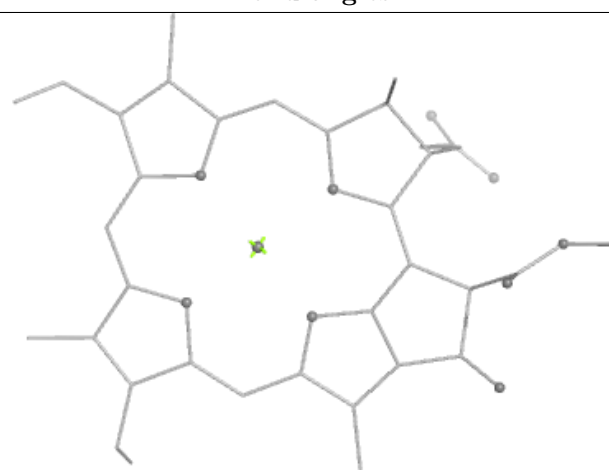
Bond lengths



Bond angles

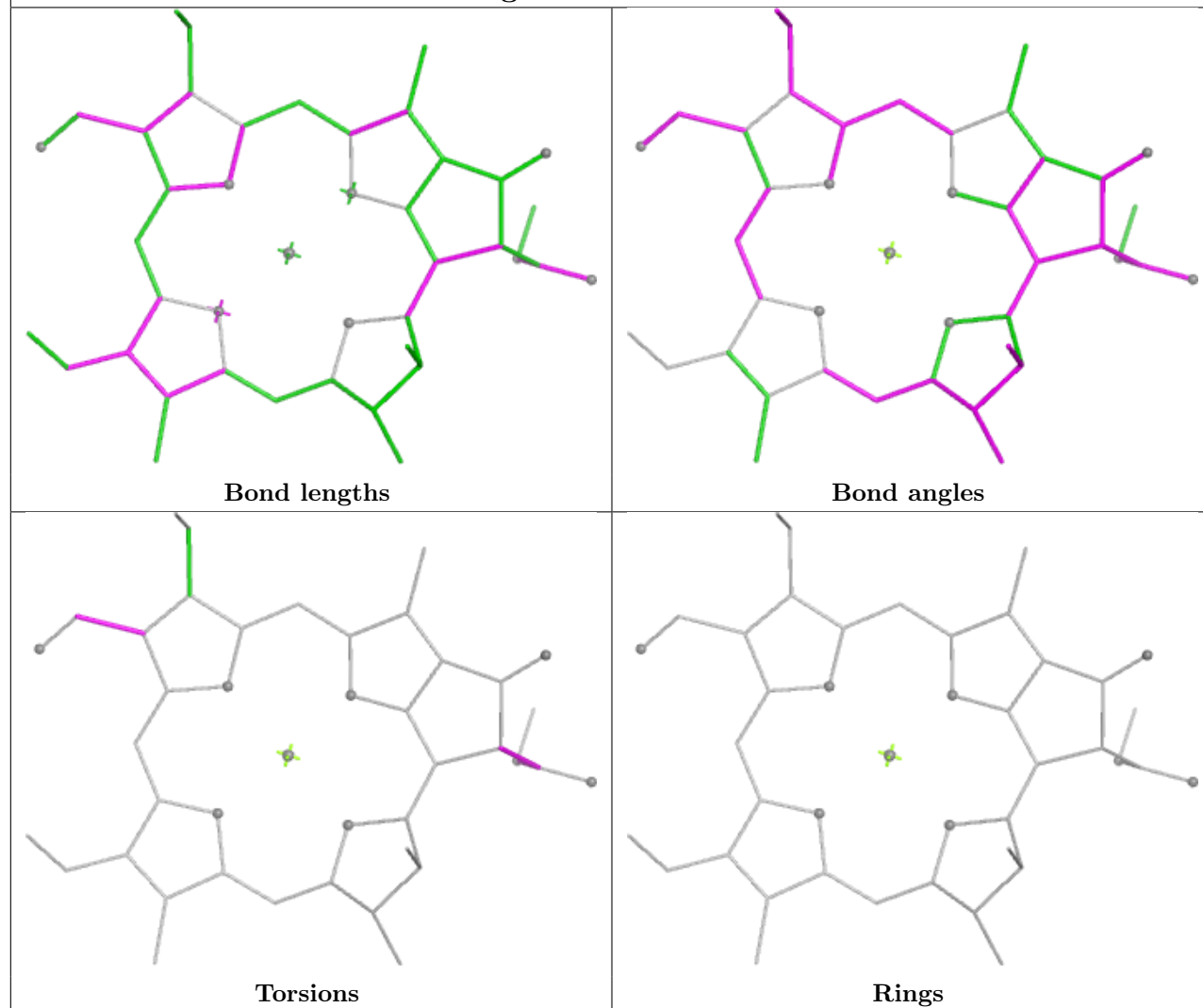


Torsions

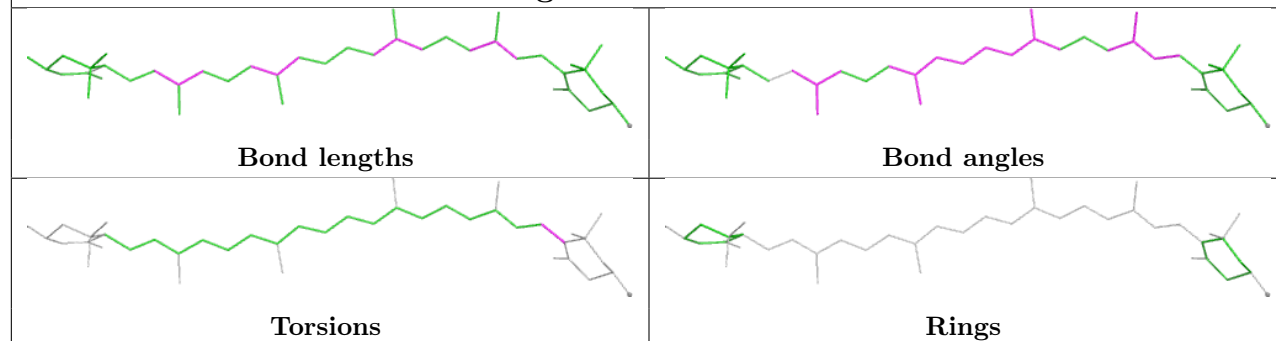


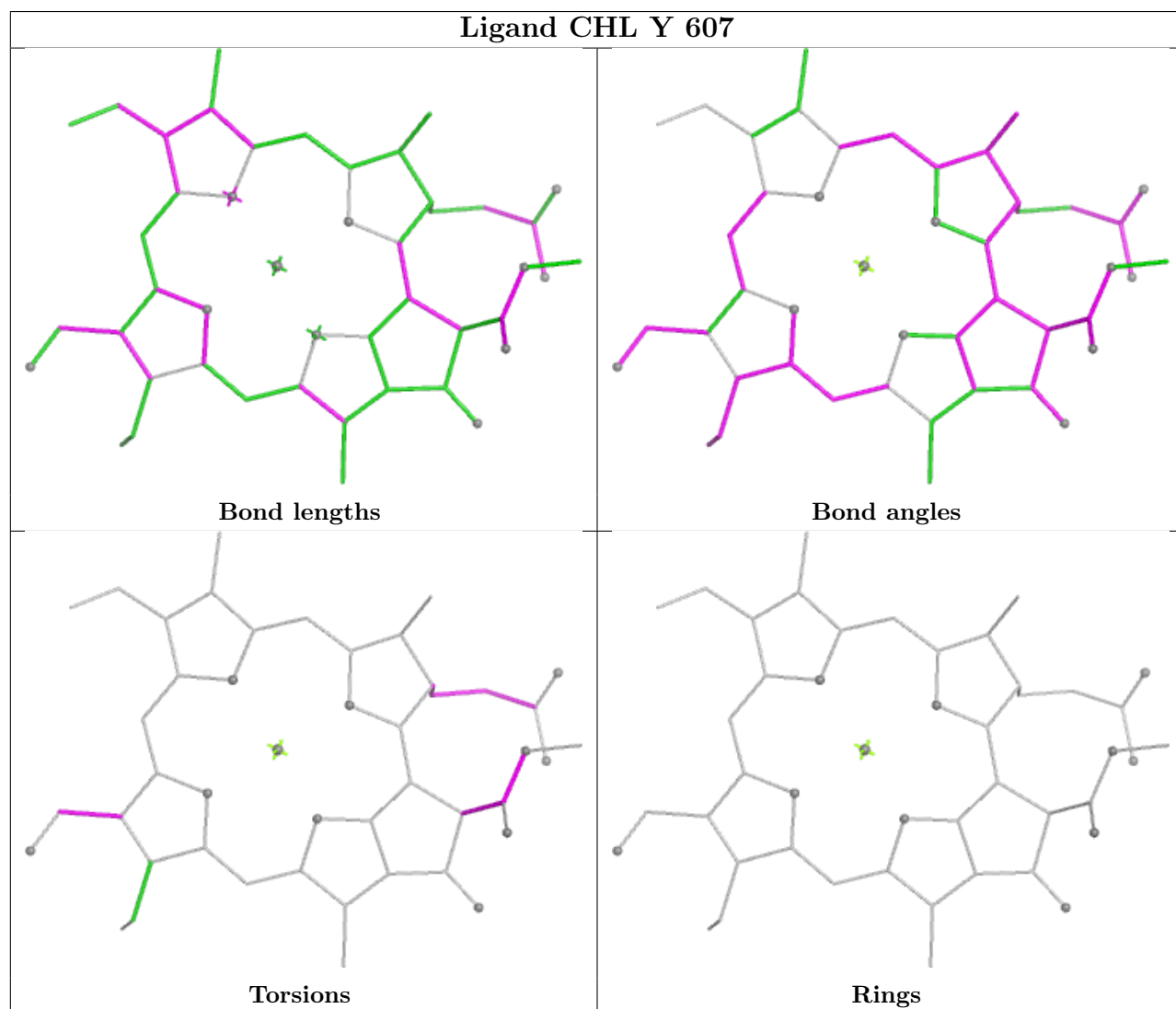
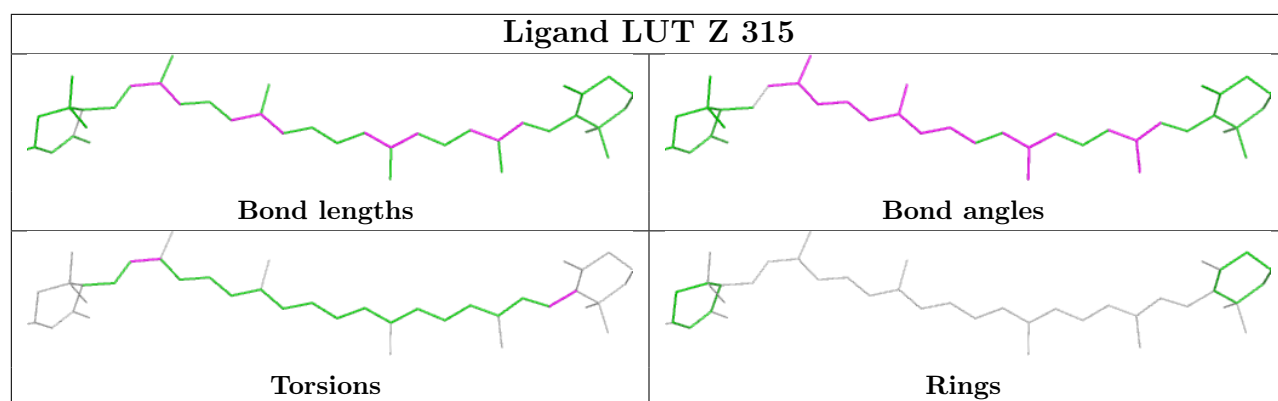
Rings

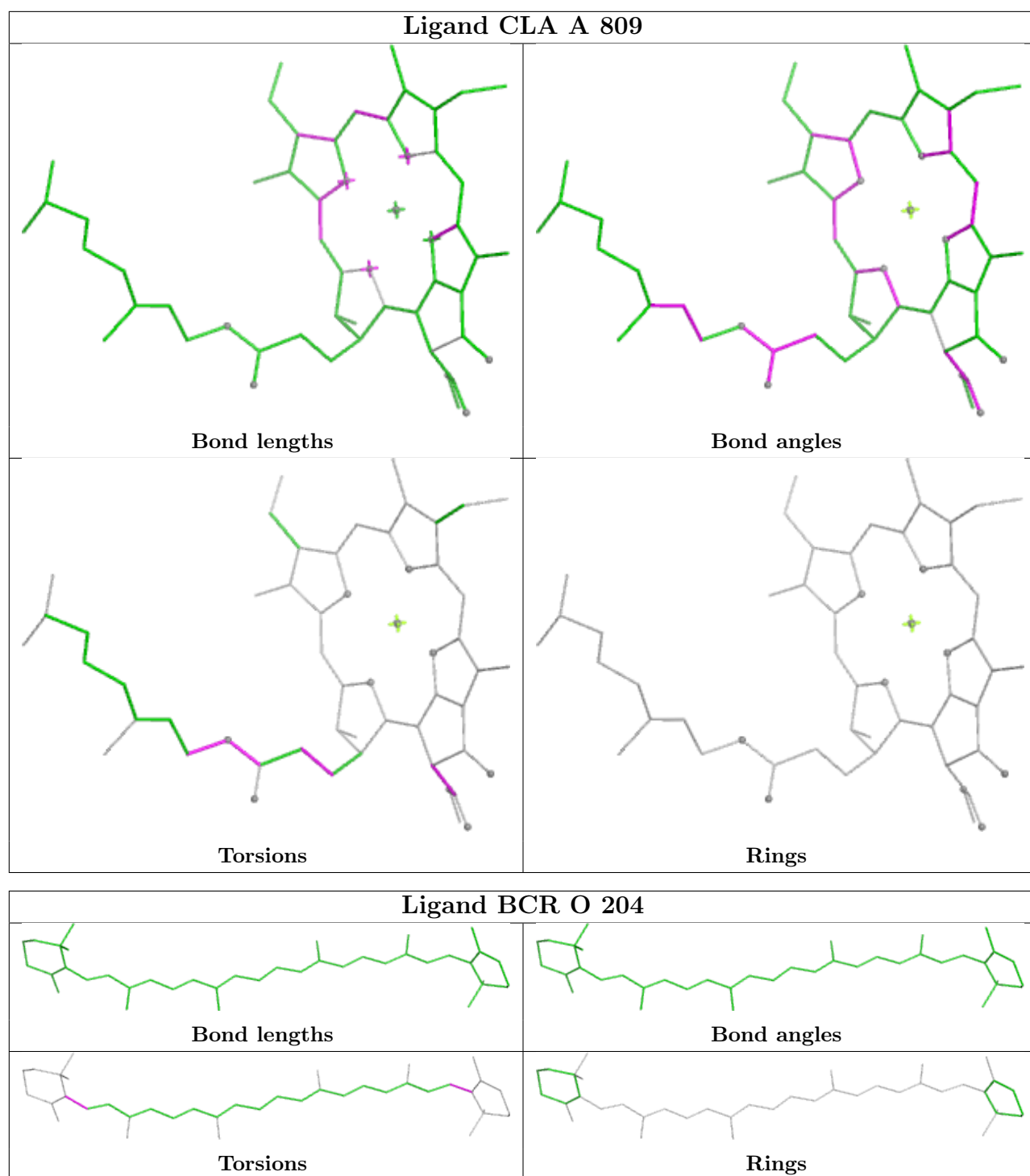
Ligand CHL Y 605



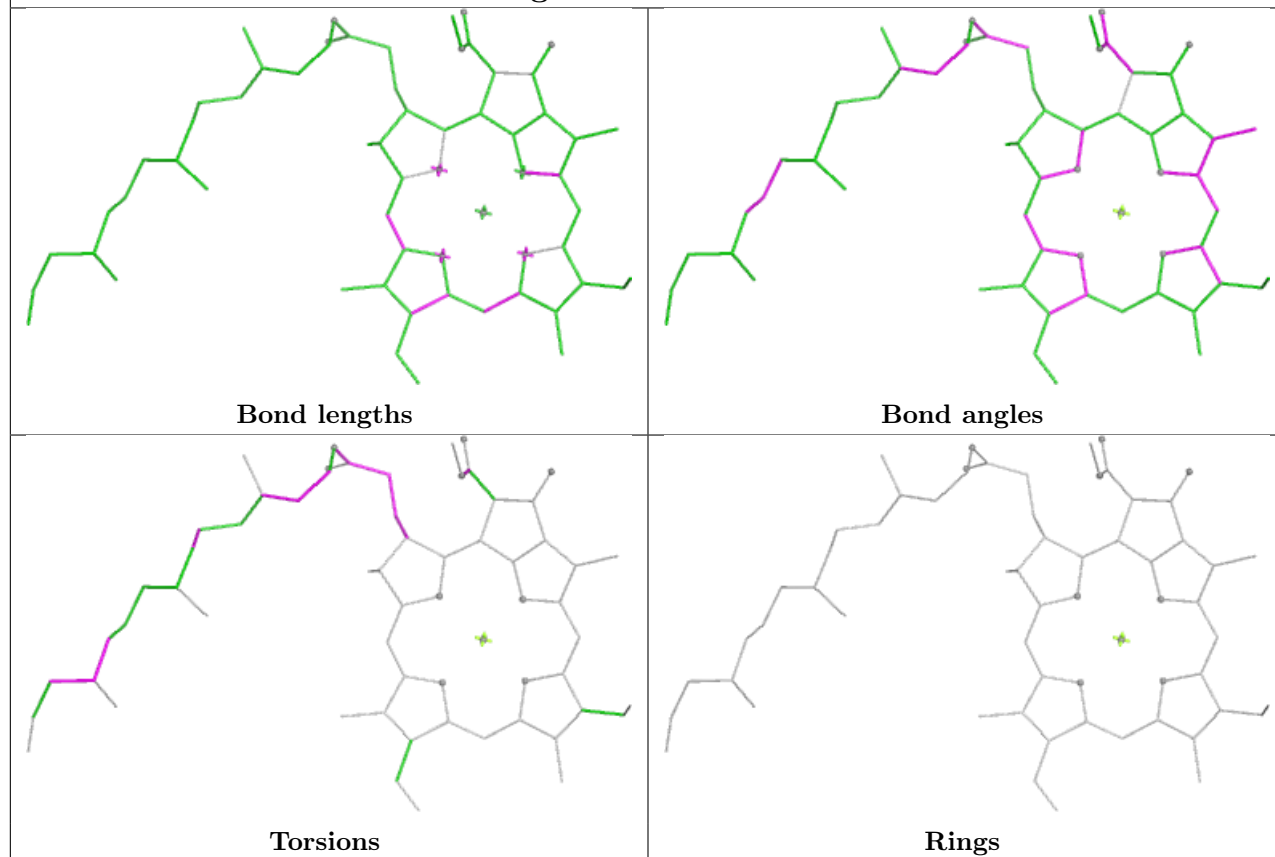
Ligand LUT 6 616



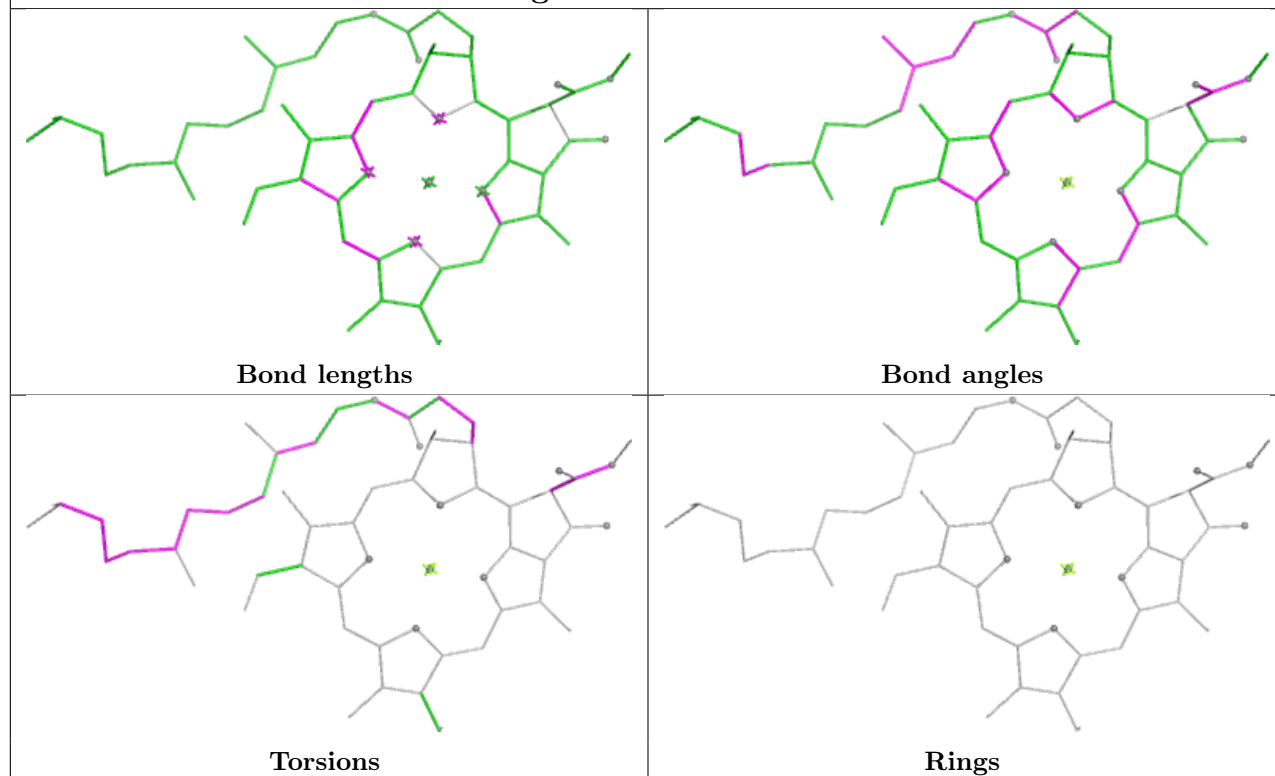




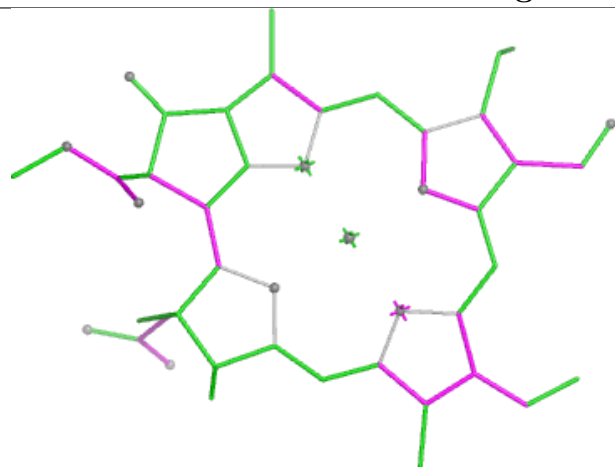
Ligand CLA O 203



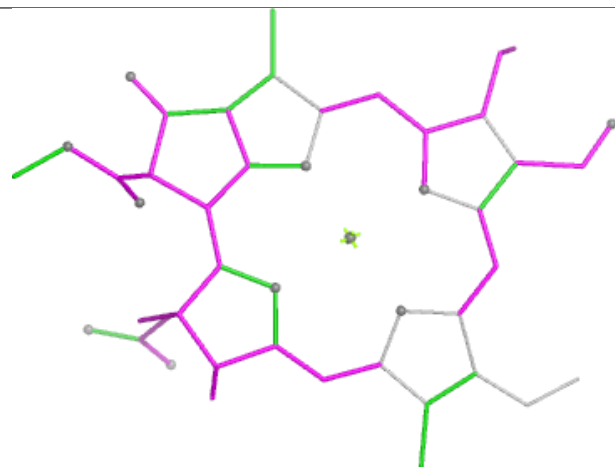
Ligand CLA B 817



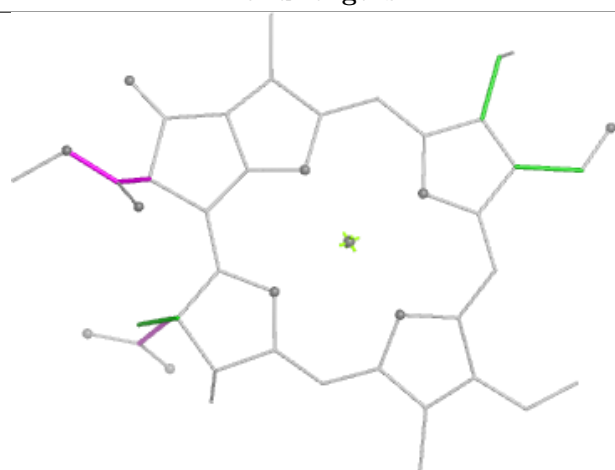
Ligand CHL Y 609



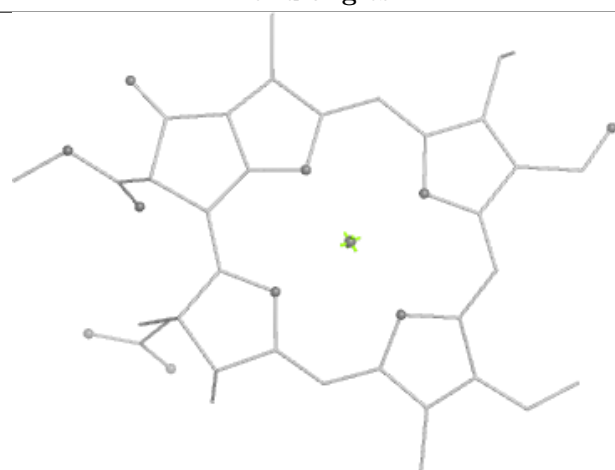
Bond lengths



Bond angles

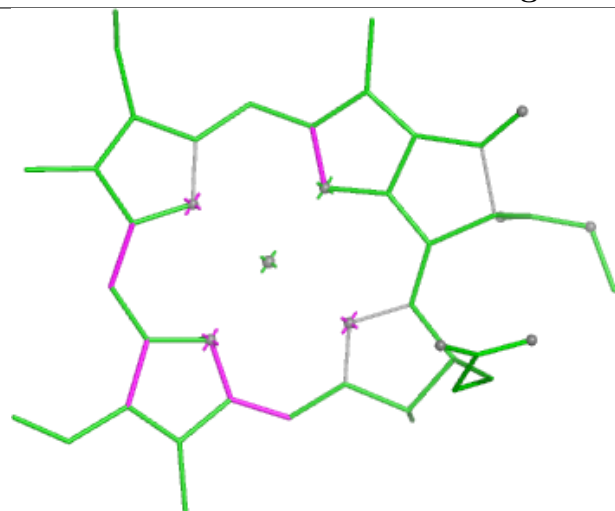


Torsions

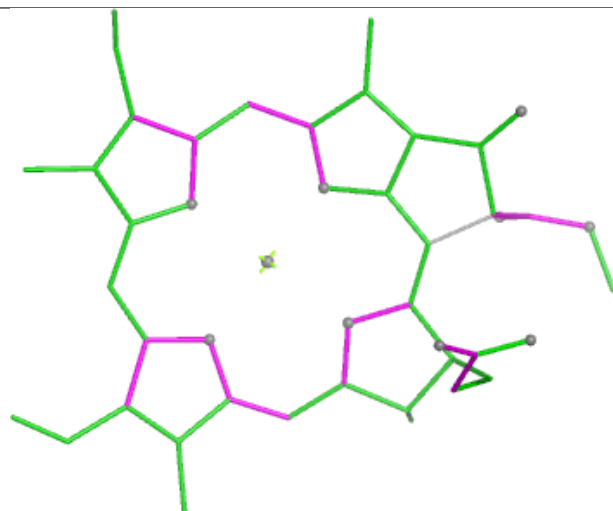


Rings

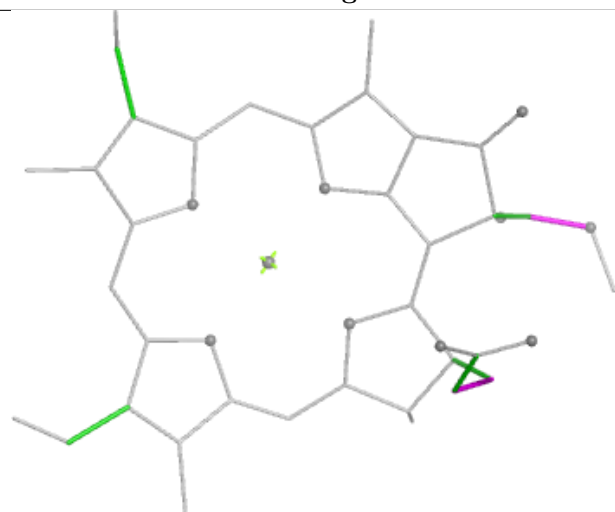
Ligand CLA 5 610



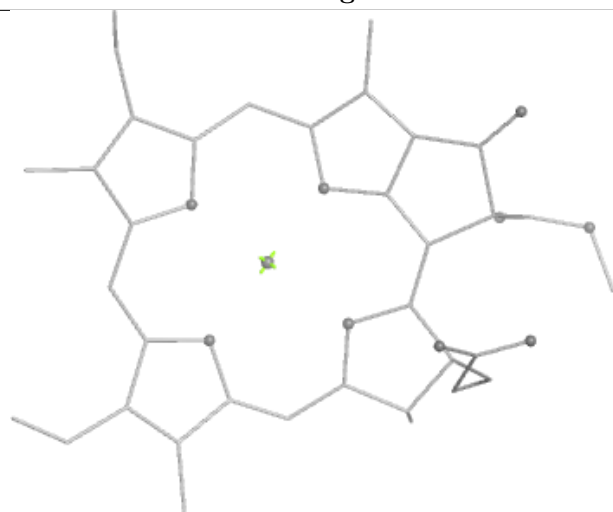
Bond lengths



Bond angles

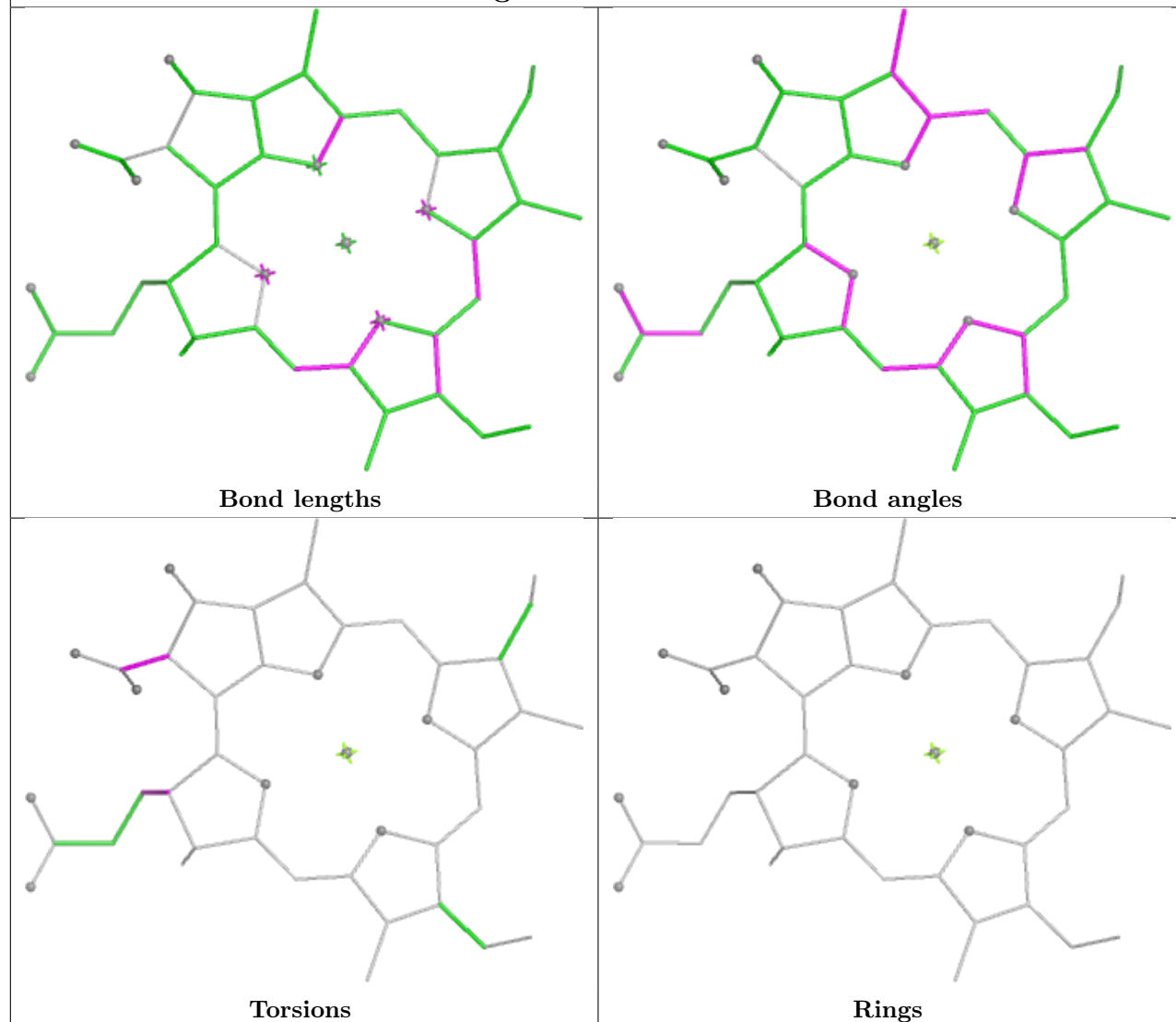


Torsions

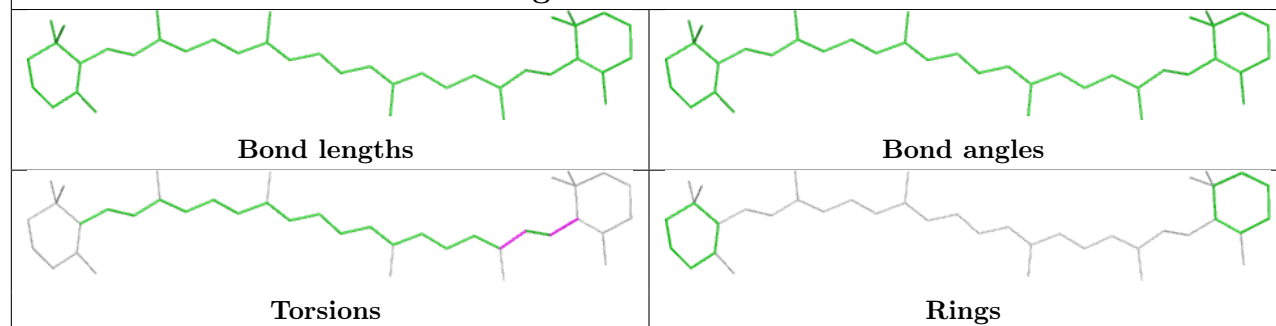


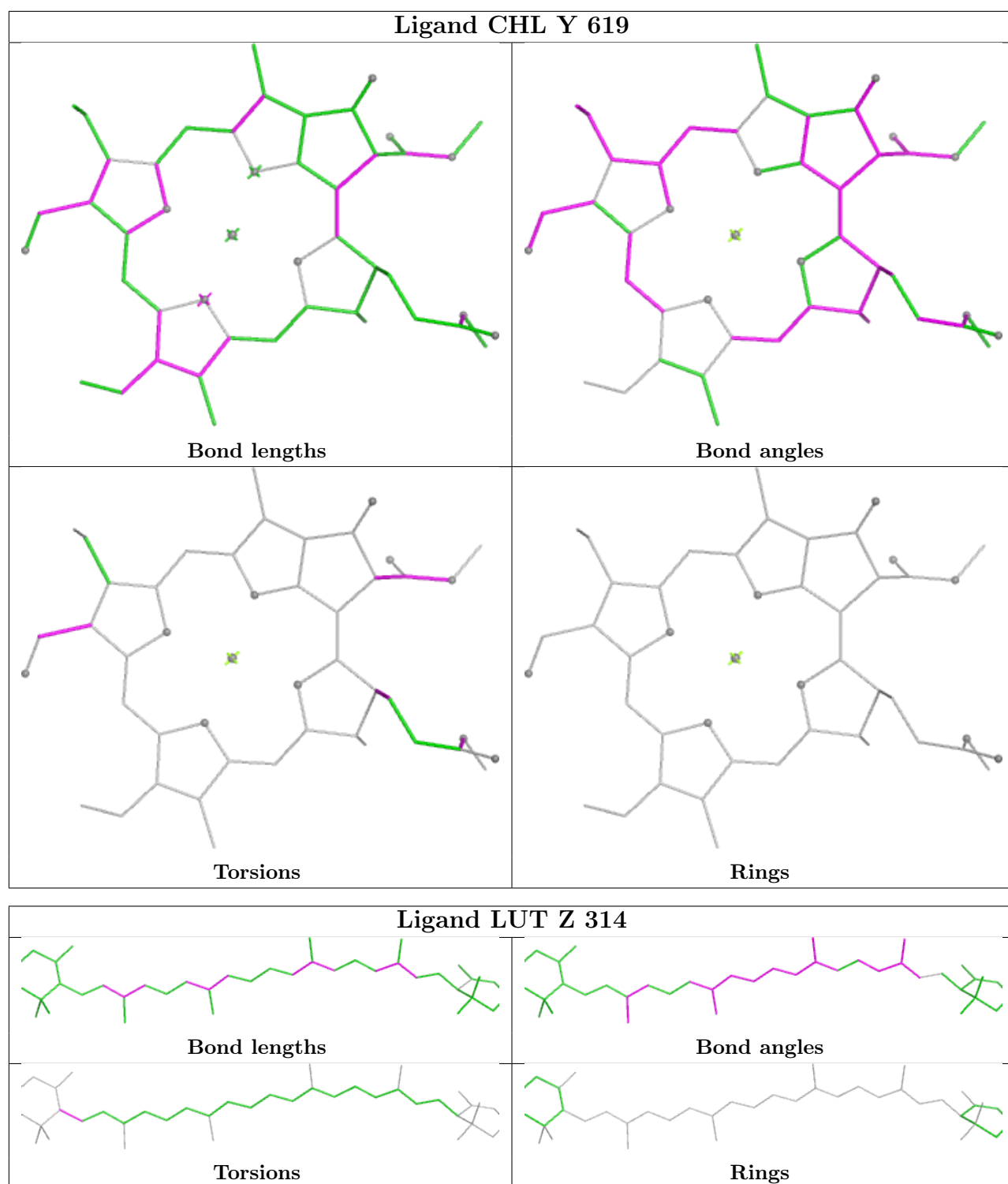
Rings

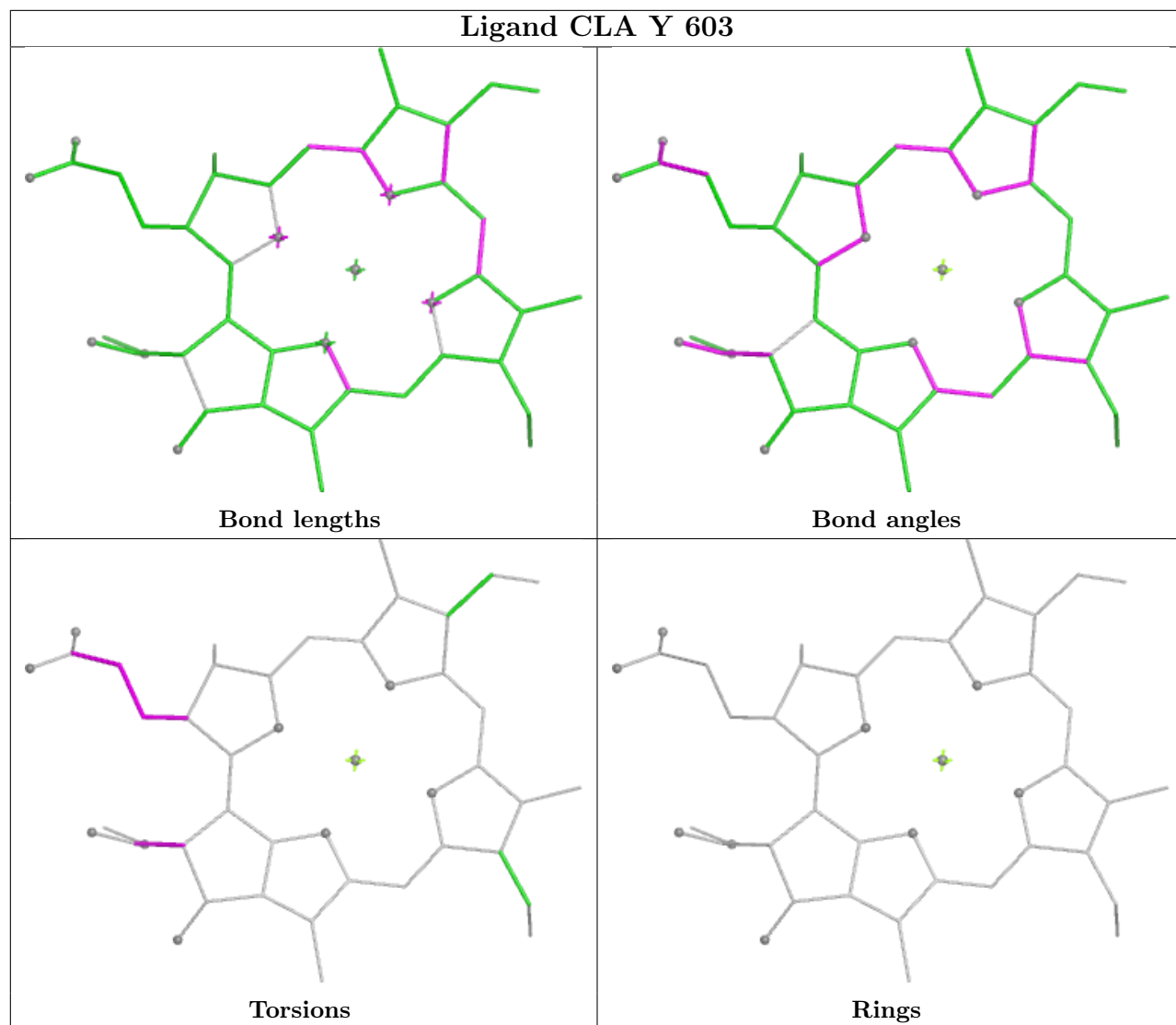
Ligand CLA 2 603

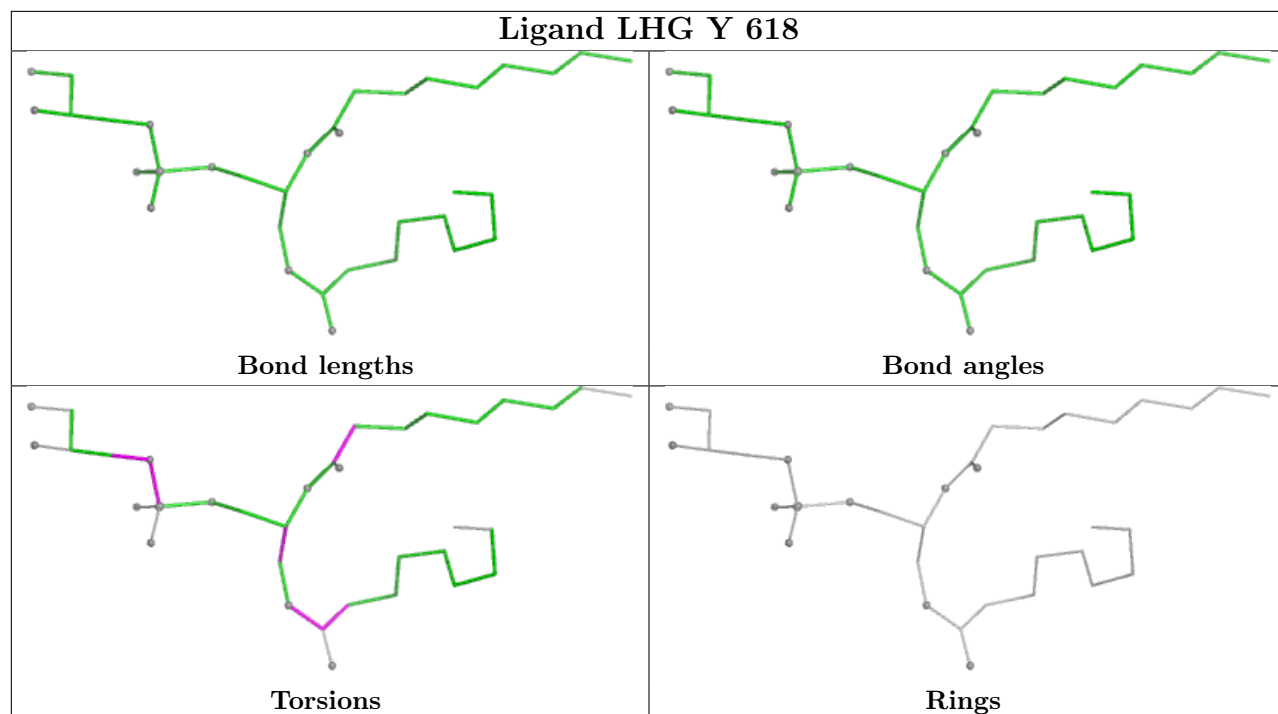


Ligand BCR L 306

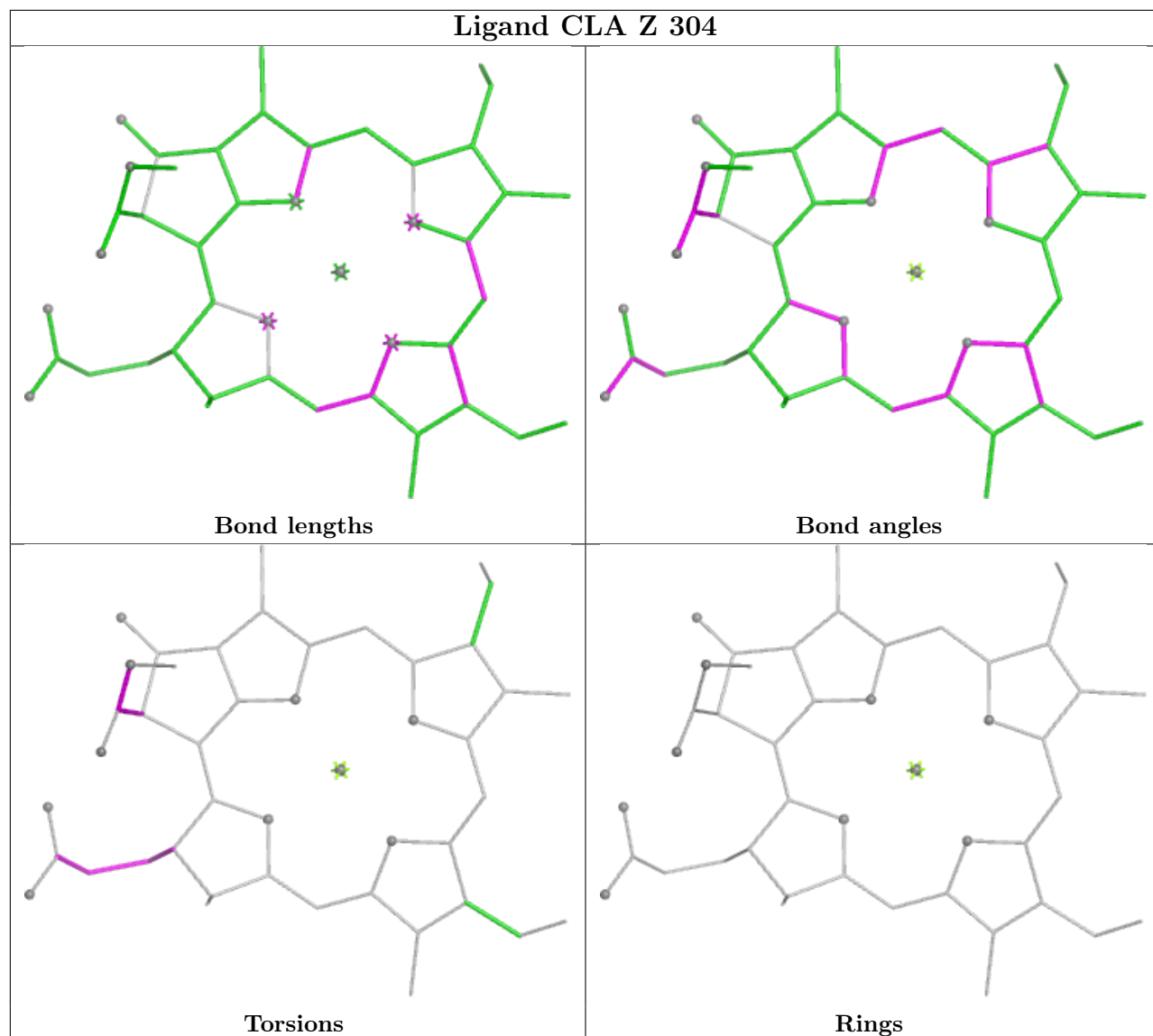


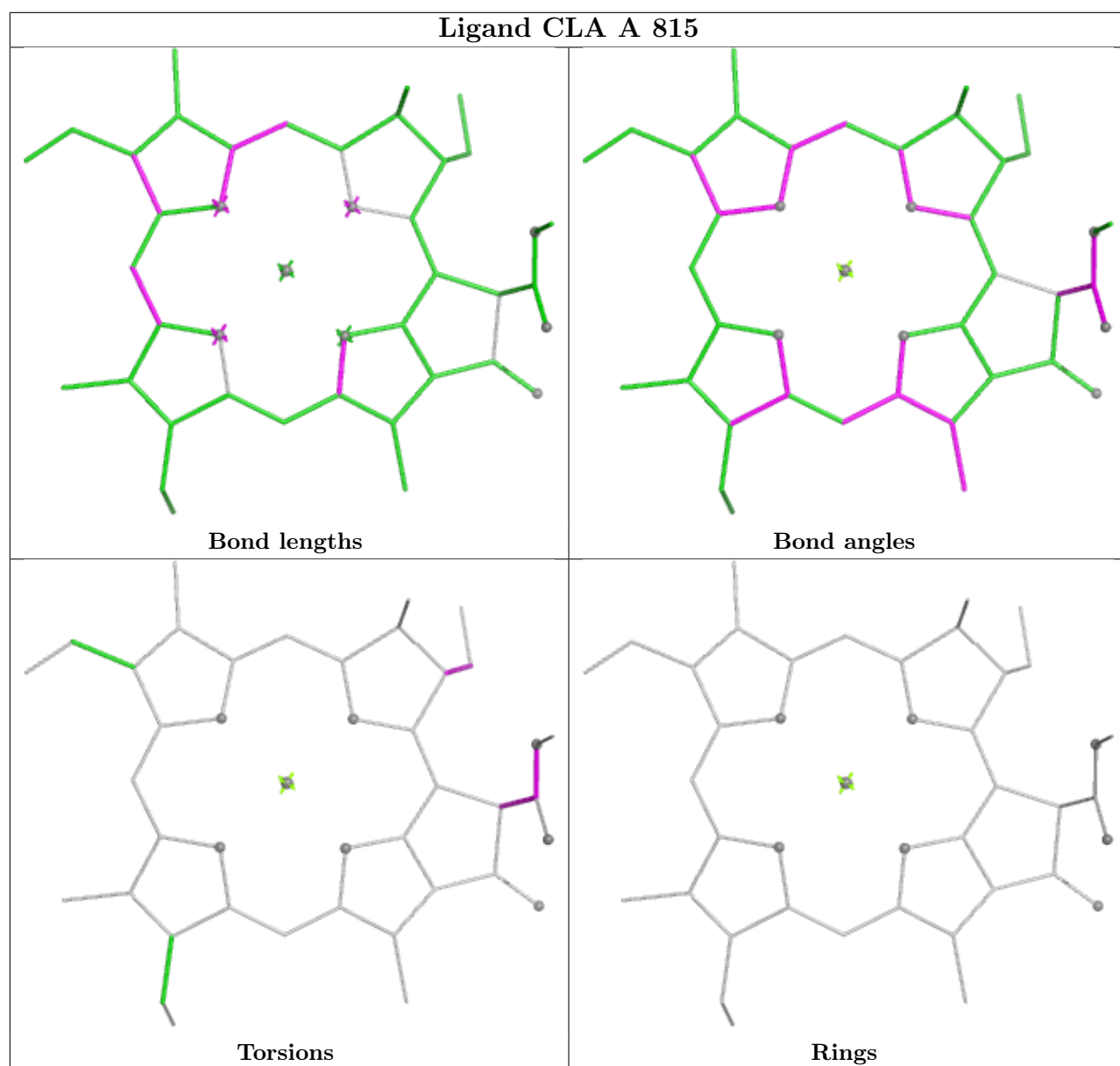


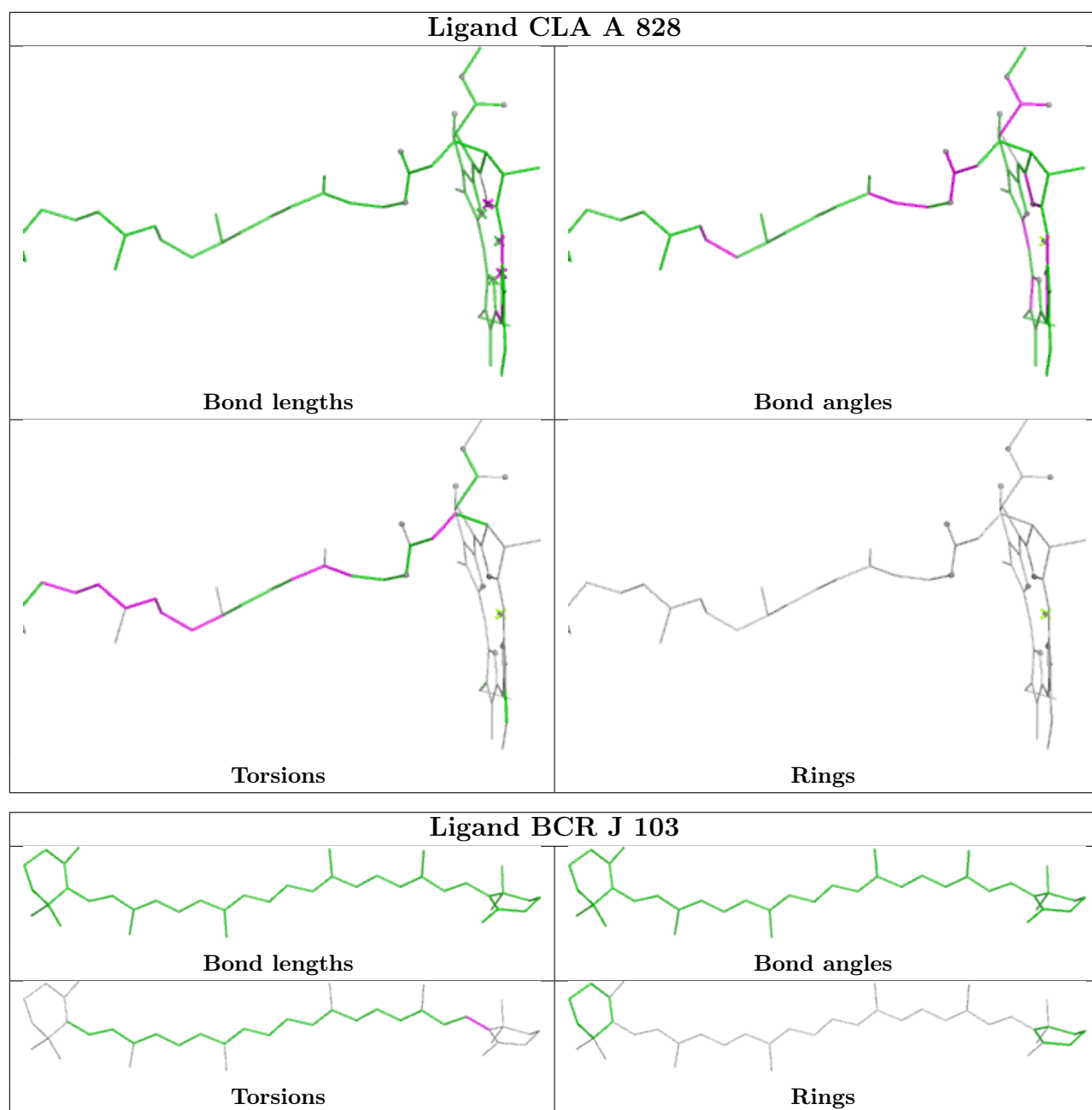


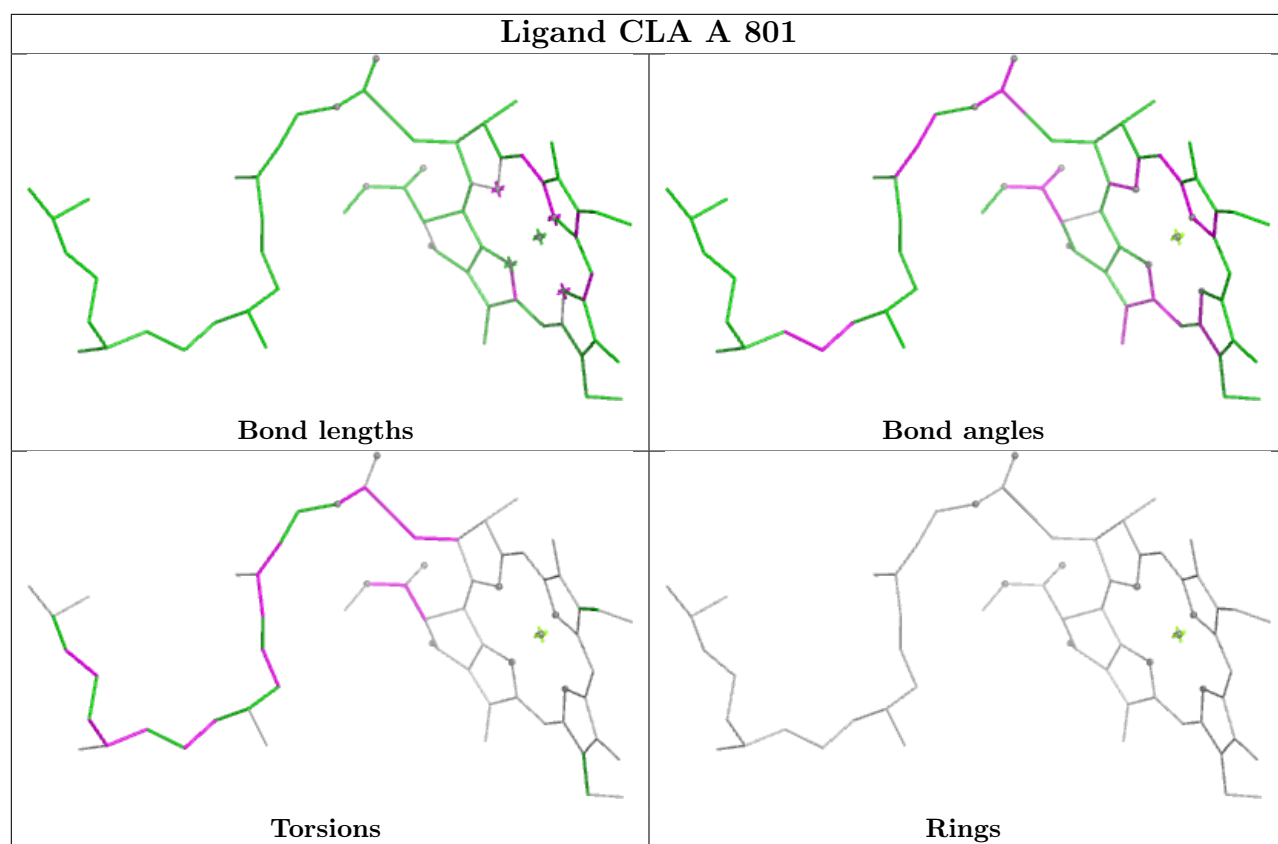


Ligand CLA Z 304

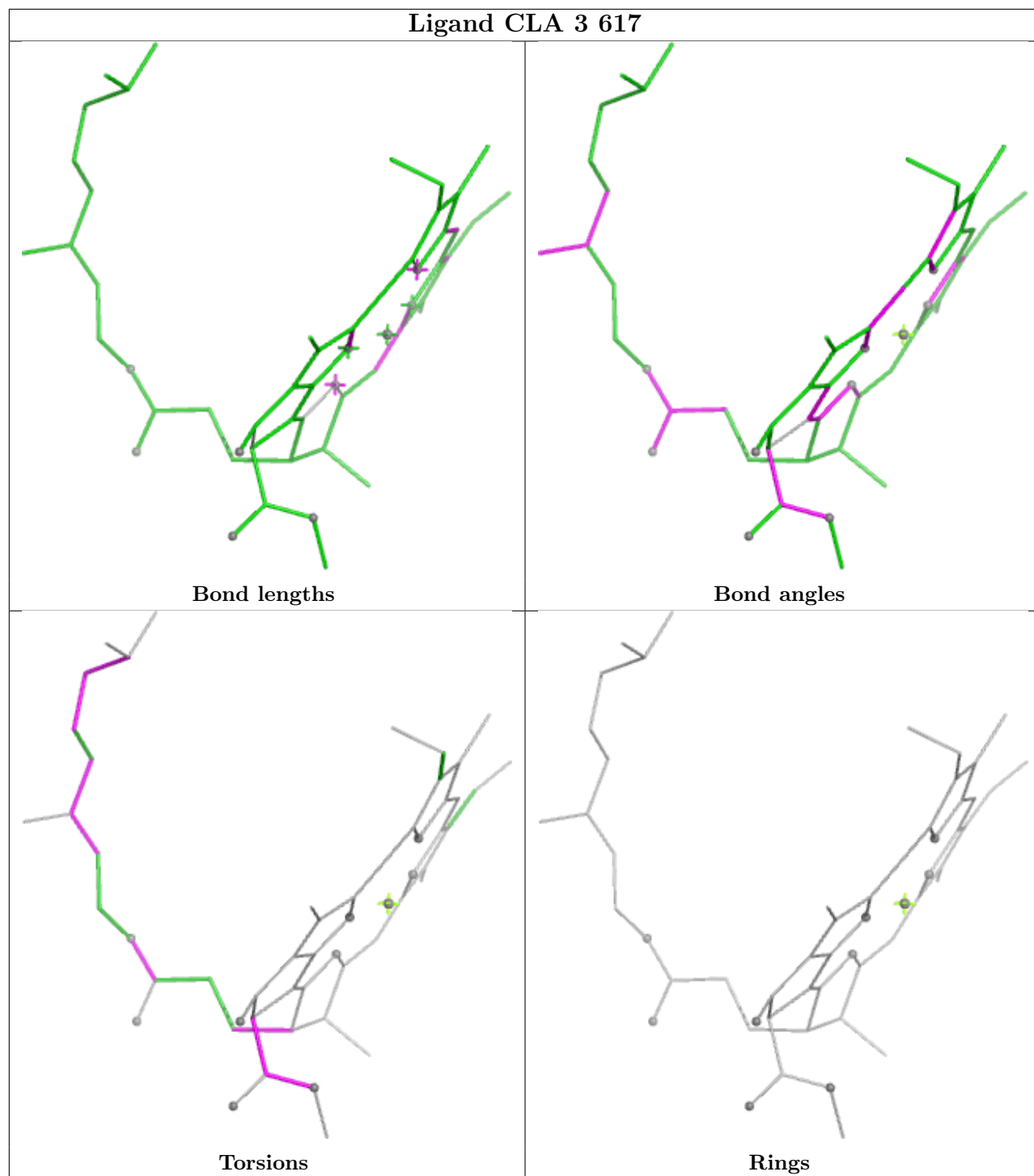




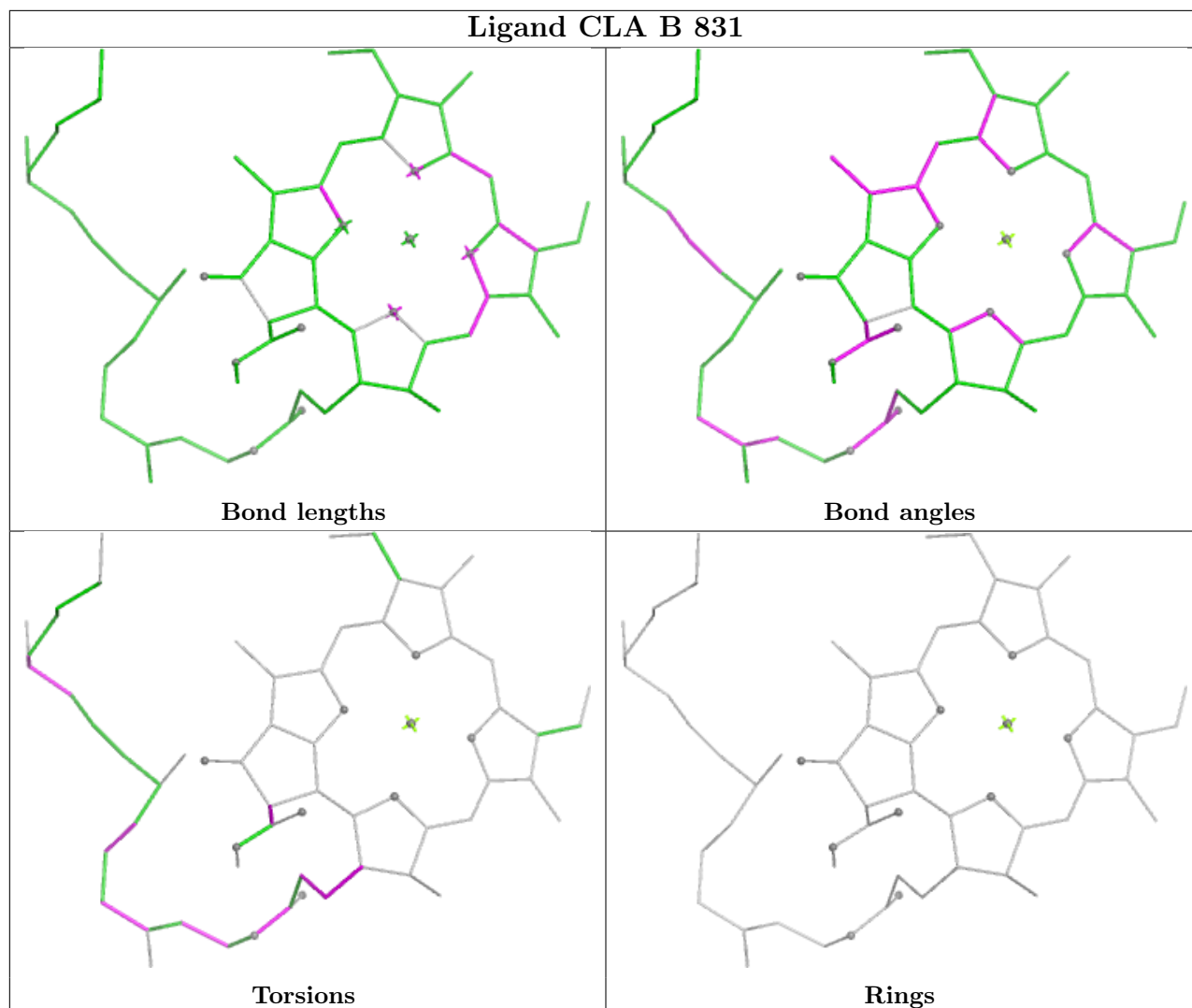




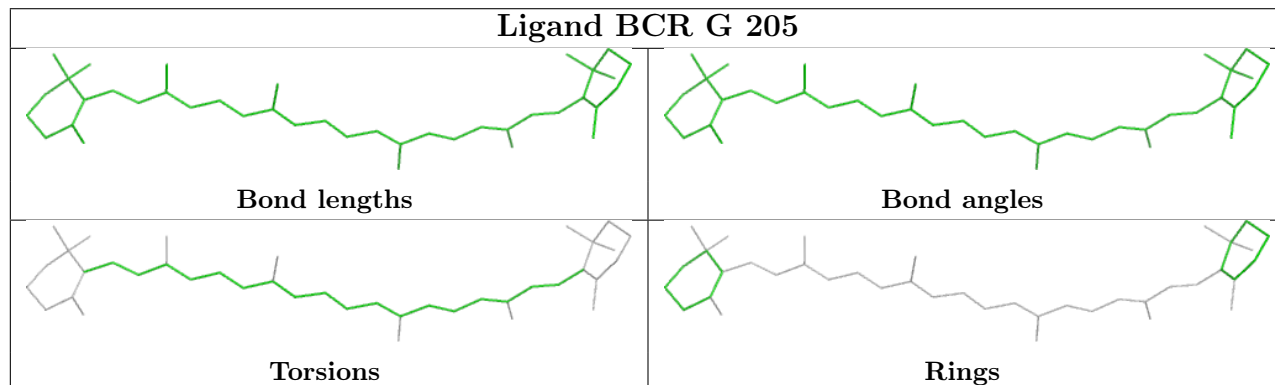
Ligand CLA 3 617



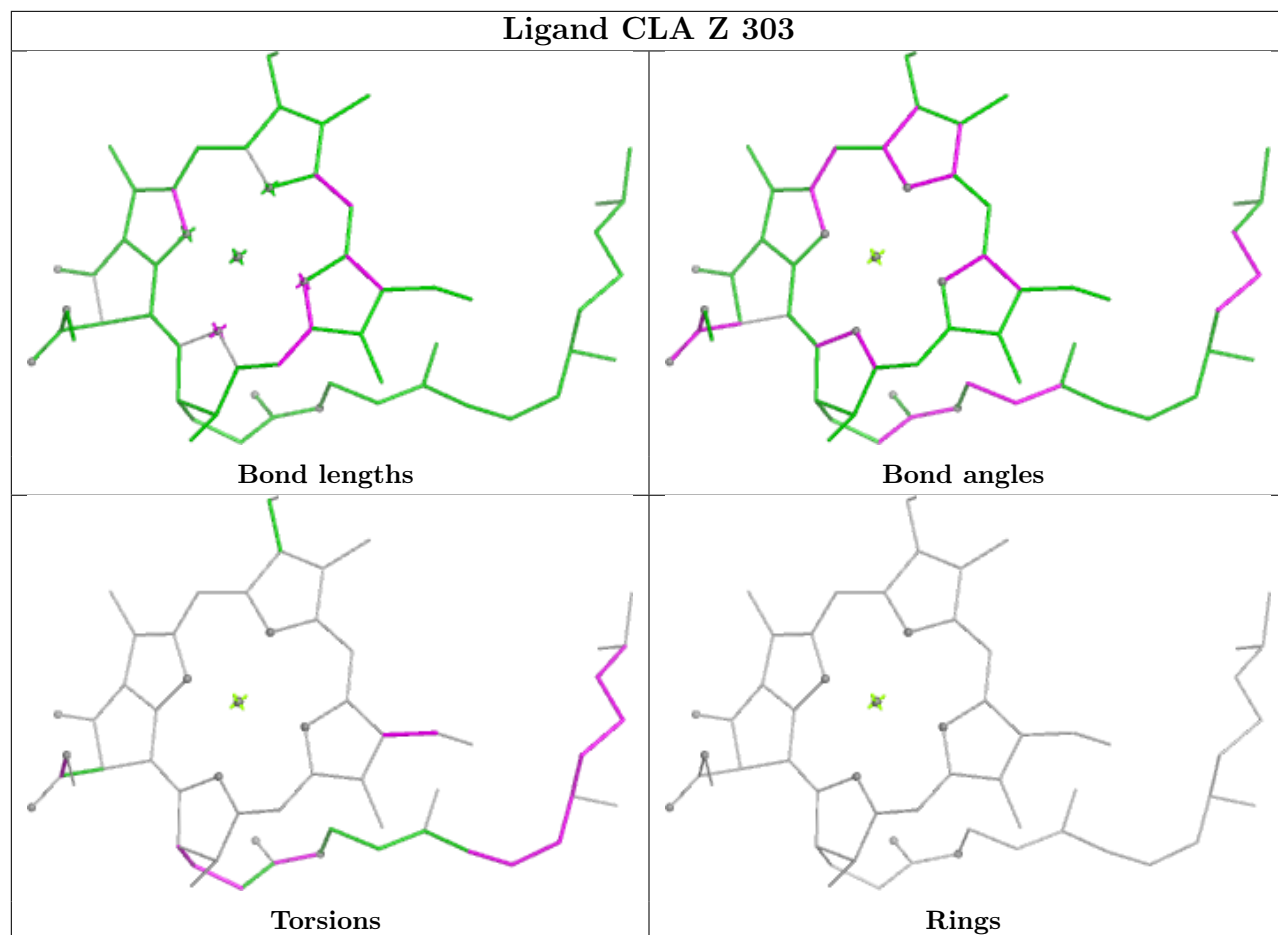
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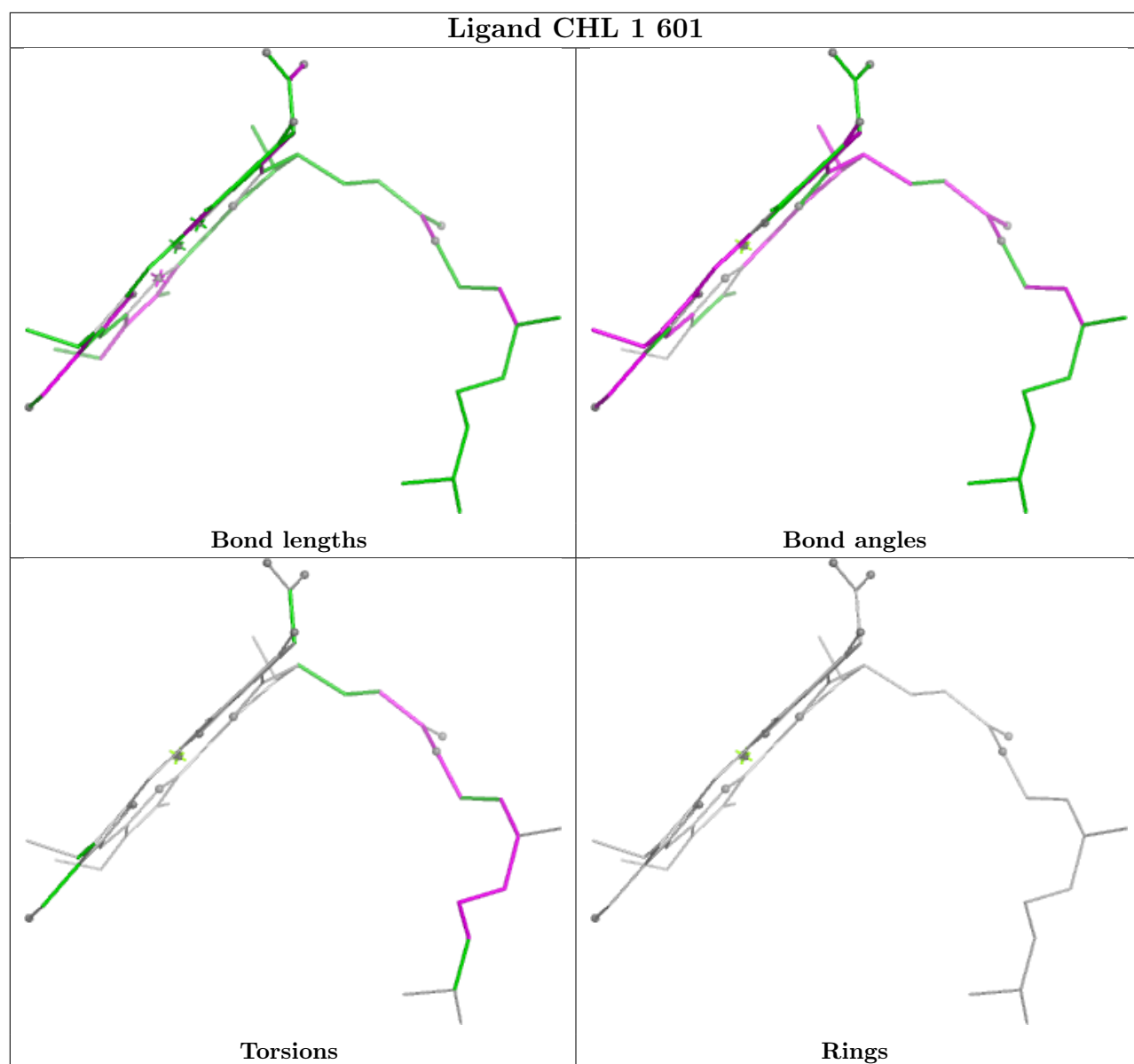


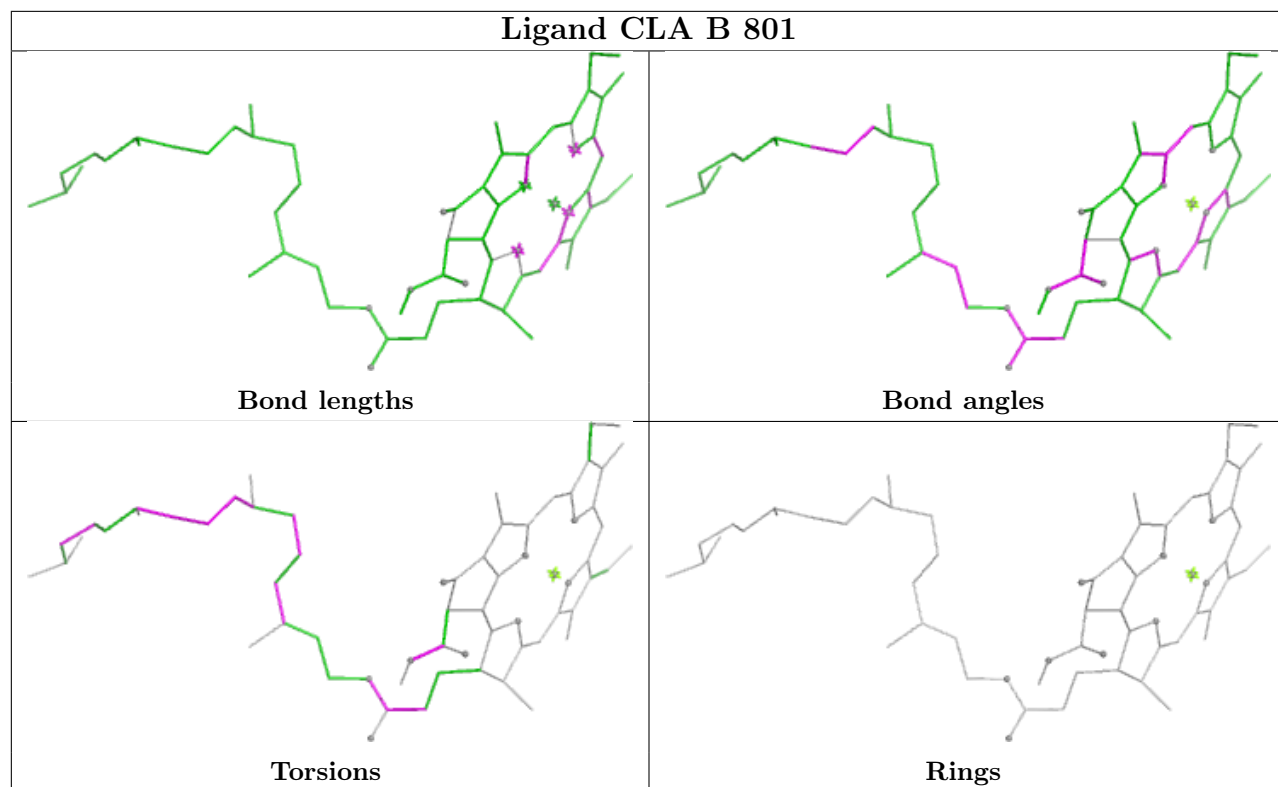
Ligand BCR G 205



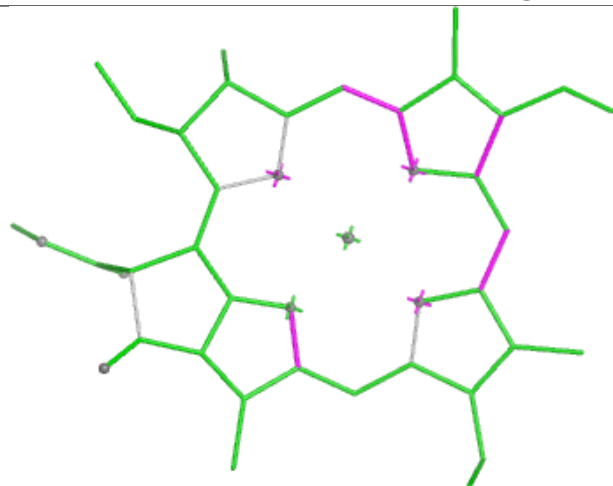
Ligand CLA Z 303



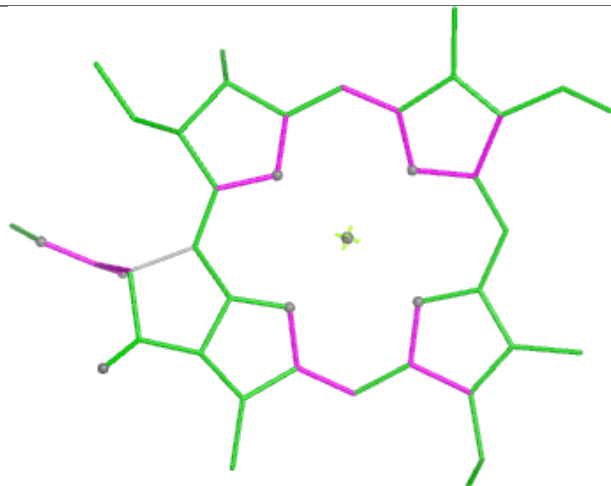




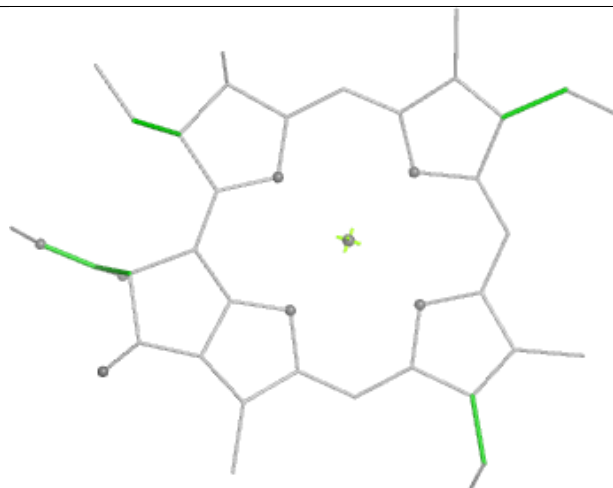
Ligand CLA J 101



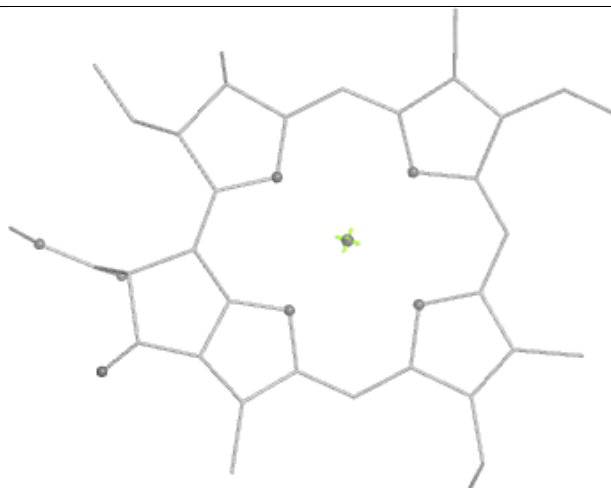
Bond lengths



Bond angles

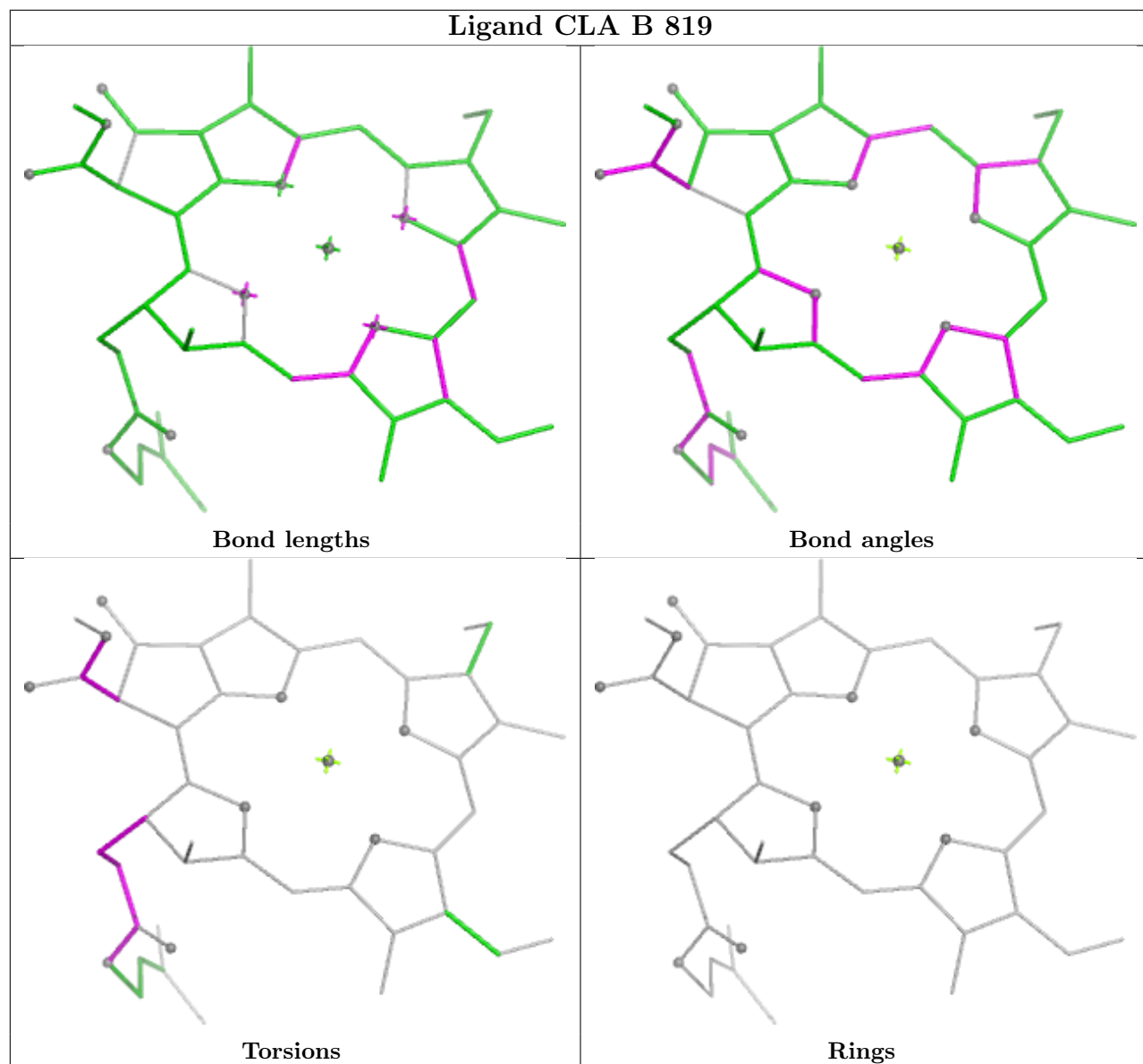


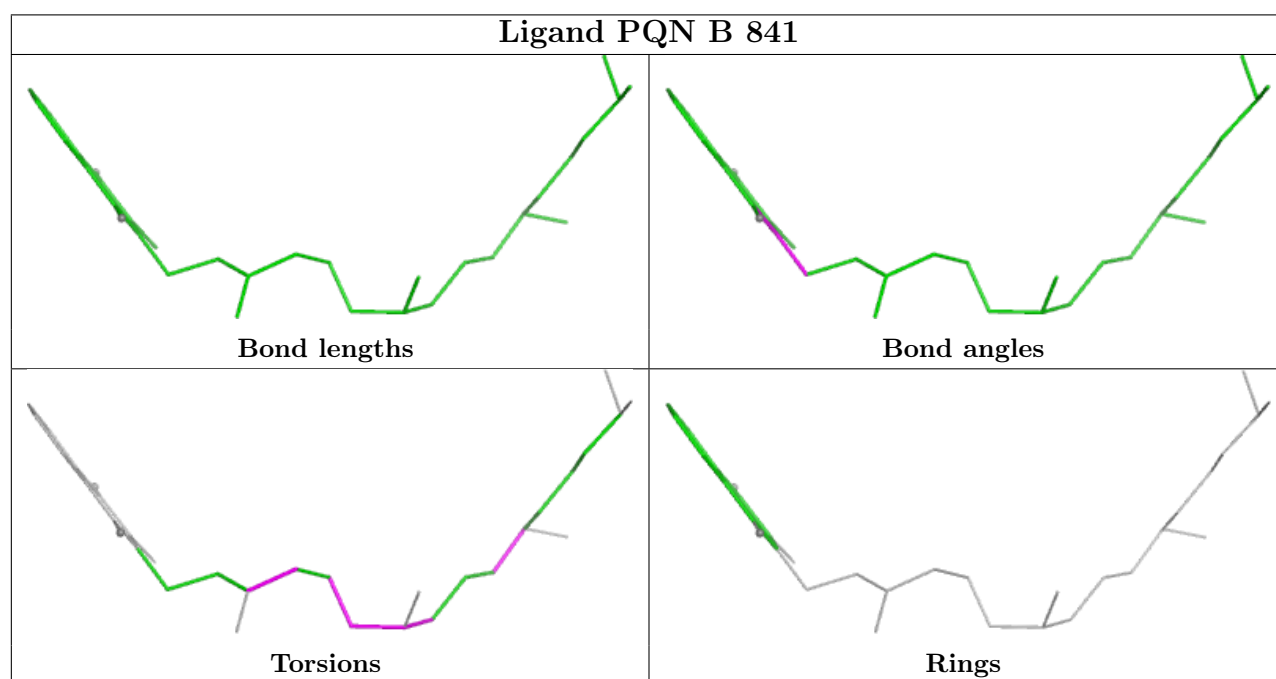
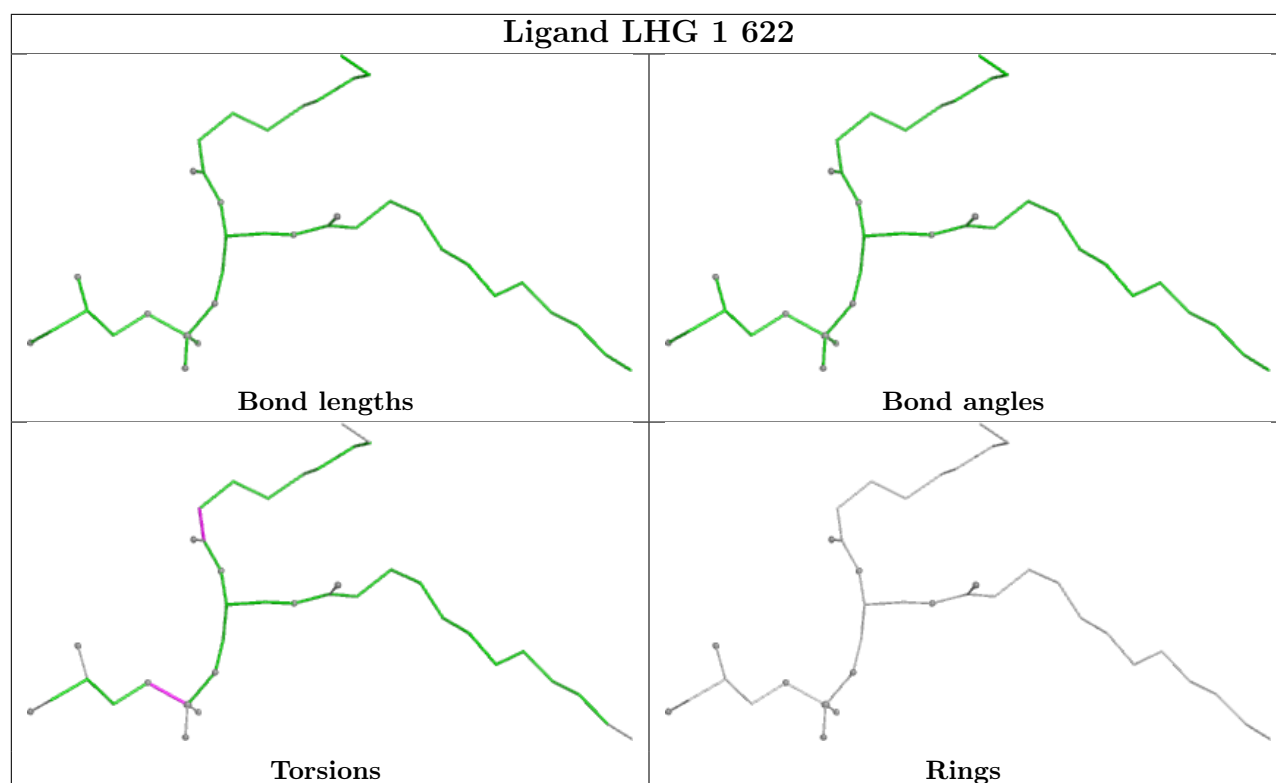
Torsions



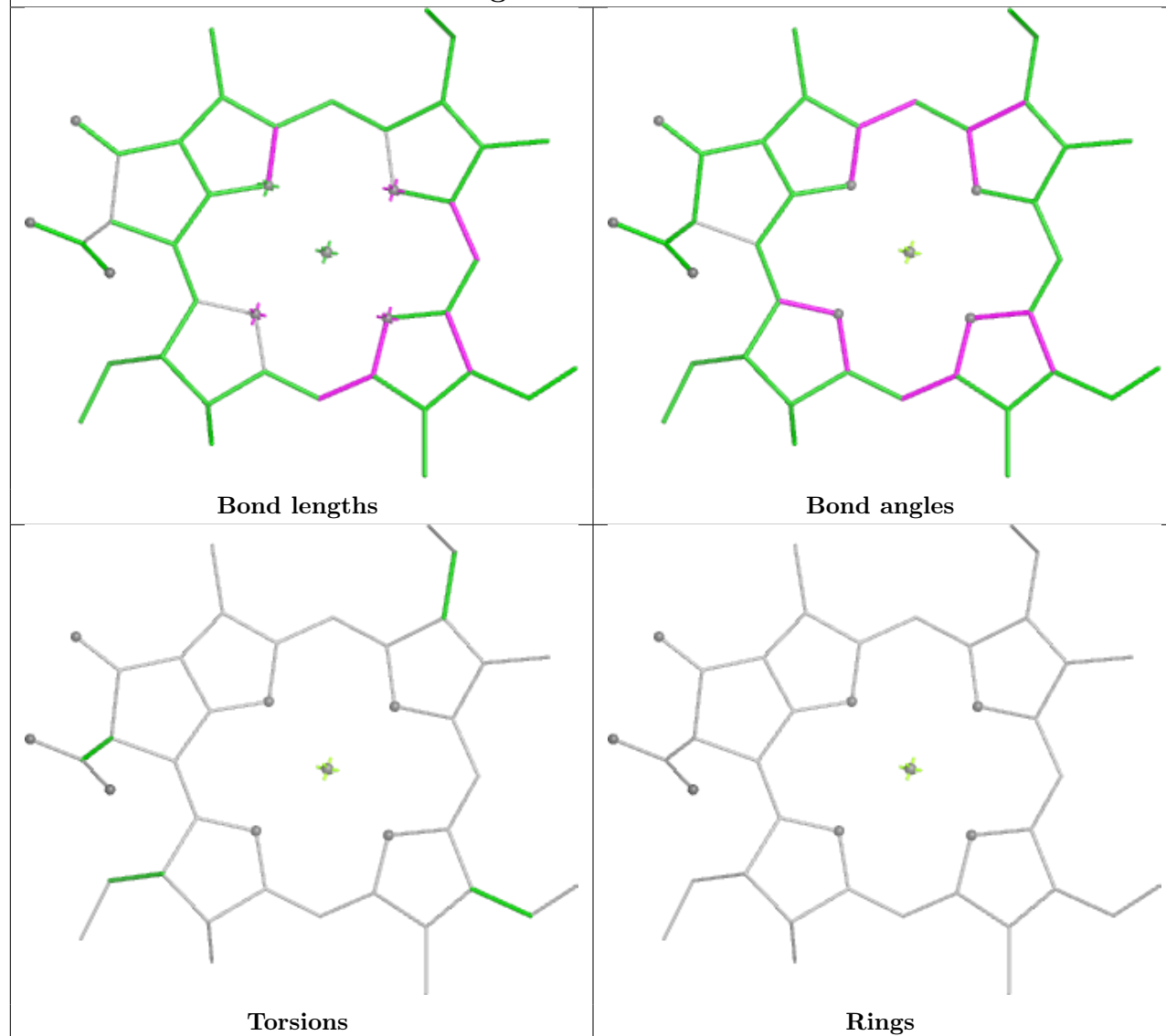
Rings

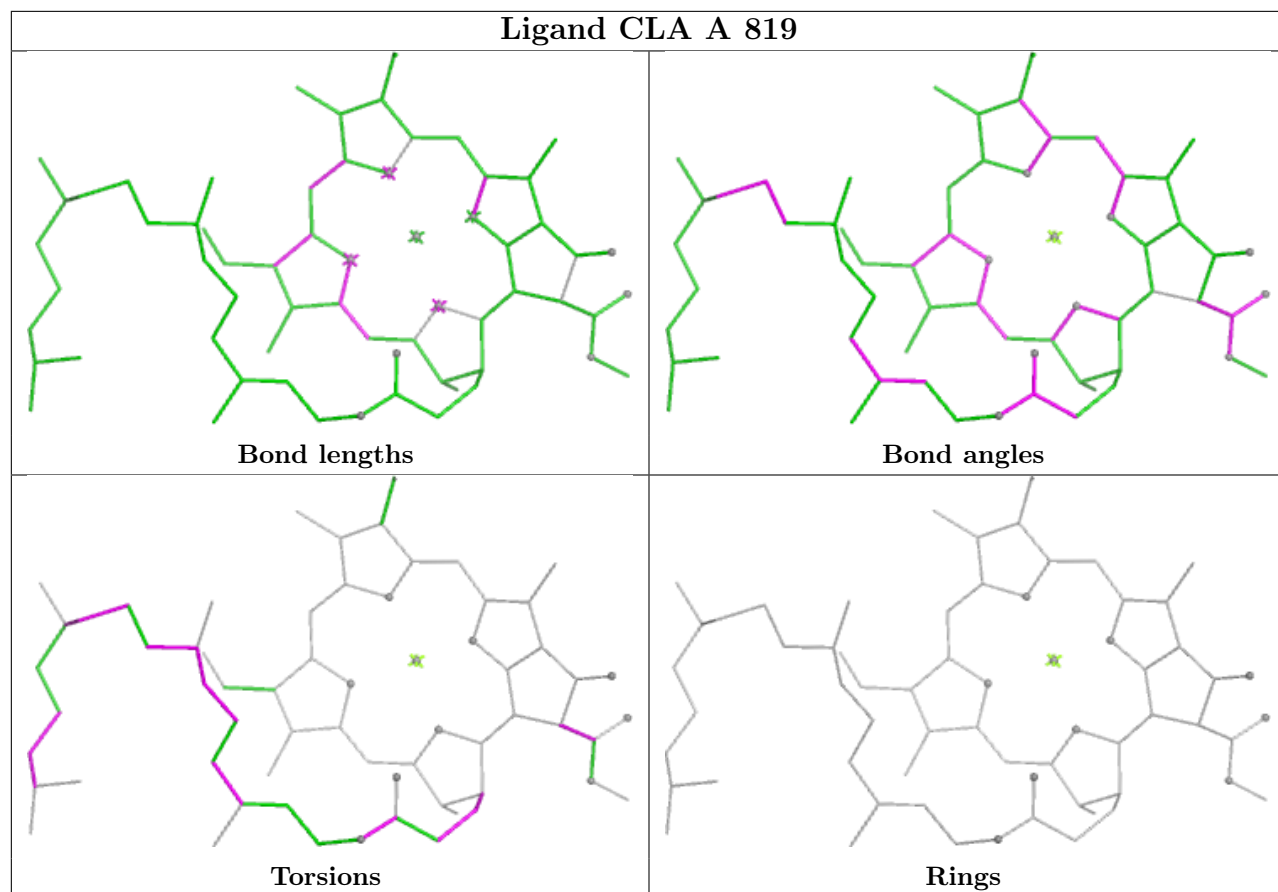
Ligand CLA B 819

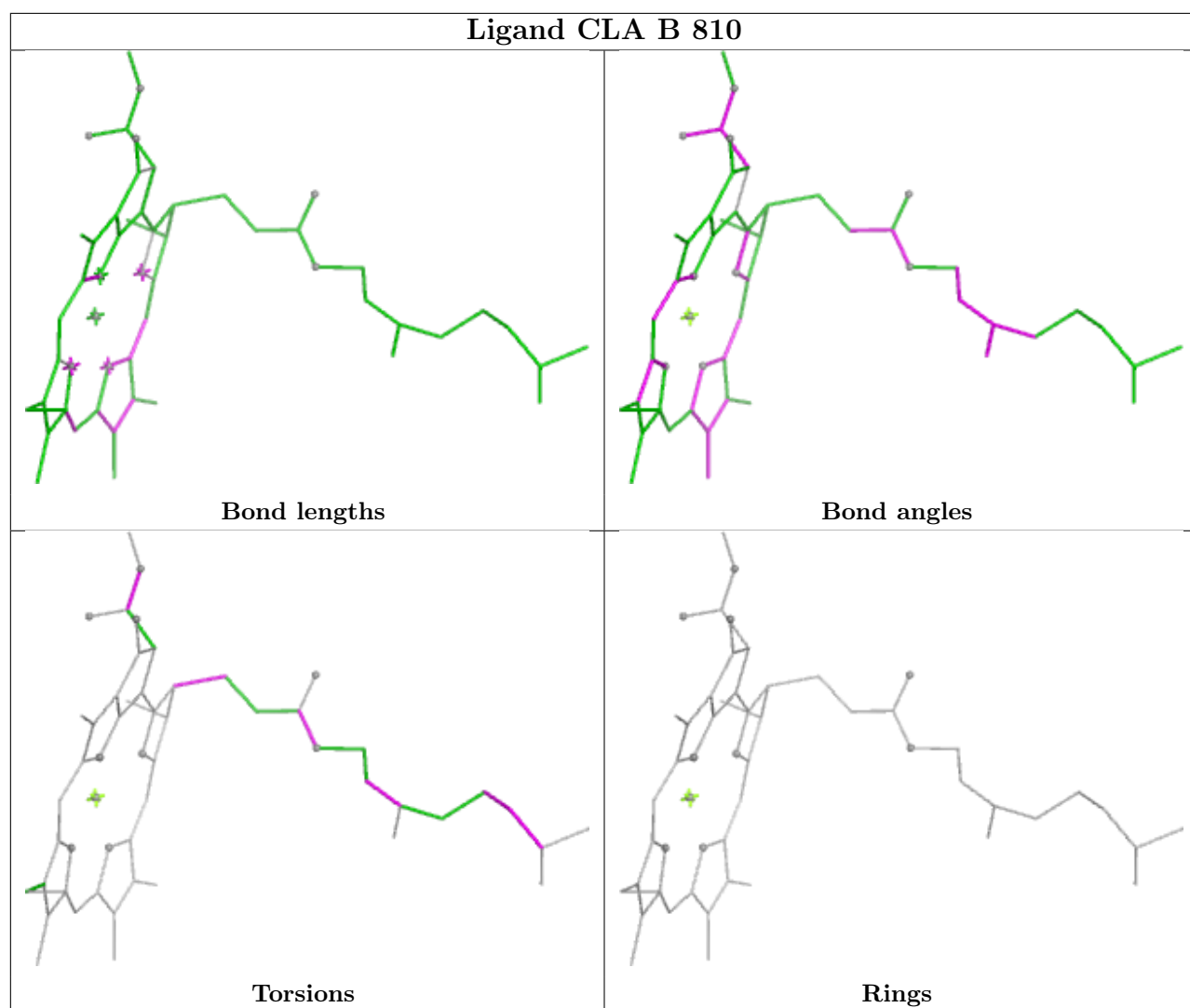


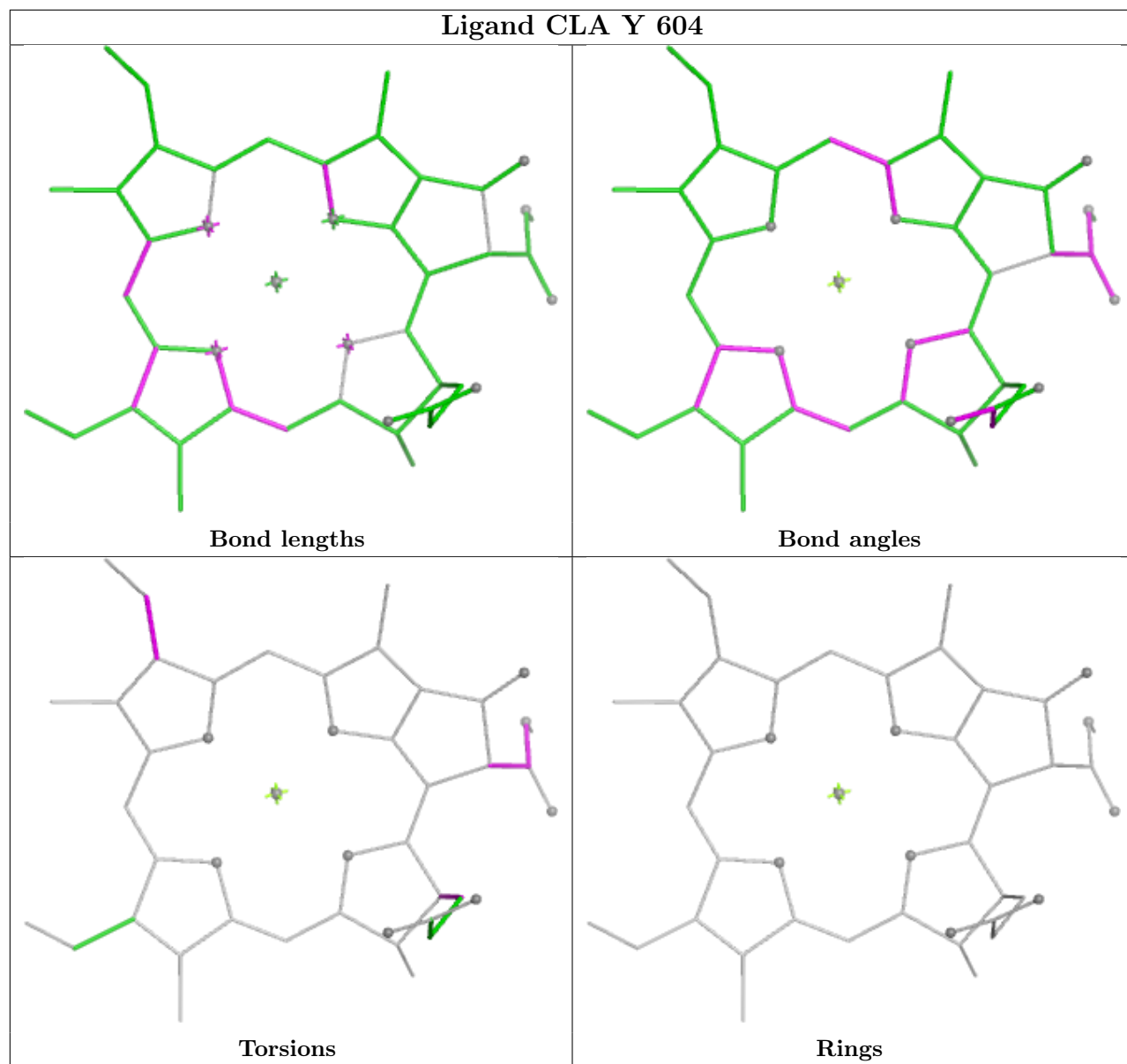


Ligand CLA 6 611

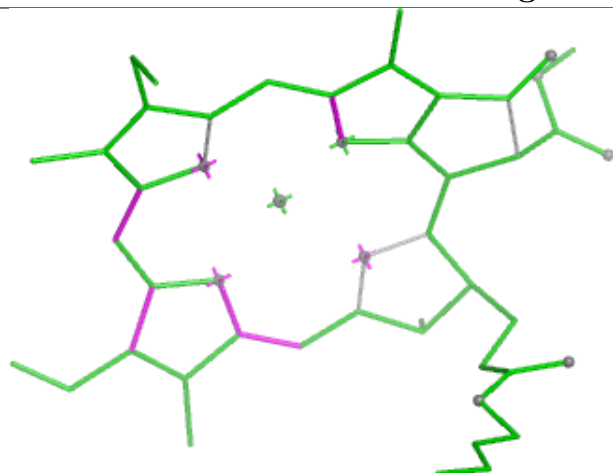




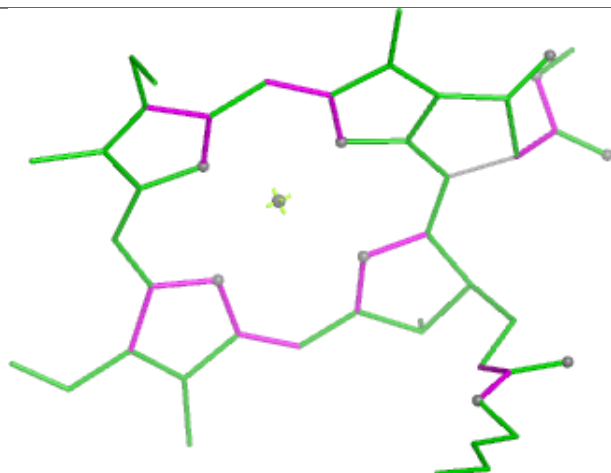




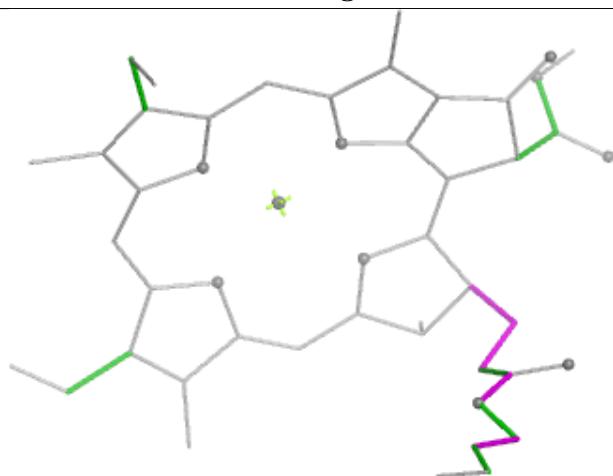
Ligand CLA 1 604



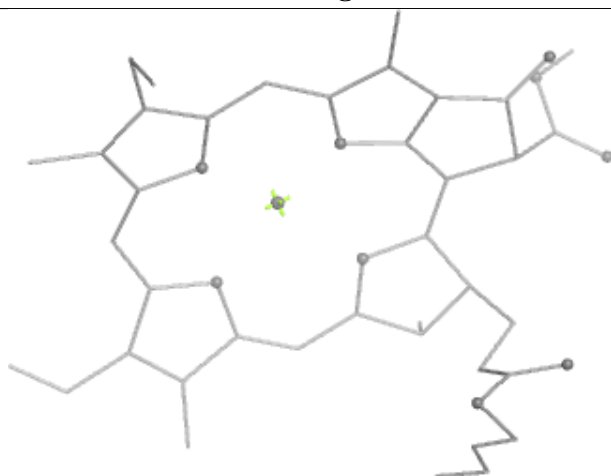
Bond lengths



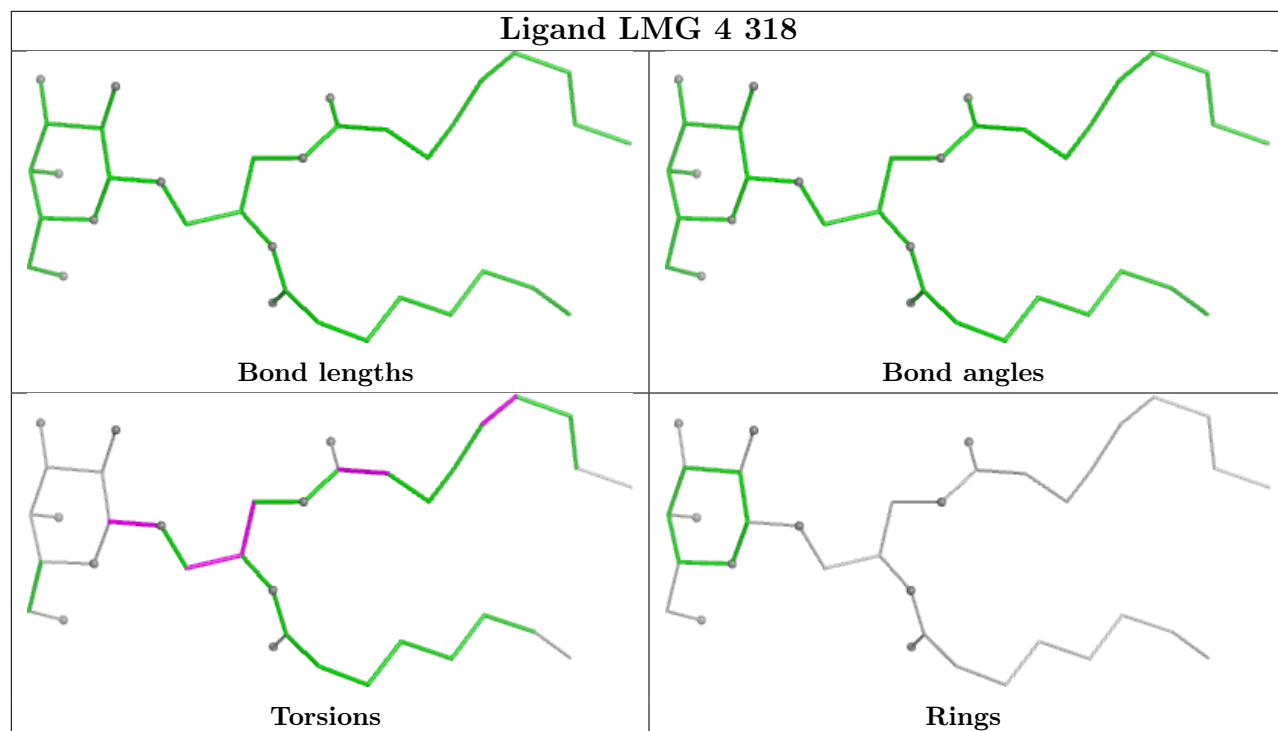
Bond angles

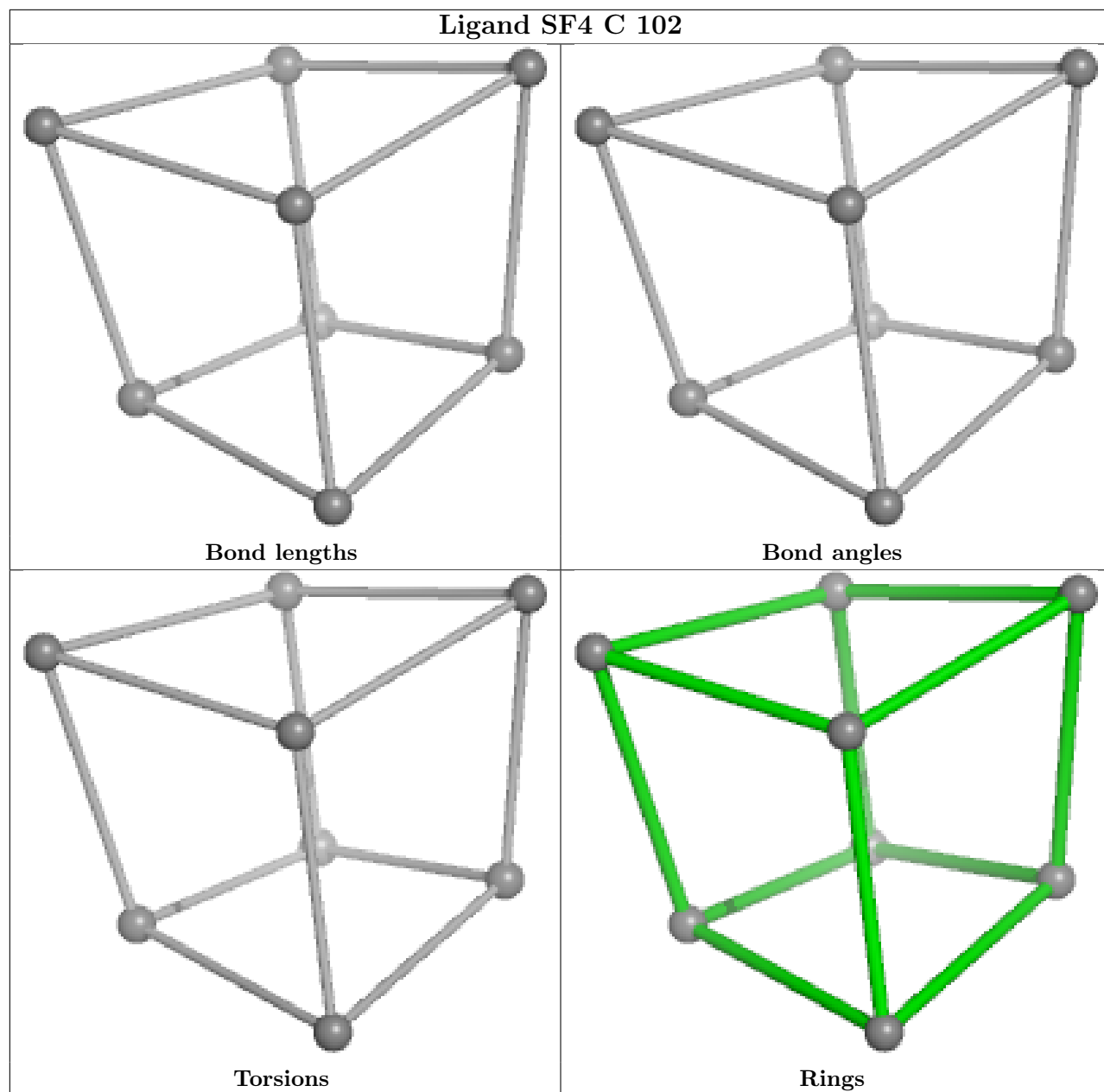


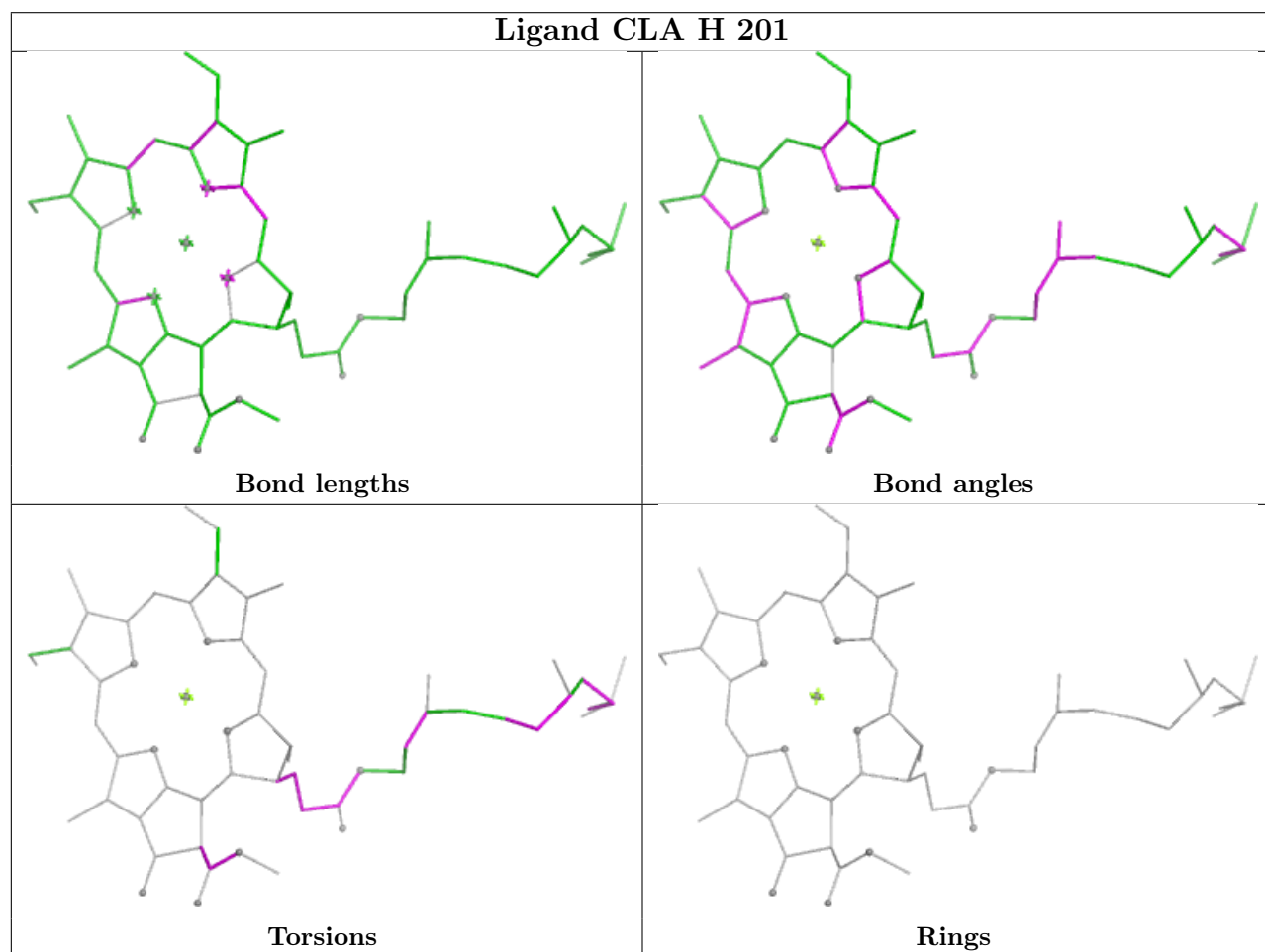
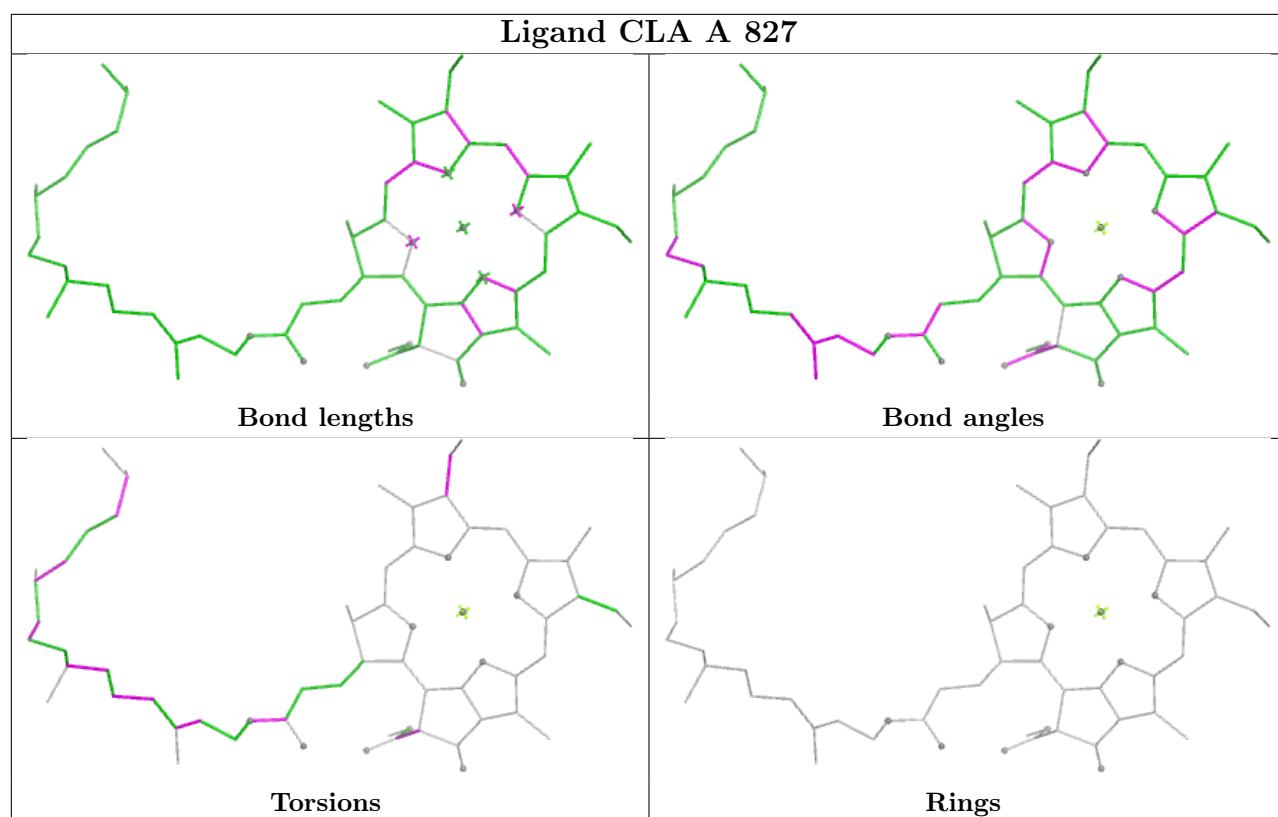
Torsions

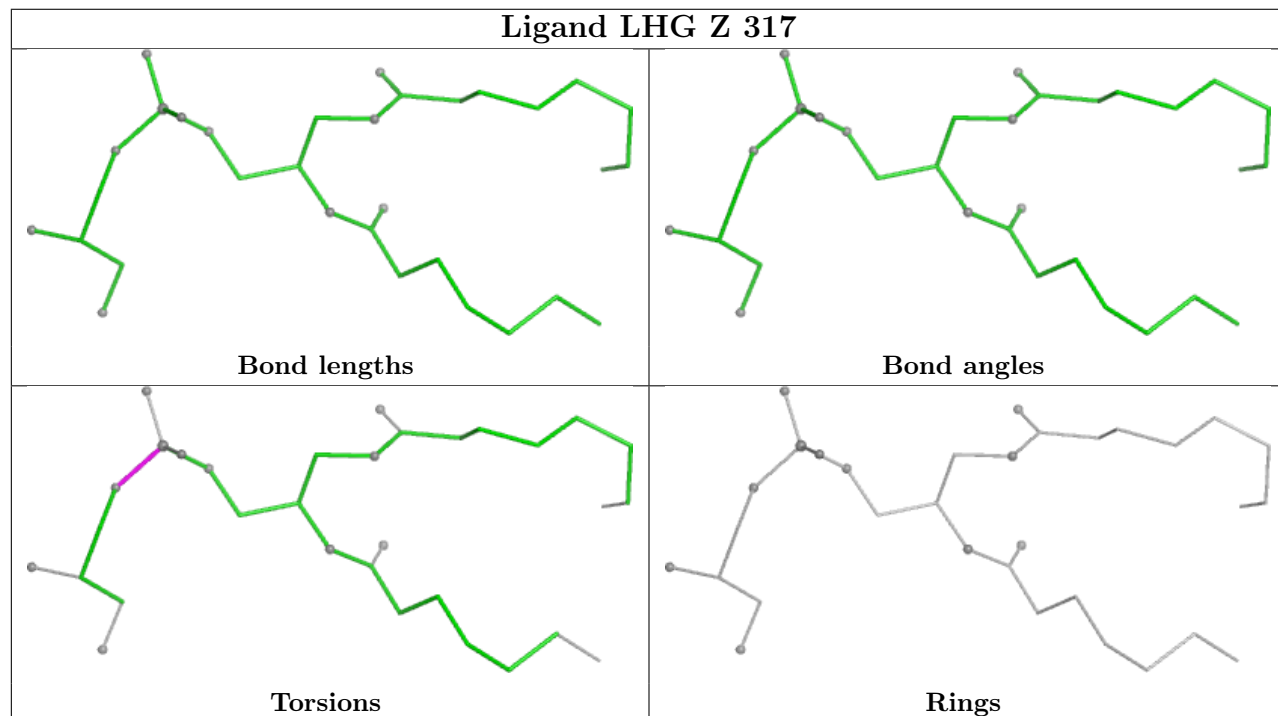
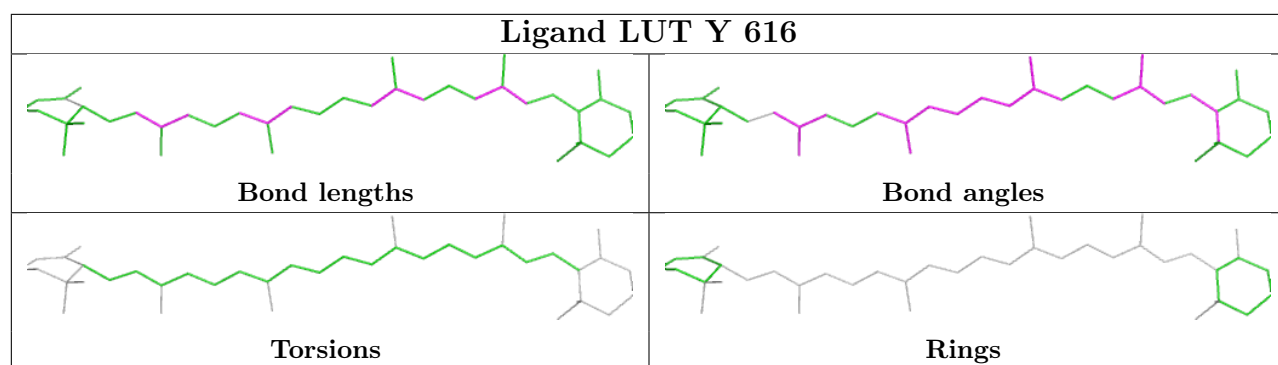


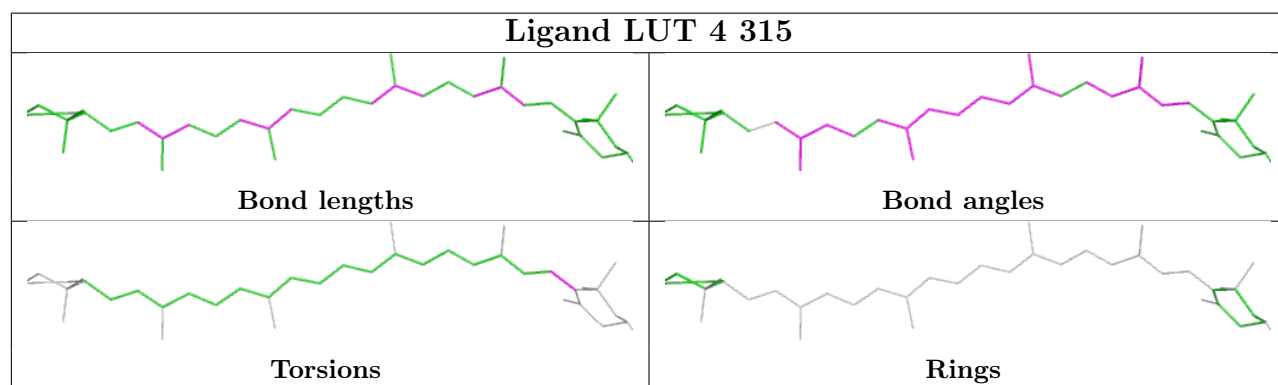
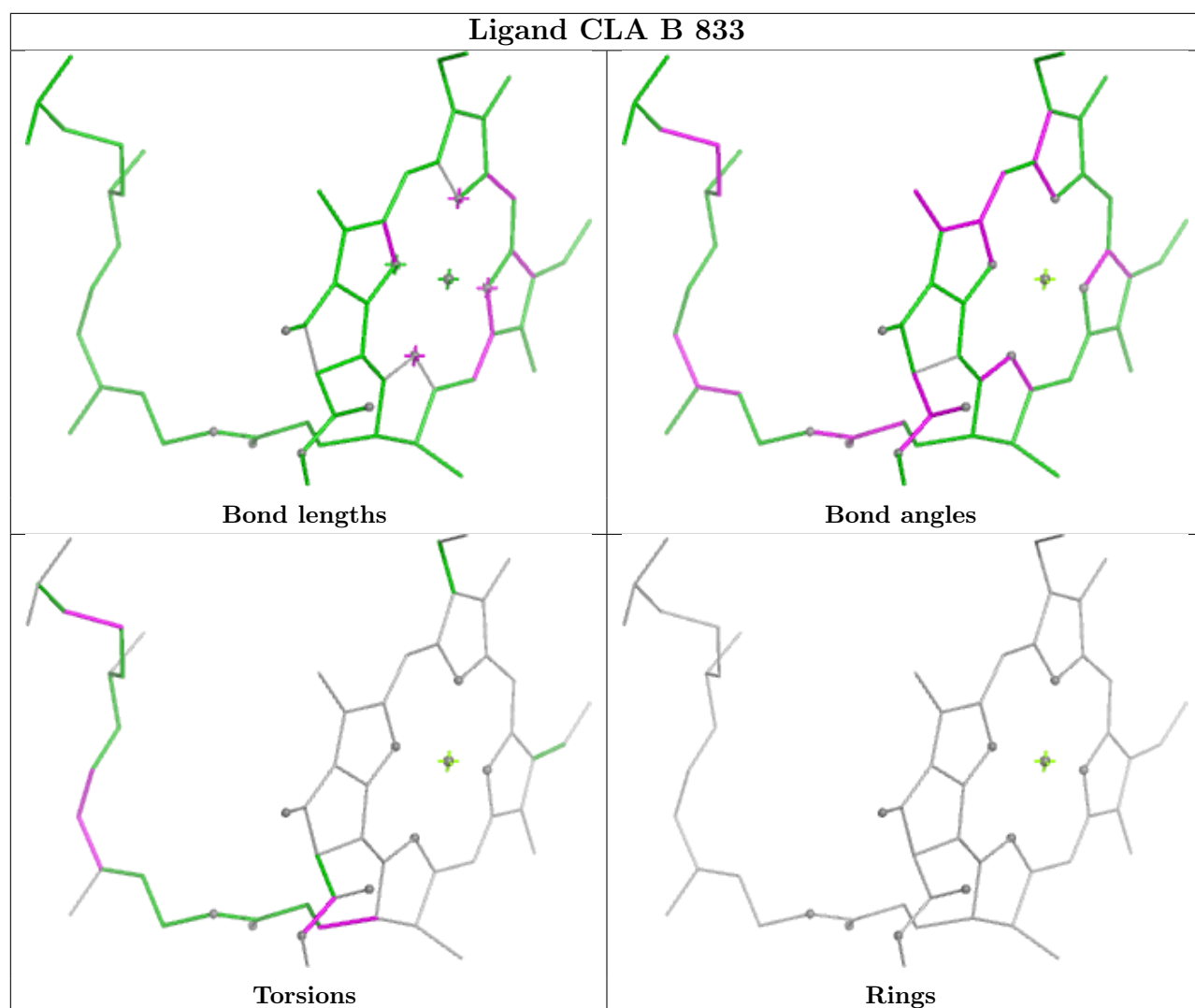
Rings

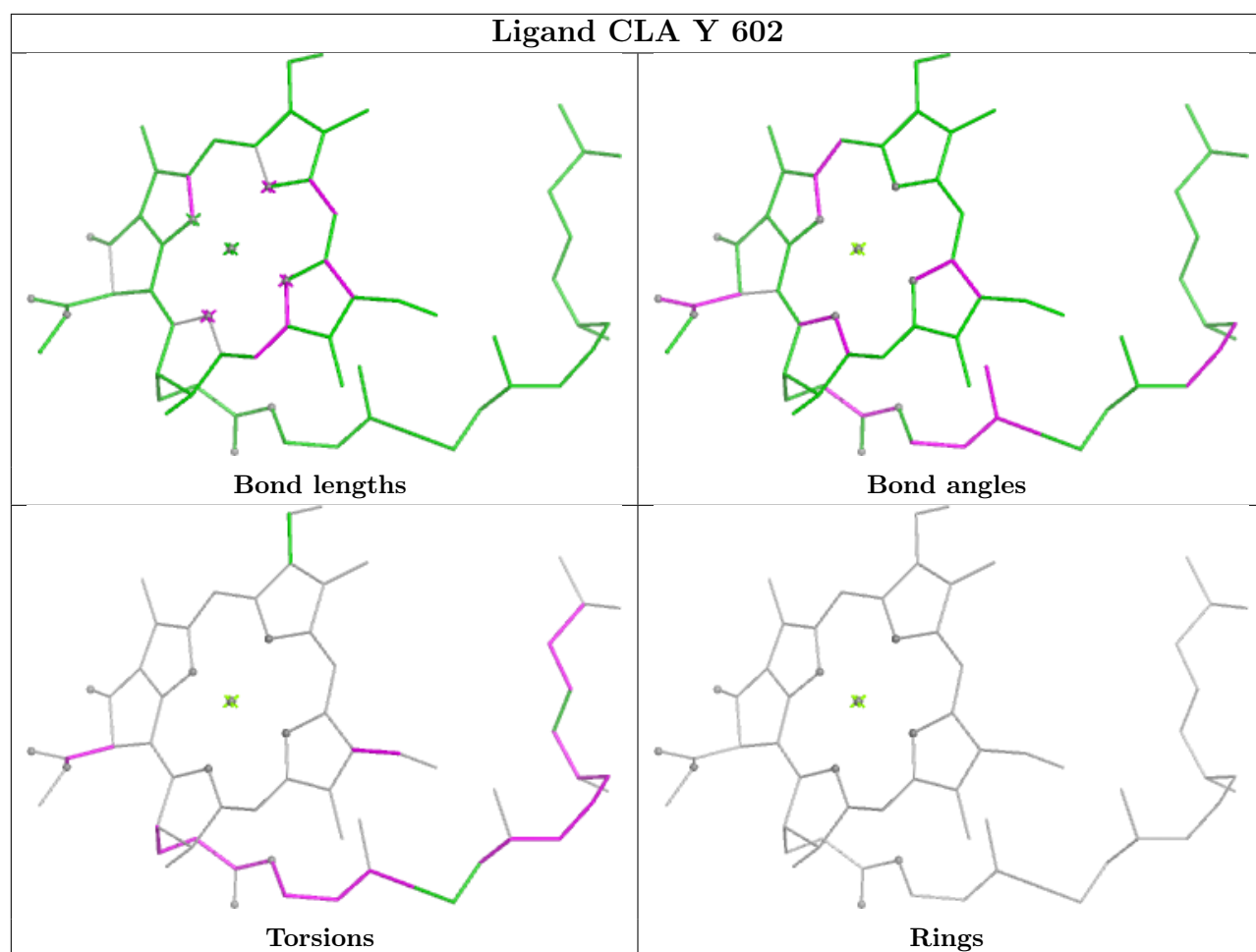


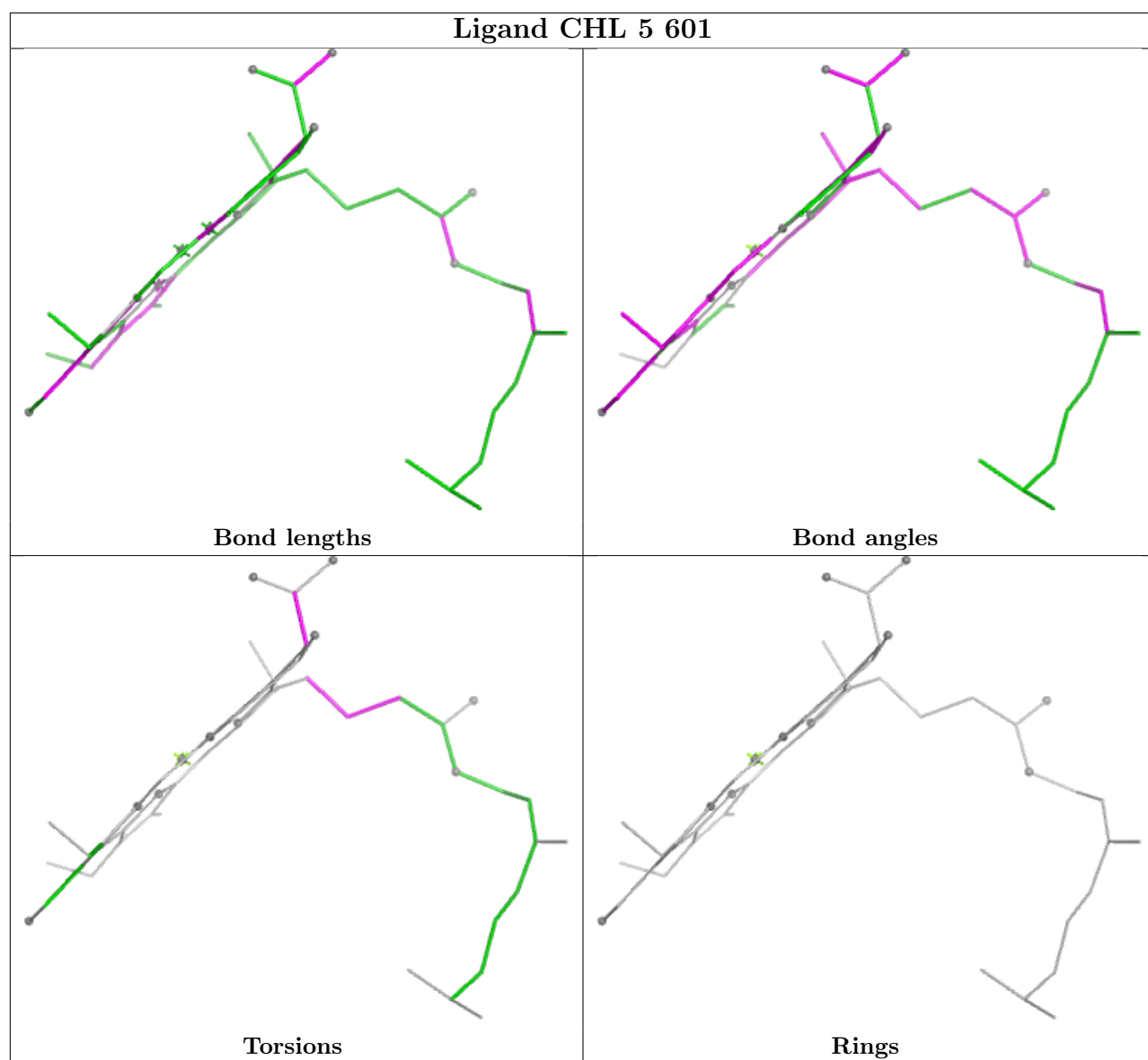


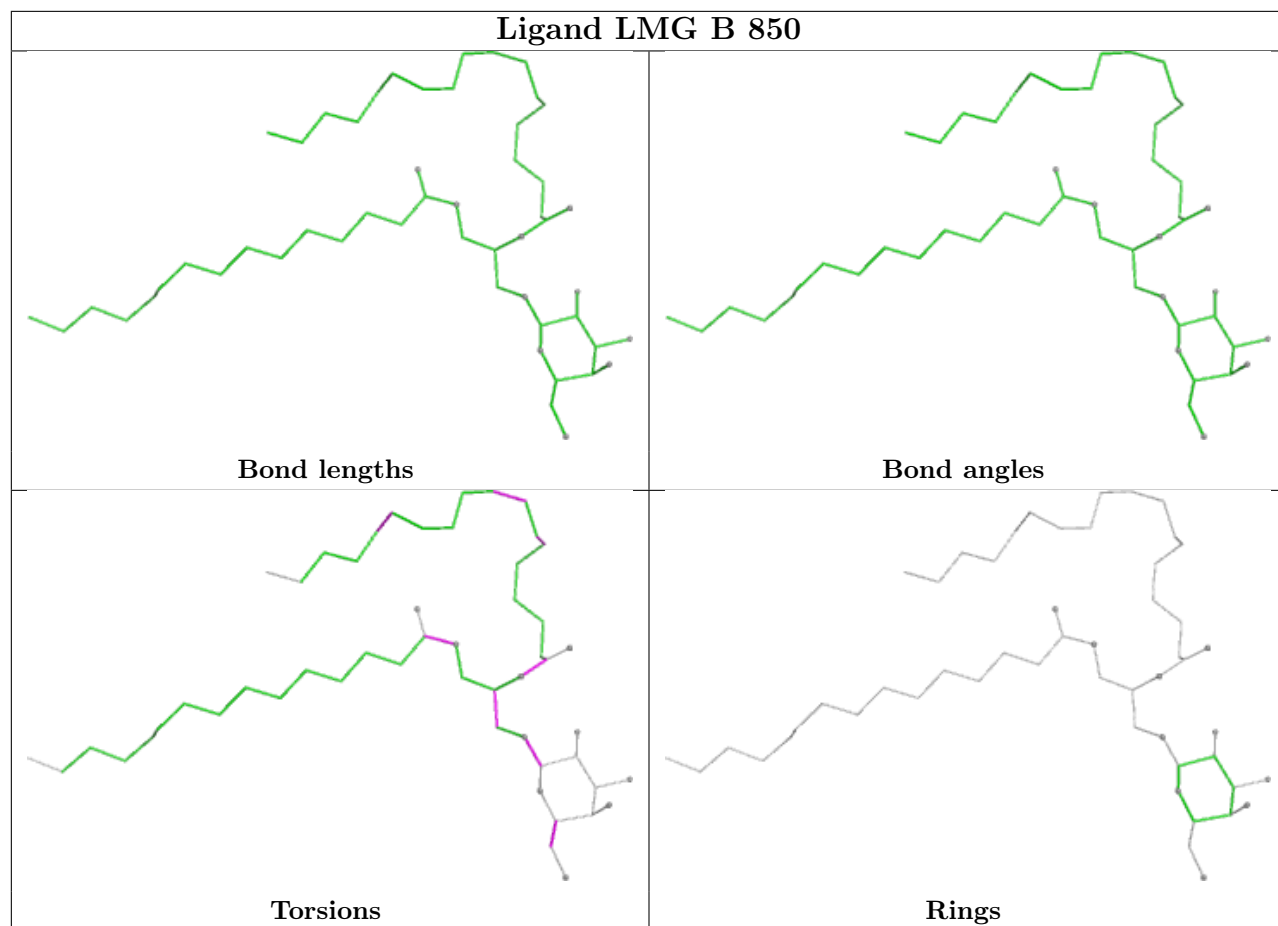




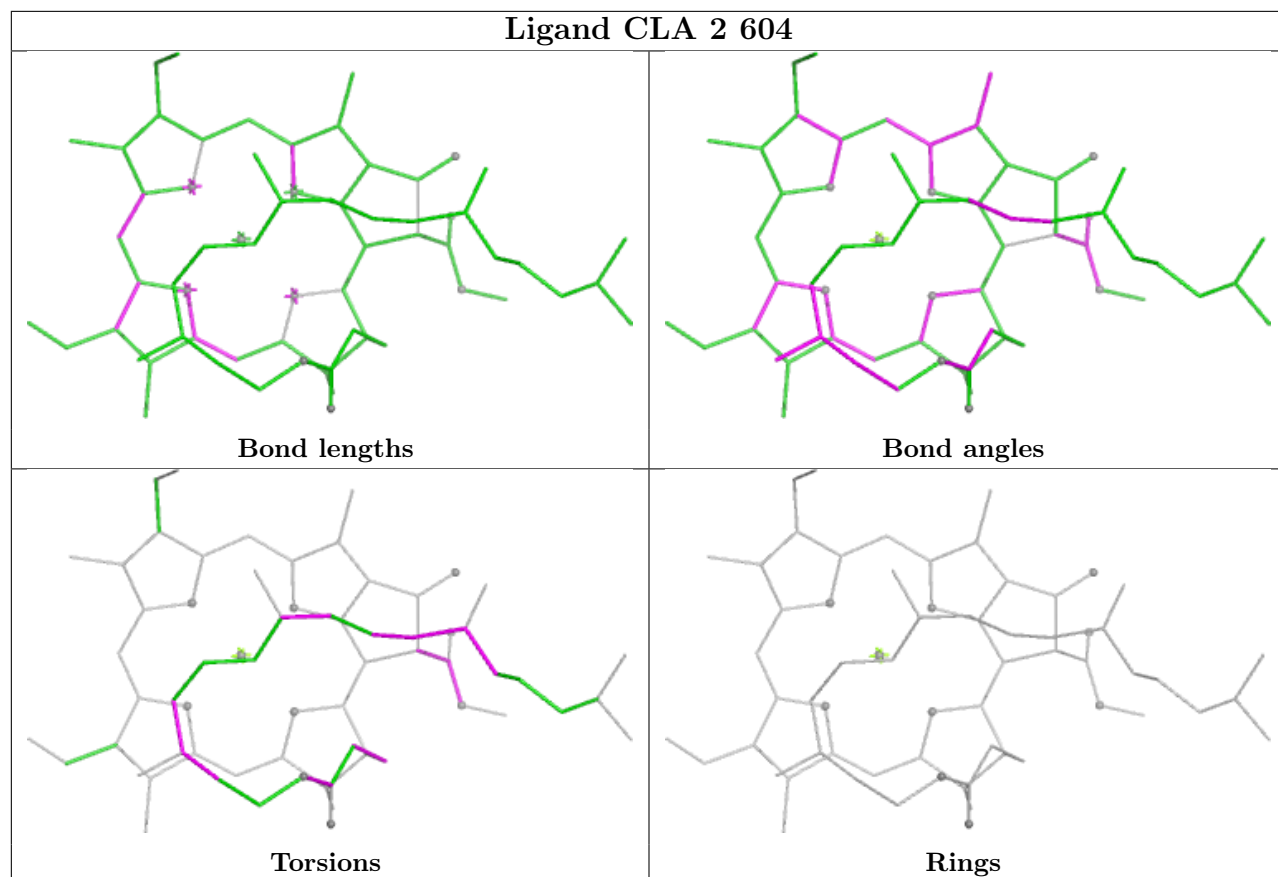




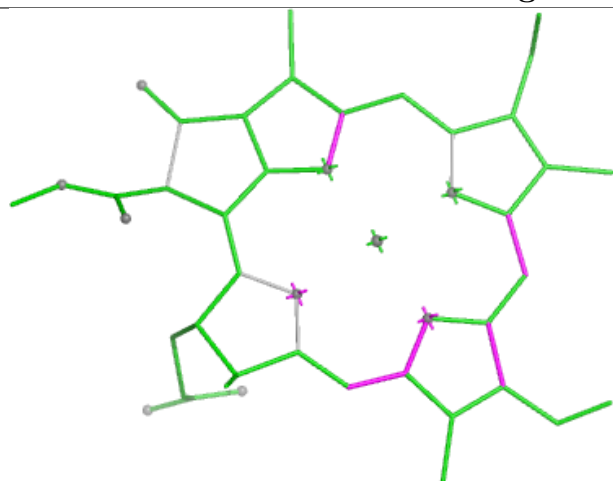




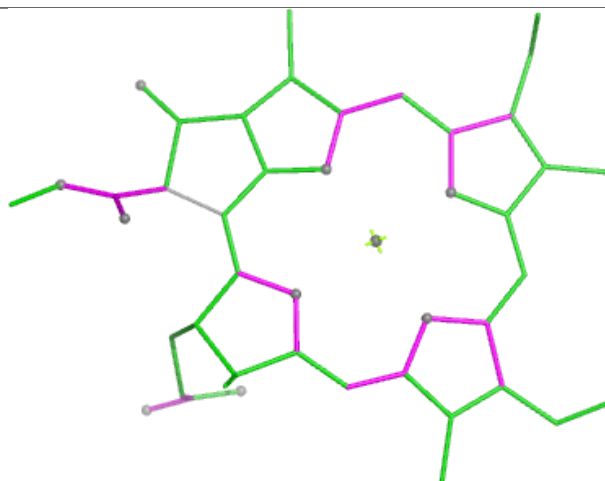
Ligand CLA 2 604



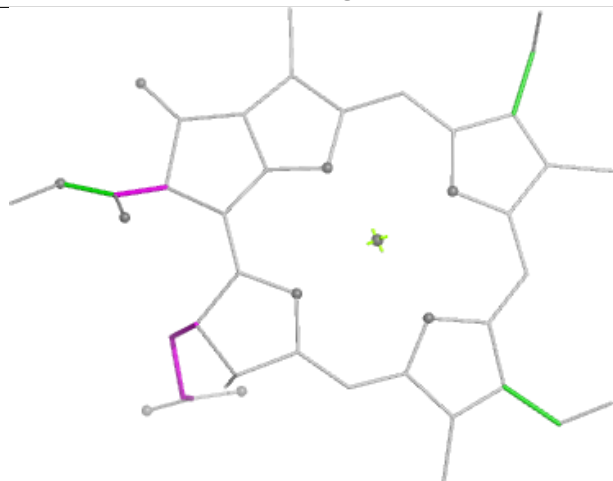
Ligand CLA 2 608



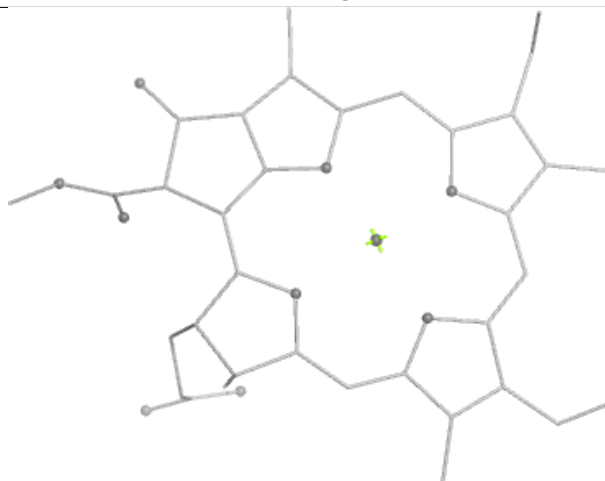
Bond lengths



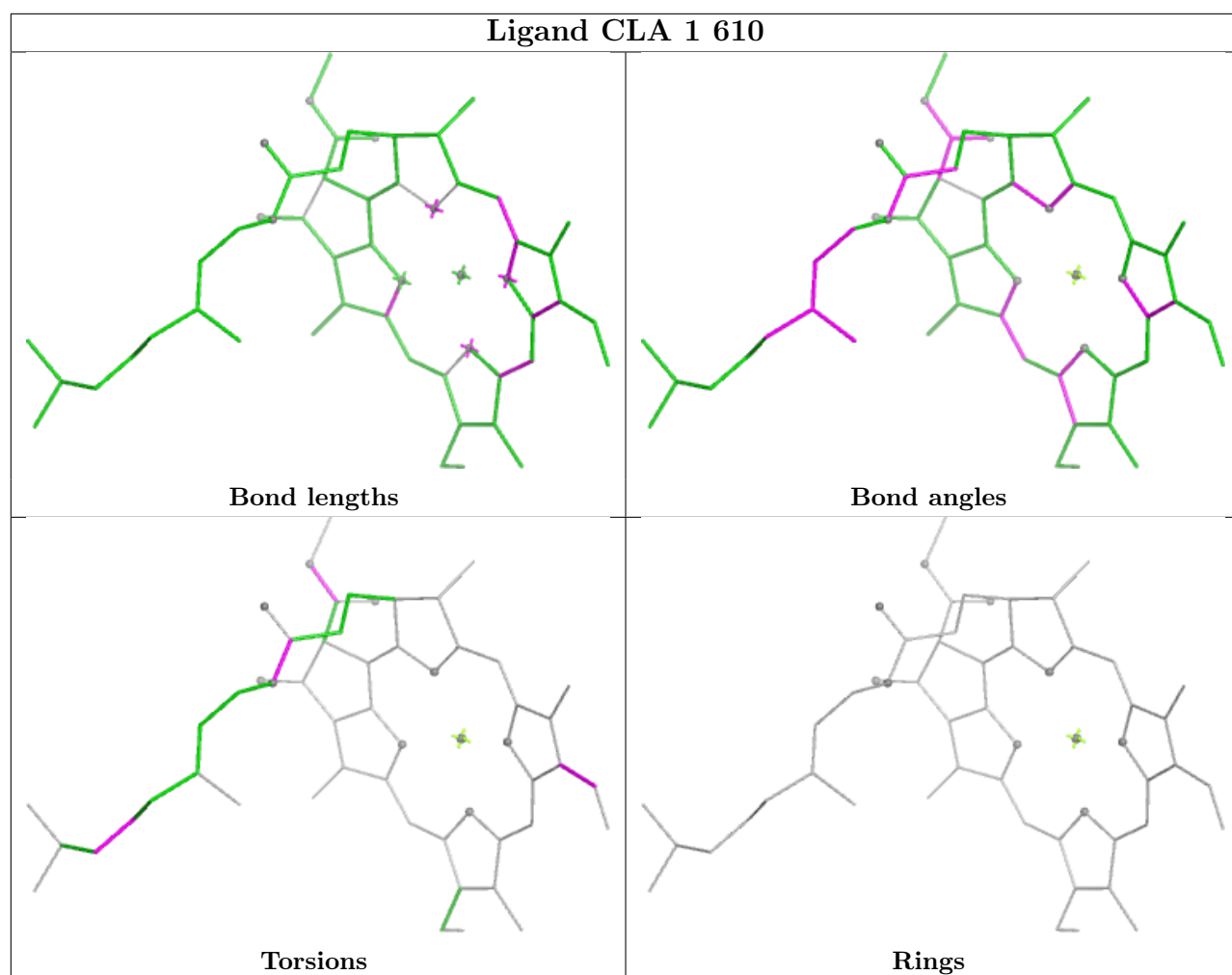
Bond angles

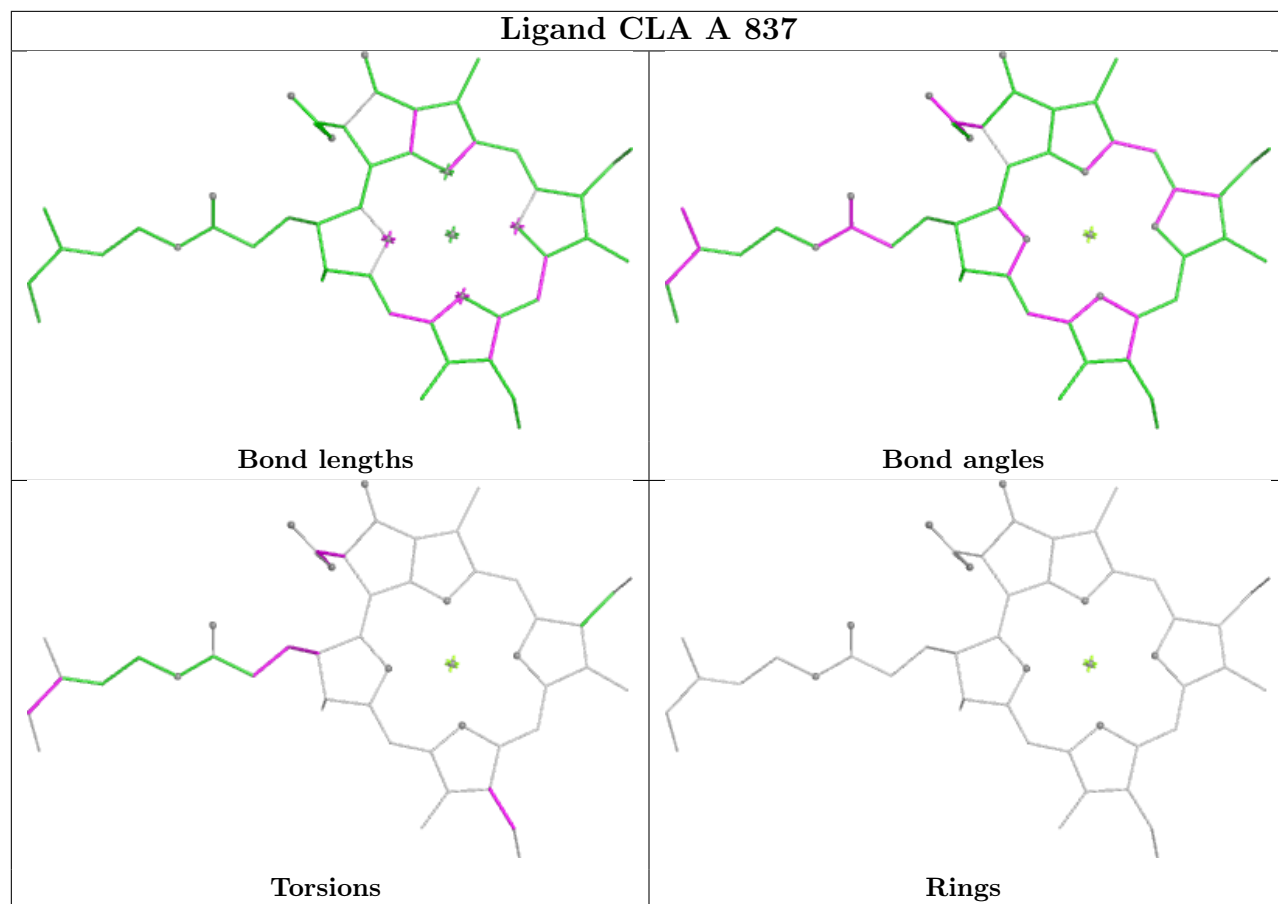


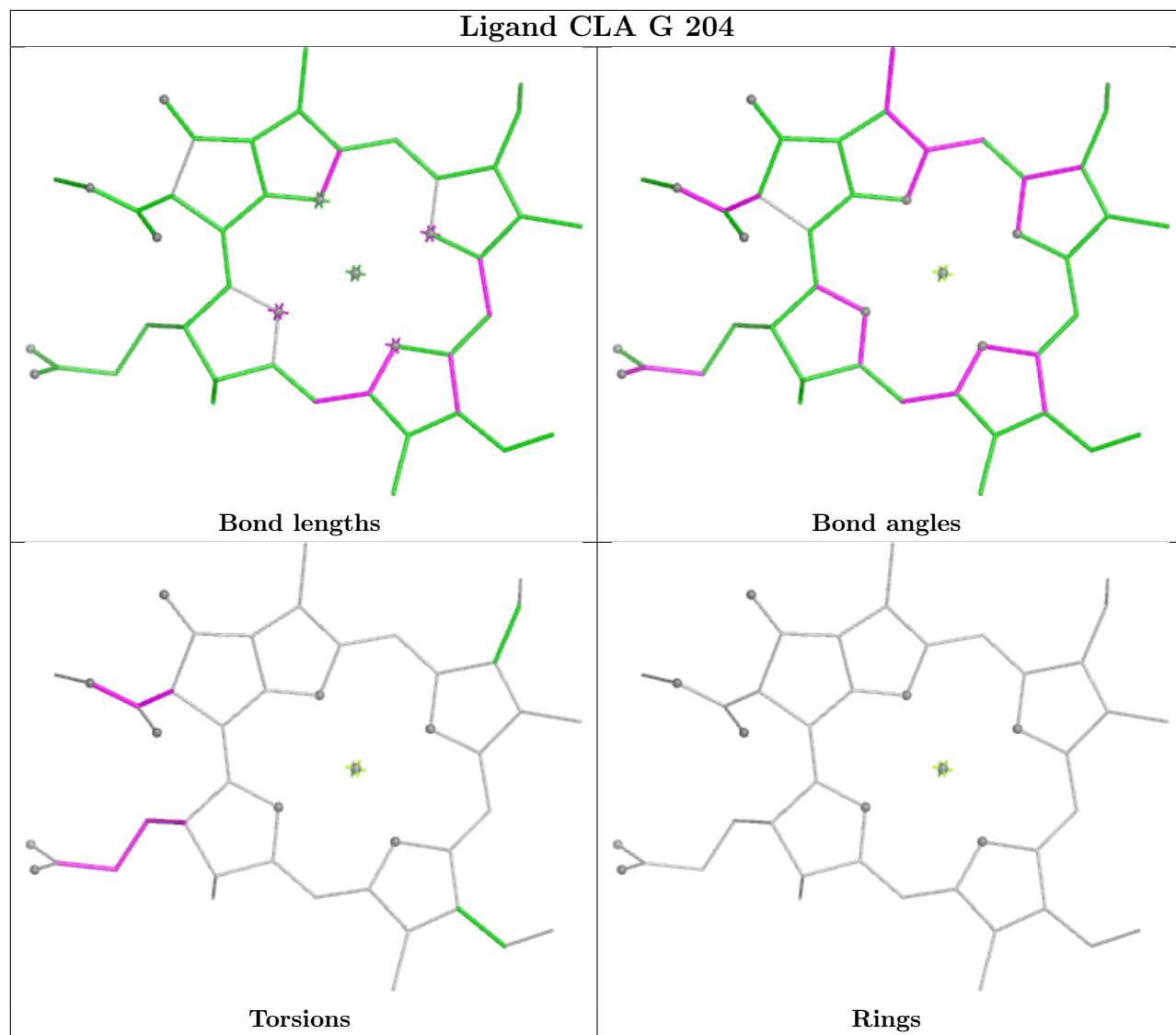
Torsions

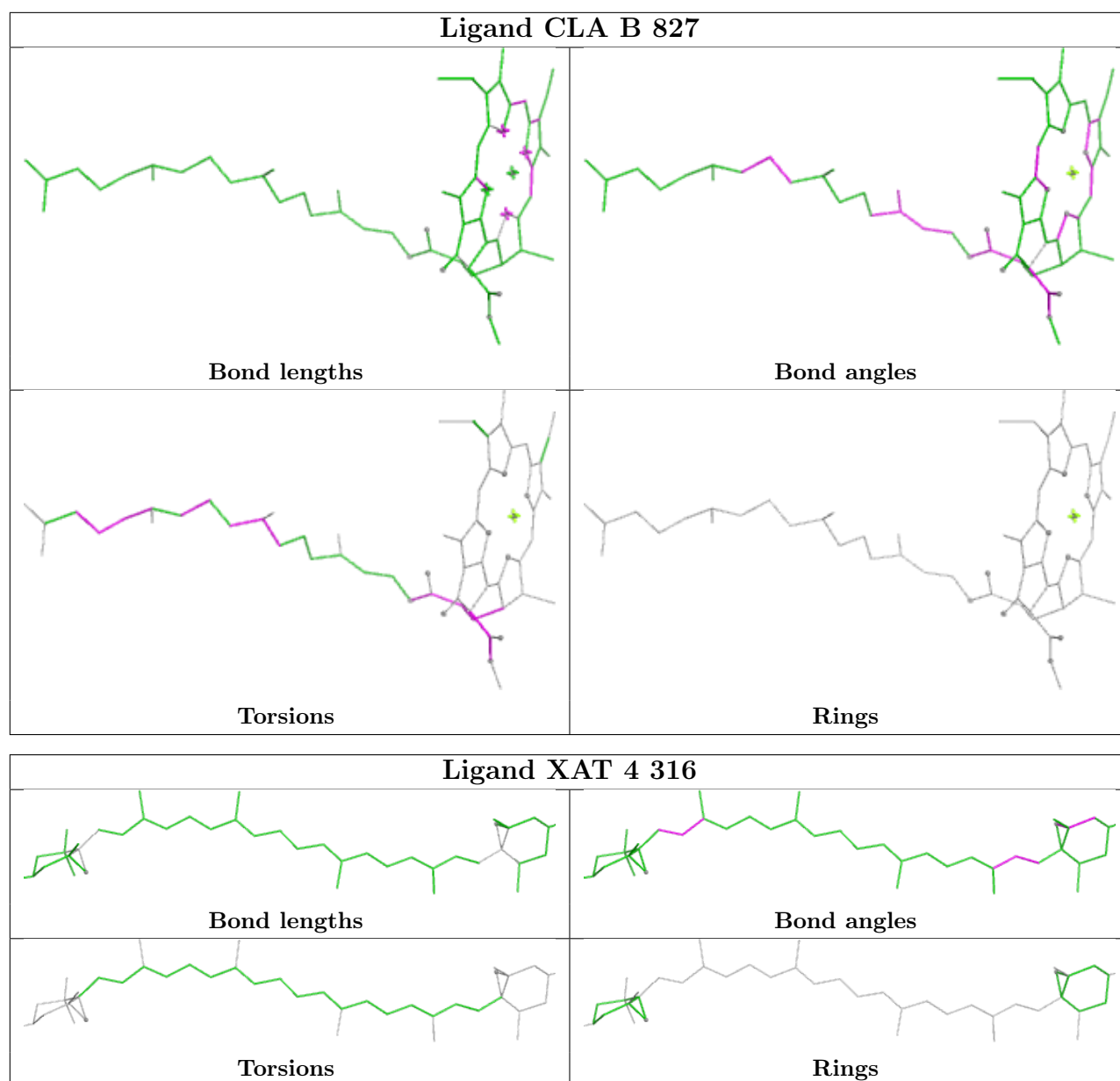


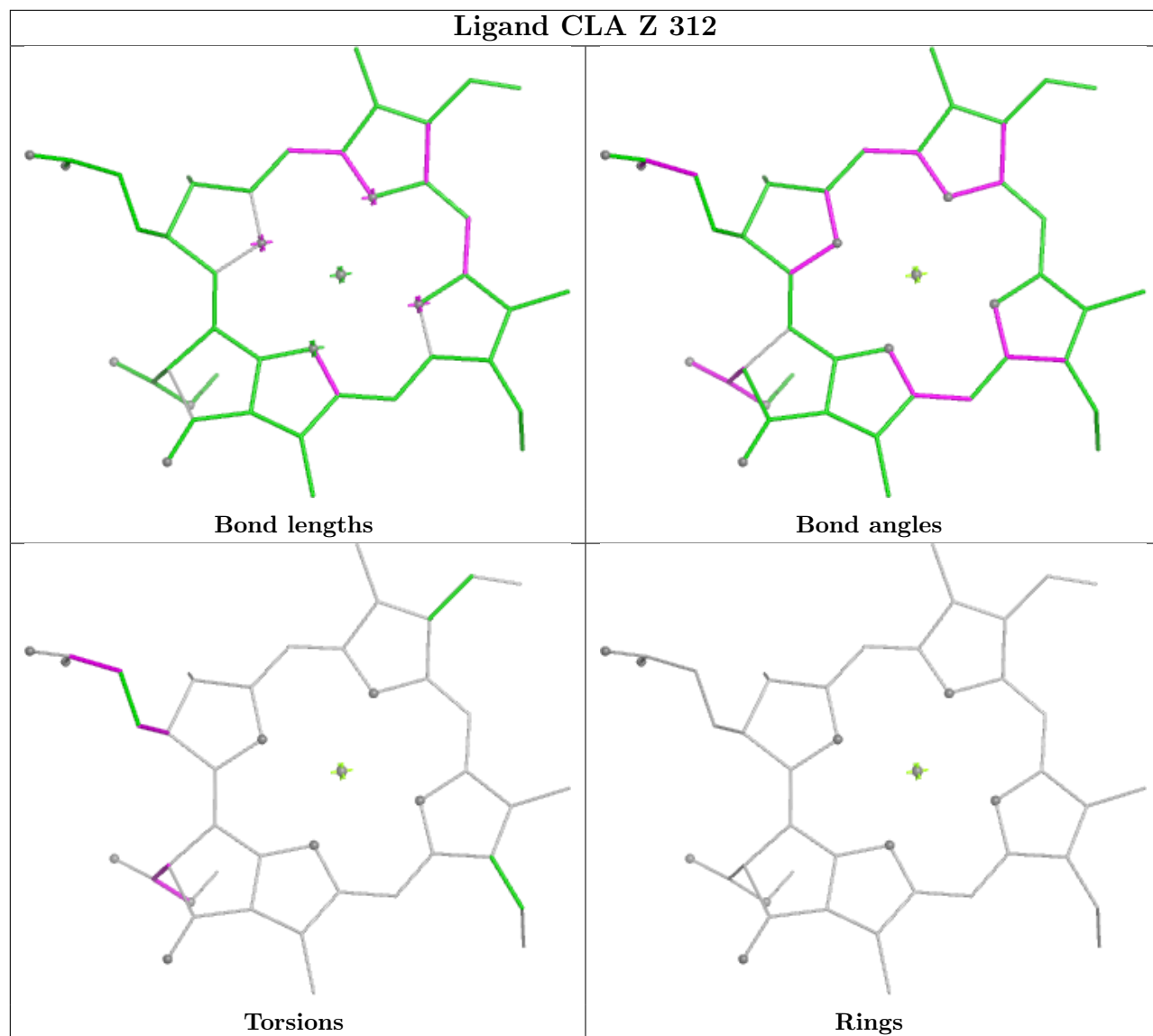
Rings



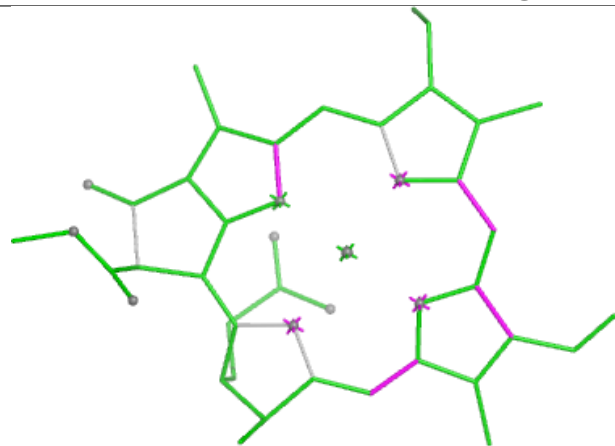




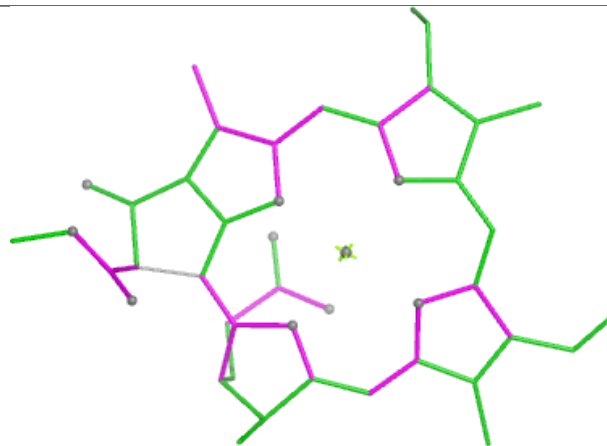




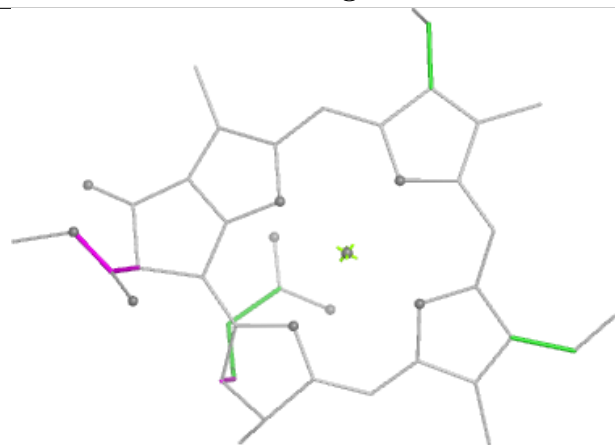
Ligand CLA X 612



Bond lengths



Bond angles



Torsions

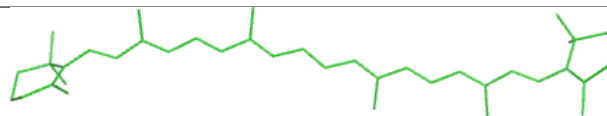


Rings

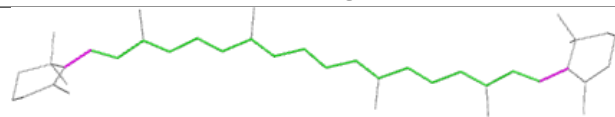
Ligand BCR A 845



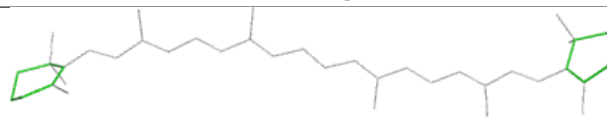
Bond lengths



Bond angles

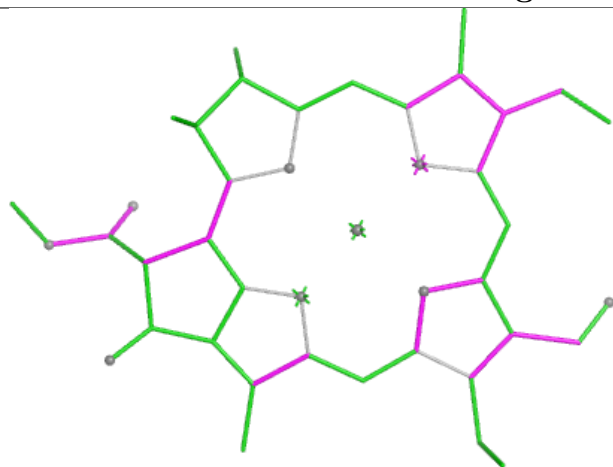


Torsions

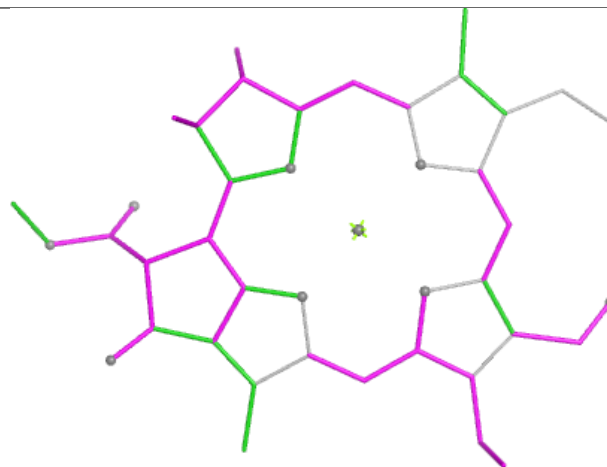


Rings

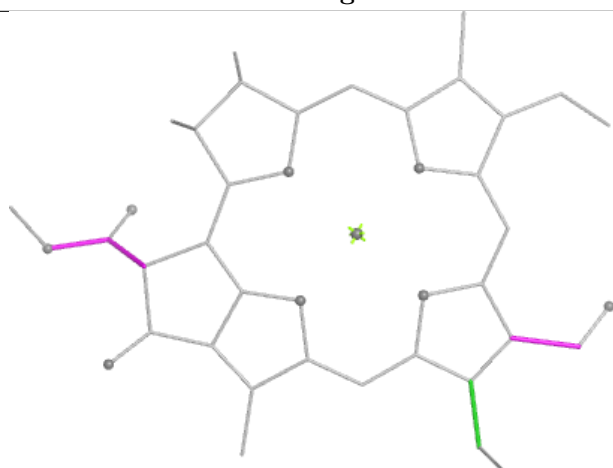
Ligand CHL Z 308



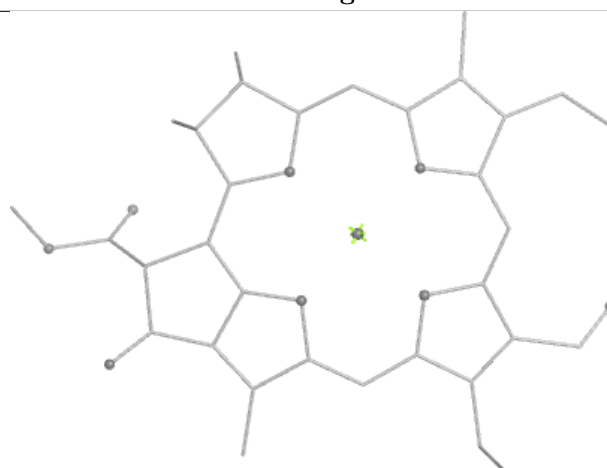
Bond lengths



Bond angles

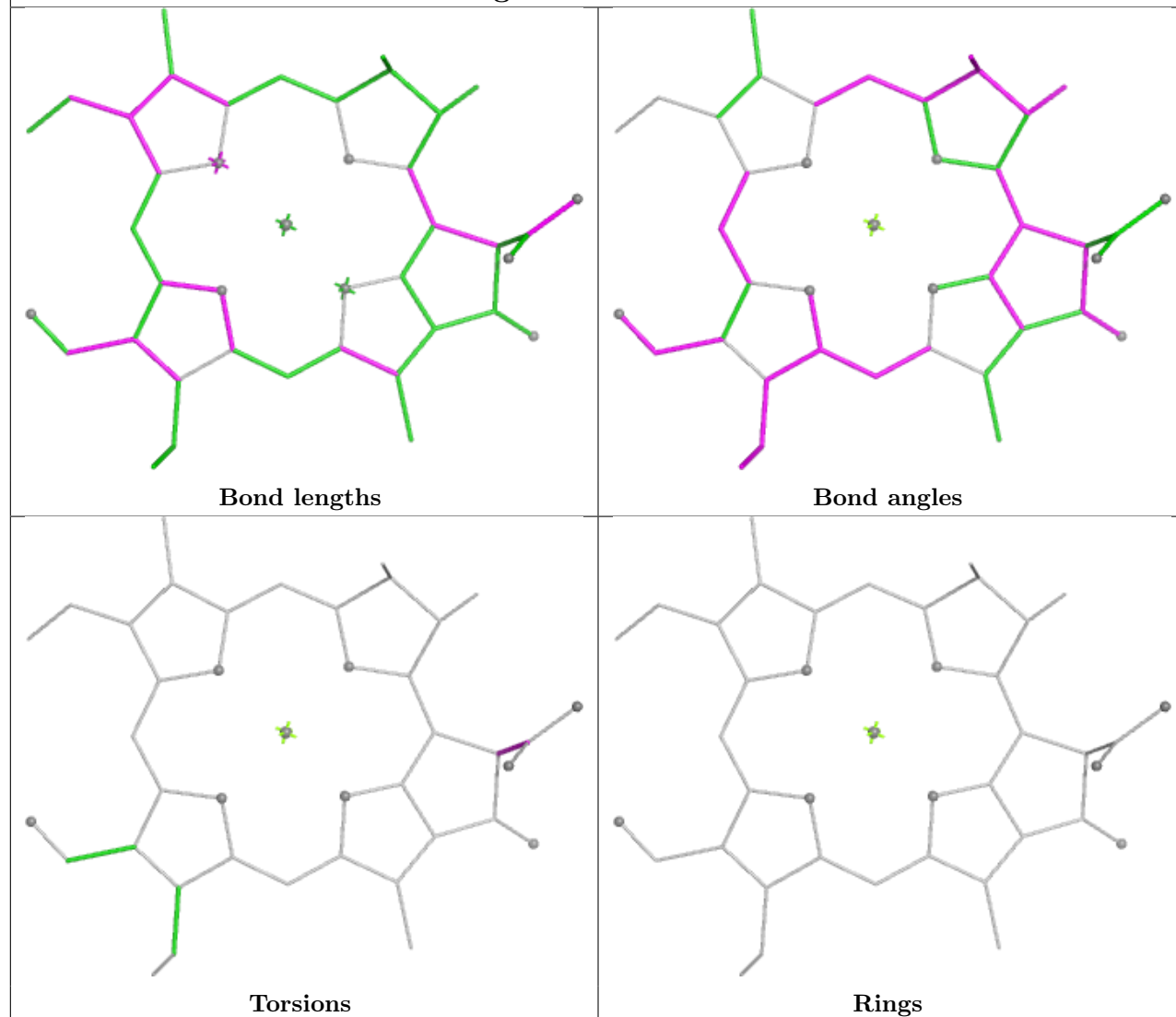


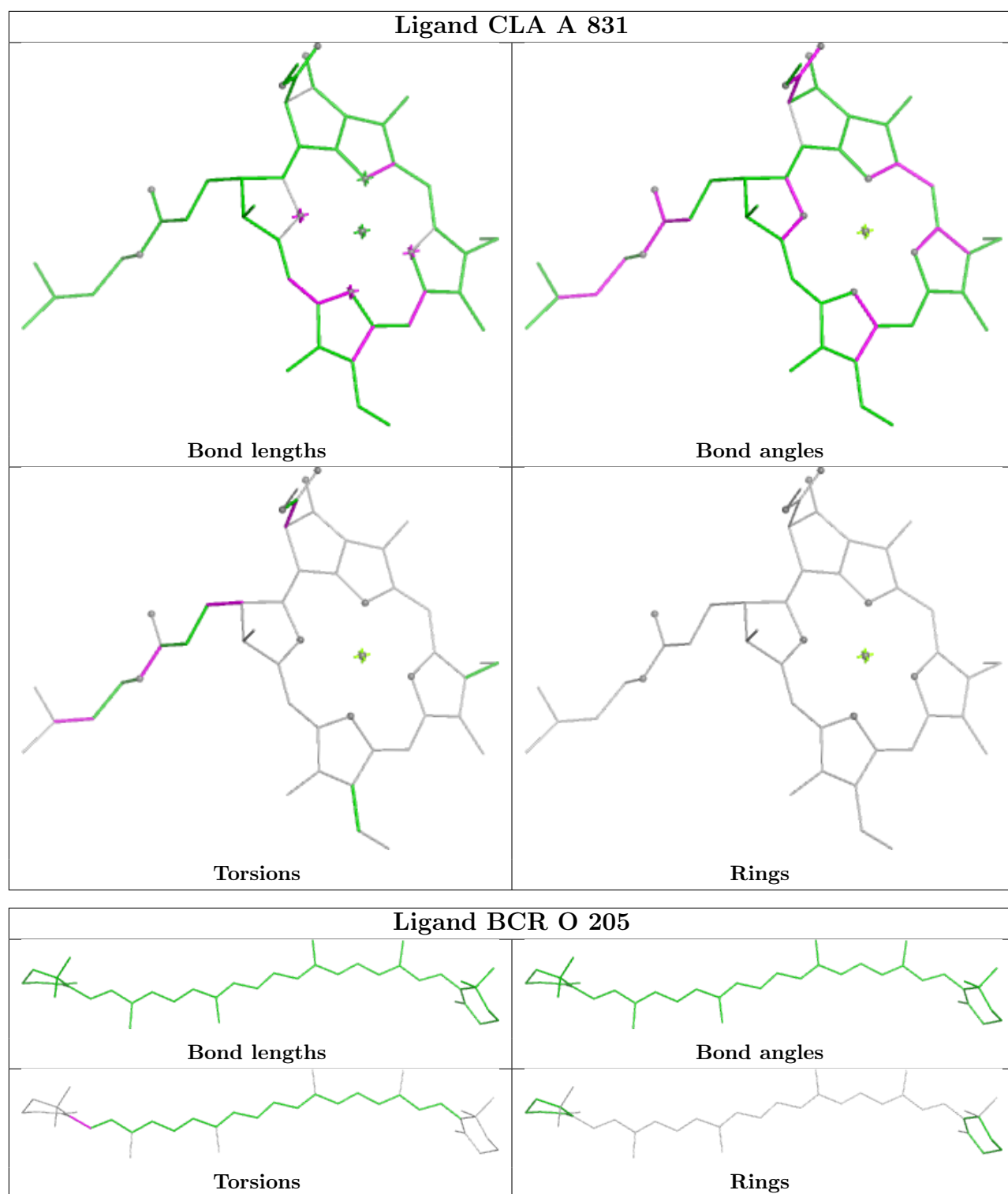
Torsions



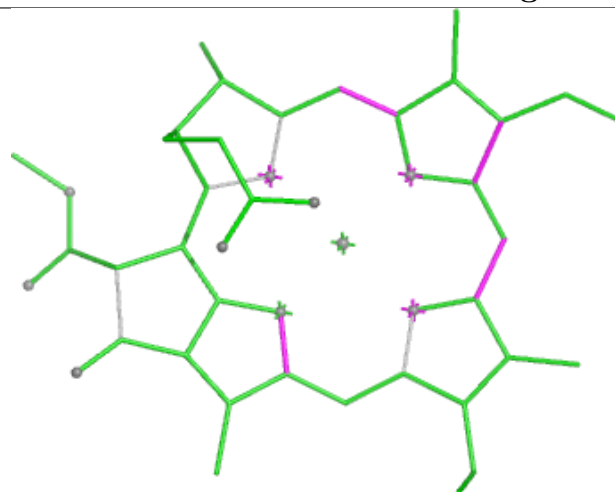
Rings

Ligand CHL 5 606

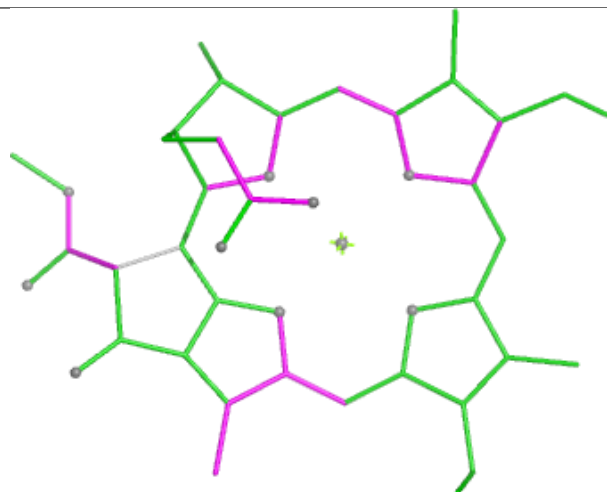




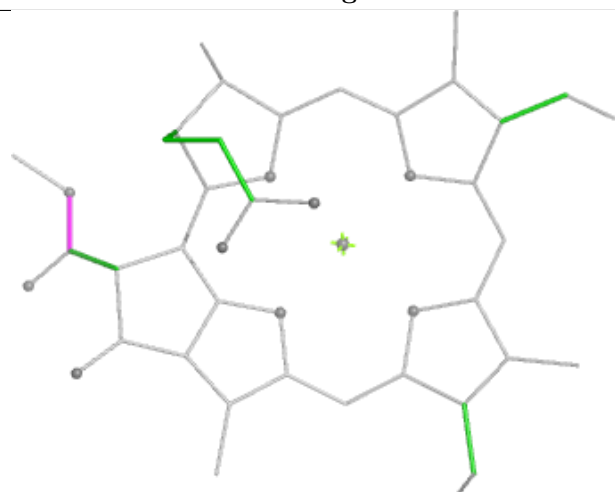
Ligand CLA 5 613



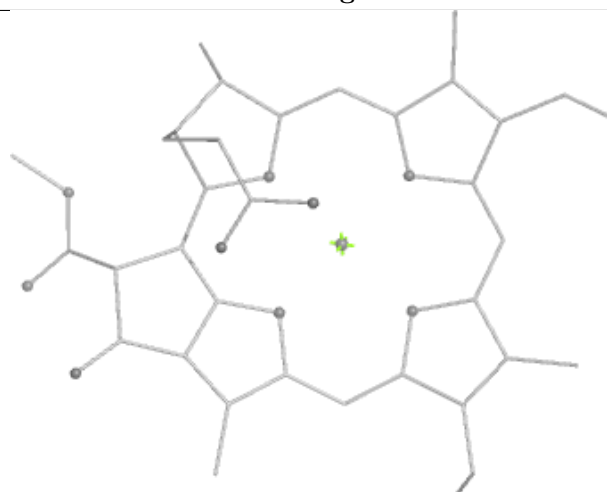
Bond lengths



Bond angles

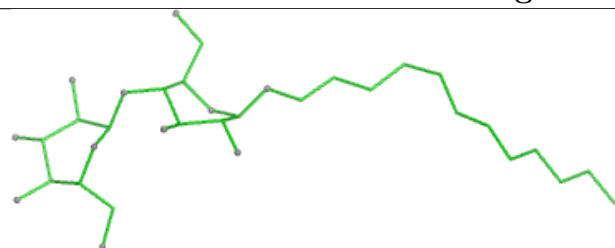


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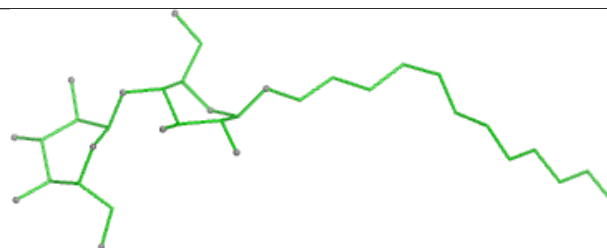


Rings

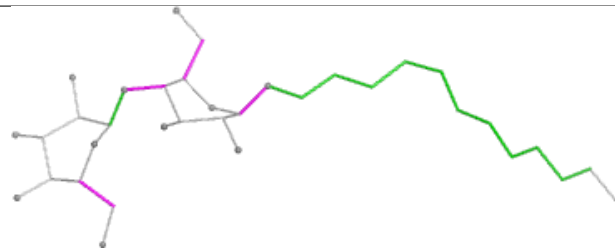
Ligand LMT F 303



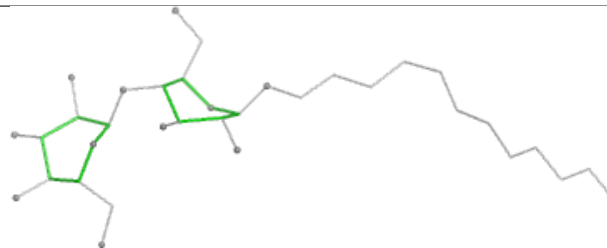
Bond lengths



Bond angles

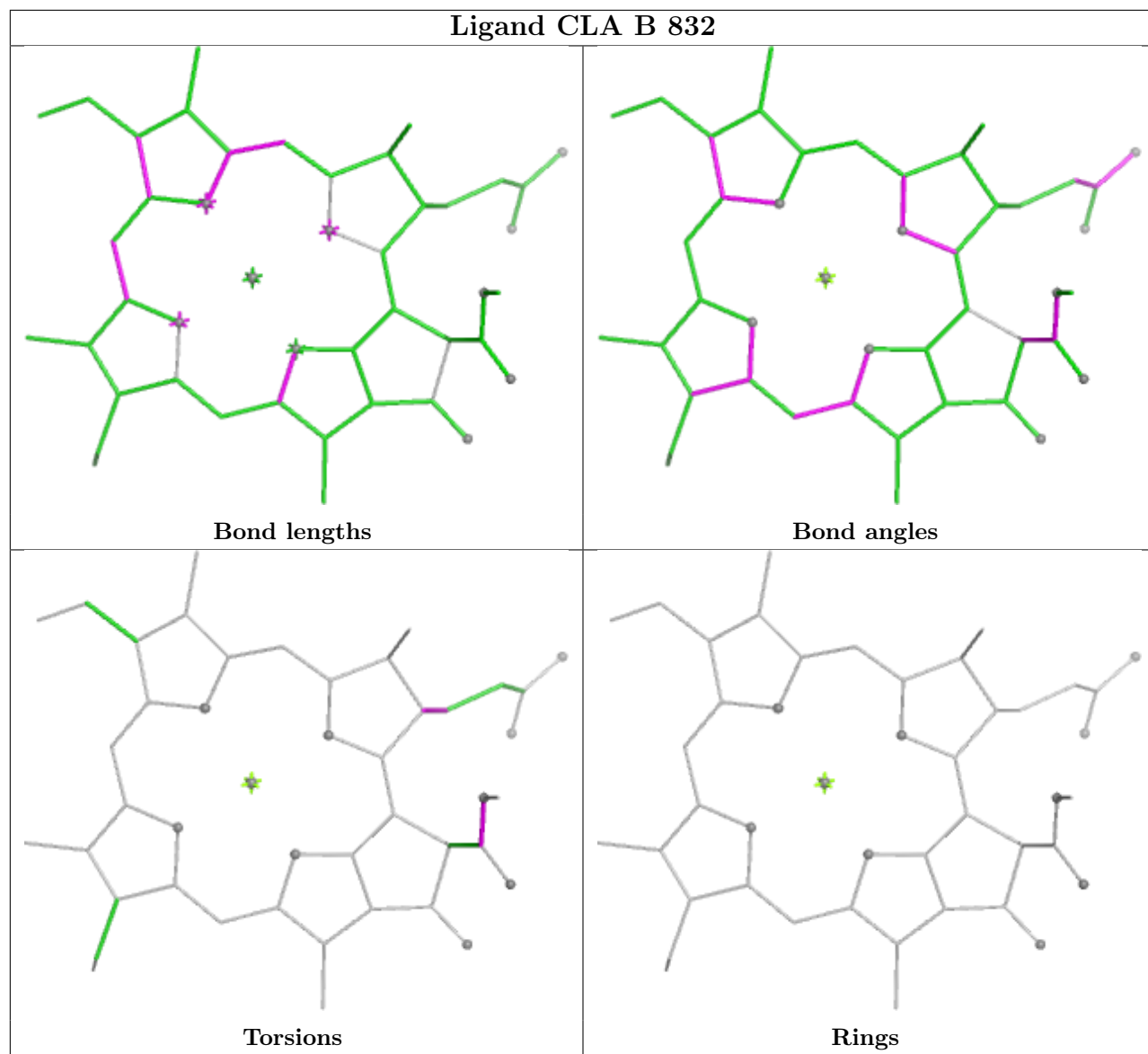


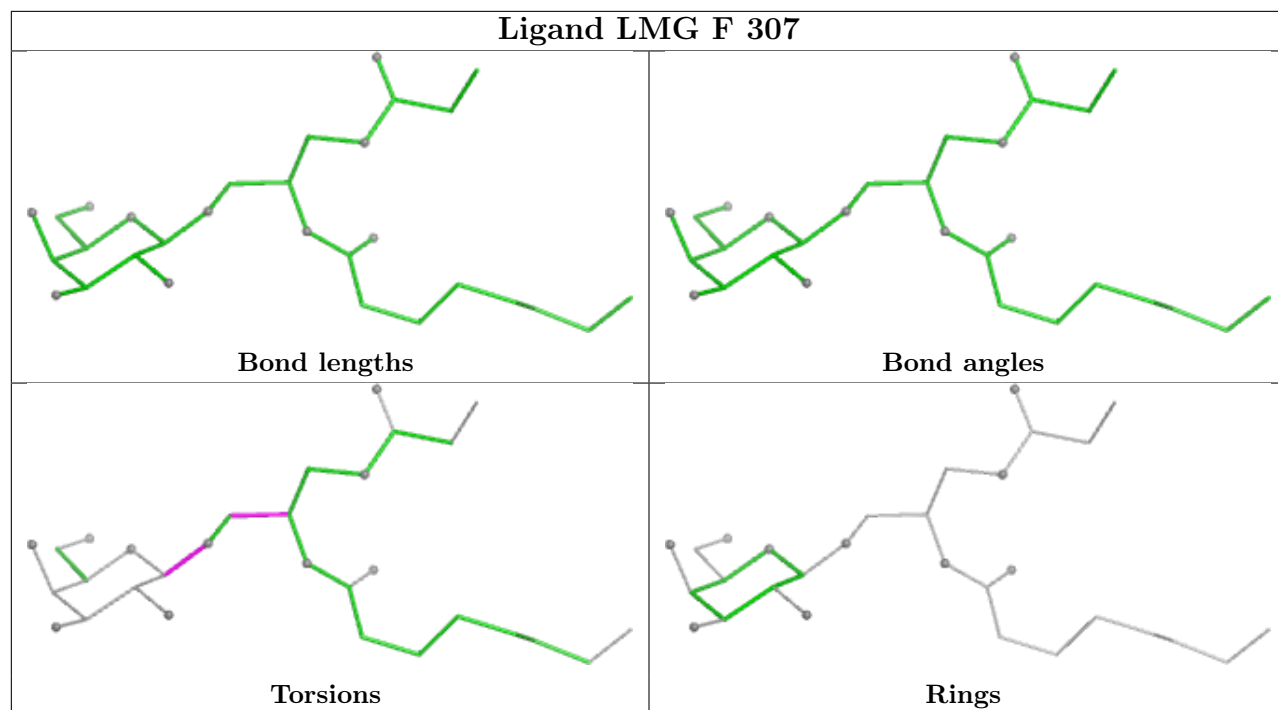
Torsions



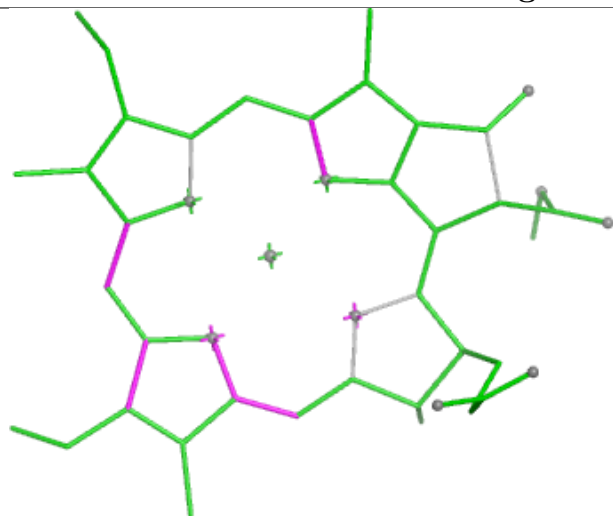
Rings

Ligand CLA B 832

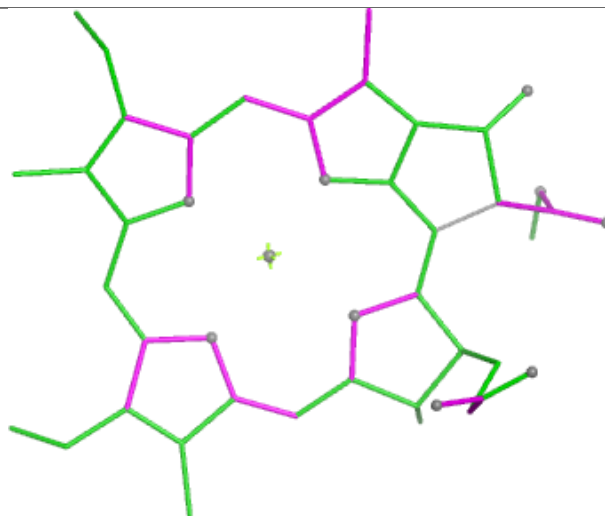




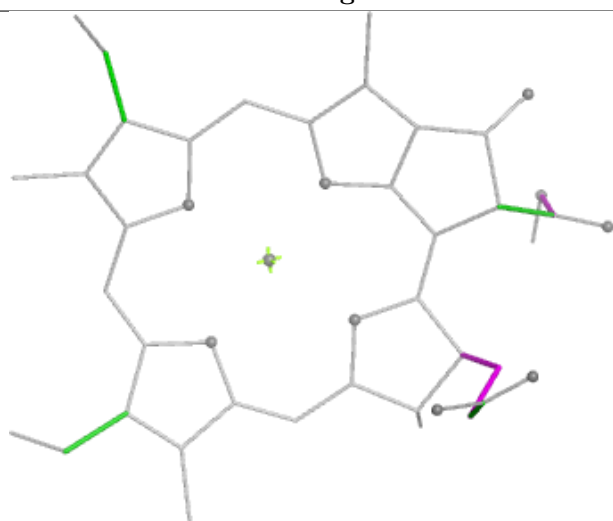
Ligand CLA 4 303



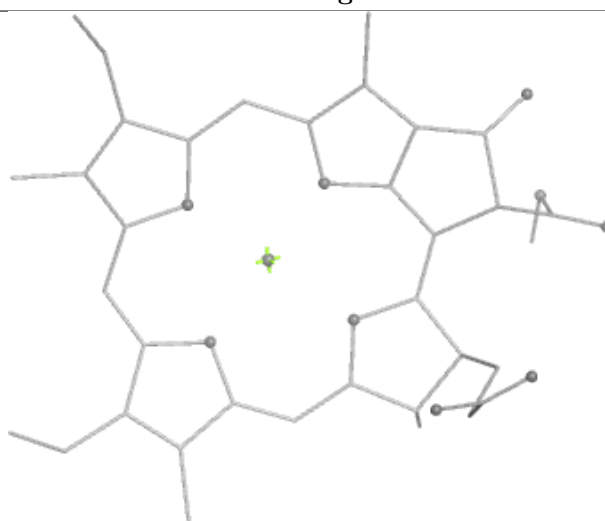
Bond lengths



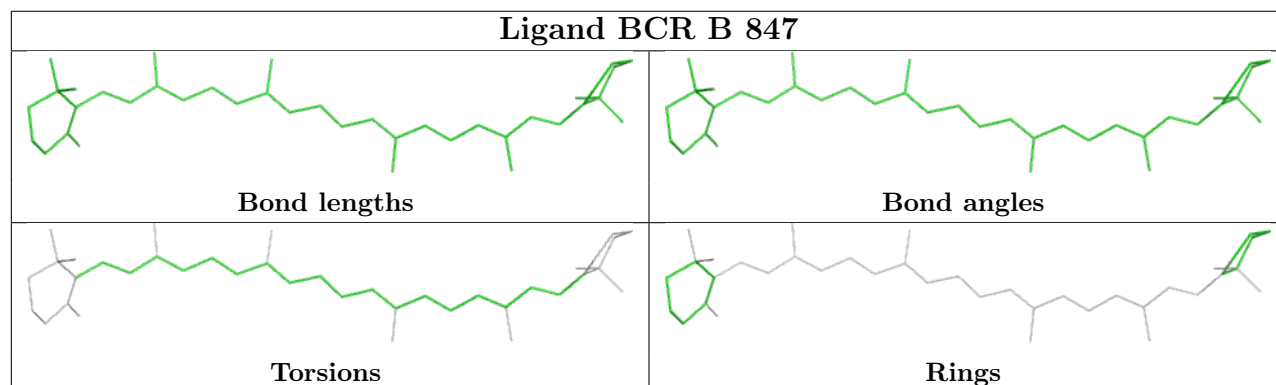
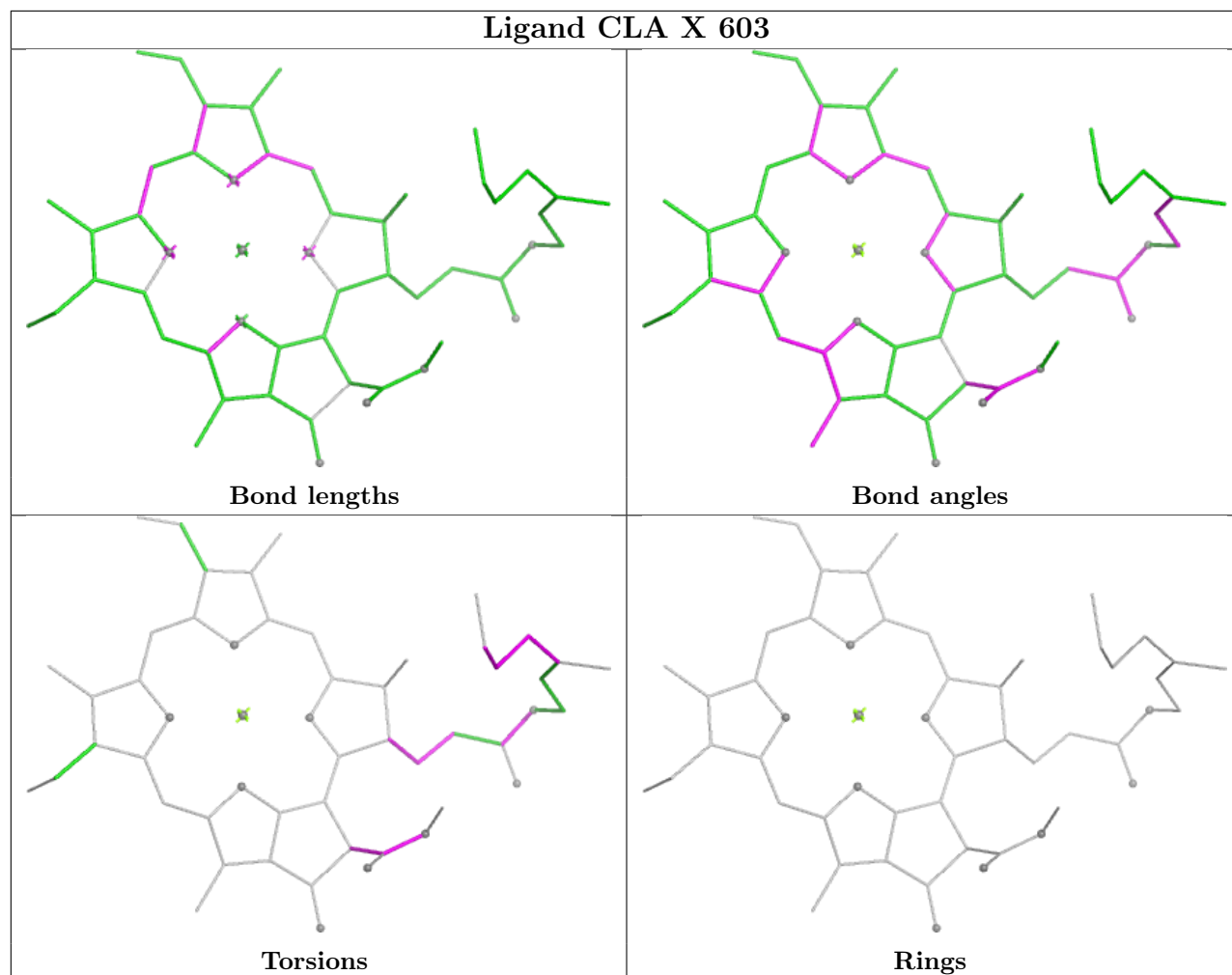
Bond angles



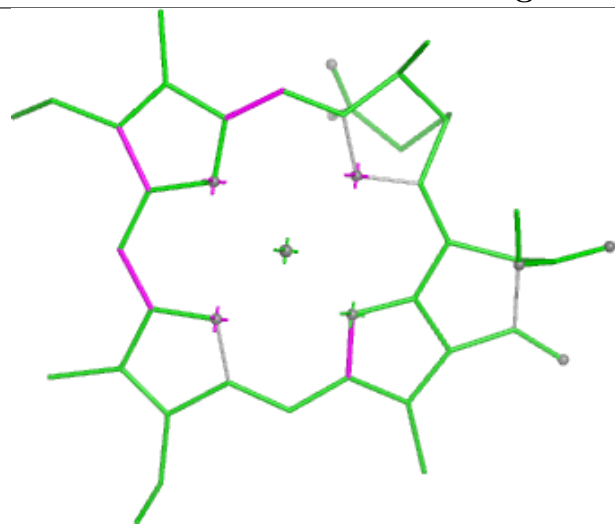
Torsions



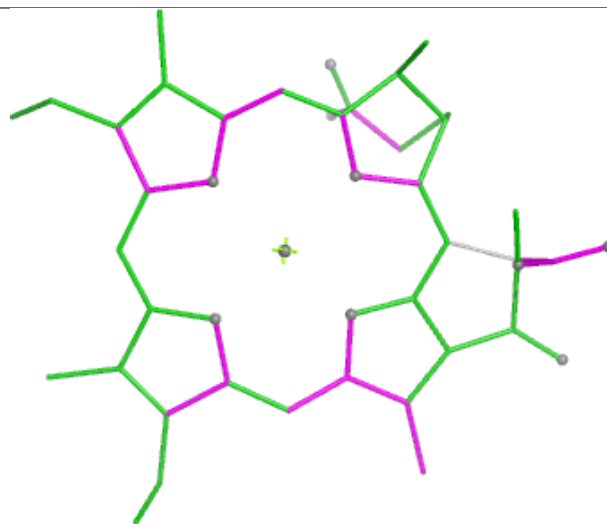
Rings



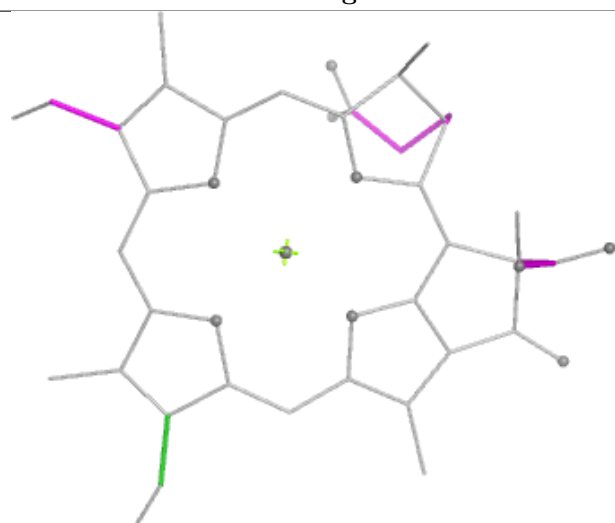
Ligand CLA X 604



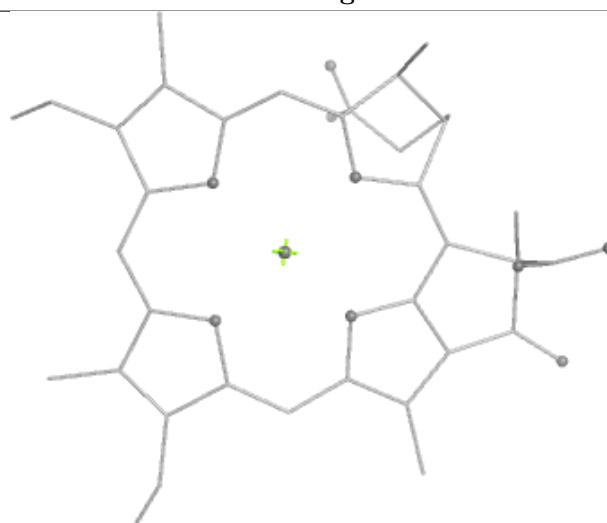
Bond lengths



Bond angles

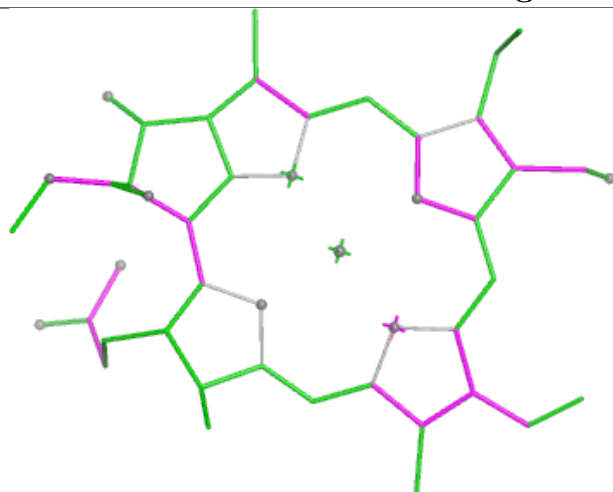


Torsions

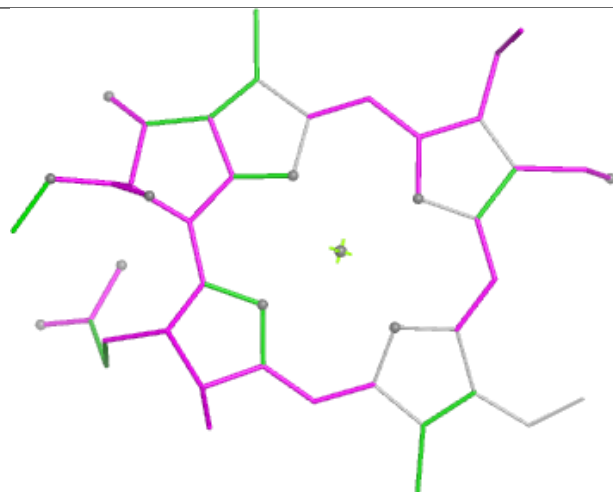


Rings

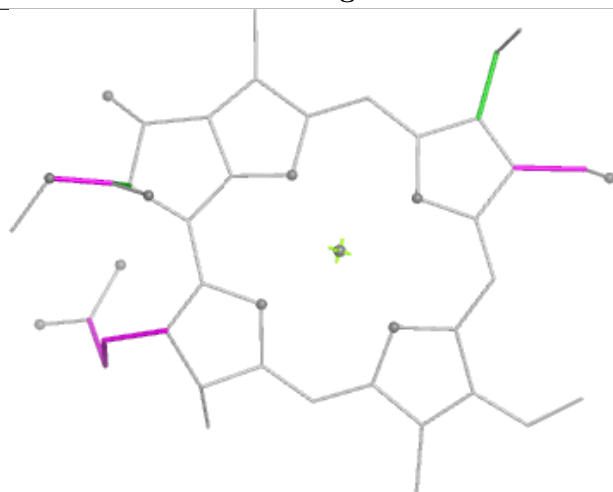
Ligand CHL Z 307



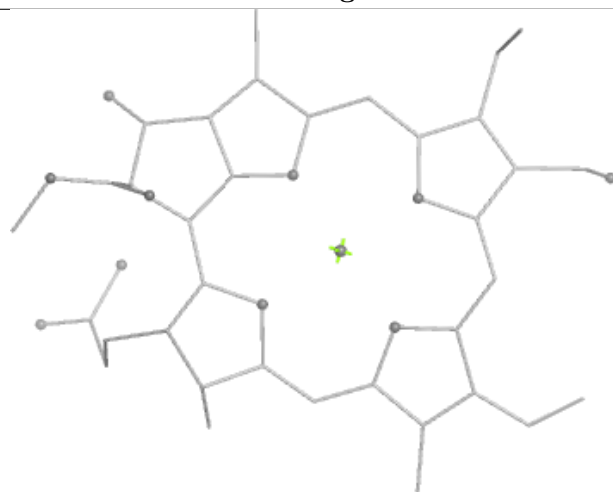
Bond lengths



Bond angles

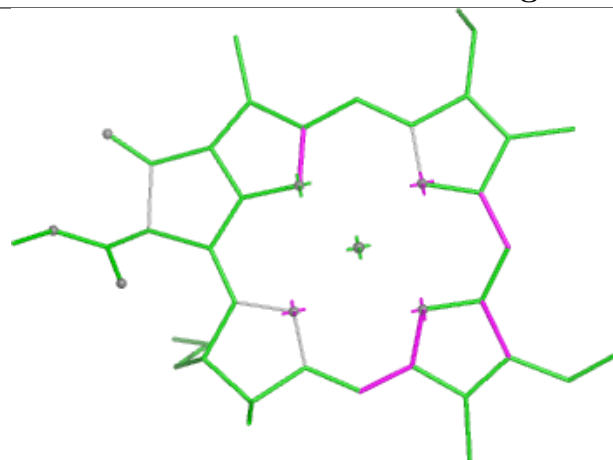


Torsions

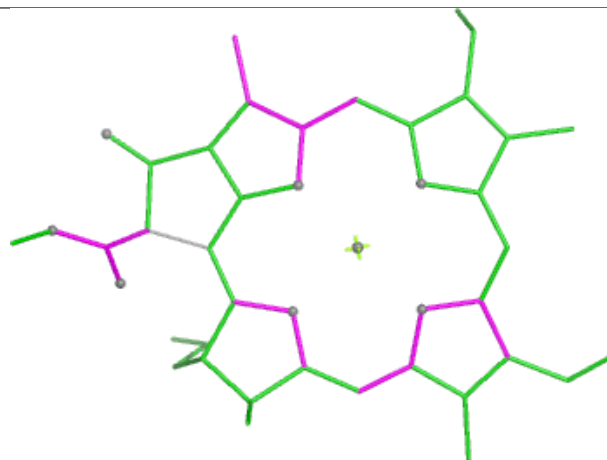


Rings

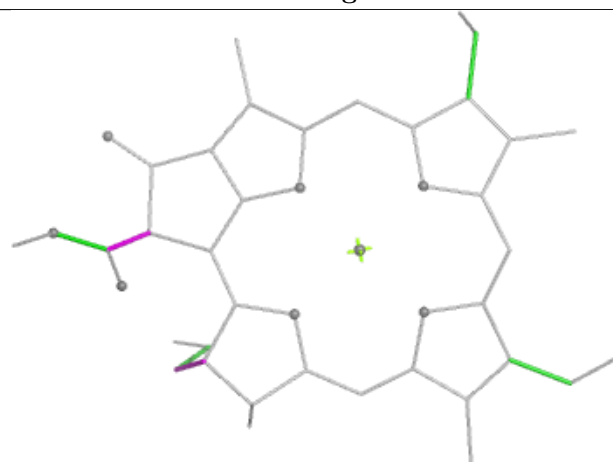
Ligand CLA 2 613



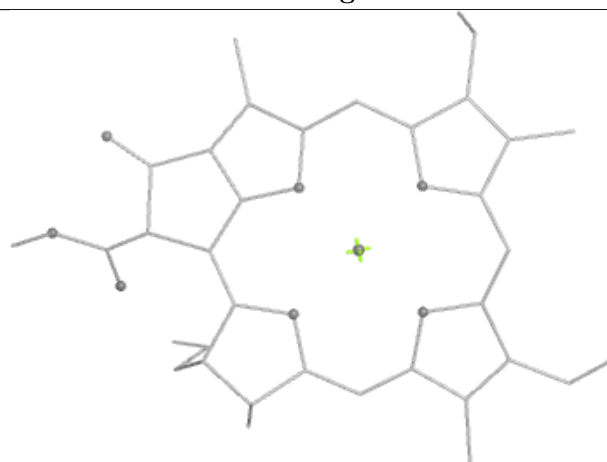
Bond lengths



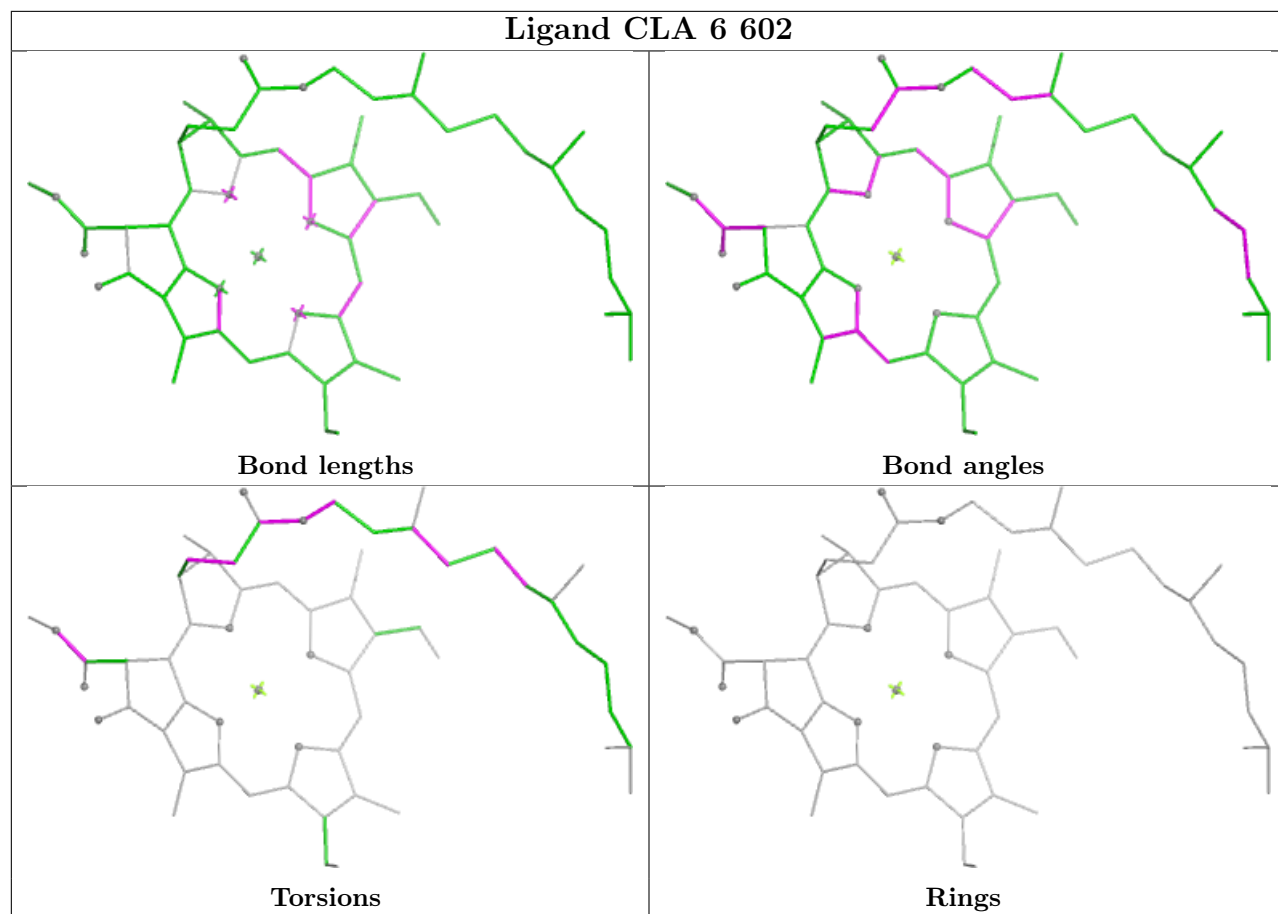
Bond angles

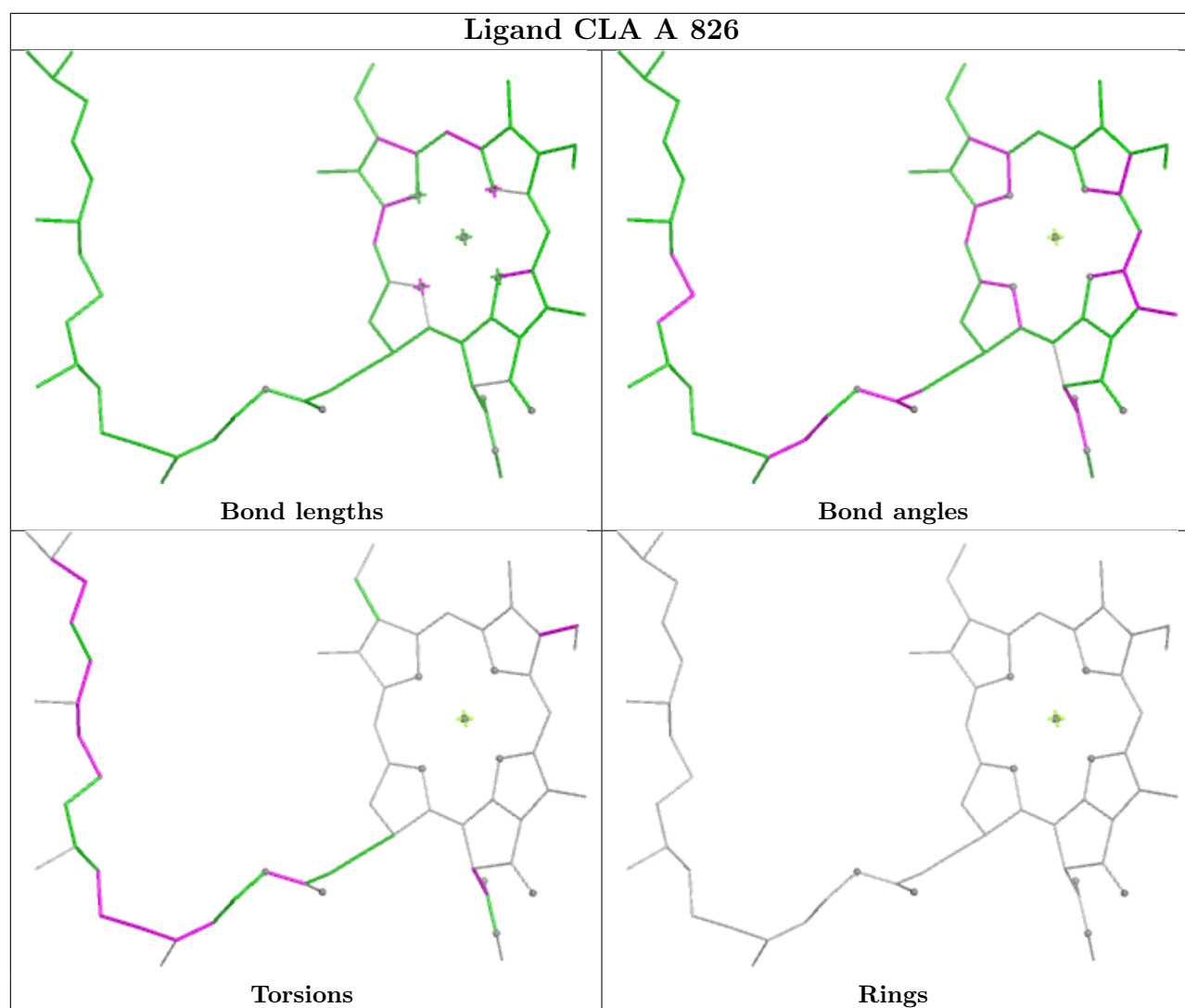


Torsions

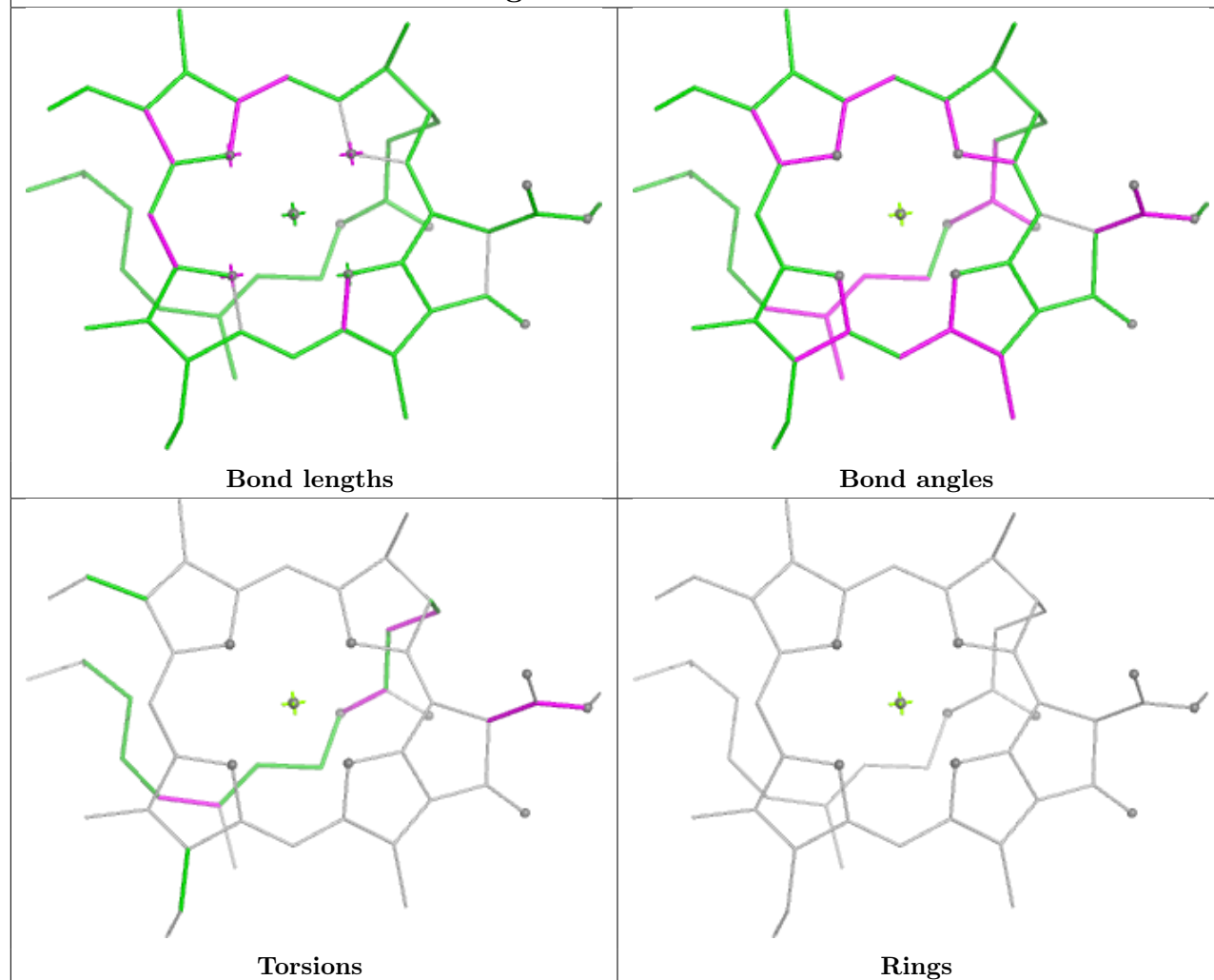


Rings

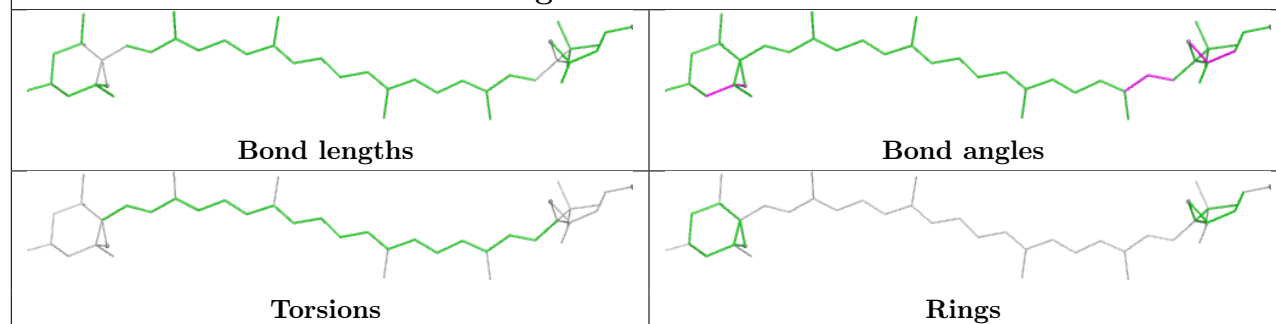


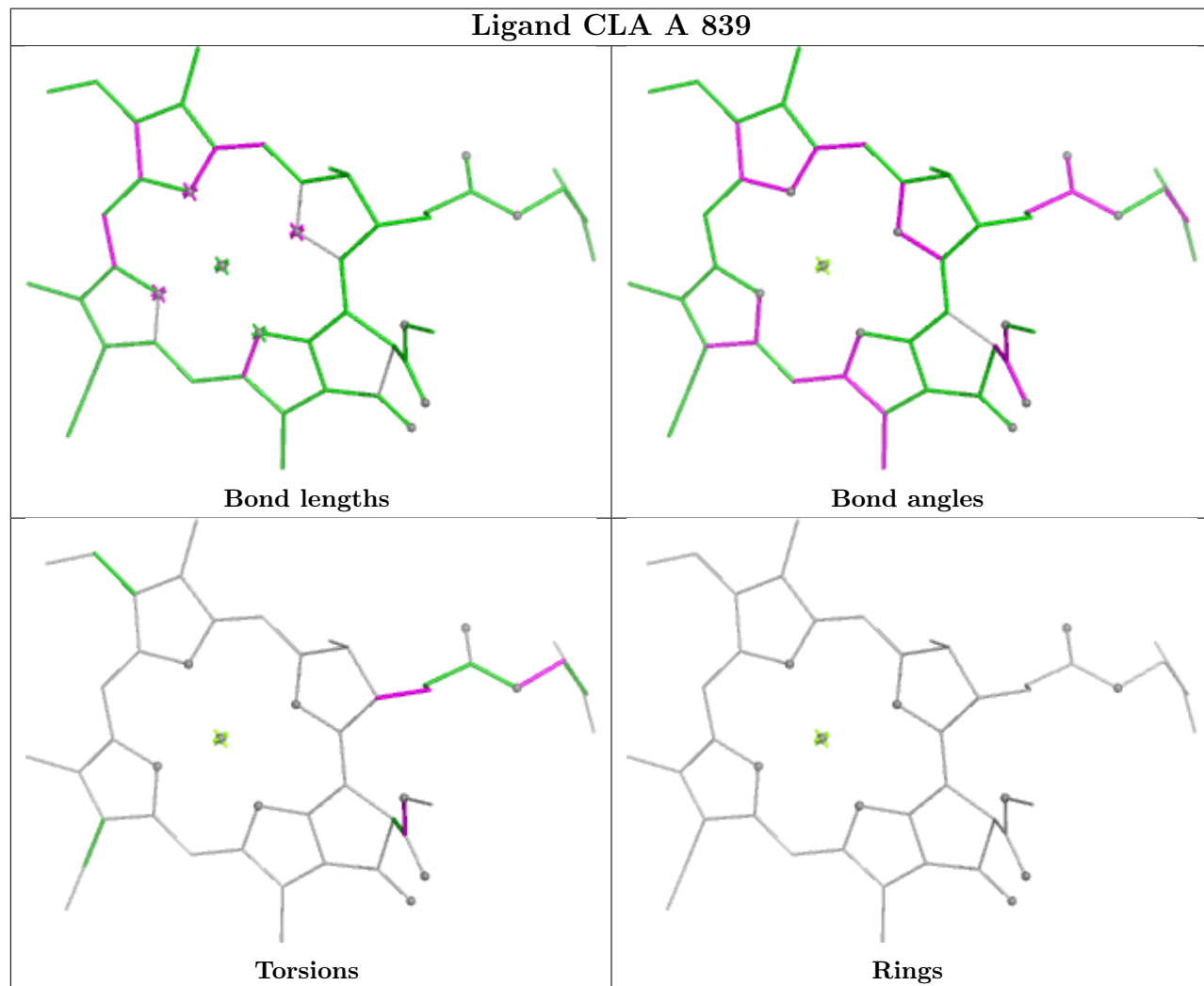
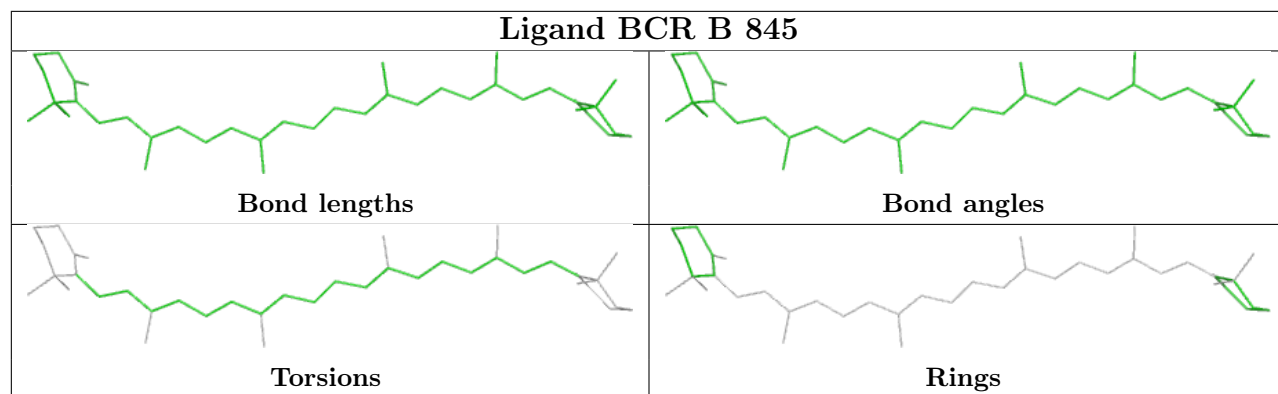


Ligand CLA Y 613

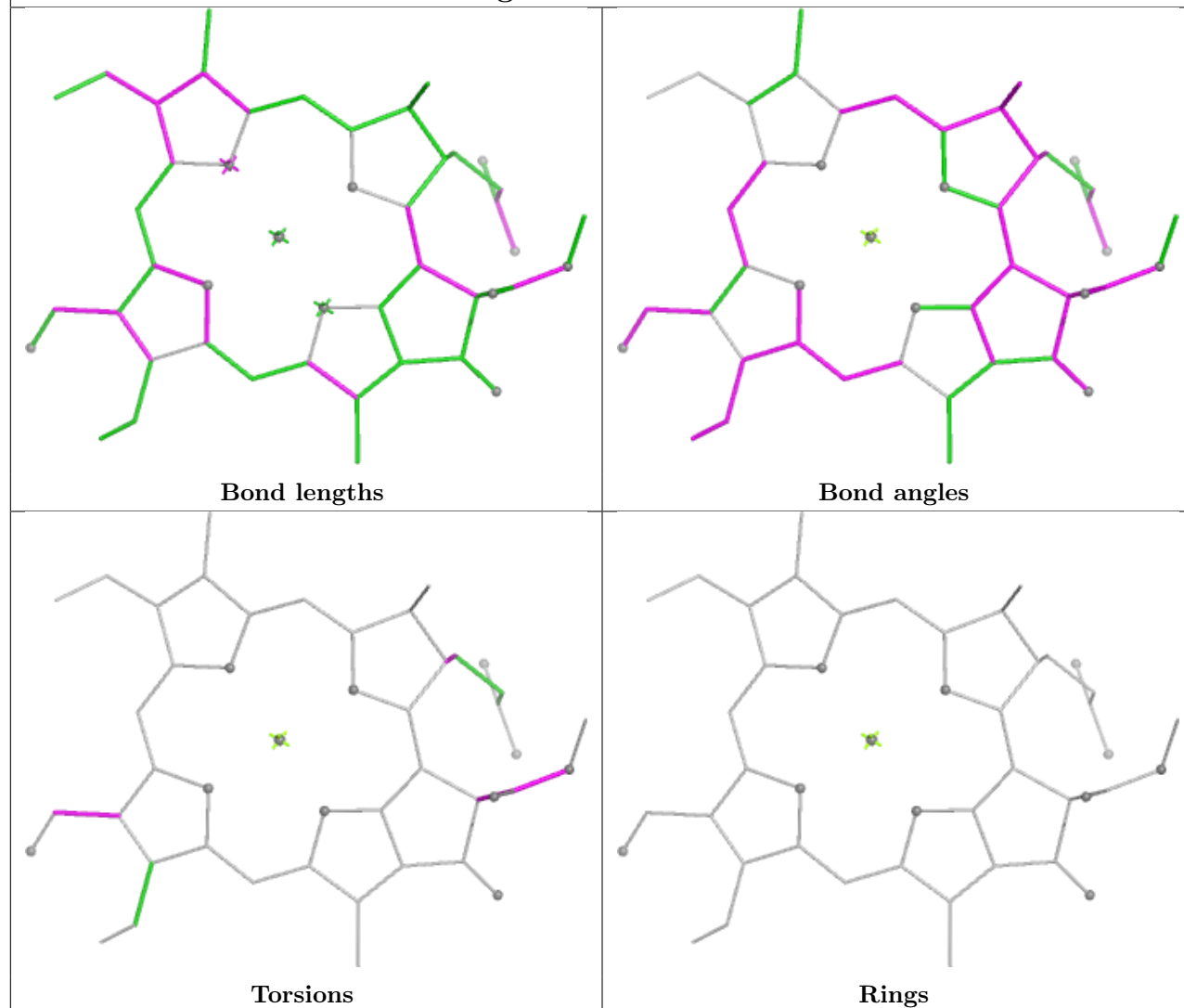


Ligand XAT 6 617

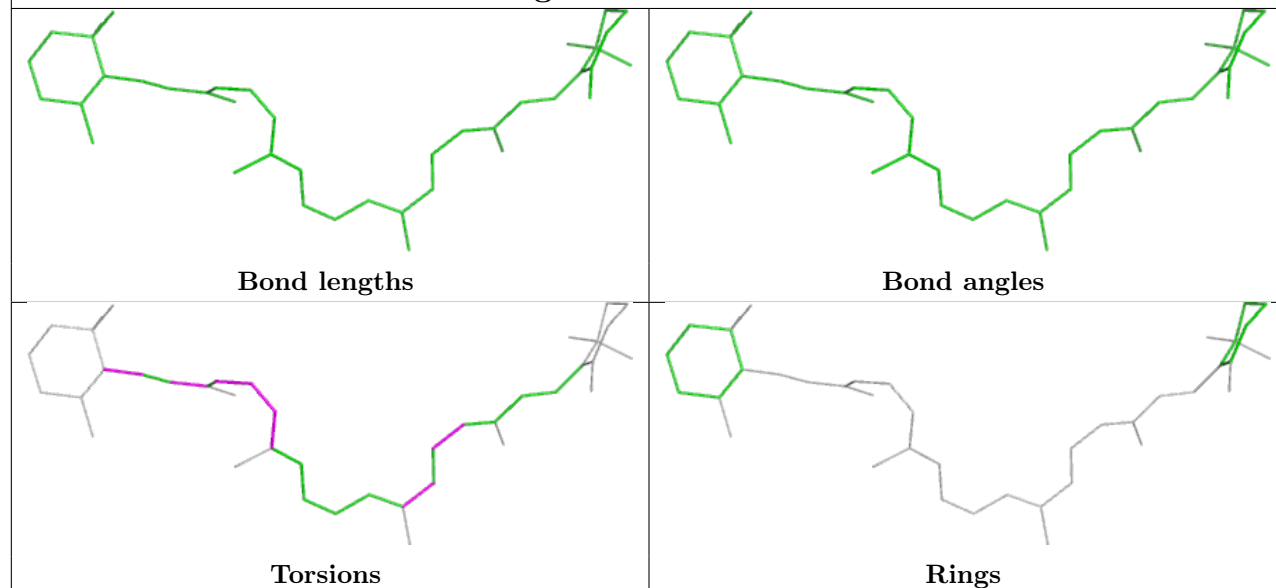


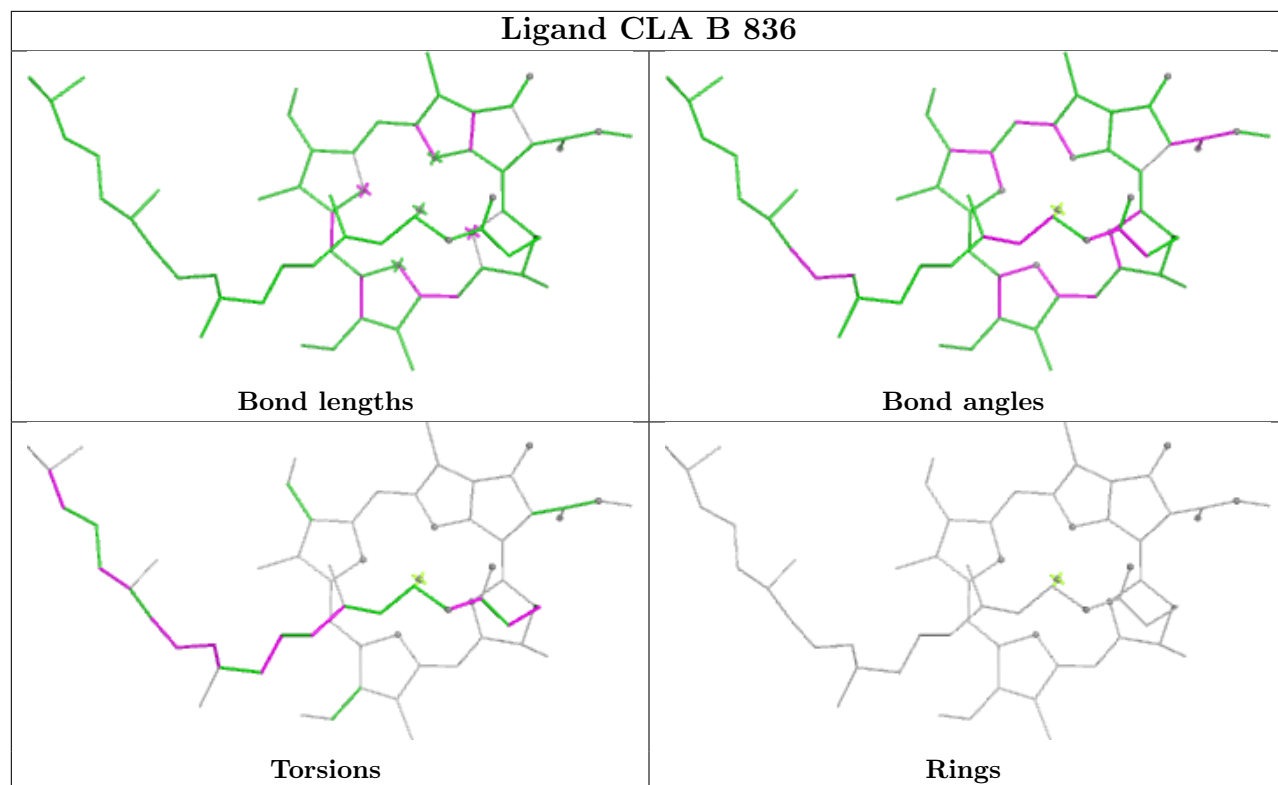


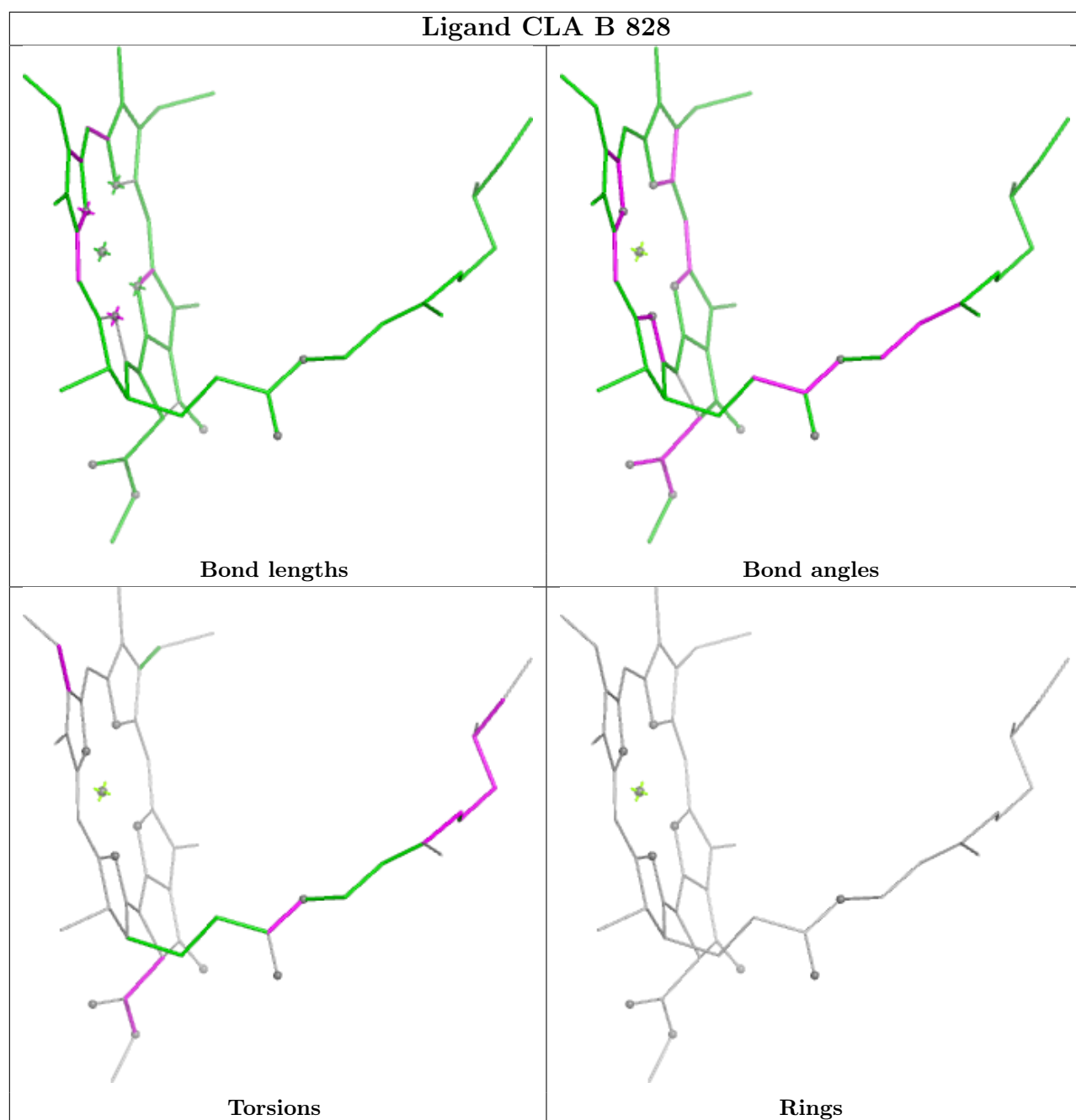
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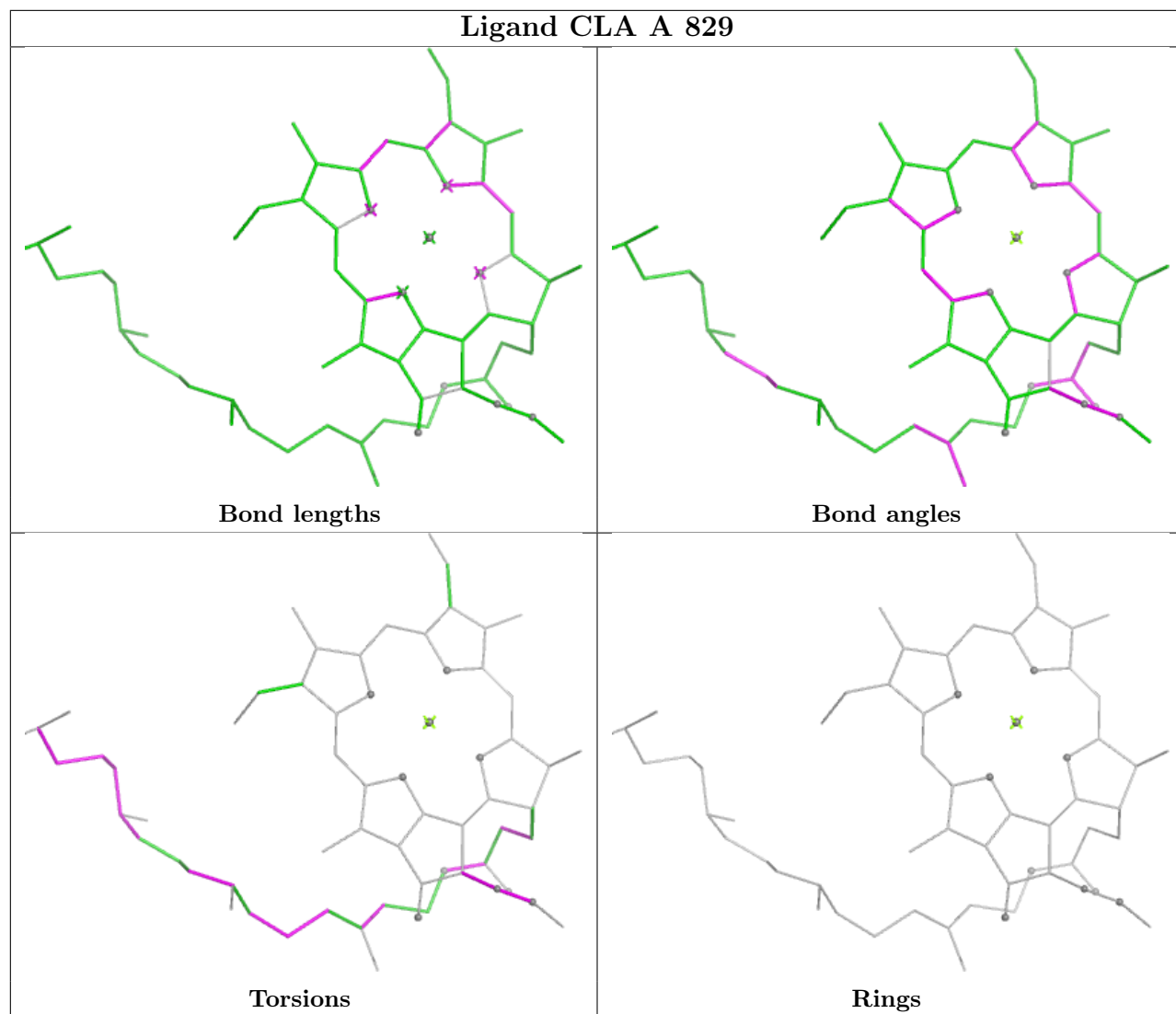


Ligand BCR 6 620

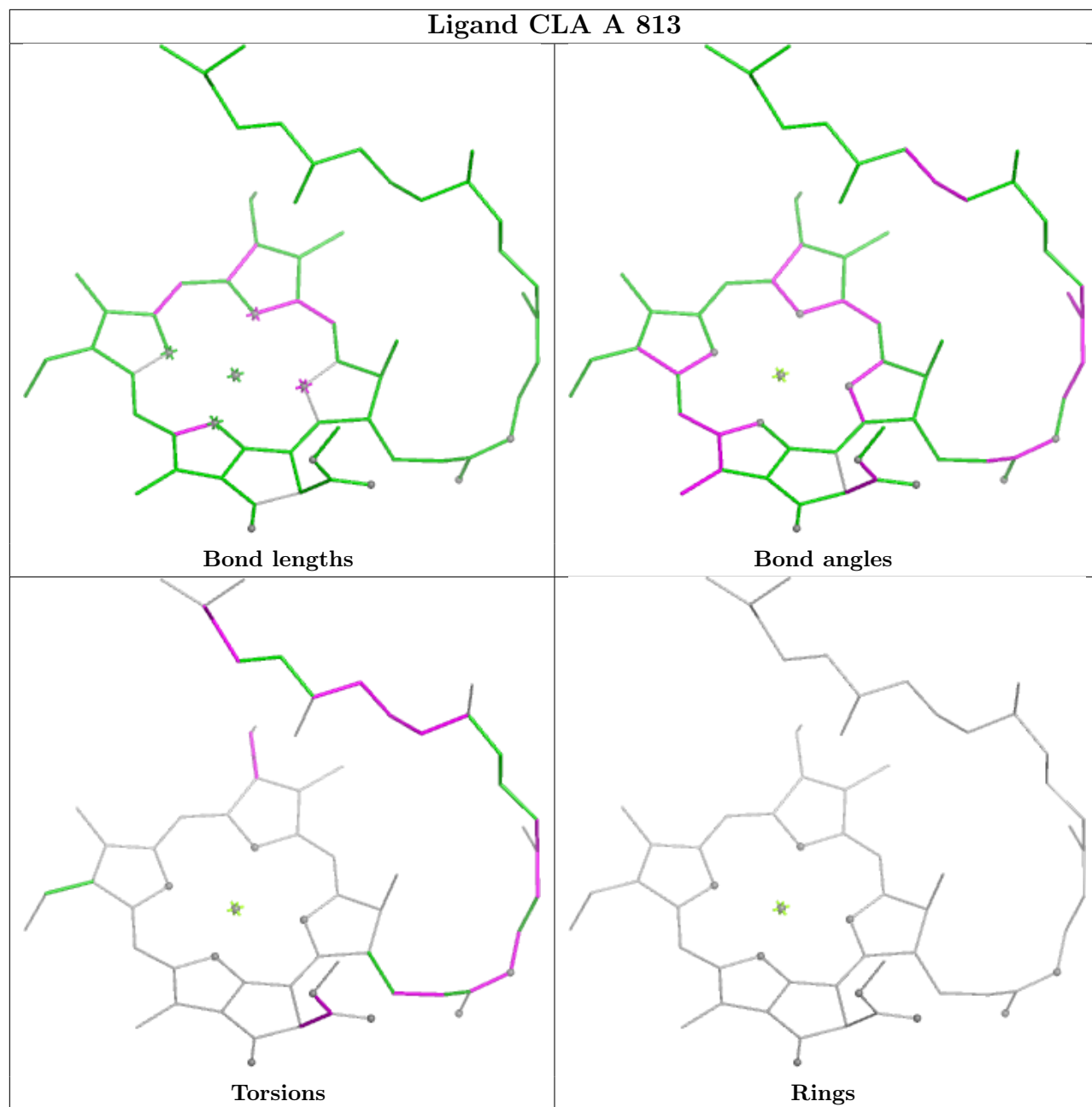


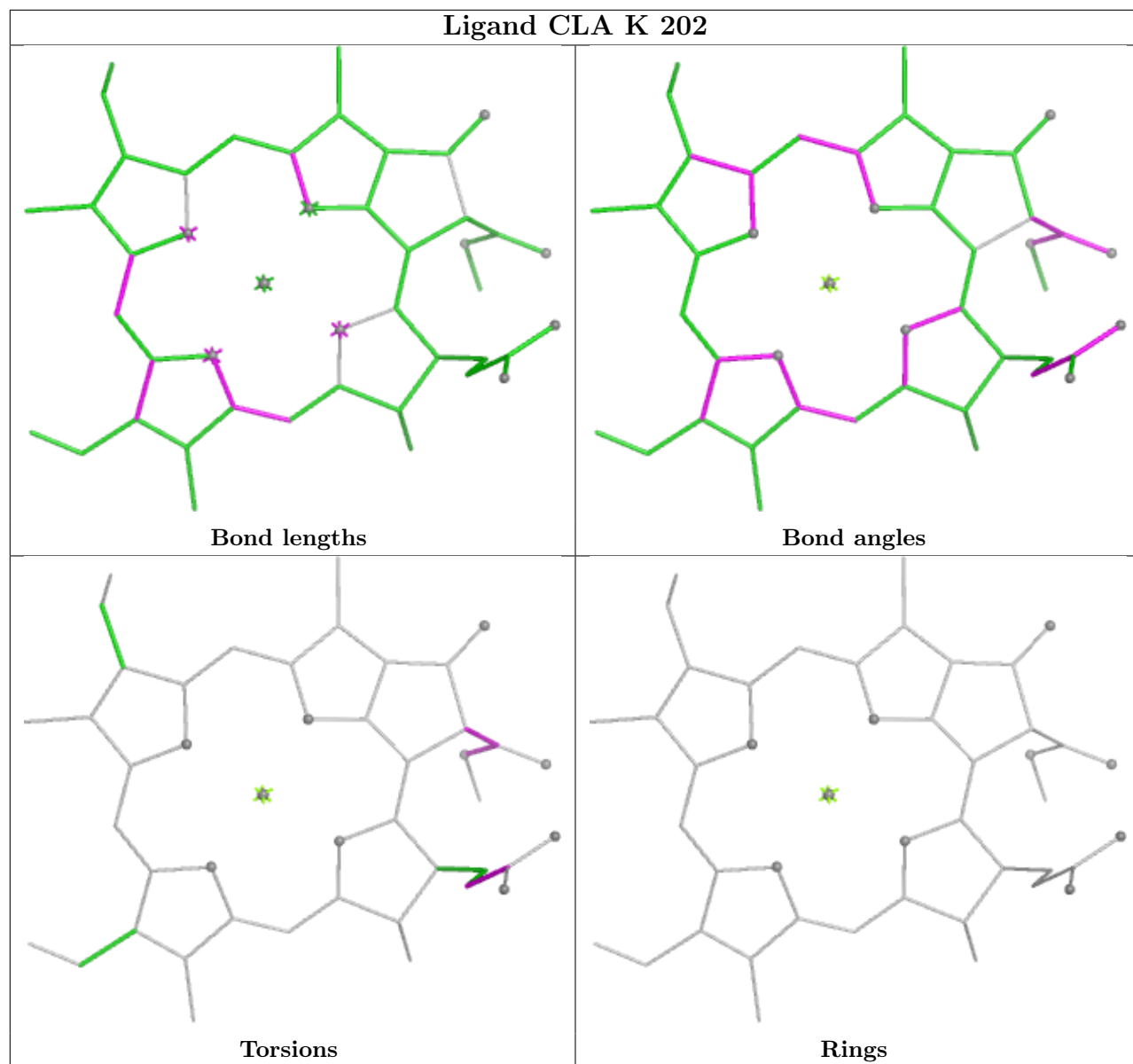




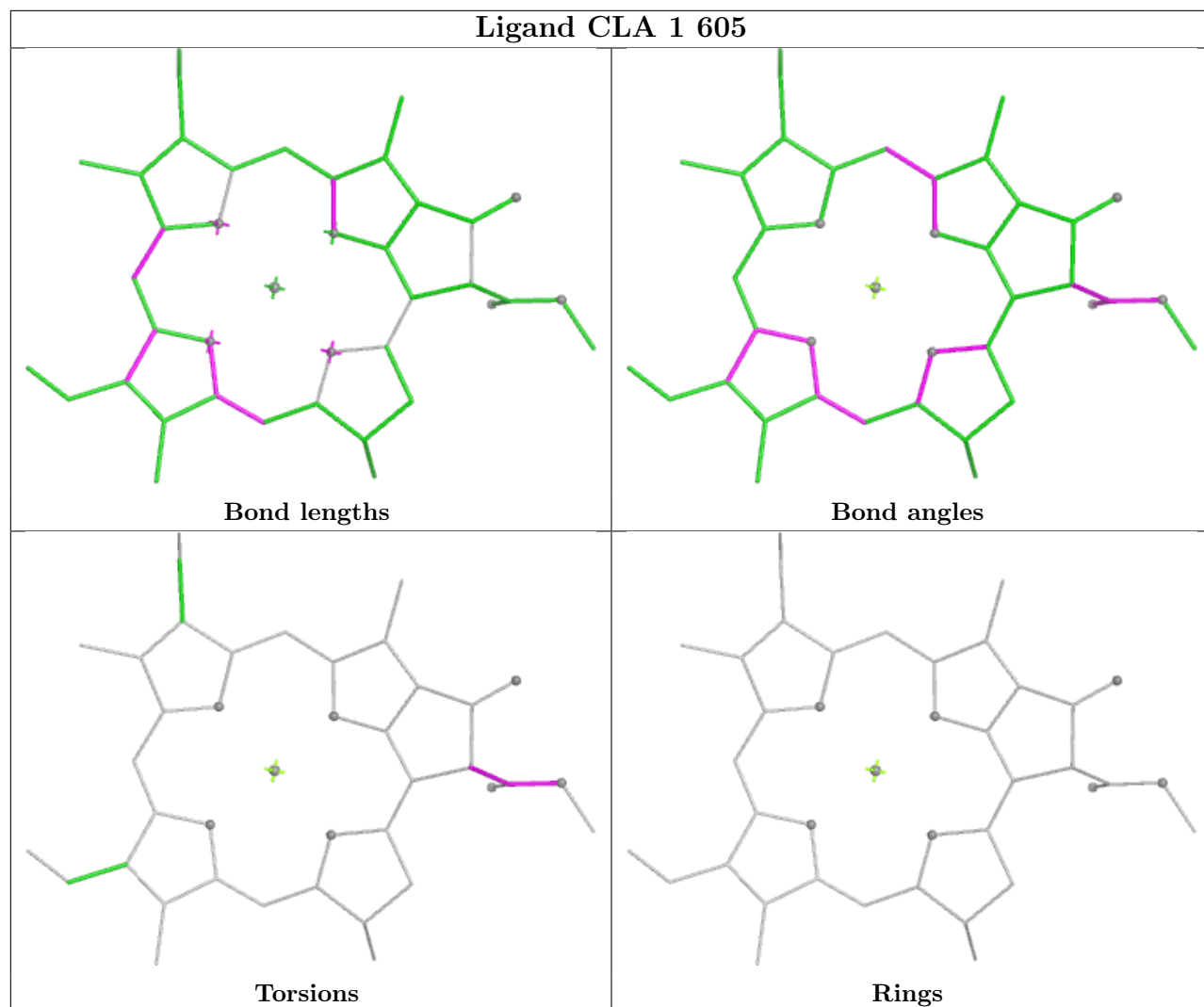


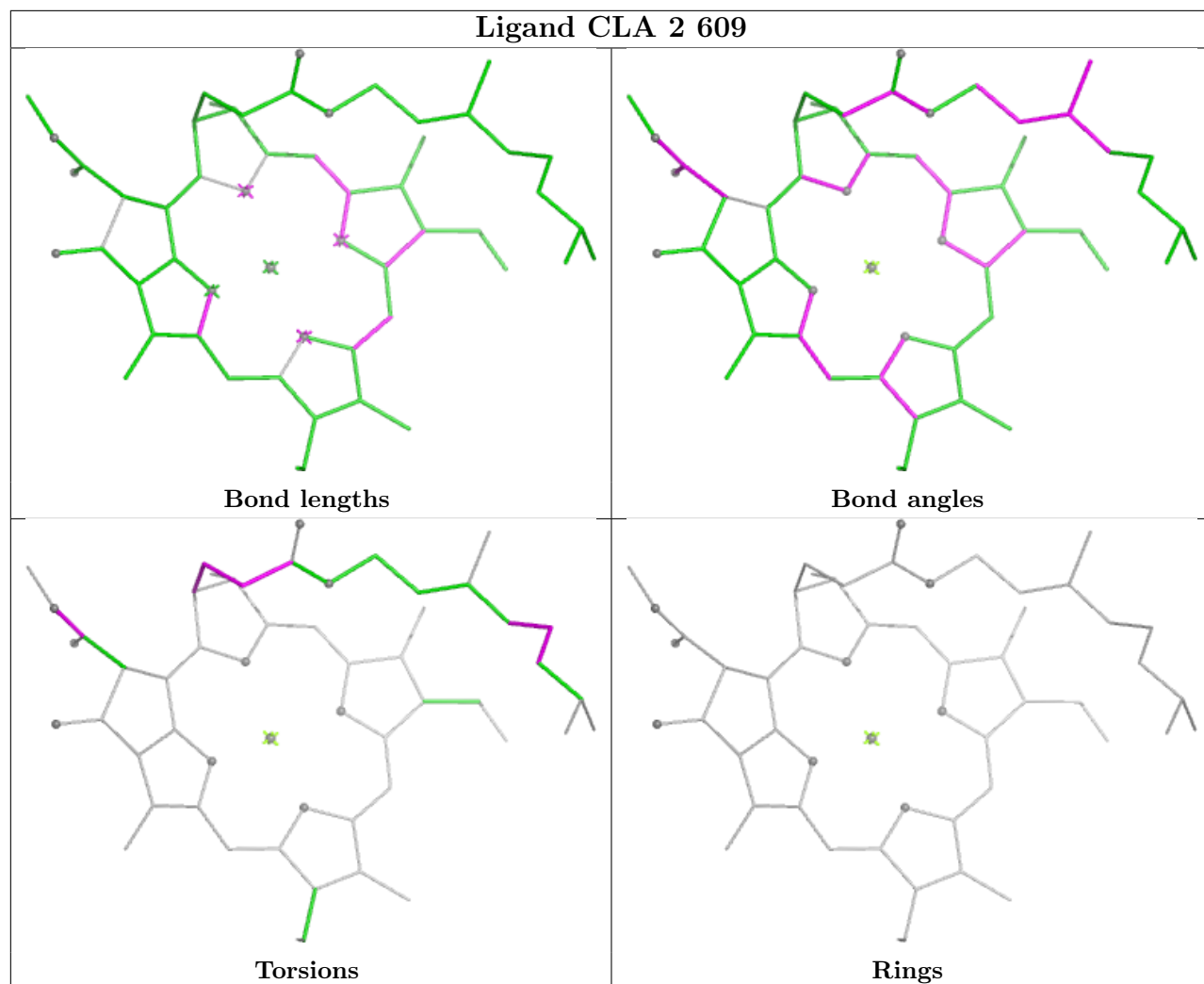
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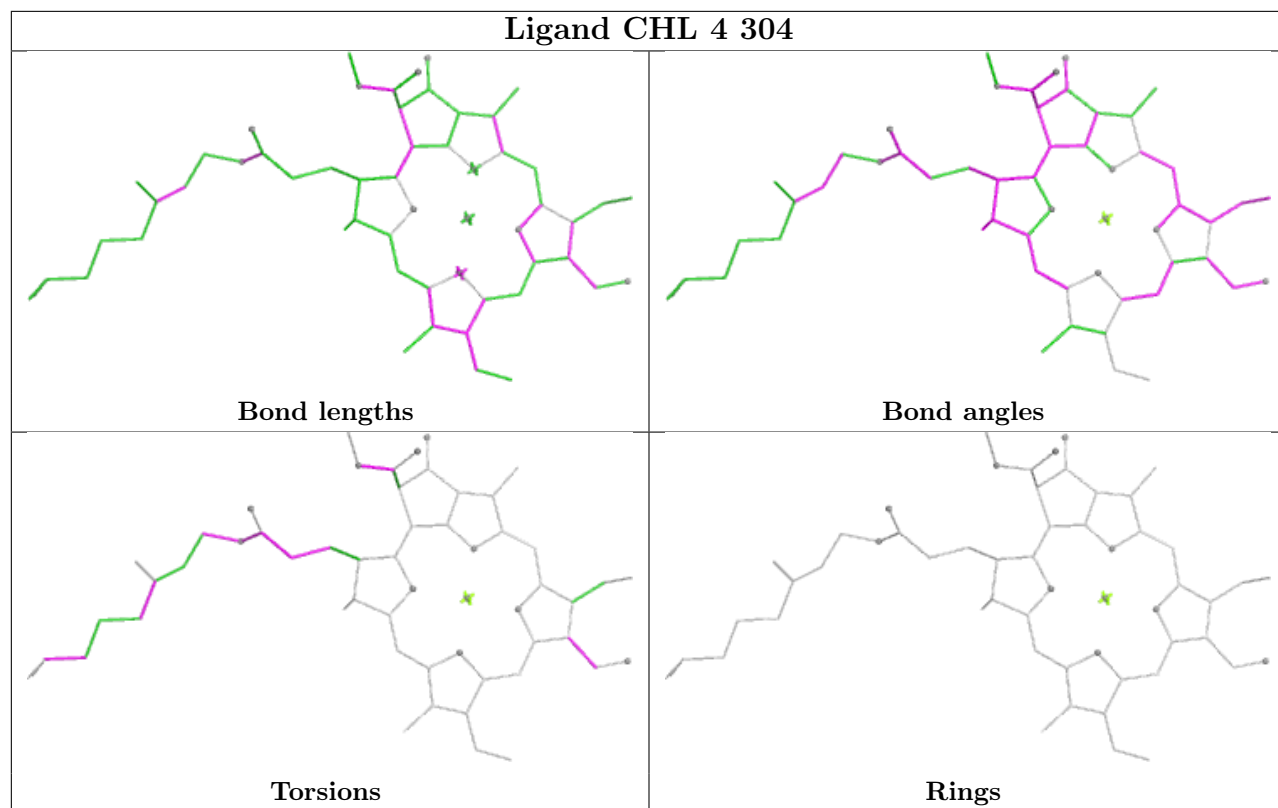




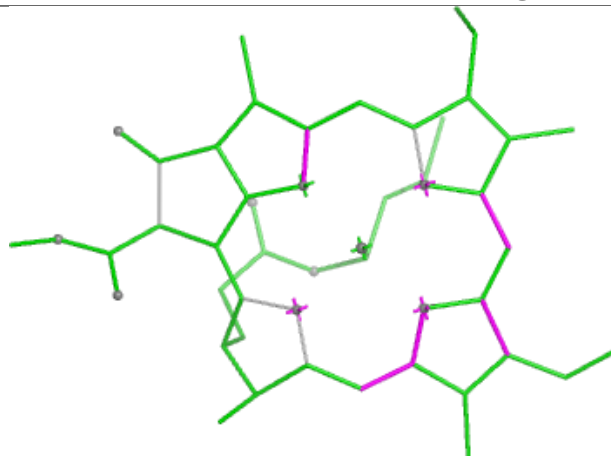
Ligand CLA 1 605



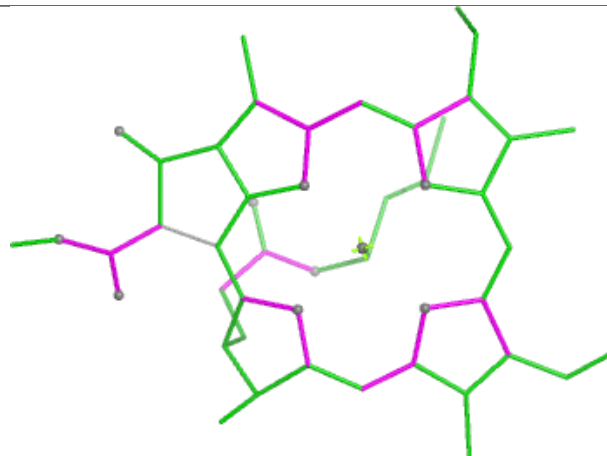




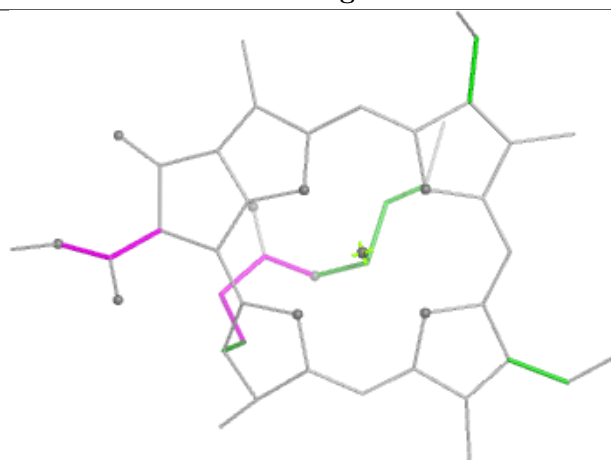
Ligand CLA O 206



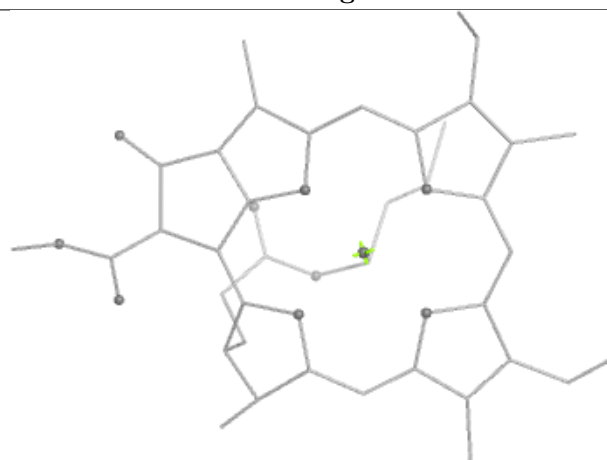
Bond lengths



Bond angles

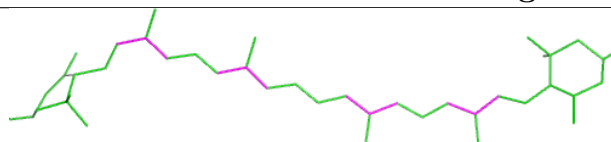


Torsions



Rings

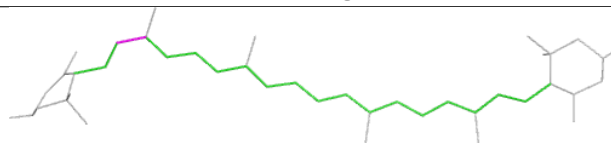
Ligand LUT 3 615



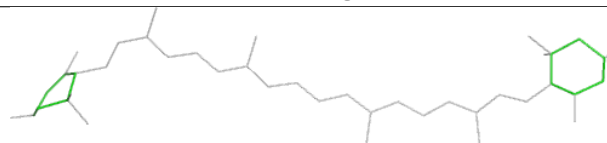
Bond lengths



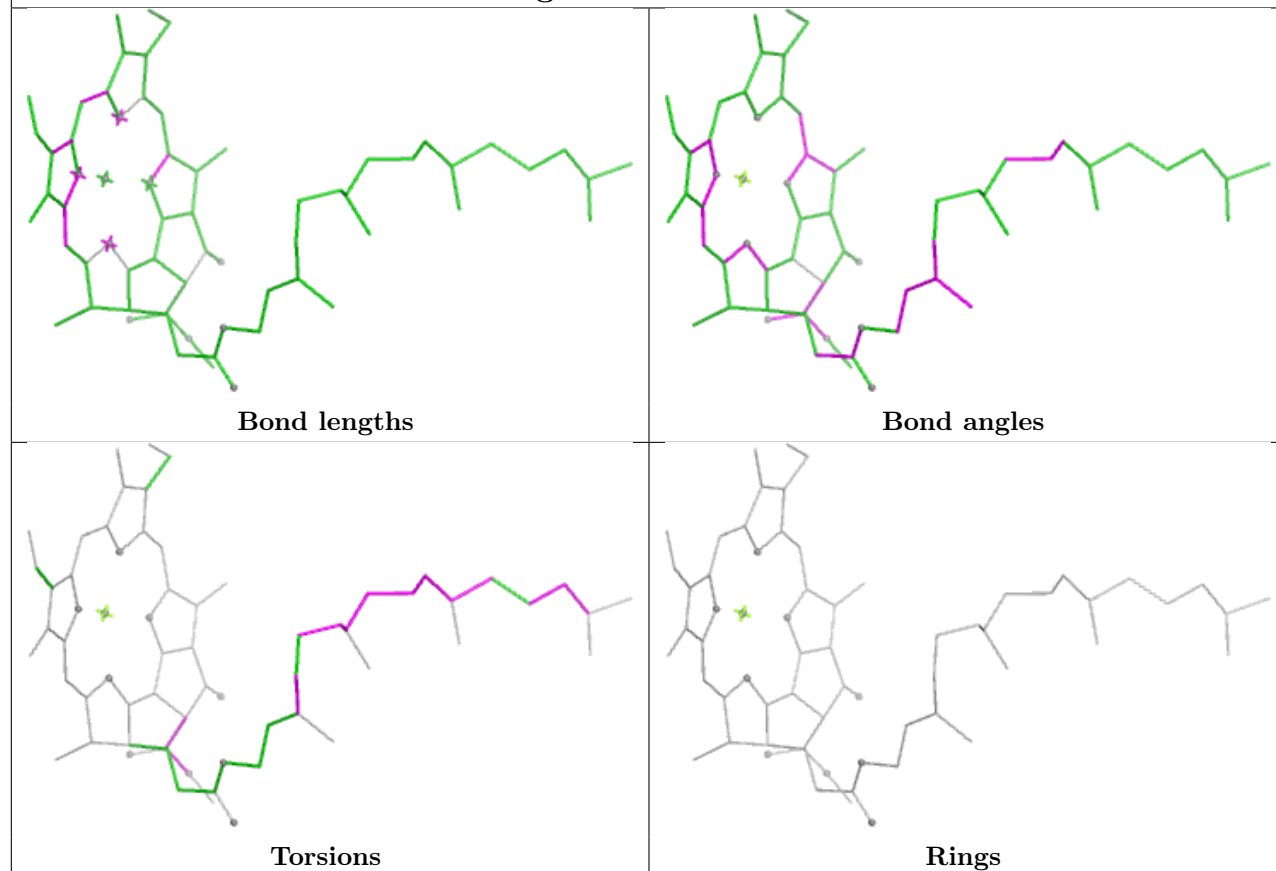
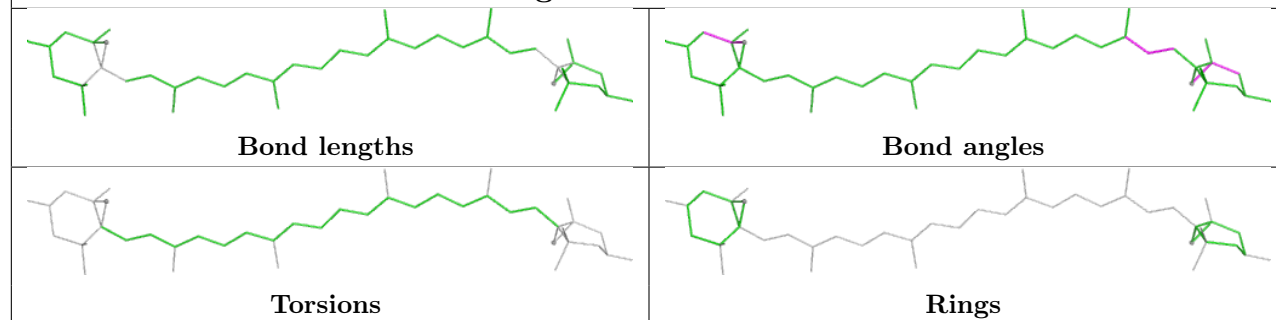
Bond angles



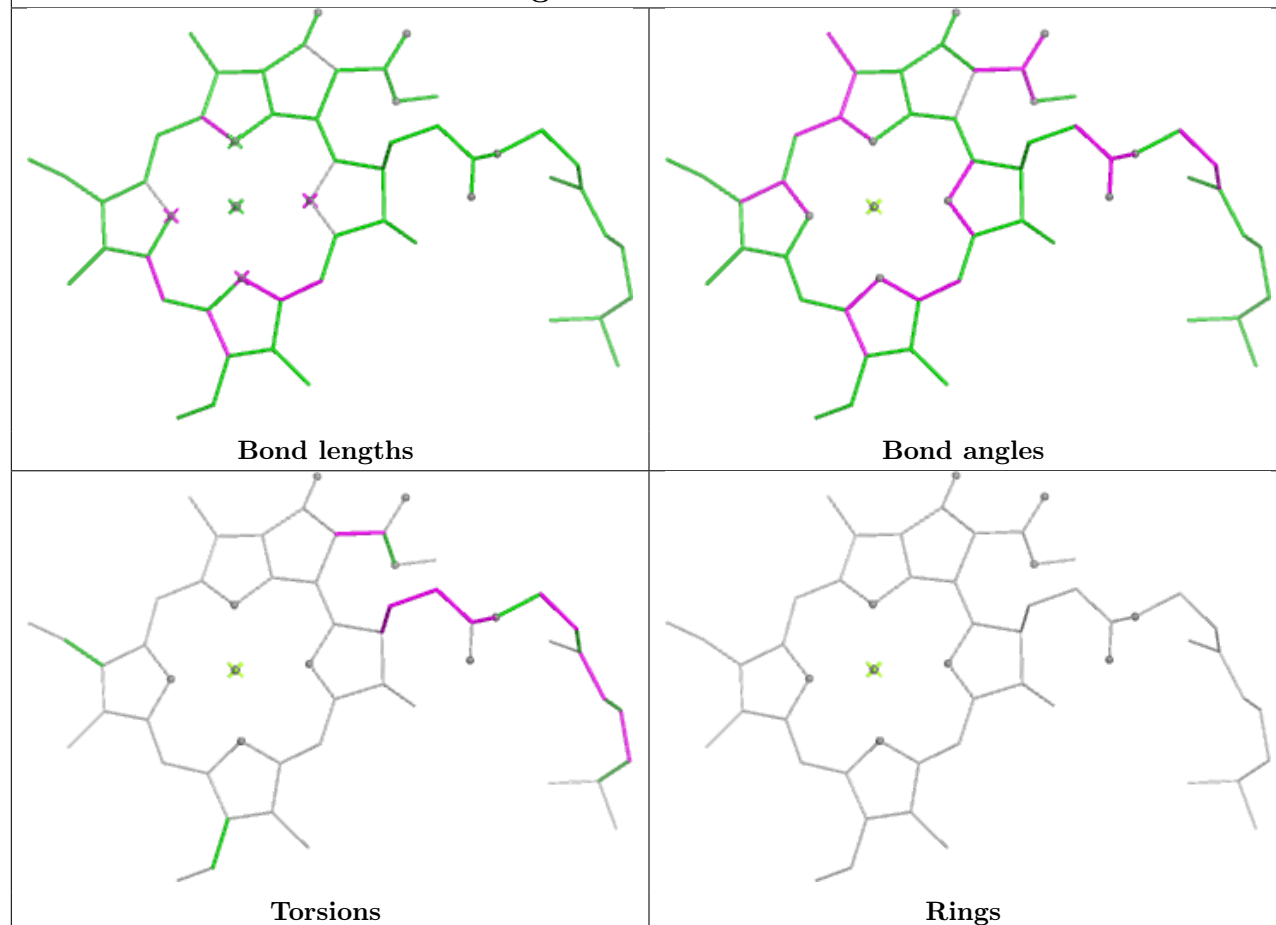
Torsions



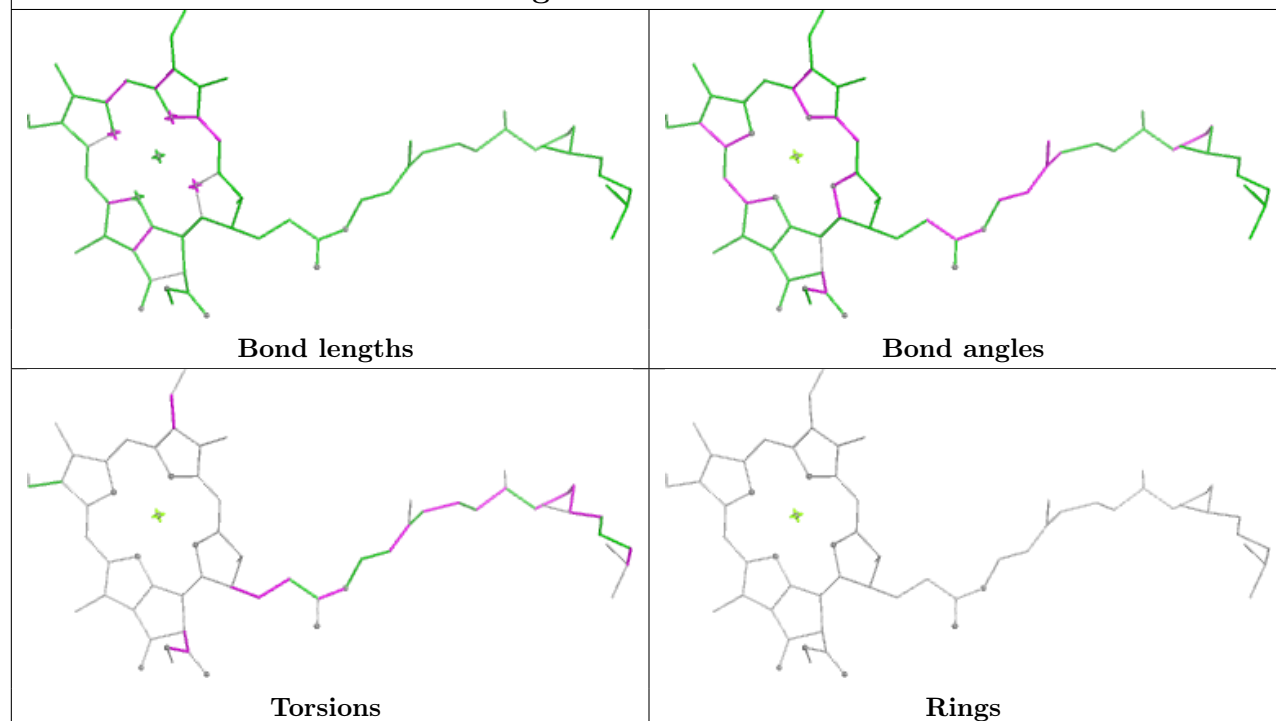
Rings

Ligand CLA 1 608**Ligand XAT 2 616**

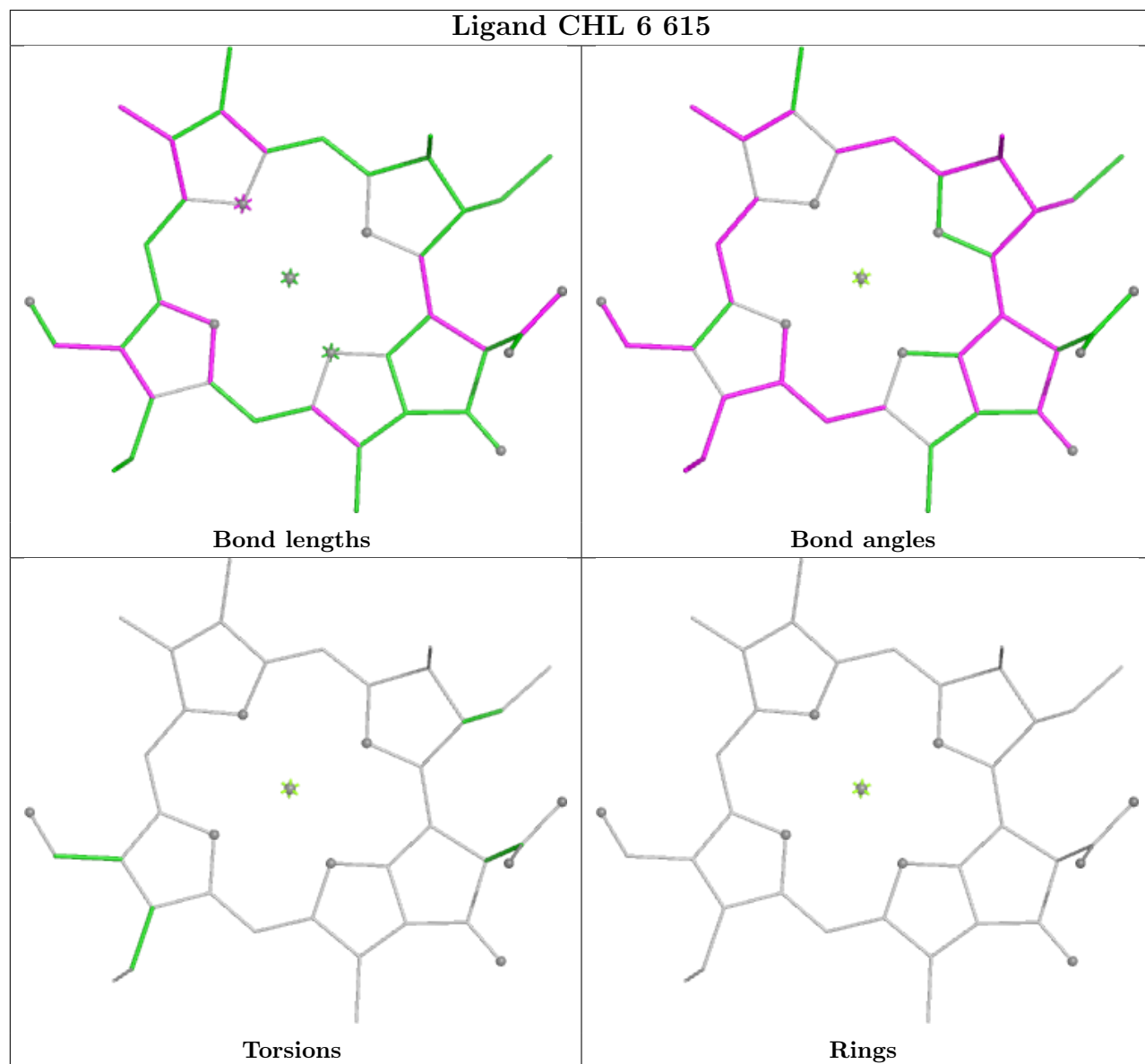
Ligand CLA A 804



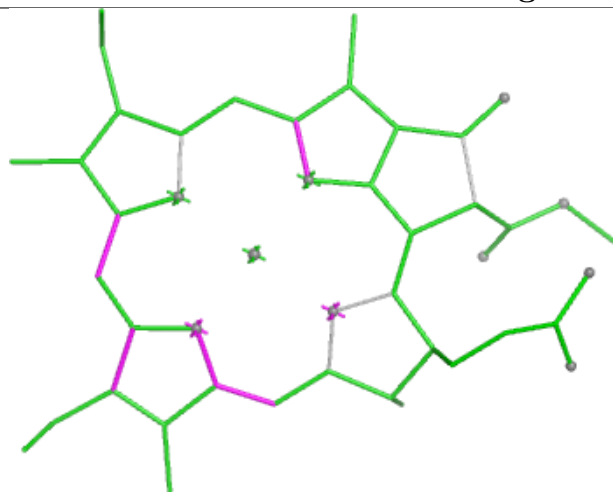
Ligand CLA B 812



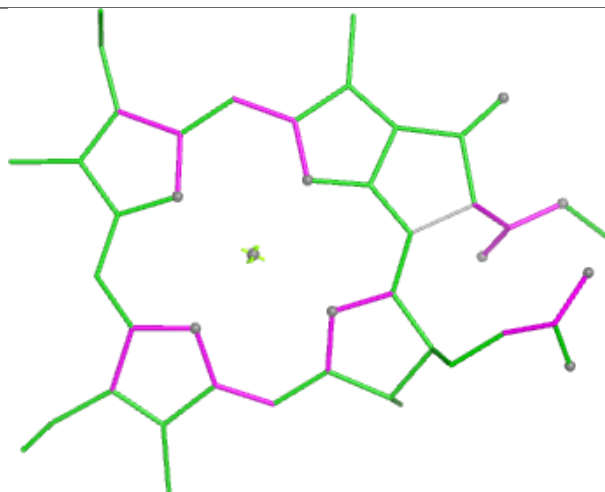
Ligand CHL 6 615



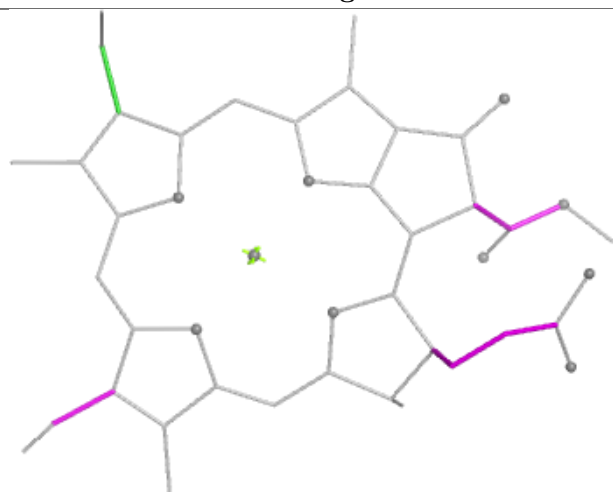
Ligand CLA 5 614



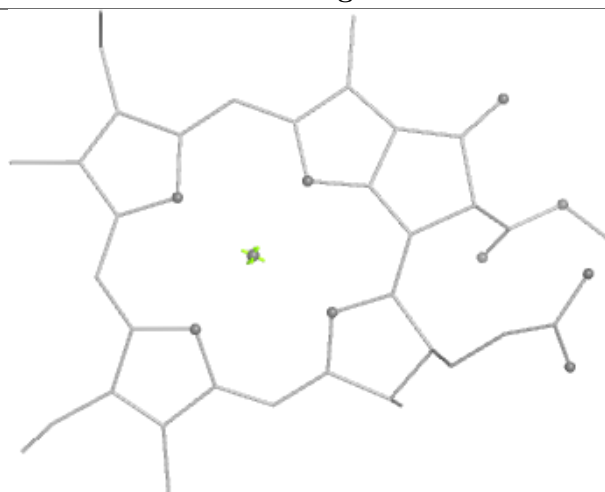
Bond lengths



Bond angles

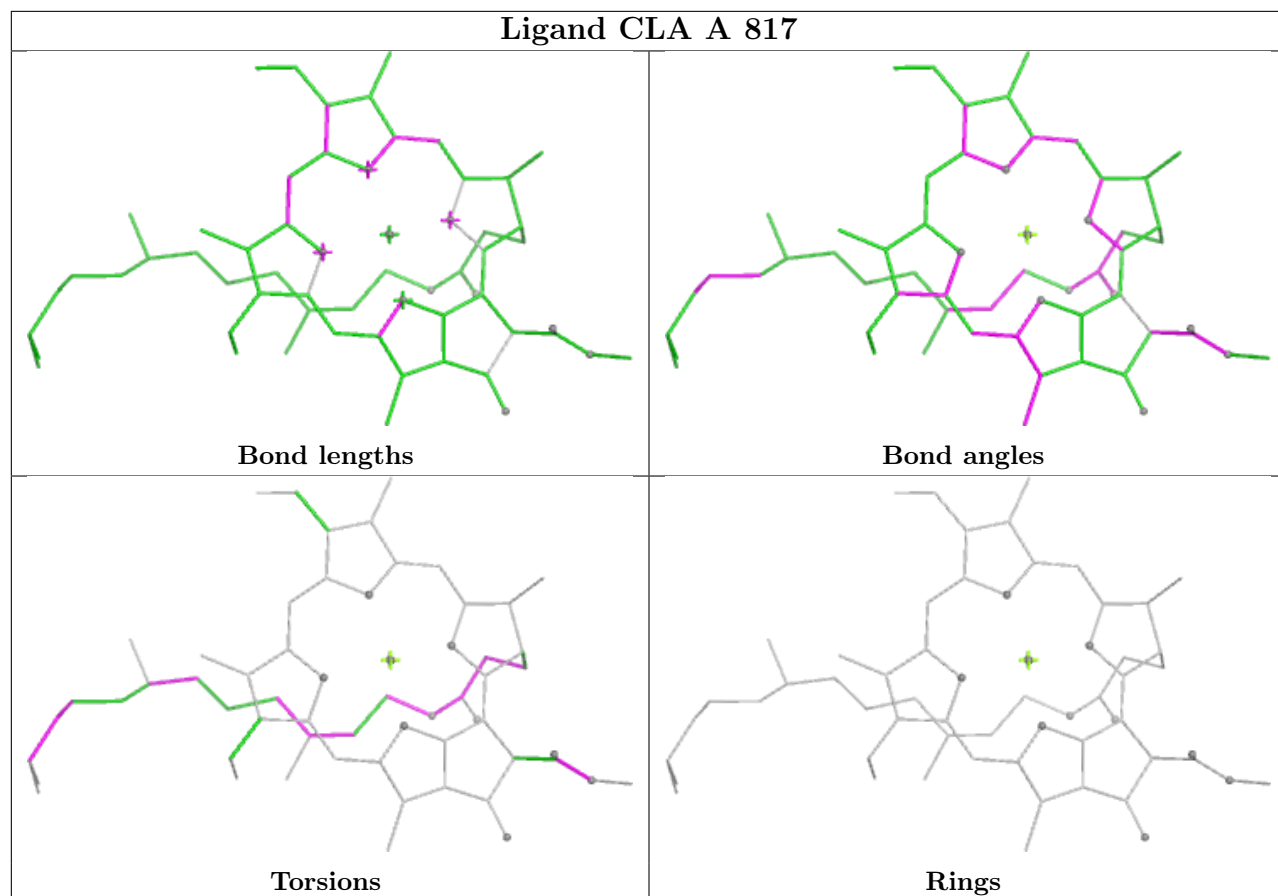


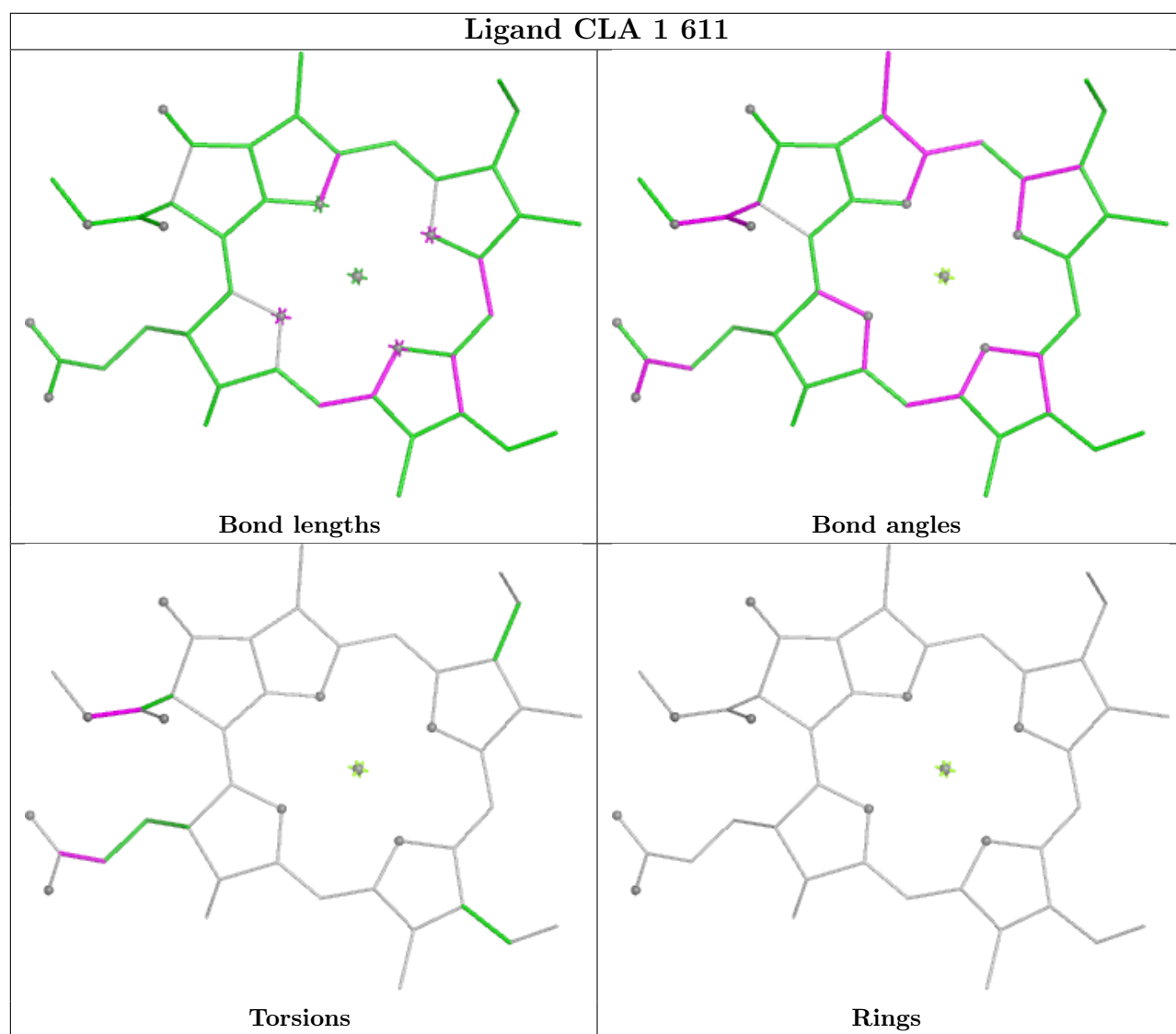
Torsions

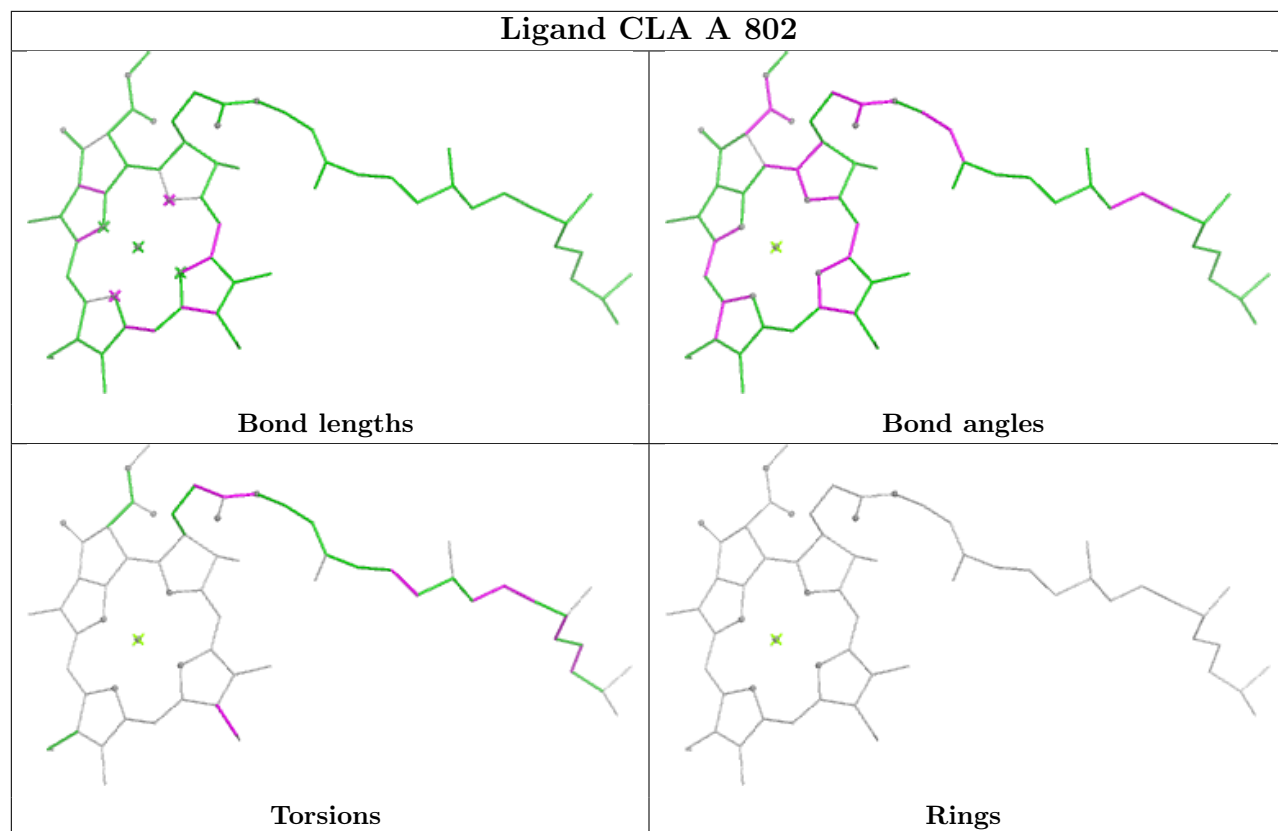


Rings

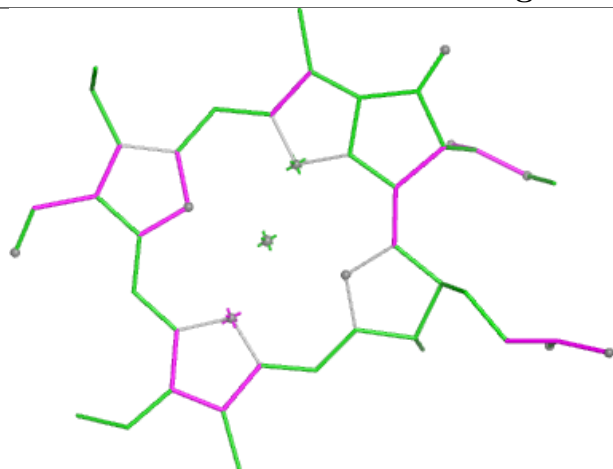
Ligand CLA A 817



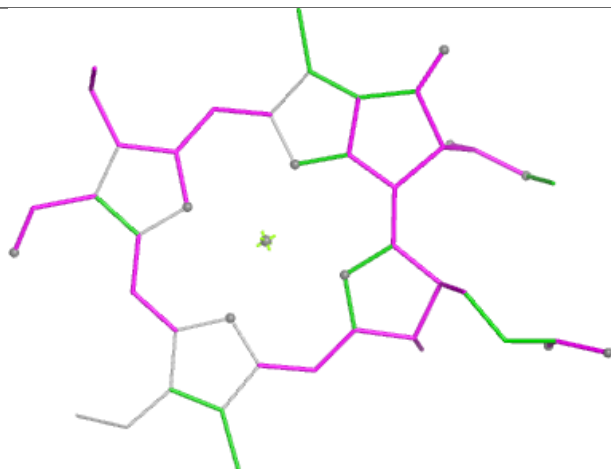




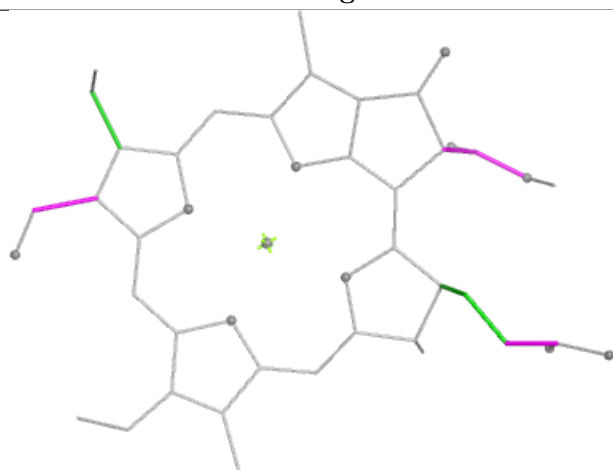
Ligand CHL Z 302



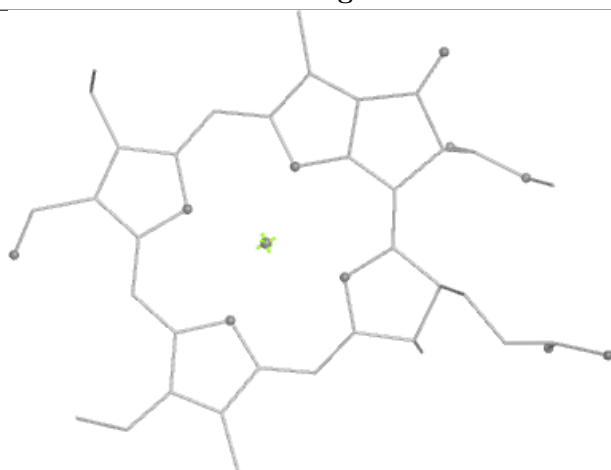
Bond lengths



Bond angles

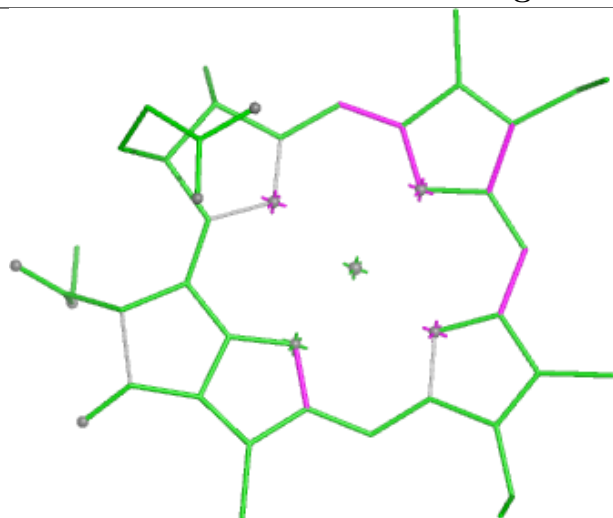


Torsions

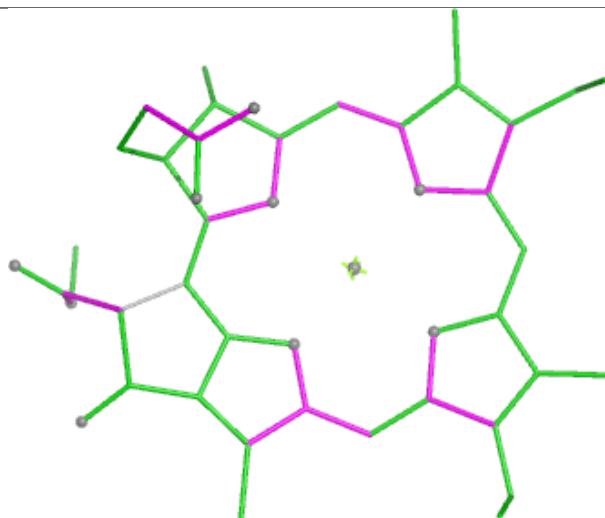


Rings

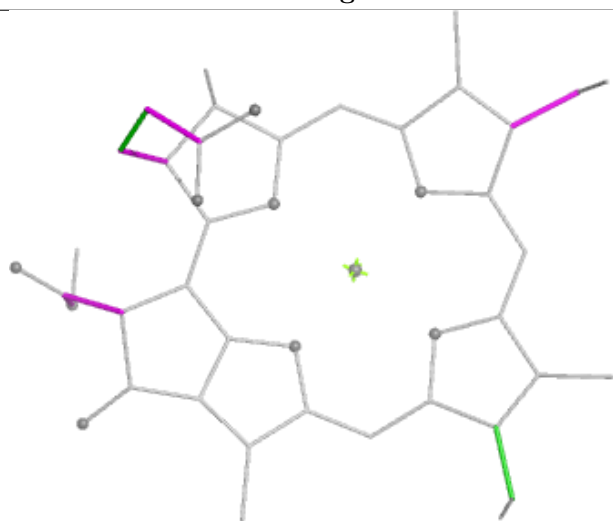
Ligand CLA X 602



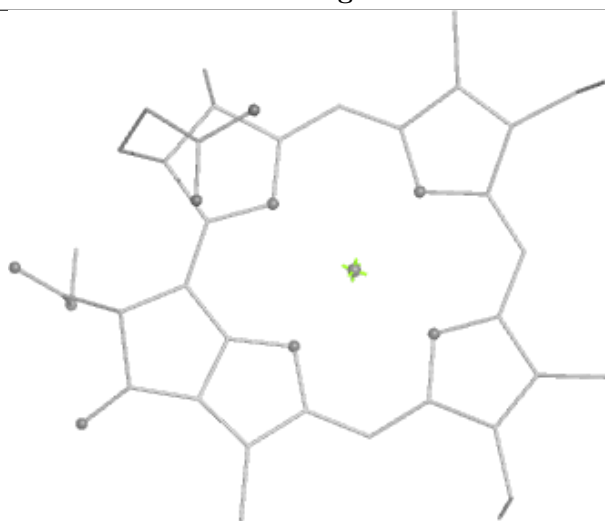
Bond lengths



Bond angles

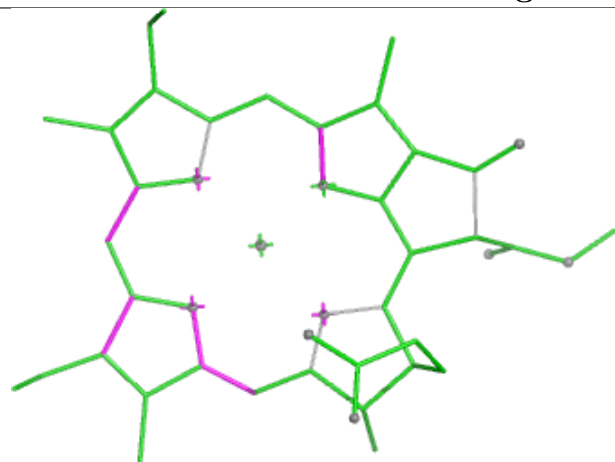


Torsions

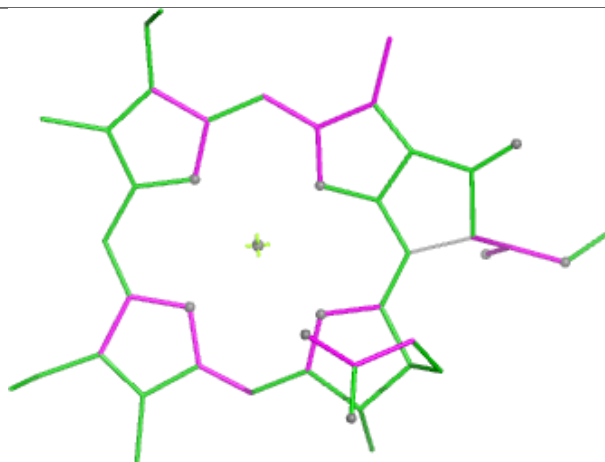


Rings

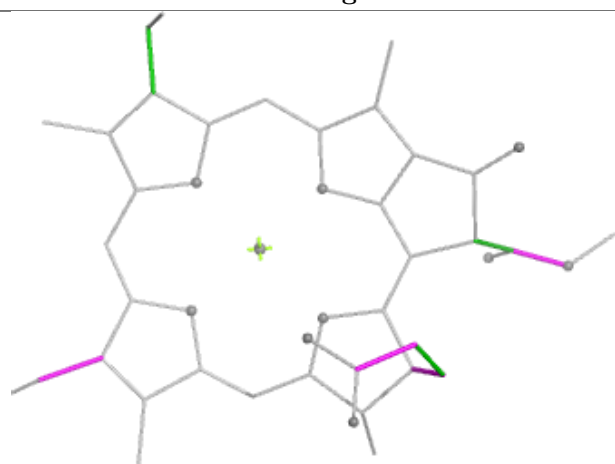
Ligand CLA X 613



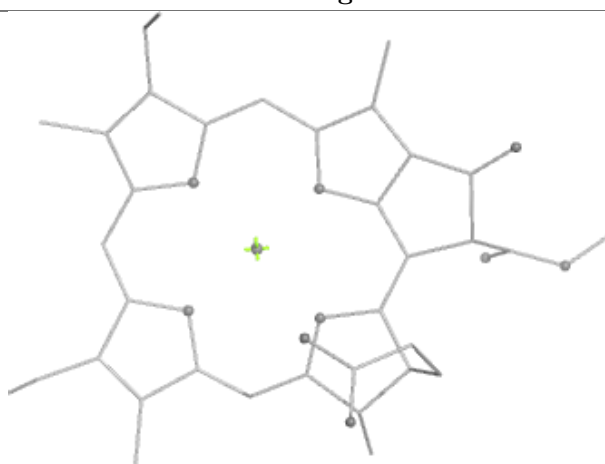
Bond lengths



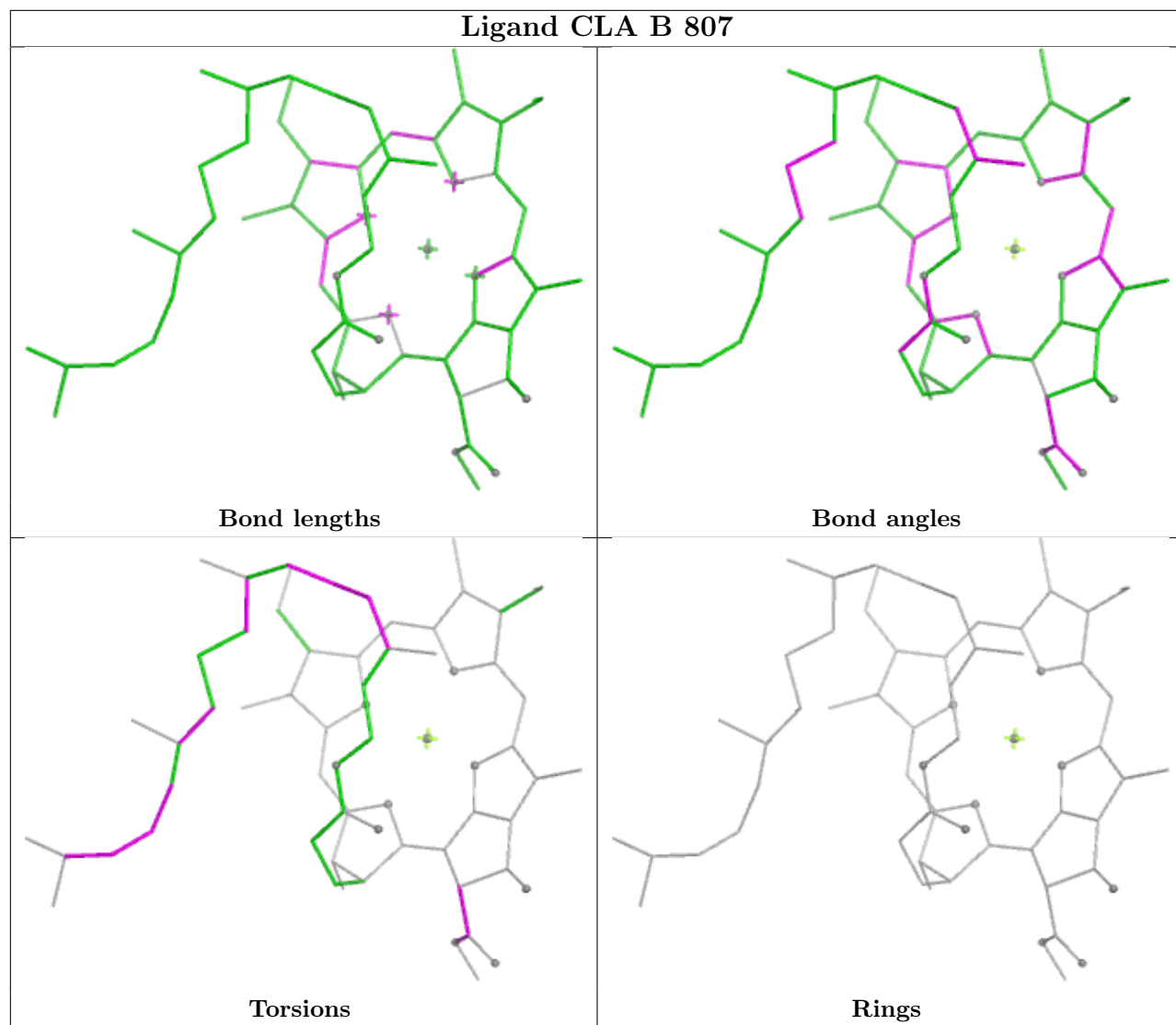
Bond angles



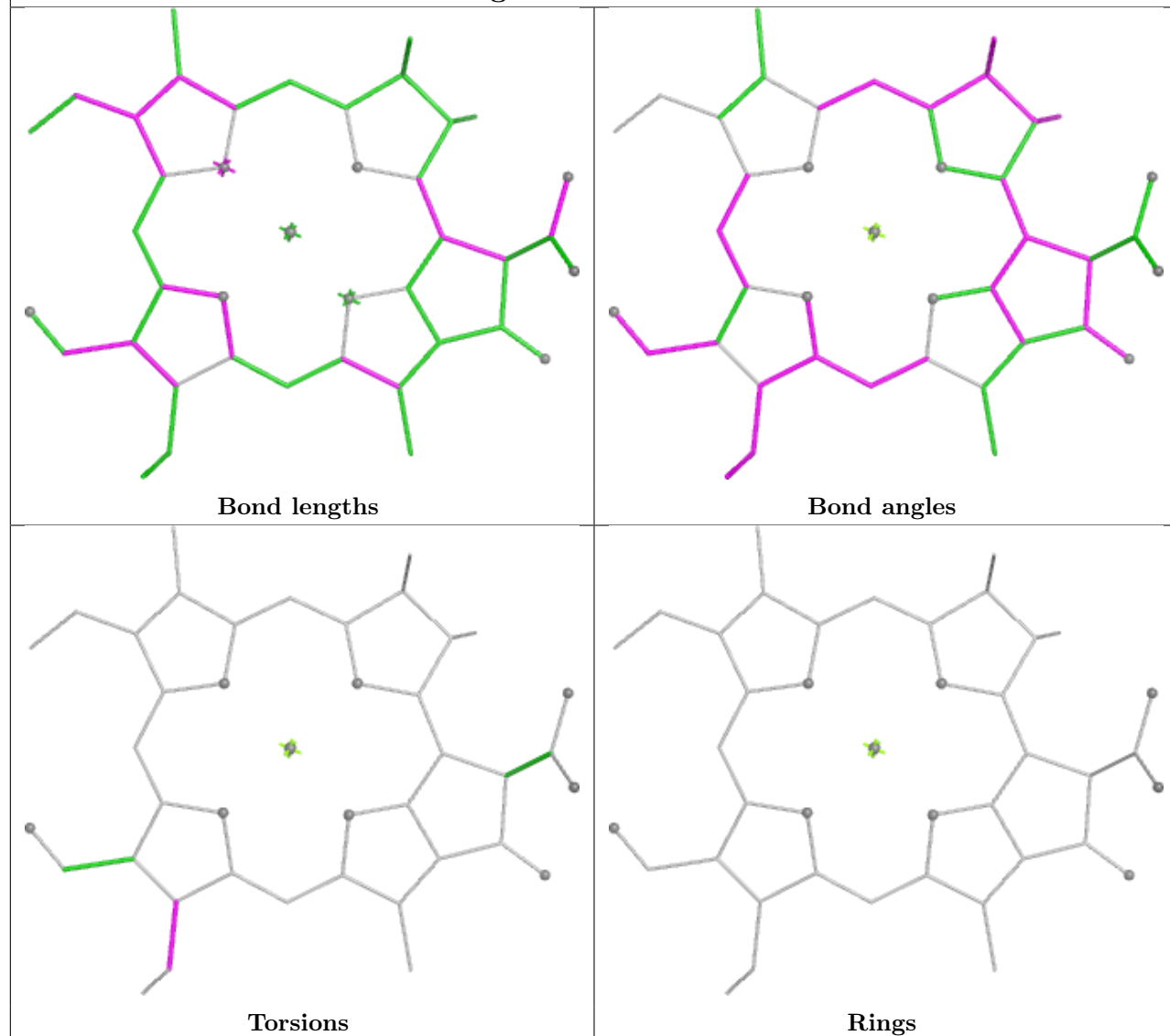
Torsions



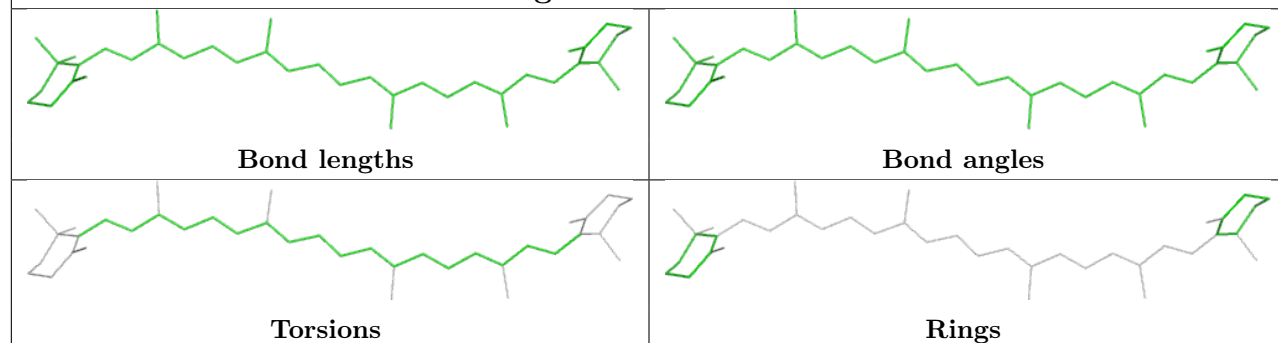
Rings



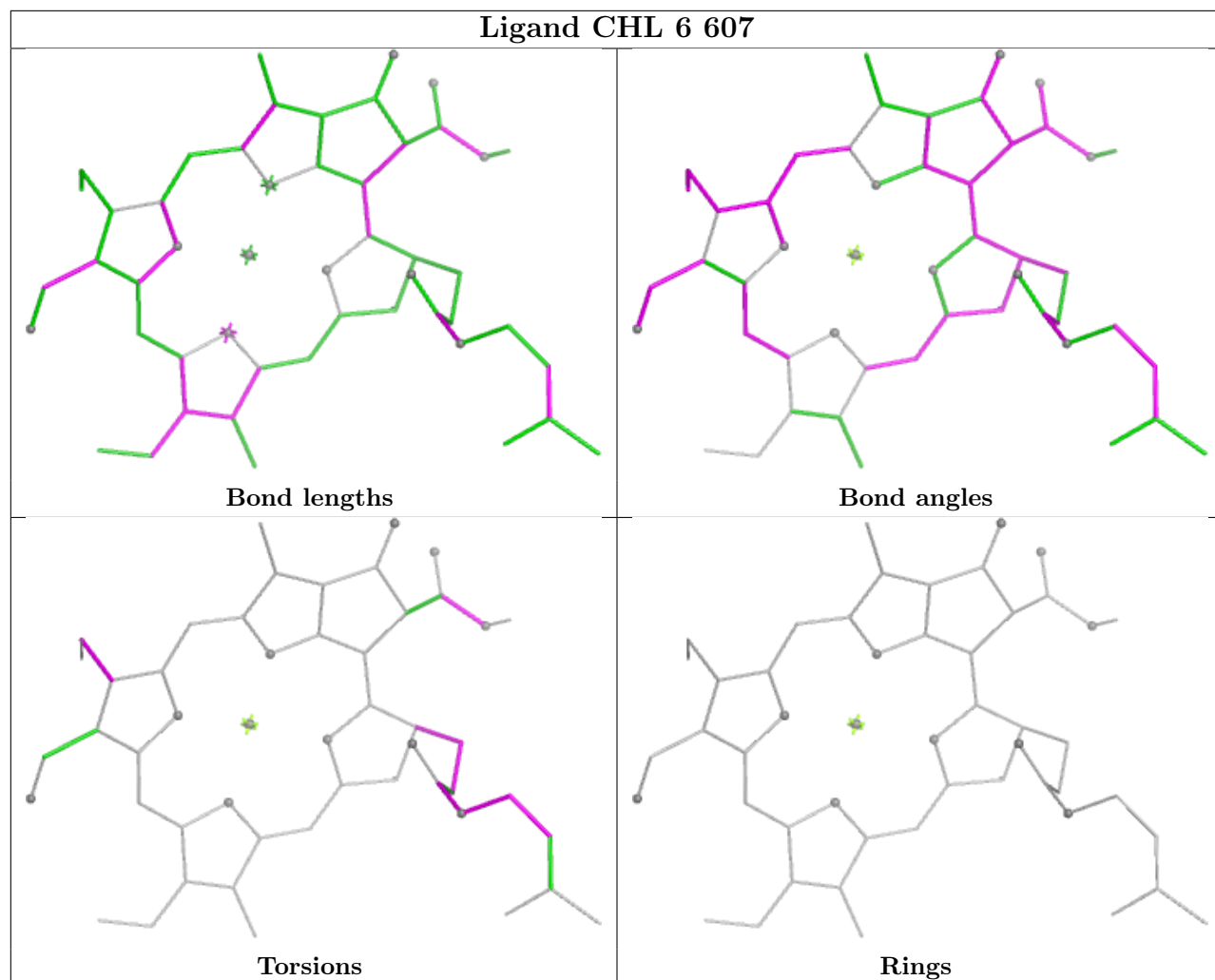
Ligand CHL 1 606



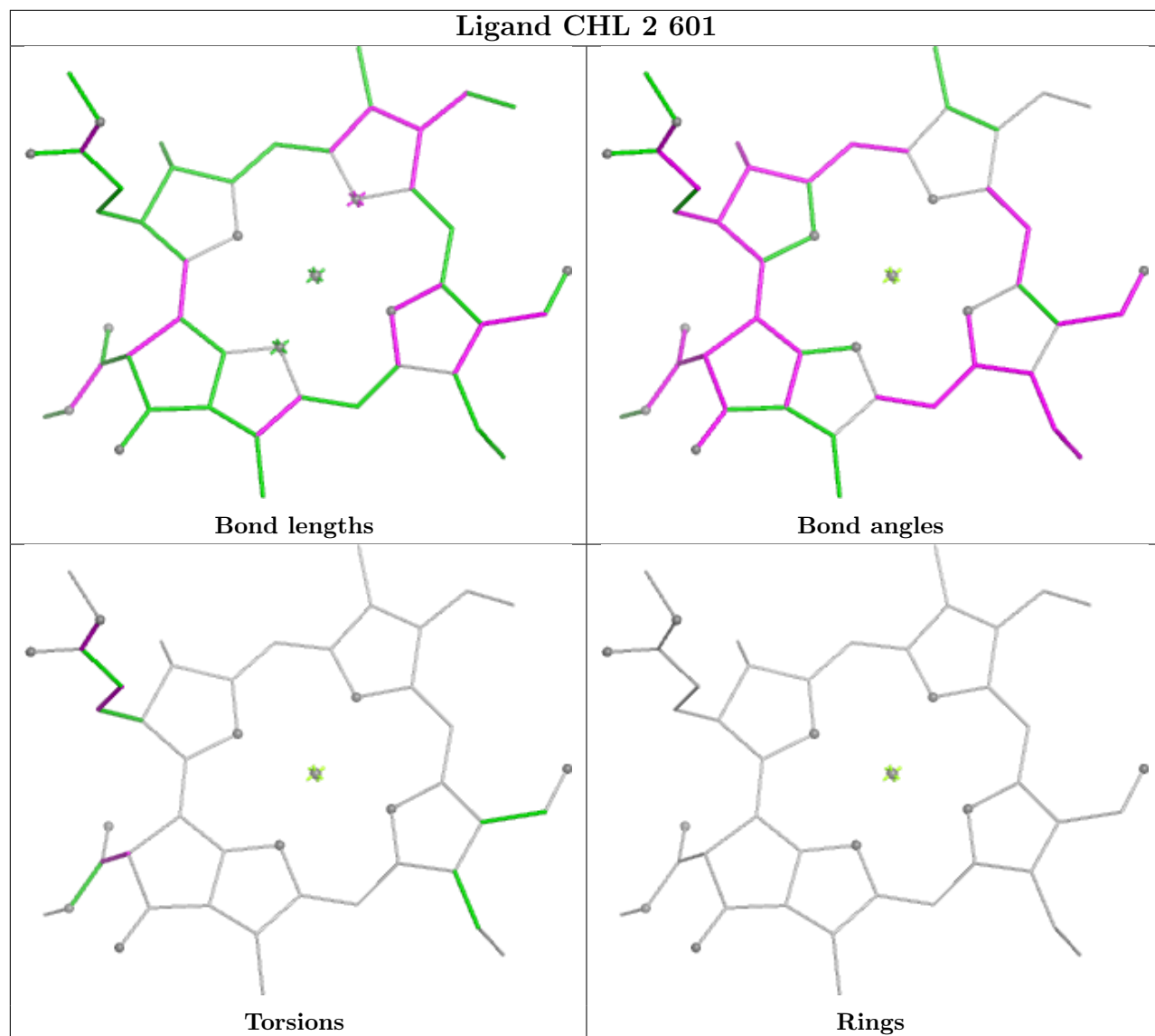
Ligand BCR 3 601



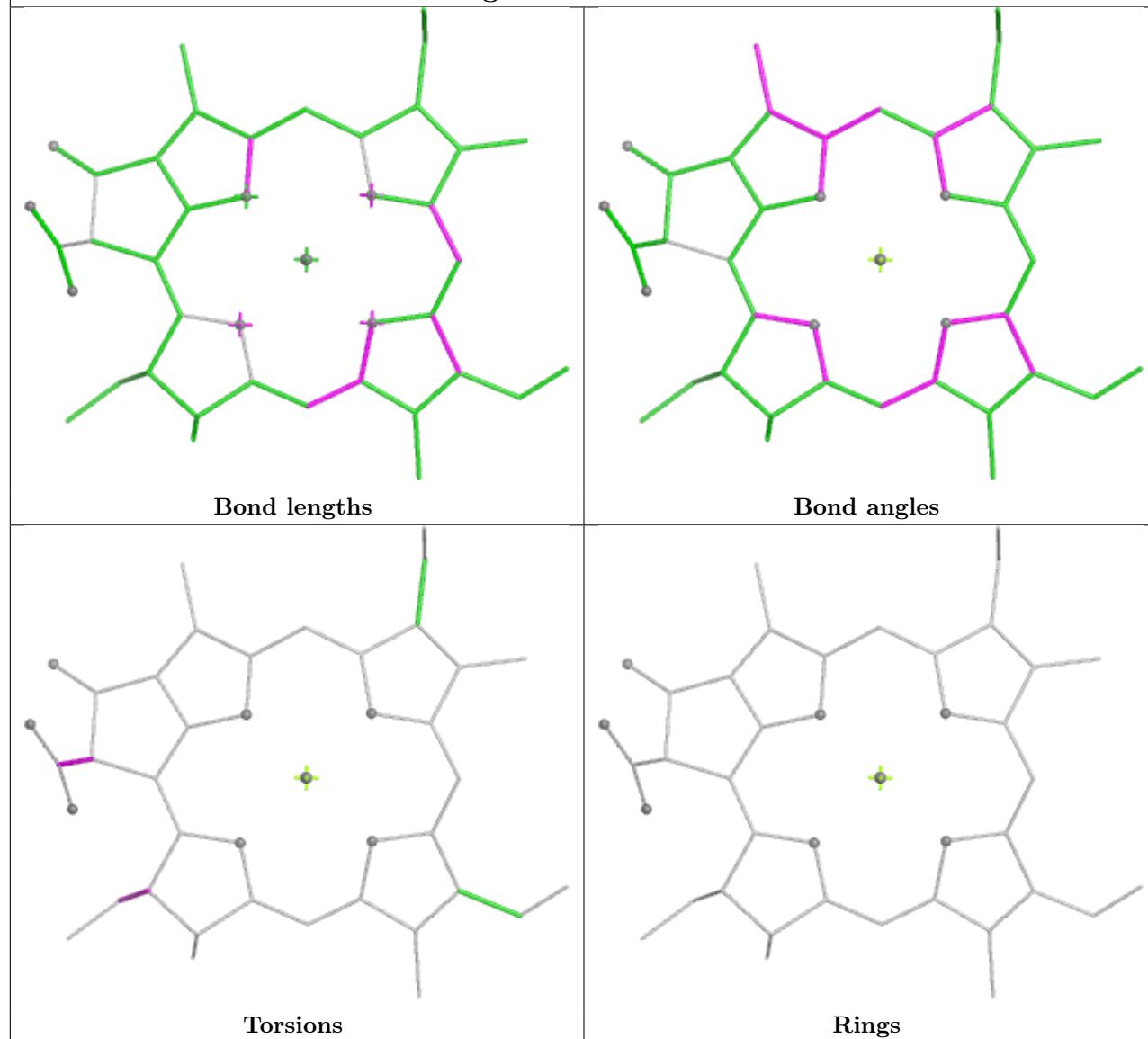
Ligand CHL 6 607

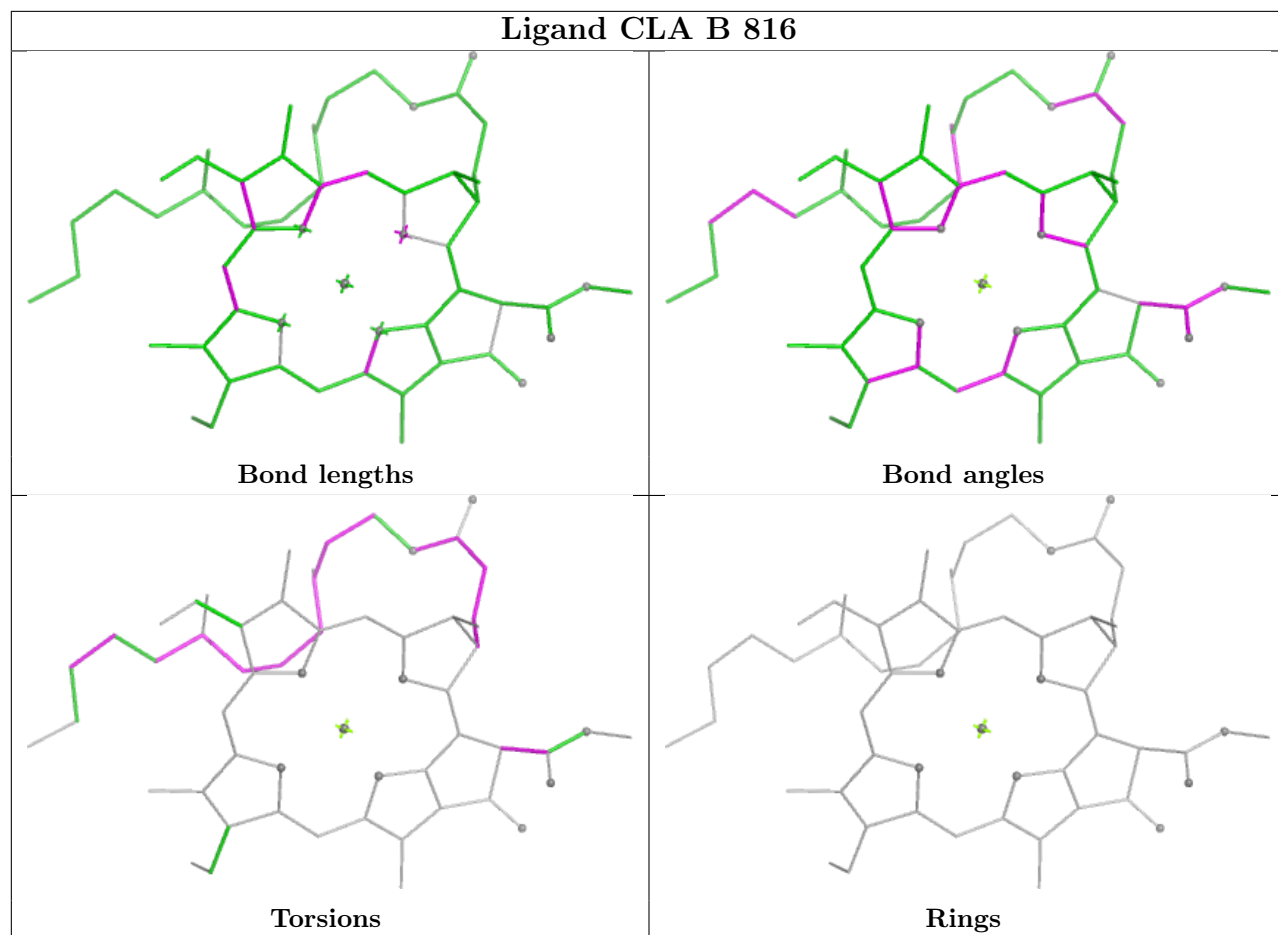


Ligand CHL 2 601

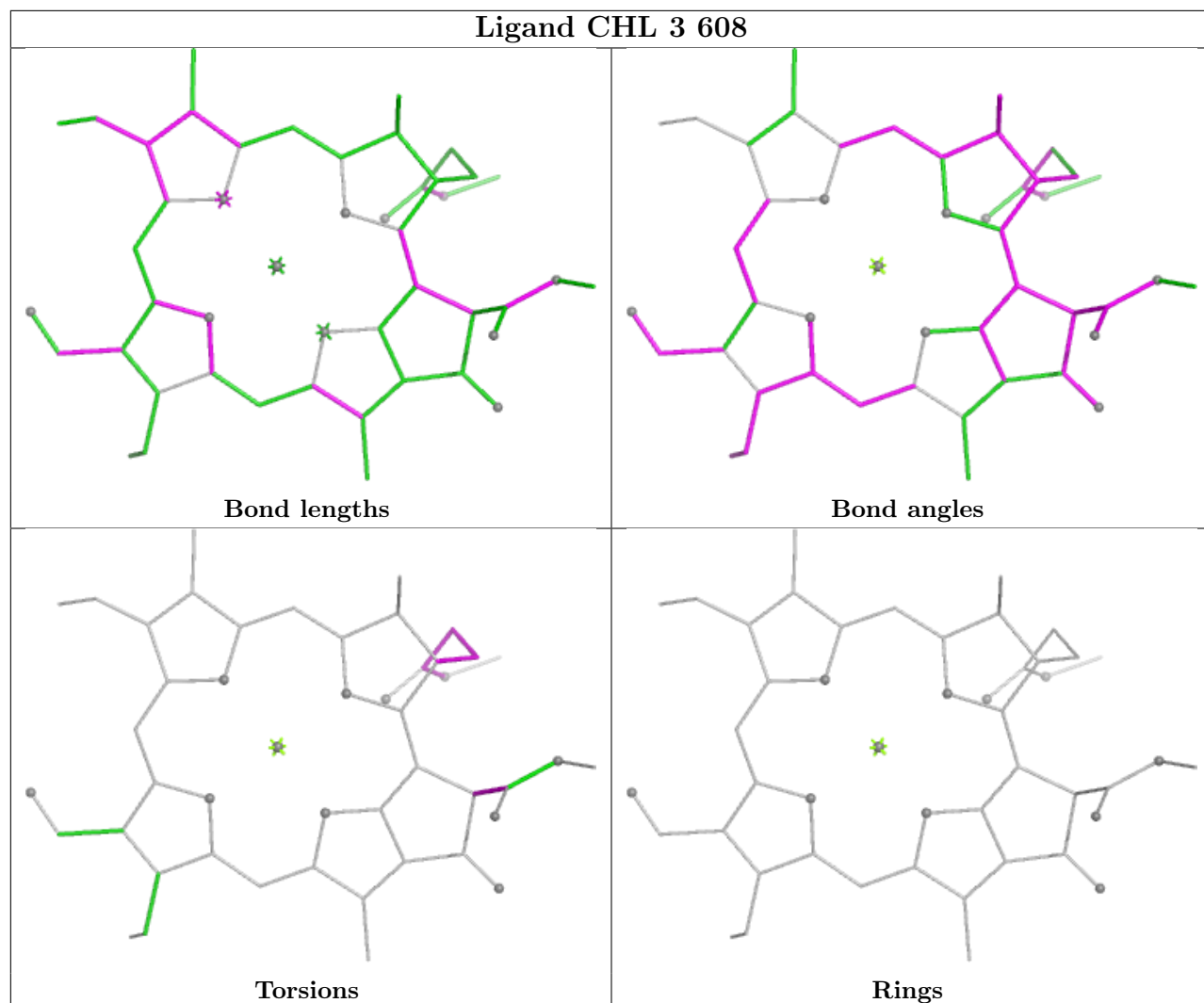


Ligand CLA 3 606

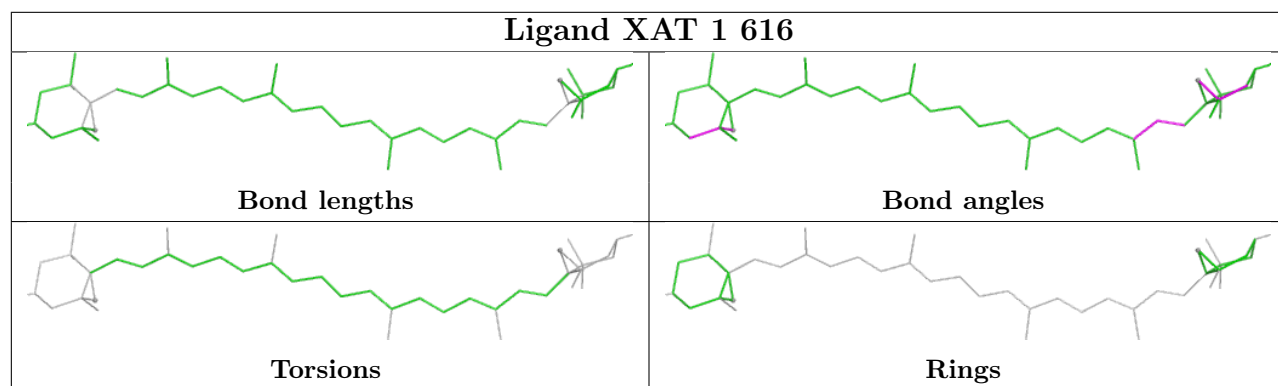


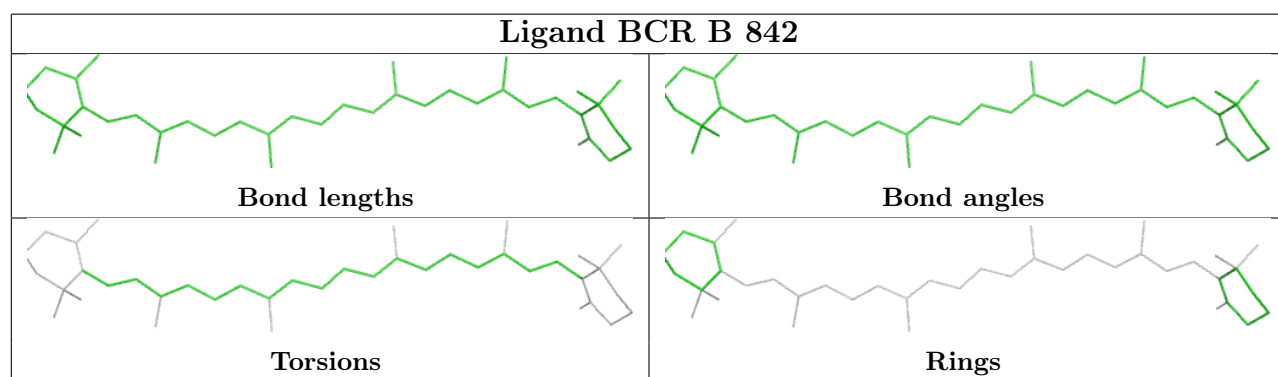
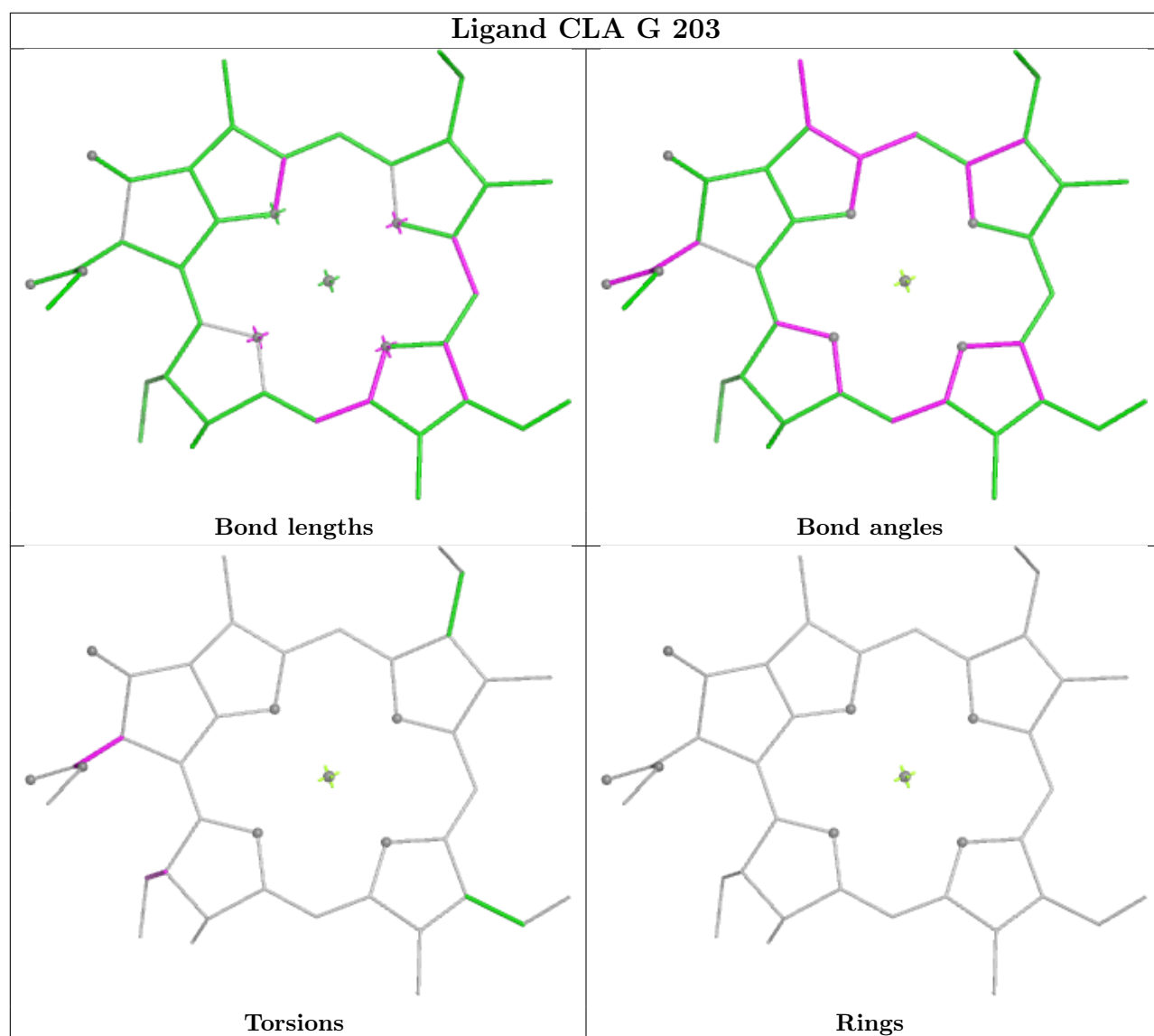


Ligand CHL 3 608

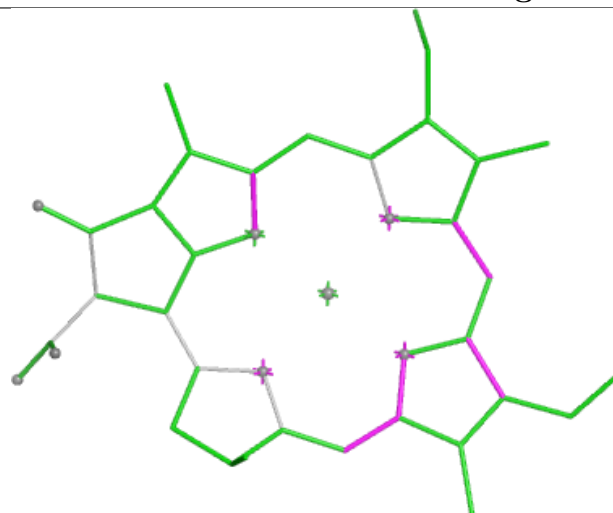


Ligand XAT 1 616

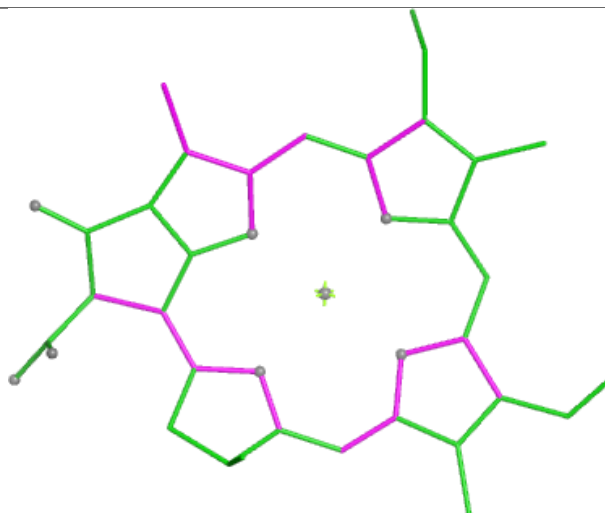




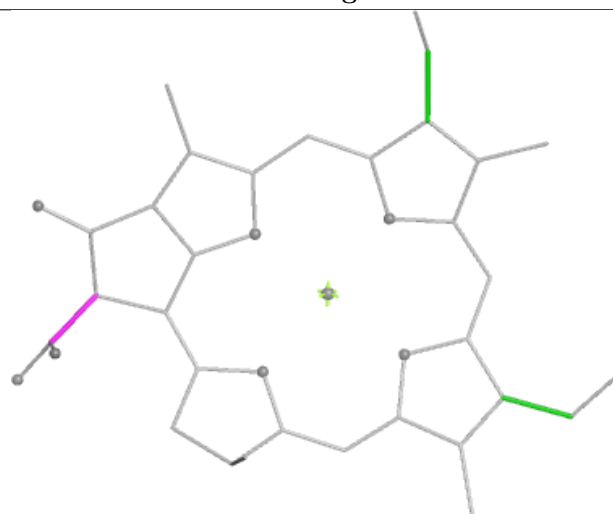
Ligand CLA K 204



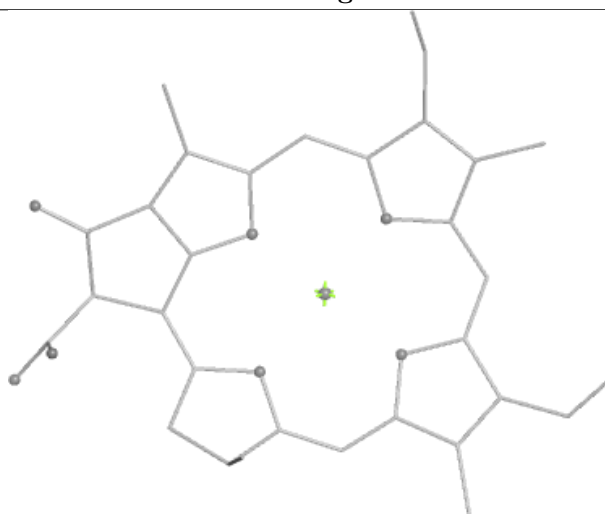
Bond lengths



Bond angles

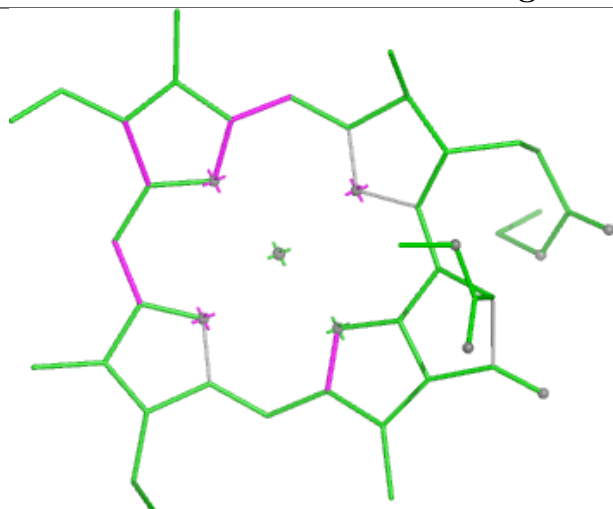


Torsions

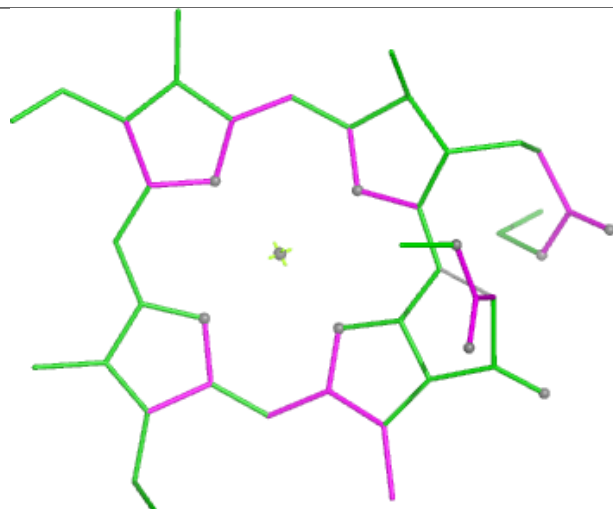


Rings

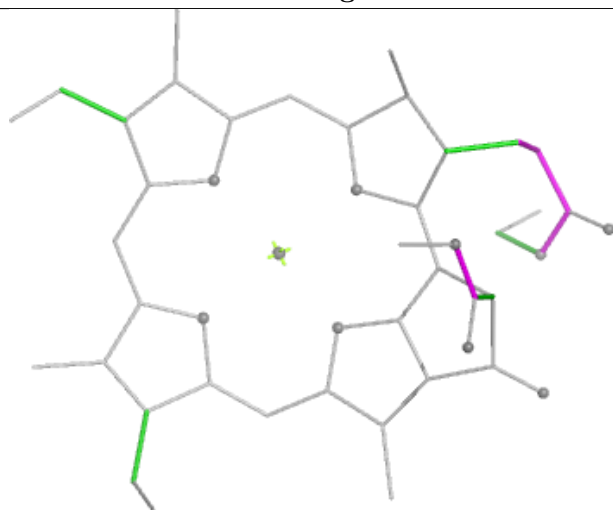
Ligand CLA 3 605



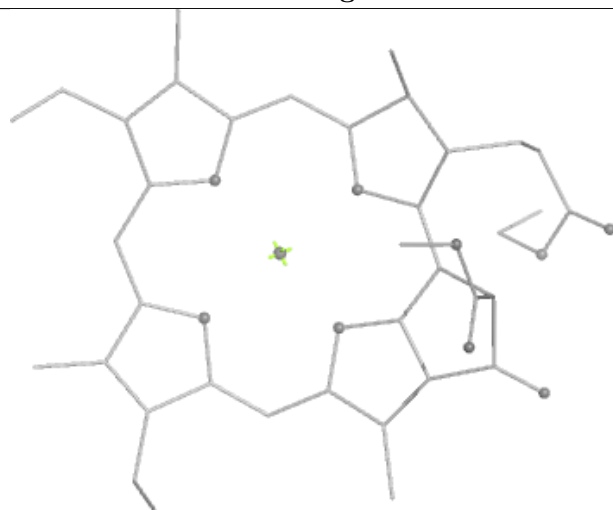
Bond lengths



Bond angles

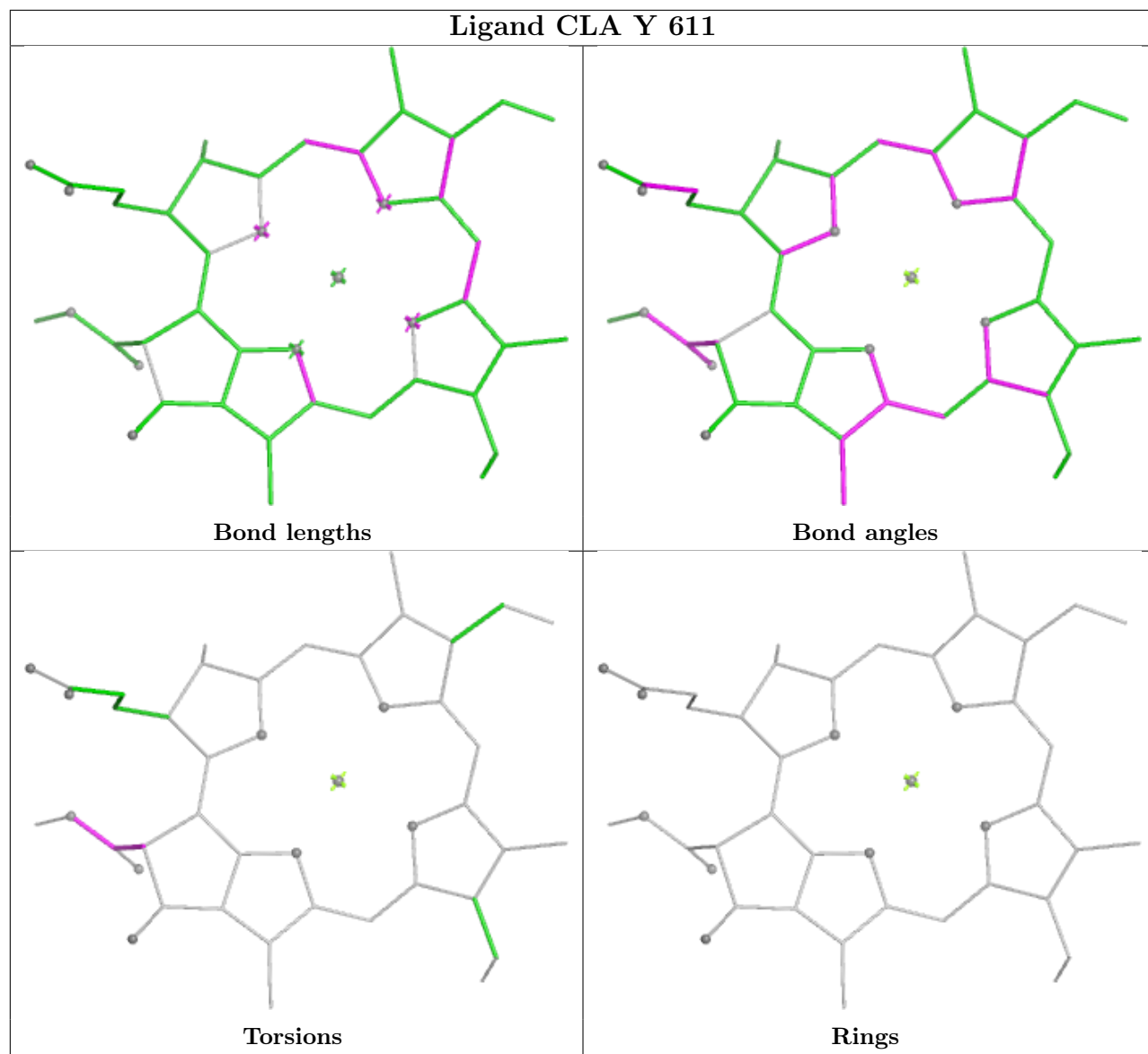


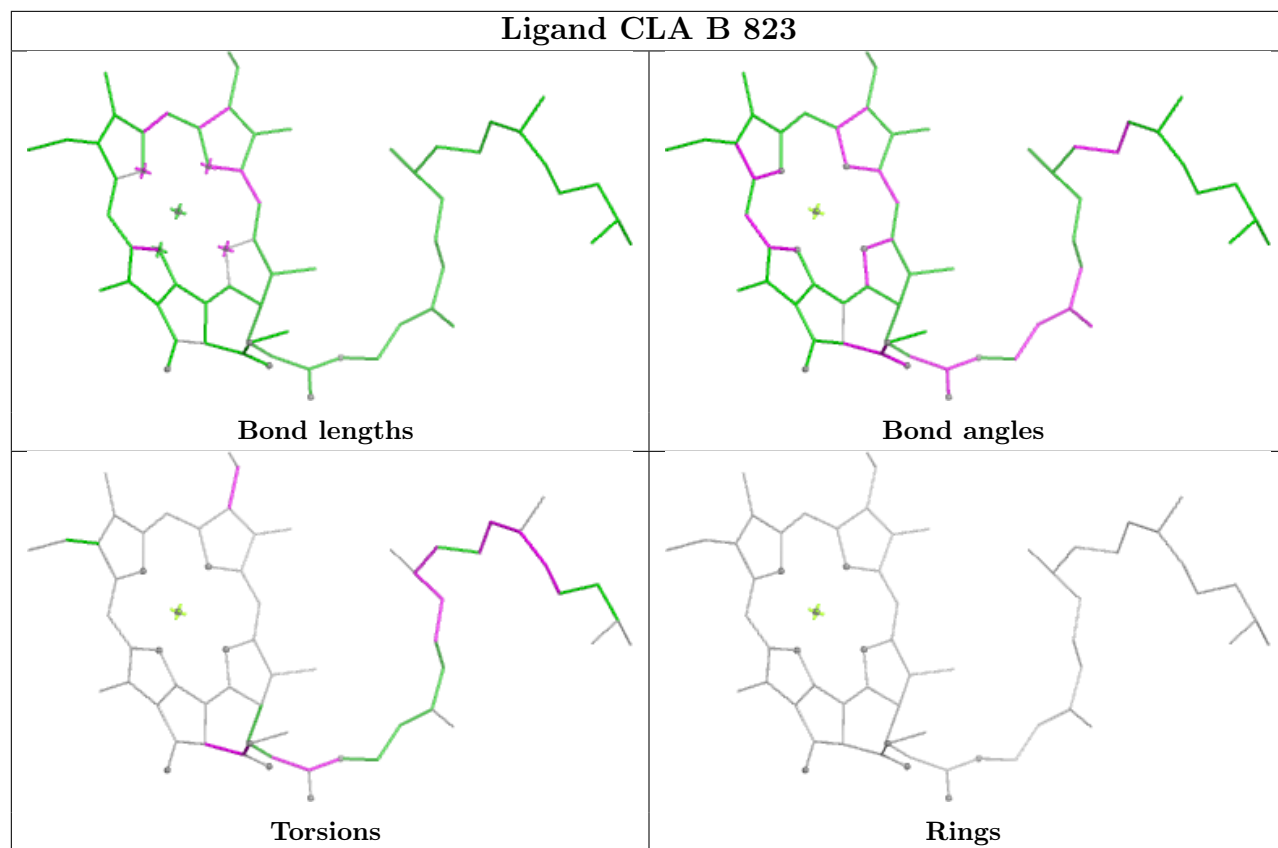
Torsions

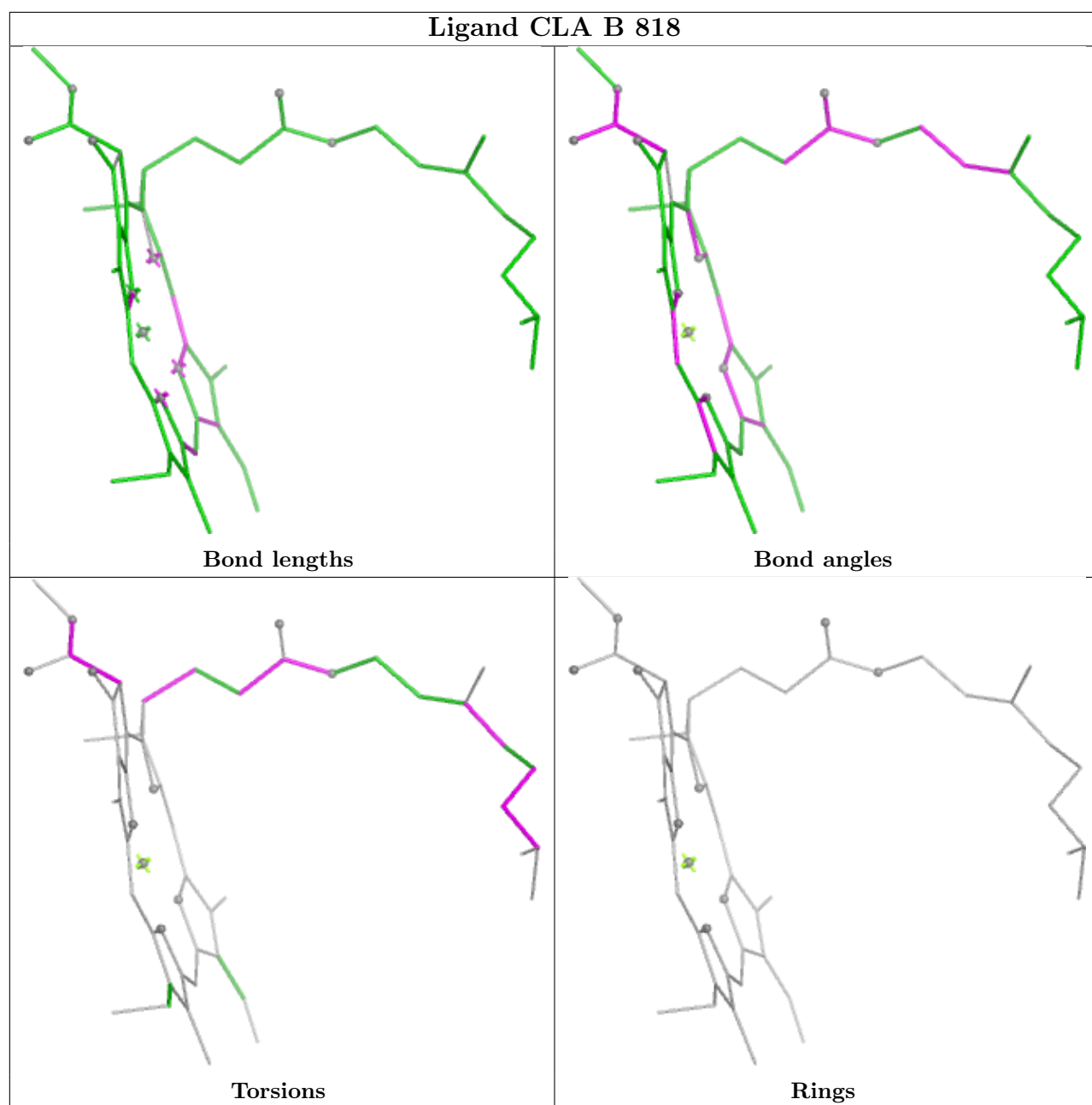


Rings

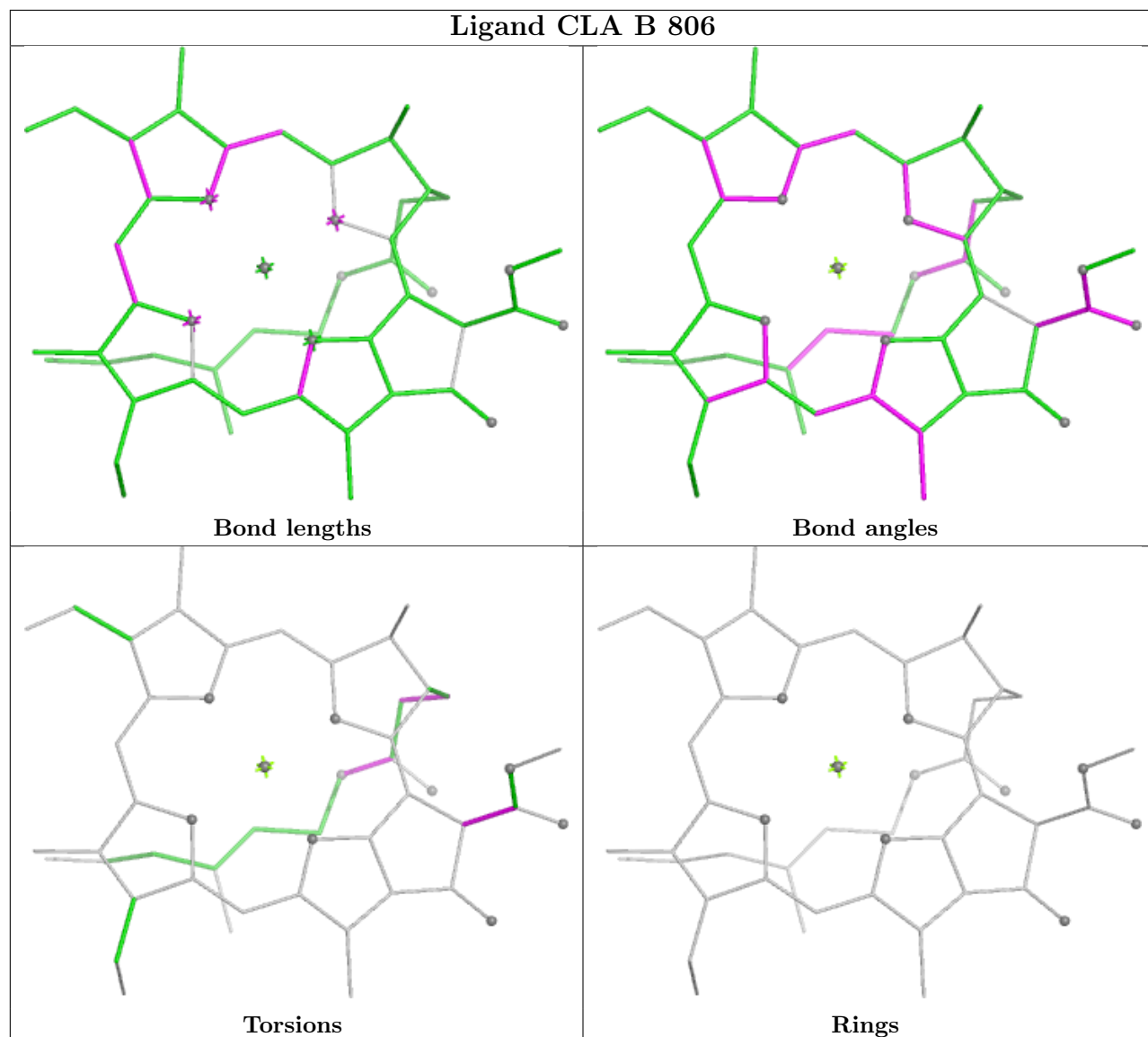
Ligand CLA Y 611



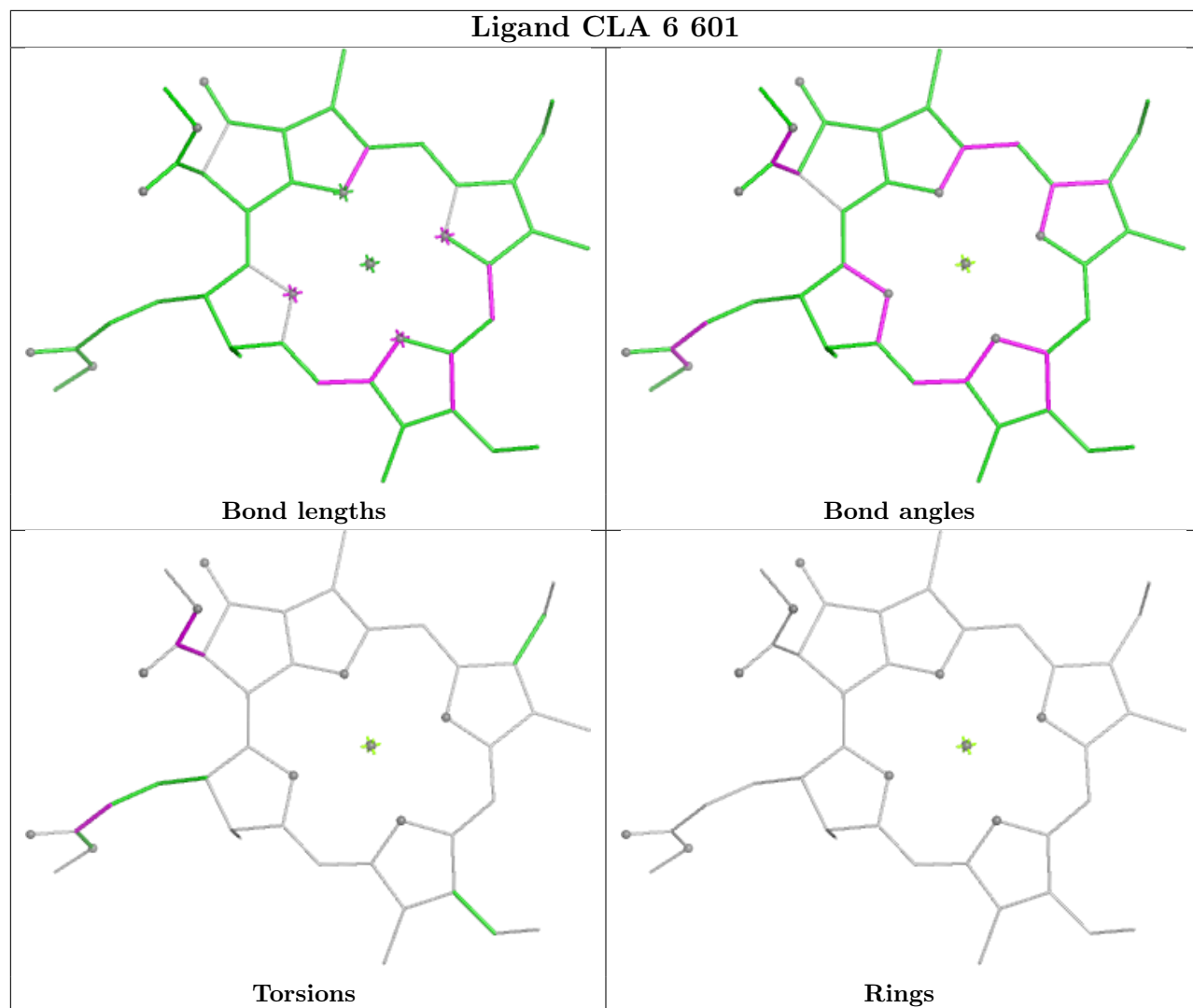


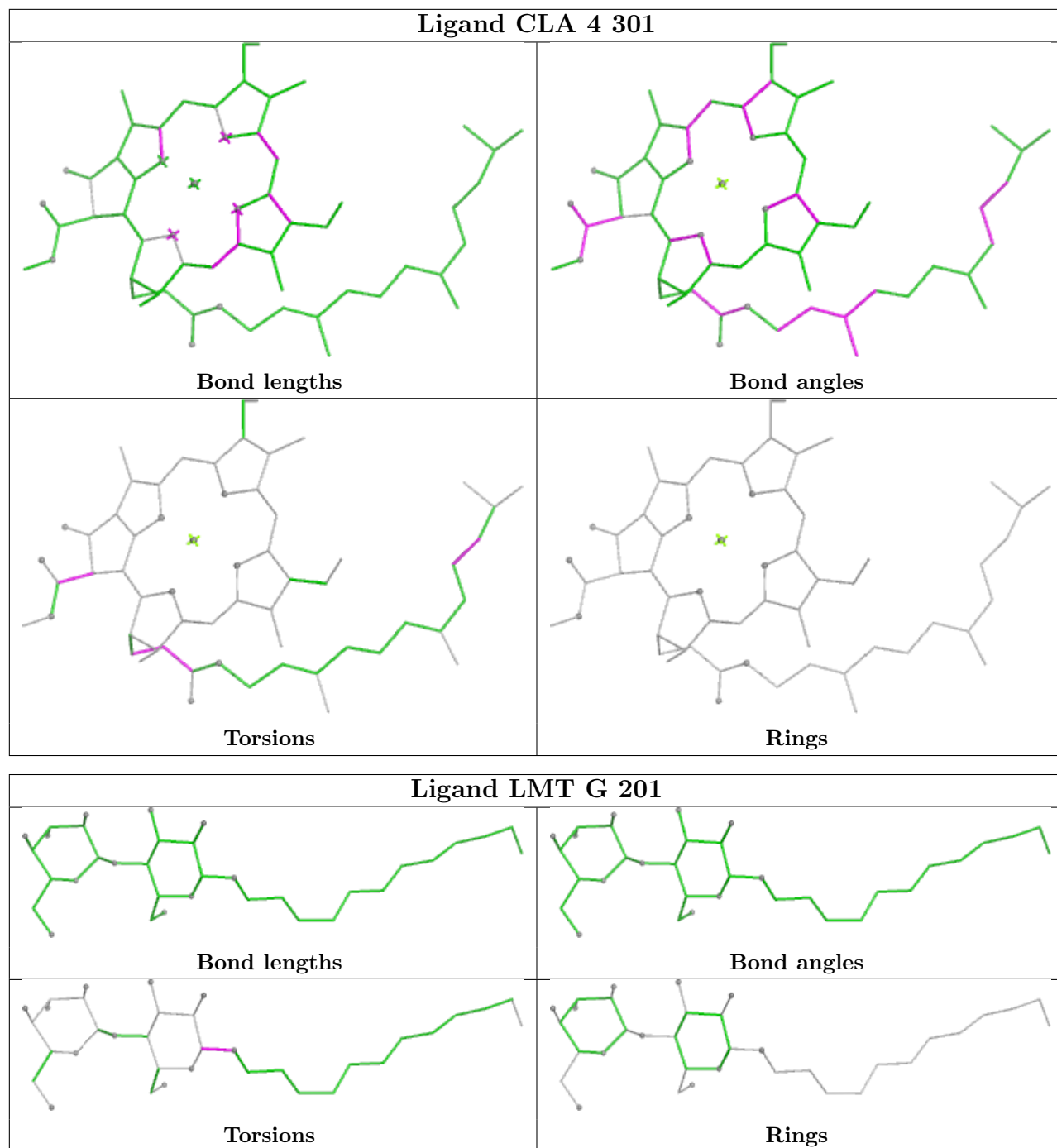


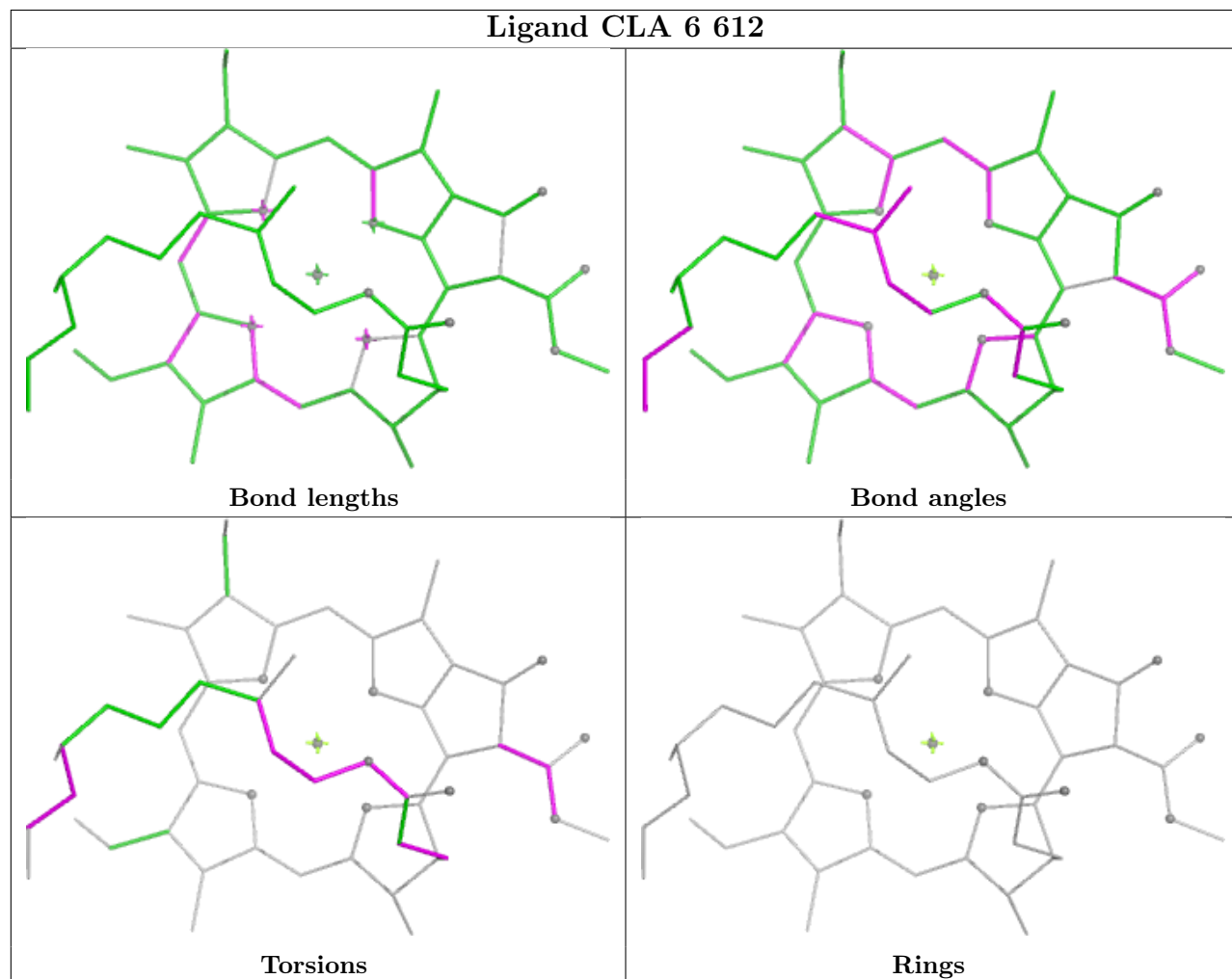
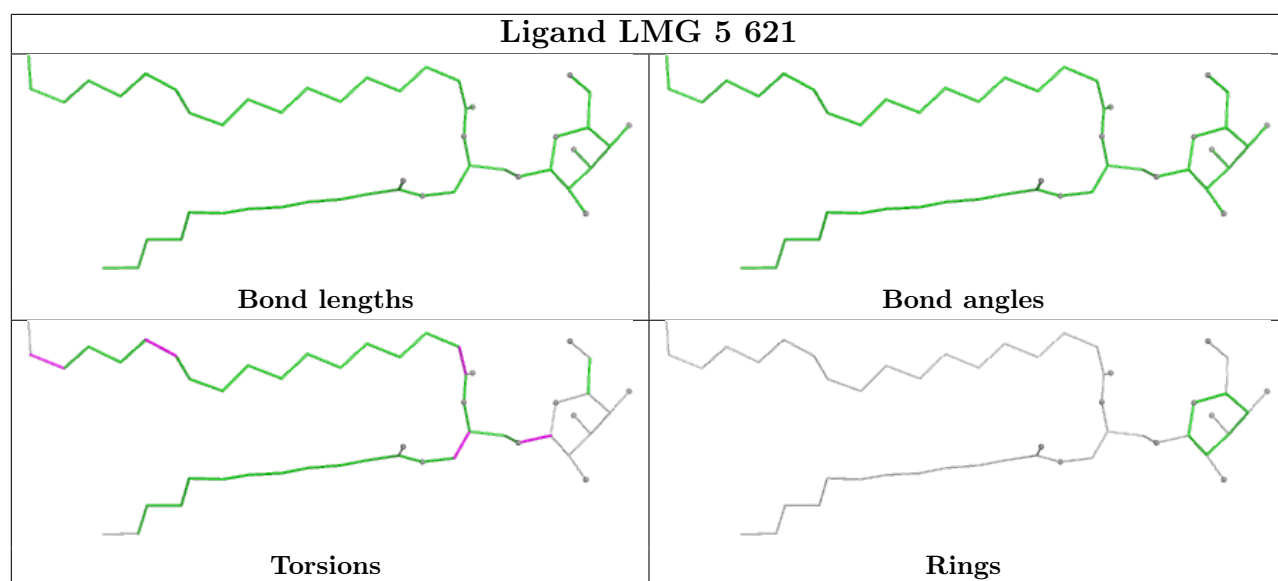
Ligand CLA B 806

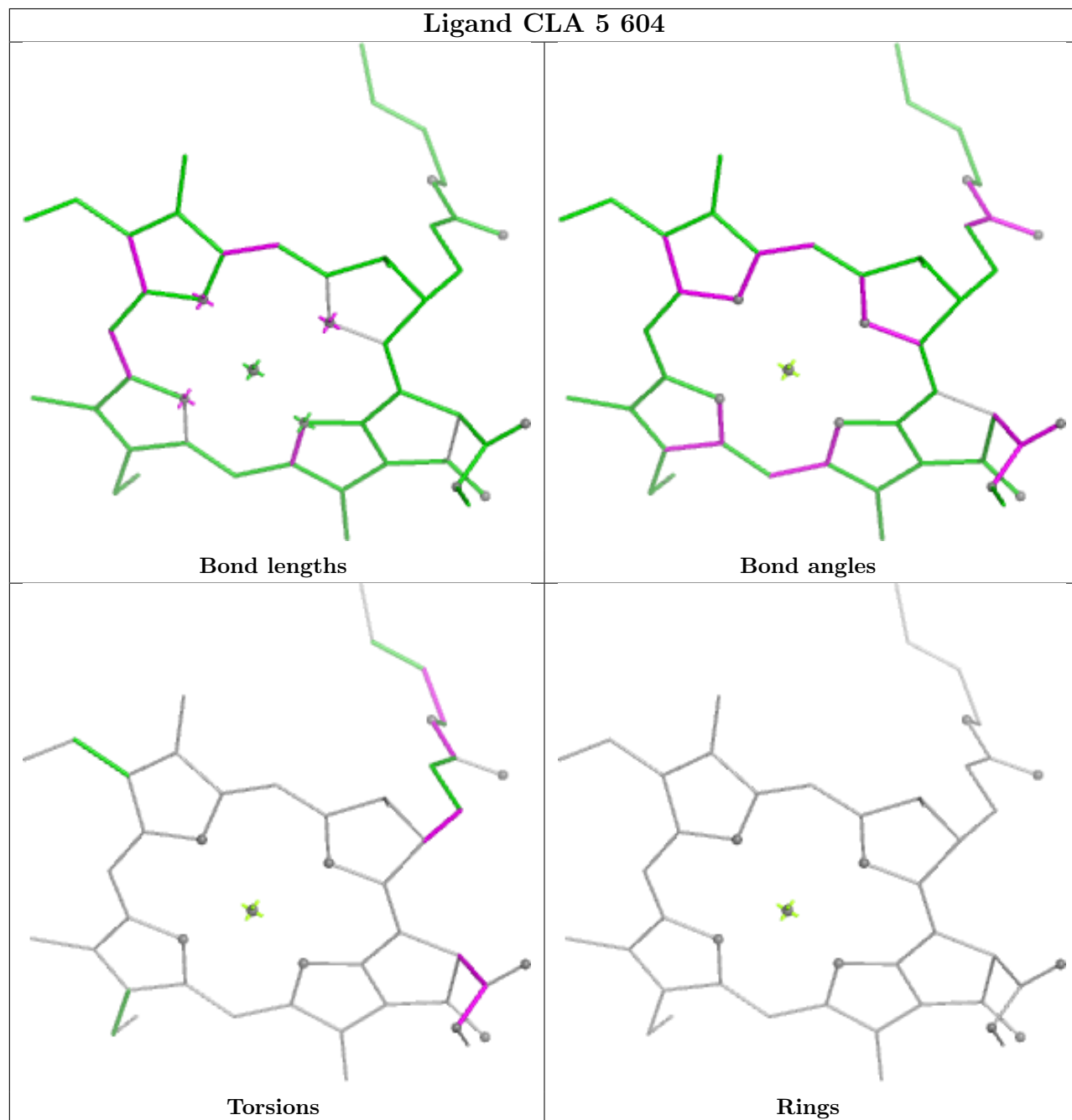
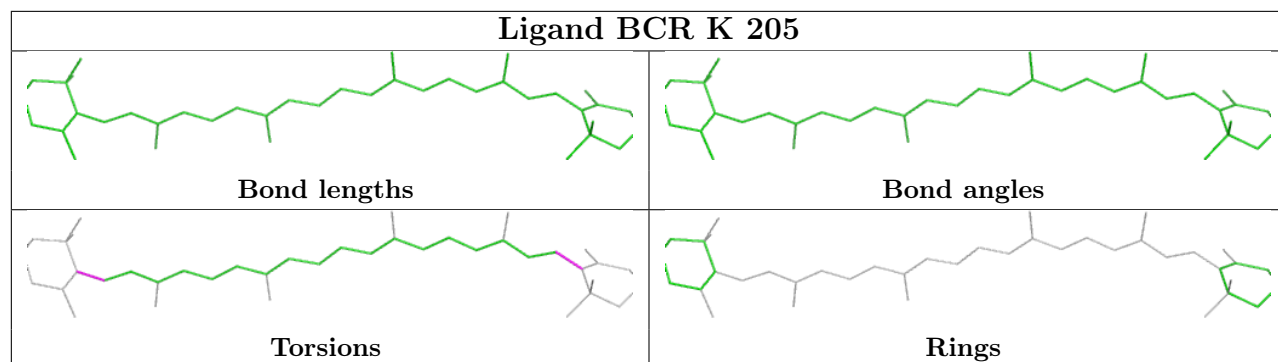


Ligand CLA 6 601

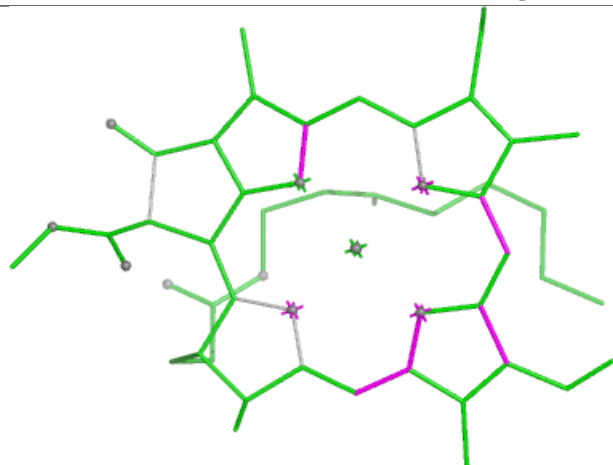




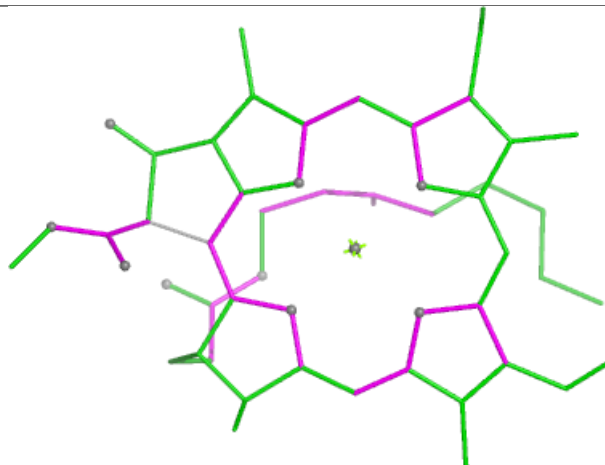




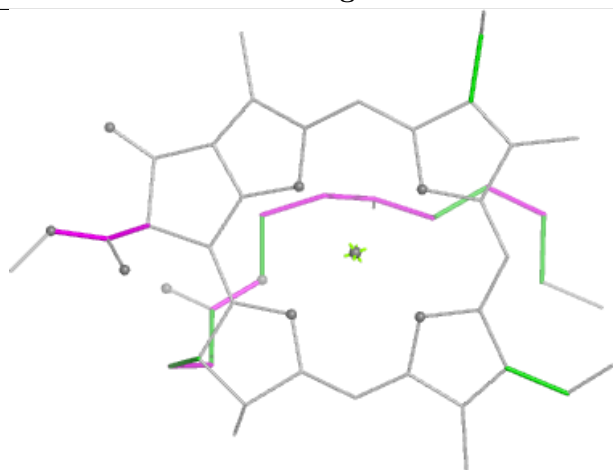
Ligand CLA A 812



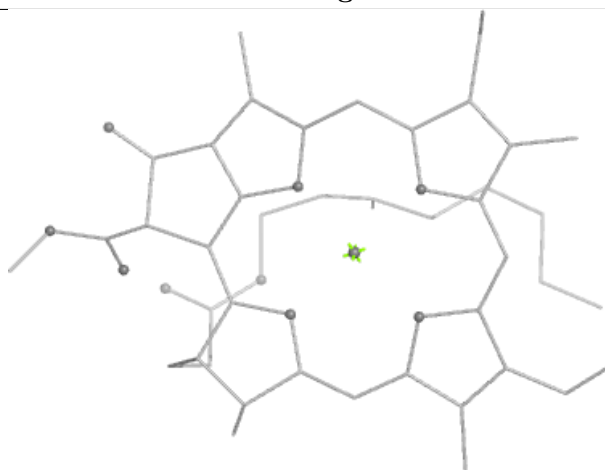
Bond lengths



Bond angles

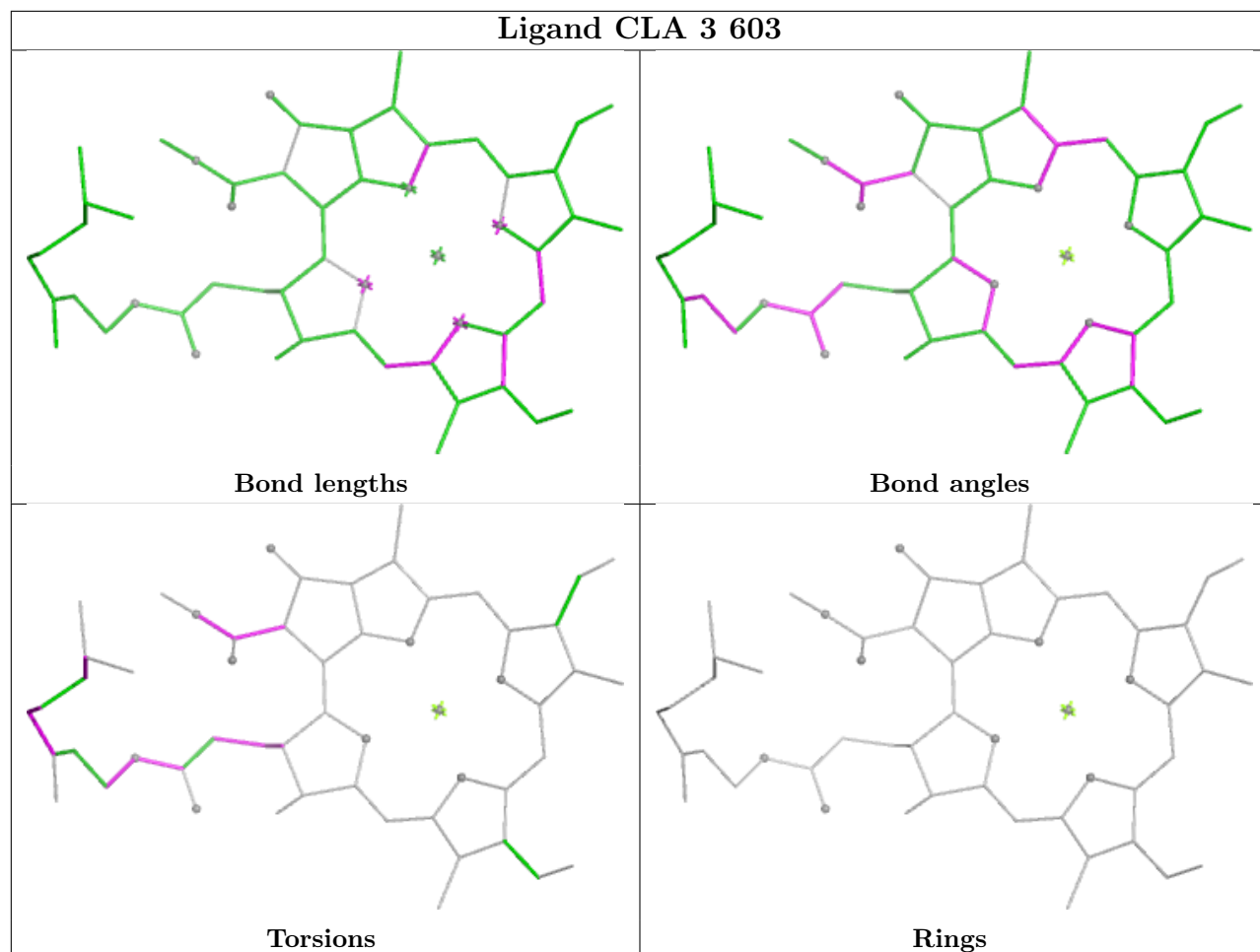


Torsions

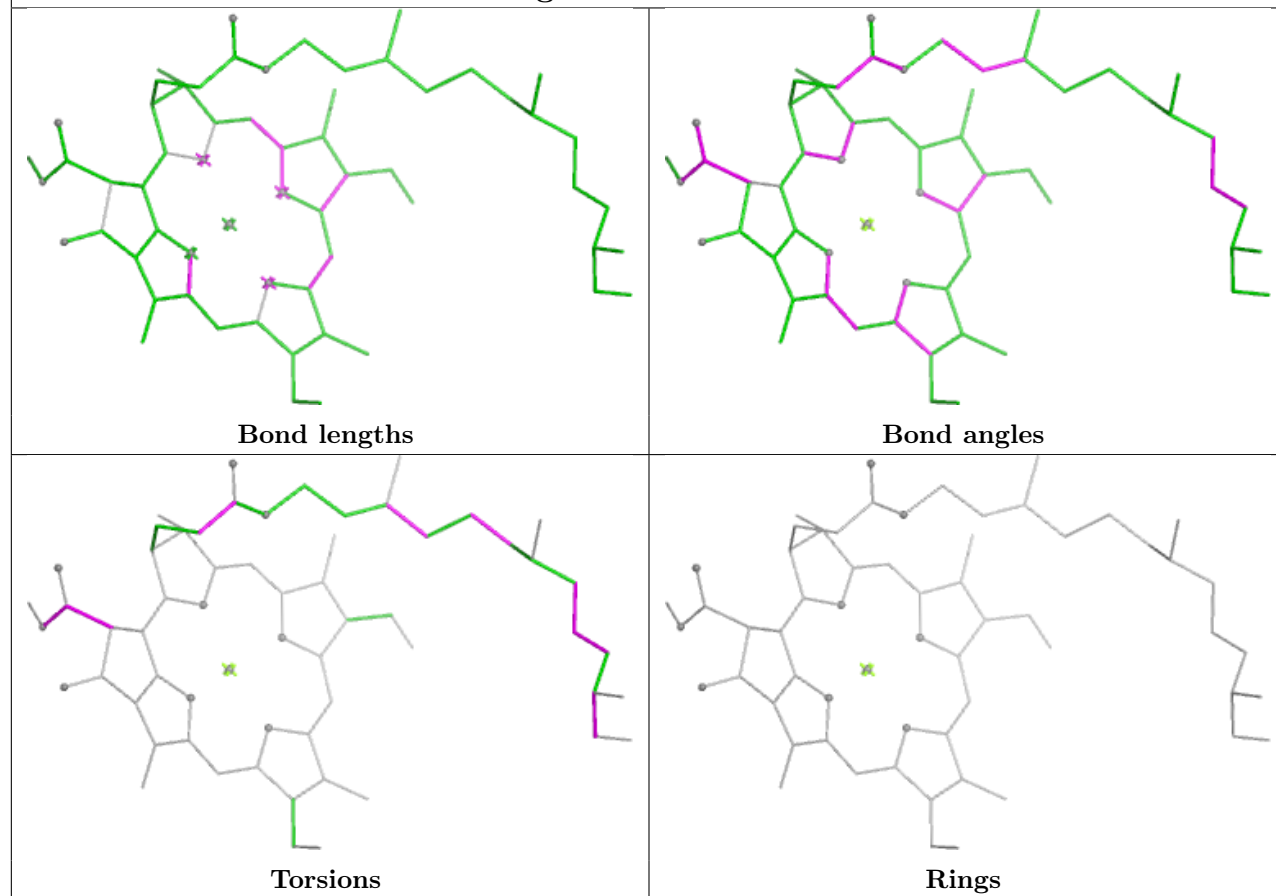


Rings

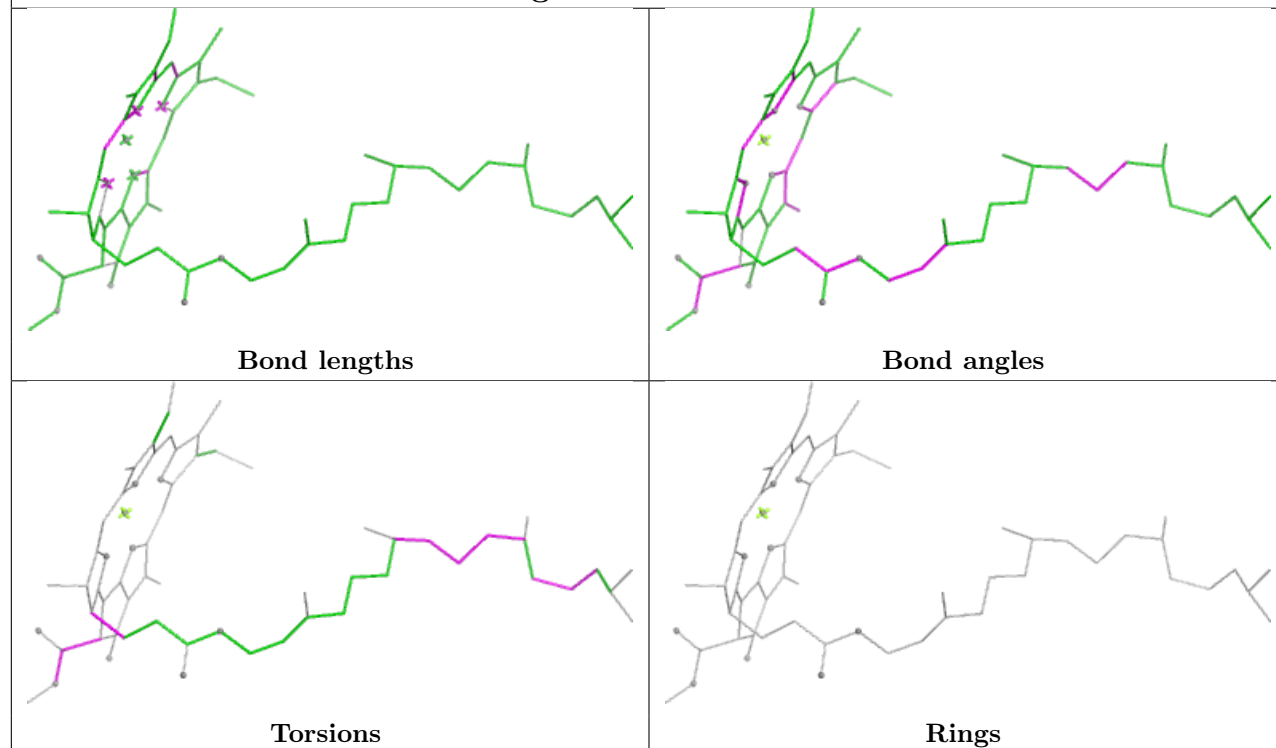
Ligand CLA 3 603

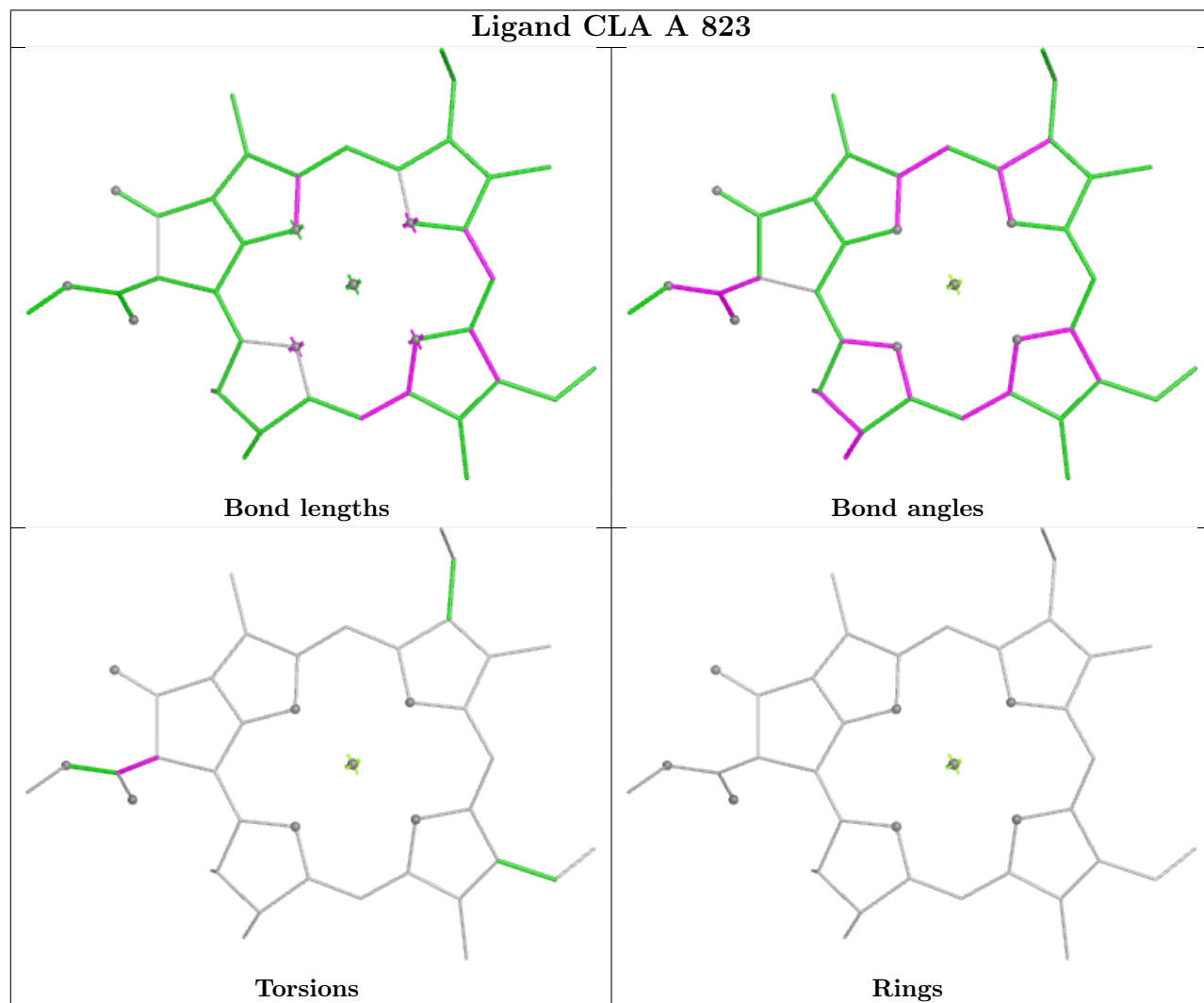
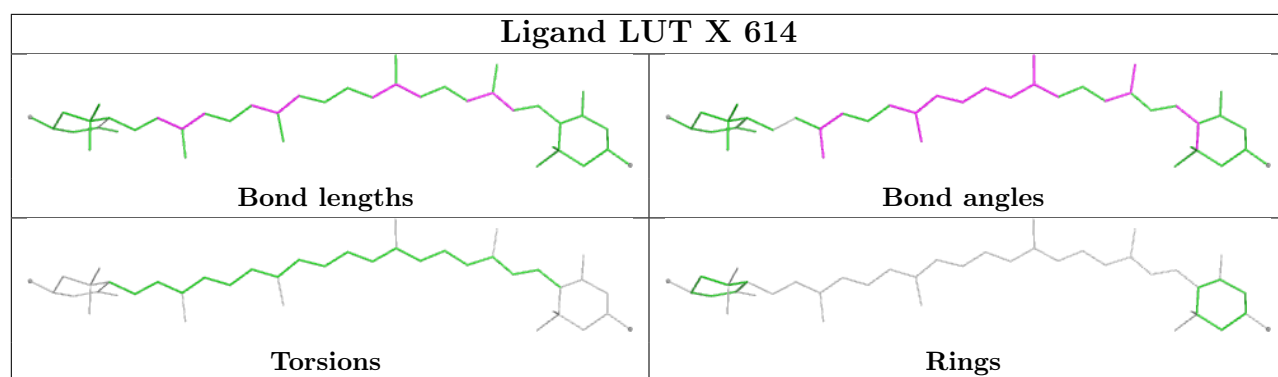


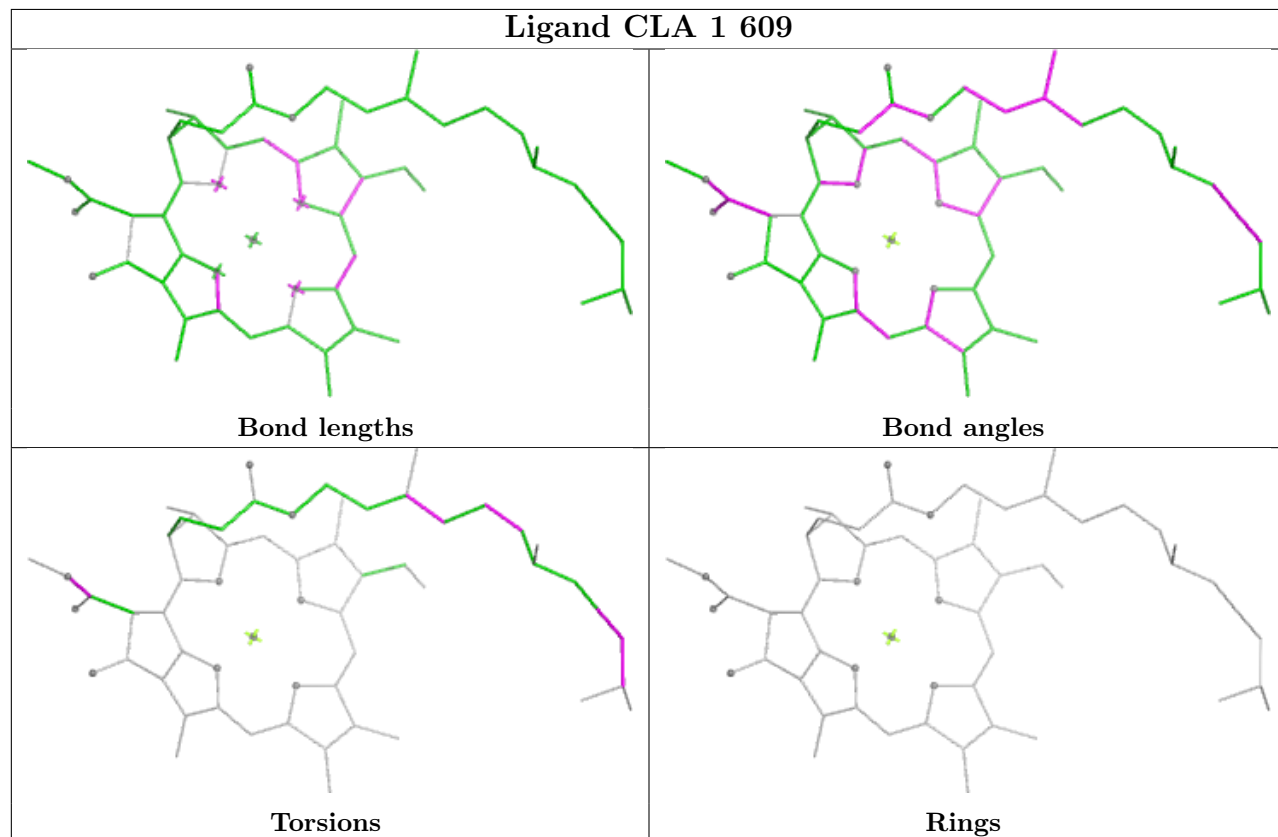
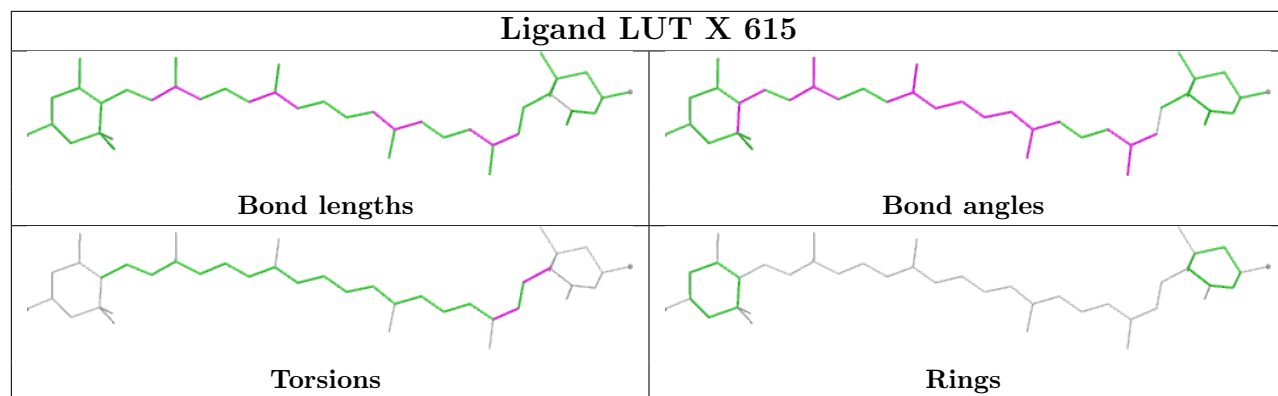
Ligand CLA 5 602



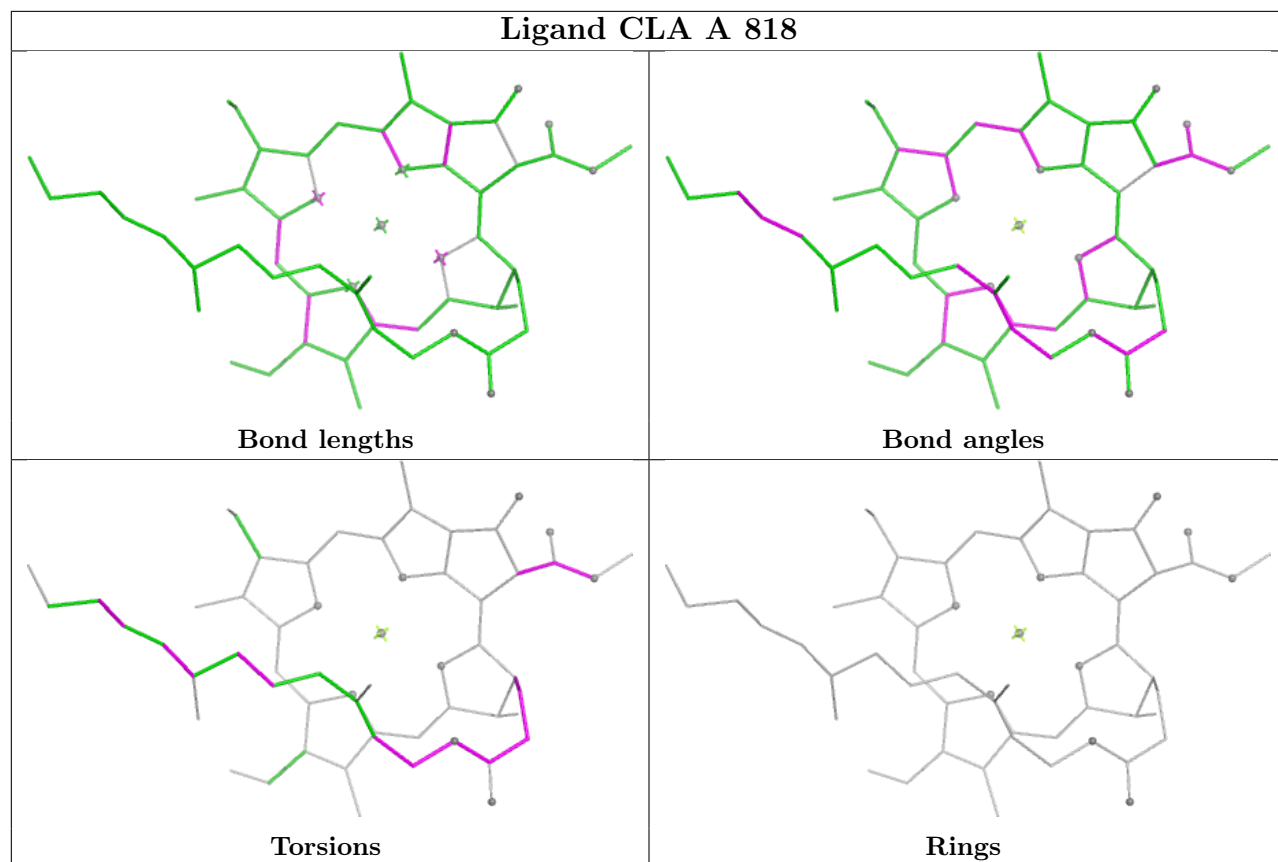
Ligand CLA A 811



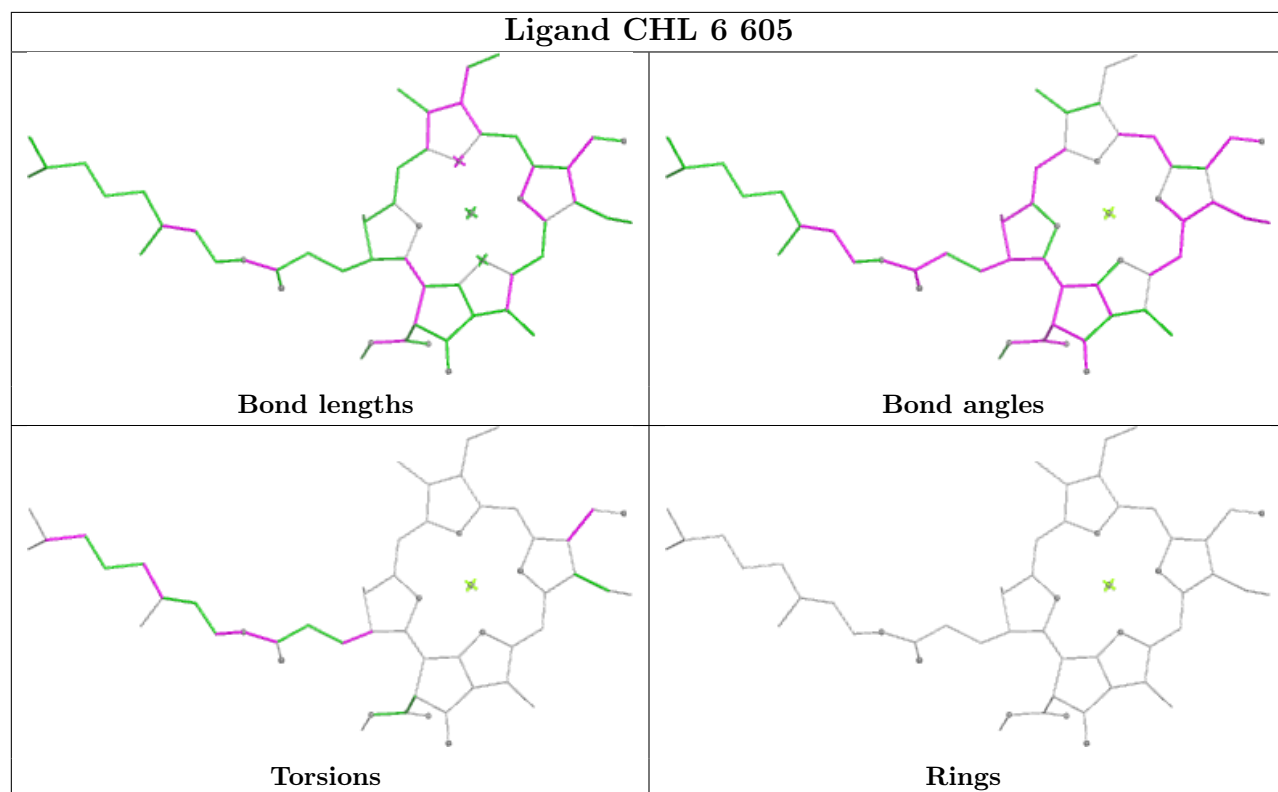


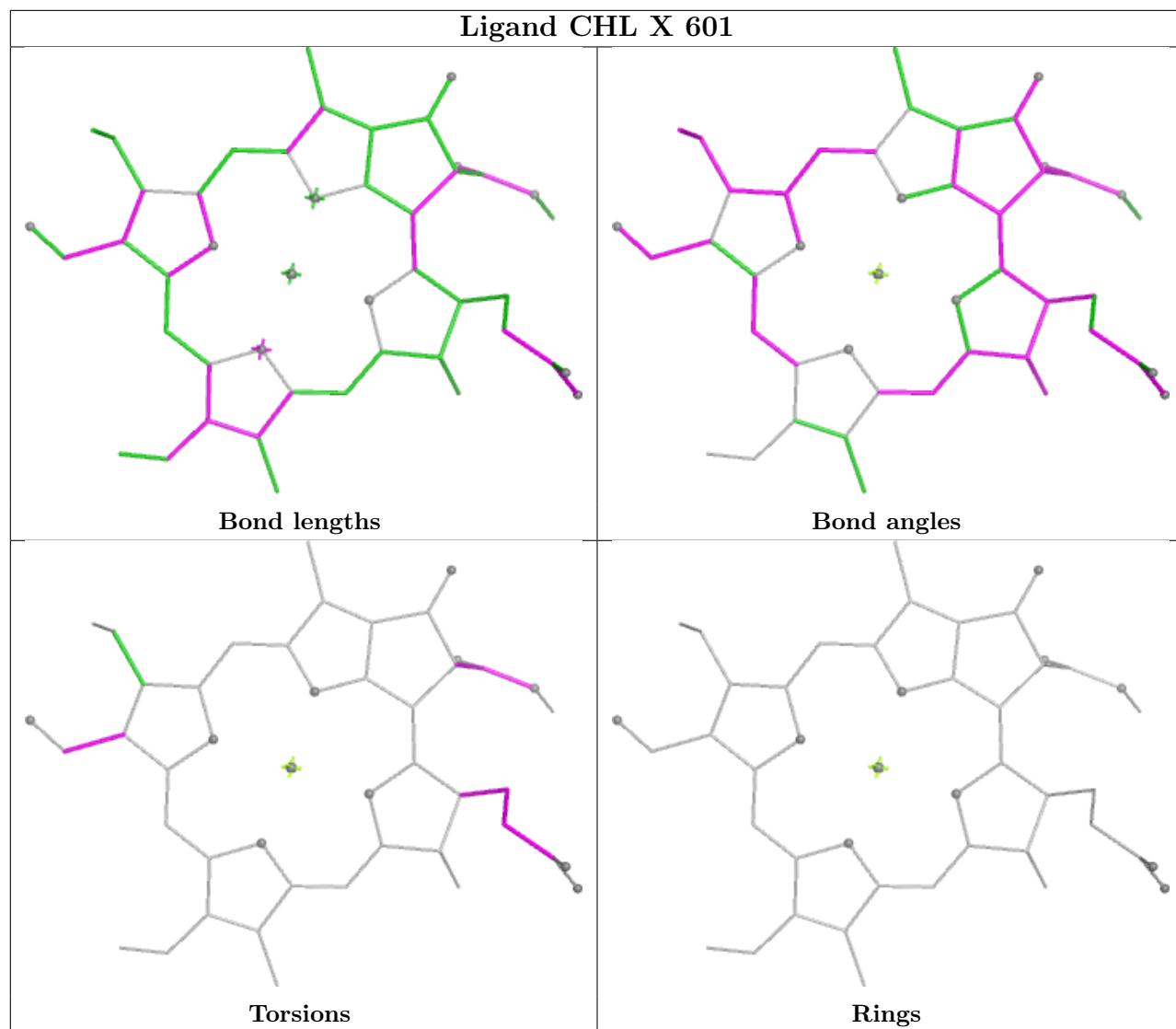


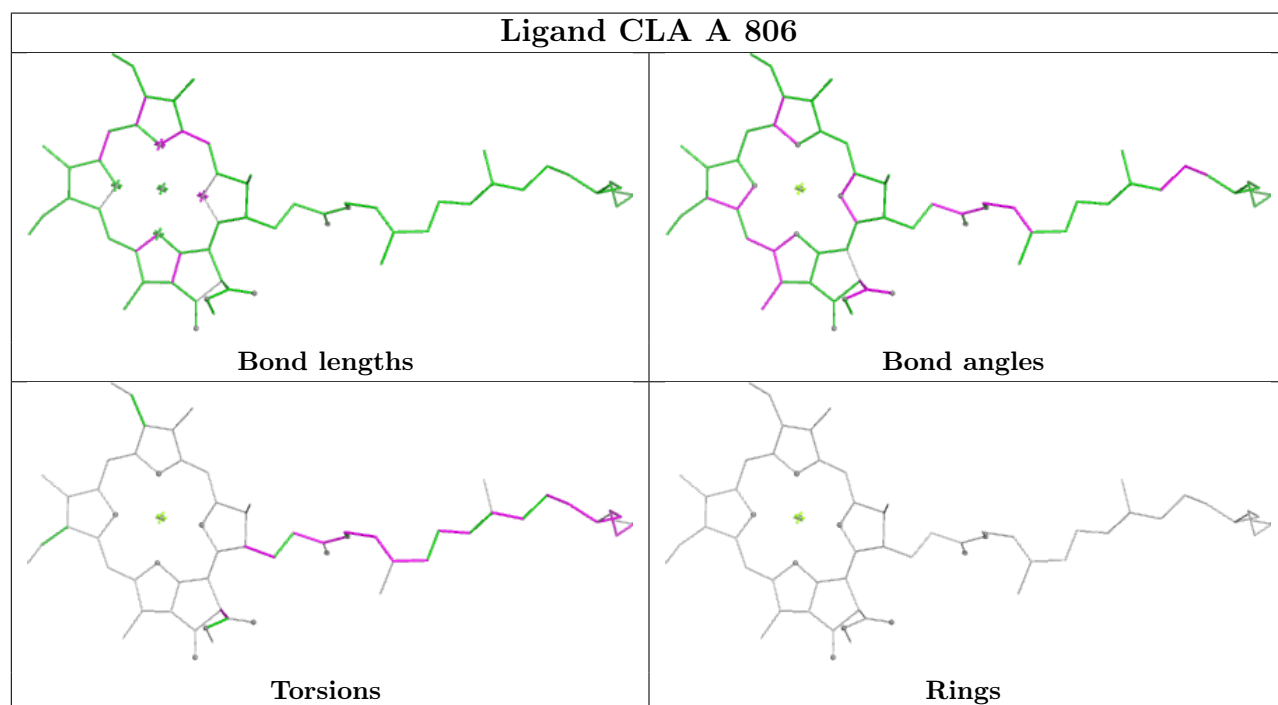
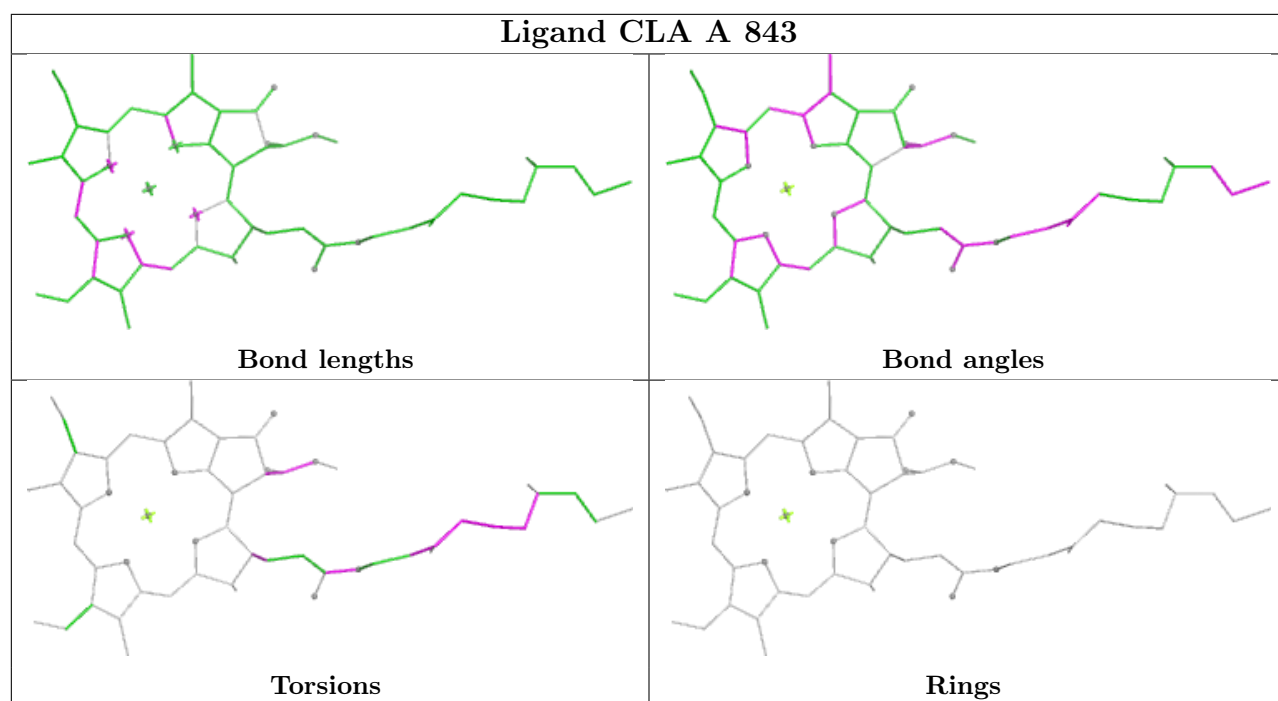
Ligand CLA A 818

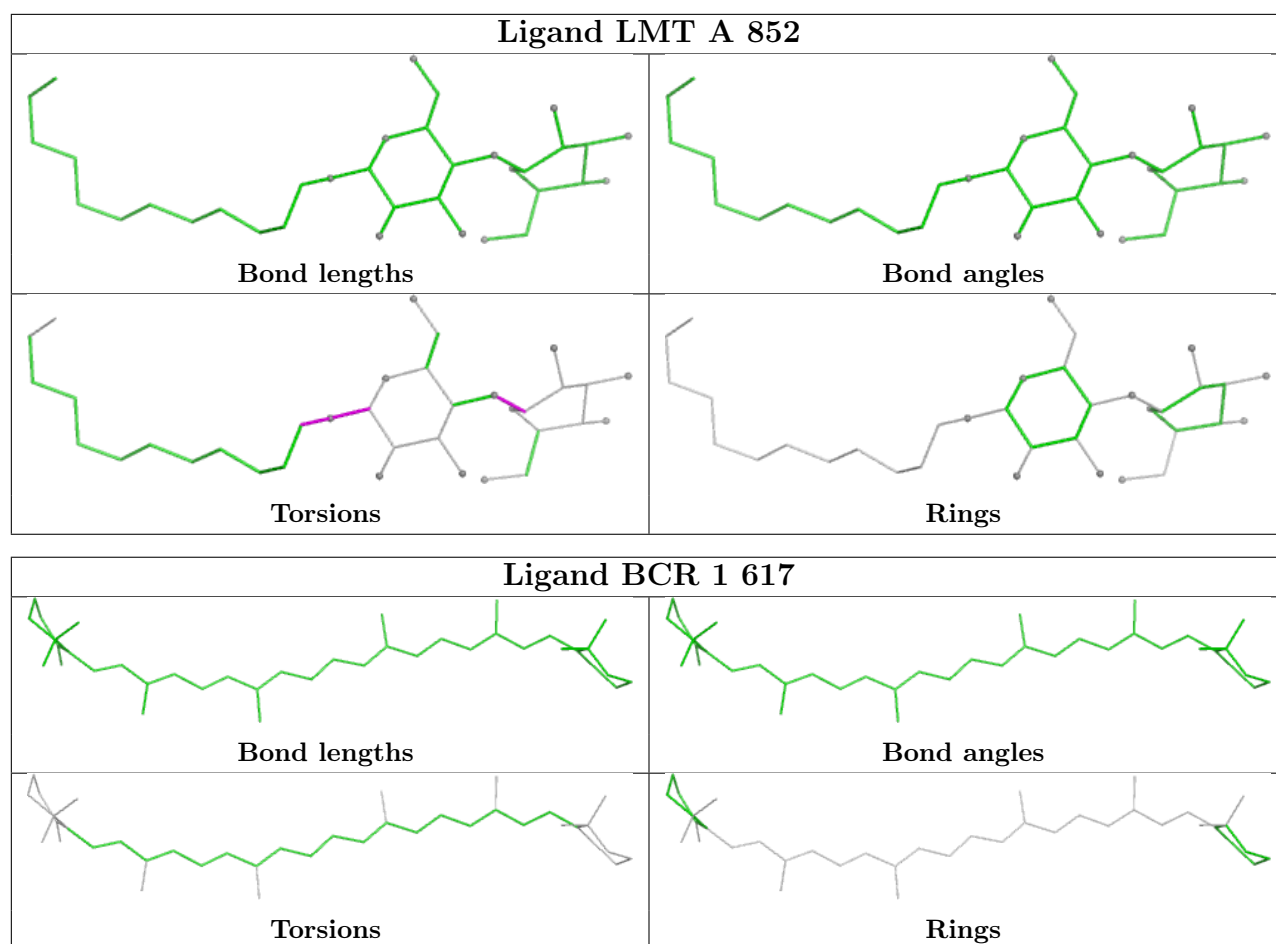


Ligand CHL 6 605









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.

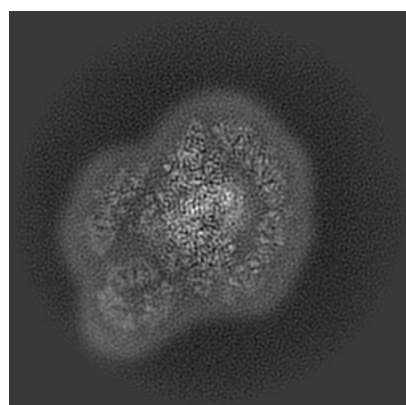
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54456. These allow visual inspection of the internal detail of the map and identification of artifacts.

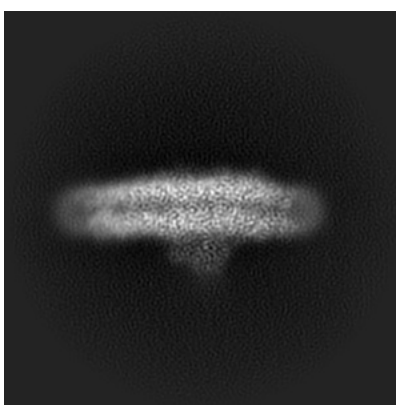
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

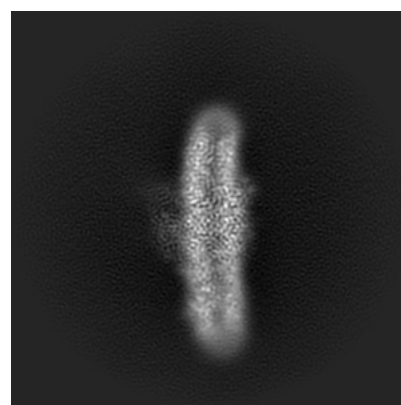
6.1.1 Primary map



X



Y

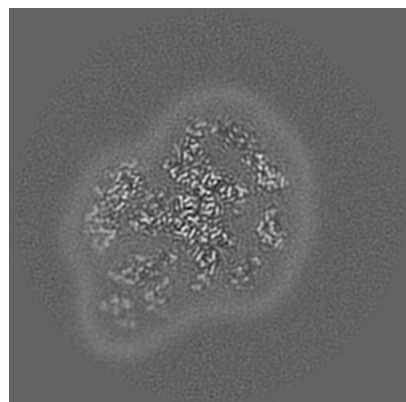


Z

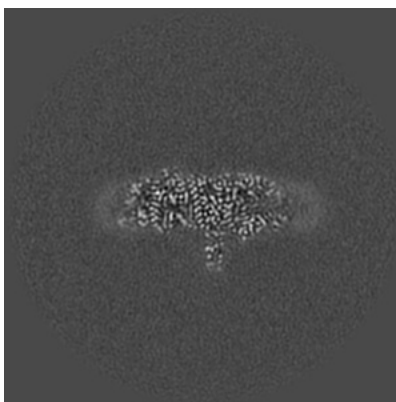
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

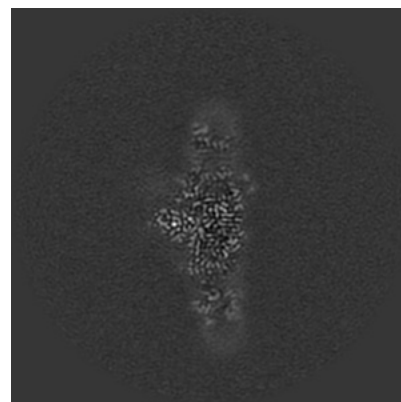
6.2.1 Primary map



X Index: 200



Y Index: 200

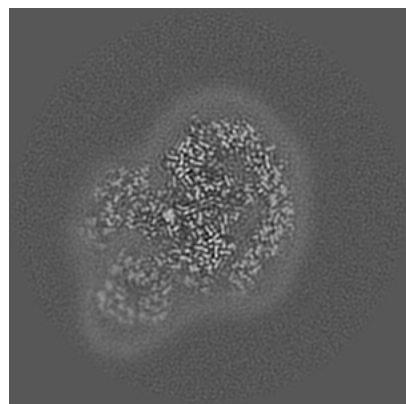


Z Index: 200

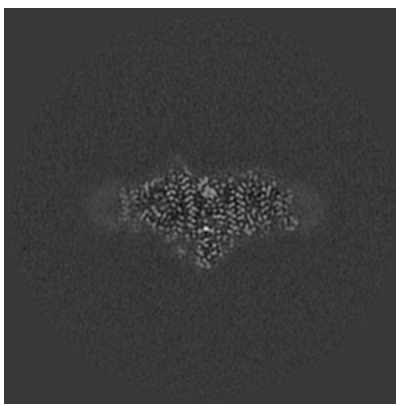
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

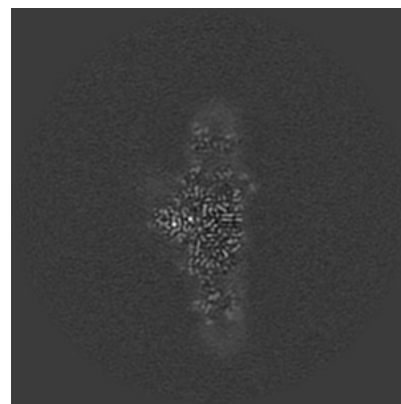
6.3.1 Primary map



X Index: 191



Y Index: 188

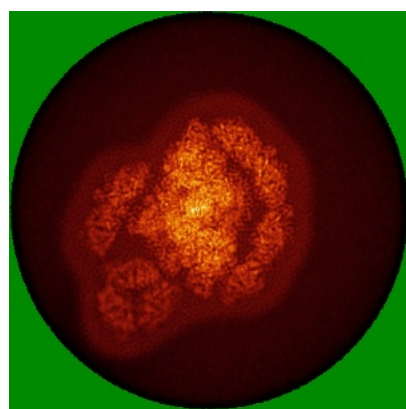


Z Index: 201

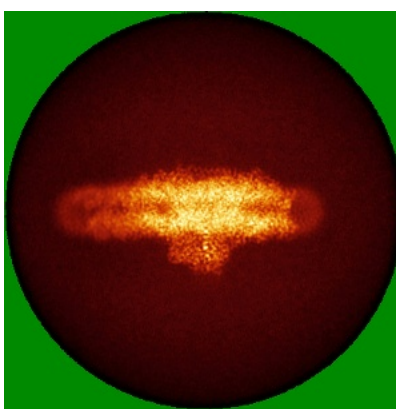
The images above show the largest variance slices of the map in three orthogonal directions.

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

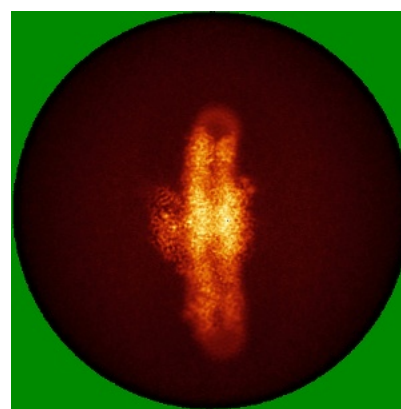
6.4.1 Primary map



X



Y

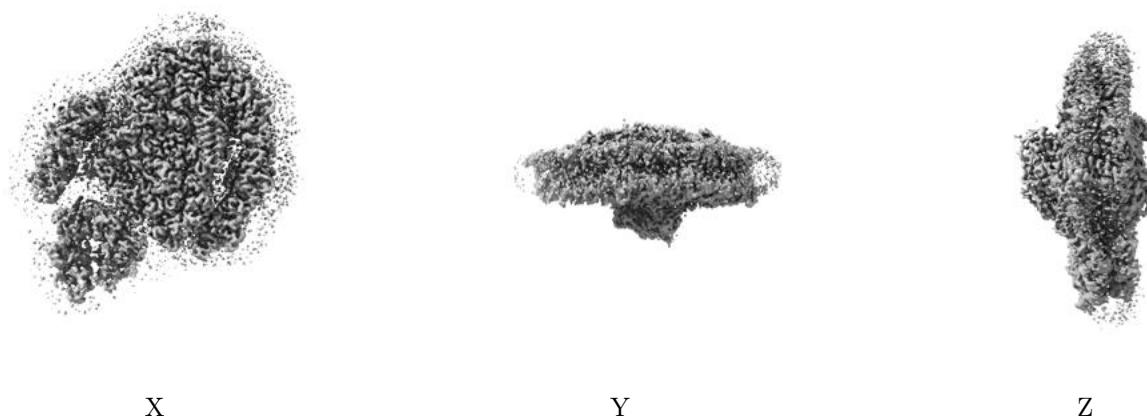


Z

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 4.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

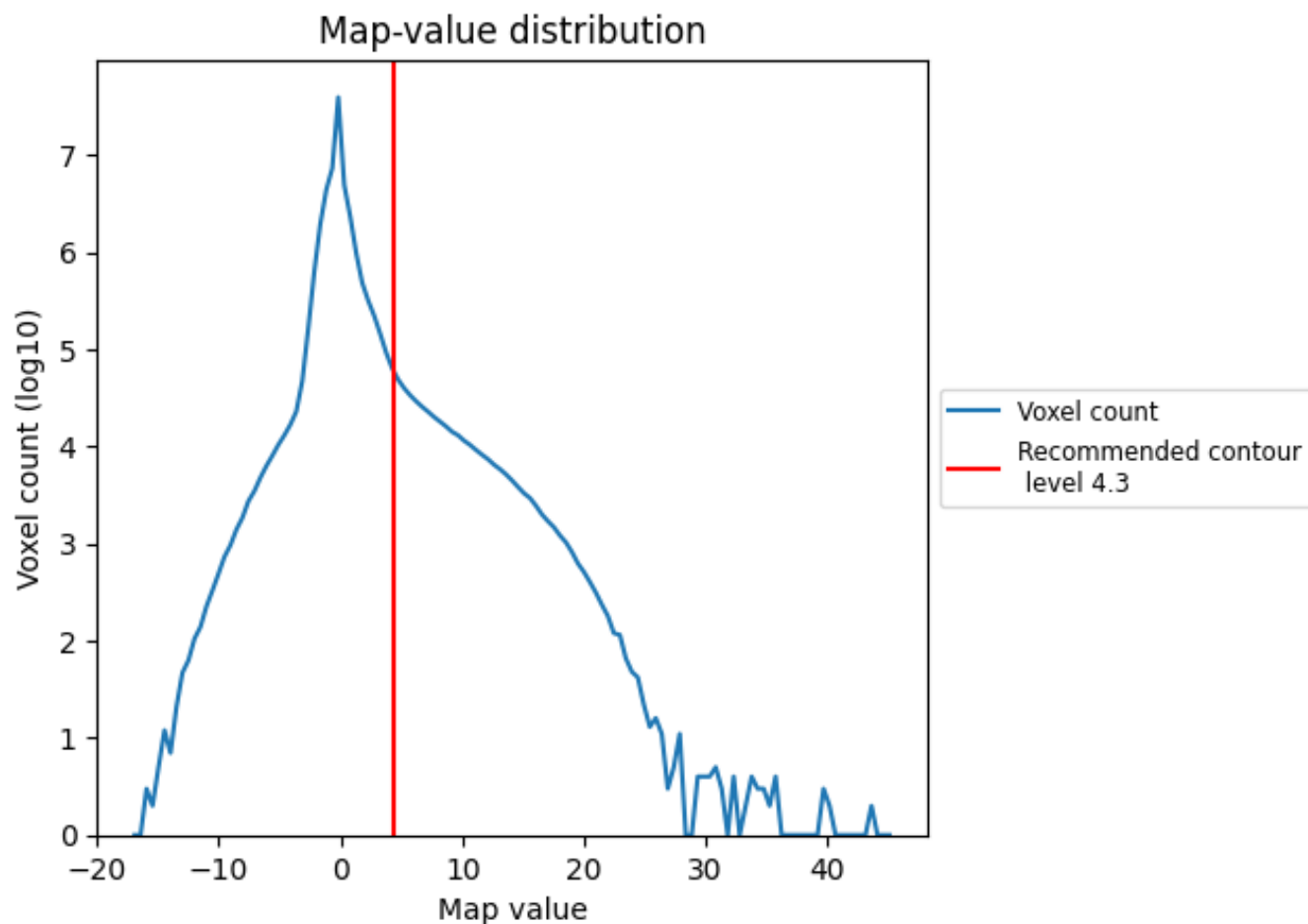
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

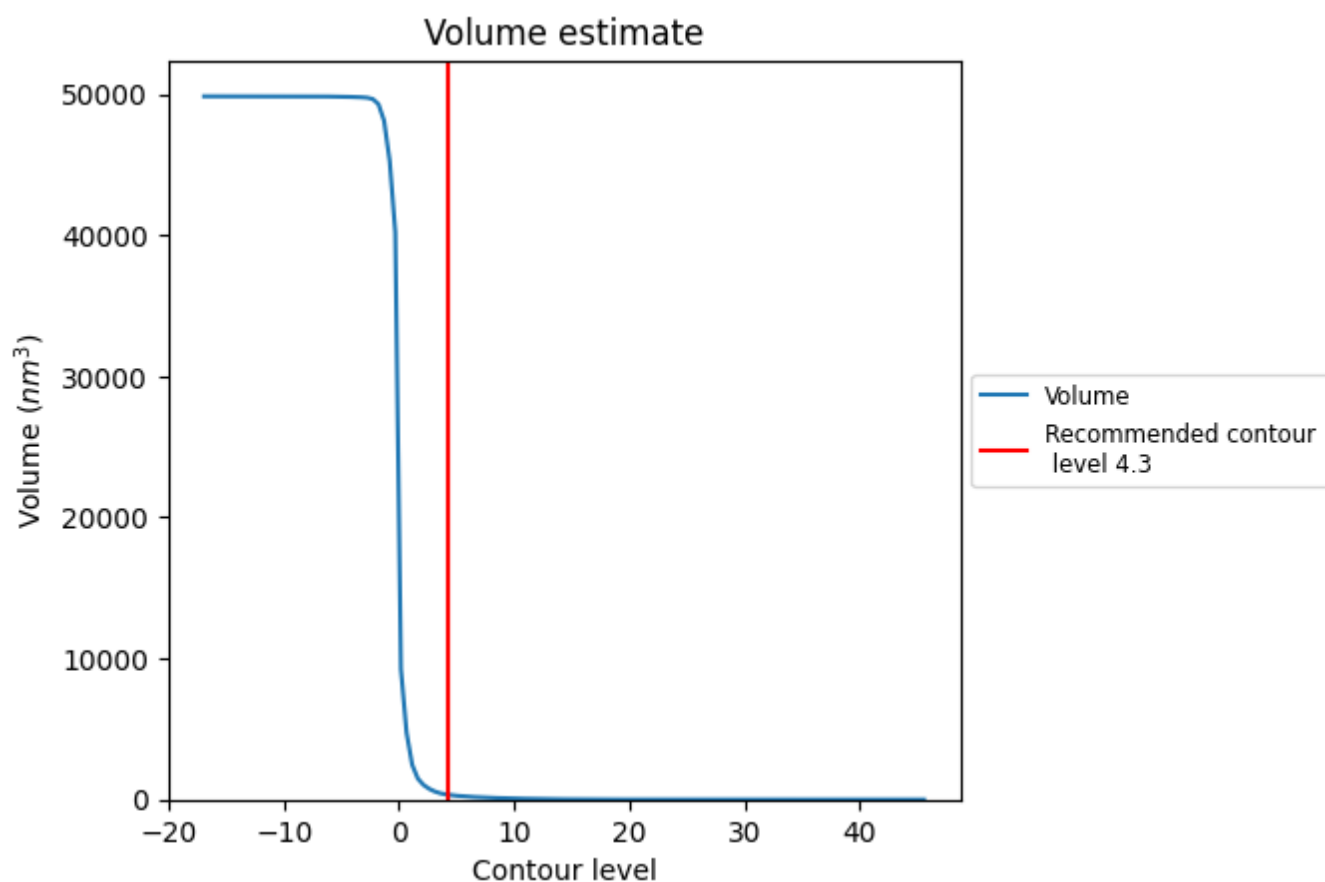
This section contains the results of statistical analysis of the map.

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.

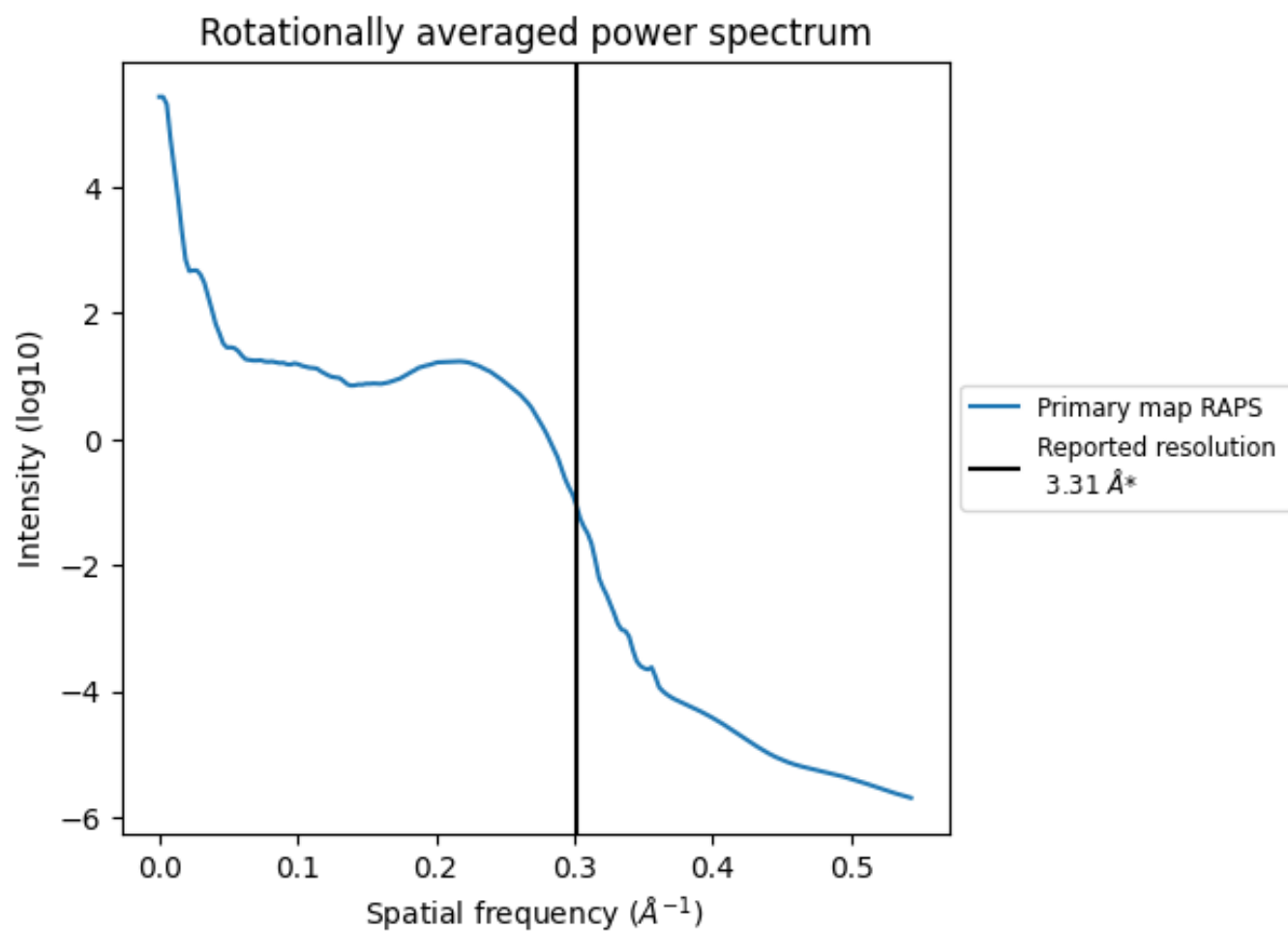
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 337 nm³; this corresponds to an approximate mass of 304 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 0.302 Å⁻¹

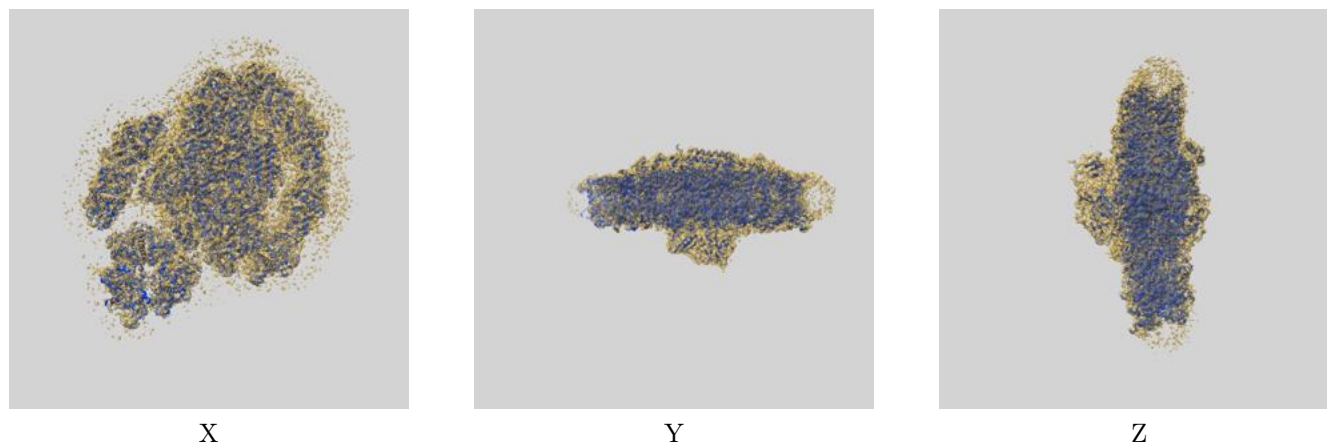
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

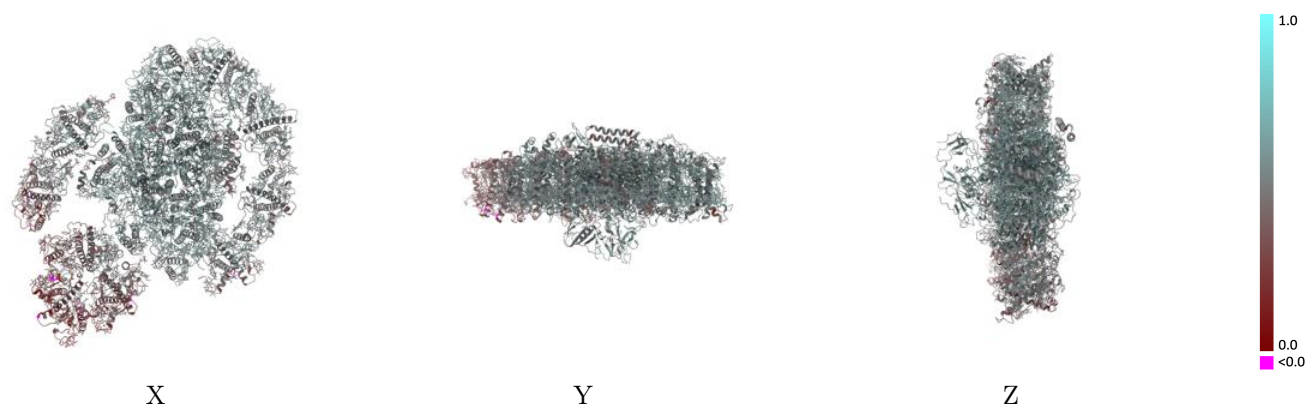
This section contains information regarding the fit between EMDB map EMD-54456 and PDB model 9S1M. Per-residue inclusion information can be found in section [3](#) on page [29](#).

9.1 Map-model overlay [i](#)



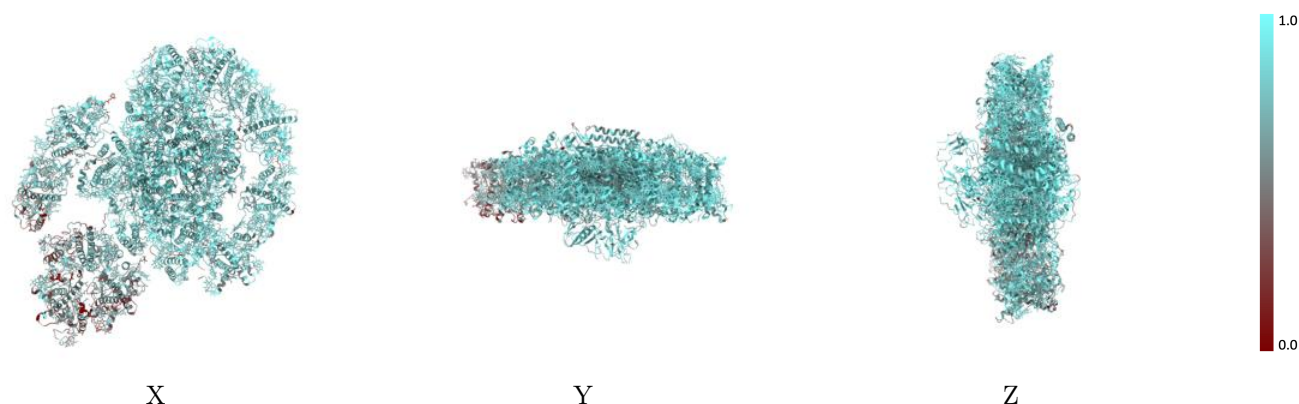
The images above show the 3D surface view of the map at the recommended contour level 4.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



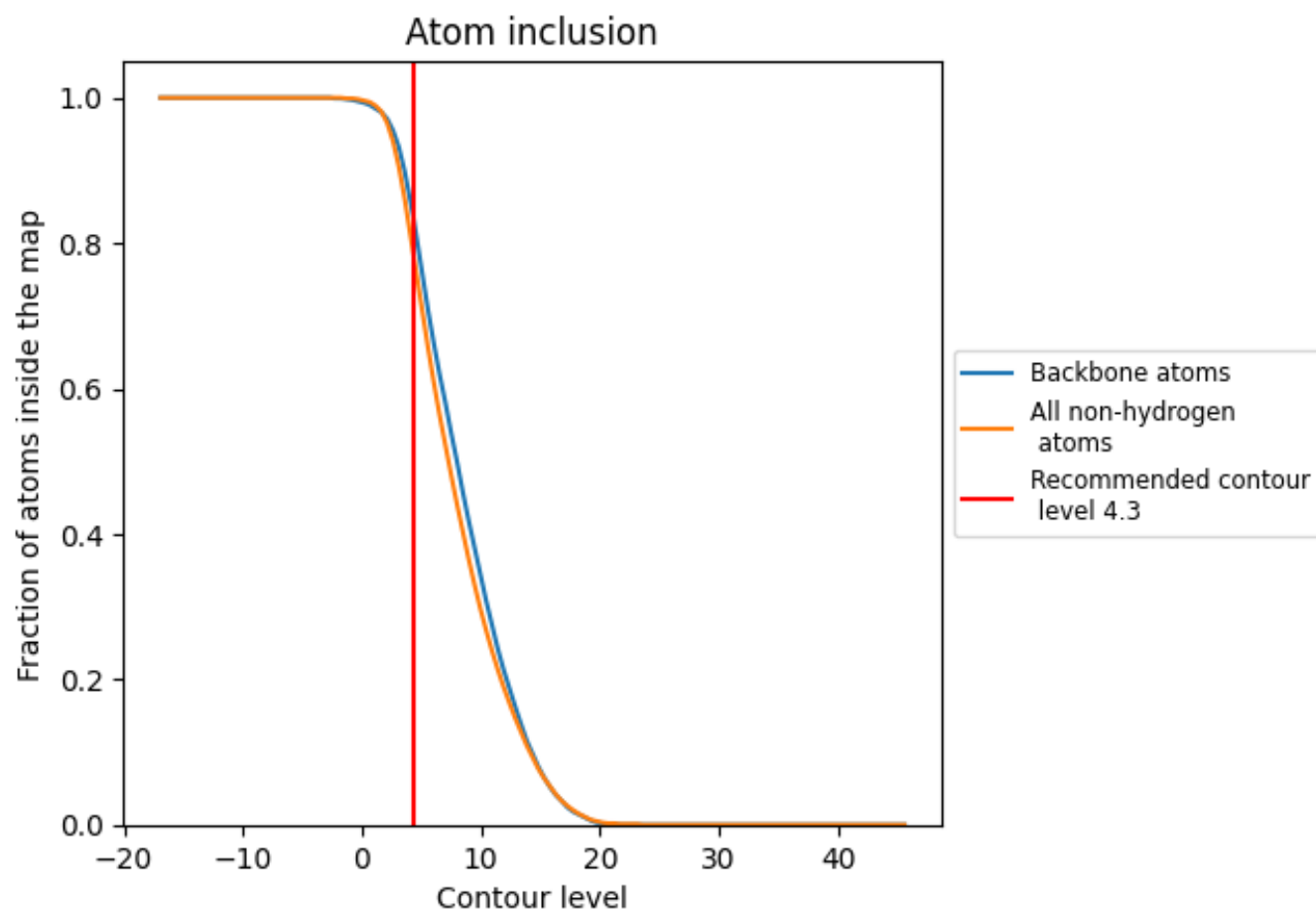
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 79% 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 (4.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7880	 0.4930
1	 0.8350	 0.5180
2	 0.8140	 0.4840
3	 0.7400	 0.4600
4	 0.8620	 0.5100
5	 0.6240	 0.4050
6	 0.7770	 0.4890
A	 0.8810	 0.5520
B	 0.8990	 0.5550
C	 0.9140	 0.5450
D	 0.8550	 0.5360
E	 0.8210	 0.5350
F	 0.7850	 0.5050
G	 0.8270	 0.5140
H	 0.7990	 0.5020
I	 0.8710	 0.5380
J	 0.7060	 0.4890
K	 0.7150	 0.4700
L	 0.8570	 0.5360
O	 0.8010	 0.5230
X	 0.5110	 0.2930
Y	 0.6080	 0.4050
Z	 0.5120	 0.3490

