



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 01:53 PM JST

PDB ID : 7WYI / pdb_00007wyi
EMDB ID : EMD-32892
Title : Native Photosystem I of Chlamydomonas reinhardtii
Authors : Kurisu, G.; Gerle, C.; Mitsuoka, K.; Kawamoto, A.; Tanaka, H.
Deposited on : 2022-02-16
Resolution : 3.90 Å(reported)
Based on initial model : 6JO5

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 : 1.8.5 (274361), CSD as541be (2020)
MolProbity : **FAILED**
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

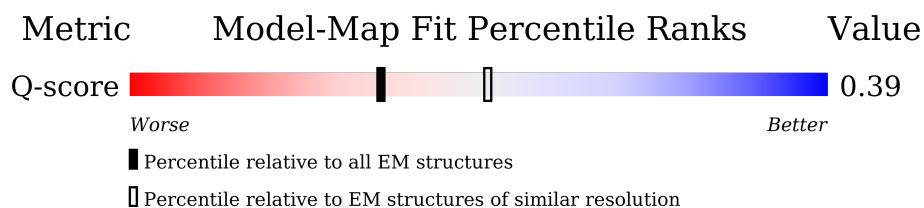
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Q-score	25397	8855 (3.40 - 4.40)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 25007 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	738	Total	C	N	O	0	0
			3628	2151	739	738		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	732	Total	C	N	O	0	0
			3601	2137	733	731		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	80	Total	C	N	O	0	0
			395	235	80	80		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	144	Total	C	N	O	0	0
			706	418	144	144		

- Molecule 5 is a protein called Photosystem I reaction center subunit IV, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	61	Total	C	N	O	0	0
			300	178	61	61		

- Molecule 6 is a protein called Photosystem I reaction center subunit III, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	165	Total	C	N	O	0	0
			810	480	165	165		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
7	J	39	Total	C	N	O	0	0
			194	116	39	39		

- Molecule 8 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	1	194	Total	C	N	O	0	0
			942	554	194	194		

- Molecule 9 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	3	202	Total	C	N	O	0	0
			985	581	202	202		

- Molecule 10 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	7	212	Total	C	N	O	0	0
			1033	609	212	212		

- Molecule 11 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	8	217	Total	C	N	O	0	0
			1059	625	217	217		

- Molecule 12 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	Z	192	Total	C	N	O	0	0
			934	550	192	192		

- Molecule 13 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	4	203	Total	C	N	O	0	0
			992	586	203	203		

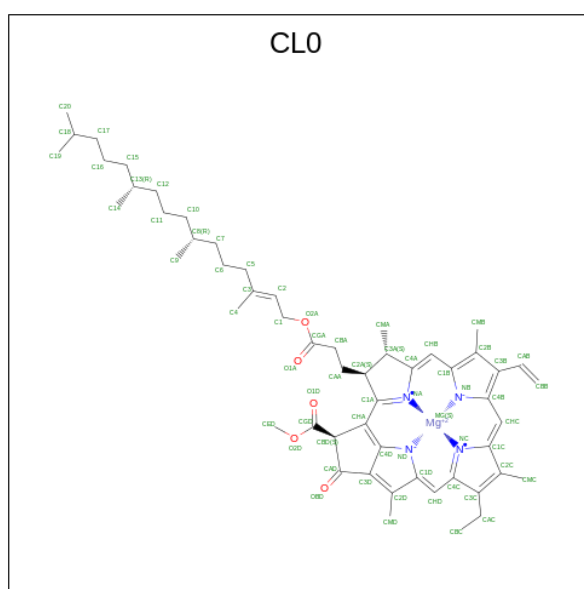
- Molecule 14 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	5	223	Total	C	N	O	0	0
			1091	645	223	223		

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

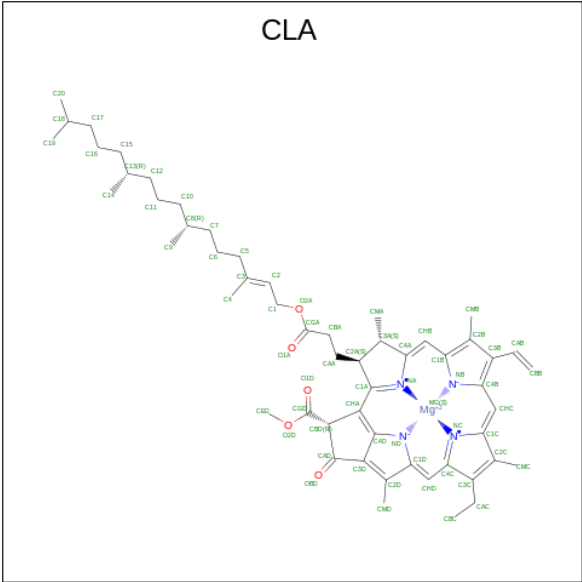
Mol	Chain	Residues	Atoms				AltConf	Trace
15	6	229	Total	C	N	O	0	0
			1122	664	229	229		

- Molecule 16 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
16	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

- Molecule 17 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
17	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	A	1	Total 42	C 34	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
17	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
17	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
17	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			39	33	1	4	1	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
17	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
17	B	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	B	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	F	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	F	1	Total 62	C 52	Mg 1	N 4	O 5	0
17	J	1	Total 43	C 35	Mg 1	N 4	O 3	0
17	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	1	1	Total 43	C 35	Mg 1	N 4	O 3	0
17	1	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	1	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	1	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	1	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	1	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	1	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	1	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	1	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	1	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	3	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	3	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	3	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	3	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	3	1	Total 42	C 34	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
17	3	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	3	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	3	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	3	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	7	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	7	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	7	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	7	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	7	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	7	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	7	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	7	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	7	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	7	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
17	7	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	8	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	8	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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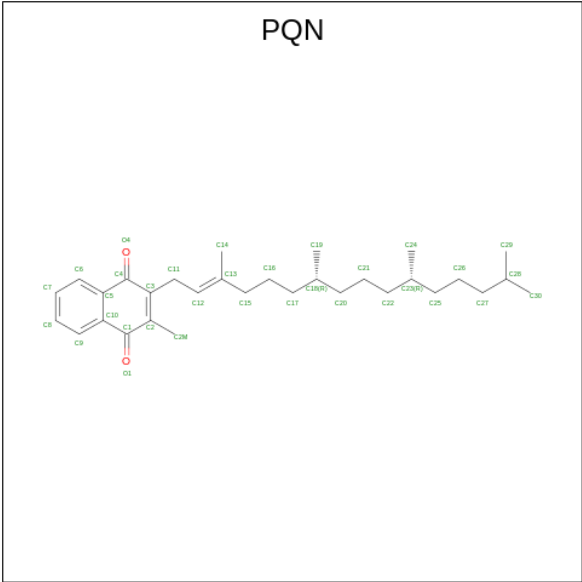
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17	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	8	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	8	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	8	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	8	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	8	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	8	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	8	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	8	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
17	8	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	8	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	4	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	4	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	4	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	5	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	5	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	5	1	Total 48	C 38	Mg 1	N 4	O 5	0
17	5	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	5	1	Total 50	C 40	Mg 1	N 4	O 5	0

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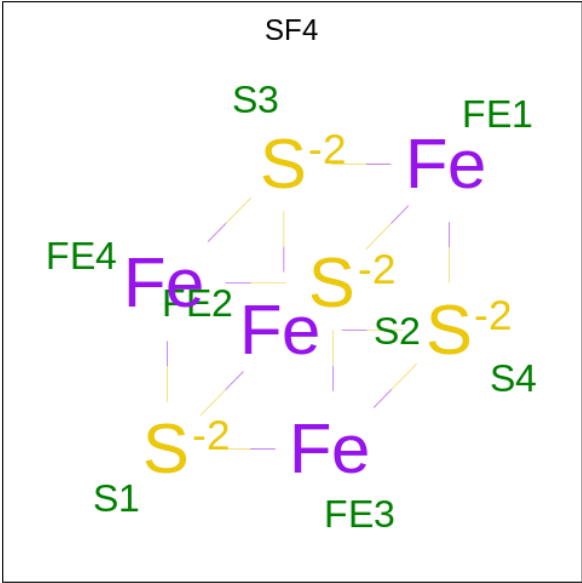
Mol	Chain	Residues	Atoms					AltConf
17	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	6	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	6	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	6	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	6	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 18 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 19 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



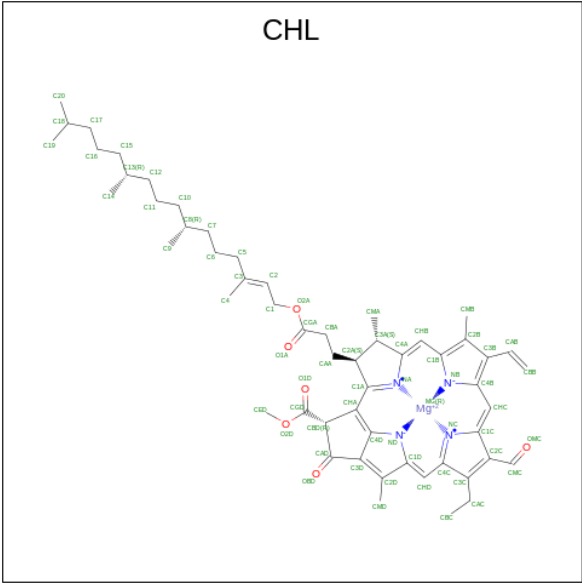
Mol	Chain	Residues	Atoms			AltConf
19	B	1	Total	Fe	S	0
			8	4	4	

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

- Molecule 20 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
20	1	1	53	42	1	4	6	0
20	3	1	46	35	1	4	6	0
20	7	1	43	34	1	4	4	0
20	8	1	43	34	1	4	4	0
20	Z	1	43	34	1	4	4	0
20	5	1	46	35	1	4	6	0
20	5	1	43	34	1	4	4	0
20	6	1	43	34	1	4	4	0
20	6	1	43	34	1	4	4	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
20	6	1	43	34	1	4	4	0

MolProbity failed to run properly - this section is therefore empty.

3 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	47618	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45.5	Depositor
Minimum defocus (nm)	1250	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	3.382	Depositor
Minimum map value	-0.724	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.102	Depositor
Recommended contour level	0.5	Depositor
Map size ($\text{\AA}$)	431.2, 431.2, 431.2	wwPDB
Map dimensions	392, 392, 392	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	Depositor

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

171 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
17	CLA	8	610	-	46,50,73	2.09	9 (19%)	55,85,113	1.56	9 (16%)
17	CLA	A	805	-	46,50,73	2.20	9 (19%)	55,85,113	1.63	9 (16%)
17	CLA	A	838	-	46,50,73	2.19	8 (17%)	55,85,113	1.61	9 (16%)
17	CLA	7	611	-	46,50,73	2.13	11 (23%)	55,85,113	1.50	8 (14%)
17	CLA	5	315	-	49,53,73	2.06	10 (20%)	59,89,113	1.47	8 (13%)
17	CLA	A	812	-	46,50,73	2.15	10 (21%)	55,85,113	1.46	8 (14%)
17	CLA	4	603	-	46,50,73	2.21	9 (19%)	55,85,113	1.82	9 (16%)
17	CLA	B	835	-	47,51,73	2.07	8 (17%)	56,86,113	1.44	8 (14%)
17	CLA	1	610	-	46,50,73	2.12	9 (19%)	55,85,113	1.41	8 (14%)
17	CLA	8	604	-	46,50,73	2.15	11 (23%)	55,85,113	1.42	8 (14%)
17	CLA	7	603	-	46,50,73	2.22	9 (19%)	55,85,113	1.67	10 (18%)
18	PQN	B	840	-	34,34,34	0.23	0	42,45,45	0.23	0
17	CLA	1	605	-	46,50,73	2.14	11 (23%)	55,85,113	1.47	8 (14%)
17	CLA	B	815	-	69,73,73	1.82	9 (13%)	83,113,113	1.57	13 (15%)
17	CLA	A	811	-	46,50,73	2.11	10 (21%)	55,85,113	1.47	8 (14%)
17	CLA	3	301	-	46,50,73	2.19	9 (19%)	55,85,113	1.56	9 (16%)
20	CHL	5	305	-	50,54,74	2.06	9 (18%)	56,90,114	1.73	9 (16%)
17	CLA	1	608	-	46,50,73	2.14	9 (19%)	55,85,113	1.49	9 (16%)
17	CLA	8	605	-	46,50,73	2.07	10 (21%)	55,85,113	1.40	8 (14%)
17	CLA	A	819	-	46,50,73	2.08	9 (19%)	55,85,113	1.41	9 (16%)
17	CLA	6	604	-	46,50,73	2.07	10 (21%)	55,85,113	1.41	9 (16%)
17	CLA	6	609	15	50,54,73	2.05	10 (20%)	60,90,113	1.41	8 (13%)
17	CLA	A	820	-	46,50,73	2.14	10 (21%)	55,85,113	1.48	7 (12%)
17	CLA	A	830	-	46,50,73	2.12	10 (21%)	55,85,113	1.54	10 (18%)
17	CLA	B	827	-	46,50,73	2.09	9 (19%)	55,85,113	1.42	8 (14%)
17	CLA	5	311	-	46,50,73	2.08	10 (21%)	55,85,113	1.48	8 (14%)
17	CLA	3	302	-	46,50,73	2.14	10 (21%)	55,85,113	1.42	9 (16%)
17	CLA	B	825	-	46,50,73	2.12	9 (19%)	55,85,113	1.41	8 (14%)
17	CLA	4	605	-	49,53,73	2.06	10 (20%)	59,89,113	1.34	8 (13%)
17	CLA	A	829	-	46,50,73	2.10	8 (17%)	55,85,113	1.52	9 (16%)
17	CLA	7	614	10	46,50,73	2.18	10 (21%)	55,85,113	1.79	11 (20%)
17	CLA	A	817	-	46,50,73	2.17	9 (19%)	55,85,113	1.66	10 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	8	612	-	50,54,73	2.06	11 (22%)	60,90,113	1.37	8 (13%)
17	CLA	5	306	17	54,58,73	1.99	8 (14%)	65,95,113	1.35	7 (10%)
16	CL0	A	801	-	46,50,73	2.10	9 (19%)	55,85,113	1.60	9 (16%)
17	CLA	7	613	-	47,51,73	2.12	10 (21%)	56,86,113	1.40	8 (14%)
17	CLA	B	832	-	46,50,73	2.17	10 (21%)	55,85,113	1.49	8 (14%)
17	CLA	J	102	-	46,50,73	2.16	10 (21%)	55,85,113	1.55	9 (16%)
17	CLA	A	821	-	55,59,73	1.99	8 (14%)	66,96,113	1.53	11 (16%)
17	CLA	B	822	-	46,50,73	2.07	9 (19%)	55,85,113	1.48	9 (16%)
17	CLA	3	310	-	45,49,73	2.27	9 (20%)	54,84,113	2.05	15 (27%)
17	CLA	A	807	-	46,50,73	2.20	10 (21%)	55,85,113	1.69	10 (18%)
19	SF4	C	102	-	0,12,12	-	-	-	-	-
17	CLA	1	609	-	46,50,73	2.16	9 (19%)	55,85,113	1.39	8 (14%)
17	CLA	1	603	-	46,50,73	2.10	11 (23%)	55,85,113	1.42	8 (14%)
17	CLA	8	609	-	46,50,73	2.07	8 (17%)	55,85,113	1.41	8 (14%)
17	CLA	3	309	-	49,53,73	2.00	8 (16%)	59,89,113	1.43	7 (11%)
17	CLA	A	802	-	46,50,73	2.23	9 (19%)	55,85,113	1.68	9 (16%)
20	CHL	5	313	-	47,51,74	2.11	9 (19%)	52,86,114	1.65	8 (15%)
20	CHL	6	606	-	47,51,74	2.14	9 (19%)	52,86,114	1.73	9 (17%)
17	CLA	A	841	-	56,60,73	2.00	9 (16%)	67,97,113	1.44	10 (14%)
17	CLA	A	810	-	46,50,73	2.15	9 (19%)	55,85,113	1.49	9 (16%)
17	CLA	B	818	-	46,50,73	2.09	9 (19%)	55,85,113	1.59	9 (16%)
17	CLA	8	614	11	46,50,73	2.19	11 (23%)	55,85,113	1.59	8 (14%)
19	SF4	B	803	-	0,12,12	-	-	-	-	-
17	CLA	A	831	-	46,50,73	2.11	11 (23%)	55,85,113	1.46	10 (18%)
17	CLA	8	608	-	46,50,73	2.20	10 (21%)	55,85,113	1.58	10 (18%)
17	CLA	B	834	-	46,50,73	2.13	9 (19%)	55,85,113	1.56	8 (14%)
17	CLA	5	309	-	46,50,73	2.12	9 (19%)	55,85,113	1.60	9 (16%)
17	CLA	6	602	-	46,50,73	2.11	10 (21%)	55,85,113	1.46	8 (14%)
17	CLA	6	603	-	46,50,73	2.11	9 (19%)	55,85,113	1.55	8 (14%)
17	CLA	B	811	-	46,50,73	2.09	9 (19%)	55,85,113	1.46	10 (18%)
17	CLA	3	313	-	46,50,73	2.18	9 (19%)	55,85,113	1.70	11 (20%)
20	CHL	6	607	-	47,51,74	2.17	9 (19%)	52,86,114	1.60	9 (17%)
17	CLA	3	311	-	46,50,73	2.16	10 (21%)	55,85,113	1.42	8 (14%)
17	CLA	B	808	-	46,50,73	2.08	9 (19%)	55,85,113	1.49	8 (14%)
17	CLA	B	829	-	47,51,73	2.07	8 (17%)	56,86,113	1.55	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	1	606	-	46,50,73	2.11	8 (17%)	55,85,113	1.69	9 (16%)
17	CLA	B	824	-	45,49,73	2.30	9 (20%)	54,84,113	1.69	11 (20%)
17	CLA	B	831	-	46,50,73	2.26	11 (23%)	55,85,113	1.71	9 (16%)
17	CLA	3	304	-	49,53,73	2.03	10 (20%)	59,89,113	1.35	8 (13%)
17	CLA	B	837	-	46,50,73	2.21	9 (19%)	55,85,113	1.55	9 (16%)
17	CLA	5	303	-	52,56,73	1.94	8 (15%)	62,92,113	1.32	9 (14%)
17	CLA	4	602	-	49,53,73	2.03	8 (16%)	59,89,113	1.41	8 (13%)
17	CLA	7	602	-	46,50,73	2.08	9 (19%)	55,85,113	1.47	9 (16%)
17	CLA	B	820	-	46,50,73	2.05	9 (19%)	55,85,113	1.56	10 (18%)
17	CLA	8	602	-	46,50,73	2.07	9 (19%)	55,85,113	1.46	8 (14%)
17	CLA	7	610	-	45,49,73	2.39	9 (20%)	54,84,113	1.91	12 (22%)
17	CLA	B	830	-	46,50,73	2.11	8 (17%)	55,85,113	1.52	8 (14%)
17	CLA	A	828	-	46,50,73	2.09	9 (19%)	55,85,113	1.39	9 (16%)
17	CLA	7	609	-	46,50,73	2.07	9 (19%)	55,85,113	1.48	9 (16%)
17	CLA	B	819	-	46,50,73	2.13	8 (17%)	55,85,113	1.68	11 (20%)
17	CLA	A	818	-	49,53,73	2.09	11 (22%)	59,89,113	1.43	8 (13%)
20	CHL	Z	601	12	47,51,74	2.18	9 (19%)	52,86,114	1.58	8 (15%)
17	CLA	B	814	-	42,47,73	2.20	8 (19%)	52,81,113	1.46	8 (15%)
17	CLA	B	823	-	46,50,73	2.17	10 (21%)	55,85,113	1.52	9 (16%)
17	CLA	A	832	-	45,48,73	2.33	11 (24%)	53,82,113	2.03	11 (20%)
17	CLA	A	839	-	46,50,73	2.20	11 (23%)	55,85,113	1.49	9 (16%)
17	CLA	5	308	-	46,50,73	1.97	8 (17%)	55,85,113	1.52	10 (18%)
17	CLA	B	809	-	46,50,73	2.16	11 (23%)	55,85,113	1.55	8 (14%)
17	CLA	7	612	-	49,53,73	2.06	11 (22%)	59,89,113	1.35	8 (13%)
17	CLA	A	809	-	46,50,73	2.17	8 (17%)	55,85,113	1.49	8 (14%)
17	CLA	B	817	-	46,50,73	2.14	10 (21%)	55,85,113	1.51	9 (16%)
17	CLA	B	801	-	46,50,73	2.11	8 (17%)	55,85,113	1.69	11 (20%)
17	CLA	B	813	-	45,49,73	2.06	9 (20%)	57,84,113	1.49	8 (14%)
17	CLA	5	312	-	46,50,73	2.11	9 (19%)	55,85,113	1.42	9 (16%)
17	CLA	A	813	-	46,50,73	2.15	11 (23%)	55,85,113	1.48	9 (16%)
17	CLA	7	604	-	46,50,73	2.27	10 (21%)	55,85,113	1.54	10 (18%)
17	CLA	7	608	-	46,50,73	2.08	8 (17%)	55,85,113	1.57	9 (16%)
17	CLA	A	842	-	46,50,73	2.14	7 (15%)	55,85,113	1.35	9 (16%)
17	CLA	6	608	-	46,50,73	2.05	8 (17%)	55,85,113	1.53	11 (20%)
17	CLA	A	814	-	46,50,73	2.14	10 (21%)	55,85,113	1.43	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	A	833	-	46,50,73	2.12	10 (21%)	55,85,113	1.53	8 (14%)
17	CLA	1	602	-	46,50,73	2.03	9 (19%)	55,85,113	1.49	8 (14%)
17	CLA	8	603	-	49,53,73	2.13	10 (20%)	59,89,113	1.46	8 (13%)
17	CLA	A	823	-	46,50,73	2.16	9 (19%)	55,85,113	1.56	9 (16%)
17	CLA	A	806	-	46,50,73	2.18	10 (21%)	55,85,113	1.45	7 (12%)
20	CHL	3	307	-	50,54,74	2.08	10 (20%)	56,90,114	1.63	9 (16%)
17	CLA	B	838	-	46,50,73	2.06	10 (21%)	55,85,113	1.49	8 (14%)
19	SF4	C	101	-	0,12,12	-	-	-	-	-
17	CLA	3	308	-	46,50,73	2.18	9 (19%)	55,85,113	1.84	10 (18%)
17	CLA	B	810	-	50,54,73	2.07	8 (16%)	59,89,113	1.51	9 (15%)
17	CLA	B	802	-	49,53,73	2.10	7 (14%)	59,89,113	1.68	9 (15%)
17	CLA	5	302	14	46,50,73	2.16	10 (21%)	55,85,113	1.45	8 (14%)
17	CLA	A	837	-	46,50,73	2.15	10 (21%)	55,85,113	1.44	8 (14%)
17	CLA	7	601	10	46,50,73	2.11	10 (21%)	55,85,113	1.52	8 (14%)
18	PQN	A	840	-	34,34,34	0.21	0	42,45,45	0.26	0
17	CLA	A	827	-	46,50,73	2.06	10 (21%)	55,85,113	1.47	9 (16%)
17	CLA	B	836	-	46,50,73	2.13	10 (21%)	55,85,113	1.57	8 (14%)
20	CHL	8	606	-	47,51,74	2.10	9 (19%)	52,86,114	1.67	7 (13%)
20	CHL	7	606	-	47,51,74	2.15	9 (19%)	52,86,114	1.72	9 (17%)
17	CLA	B	821	-	50,54,73	2.01	11 (22%)	60,90,113	1.33	7 (11%)
17	CLA	A	826	-	46,50,73	2.06	8 (17%)	55,85,113	1.42	8 (14%)
17	CLA	1	604	-	46,50,73	2.14	8 (17%)	55,85,113	1.38	9 (16%)
20	CHL	1	601	8	57,61,74	1.98	9 (15%)	64,98,114	1.42	7 (10%)
17	CLA	A	836	-	46,50,73	2.10	10 (21%)	55,85,113	1.53	10 (18%)
17	CLA	A	804	-	46,50,73	2.18	8 (17%)	55,85,113	1.91	11 (20%)
17	CLA	B	804	-	46,50,73	2.18	8 (17%)	55,85,113	1.67	9 (16%)
17	CLA	3	305	-	46,50,73	2.07	8 (17%)	55,85,113	1.58	10 (18%)
17	CLA	A	835	-	46,50,73	2.12	11 (23%)	55,85,113	1.41	8 (14%)
17	CLA	4	604	-	46,50,73	2.16	10 (21%)	55,85,113	1.42	7 (12%)
17	CLA	3	303	-	46,50,73	2.21	10 (21%)	55,85,113	1.47	8 (14%)
17	CLA	8	611	-	46,50,73	2.14	10 (21%)	55,85,113	1.53	7 (12%)
17	CLA	6	601	15	46,50,73	2.13	9 (19%)	55,85,113	1.44	9 (16%)
17	CLA	5	301	-	46,50,73	2.08	9 (19%)	55,85,113	1.43	8 (14%)
17	CLA	5	304	-	46,50,73	2.13	9 (19%)	55,85,113	1.37	8 (14%)
17	CLA	A	843	-	46,50,73	2.11	10 (21%)	55,85,113	1.39	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	A	825	-	46,50,73	2.03	9 (19%)	55,85,113	1.62	10 (18%)
17	CLA	A	834	1	46,50,73	2.11	8 (17%)	55,85,113	1.53	8 (14%)
17	CLA	B	826	-	46,50,73	2.18	8 (17%)	55,85,113	1.71	8 (14%)
17	CLA	5	307	-	46,50,73	2.12	8 (17%)	55,85,113	1.45	8 (14%)
17	CLA	8	607	-	46,50,73	2.10	11 (23%)	55,85,113	1.52	9 (16%)
17	CLA	6	610	-	49,53,73	2.10	10 (20%)	59,89,113	1.42	9 (15%)
17	CLA	A	803	-	46,50,73	2.15	10 (21%)	55,85,113	1.56	8 (14%)
17	CLA	5	314	17	50,54,73	2.04	9 (18%)	60,90,113	1.62	11 (18%)
17	CLA	B	805	-	46,50,73	2.21	7 (15%)	55,85,113	1.51	9 (16%)
17	CLA	1	607	-	46,50,73	2.23	9 (19%)	55,85,113	1.84	9 (16%)
17	CLA	B	828	-	47,51,73	2.15	9 (19%)	56,86,113	1.44	7 (12%)
17	CLA	F	302	-	66,70,73	1.75	9 (13%)	79,109,113	1.25	9 (11%)
17	CLA	J	101	-	46,50,73	2.19	10 (21%)	55,85,113	1.58	8 (14%)
17	CLA	A	816	-	46,50,73	2.03	8 (17%)	55,85,113	1.43	9 (16%)
17	CLA	3	312	-	46,50,73	2.10	9 (19%)	55,85,113	1.57	9 (16%)
17	CLA	B	839	-	46,50,73	2.10	9 (19%)	55,85,113	1.46	9 (16%)
17	CLA	A	822	-	46,50,73	2.19	9 (19%)	55,85,113	1.56	8 (14%)
20	CHL	6	605	-	47,51,74	2.13	9 (19%)	52,86,114	1.63	10 (19%)
17	CLA	A	824	-	46,50,73	2.11	9 (19%)	55,85,113	1.66	10 (18%)
17	CLA	A	808	-	46,50,73	2.15	11 (23%)	55,85,113	1.43	8 (14%)
17	CLA	7	605	-	46,50,73	2.15	11 (23%)	55,85,113	1.43	9 (16%)
17	CLA	8	601	11	46,50,73	2.14	11 (23%)	55,85,113	1.48	8 (14%)
17	CLA	8	613	-	46,50,73	2.11	9 (19%)	55,85,113	1.47	8 (14%)
17	CLA	B	812	-	46,50,73	2.21	10 (21%)	55,85,113	1.93	11 (20%)
17	CLA	A	815	-	46,50,73	2.25	9 (19%)	55,85,113	1.49	8 (14%)
17	CLA	F	301	-	46,50,73	2.12	9 (19%)	55,85,113	1.57	10 (18%)
17	CLA	7	607	-	46,50,73	2.12	9 (19%)	55,85,113	1.46	9 (16%)
17	CLA	4	601	-	46,50,73	2.15	11 (23%)	55,85,113	1.48	8 (14%)
17	CLA	B	816	-	46,50,73	2.14	10 (21%)	55,85,113	1.50	8 (14%)
17	CLA	B	833	-	46,50,73	2.09	8 (17%)	55,85,113	1.49	9 (16%)
17	CLA	5	310	-	46,50,73	2.19	11 (23%)	55,85,113	1.38	8 (14%)
17	CLA	B	807	-	46,50,73	2.18	9 (19%)	55,85,113	1.79	9 (16%)
17	CLA	B	806	-	46,50,73	2.24	10 (21%)	55,85,113	1.91	12 (21%)
17	CLA	3	306	-	46,50,73	2.14	9 (19%)	55,85,113	1.88	14 (25%)

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
17	CLA	8	610	-	-	3/12/88/115	-
17	CLA	A	805	-	-	4/12/88/115	-
17	CLA	A	838	-	-	2/12/88/115	-
17	CLA	7	611	-	-	3/12/88/115	-
17	CLA	5	315	-	-	6/15/91/115	-
17	CLA	A	812	-	-	2/12/88/115	-
17	CLA	4	603	-	-	6/12/88/115	-
17	CLA	B	835	-	-	5/13/89/115	-
17	CLA	1	610	-	-	3/12/88/115	-
17	CLA	8	604	-	-	0/12/88/115	-
17	CLA	7	603	-	-	4/12/88/115	-
18	PQN	B	840	-	-	4/23/43/43	0/2/2/2
17	CLA	1	605	-	-	3/12/88/115	-
17	CLA	B	815	-	-	12/39/115/115	-
17	CLA	A	811	-	-	4/12/88/115	-
17	CLA	3	301	-	-	3/12/88/115	-
20	CHL	5	305	-	-	5/17/93/117	-
17	CLA	1	608	-	-	3/12/88/115	-
17	CLA	8	605	-	-	4/12/88/115	-
17	CLA	A	819	-	-	4/12/88/115	-
17	CLA	6	604	-	-	2/12/88/115	-
17	CLA	6	609	15	-	3/17/93/115	-
17	CLA	A	820	-	-	6/12/88/115	-
17	CLA	A	830	-	-	2/12/88/115	-
17	CLA	B	827	-	-	6/12/88/115	-
17	CLA	5	311	-	-	5/12/88/115	-
17	CLA	3	302	-	-	4/12/88/115	-
17	CLA	B	825	-	-	6/12/88/115	-
17	CLA	4	605	-	-	3/15/91/115	-
17	CLA	A	829	-	-	5/12/88/115	-
17	CLA	7	614	10	-	4/12/88/115	-
17	CLA	A	817	-	-	4/12/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	8	612	-	-	0/17/93/115	-
17	CLA	5	306	17	-	4/21/97/115	-
16	CL0	A	801	-	-	5/12/88/115	-
17	CLA	7	613	-	-	3/13/89/115	-
17	CLA	B	832	-	-	3/12/88/115	-
17	CLA	J	102	-	-	4/12/88/115	-
17	CLA	A	821	-	-	7/23/99/115	-
17	CLA	B	822	-	-	3/12/88/115	-
17	CLA	3	310	-	-	2/10/86/115	-
17	CLA	A	807	-	-	4/12/88/115	-
19	SF4	C	102	-	-	-	0/6/5/5
17	CLA	1	609	-	-	2/12/88/115	-
17	CLA	1	603	-	-	4/12/88/115	-
17	CLA	8	609	-	-	3/12/88/115	-
17	CLA	3	309	-	-	0/15/91/115	-
17	CLA	A	802	-	-	4/12/88/115	-
20	CHL	5	313	-	-	2/14/90/117	-
20	CHL	6	606	-	-	5/14/90/117	-
17	CLA	A	841	-	-	9/24/100/115	-
17	CLA	A	810	-	-	3/12/88/115	-
17	CLA	B	818	-	-	5/12/88/115	-
17	CLA	8	614	11	-	2/12/88/115	-
19	SF4	B	803	-	-	-	0/6/5/5
17	CLA	A	831	-	-	3/12/88/115	-
17	CLA	8	608	-	-	0/12/88/115	-
17	CLA	B	834	-	-	7/12/88/115	-
17	CLA	5	309	-	-	3/12/88/115	-
17	CLA	6	602	-	-	5/12/88/115	-
17	CLA	6	603	-	-	4/12/88/115	-
17	CLA	B	811	-	-	2/12/88/115	-
17	CLA	3	313	-	-	3/12/88/115	-
20	CHL	6	607	-	-	4/14/90/117	-
17	CLA	3	311	-	-	3/12/88/115	-
17	CLA	B	808	-	-	3/12/88/115	-
17	CLA	B	829	-	-	7/13/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	1	606	-	-	0/12/88/115	-
17	CLA	B	824	-	-	3/10/86/115	-
17	CLA	B	831	-	-	2/12/88/115	-
17	CLA	3	304	-	-	4/15/91/115	-
17	CLA	B	837	-	-	2/12/88/115	-
17	CLA	5	303	-	-	7/19/95/115	-
17	CLA	4	602	-	-	4/15/91/115	-
17	CLA	7	602	-	-	5/12/88/115	-
17	CLA	B	820	-	-	5/12/88/115	-
17	CLA	8	602	-	-	5/12/88/115	-
17	CLA	7	610	-	-	5/10/86/115	-
17	CLA	B	830	-	-	4/12/88/115	-
17	CLA	A	828	-	-	3/12/88/115	-
17	CLA	7	609	-	-	3/12/88/115	-
17	CLA	B	819	-	-	4/12/88/115	-
17	CLA	A	818	-	-	5/15/91/115	-
20	CHL	Z	601	12	-	3/14/90/117	-
17	CLA	B	814	-	-	0/6/82/115	-
17	CLA	B	823	-	-	4/12/88/115	-
17	CLA	A	832	-	-	5/10/86/115	-
17	CLA	A	839	-	-	3/12/88/115	-
17	CLA	5	308	-	-	5/12/88/115	-
17	CLA	B	809	-	-	6/12/88/115	-
17	CLA	7	612	-	-	4/15/91/115	-
17	CLA	A	809	-	-	4/12/88/115	-
17	CLA	B	817	-	-	5/12/88/115	-
17	CLA	B	801	-	-	3/12/88/115	-
17	CLA	B	813	-	-	1/10/86/115	-
17	CLA	5	312	-	-	3/12/88/115	-
17	CLA	A	813	-	-	3/12/88/115	-
17	CLA	7	604	-	-	1/12/88/115	-
17	CLA	7	608	-	-	1/12/88/115	-
17	CLA	A	842	-	-	3/12/88/115	-
17	CLA	6	608	-	-	2/12/88/115	-
17	CLA	A	814	-	-	3/12/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	A	833	-	-	3/12/88/115	-
17	CLA	1	602	-	-	5/12/88/115	-
17	CLA	8	603	-	-	2/15/91/115	-
17	CLA	A	823	-	-	3/12/88/115	-
17	CLA	A	806	-	-	3/12/88/115	-
20	CHL	3	307	-	-	7/17/93/117	-
17	CLA	B	838	-	-	4/12/88/115	-
19	SF4	C	101	-	-	-	0/6/5/5
17	CLA	3	308	-	-	3/12/88/115	-
17	CLA	B	810	-	-	5/15/91/115	-
17	CLA	B	802	-	-	7/15/91/115	-
17	CLA	5	302	14	-	4/12/88/115	-
17	CLA	A	837	-	-	5/12/88/115	-
17	CLA	7	601	10	-	5/12/88/115	-
18	PQN	A	840	-	-	5/23/43/43	0/2/2/2
17	CLA	A	827	-	-	2/12/88/115	-
17	CLA	B	836	-	-	2/12/88/115	-
20	CHL	8	606	-	-	2/14/90/117	-
20	CHL	7	606	-	-	2/14/90/117	-
17	CLA	B	821	-	-	3/17/93/115	-
17	CLA	A	826	-	-	2/12/88/115	-
17	CLA	1	604	-	-	3/12/88/115	-
20	CHL	1	601	8	-	6/26/102/117	-
17	CLA	A	836	-	-	2/12/88/115	-
17	CLA	A	804	-	-	3/12/88/115	-
17	CLA	B	804	-	-	1/12/88/115	-
17	CLA	3	305	-	-	3/12/88/115	-
17	CLA	A	835	-	-	6/12/88/115	-
17	CLA	4	604	-	-	3/12/88/115	-
17	CLA	3	303	-	-	0/12/88/115	-
17	CLA	8	611	-	-	5/12/88/115	-
17	CLA	6	601	15	-	5/12/88/115	-
17	CLA	5	301	-	-	4/12/88/115	-
17	CLA	5	304	-	-	4/12/88/115	-
17	CLA	A	843	-	-	4/12/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	A	825	-	-	2/12/88/115	-
17	CLA	A	834	1	-	0/12/88/115	-
17	CLA	B	826	-	-	2/12/88/115	-
17	CLA	5	307	-	-	5/12/88/115	-
17	CLA	8	607	-	-	4/12/88/115	-
17	CLA	6	610	-	-	5/15/91/115	-
17	CLA	A	803	-	-	4/12/88/115	-
17	CLA	5	314	17	-	9/17/93/115	-
17	CLA	B	805	-	-	0/12/88/115	-
17	CLA	1	607	-	-	5/12/88/115	-
17	CLA	B	828	-	-	1/13/89/115	-
17	CLA	F	302	-	-	8/36/112/115	-
17	CLA	J	101	-	-	4/12/88/115	-
17	CLA	A	816	-	-	5/12/88/115	-
17	CLA	3	312	-	-	3/12/88/115	-
17	CLA	B	839	-	-	3/12/88/115	-
17	CLA	A	822	-	-	4/12/88/115	-
20	CHL	6	605	-	-	3/14/90/117	-
17	CLA	A	824	-	-	2/12/88/115	-
17	CLA	A	808	-	-	2/12/88/115	-
17	CLA	7	605	-	-	3/12/88/115	-
17	CLA	8	601	11	-	3/12/88/115	-
17	CLA	8	613	-	-	5/12/88/115	-
17	CLA	B	812	-	-	6/12/88/115	-
17	CLA	A	815	-	-	2/12/88/115	-
17	CLA	F	301	-	-	3/12/88/115	-
17	CLA	7	607	-	-	3/12/88/115	-
17	CLA	4	601	-	-	2/12/88/115	-
17	CLA	B	816	-	-	5/12/88/115	-
17	CLA	B	833	-	-	1/12/88/115	-
17	CLA	5	310	-	-	2/12/88/115	-
17	CLA	B	807	-	-	4/12/88/115	-
17	CLA	B	806	-	-	4/12/88/115	-
17	CLA	3	306	-	-	4/12/88/115	-

All (1547) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	608	CLA	C4B-NB	8.72	1.48	1.37
17	7	604	CLA	C4B-NB	8.40	1.48	1.37
17	B	821	CLA	C4B-NB	8.29	1.48	1.37
17	B	814	CLA	C4B-NB	8.28	1.48	1.37
17	1	609	CLA	C4B-NB	8.18	1.47	1.37
17	1	605	CLA	C4B-NB	8.07	1.47	1.37
17	8	603	CLA	C4B-NB	8.02	1.47	1.37
17	3	311	CLA	C4B-NB	8.02	1.47	1.37
17	4	604	CLA	C4B-NB	8.02	1.47	1.37
17	6	609	CLA	C4B-NB	8.02	1.47	1.37
17	A	815	CLA	C4B-NB	7.96	1.47	1.37
17	8	604	CLA	C4B-NB	7.95	1.47	1.37
17	A	831	CLA	C4B-NB	7.95	1.47	1.37
17	A	820	CLA	C4B-NB	7.95	1.47	1.37
17	A	806	CLA	C4B-NB	7.93	1.47	1.37
17	A	823	CLA	C4B-NB	7.92	1.47	1.37
17	5	304	CLA	C4B-NB	7.91	1.47	1.37
17	3	303	CLA	C4B-NB	7.85	1.47	1.37
17	A	810	CLA	C4B-NB	7.84	1.47	1.37
17	J	101	CLA	C4B-NB	7.80	1.47	1.37
17	7	611	CLA	C4B-NB	7.78	1.47	1.37
17	6	601	CLA	C4B-NB	7.76	1.47	1.37
17	4	602	CLA	C4B-NB	7.72	1.47	1.37
17	7	605	CLA	C4B-NB	7.71	1.47	1.37
17	7	612	CLA	C4B-NB	7.70	1.47	1.37
17	6	610	CLA	C4B-NB	7.69	1.47	1.37
17	8	612	CLA	C4B-NB	7.69	1.47	1.37
17	7	608	CLA	C4B-NB	7.67	1.47	1.37
17	B	809	CLA	C4B-NB	7.66	1.47	1.37
17	J	102	CLA	C4B-NB	7.65	1.47	1.37
17	B	828	CLA	C4B-NB	7.64	1.47	1.37
17	B	817	CLA	C4B-NB	7.61	1.47	1.37
17	8	605	CLA	C4B-NB	7.61	1.47	1.37
17	7	607	CLA	C4B-NB	7.61	1.47	1.37
17	B	816	CLA	C4B-NB	7.60	1.47	1.37
17	1	610	CLA	C4B-NB	7.59	1.47	1.37
17	A	813	CLA	C4B-NB	7.58	1.47	1.37
17	B	823	CLA	C4B-NB	7.58	1.47	1.37
17	1	603	CLA	C4B-NB	7.58	1.47	1.37
17	B	832	CLA	C4B-NB	7.55	1.47	1.37
17	3	302	CLA	C4B-NB	7.55	1.47	1.37
17	A	811	CLA	C4B-NB	7.54	1.47	1.37
17	5	307	CLA	C4B-NB	7.53	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	5	310	CLA	C4B-NB	7.50	1.47	1.37
17	B	811	CLA	C4B-NB	7.47	1.47	1.37
17	A	812	CLA	C4B-NB	7.47	1.47	1.37
17	A	807	CLA	C4B-NB	7.47	1.47	1.37
17	A	828	CLA	C4B-NB	7.46	1.47	1.37
17	B	822	CLA	C4B-NB	7.45	1.46	1.37
17	1	606	CLA	C4B-NB	7.45	1.46	1.37
17	B	815	CLA	C4B-NB	7.44	1.46	1.37
17	A	819	CLA	C4B-NB	7.44	1.46	1.37
17	5	311	CLA	C4B-NB	7.42	1.46	1.37
17	A	805	CLA	C4B-NB	7.41	1.46	1.37
17	B	825	CLA	C4B-NB	7.41	1.46	1.37
17	7	601	CLA	C4B-NB	7.40	1.46	1.37
17	5	302	CLA	C4B-NB	7.40	1.46	1.37
17	A	836	CLA	C4B-NB	7.37	1.46	1.37
17	6	604	CLA	C4B-NB	7.37	1.46	1.37
17	8	601	CLA	C4B-NB	7.36	1.46	1.37
17	B	836	CLA	C4B-NB	7.36	1.46	1.37
17	8	614	CLA	C4B-NB	7.34	1.46	1.37
17	3	301	CLA	C4B-NB	7.33	1.46	1.37
17	A	834	CLA	C4B-NB	7.33	1.46	1.37
17	8	602	CLA	C4B-NB	7.32	1.46	1.37
17	A	843	CLA	C4B-NB	7.32	1.46	1.37
17	7	609	CLA	C4B-NB	7.32	1.46	1.37
17	8	608	CLA	C4B-NB	7.32	1.46	1.37
17	1	604	CLA	C4B-NB	7.31	1.46	1.37
17	5	306	CLA	C4B-NB	7.31	1.46	1.37
17	6	602	CLA	C4B-NB	7.31	1.46	1.37
17	5	312	CLA	C4B-NB	7.31	1.46	1.37
17	A	803	CLA	C4B-NB	7.30	1.46	1.37
17	6	603	CLA	C4B-NB	7.28	1.46	1.37
17	5	301	CLA	C4B-NB	7.26	1.46	1.37
17	A	808	CLA	C4B-NB	7.26	1.46	1.37
17	8	607	CLA	C4B-NB	7.23	1.46	1.37
17	B	831	CLA	C4B-NB	7.22	1.46	1.37
17	A	829	CLA	C4B-NB	7.21	1.46	1.37
17	B	818	CLA	C4B-NB	7.21	1.46	1.37
20	5	305	CHL	MG-NB	-7.20	1.91	2.05
17	7	602	CLA	C4B-NB	7.19	1.46	1.37
20	7	606	CHL	MG-NB	-7.19	1.91	2.05
17	7	603	CLA	C4B-NB	7.18	1.46	1.37
17	8	611	CLA	C4B-NB	7.17	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	808	CLA	C4B-NB	7.17	1.46	1.37
17	7	613	CLA	C4B-NB	7.17	1.46	1.37
17	B	827	CLA	C4B-NB	7.15	1.46	1.37
17	A	818	CLA	C4B-NB	7.15	1.46	1.37
17	B	830	CLA	C4B-NB	7.15	1.46	1.37
17	A	842	CLA	C4B-NB	7.14	1.46	1.37
17	A	832	CLA	C4B-NB	7.14	1.46	1.37
17	B	839	CLA	C4B-NB	7.13	1.46	1.37
20	Z	601	CHL	MG-NB	-7.12	1.91	2.05
17	4	601	CLA	C4B-NB	7.11	1.46	1.37
17	A	837	CLA	C4B-NB	7.10	1.46	1.37
17	B	838	CLA	C4B-NB	7.10	1.46	1.37
17	B	804	CLA	C4B-NB	7.09	1.46	1.37
20	6	607	CHL	MG-NB	-7.09	1.91	2.05
20	6	606	CHL	MG-NB	-7.09	1.91	2.05
20	1	601	CHL	MG-NB	-7.08	1.91	2.05
17	A	838	CLA	C4B-NB	7.08	1.46	1.37
17	A	809	CLA	C4B-NB	7.06	1.46	1.37
17	5	309	CLA	C4B-NB	7.06	1.46	1.37
17	B	833	CLA	C4B-NB	7.04	1.46	1.37
17	A	841	CLA	C4B-NB	7.04	1.46	1.37
17	A	833	CLA	C4B-NB	7.04	1.46	1.37
17	1	602	CLA	C4B-NB	7.03	1.46	1.37
17	1	607	CLA	C4B-NB	7.03	1.46	1.37
17	8	609	CLA	C4B-NB	7.03	1.46	1.37
17	5	315	CLA	C4B-NB	7.02	1.46	1.37
17	A	817	CLA	C4B-NB	7.01	1.46	1.37
17	B	837	CLA	C4B-NB	7.01	1.46	1.37
17	5	303	CLA	C4B-NB	7.01	1.46	1.37
17	5	314	CLA	MG-NB	-7.00	1.91	2.05
20	5	313	CHL	MG-NB	-7.00	1.91	2.05
17	A	830	CLA	C4B-NB	6.99	1.46	1.37
17	B	820	CLA	C4B-NB	6.98	1.46	1.37
17	A	816	CLA	C4B-NB	6.97	1.46	1.37
17	7	610	CLA	C3A-C2A	-6.97	1.48	1.54
17	4	603	CLA	C4B-NB	6.97	1.46	1.37
20	3	307	CHL	MG-NB	-6.95	1.92	2.05
16	A	801	CL0	C4B-NB	6.95	1.46	1.37
20	6	605	CHL	MG-NB	-6.93	1.92	2.05
17	B	824	CLA	C4B-NB	6.93	1.46	1.37
20	8	606	CHL	MG-NB	-6.93	1.92	2.05
17	A	835	CLA	C4B-NB	6.92	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	7	604	CLA	MG-ND	-6.92	1.92	2.05
17	B	806	CLA	C4B-NB	6.92	1.46	1.37
17	A	826	CLA	C4B-NB	6.91	1.46	1.37
17	F	301	CLA	C4B-NB	6.91	1.46	1.37
17	B	819	CLA	C4B-NB	6.90	1.46	1.37
17	B	805	CLA	MG-NB	-6.90	1.92	2.05
17	A	802	CLA	C4B-NB	6.90	1.46	1.37
17	B	805	CLA	C4B-NB	6.90	1.46	1.37
17	B	834	CLA	C4B-NB	6.90	1.46	1.37
17	B	801	CLA	MG-NB	-6.89	1.92	2.05
17	B	835	CLA	C4B-NB	6.89	1.46	1.37
17	3	312	CLA	C4B-NB	6.89	1.46	1.37
17	3	313	CLA	C4B-NB	6.88	1.46	1.37
17	A	822	CLA	C4B-NB	6.88	1.46	1.37
17	A	821	CLA	C4B-NB	6.87	1.46	1.37
17	A	814	CLA	C4B-NB	6.86	1.46	1.37
17	3	309	CLA	C4B-NB	6.85	1.46	1.37
17	3	306	CLA	C4B-NB	6.84	1.46	1.37
17	A	827	CLA	C4B-NB	6.84	1.46	1.37
17	F	302	CLA	C4B-NB	6.82	1.46	1.37
17	B	802	CLA	MG-NB	-6.79	1.92	2.05
17	8	613	CLA	C4B-NB	6.79	1.46	1.37
17	7	614	CLA	C4B-NB	6.77	1.46	1.37
17	B	813	CLA	C4B-NB	6.76	1.46	1.37
20	6	605	CHL	C4B-NB	6.76	1.46	1.37
17	3	308	CLA	C4B-NB	6.75	1.46	1.37
17	3	304	CLA	C4B-NB	6.75	1.46	1.37
17	A	832	CLA	C4C-NC	6.73	1.48	1.37
20	Z	601	CHL	MG-ND	-6.72	1.92	2.05
20	1	601	CHL	MG-ND	-6.70	1.92	2.05
17	4	605	CLA	C4B-NB	6.68	1.46	1.37
17	3	305	CLA	C4B-NB	6.66	1.46	1.37
17	A	825	CLA	C4B-NB	6.66	1.46	1.37
17	A	804	CLA	MG-NB	-6.64	1.92	2.05
20	5	305	CHL	MG-ND	-6.60	1.92	2.05
17	A	842	CLA	MG-NB	-6.59	1.92	2.05
17	7	610	CLA	C4B-NB	6.59	1.45	1.37
17	B	805	CLA	MG-ND	-6.58	1.92	2.05
17	B	807	CLA	C4B-NB	6.58	1.45	1.37
17	A	839	CLA	C4B-NB	6.58	1.45	1.37
17	B	826	CLA	MG-NB	-6.58	1.92	2.05
17	3	310	CLA	MG-NB	-6.57	1.92	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	7	606	CHL	MG-ND	-6.54	1.92	2.05
17	6	608	CLA	C4B-NB	6.53	1.45	1.37
20	3	307	CHL	MG-ND	-6.49	1.92	2.05
17	B	824	CLA	MG-NB	-6.48	1.92	2.05
17	B	837	CLA	MG-NB	-6.46	1.93	2.05
17	A	842	CLA	MG-ND	-6.46	1.93	2.05
17	B	812	CLA	C4B-NB	6.46	1.45	1.37
17	B	812	CLA	MG-NB	-6.45	1.93	2.05
17	3	305	CLA	MG-NB	-6.45	1.93	2.05
17	7	610	CLA	MG-NB	-6.44	1.93	2.05
17	7	603	CLA	MG-NB	-6.43	1.93	2.05
20	8	606	CHL	MG-ND	-6.43	1.93	2.05
17	B	802	CLA	MG-ND	-6.43	1.93	2.05
17	B	826	CLA	C4B-NB	6.42	1.45	1.37
20	6	607	CHL	MG-ND	-6.42	1.93	2.05
17	8	610	CLA	C4B-NB	6.41	1.45	1.37
17	3	308	CLA	MG-NB	-6.41	1.93	2.05
17	B	804	CLA	MG-NB	-6.40	1.93	2.05
17	B	801	CLA	MG-ND	-6.39	1.93	2.05
17	A	839	CLA	MG-NB	-6.38	1.93	2.05
17	A	839	CLA	MG-ND	-6.37	1.93	2.05
17	A	824	CLA	C4B-NB	6.37	1.45	1.37
17	A	841	CLA	MG-NB	-6.37	1.93	2.05
17	B	831	CLA	MG-ND	-6.36	1.93	2.05
17	5	308	CLA	C4B-NB	6.36	1.45	1.37
17	3	310	CLA	C4B-NB	6.35	1.45	1.37
17	6	608	CLA	MG-NB	-6.35	1.93	2.05
17	7	614	CLA	MG-NB	-6.34	1.93	2.05
17	8	610	CLA	MG-NB	-6.33	1.93	2.05
20	6	606	CHL	MG-ND	-6.33	1.93	2.05
17	B	809	CLA	MG-ND	-6.33	1.93	2.05
20	5	313	CHL	C4B-NB	6.33	1.45	1.37
17	A	841	CLA	MG-ND	-6.32	1.93	2.05
17	B	810	CLA	MG-NB	-6.32	1.93	2.05
20	8	606	CHL	C4B-NB	6.31	1.45	1.37
17	B	829	CLA	C4B-NB	6.29	1.45	1.37
17	A	822	CLA	MG-NB	-6.29	1.93	2.05
17	A	809	CLA	MG-NB	-6.29	1.93	2.05
20	5	313	CHL	MG-ND	-6.29	1.93	2.05
17	A	838	CLA	MG-ND	-6.27	1.93	2.05
20	6	605	CHL	MG-ND	-6.26	1.93	2.05
17	A	807	CLA	MG-NB	-6.25	1.93	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	5	314	CLA	MG-ND	-6.25	1.93	2.05
17	B	830	CLA	MG-NB	-6.25	1.93	2.05
17	3	313	CLA	MG-ND	-6.23	1.93	2.05
17	B	831	CLA	MG-NB	-6.23	1.93	2.05
17	A	812	CLA	MG-ND	-6.22	1.93	2.05
17	B	807	CLA	MG-NB	-6.22	1.93	2.05
17	3	313	CLA	MG-NB	-6.22	1.93	2.05
17	7	604	CLA	MG-NB	-6.22	1.93	2.05
17	A	821	CLA	MG-NB	-6.21	1.93	2.05
17	A	822	CLA	MG-ND	-6.21	1.93	2.05
17	F	302	CLA	MG-NB	-6.21	1.93	2.05
17	A	824	CLA	MG-NB	-6.21	1.93	2.05
17	4	605	CLA	MG-NB	-6.20	1.93	2.05
17	B	829	CLA	MG-NB	-6.19	1.93	2.05
17	1	607	CLA	MG-NA	-6.19	1.91	2.06
17	A	838	CLA	MG-NB	-6.19	1.93	2.05
17	F	301	CLA	MG-NB	-6.18	1.93	2.05
17	B	802	CLA	C4B-NB	6.18	1.45	1.37
17	1	607	CLA	MG-NB	-6.18	1.93	2.05
17	B	829	CLA	MG-ND	-6.18	1.93	2.05
17	5	302	CLA	MG-NB	-6.16	1.93	2.05
17	A	815	CLA	MG-ND	-6.16	1.93	2.05
17	B	807	CLA	MG-ND	-6.16	1.93	2.05
17	A	802	CLA	MG-NB	-6.16	1.93	2.05
17	B	834	CLA	MG-NB	-6.16	1.93	2.05
17	B	824	CLA	MG-ND	-6.15	1.93	2.05
17	3	303	CLA	MG-NB	-6.15	1.93	2.05
17	B	810	CLA	C4B-NB	6.14	1.45	1.37
20	7	606	CHL	C4B-NB	6.13	1.45	1.37
17	8	614	CLA	MG-NB	-6.13	1.93	2.05
17	A	803	CLA	MG-NB	-6.13	1.93	2.05
17	A	814	CLA	MG-NB	-6.13	1.93	2.05
17	5	302	CLA	MG-ND	-6.13	1.93	2.05
17	4	605	CLA	MG-ND	-6.13	1.93	2.05
17	B	810	CLA	MG-ND	-6.12	1.93	2.05
17	3	312	CLA	MG-NB	-6.10	1.93	2.05
17	A	821	CLA	MG-ND	-6.09	1.93	2.05
17	4	603	CLA	MG-NB	-6.09	1.93	2.05
20	6	607	CHL	C4B-NB	6.09	1.45	1.37
17	A	817	CLA	MG-NB	-6.09	1.93	2.05
17	8	608	CLA	MG-NB	-6.08	1.93	2.05
17	B	804	CLA	MG-ND	-6.08	1.93	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	812	CLA	MG-ND	-6.08	1.93	2.05
17	8	610	CLA	MG-ND	-6.07	1.93	2.05
17	A	818	CLA	MG-NB	-6.07	1.93	2.05
17	B	837	CLA	MG-ND	-6.07	1.93	2.05
17	5	304	CLA	MG-ND	-6.07	1.93	2.05
17	A	805	CLA	MG-NB	-6.06	1.93	2.05
17	A	837	CLA	MG-NB	-6.06	1.93	2.05
17	3	308	CLA	MG-ND	-6.06	1.93	2.05
20	Z	601	CHL	C4B-NB	6.04	1.45	1.37
17	8	614	CLA	MG-ND	-6.04	1.93	2.05
17	A	803	CLA	MG-ND	-6.04	1.93	2.05
17	3	301	CLA	MG-ND	-6.03	1.93	2.05
17	A	835	CLA	MG-NB	-6.03	1.93	2.05
17	8	601	CLA	MG-ND	-6.03	1.93	2.05
17	B	801	CLA	C4B-NB	6.03	1.45	1.37
17	7	605	CLA	MG-ND	-6.02	1.93	2.05
17	B	806	CLA	MG-NA	-6.02	1.92	2.06
20	1	601	CHL	C4B-NB	6.01	1.45	1.37
17	A	830	CLA	MG-NB	-6.01	1.93	2.05
17	A	809	CLA	MG-ND	-6.01	1.93	2.05
17	B	823	CLA	MG-ND	-6.01	1.93	2.05
17	F	301	CLA	MG-ND	-6.00	1.93	2.05
17	F	302	CLA	MG-ND	-6.00	1.93	2.05
17	A	837	CLA	MG-ND	-6.00	1.93	2.05
17	A	807	CLA	MG-ND	-6.00	1.93	2.05
17	1	604	CLA	MG-NB	-6.00	1.93	2.05
17	6	610	CLA	MG-ND	-5.99	1.93	2.05
17	3	301	CLA	MG-NB	-5.99	1.93	2.05
17	7	601	CLA	MG-ND	-5.99	1.93	2.05
17	3	309	CLA	MG-NB	-5.99	1.93	2.05
17	B	836	CLA	MG-NB	-5.99	1.93	2.05
17	8	601	CLA	MG-NB	-5.99	1.93	2.05
17	A	804	CLA	C4B-NB	5.99	1.45	1.37
17	3	306	CLA	MG-NB	-5.98	1.93	2.05
17	B	839	CLA	MG-NB	-5.98	1.93	2.05
17	7	610	CLA	MG-ND	-5.98	1.93	2.05
17	A	824	CLA	MG-ND	-5.98	1.93	2.05
17	3	305	CLA	MG-ND	-5.97	1.93	2.05
17	A	804	CLA	MG-ND	-5.97	1.93	2.05
17	A	826	CLA	MG-ND	-5.97	1.93	2.05
17	5	309	CLA	MG-NB	-5.97	1.94	2.05
17	3	303	CLA	MG-ND	-5.96	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	835	CLA	MG-ND	-5.96	1.94	2.05
17	5	312	CLA	MG-ND	-5.96	1.94	2.05
17	B	806	CLA	MG-NB	-5.96	1.94	2.05
17	4	601	CLA	MG-NB	-5.95	1.94	2.05
17	B	815	CLA	MG-NA	-5.95	1.92	2.06
17	5	310	CLA	MG-ND	-5.95	1.94	2.05
17	B	836	CLA	MG-ND	-5.94	1.94	2.05
17	8	608	CLA	MG-ND	-5.94	1.94	2.05
17	B	825	CLA	MG-ND	-5.94	1.94	2.05
17	B	826	CLA	MG-ND	-5.93	1.94	2.05
17	5	312	CLA	MG-NB	-5.93	1.94	2.05
17	A	806	CLA	MG-ND	-5.93	1.94	2.05
17	5	310	CLA	MG-NB	-5.93	1.94	2.05
17	A	829	CLA	MG-NB	-5.93	1.94	2.05
17	B	823	CLA	MG-NB	-5.92	1.94	2.05
17	8	613	CLA	MG-NB	-5.92	1.94	2.05
17	A	802	CLA	MG-ND	-5.91	1.94	2.05
20	3	307	CHL	C4B-NB	5.90	1.45	1.37
17	B	835	CLA	MG-ND	-5.90	1.94	2.05
17	B	812	CLA	MG-NA	-5.90	1.92	2.06
17	A	815	CLA	MG-NB	-5.90	1.94	2.05
17	A	817	CLA	MG-ND	-5.89	1.94	2.05
17	4	604	CLA	MG-NB	-5.89	1.94	2.05
17	B	835	CLA	MG-NB	-5.89	1.94	2.05
17	4	601	CLA	MG-ND	-5.88	1.94	2.05
17	A	833	CLA	MG-NB	-5.88	1.94	2.05
17	7	613	CLA	MG-NB	-5.88	1.94	2.05
17	4	603	CLA	MG-NA	-5.88	1.92	2.06
17	6	603	CLA	MG-NB	-5.88	1.94	2.05
17	7	605	CLA	MG-NB	-5.87	1.94	2.05
17	3	310	CLA	MG-ND	-5.87	1.94	2.05
20	6	606	CHL	C4B-NB	5.87	1.45	1.37
17	B	809	CLA	MG-NB	-5.87	1.94	2.05
17	5	315	CLA	MG-NB	-5.86	1.94	2.05
17	8	613	CLA	MG-ND	-5.86	1.94	2.05
17	J	101	CLA	MG-ND	-5.86	1.94	2.05
17	B	808	CLA	MG-NB	-5.86	1.94	2.05
17	A	808	CLA	MG-ND	-5.86	1.94	2.05
17	3	302	CLA	MG-NB	-5.86	1.94	2.05
17	B	820	CLA	MG-NB	-5.85	1.94	2.05
17	A	812	CLA	MG-NB	-5.85	1.94	2.05
17	A	808	CLA	MG-NB	-5.85	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	838	CLA	MG-ND	-5.85	1.94	2.05
17	B	833	CLA	MG-NB	-5.85	1.94	2.05
17	A	826	CLA	MG-NB	-5.84	1.94	2.05
17	J	101	CLA	MG-NB	-5.83	1.94	2.05
17	1	607	CLA	MG-ND	-5.83	1.94	2.05
17	8	612	CLA	MG-NB	-5.83	1.94	2.05
17	5	308	CLA	MG-NB	-5.83	1.94	2.05
17	B	817	CLA	MG-ND	-5.83	1.94	2.05
17	3	304	CLA	MG-ND	-5.83	1.94	2.05
17	B	827	CLA	MG-NB	-5.83	1.94	2.05
17	A	843	CLA	MG-ND	-5.82	1.94	2.05
17	7	613	CLA	MG-ND	-5.81	1.94	2.05
17	B	815	CLA	MG-ND	-5.81	1.94	2.05
17	5	314	CLA	C4B-NB	5.80	1.44	1.37
16	A	801	CL0	MG-NB	-5.80	1.94	2.05
17	6	602	CLA	MG-NB	-5.80	1.94	2.05
17	3	311	CLA	MG-NB	-5.80	1.94	2.05
17	A	819	CLA	MG-NB	-5.80	1.94	2.05
17	5	307	CLA	MG-ND	-5.79	1.94	2.05
17	B	822	CLA	MG-ND	-5.79	1.94	2.05
17	J	102	CLA	MG-NB	-5.79	1.94	2.05
17	7	602	CLA	MG-ND	-5.79	1.94	2.05
17	B	833	CLA	MG-ND	-5.79	1.94	2.05
17	5	307	CLA	MG-NB	-5.79	1.94	2.05
17	3	306	CLA	MG-ND	-5.79	1.94	2.05
17	B	816	CLA	MG-ND	-5.78	1.94	2.05
17	8	609	CLA	MG-NB	-5.78	1.94	2.05
17	A	814	CLA	MG-ND	-5.78	1.94	2.05
17	7	614	CLA	MG-ND	-5.78	1.94	2.05
17	7	612	CLA	MG-ND	-5.78	1.94	2.05
17	B	817	CLA	MG-NB	-5.77	1.94	2.05
17	A	805	CLA	MG-ND	-5.77	1.94	2.05
17	B	832	CLA	MG-ND	-5.76	1.94	2.05
17	5	303	CLA	MG-NB	-5.76	1.94	2.05
17	B	828	CLA	MG-ND	-5.76	1.94	2.05
17	6	608	CLA	MG-ND	-5.76	1.94	2.05
17	A	802	CLA	MG-NA	-5.76	1.92	2.06
17	B	815	CLA	MG-NB	-5.75	1.94	2.05
17	B	818	CLA	MG-NB	-5.75	1.94	2.05
17	B	828	CLA	MG-NB	-5.75	1.94	2.05
17	A	823	CLA	MG-ND	-5.74	1.94	2.05
17	7	607	CLA	MG-NB	-5.74	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	7	601	CLA	MG-NB	-5.74	1.94	2.05
17	6	601	CLA	MG-NB	-5.73	1.94	2.05
17	3	310	CLA	C3A-C2A	-5.73	1.49	1.54
17	B	838	CLA	MG-NB	-5.72	1.94	2.05
17	B	811	CLA	MG-NB	-5.72	1.94	2.05
17	3	302	CLA	MG-ND	-5.71	1.94	2.05
17	B	810	CLA	MG-NA	-5.71	1.92	2.06
17	4	603	CLA	MG-ND	-5.71	1.94	2.05
17	A	813	CLA	MG-NB	-5.70	1.94	2.05
17	7	607	CLA	MG-ND	-5.70	1.94	2.05
17	A	818	CLA	MG-ND	-5.70	1.94	2.05
17	1	602	CLA	MG-NB	-5.70	1.94	2.05
17	B	819	CLA	MG-NA	-5.69	1.92	2.06
17	B	818	CLA	MG-ND	-5.69	1.94	2.05
17	1	605	CLA	MG-ND	-5.69	1.94	2.05
17	3	304	CLA	MG-NB	-5.69	1.94	2.05
17	A	834	CLA	MG-NB	-5.69	1.94	2.05
17	5	311	CLA	MG-ND	-5.68	1.94	2.05
17	A	806	CLA	MG-NB	-5.68	1.94	2.05
17	B	824	CLA	C3A-C2A	-5.68	1.49	1.54
17	7	603	CLA	MG-NA	-5.67	1.92	2.06
17	1	605	CLA	MG-NB	-5.67	1.94	2.05
17	8	603	CLA	MG-ND	-5.67	1.94	2.05
17	6	602	CLA	MG-ND	-5.66	1.94	2.05
17	1	606	CLA	MG-NB	-5.66	1.94	2.05
17	8	603	CLA	MG-NB	-5.65	1.94	2.05
17	8	604	CLA	MG-ND	-5.65	1.94	2.05
17	5	304	CLA	MG-NB	-5.65	1.94	2.05
17	B	822	CLA	MG-NB	-5.65	1.94	2.05
17	A	830	CLA	MG-ND	-5.65	1.94	2.05
17	B	839	CLA	MG-ND	-5.65	1.94	2.05
17	5	315	CLA	MG-ND	-5.65	1.94	2.05
17	J	102	CLA	MG-ND	-5.65	1.94	2.05
17	4	604	CLA	MG-ND	-5.64	1.94	2.05
17	5	303	CLA	MG-ND	-5.64	1.94	2.05
17	8	607	CLA	MG-NB	-5.64	1.94	2.05
17	A	823	CLA	MG-NB	-5.63	1.94	2.05
17	B	811	CLA	MG-ND	-5.63	1.94	2.05
17	B	834	CLA	MG-ND	-5.63	1.94	2.05
17	A	810	CLA	MG-ND	-5.63	1.94	2.05
17	A	836	CLA	MG-ND	-5.63	1.94	2.05
17	A	843	CLA	MG-NB	-5.62	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	827	CLA	MG-ND	-5.62	1.94	2.05
17	A	825	CLA	MG-NB	-5.61	1.94	2.05
17	8	611	CLA	MG-NB	-5.61	1.94	2.05
17	5	306	CLA	MG-NB	-5.61	1.94	2.05
16	A	801	CL0	MG-ND	-5.61	1.94	2.05
17	A	813	CLA	MG-ND	-5.61	1.94	2.05
17	A	828	CLA	MG-NB	-5.59	1.94	2.05
17	8	607	CLA	MG-ND	-5.59	1.94	2.05
17	B	819	CLA	MG-ND	-5.59	1.94	2.05
17	B	808	CLA	MG-ND	-5.59	1.94	2.05
17	A	836	CLA	MG-NB	-5.59	1.94	2.05
17	8	604	CLA	MG-NB	-5.59	1.94	2.05
17	B	832	CLA	MG-NB	-5.57	1.94	2.05
17	3	312	CLA	MG-ND	-5.57	1.94	2.05
17	B	827	CLA	MG-ND	-5.57	1.94	2.05
17	B	820	CLA	MG-ND	-5.57	1.94	2.05
17	1	603	CLA	MG-NB	-5.56	1.94	2.05
17	A	829	CLA	MG-ND	-5.55	1.94	2.05
17	3	313	CLA	MG-NA	-5.55	1.93	2.06
17	1	603	CLA	MG-ND	-5.55	1.94	2.05
17	6	601	CLA	MG-ND	-5.54	1.94	2.05
17	6	609	CLA	MG-ND	-5.54	1.94	2.05
17	A	834	CLA	MG-ND	-5.54	1.94	2.05
17	A	811	CLA	MG-ND	-5.54	1.94	2.05
20	5	305	CHL	C4B-NB	5.54	1.44	1.37
17	A	828	CLA	MG-ND	-5.54	1.94	2.05
17	3	311	CLA	MG-ND	-5.53	1.94	2.05
17	4	602	CLA	MG-NB	-5.53	1.94	2.05
17	A	819	CLA	MG-ND	-5.53	1.94	2.05
17	A	832	CLA	MG-ND	-5.53	1.94	2.05
17	7	602	CLA	MG-NB	-5.53	1.94	2.05
17	8	609	CLA	MG-ND	-5.53	1.94	2.05
17	5	306	CLA	MG-ND	-5.53	1.94	2.05
17	5	311	CLA	MG-NB	-5.52	1.94	2.05
17	8	612	CLA	MG-ND	-5.51	1.94	2.05
17	5	301	CLA	MG-ND	-5.51	1.94	2.05
17	B	816	CLA	MG-NB	-5.51	1.94	2.05
17	A	811	CLA	MG-NB	-5.51	1.94	2.05
17	A	804	CLA	MG-NA	-5.50	1.93	2.06
17	6	610	CLA	MG-NB	-5.50	1.94	2.05
17	8	602	CLA	MG-NB	-5.50	1.94	2.05
17	8	611	CLA	MG-ND	-5.50	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	5	308	CLA	MG-ND	-5.50	1.94	2.05
17	A	827	CLA	MG-NB	-5.50	1.94	2.05
17	A	820	CLA	MG-ND	-5.49	1.94	2.05
17	8	605	CLA	MG-ND	-5.49	1.94	2.05
17	1	604	CLA	MG-ND	-5.48	1.94	2.05
17	7	603	CLA	MG-ND	-5.48	1.94	2.05
17	A	833	CLA	MG-ND	-5.48	1.94	2.05
17	8	602	CLA	MG-ND	-5.47	1.94	2.05
17	8	605	CLA	MG-NB	-5.47	1.94	2.05
17	5	301	CLA	MG-NB	-5.47	1.94	2.05
17	B	806	CLA	MG-ND	-5.46	1.95	2.05
17	A	832	CLA	MG-NB	-5.45	1.95	2.05
17	A	831	CLA	MG-ND	-5.44	1.95	2.05
17	B	813	CLA	MG-NB	-5.44	1.95	2.05
17	B	830	CLA	MG-ND	-5.44	1.95	2.05
17	1	609	CLA	MG-NB	-5.43	1.95	2.05
17	A	821	CLA	MG-NA	-5.43	1.93	2.06
17	A	816	CLA	MG-NB	-5.43	1.95	2.05
17	1	606	CLA	MG-ND	-5.42	1.95	2.05
17	B	802	CLA	MG-NA	-5.41	1.93	2.06
17	6	603	CLA	MG-ND	-5.41	1.95	2.05
17	7	610	CLA	MG-NA	-5.41	1.93	2.06
17	A	817	CLA	MG-NA	-5.40	1.93	2.06
17	1	610	CLA	MG-ND	-5.40	1.95	2.05
17	A	810	CLA	MG-NB	-5.40	1.95	2.05
17	1	609	CLA	MG-ND	-5.39	1.95	2.05
17	6	604	CLA	MG-ND	-5.38	1.95	2.05
17	A	816	CLA	MG-ND	-5.38	1.95	2.05
17	A	825	CLA	MG-ND	-5.37	1.95	2.05
17	3	309	CLA	MG-ND	-5.36	1.95	2.05
17	3	301	CLA	MG-NA	-5.36	1.93	2.06
17	7	609	CLA	MG-NB	-5.35	1.95	2.05
17	3	310	CLA	MG-NA	-5.35	1.93	2.06
17	1	610	CLA	MG-NB	-5.35	1.95	2.05
17	B	831	CLA	MG-NA	-5.34	1.93	2.06
17	B	826	CLA	MG-NA	-5.34	1.93	2.06
17	7	614	CLA	MG-NA	-5.32	1.93	2.06
17	3	306	CLA	MG-NA	-5.32	1.93	2.06
17	3	308	CLA	MG-NA	-5.32	1.93	2.06
17	B	804	CLA	MG-NA	-5.30	1.93	2.06
17	A	822	CLA	MG-NA	-5.29	1.93	2.06
17	7	612	CLA	MG-NB	-5.29	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	805	CLA	MG-NA	-5.29	1.93	2.06
17	B	813	CLA	MG-ND	-5.28	1.95	2.05
17	5	309	CLA	MG-ND	-5.28	1.95	2.05
17	6	604	CLA	MG-NB	-5.26	1.95	2.05
17	6	609	CLA	MG-NB	-5.24	1.95	2.05
17	7	609	CLA	MG-ND	-5.24	1.95	2.05
17	B	825	CLA	MG-NB	-5.22	1.95	2.05
17	B	807	CLA	MG-NA	-5.22	1.93	2.06
17	5	309	CLA	MG-NA	-5.22	1.93	2.06
17	A	831	CLA	MG-NB	-5.20	1.95	2.05
17	1	606	CLA	MG-NA	-5.19	1.93	2.06
17	B	837	CLA	MG-NA	-5.19	1.93	2.06
17	A	809	CLA	MG-NA	-5.18	1.94	2.06
17	7	608	CLA	MG-ND	-5.15	1.95	2.05
17	A	820	CLA	MG-NB	-5.15	1.95	2.05
17	B	806	CLA	MG-NC	-5.15	1.94	2.06
17	1	607	CLA	MG-NC	-5.13	1.94	2.06
17	7	608	CLA	MG-NB	-5.13	1.95	2.05
17	B	829	CLA	MG-NA	-5.13	1.94	2.06
17	B	814	CLA	MG-NB	-5.11	1.95	2.05
17	4	602	CLA	MG-ND	-5.11	1.95	2.05
17	5	306	CLA	MG-NA	-5.10	1.94	2.06
17	7	611	CLA	MG-NB	-5.10	1.95	2.05
17	B	824	CLA	MG-NA	-5.09	1.94	2.06
17	A	802	CLA	MG-NC	-5.07	1.94	2.06
17	7	611	CLA	MG-ND	-5.07	1.95	2.05
17	1	608	CLA	MG-ND	-5.06	1.95	2.05
17	A	838	CLA	MG-NA	-5.05	1.94	2.06
17	3	303	CLA	MG-NA	-5.04	1.94	2.06
17	4	603	CLA	MG-NC	-5.03	1.94	2.06
17	B	821	CLA	MG-NB	-5.03	1.95	2.05
17	A	815	CLA	MG-NA	-5.03	1.94	2.06
17	5	314	CLA	MG-NA	-5.02	1.94	2.06
17	F	301	CLA	MG-NA	-5.01	1.94	2.06
17	B	827	CLA	MG-NA	-5.00	1.94	2.06
17	8	608	CLA	MG-NA	-5.00	1.94	2.06
17	A	807	CLA	MG-NA	-4.97	1.94	2.06
17	A	841	CLA	MG-NA	-4.94	1.94	2.06
17	7	608	CLA	MG-NA	-4.93	1.94	2.06
20	Z	601	CHL	MG-NA	-4.92	1.94	2.06
17	7	603	CLA	MG-NC	-4.92	1.94	2.06
20	6	607	CHL	MG-NC	-4.92	1.94	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	831	CLA	MG-NC	-4.92	1.94	2.06
17	8	610	CLA	MG-NA	-4.91	1.94	2.06
17	B	814	CLA	MG-ND	-4.90	1.96	2.05
17	B	832	CLA	MG-NA	-4.90	1.94	2.06
17	B	804	CLA	MG-NC	-4.89	1.94	2.06
17	1	602	CLA	MG-ND	-4.89	1.96	2.05
17	8	614	CLA	MG-NA	-4.89	1.94	2.06
20	1	601	CHL	MG-NA	-4.89	1.94	2.06
17	A	839	CLA	MG-NA	-4.88	1.94	2.06
17	3	309	CLA	MG-NA	-4.88	1.94	2.06
17	B	819	CLA	MG-NB	-4.88	1.96	2.05
17	B	821	CLA	MG-ND	-4.87	1.96	2.05
17	A	805	CLA	MG-NA	-4.86	1.94	2.06
17	A	816	CLA	MG-NA	-4.86	1.94	2.06
17	A	821	CLA	MG-NC	-4.83	1.94	2.06
17	A	804	CLA	MG-NC	-4.82	1.94	2.06
17	B	825	CLA	MG-NA	-4.82	1.94	2.06
17	4	605	CLA	MG-NA	-4.82	1.94	2.06
17	A	825	CLA	MG-NA	-4.81	1.94	2.06
17	B	820	CLA	MG-NA	-4.80	1.94	2.06
17	B	833	CLA	MG-NA	-4.80	1.94	2.06
17	3	302	CLA	MG-NA	-4.80	1.94	2.06
17	7	609	CLA	MG-NA	-4.78	1.94	2.06
17	5	315	CLA	MG-NA	-4.78	1.94	2.06
17	A	834	CLA	MG-NA	-4.77	1.94	2.06
17	B	818	CLA	MG-NA	-4.77	1.94	2.06
17	B	823	CLA	MG-NA	-4.76	1.95	2.06
17	8	603	CLA	MG-NA	-4.76	1.95	2.06
17	8	613	CLA	MG-NA	-4.76	1.95	2.06
17	5	307	CLA	MG-NA	-4.76	1.95	2.06
17	B	835	CLA	MG-NA	-4.76	1.95	2.06
17	4	601	CLA	MG-NA	-4.76	1.95	2.06
17	B	802	CLA	MG-NC	-4.75	1.95	2.06
17	1	608	CLA	MG-NB	-4.75	1.96	2.05
17	B	828	CLA	MG-NA	-4.74	1.95	2.06
17	7	611	CLA	MG-NA	-4.74	1.95	2.06
20	6	607	CHL	MG-NA	-4.73	1.95	2.06
17	6	603	CLA	MG-NA	-4.73	1.95	2.06
17	B	801	CLA	MG-NA	-4.72	1.95	2.06
17	B	837	CLA	MG-NC	-4.72	1.95	2.06
17	A	813	CLA	MG-NA	-4.72	1.95	2.06
17	8	603	CLA	MG-NC	-4.71	1.95	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	5	308	CLA	MG-NA	-4.71	1.95	2.06
20	5	305	CHL	MG-NA	-4.71	1.95	2.06
17	B	810	CLA	MG-NC	-4.71	1.95	2.06
17	7	613	CLA	MG-NA	-4.71	1.95	2.06
17	B	826	CLA	MG-NC	-4.70	1.95	2.06
17	J	102	CLA	MG-NA	-4.70	1.95	2.06
17	A	830	CLA	MG-NA	-4.69	1.95	2.06
17	A	811	CLA	MG-NA	-4.69	1.95	2.06
17	B	830	CLA	MG-NA	-4.69	1.95	2.06
17	B	812	CLA	MG-NC	-4.69	1.95	2.06
17	8	609	CLA	MG-NA	-4.69	1.95	2.06
17	8	611	CLA	MG-NA	-4.68	1.95	2.06
16	A	801	CL0	MG-NA	-4.68	1.95	2.06
17	A	814	CLA	MG-NA	-4.68	1.95	2.06
17	B	805	CLA	MG-NC	-4.68	1.95	2.06
17	1	604	CLA	MG-NA	-4.68	1.95	2.06
17	7	614	CLA	MG-NC	-4.67	1.95	2.06
17	3	301	CLA	MG-NC	-4.67	1.95	2.06
17	A	824	CLA	MG-NA	-4.66	1.95	2.06
17	A	806	CLA	MG-NA	-4.66	1.95	2.06
17	6	610	CLA	MG-NA	-4.66	1.95	2.06
17	B	815	CLA	MG-NC	-4.66	1.95	2.06
17	3	312	CLA	MG-NA	-4.65	1.95	2.06
17	7	610	CLA	MG-NC	-4.65	1.95	2.06
17	A	815	CLA	MG-NC	-4.65	1.95	2.06
17	B	819	CLA	MG-NC	-4.64	1.95	2.06
17	5	310	CLA	MG-NA	-4.64	1.95	2.06
17	A	823	CLA	MG-NA	-4.64	1.95	2.06
17	A	836	CLA	MG-NA	-4.63	1.95	2.06
17	8	612	CLA	MG-NA	-4.63	1.95	2.06
20	1	601	CHL	MG-NC	-4.63	1.95	2.06
17	8	602	CLA	MG-NA	-4.63	1.95	2.06
17	A	829	CLA	MG-NA	-4.63	1.95	2.06
17	A	820	CLA	MG-NA	-4.62	1.95	2.06
20	5	305	CHL	MG-NC	-4.62	1.95	2.06
17	J	101	CLA	MG-NC	-4.61	1.95	2.06
17	A	818	CLA	MG-NA	-4.61	1.95	2.06
17	A	842	CLA	MG-NA	-4.61	1.95	2.06
17	A	832	CLA	MG-NA	-4.61	1.95	2.06
17	3	304	CLA	MG-NA	-4.60	1.95	2.06
17	3	308	CLA	MG-NC	-4.60	1.95	2.06
20	Z	601	CHL	MG-NC	-4.60	1.95	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	826	CLA	MG-NA	-4.59	1.95	2.06
17	A	814	CLA	MG-NC	-4.59	1.95	2.06
17	A	819	CLA	MG-NA	-4.59	1.95	2.06
17	1	609	CLA	MG-NA	-4.59	1.95	2.06
17	B	809	CLA	MG-NA	-4.58	1.95	2.06
20	6	606	CHL	MG-NA	-4.57	1.95	2.06
17	6	601	CLA	MG-NA	-4.57	1.95	2.06
17	A	812	CLA	MG-NA	-4.57	1.95	2.06
17	A	843	CLA	MG-NA	-4.57	1.95	2.06
17	B	834	CLA	MG-NA	-4.56	1.95	2.06
17	3	306	CLA	MG-NC	-4.56	1.95	2.06
17	8	608	CLA	MG-NC	-4.56	1.95	2.06
17	J	101	CLA	MG-NA	-4.55	1.95	2.06
17	3	305	CLA	MG-NA	-4.55	1.95	2.06
17	7	608	CLA	MG-NC	-4.55	1.95	2.06
17	A	827	CLA	MG-NA	-4.55	1.95	2.06
17	B	828	CLA	MG-NC	-4.54	1.95	2.06
17	A	833	CLA	MG-NA	-4.54	1.95	2.06
17	5	303	CLA	MG-NA	-4.54	1.95	2.06
17	A	839	CLA	MG-NC	-4.54	1.95	2.06
17	5	311	CLA	MG-NA	-4.53	1.95	2.06
17	4	602	CLA	MG-NA	-4.53	1.95	2.06
17	1	602	CLA	MG-NA	-4.53	1.95	2.06
17	1	603	CLA	MG-NA	-4.52	1.95	2.06
17	A	841	CLA	MG-NC	-4.52	1.95	2.06
17	B	839	CLA	MG-NA	-4.52	1.95	2.06
17	B	813	CLA	MG-NA	-4.52	1.95	2.06
17	6	602	CLA	MG-NA	-4.51	1.95	2.06
17	7	607	CLA	MG-NA	-4.51	1.95	2.06
17	B	811	CLA	MG-NA	-4.51	1.95	2.06
17	5	301	CLA	MG-NA	-4.50	1.95	2.06
17	3	313	CLA	MG-NC	-4.50	1.95	2.06
17	7	602	CLA	MG-NA	-4.49	1.95	2.06
20	6	606	CHL	MG-NC	-4.49	1.95	2.06
17	4	604	CLA	MG-NA	-4.49	1.95	2.06
17	5	306	CLA	MG-NC	-4.49	1.95	2.06
17	A	810	CLA	MG-NA	-4.49	1.95	2.06
17	B	829	CLA	MG-NC	-4.48	1.95	2.06
17	A	822	CLA	MG-NC	-4.47	1.95	2.06
17	A	808	CLA	MG-NA	-4.47	1.95	2.06
17	F	302	CLA	MG-NA	-4.45	1.95	2.06
17	A	835	CLA	MG-NA	-4.44	1.95	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	834	CLA	MG-NC	-4.44	1.95	2.06
17	B	816	CLA	MG-NA	-4.44	1.95	2.06
20	7	606	CHL	MG-NC	-4.43	1.95	2.06
17	1	610	CLA	MG-NA	-4.43	1.95	2.06
17	3	303	CLA	MG-NC	-4.43	1.95	2.06
17	A	820	CLA	MG-NC	-4.42	1.95	2.06
17	8	607	CLA	MG-NA	-4.42	1.95	2.06
17	A	823	CLA	MG-NC	-4.41	1.95	2.06
17	5	312	CLA	MG-NA	-4.41	1.95	2.06
20	3	307	CHL	MG-NA	-4.41	1.95	2.06
17	A	817	CLA	MG-NC	-4.40	1.95	2.06
17	6	604	CLA	MG-NA	-4.40	1.95	2.06
17	6	608	CLA	MG-NA	-4.40	1.95	2.06
17	8	601	CLA	MG-NA	-4.39	1.95	2.06
17	B	817	CLA	MG-NA	-4.39	1.95	2.06
17	B	823	CLA	MG-NC	-4.39	1.95	2.06
20	8	606	CHL	MG-NA	-4.39	1.95	2.06
17	A	837	CLA	MG-NA	-4.39	1.95	2.06
17	A	825	CLA	MG-NC	-4.39	1.95	2.06
17	A	828	CLA	MG-NA	-4.38	1.95	2.06
20	3	307	CHL	MG-NC	-4.38	1.95	2.06
17	A	831	CLA	MG-NA	-4.38	1.95	2.06
17	B	822	CLA	MG-NA	-4.38	1.95	2.06
17	4	601	CLA	MG-NC	-4.38	1.95	2.06
17	3	312	CLA	MG-NC	-4.38	1.95	2.06
17	5	309	CLA	MG-NC	-4.38	1.95	2.06
17	A	803	CLA	MG-NA	-4.38	1.95	2.06
17	1	609	CLA	MG-NC	-4.37	1.95	2.06
17	A	805	CLA	MG-NC	-4.37	1.95	2.06
17	7	612	CLA	MG-NA	-4.36	1.95	2.06
17	B	836	CLA	MG-NA	-4.36	1.95	2.06
17	B	808	CLA	MG-NA	-4.36	1.95	2.06
17	A	818	CLA	MG-NC	-4.36	1.95	2.06
17	A	810	CLA	MG-NC	-4.35	1.95	2.06
17	B	814	CLA	MG-NA	-4.35	1.95	2.06
17	6	609	CLA	MG-NA	-4.35	1.95	2.06
17	3	311	CLA	MG-NA	-4.34	1.95	2.06
17	5	304	CLA	MG-NA	-4.34	1.96	2.06
17	5	302	CLA	MG-NA	-4.34	1.96	2.06
17	7	613	CLA	MG-NC	-4.34	1.96	2.06
17	J	102	CLA	MG-NC	-4.34	1.96	2.06
16	A	801	CL0	MG-NC	-4.33	1.96	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	5	314	CLA	MG-NC	-4.33	1.96	2.06
17	A	838	CLA	MG-NC	-4.33	1.96	2.06
17	1	604	CLA	MG-NC	-4.32	1.96	2.06
20	5	313	CHL	MG-NC	-4.32	1.96	2.06
17	7	605	CLA	MG-NA	-4.32	1.96	2.06
17	8	614	CLA	MG-NC	-4.31	1.96	2.06
17	6	603	CLA	MG-NC	-4.31	1.96	2.06
20	5	313	CHL	MG-NA	-4.31	1.96	2.06
17	3	304	CLA	MG-NC	-4.30	1.96	2.06
17	8	604	CLA	MG-NA	-4.30	1.96	2.06
17	B	825	CLA	MG-NC	-4.30	1.96	2.06
17	A	808	CLA	MG-NC	-4.29	1.96	2.06
17	B	834	CLA	MG-NC	-4.29	1.96	2.06
17	3	302	CLA	MG-NC	-4.28	1.96	2.06
20	7	606	CHL	MG-NA	-4.28	1.96	2.06
17	8	611	CLA	MG-NC	-4.27	1.96	2.06
17	A	809	CLA	MG-NC	-4.27	1.96	2.06
17	B	816	CLA	MG-NC	-4.27	1.96	2.06
17	3	310	CLA	MG-NC	-4.26	1.96	2.06
17	7	601	CLA	MG-NA	-4.26	1.96	2.06
17	A	830	CLA	MG-NC	-4.26	1.96	2.06
17	A	813	CLA	MG-NC	-4.24	1.96	2.06
17	A	811	CLA	MG-NC	-4.24	1.96	2.06
17	7	611	CLA	MG-NC	-4.24	1.96	2.06
17	1	608	CLA	MG-NA	-4.24	1.96	2.06
17	A	807	CLA	MG-NC	-4.23	1.96	2.06
17	4	602	CLA	MG-NC	-4.23	1.96	2.06
17	B	807	CLA	MG-NC	-4.23	1.96	2.06
17	3	311	CLA	MG-NC	-4.23	1.96	2.06
20	8	606	CHL	MG-NC	-4.22	1.96	2.06
17	F	301	CLA	MG-NC	-4.22	1.96	2.06
17	7	607	CLA	MG-NC	-4.21	1.96	2.06
17	8	605	CLA	MG-NA	-4.21	1.96	2.06
17	A	816	CLA	MG-NC	-4.21	1.96	2.06
17	B	830	CLA	MG-NC	-4.20	1.96	2.06
17	B	813	CLA	MG-NC	-4.20	1.96	2.06
17	5	315	CLA	MG-NC	-4.19	1.96	2.06
17	5	302	CLA	MG-NC	-4.19	1.96	2.06
17	A	829	CLA	MG-NC	-4.19	1.96	2.06
17	5	310	CLA	MG-NC	-4.18	1.96	2.06
17	A	837	CLA	MG-NC	-4.18	1.96	2.06
17	8	607	CLA	MG-NC	-4.17	1.96	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	8	610	CLA	MG-NC	-4.16	1.96	2.06
17	B	814	CLA	MG-NC	-4.16	1.96	2.06
17	4	605	CLA	MG-NC	-4.16	1.96	2.06
17	1	606	CLA	MG-NC	-4.15	1.96	2.06
17	A	806	CLA	MG-NC	-4.15	1.96	2.06
17	A	832	CLA	MG-NC	-4.15	1.96	2.06
17	B	820	CLA	MG-NC	-4.15	1.96	2.06
17	A	833	CLA	MG-NC	-4.14	1.96	2.06
17	B	832	CLA	MG-NC	-4.14	1.96	2.06
17	5	301	CLA	MG-NC	-4.14	1.96	2.06
17	7	602	CLA	MG-NC	-4.13	1.96	2.06
17	A	836	CLA	MG-NC	-4.12	1.96	2.06
17	B	821	CLA	MG-NA	-4.12	1.96	2.06
17	B	833	CLA	MG-NC	-4.11	1.96	2.06
20	6	605	CHL	MG-NC	-4.11	1.96	2.06
17	1	602	CLA	MG-NC	-4.11	1.96	2.06
17	A	842	CLA	MG-NC	-4.11	1.96	2.06
17	8	601	CLA	MG-NC	-4.10	1.96	2.06
17	8	602	CLA	MG-NC	-4.10	1.96	2.06
20	6	605	CHL	MG-NA	-4.09	1.96	2.06
17	3	309	CLA	MG-NC	-4.09	1.96	2.06
17	6	608	CLA	MG-NC	-4.07	1.96	2.06
17	B	817	CLA	MG-NC	-4.07	1.96	2.06
17	8	613	CLA	MG-NC	-4.06	1.96	2.06
17	B	824	CLA	MG-NC	-4.06	1.96	2.06
17	1	605	CLA	MG-NA	-4.06	1.96	2.06
17	6	610	CLA	MG-NC	-4.06	1.96	2.06
17	6	609	CLA	MG-NC	-4.06	1.96	2.06
17	6	602	CLA	MG-NC	-4.04	1.96	2.06
17	B	835	CLA	MG-NC	-4.04	1.96	2.06
17	5	307	CLA	MG-NC	-4.04	1.96	2.06
17	B	838	CLA	MG-NA	-4.04	1.96	2.06
17	5	311	CLA	MG-NC	-4.03	1.96	2.06
17	A	826	CLA	MG-NC	-4.03	1.96	2.06
17	B	839	CLA	MG-NC	-4.03	1.96	2.06
17	A	819	CLA	MG-NC	-4.01	1.96	2.06
17	A	827	CLA	MG-NC	-4.01	1.96	2.06
17	8	612	CLA	MG-NC	-4.00	1.96	2.06
17	6	601	CLA	MG-NC	-4.00	1.96	2.06
17	A	843	CLA	MG-NC	-3.99	1.96	2.06
17	1	610	CLA	MG-NC	-3.99	1.96	2.06
17	B	827	CLA	MG-NC	-3.96	1.96	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	7	609	CLA	MG-NC	-3.96	1.96	2.06
17	8	604	CLA	MG-NC	-3.96	1.96	2.06
17	B	801	CLA	MG-NC	-3.96	1.96	2.06
17	7	604	CLA	MG-NA	-3.95	1.96	2.06
17	5	308	CLA	MG-NC	-3.95	1.96	2.06
17	B	822	CLA	MG-NC	-3.94	1.96	2.06
17	A	831	CLA	MG-NC	-3.94	1.96	2.06
17	A	828	CLA	MG-NC	-3.93	1.96	2.06
17	8	609	CLA	MG-NC	-3.92	1.97	2.06
17	A	803	CLA	MG-NC	-3.90	1.97	2.06
17	5	303	CLA	MG-NC	-3.90	1.97	2.06
17	5	304	CLA	MG-NC	-3.89	1.97	2.06
17	7	612	CLA	MG-NC	-3.89	1.97	2.06
17	B	818	CLA	MG-NC	-3.88	1.97	2.06
17	B	808	CLA	MG-NC	-3.88	1.97	2.06
17	B	811	CLA	MG-NC	-3.88	1.97	2.06
17	1	610	CLA	C1D-ND	3.87	1.42	1.37
17	7	601	CLA	MG-NC	-3.85	1.97	2.06
17	B	836	CLA	MG-NC	-3.85	1.97	2.06
17	A	835	CLA	MG-NC	-3.84	1.97	2.06
17	A	812	CLA	MG-NC	-3.84	1.97	2.06
17	1	605	CLA	MG-NC	-3.83	1.97	2.06
17	7	605	CLA	MG-NC	-3.83	1.97	2.06
17	A	824	CLA	MG-NC	-3.83	1.97	2.06
17	F	302	CLA	MG-NC	-3.82	1.97	2.06
17	B	809	CLA	MG-NC	-3.81	1.97	2.06
17	1	608	CLA	MG-NC	-3.80	1.97	2.06
17	1	603	CLA	MG-NC	-3.78	1.97	2.06
17	B	838	CLA	MG-NC	-3.78	1.97	2.06
17	1	608	CLA	C1D-ND	3.77	1.42	1.37
17	3	305	CLA	MG-NC	-3.75	1.97	2.06
17	5	312	CLA	MG-NC	-3.71	1.97	2.06
17	B	821	CLA	C1D-ND	3.71	1.42	1.37
17	6	604	CLA	MG-NC	-3.71	1.97	2.06
17	7	604	CLA	MG-NC	-3.68	1.97	2.06
17	4	604	CLA	MG-NC	-3.61	1.97	2.06
17	6	604	CLA	C1D-ND	3.61	1.42	1.37
17	1	604	CLA	C1D-ND	3.58	1.42	1.37
17	8	605	CLA	MG-NC	-3.58	1.97	2.06
17	B	821	CLA	MG-NC	-3.51	1.97	2.06
17	A	804	CLA	C3A-C2A	-3.36	1.45	1.54
17	5	306	CLA	C1D-ND	3.35	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	814	CLA	C1D-ND	3.30	1.41	1.37
17	6	609	CLA	C1D-ND	3.26	1.41	1.37
17	3	311	CLA	C1D-ND	3.26	1.41	1.37
17	B	828	CLA	C1D-ND	3.26	1.41	1.37
17	A	833	CLA	C1D-ND	3.25	1.41	1.37
17	A	831	CLA	C1D-ND	3.24	1.41	1.37
17	B	815	CLA	C3A-C2A	-3.22	1.45	1.54
20	6	606	CHL	CHB-C4A	-3.22	1.30	1.37
17	1	605	CLA	C1D-ND	3.20	1.41	1.37
17	8	605	CLA	C1D-ND	3.19	1.41	1.37
17	7	614	CLA	C1D-ND	3.18	1.41	1.37
17	8	604	CLA	C1D-ND	3.18	1.41	1.37
16	A	801	CL0	C1D-ND	3.17	1.41	1.37
17	4	602	CLA	C1D-ND	3.16	1.41	1.37
17	8	609	CLA	C1D-ND	3.14	1.41	1.37
17	7	611	CLA	C1D-ND	3.13	1.41	1.37
17	1	609	CLA	C1D-ND	3.12	1.41	1.37
17	5	301	CLA	C1D-ND	3.12	1.41	1.37
17	4	604	CLA	C1D-ND	3.12	1.41	1.37
17	A	820	CLA	C1D-ND	3.12	1.41	1.37
17	5	310	CLA	C1D-ND	3.11	1.41	1.37
17	8	612	CLA	C1D-ND	3.09	1.41	1.37
17	B	808	CLA	C1D-ND	3.09	1.41	1.37
17	4	603	CLA	C1B-NB	3.08	1.41	1.37
17	A	818	CLA	C1D-ND	3.07	1.41	1.37
17	B	834	CLA	C1D-ND	3.05	1.41	1.37
17	B	836	CLA	C1D-ND	3.04	1.41	1.37
17	A	830	CLA	C1D-ND	3.04	1.41	1.37
17	8	607	CLA	C1D-ND	3.04	1.41	1.37
17	6	601	CLA	C1D-ND	3.03	1.41	1.37
17	A	814	CLA	C1D-ND	3.03	1.41	1.37
17	1	603	CLA	C1D-ND	3.01	1.41	1.37
17	B	807	CLA	C1D-ND	3.01	1.41	1.37
17	A	828	CLA	C1D-ND	2.99	1.41	1.37
17	3	312	CLA	C1D-ND	2.99	1.41	1.37
17	7	609	CLA	C1D-ND	2.99	1.41	1.37
17	B	832	CLA	C1D-ND	2.98	1.41	1.37
17	5	315	CLA	C1D-ND	2.98	1.41	1.37
17	7	613	CLA	C1D-ND	2.98	1.41	1.37
17	B	839	CLA	C1D-ND	2.97	1.41	1.37
17	8	613	CLA	C1D-ND	2.97	1.41	1.37
17	7	612	CLA	C1D-ND	2.97	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	5	309	CLA	C1D-ND	2.95	1.41	1.37
17	A	805	CLA	C3A-C2A	-2.94	1.46	1.54
17	A	810	CLA	C1D-ND	2.93	1.41	1.37
17	B	833	CLA	C1D-ND	2.93	1.41	1.37
20	3	307	CHL	CHB-C4A	-2.92	1.30	1.37
17	8	611	CLA	C3A-C2A	-2.90	1.46	1.54
17	1	602	CLA	C1D-ND	2.89	1.41	1.37
17	5	302	CLA	C1D-ND	2.89	1.41	1.37
17	A	824	CLA	C3A-C2A	-2.88	1.46	1.54
17	B	819	CLA	C1D-C2D	-2.88	1.39	1.45
17	6	610	CLA	C1D-C2D	-2.87	1.39	1.45
17	7	604	CLA	C1D-ND	2.87	1.41	1.37
17	J	102	CLA	C1D-ND	2.84	1.41	1.37
17	A	805	CLA	C1D-ND	2.83	1.41	1.37
17	8	603	CLA	C1D-ND	2.83	1.41	1.37
17	A	835	CLA	C1D-ND	2.82	1.41	1.37
17	A	823	CLA	C1D-ND	2.82	1.41	1.37
17	5	308	CLA	C1D-ND	2.82	1.41	1.37
17	3	309	CLA	C1D-ND	2.82	1.41	1.37
17	B	813	CLA	C1D-ND	2.81	1.41	1.37
17	A	824	CLA	C1D-ND	2.81	1.41	1.37
17	1	607	CLA	C1B-NB	2.80	1.41	1.37
17	A	837	CLA	C3A-C2A	-2.80	1.46	1.54
17	8	611	CLA	C1D-ND	2.80	1.41	1.37
17	A	808	CLA	C1D-ND	2.80	1.41	1.37
17	B	838	CLA	C1D-C2D	-2.79	1.39	1.45
17	B	825	CLA	C1D-ND	2.79	1.41	1.37
17	A	836	CLA	C1D-ND	2.78	1.41	1.37
17	6	603	CLA	C1D-ND	2.77	1.41	1.37
17	B	816	CLA	C1D-ND	2.77	1.41	1.37
17	5	304	CLA	C1D-ND	2.77	1.41	1.37
17	6	610	CLA	C3A-C2A	-2.76	1.46	1.54
17	A	837	CLA	C1D-ND	2.75	1.41	1.37
17	B	811	CLA	C1D-ND	2.75	1.41	1.37
17	A	813	CLA	C1D-ND	2.75	1.41	1.37
17	B	817	CLA	C1D-ND	2.75	1.41	1.37
17	A	820	CLA	C1B-NB	2.75	1.41	1.37
17	8	607	CLA	C3A-C2A	-2.75	1.46	1.54
17	5	307	CLA	C1D-ND	2.74	1.41	1.37
17	A	808	CLA	C1D-C2D	-2.74	1.39	1.45
17	4	605	CLA	C1D-C2D	-2.74	1.39	1.45
17	A	841	CLA	C1D-ND	2.73	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	6	605	CHL	CHB-C4A	-2.73	1.31	1.37
20	7	606	CHL	CHB-C4A	-2.73	1.31	1.37
17	5	303	CLA	C1D-ND	2.73	1.41	1.37
17	A	843	CLA	C1D-C2D	-2.72	1.39	1.45
17	A	815	CLA	C1D-C2D	-2.72	1.40	1.45
17	B	812	CLA	C1D-ND	2.72	1.41	1.37
17	8	601	CLA	C1D-ND	2.71	1.41	1.37
17	B	823	CLA	C1D-ND	2.71	1.41	1.37
17	B	821	CLA	C1B-NB	2.71	1.41	1.37
17	A	827	CLA	C3A-C2A	-2.70	1.46	1.54
17	6	602	CLA	C1D-ND	2.70	1.41	1.37
17	5	304	CLA	C1D-C2D	-2.70	1.40	1.45
17	A	803	CLA	C3A-C2A	-2.70	1.46	1.54
17	1	606	CLA	C1B-NB	2.70	1.41	1.37
17	1	605	CLA	C1B-NB	2.69	1.41	1.37
17	A	837	CLA	C1D-C2D	-2.69	1.40	1.45
17	7	607	CLA	C1D-ND	2.68	1.41	1.37
17	5	312	CLA	C1D-ND	2.67	1.41	1.37
17	A	843	CLA	C1D-ND	2.67	1.41	1.37
17	6	610	CLA	C1D-ND	2.66	1.41	1.37
17	A	827	CLA	C1D-C2D	-2.66	1.40	1.45
17	A	838	CLA	C1D-ND	2.66	1.41	1.37
17	4	601	CLA	C1D-ND	2.66	1.41	1.37
17	7	611	CLA	C3A-C2A	-2.66	1.47	1.54
17	6	609	CLA	C1D-C2D	-2.65	1.40	1.45
17	A	839	CLA	C1D-ND	2.65	1.41	1.37
17	A	827	CLA	C1D-ND	2.65	1.41	1.37
17	1	603	CLA	C1D-C2D	-2.65	1.40	1.45
17	1	609	CLA	C1D-C2D	-2.65	1.40	1.45
17	A	832	CLA	C1D-ND	2.64	1.41	1.37
17	7	612	CLA	C1D-C2D	-2.64	1.40	1.45
17	5	312	CLA	C1D-C2D	-2.64	1.40	1.45
17	A	814	CLA	C1D-C2D	-2.64	1.40	1.45
17	7	604	CLA	C3D-C4D	-2.64	1.38	1.44
17	5	310	CLA	C1D-C2D	-2.63	1.40	1.45
17	A	831	CLA	C1D-C2D	-2.63	1.40	1.45
17	A	835	CLA	C1D-C2D	-2.63	1.40	1.45
20	5	313	CHL	CHB-C4A	-2.63	1.31	1.37
17	1	605	CLA	C1D-C2D	-2.63	1.40	1.45
17	J	101	CLA	C1D-C2D	-2.62	1.40	1.45
17	A	839	CLA	C1D-C2D	-2.62	1.40	1.45
17	B	806	CLA	C1D-ND	2.62	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	8	602	CLA	C1D-ND	2.62	1.41	1.37
17	J	101	CLA	C3A-C2A	-2.62	1.47	1.54
17	A	803	CLA	C1D-C2D	-2.62	1.40	1.45
17	A	802	CLA	C1D-C2D	-2.62	1.40	1.45
17	A	834	CLA	C1D-ND	2.62	1.41	1.37
17	7	601	CLA	C3A-C2A	-2.61	1.47	1.54
17	A	828	CLA	C1D-C2D	-2.61	1.40	1.45
17	B	816	CLA	C1B-NB	2.61	1.41	1.37
17	7	612	CLA	C3A-C2A	-2.61	1.47	1.54
17	A	806	CLA	C1D-C2D	-2.61	1.40	1.45
17	3	302	CLA	C1D-C2D	-2.60	1.40	1.45
17	8	611	CLA	C1B-NB	2.60	1.41	1.37
17	3	308	CLA	C3A-C2A	-2.60	1.47	1.54
17	6	602	CLA	C1D-C2D	-2.60	1.40	1.45
17	A	821	CLA	C1D-ND	2.59	1.41	1.37
20	6	605	CHL	C1D-ND	2.59	1.41	1.37
17	B	823	CLA	C3A-C2A	-2.59	1.47	1.54
17	B	832	CLA	C1D-C2D	-2.59	1.40	1.45
17	A	826	CLA	C1D-C2D	-2.59	1.40	1.45
17	1	610	CLA	C1D-C2D	-2.58	1.40	1.45
17	7	601	CLA	C1D-ND	2.58	1.41	1.37
17	A	823	CLA	C3A-C2A	-2.58	1.47	1.54
17	5	302	CLA	C1D-C2D	-2.58	1.40	1.45
17	6	604	CLA	C1D-C2D	-2.58	1.40	1.45
17	5	311	CLA	C1D-C2D	-2.58	1.40	1.45
17	A	807	CLA	C1D-C2D	-2.57	1.40	1.45
17	A	816	CLA	C1D-C2D	-2.57	1.40	1.45
17	5	303	CLA	C1D-C2D	-2.57	1.40	1.45
20	6	606	CHL	C1D-ND	2.57	1.40	1.37
17	A	810	CLA	C1D-C2D	-2.57	1.40	1.45
17	A	813	CLA	C1D-C2D	-2.57	1.40	1.45
17	7	605	CLA	C1D-C2D	-2.57	1.40	1.45
17	1	608	CLA	C1D-C2D	-2.56	1.40	1.45
17	6	601	CLA	C1D-C2D	-2.56	1.40	1.45
17	A	812	CLA	C1D-C2D	-2.56	1.40	1.45
17	4	604	CLA	C1D-C2D	-2.56	1.40	1.45
17	7	607	CLA	C1D-C2D	-2.56	1.40	1.45
17	7	603	CLA	C1D-ND	2.56	1.40	1.37
17	7	613	CLA	C1D-C2D	-2.56	1.40	1.45
17	F	302	CLA	C1D-ND	2.56	1.40	1.37
17	A	829	CLA	C1D-C2D	-2.56	1.40	1.45
17	B	835	CLA	C1D-C2D	-2.56	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	834	CLA	C1D-C2D	-2.55	1.40	1.45
17	A	842	CLA	C1D-C2D	-2.55	1.40	1.45
17	B	822	CLA	C1D-C2D	-2.55	1.40	1.45
17	7	604	CLA	C1D-C2D	-2.55	1.40	1.45
17	A	803	CLA	C1D-ND	2.55	1.40	1.37
17	8	601	CLA	C1D-C2D	-2.55	1.40	1.45
17	8	604	CLA	C1D-C2D	-2.55	1.40	1.45
17	4	603	CLA	C1D-ND	2.54	1.40	1.37
20	6	607	CHL	C1D-ND	2.54	1.40	1.37
17	8	613	CLA	C1D-C2D	-2.54	1.40	1.45
17	B	821	CLA	C1D-C2D	-2.54	1.40	1.45
17	8	607	CLA	C1D-C2D	-2.54	1.40	1.45
17	A	806	CLA	C1D-ND	2.54	1.40	1.37
17	7	601	CLA	C1D-C2D	-2.53	1.40	1.45
17	3	306	CLA	C1D-ND	2.53	1.40	1.37
17	5	311	CLA	C1D-ND	2.53	1.40	1.37
17	1	602	CLA	C1D-C2D	-2.53	1.40	1.45
17	4	601	CLA	C1D-C2D	-2.53	1.40	1.45
17	B	816	CLA	C3A-C2A	-2.53	1.47	1.54
17	7	609	CLA	C1D-C2D	-2.53	1.40	1.45
17	A	836	CLA	C1D-C2D	-2.53	1.40	1.45
17	B	818	CLA	C1D-C2D	-2.53	1.40	1.45
17	B	830	CLA	C1D-ND	2.52	1.40	1.37
17	8	612	CLA	C1D-C2D	-2.52	1.40	1.45
20	6	607	CHL	CHB-C4A	-2.52	1.31	1.37
17	1	606	CLA	C3D-C4D	-2.52	1.38	1.44
17	B	822	CLA	C1D-ND	2.52	1.40	1.37
17	B	805	CLA	C1D-C2D	-2.52	1.40	1.45
17	1	608	CLA	C1B-NB	2.52	1.40	1.37
17	B	808	CLA	C1D-C2D	-2.52	1.40	1.45
17	7	608	CLA	C1D-ND	2.52	1.40	1.37
17	3	304	CLA	C1D-C2D	-2.52	1.40	1.45
17	3	303	CLA	C1D-ND	2.52	1.40	1.37
17	3	311	CLA	C1D-C2D	-2.52	1.40	1.45
17	B	823	CLA	C1D-C2D	-2.51	1.40	1.45
17	5	301	CLA	C1D-C2D	-2.51	1.40	1.45
17	B	830	CLA	C1D-C2D	-2.51	1.40	1.45
17	A	833	CLA	C1D-C2D	-2.51	1.40	1.45
17	B	825	CLA	C1D-C2D	-2.51	1.40	1.45
17	A	822	CLA	C1D-C2D	-2.51	1.40	1.45
17	8	614	CLA	C1D-C2D	-2.51	1.40	1.45
20	5	313	CHL	C1D-ND	2.51	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	830	CLA	C1D-C2D	-2.51	1.40	1.45
17	7	602	CLA	C1D-C2D	-2.51	1.40	1.45
17	A	811	CLA	C1D-ND	2.51	1.40	1.37
17	A	810	CLA	C3A-C2A	-2.50	1.47	1.54
17	B	809	CLA	C1D-C2D	-2.50	1.40	1.45
20	1	601	CHL	CHB-C4A	-2.50	1.31	1.37
17	B	804	CLA	C1D-C2D	-2.50	1.40	1.45
17	A	832	CLA	C1D-C2D	-2.50	1.40	1.45
17	A	835	CLA	C3A-C2A	-2.50	1.47	1.54
17	8	609	CLA	C1D-C2D	-2.50	1.40	1.45
20	8	606	CHL	C1D-C2D	-2.49	1.40	1.45
17	B	810	CLA	C1D-ND	2.49	1.40	1.37
17	B	819	CLA	C3D-C4D	-2.49	1.38	1.44
17	8	611	CLA	C1D-C2D	-2.49	1.40	1.45
17	3	302	CLA	C1D-ND	2.49	1.40	1.37
17	F	302	CLA	C1D-C2D	-2.49	1.40	1.45
17	5	307	CLA	C1D-C2D	-2.49	1.40	1.45
17	B	839	CLA	C1D-C2D	-2.49	1.40	1.45
17	8	605	CLA	C1D-C2D	-2.49	1.40	1.45
17	B	831	CLA	C3A-C2A	-2.49	1.47	1.54
17	8	608	CLA	C1D-C2D	-2.49	1.40	1.45
17	7	611	CLA	C1D-C2D	-2.49	1.40	1.45
17	B	826	CLA	C1D-C2D	-2.49	1.40	1.45
17	3	310	CLA	C1D-ND	2.48	1.40	1.37
17	A	809	CLA	C1D-C2D	-2.48	1.40	1.45
17	A	818	CLA	C1D-C2D	-2.48	1.40	1.45
20	5	305	CHL	C1D-C2D	-2.48	1.40	1.45
17	A	817	CLA	C1D-C2D	-2.48	1.40	1.45
17	B	816	CLA	C1D-C2D	-2.48	1.40	1.45
20	3	307	CHL	C1D-C2D	-2.48	1.40	1.45
17	B	827	CLA	C1D-C2D	-2.48	1.40	1.45
17	A	805	CLA	C1D-C2D	-2.48	1.40	1.45
17	3	305	CLA	C1D-C2D	-2.48	1.40	1.45
17	3	308	CLA	C1D-ND	2.48	1.40	1.37
17	A	823	CLA	C1D-C2D	-2.48	1.40	1.45
17	3	304	CLA	C1D-ND	2.48	1.40	1.37
17	1	604	CLA	C1B-NB	2.47	1.40	1.37
17	B	827	CLA	C1D-ND	2.47	1.40	1.37
17	3	306	CLA	C1D-C2D	-2.47	1.40	1.45
17	B	817	CLA	C1D-C2D	-2.47	1.40	1.45
17	B	820	CLA	C1D-C2D	-2.47	1.40	1.45
17	A	807	CLA	C3A-C2A	-2.46	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	Z	601	CHL	CHB-C4A	-2.46	1.31	1.37
20	5	305	CHL	CHB-C4A	-2.46	1.31	1.37
17	3	308	CLA	C1D-C2D	-2.46	1.40	1.45
17	A	838	CLA	C1D-C2D	-2.46	1.40	1.45
17	B	806	CLA	C3A-C2A	-2.45	1.47	1.54
17	B	801	CLA	C3D-C4D	-2.45	1.38	1.44
17	J	102	CLA	C1D-C2D	-2.45	1.40	1.45
17	B	831	CLA	C1D-C2D	-2.45	1.40	1.45
17	8	603	CLA	C1D-C2D	-2.45	1.40	1.45
17	B	832	CLA	C3A-C2A	-2.45	1.47	1.54
17	8	602	CLA	C1D-C2D	-2.45	1.40	1.45
17	B	802	CLA	C1D-C2D	-2.45	1.40	1.45
17	F	301	CLA	C1D-C2D	-2.45	1.40	1.45
17	5	314	CLA	C1D-C2D	-2.45	1.40	1.45
17	B	828	CLA	C1D-C2D	-2.44	1.40	1.45
17	A	824	CLA	C1D-C2D	-2.44	1.40	1.45
17	A	819	CLA	C1D-C2D	-2.44	1.40	1.45
17	7	607	CLA	C3A-C2A	-2.44	1.47	1.54
17	B	811	CLA	C1D-C2D	-2.44	1.40	1.45
17	B	836	CLA	C1D-C2D	-2.44	1.40	1.45
17	B	814	CLA	C1D-C2D	-2.44	1.40	1.45
17	A	838	CLA	C3D-C4D	-2.44	1.38	1.44
17	A	820	CLA	C1D-C2D	-2.44	1.40	1.45
17	6	608	CLA	C1D-ND	2.43	1.40	1.37
17	A	821	CLA	C1D-C2D	-2.43	1.40	1.45
20	7	606	CHL	C1D-C2D	-2.43	1.40	1.45
17	4	602	CLA	C1B-NB	2.43	1.40	1.37
20	3	307	CHL	C3A-C2A	-2.43	1.47	1.54
20	6	607	CHL	C1D-C2D	-2.43	1.40	1.45
17	3	313	CLA	C1D-C2D	-2.43	1.40	1.45
17	A	833	CLA	C1B-NB	2.43	1.40	1.37
17	A	841	CLA	C1D-C2D	-2.43	1.40	1.45
17	A	809	CLA	C1D-ND	2.43	1.40	1.37
17	B	837	CLA	C1D-C2D	-2.42	1.40	1.45
17	1	604	CLA	C1D-C2D	-2.42	1.40	1.45
17	B	829	CLA	C1D-C2D	-2.42	1.40	1.45
17	7	605	CLA	C3A-C2A	-2.42	1.47	1.54
17	B	810	CLA	C1D-C2D	-2.42	1.40	1.45
17	B	813	CLA	C1D-C2D	-2.42	1.40	1.45
17	4	604	CLA	C3A-C2A	-2.41	1.47	1.54
17	5	306	CLA	C1D-C2D	-2.41	1.40	1.45
17	A	808	CLA	C3A-C2A	-2.41	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	825	CLA	C1D-ND	2.41	1.40	1.37
17	A	818	CLA	C3A-C2A	-2.41	1.47	1.54
17	3	309	CLA	C1D-C2D	-2.41	1.40	1.45
17	A	825	CLA	C1D-C2D	-2.41	1.40	1.45
17	A	834	CLA	C1D-C2D	-2.41	1.40	1.45
17	1	609	CLA	C1B-NB	2.40	1.40	1.37
17	B	821	CLA	C1C-C2C	2.40	1.49	1.44
20	8	606	CHL	C1D-ND	2.40	1.40	1.37
17	1	610	CLA	C1B-NB	2.40	1.40	1.37
17	8	610	CLA	C1D-C2D	-2.40	1.40	1.45
17	8	613	CLA	C3A-C2A	-2.39	1.47	1.54
17	B	829	CLA	C3D-C4D	-2.39	1.38	1.44
17	7	602	CLA	C1D-ND	2.39	1.40	1.37
20	5	313	CHL	C1D-C2D	-2.39	1.40	1.45
17	8	608	CLA	C1D-ND	2.38	1.40	1.37
17	7	610	CLA	C1D-C2D	-2.38	1.40	1.45
17	A	816	CLA	C1D-ND	2.38	1.40	1.37
20	1	601	CHL	C1D-C2D	-2.38	1.40	1.45
17	A	811	CLA	C1D-C2D	-2.38	1.40	1.45
20	Z	601	CHL	C1D-C2D	-2.38	1.40	1.45
20	6	605	CHL	C1D-C2D	-2.37	1.40	1.45
17	6	609	CLA	C3A-C2A	-2.37	1.47	1.54
17	B	806	CLA	C1D-C2D	-2.37	1.40	1.45
17	5	312	CLA	C3A-C2A	-2.37	1.47	1.54
17	B	833	CLA	C1D-C2D	-2.37	1.40	1.45
17	B	824	CLA	C1D-C2D	-2.37	1.40	1.45
17	3	303	CLA	C1D-C2D	-2.37	1.40	1.45
17	A	804	CLA	C1D-C2D	-2.37	1.40	1.45
17	B	811	CLA	C3A-C2A	-2.36	1.47	1.54
17	A	819	CLA	C1D-ND	2.36	1.40	1.37
17	B	838	CLA	C3A-C2A	-2.36	1.47	1.54
17	A	812	CLA	C1D-ND	2.36	1.40	1.37
17	A	836	CLA	C3A-C2A	-2.36	1.47	1.54
17	7	610	CLA	C3D-C4D	-2.36	1.38	1.44
17	B	824	CLA	C3D-C4D	-2.36	1.38	1.44
17	8	614	CLA	C1D-ND	2.36	1.40	1.37
17	6	608	CLA	C1D-C2D	-2.35	1.40	1.45
17	5	315	CLA	C1D-C2D	-2.35	1.40	1.45
20	8	606	CHL	CHB-C4A	-2.35	1.32	1.37
17	A	812	CLA	C3D-C4D	-2.35	1.38	1.44
17	B	839	CLA	C3A-C2A	-2.35	1.47	1.54
17	3	301	CLA	C1D-C2D	-2.35	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	8	614	CLA	C3A-C2A	-2.35	1.47	1.54
20	1	601	CHL	C1D-ND	2.35	1.40	1.37
17	3	301	CLA	C3D-C4D	-2.34	1.38	1.44
17	7	608	CLA	C1D-C2D	-2.34	1.40	1.45
17	3	312	CLA	C1D-C2D	-2.34	1.40	1.45
17	A	815	CLA	CHD-C4C	-2.34	1.33	1.39
17	4	602	CLA	C1D-C2D	-2.34	1.40	1.45
17	1	607	CLA	C1D-C2D	-2.34	1.40	1.45
17	8	612	CLA	C3A-C2A	-2.34	1.47	1.54
17	B	837	CLA	C3D-C4D	-2.34	1.38	1.44
17	8	614	CLA	C3D-C4D	-2.34	1.38	1.44
17	7	611	CLA	C1B-NB	2.33	1.40	1.37
17	B	820	CLA	C1D-ND	2.33	1.40	1.37
17	6	603	CLA	C1D-C2D	-2.33	1.40	1.45
17	B	806	CLA	C3D-C4D	-2.33	1.38	1.44
17	A	829	CLA	C1D-ND	2.32	1.40	1.37
17	A	824	CLA	C3D-C4D	-2.32	1.38	1.44
17	B	826	CLA	C3D-C4D	-2.32	1.38	1.44
17	3	306	CLA	C3A-C2A	-2.32	1.48	1.54
20	1	601	CHL	C3D-C4D	-2.32	1.38	1.44
17	8	608	CLA	C3D-C4D	-2.32	1.38	1.44
17	J	102	CLA	C1B-NB	2.32	1.40	1.37
17	5	309	CLA	C1D-C2D	-2.32	1.40	1.45
17	A	829	CLA	C3D-C4D	-2.32	1.38	1.44
17	5	314	CLA	C3D-C4D	-2.32	1.38	1.44
17	A	822	CLA	C3D-C4D	-2.32	1.38	1.44
17	7	603	CLA	C1D-C2D	-2.32	1.40	1.45
17	3	304	CLA	C3D-C4D	-2.32	1.38	1.44
20	6	606	CHL	C1D-C2D	-2.31	1.40	1.45
20	Z	601	CHL	C3D-C4D	-2.31	1.39	1.44
17	6	602	CLA	C1B-NB	2.31	1.40	1.37
17	B	835	CLA	C1D-ND	2.31	1.40	1.37
17	7	614	CLA	C1B-NB	2.31	1.40	1.37
17	A	802	CLA	C3A-C2A	-2.31	1.48	1.54
17	6	610	CLA	CHD-C4C	-2.31	1.33	1.39
17	A	804	CLA	C3D-C4D	-2.31	1.39	1.44
17	A	817	CLA	C3D-C4D	-2.31	1.39	1.44
17	B	812	CLA	C1D-C2D	-2.30	1.40	1.45
17	7	605	CLA	C3D-C4D	-2.30	1.39	1.44
17	4	603	CLA	C1D-C2D	-2.30	1.40	1.45
17	A	839	CLA	C3A-C2A	-2.29	1.48	1.54
16	A	801	CL0	C3D-C4D	-2.29	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	5	309	CLA	C3A-C2A	-2.29	1.48	1.54
17	A	807	CLA	C3D-C4D	-2.29	1.39	1.44
20	Z	601	CHL	C1D-ND	2.29	1.40	1.37
17	J	101	CLA	C3D-C4D	-2.29	1.39	1.44
17	7	612	CLA	C3D-C4D	-2.29	1.39	1.44
17	B	838	CLA	C3D-C4D	-2.29	1.39	1.44
17	A	815	CLA	C3D-C4D	-2.29	1.39	1.44
17	5	308	CLA	C1D-C2D	-2.28	1.40	1.45
17	3	305	CLA	C3D-C4D	-2.28	1.39	1.44
17	7	603	CLA	C3A-C2A	-2.28	1.48	1.54
17	A	841	CLA	C3D-C4D	-2.28	1.39	1.44
17	A	833	CLA	C3A-C2A	-2.28	1.48	1.54
17	3	308	CLA	C3D-C4D	-2.28	1.39	1.44
17	B	804	CLA	C3D-C4D	-2.28	1.39	1.44
17	A	831	CLA	C1B-NB	2.28	1.40	1.37
17	A	842	CLA	C3D-C4D	-2.28	1.39	1.44
17	B	831	CLA	C3D-C4D	-2.28	1.39	1.44
17	B	807	CLA	C1D-C2D	-2.27	1.40	1.45
17	B	831	CLA	C1D-ND	2.27	1.40	1.37
17	A	843	CLA	C3A-C2A	-2.27	1.48	1.54
17	B	808	CLA	C3A-C2A	-2.27	1.48	1.54
17	A	806	CLA	C3A-C2A	-2.27	1.48	1.54
17	B	806	CLA	C1B-NB	2.27	1.40	1.37
17	1	607	CLA	C1D-ND	2.27	1.40	1.37
17	4	604	CLA	C1B-NB	2.27	1.40	1.37
17	A	821	CLA	C3D-C4D	-2.27	1.39	1.44
17	7	614	CLA	C1D-C2D	-2.27	1.40	1.45
20	6	605	CHL	C3D-C4D	-2.26	1.39	1.44
17	B	830	CLA	C3D-C4D	-2.26	1.39	1.44
17	A	807	CLA	C1D-ND	2.26	1.40	1.37
17	B	809	CLA	C1B-NB	2.26	1.40	1.37
17	A	831	CLA	C3A-C2A	-2.26	1.48	1.54
17	1	602	CLA	C1B-NB	2.26	1.40	1.37
17	A	834	CLA	C3D-C4D	-2.25	1.39	1.44
17	B	817	CLA	C1B-NB	2.25	1.40	1.37
17	5	314	CLA	C3A-C2A	-2.25	1.48	1.54
17	B	818	CLA	C1D-ND	2.25	1.40	1.37
17	A	839	CLA	C3D-C4D	-2.25	1.39	1.44
20	7	606	CHL	C3D-C4D	-2.25	1.39	1.44
17	B	834	CLA	C3A-C2A	-2.25	1.48	1.54
17	B	804	CLA	C3A-C2A	-2.25	1.48	1.54
16	A	801	CL0	C1D-C2D	-2.25	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	826	CLA	C1D-ND	2.24	1.40	1.37
20	7	606	CHL	C1D-ND	2.24	1.40	1.37
17	B	836	CLA	C3A-C2A	-2.24	1.48	1.54
20	8	606	CHL	C3D-C4D	-2.24	1.39	1.44
17	8	608	CLA	C1B-NB	2.24	1.40	1.37
17	F	301	CLA	C3D-C4D	-2.24	1.39	1.44
17	A	839	CLA	CHC-C1C	-2.24	1.34	1.38
17	3	313	CLA	C3D-C4D	-2.24	1.39	1.44
17	B	827	CLA	C3D-C4D	-2.24	1.39	1.44
17	A	812	CLA	C3A-C2A	-2.24	1.48	1.54
17	B	835	CLA	C3D-C4D	-2.24	1.39	1.44
17	5	315	CLA	C1B-NB	2.24	1.40	1.37
17	A	817	CLA	C1B-NB	2.23	1.40	1.37
17	8	601	CLA	CHC-C1C	-2.23	1.34	1.38
17	8	610	CLA	C3D-C4D	-2.23	1.39	1.44
17	7	601	CLA	C3D-C4D	-2.23	1.39	1.44
17	3	310	CLA	C1D-C2D	-2.23	1.40	1.45
17	7	603	CLA	C3D-C4D	-2.23	1.39	1.44
17	3	306	CLA	C3D-C4D	-2.23	1.39	1.44
17	7	608	CLA	C3D-C4D	-2.23	1.39	1.44
17	8	603	CLA	C3D-C4D	-2.23	1.39	1.44
20	3	307	CHL	C3D-C4D	-2.23	1.39	1.44
17	B	815	CLA	C1D-C2D	-2.23	1.40	1.45
17	B	832	CLA	C3D-C4D	-2.23	1.39	1.44
17	5	308	CLA	C3D-C4D	-2.23	1.39	1.44
17	B	807	CLA	C3D-C4D	-2.23	1.39	1.44
17	A	830	CLA	C3D-C4D	-2.23	1.39	1.44
17	7	610	CLA	C1D-ND	2.23	1.40	1.37
20	6	606	CHL	C3D-C4D	-2.23	1.39	1.44
17	A	809	CLA	C3D-C4D	-2.22	1.39	1.44
17	A	807	CLA	C1B-NB	2.22	1.40	1.37
17	8	613	CLA	C3D-C4D	-2.22	1.39	1.44
17	A	803	CLA	C3D-C4D	-2.22	1.39	1.44
20	5	313	CHL	C3D-C4D	-2.22	1.39	1.44
17	4	605	CLA	C3D-C4D	-2.22	1.39	1.44
17	A	839	CLA	CHD-C4C	-2.21	1.34	1.39
17	A	815	CLA	C1D-ND	2.21	1.40	1.37
17	B	817	CLA	C3D-C4D	-2.21	1.39	1.44
17	A	835	CLA	C3D-C4D	-2.21	1.39	1.44
17	4	601	CLA	C3D-C4D	-2.21	1.39	1.44
17	B	801	CLA	C1D-C2D	-2.21	1.41	1.45
17	B	807	CLA	C3A-C2A	-2.21	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	802	CLA	CHD-C4C	-2.21	1.34	1.39
17	5	303	CLA	C3D-C4D	-2.21	1.39	1.44
17	A	837	CLA	C3D-C4D	-2.21	1.39	1.44
17	8	611	CLA	C3D-C4D	-2.21	1.39	1.44
17	B	832	CLA	CHD-C4C	-2.21	1.34	1.39
17	B	838	CLA	C1D-ND	2.20	1.40	1.37
17	7	605	CLA	C1D-ND	2.20	1.40	1.37
17	B	802	CLA	C3D-C4D	-2.20	1.39	1.44
17	7	613	CLA	C3D-C4D	-2.20	1.39	1.44
17	B	831	CLA	C1B-NB	2.20	1.40	1.37
17	A	822	CLA	C3A-C2A	-2.20	1.48	1.54
17	F	301	CLA	C1D-ND	2.20	1.40	1.37
17	A	833	CLA	C3D-C4D	-2.20	1.39	1.44
17	F	302	CLA	C3D-C4D	-2.20	1.39	1.44
17	6	603	CLA	C3D-C4D	-2.20	1.39	1.44
17	A	806	CLA	C3D-C4D	-2.20	1.39	1.44
17	6	602	CLA	C3D-C4D	-2.20	1.39	1.44
17	B	805	CLA	C3D-C4D	-2.20	1.39	1.44
17	5	302	CLA	C3D-C4D	-2.20	1.39	1.44
17	B	815	CLA	C1B-NB	2.20	1.40	1.37
17	4	601	CLA	CHC-C1C	-2.20	1.34	1.38
17	8	602	CLA	C3D-C4D	-2.19	1.39	1.44
17	B	819	CLA	C3A-C2A	-2.19	1.48	1.54
17	A	832	CLA	C3C-C4C	2.19	1.43	1.40
17	5	310	CLA	C3A-C2A	-2.19	1.48	1.54
17	B	810	CLA	C3D-C4D	-2.19	1.39	1.44
17	A	831	CLA	CHD-C4C	-2.19	1.34	1.39
17	A	811	CLA	C3D-C4D	-2.19	1.39	1.44
17	8	609	CLA	C3D-C4D	-2.19	1.39	1.44
17	B	809	CLA	CHC-C1C	-2.19	1.34	1.38
17	B	813	CLA	C3D-C4D	-2.19	1.39	1.44
17	B	820	CLA	C3D-C4D	-2.19	1.39	1.44
17	8	610	CLA	C3A-C2A	-2.19	1.48	1.54
17	A	832	CLA	C3D-C4D	-2.19	1.39	1.44
17	B	834	CLA	C3D-C4D	-2.19	1.39	1.44
17	8	604	CLA	C1B-NB	2.19	1.40	1.37
17	4	605	CLA	CHD-C4C	-2.19	1.34	1.39
17	6	608	CLA	C3D-C4D	-2.18	1.39	1.44
17	5	304	CLA	C3D-C4D	-2.18	1.39	1.44
17	4	605	CLA	C1D-ND	2.18	1.40	1.37
17	A	825	CLA	C3D-C4D	-2.18	1.39	1.44
17	B	812	CLA	C3D-C4D	-2.18	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	302	CLA	C3D-C4D	-2.18	1.39	1.44
17	A	813	CLA	C3D-C4D	-2.18	1.39	1.44
17	A	808	CLA	CHD-C4C	-2.18	1.34	1.39
17	J	101	CLA	C1D-ND	2.18	1.40	1.37
17	J	102	CLA	C3A-C2A	-2.18	1.48	1.54
17	B	818	CLA	C3D-C4D	-2.18	1.39	1.44
17	A	817	CLA	C1D-ND	2.18	1.40	1.37
17	A	802	CLA	C3D-C4D	-2.18	1.39	1.44
17	A	836	CLA	C3D-C4D	-2.18	1.39	1.44
17	7	602	CLA	C3D-C4D	-2.18	1.39	1.44
17	5	315	CLA	C3D-C4D	-2.18	1.39	1.44
17	A	808	CLA	C3D-C4D	-2.18	1.39	1.44
17	B	811	CLA	C3D-C4D	-2.18	1.39	1.44
17	1	607	CLA	C3D-C4D	-2.18	1.39	1.44
17	A	805	CLA	C3D-C4D	-2.18	1.39	1.44
17	3	310	CLA	C3D-C4D	-2.18	1.39	1.44
17	B	808	CLA	C3D-C4D	-2.17	1.39	1.44
17	A	810	CLA	C3D-C4D	-2.17	1.39	1.44
17	J	102	CLA	C3D-C4D	-2.17	1.39	1.44
17	5	302	CLA	CHC-C1C	-2.17	1.34	1.38
17	7	609	CLA	C1B-NB	2.17	1.40	1.37
17	B	801	CLA	C3A-C2A	-2.17	1.48	1.54
17	B	836	CLA	C3D-C4D	-2.17	1.39	1.44
17	5	310	CLA	C1B-NB	2.17	1.40	1.37
17	8	604	CLA	C3A-C2A	-2.17	1.48	1.54
17	8	612	CLA	C1B-NB	2.17	1.40	1.37
17	7	614	CLA	C3A-C2A	-2.16	1.48	1.54
17	5	309	CLA	C3D-C4D	-2.16	1.39	1.44
17	A	825	CLA	C3A-C2A	-2.16	1.48	1.54
17	5	314	CLA	C1D-ND	2.16	1.40	1.37
17	B	809	CLA	C3D-C4D	-2.16	1.39	1.44
17	A	819	CLA	C3D-C4D	-2.16	1.39	1.44
20	5	305	CHL	C1D-ND	2.16	1.40	1.37
17	3	309	CLA	C3D-C4D	-2.16	1.39	1.44
17	3	312	CLA	C3D-C4D	-2.16	1.39	1.44
17	6	609	CLA	C1B-NB	2.16	1.40	1.37
17	8	614	CLA	C1B-NB	2.15	1.40	1.37
17	A	841	CLA	C1B-NB	2.15	1.40	1.37
17	A	826	CLA	C3D-C4D	-2.15	1.39	1.44
17	A	836	CLA	C1B-NB	2.15	1.40	1.37
17	7	611	CLA	C3D-C4D	-2.15	1.39	1.44
20	5	305	CHL	C3D-C4D	-2.15	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	608	CLA	C3A-C2A	-2.15	1.48	1.54
17	3	303	CLA	C3D-C4D	-2.14	1.39	1.44
17	A	818	CLA	CHC-C1C	-2.14	1.34	1.38
17	6	603	CLA	C3A-C2A	-2.14	1.48	1.54
17	A	827	CLA	C3D-C4D	-2.14	1.39	1.44
17	B	833	CLA	C3D-C4D	-2.14	1.39	1.44
17	5	306	CLA	C3D-C4D	-2.14	1.39	1.44
17	8	612	CLA	C3D-C4D	-2.14	1.39	1.44
17	1	606	CLA	C1D-C2D	-2.14	1.41	1.45
17	B	828	CLA	C3D-C4D	-2.14	1.39	1.44
17	5	301	CLA	C3D-C4D	-2.13	1.39	1.44
17	B	812	CLA	C1B-NB	2.13	1.40	1.37
17	6	604	CLA	C1B-NB	2.13	1.40	1.37
17	A	830	CLA	C1B-NB	2.13	1.40	1.37
17	3	305	CLA	C3A-C2A	-2.13	1.48	1.54
17	5	310	CLA	C3D-C4D	-2.13	1.39	1.44
17	8	601	CLA	C3D-C4D	-2.13	1.39	1.44
17	B	825	CLA	CHD-C4C	-2.13	1.34	1.39
17	B	812	CLA	C3A-C2A	-2.12	1.48	1.54
17	A	813	CLA	C1B-NB	2.12	1.40	1.37
17	F	301	CLA	C3A-C2A	-2.12	1.48	1.54
17	A	811	CLA	C3A-C2A	-2.12	1.48	1.54
17	4	601	CLA	C3A-C2A	-2.12	1.48	1.54
17	B	838	CLA	CHD-C4C	-2.12	1.34	1.39
17	5	315	CLA	C3A-C2A	-2.12	1.48	1.54
17	5	312	CLA	C3D-C4D	-2.12	1.39	1.44
17	4	603	CLA	C3D-C4D	-2.12	1.39	1.44
17	A	828	CLA	C3D-C4D	-2.12	1.39	1.44
17	A	814	CLA	C3D-C4D	-2.12	1.39	1.44
17	8	604	CLA	C3D-C4D	-2.12	1.39	1.44
17	J	101	CLA	CHD-C4C	-2.12	1.34	1.39
17	5	302	CLA	CHD-C4C	-2.11	1.34	1.39
17	3	301	CLA	C1D-ND	2.11	1.40	1.37
17	A	843	CLA	C3D-C4D	-2.11	1.39	1.44
17	7	609	CLA	C3D-C4D	-2.11	1.39	1.44
17	7	607	CLA	C3D-C4D	-2.11	1.39	1.44
17	B	809	CLA	C3A-C2A	-2.11	1.48	1.54
17	B	818	CLA	C1B-NB	2.11	1.40	1.37
17	B	822	CLA	C3D-C4D	-2.11	1.39	1.44
17	6	609	CLA	CHD-C4C	-2.11	1.34	1.39
17	B	816	CLA	C3D-C4D	-2.11	1.39	1.44
17	1	605	CLA	CHC-C1C	-2.11	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	605	CLA	C3A-C2A	-2.11	1.48	1.54
17	5	311	CLA	C3D-C4D	-2.11	1.39	1.44
17	3	313	CLA	C3A-C2A	-2.11	1.48	1.54
17	7	613	CLA	C3A-C2A	-2.11	1.48	1.54
17	3	302	CLA	C1B-NB	2.10	1.40	1.37
17	8	610	CLA	C1D-ND	2.10	1.40	1.37
17	5	311	CLA	C1B-NB	2.10	1.40	1.37
17	5	307	CLA	C3D-C4D	-2.10	1.39	1.44
17	6	601	CLA	C3D-C4D	-2.10	1.39	1.44
17	8	605	CLA	C1B-NB	2.10	1.40	1.37
17	A	820	CLA	C3D-C4D	-2.10	1.39	1.44
17	B	815	CLA	C3D-C4D	-2.10	1.39	1.44
17	1	602	CLA	C3D-C4D	-2.09	1.39	1.44
17	7	605	CLA	CHD-C4C	-2.09	1.34	1.39
17	6	604	CLA	C3A-C2A	-2.09	1.48	1.54
16	A	801	CL0	C3A-C2A	-2.09	1.48	1.54
17	8	612	CLA	CHC-C1C	-2.09	1.34	1.38
17	B	814	CLA	C1B-NB	2.09	1.40	1.37
17	5	304	CLA	CHD-C4C	-2.09	1.34	1.39
17	6	601	CLA	C3A-C2A	-2.09	1.48	1.54
17	A	816	CLA	C3D-C4D	-2.09	1.39	1.44
17	3	313	CLA	C1D-ND	2.09	1.40	1.37
17	8	602	CLA	C1B-NB	2.09	1.40	1.37
17	8	605	CLA	C3A-C2A	-2.09	1.48	1.54
17	A	808	CLA	CHC-C1C	-2.09	1.34	1.38
17	B	821	CLA	CHD-C4C	-2.09	1.34	1.39
17	8	601	CLA	C3A-C2A	-2.09	1.48	1.54
17	8	607	CLA	C3D-C4D	-2.08	1.39	1.44
17	3	311	CLA	C3D-C4D	-2.08	1.39	1.44
20	6	607	CHL	C3D-C4D	-2.08	1.39	1.44
17	7	614	CLA	C3D-C4D	-2.08	1.39	1.44
17	4	604	CLA	C3D-C4D	-2.08	1.39	1.44
17	1	603	CLA	C3D-C4D	-2.08	1.39	1.44
17	A	823	CLA	C3D-C4D	-2.08	1.39	1.44
17	B	813	CLA	CAB-C3B	-2.08	1.46	1.50
17	8	608	CLA	CHC-C1C	-2.07	1.34	1.38
17	B	825	CLA	C3D-C4D	-2.07	1.39	1.44
17	8	607	CLA	CHD-C4C	-2.07	1.34	1.39
17	B	837	CLA	CHC-C1C	-2.07	1.34	1.38
17	8	607	CLA	CHC-C1C	-2.07	1.34	1.38
17	A	843	CLA	CHD-C4C	-2.07	1.34	1.39
17	A	803	CLA	CHC-C1C	-2.07	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	827	CLA	C3A-C2A	-2.06	1.48	1.54
17	7	604	CLA	CHC-C1C	-2.06	1.34	1.38
17	6	610	CLA	C3D-C4D	-2.06	1.39	1.44
17	A	818	CLA	C3D-C4D	-2.06	1.39	1.44
17	A	811	CLA	CHD-C4C	-2.06	1.34	1.39
17	1	603	CLA	C3A-C2A	-2.06	1.48	1.54
17	B	839	CLA	C3D-C4D	-2.05	1.39	1.44
17	1	610	CLA	C3D-C4D	-2.05	1.39	1.44
17	3	303	CLA	CHC-C1C	-2.05	1.34	1.38
17	A	826	CLA	C3A-C2A	-2.05	1.48	1.54
17	3	311	CLA	CHC-C1C	-2.05	1.34	1.38
17	6	604	CLA	C3D-C4D	-2.05	1.39	1.44
17	5	301	CLA	CHD-C4C	-2.05	1.34	1.39
17	B	837	CLA	C1D-ND	2.05	1.40	1.37
17	5	310	CLA	CHD-C4C	-2.05	1.34	1.39
17	B	822	CLA	C3A-C2A	-2.05	1.48	1.54
17	A	819	CLA	C1B-NB	2.05	1.40	1.37
17	A	832	CLA	C3A-C2A	-2.05	1.48	1.54
17	7	601	CLA	CHC-C1C	-2.04	1.34	1.38
17	A	835	CLA	CHC-C1C	-2.04	1.34	1.38
17	A	813	CLA	C3A-C2A	-2.04	1.48	1.54
17	A	828	CLA	C3A-C2A	-2.04	1.48	1.54
17	B	824	CLA	C1D-ND	2.04	1.40	1.37
17	A	837	CLA	CHD-C4C	-2.04	1.34	1.39
17	B	817	CLA	CHC-C1C	-2.04	1.34	1.38
17	A	820	CLA	CHD-C4C	-2.04	1.34	1.39
17	3	301	CLA	C3A-C2A	-2.04	1.48	1.54
17	3	302	CLA	CHD-C4C	-2.03	1.34	1.39
17	8	601	CLA	CHD-C4C	-2.03	1.34	1.39
17	8	603	CLA	C3A-C2A	-2.03	1.48	1.54
17	A	806	CLA	CHD-C4C	-2.03	1.34	1.39
17	7	612	CLA	C1B-NB	2.03	1.40	1.37
17	3	304	CLA	CHC-C1C	-2.03	1.34	1.38
17	A	822	CLA	C1D-ND	2.03	1.40	1.37
17	3	312	CLA	C1B-NB	2.03	1.40	1.37
17	B	820	CLA	C1B-NB	2.03	1.40	1.37
17	A	835	CLA	CHD-C4C	-2.03	1.34	1.39
17	1	609	CLA	CHC-C1C	-2.03	1.34	1.38
17	A	813	CLA	CHD-C4C	-2.02	1.34	1.39
17	B	836	CLA	CHC-C1C	-2.02	1.34	1.38
17	8	605	CLA	C3D-C4D	-2.02	1.39	1.44
17	B	829	CLA	C1D-ND	2.02	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	7	612	CLA	CHC-C1C	-2.02	1.34	1.38
17	5	311	CLA	CHD-C4C	-2.02	1.34	1.39
17	1	605	CLA	C3D-C4D	-2.02	1.39	1.44
17	B	831	CLA	CHC-C1C	-2.02	1.34	1.38
17	7	604	CLA	C3A-C2A	-2.02	1.48	1.54
17	A	812	CLA	CHD-C4C	-2.02	1.34	1.39
17	A	814	CLA	CHD-C4C	-2.02	1.34	1.39
17	1	603	CLA	C1B-NB	2.02	1.40	1.37
17	3	304	CLA	C1B-NB	2.02	1.40	1.37
17	8	604	CLA	CHD-C4C	-2.02	1.34	1.39
17	3	303	CLA	C3A-C2A	-2.01	1.48	1.54
17	A	818	CLA	C1B-NB	2.01	1.40	1.37
17	B	809	CLA	C1D-ND	2.01	1.40	1.37
17	7	605	CLA	CHC-C1C	-2.01	1.34	1.38
17	B	821	CLA	C3D-C4D	-2.01	1.39	1.44
17	A	831	CLA	C3D-C4D	-2.01	1.39	1.44
17	1	603	CLA	CHD-C4C	-2.01	1.34	1.39
17	4	605	CLA	CHC-C1C	-2.01	1.34	1.38
17	B	828	CLA	C3A-C2A	-2.01	1.48	1.54
17	4	601	CLA	C1B-NB	2.01	1.40	1.37
17	B	823	CLA	C3D-C4D	-2.01	1.39	1.44
20	3	307	CHL	C1D-ND	2.01	1.40	1.37
17	8	614	CLA	CHD-C4C	-2.01	1.34	1.39
17	6	602	CLA	CHD-C4C	-2.01	1.34	1.39
17	F	302	CLA	C1B-NB	2.01	1.40	1.37
17	7	602	CLA	CHD-C4C	-2.00	1.34	1.39
17	A	830	CLA	CHD-C4C	-2.00	1.34	1.39
17	B	823	CLA	CHD-C4C	-2.00	1.34	1.39
17	7	611	CLA	CHC-C1C	-2.00	1.34	1.38
17	3	311	CLA	C3A-C2A	-2.00	1.48	1.54
17	A	827	CLA	CHD-C4C	-2.00	1.34	1.39
17	8	603	CLA	CHD-C4C	-2.00	1.34	1.39
17	7	613	CLA	CHC-C1C	-2.00	1.34	1.38
17	A	814	CLA	C3A-C2A	-2.00	1.48	1.54

All (1470) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	804	CLA	C4A-NA-C1A	-9.73	102.33	106.71
17	3	310	CLA	C4A-NA-C1A	-9.32	102.52	106.71
17	A	832	CLA	C1C-NC-C4C	-9.00	102.66	106.71
17	B	815	CLA	C4A-NA-C1A	-8.93	102.69	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	812	CLA	C4A-NA-C1A	-8.85	102.72	106.71
17	B	807	CLA	C4A-NA-C1A	-8.58	102.85	106.71
17	7	610	CLA	C4A-NA-C1A	-8.47	102.90	106.71
17	7	614	CLA	C4A-NA-C1A	-8.46	102.90	106.71
17	3	306	CLA	C4A-NA-C1A	-8.40	102.93	106.71
17	4	603	CLA	C4A-NA-C1A	-8.17	103.03	106.71
20	6	606	CHL	C4A-NA-C1A	-8.14	103.05	106.71
20	7	606	CHL	C4A-NA-C1A	-8.02	103.10	106.71
20	8	606	CHL	C4A-NA-C1A	-7.83	103.19	106.71
17	A	824	CLA	C4A-NA-C1A	-7.81	103.20	106.71
17	1	607	CLA	C4A-NA-C1A	-7.67	103.26	106.71
20	5	313	CHL	C4A-NA-C1A	-7.66	103.26	106.71
20	5	305	CHL	C4A-NA-C1A	-7.60	103.29	106.71
17	3	308	CLA	C4A-NA-C1A	-7.53	103.32	106.71
17	B	802	CLA	C4A-NA-C1A	-7.47	103.35	106.71
17	B	806	CLA	C4A-NA-C1A	-7.42	103.37	106.71
17	B	824	CLA	C4A-NA-C1A	-7.37	103.39	106.71
20	3	307	CHL	C4A-NA-C1A	-7.37	103.39	106.71
17	8	614	CLA	C4A-NA-C1A	-7.28	103.43	106.71
17	B	831	CLA	C4A-NA-C1A	-7.25	103.45	106.71
17	A	807	CLA	C4A-NA-C1A	-7.21	103.47	106.71
17	A	805	CLA	C4A-NA-C1A	-7.18	103.48	106.71
20	Z	601	CHL	C4A-NA-C1A	-7.07	103.53	106.71
17	B	834	CLA	C4A-NA-C1A	-6.98	103.57	106.71
17	3	313	CLA	C4A-NA-C1A	-6.95	103.58	106.71
20	1	601	CHL	C4A-NA-C1A	-6.95	103.58	106.71
20	6	605	CHL	C4A-NA-C1A	-6.87	103.62	106.71
17	F	301	CLA	C4A-NA-C1A	-6.84	103.63	106.71
17	3	305	CLA	C4A-NA-C1A	-6.82	103.64	106.71
17	7	603	CLA	C4A-NA-C1A	-6.80	103.65	106.71
17	A	822	CLA	C4A-NA-C1A	-6.79	103.65	106.71
17	B	820	CLA	C4A-NA-C1A	-6.72	103.69	106.71
17	B	804	CLA	C4A-NA-C1A	-6.70	103.69	106.71
17	A	803	CLA	C4A-NA-C1A	-6.67	103.71	106.71
17	A	838	CLA	C4A-NA-C1A	-6.67	103.71	106.71
17	B	819	CLA	C4A-NA-C1A	-6.65	103.72	106.71
17	A	825	CLA	C4A-NA-C1A	-6.63	103.73	106.71
17	5	314	CLA	C4A-NA-C1A	-6.53	103.77	106.71
17	B	836	CLA	C4A-NA-C1A	-6.43	103.81	106.71
17	A	802	CLA	C4A-NA-C1A	-6.41	103.83	106.71
17	5	309	CLA	C4A-NA-C1A	-6.41	103.83	106.71
17	3	312	CLA	C4A-NA-C1A	-6.39	103.83	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	841	CLA	C4A-NA-C1A	-6.37	103.84	106.71
17	A	809	CLA	C4A-NA-C1A	-6.35	103.85	106.71
17	1	606	CLA	C4A-NA-C1A	-6.34	103.86	106.71
17	B	826	CLA	C4A-NA-C1A	-6.31	103.87	106.71
17	A	821	CLA	C4A-NA-C1A	-6.29	103.88	106.71
17	B	823	CLA	C4A-NA-C1A	-6.27	103.89	106.71
17	J	102	CLA	C4A-NA-C1A	-6.15	103.94	106.71
17	J	101	CLA	C4A-NA-C1A	-6.12	103.95	106.71
17	B	826	CLA	CAA-C2A-C1A	-6.10	98.64	112.14
17	5	315	CLA	C4A-NA-C1A	-6.09	103.97	106.71
17	B	808	CLA	C4A-NA-C1A	-6.08	103.97	106.71
17	B	801	CLA	C4A-NA-C1A	-6.06	103.98	106.71
17	B	837	CLA	C4A-NA-C1A	-6.06	103.98	106.71
17	B	806	CLA	CAA-C2A-C1A	-6.00	98.86	112.14
17	B	833	CLA	C4A-NA-C1A	-5.99	104.01	106.71
17	8	611	CLA	C4A-NA-C1A	-5.98	104.02	106.71
17	8	608	CLA	C4A-NA-C1A	-5.94	104.03	106.71
17	3	301	CLA	C4A-NA-C1A	-5.91	104.05	106.71
17	4	604	CLA	C4A-NA-C1A	-5.89	104.06	106.71
17	B	829	CLA	C4A-NA-C1A	-5.85	104.08	106.71
17	B	835	CLA	C4A-NA-C1A	-5.84	104.08	106.71
17	6	603	CLA	C4A-NA-C1A	-5.84	104.08	106.71
17	B	830	CLA	C4A-NA-C1A	-5.83	104.08	106.71
17	7	601	CLA	C4A-NA-C1A	-5.82	104.09	106.71
17	A	833	CLA	C4A-NA-C1A	-5.81	104.09	106.71
17	A	817	CLA	C4A-NA-C1A	-5.78	104.11	106.71
17	B	817	CLA	C4A-NA-C1A	-5.78	104.11	106.71
17	B	818	CLA	C4A-NA-C1A	-5.77	104.11	106.71
20	6	607	CHL	C4A-NA-C1A	-5.74	104.12	106.71
17	A	836	CLA	C4A-NA-C1A	-5.73	104.13	106.71
17	5	311	CLA	C4A-NA-C1A	-5.71	104.14	106.71
17	3	309	CLA	C4A-NA-C1A	-5.65	104.17	106.71
17	A	829	CLA	C4A-NA-C1A	-5.63	104.17	106.71
17	A	837	CLA	C4A-NA-C1A	-5.59	104.19	106.71
17	1	605	CLA	C4A-NA-C1A	-5.57	104.20	106.71
17	B	816	CLA	C4A-NA-C1A	-5.57	104.20	106.71
17	B	838	CLA	C4A-NA-C1A	-5.51	104.23	106.71
17	A	806	CLA	C4A-NA-C1A	-5.49	104.24	106.71
17	B	839	CLA	C4A-NA-C1A	-5.49	104.24	106.71
17	3	303	CLA	C4A-NA-C1A	-5.46	104.25	106.71
17	1	607	CLA	C3A-C2A-C1A	-5.43	93.21	101.34
17	A	830	CLA	C4A-NA-C1A	-5.43	104.27	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	4	605	CLA	C4A-NA-C1A	-5.43	104.27	106.71
17	5	307	CLA	C4A-NA-C1A	-5.43	104.27	106.71
17	8	610	CLA	C4A-NA-C1A	-5.42	104.27	106.71
17	8	604	CLA	C4A-NA-C1A	-5.41	104.27	106.71
17	7	605	CLA	C4A-NA-C1A	-5.40	104.28	106.71
17	A	834	CLA	C4A-NA-C1A	-5.39	104.28	106.71
17	B	809	CLA	C4A-NA-C1A	-5.39	104.28	106.71
17	6	608	CLA	C4A-NA-C1A	-5.39	104.28	106.71
17	B	810	CLA	C4A-NA-C1A	-5.38	104.29	106.71
17	A	812	CLA	C4A-NA-C1A	-5.38	104.29	106.71
17	A	839	CLA	C4A-NA-C1A	-5.38	104.29	106.71
17	6	610	CLA	C4A-NA-C1A	-5.35	104.30	106.71
17	8	613	CLA	C4A-NA-C1A	-5.34	104.31	106.71
17	A	813	CLA	C4A-NA-C1A	-5.32	104.31	106.71
17	F	302	CLA	C4A-NA-C1A	-5.30	104.32	106.71
17	A	810	CLA	C4A-NA-C1A	-5.28	104.33	106.71
17	B	832	CLA	C4A-NA-C1A	-5.27	104.34	106.71
17	A	817	CLA	CAA-C2A-C1A	-5.27	100.48	112.14
17	A	823	CLA	C4A-NA-C1A	-5.26	104.34	106.71
17	7	604	CLA	C4A-NA-C1A	-5.26	104.34	106.71
17	A	818	CLA	C4A-NA-C1A	-5.26	104.34	106.71
17	B	805	CLA	C4A-NA-C1A	-5.26	104.34	106.71
17	5	312	CLA	C4A-NA-C1A	-5.21	104.36	106.71
17	A	811	CLA	C4A-NA-C1A	-5.19	104.37	106.71
17	3	308	CLA	CAA-C2A-C1A	-5.18	100.68	112.14
17	B	828	CLA	C4A-NA-C1A	-5.12	104.41	106.71
17	4	601	CLA	C4A-NA-C1A	-5.12	104.41	106.71
17	B	813	CLA	C4A-NA-C1A	-5.11	104.41	106.71
17	A	832	CLA	C4A-NA-C1A	-5.10	104.41	106.71
17	B	821	CLA	C4A-NA-C1A	-5.09	104.42	106.71
17	B	827	CLA	C4A-NA-C1A	-5.09	104.42	106.71
17	8	601	CLA	C4A-NA-C1A	-5.08	104.42	106.71
17	7	602	CLA	C4A-NA-C1A	-5.06	104.43	106.71
17	1	608	CLA	C4A-NA-C1A	-5.04	104.44	106.71
17	8	609	CLA	C4A-NA-C1A	-5.01	104.45	106.71
17	7	608	CLA	C4A-NA-C1A	-4.97	104.47	106.71
17	8	603	CLA	C4A-NA-C1A	-4.97	104.47	106.71
17	A	826	CLA	C4A-NA-C1A	-4.97	104.47	106.71
17	8	605	CLA	C4A-NA-C1A	-4.96	104.48	106.71
17	A	819	CLA	C4A-NA-C1A	-4.94	104.49	106.71
17	A	814	CLA	C4A-NA-C1A	-4.93	104.49	106.71
17	8	612	CLA	C4A-NA-C1A	-4.90	104.50	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	8	607	CLA	C4A-NA-C1A	-4.90	104.50	106.71
17	6	609	CLA	C4A-NA-C1A	-4.90	104.50	106.71
17	7	613	CLA	C4A-NA-C1A	-4.89	104.51	106.71
17	B	822	CLA	C4A-NA-C1A	-4.88	104.51	106.71
17	4	602	CLA	C4A-NA-C1A	-4.88	104.51	106.71
17	A	807	CLA	CAA-C2A-C1A	-4.85	101.40	112.14
16	A	801	CL0	C4A-NA-C1A	-4.85	104.53	106.71
17	7	612	CLA	C4A-NA-C1A	-4.83	104.54	106.71
17	6	601	CLA	C4A-NA-C1A	-4.82	104.54	106.71
17	B	811	CLA	C4A-NA-C1A	-4.82	104.54	106.71
17	6	602	CLA	C4A-NA-C1A	-4.82	104.54	106.71
17	B	801	CLA	CAA-C2A-C1A	-4.81	101.49	112.14
17	5	303	CLA	C4A-NA-C1A	-4.80	104.55	106.71
17	A	808	CLA	C4A-NA-C1A	-4.79	104.55	106.71
17	1	610	CLA	C4A-NA-C1A	-4.79	104.55	106.71
17	5	306	CLA	C4A-NA-C1A	-4.77	104.56	106.71
17	7	609	CLA	C4A-NA-C1A	-4.77	104.56	106.71
17	A	827	CLA	C4A-NA-C1A	-4.76	104.57	106.71
17	5	310	CLA	C4A-NA-C1A	-4.76	104.57	106.71
17	3	311	CLA	C4A-NA-C1A	-4.74	104.58	106.71
17	5	304	CLA	C4A-NA-C1A	-4.73	104.58	106.71
17	3	304	CLA	C4A-NA-C1A	-4.72	104.58	106.71
17	A	802	CLA	CAA-C2A-C1A	-4.71	101.71	112.14
17	A	820	CLA	C4A-NA-C1A	-4.71	104.59	106.71
17	1	602	CLA	C4A-NA-C1A	-4.71	104.59	106.71
17	A	828	CLA	C4A-NA-C1A	-4.69	104.60	106.71
17	1	606	CLA	CAA-C2A-C1A	-4.65	101.84	112.14
17	4	603	CLA	C3A-C2A-C1A	-4.64	94.39	101.34
17	A	835	CLA	C4A-NA-C1A	-4.60	104.64	106.71
17	1	603	CLA	C4A-NA-C1A	-4.59	104.64	106.71
17	7	611	CLA	C4A-NA-C1A	-4.55	104.66	106.71
17	7	603	CLA	CHD-C1D-ND	-4.55	120.27	124.45
17	7	614	CLA	CHD-C1D-ND	-4.53	120.29	124.45
17	5	301	CLA	C4A-NA-C1A	-4.52	104.67	106.71
17	A	831	CLA	C4A-NA-C1A	-4.50	104.68	106.71
17	7	608	CLA	CHD-C1D-ND	-4.49	120.33	124.45
17	A	832	CLA	CHC-C1C-C2C	-4.48	119.11	129.77
17	5	302	CLA	C4A-NA-C1A	-4.46	104.70	106.71
17	3	302	CLA	C4A-NA-C1A	-4.46	104.70	106.71
17	A	825	CLA	CHD-C1D-ND	-4.45	120.36	124.45
17	1	606	CLA	CHD-C1D-ND	-4.45	120.37	124.45
17	8	602	CLA	C4A-NA-C1A	-4.42	104.72	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	806	CLA	CHD-C1D-ND	-4.41	120.41	124.45
17	B	814	CLA	C4A-NA-C1A	-4.37	104.74	106.71
17	1	607	CLA	CHD-C1D-ND	-4.36	120.45	124.45
17	3	301	CLA	CHD-C1D-ND	-4.34	120.46	124.45
17	A	815	CLA	C4A-NA-C1A	-4.33	104.76	106.71
17	B	825	CLA	C4A-NA-C1A	-4.32	104.76	106.71
17	6	604	CLA	C4A-NA-C1A	-4.32	104.77	106.71
17	B	818	CLA	CAA-C2A-C1A	-4.30	102.62	112.14
17	4	603	CLA	CHD-C1D-ND	-4.30	120.51	124.45
17	A	804	CLA	CHD-C1D-ND	-4.29	120.51	124.45
17	A	843	CLA	C4A-NA-C1A	-4.29	104.78	106.71
17	B	801	CLA	CHD-C1D-ND	-4.26	120.53	124.45
17	7	610	CLA	CHD-C1D-ND	-4.23	120.56	124.45
17	7	607	CLA	C4A-NA-C1A	-4.22	104.81	106.71
17	3	310	CLA	C3A-C2A-C1A	-4.20	94.53	101.64
17	5	309	CLA	CHD-C1D-ND	-4.19	120.60	124.45
17	B	807	CLA	CHD-C1D-ND	-4.19	120.61	124.45
17	5	308	CLA	CHD-C1D-ND	-4.18	120.61	124.45
17	4	602	CLA	CHD-C1D-ND	-4.18	120.61	124.45
16	A	801	CL0	CHD-C1D-ND	-4.18	120.61	124.45
17	8	608	CLA	CHD-C1D-ND	-4.18	120.61	124.45
17	3	310	CLA	CHD-C1D-ND	-4.17	120.62	124.45
17	5	308	CLA	C4A-NA-C1A	-4.17	104.83	106.71
17	6	603	CLA	CHD-C1D-ND	-4.17	120.63	124.45
17	B	831	CLA	CAA-C2A-C1A	-4.14	102.98	112.14
17	A	802	CLA	CHD-C1D-ND	-4.12	120.67	124.45
17	8	610	CLA	CHD-C1D-ND	-4.10	120.69	124.45
17	B	837	CLA	CHD-C1D-ND	-4.09	120.69	124.45
17	B	805	CLA	CHD-C1D-ND	-4.09	120.69	124.45
20	5	305	CHL	C2A-C1A-CHA	4.08	130.99	123.86
17	B	812	CLA	C3A-C2A-C1A	-4.07	95.24	101.34
17	B	812	CLA	CAA-C2A-C1A	-4.07	103.14	112.14
17	1	604	CLA	C4A-NA-C1A	-4.06	104.88	106.71
17	B	826	CLA	CHD-C1D-ND	-4.05	120.73	124.45
17	B	813	CLA	CHD-C1D-ND	-4.04	120.74	124.45
17	B	831	CLA	CHD-C1D-ND	-4.04	120.75	124.45
17	8	603	CLA	CHD-C1D-ND	-4.03	120.75	124.45
17	3	312	CLA	CHD-C1D-ND	-4.03	120.75	124.45
17	B	829	CLA	CHD-C1D-ND	-4.02	120.76	124.45
17	A	819	CLA	CHD-C1D-ND	-4.02	120.76	124.45
17	B	836	CLA	CHD-C1D-ND	-4.02	120.76	124.45
17	B	804	CLA	CHD-C1D-ND	-4.01	120.77	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	5	306	CLA	CHD-C1D-ND	-4.01	120.77	124.45
17	7	611	CLA	CHD-C1D-ND	-3.99	120.78	124.45
17	J	102	CLA	CHD-C1D-ND	-3.99	120.79	124.45
17	B	812	CLA	CHD-C1D-ND	-3.97	120.81	124.45
17	5	308	CLA	C3B-C4B-NB	-3.97	106.83	110.52
17	A	834	CLA	CHD-C1D-ND	-3.97	120.81	124.45
17	A	805	CLA	CHD-C1D-ND	-3.96	120.81	124.45
17	1	602	CLA	CHD-C1D-ND	-3.96	120.82	124.45
17	3	313	CLA	CAA-C2A-C1A	-3.95	103.39	112.14
17	1	609	CLA	C4A-NA-C1A	-3.95	104.93	106.71
16	A	801	CL0	CHB-C1B-NB	-3.95	120.08	124.26
17	B	830	CLA	CHD-C1D-ND	-3.93	120.84	124.45
17	3	304	CLA	CHD-C1D-ND	-3.93	120.84	124.45
17	B	810	CLA	CHD-C1D-ND	-3.92	120.85	124.45
17	3	303	CLA	CHD-C1D-ND	-3.92	120.85	124.45
17	B	824	CLA	CHD-C1D-ND	-3.91	120.86	124.45
17	A	816	CLA	CHB-C1B-NB	-3.90	120.12	124.26
17	A	817	CLA	CHD-C1D-ND	-3.89	120.88	124.45
17	A	821	CLA	CHD-C1D-ND	-3.89	120.88	124.45
17	B	802	CLA	CHD-C1D-ND	-3.89	120.88	124.45
17	8	611	CLA	CHD-C1D-ND	-3.89	120.88	124.45
17	B	819	CLA	CHC-C1C-NC	3.88	130.09	124.20
17	3	309	CLA	CHD-C1D-ND	-3.88	120.89	124.45
17	5	314	CLA	CHD-C1D-ND	-3.88	120.89	124.45
17	3	306	CLA	CHD-C1D-ND	-3.86	120.91	124.45
17	6	608	CLA	CHD-C1D-ND	-3.85	120.92	124.45
17	A	809	CLA	CHD-C1D-ND	-3.85	120.92	124.45
17	B	815	CLA	CHD-C1D-ND	-3.84	120.92	124.45
17	A	831	CLA	CHB-C1B-NB	-3.84	120.19	124.26
17	A	833	CLA	CHD-C1D-ND	-3.84	120.92	124.45
17	B	828	CLA	CHD-C1D-ND	-3.84	120.93	124.45
17	A	836	CLA	CHD-C1D-ND	-3.84	120.93	124.45
17	A	818	CLA	CHD-C1D-ND	-3.84	120.93	124.45
17	7	610	CLA	C3A-C2A-C1A	-3.82	95.18	101.64
17	3	313	CLA	CHD-C1D-ND	-3.82	120.95	124.45
17	5	307	CLA	CHD-C1D-ND	-3.82	120.95	124.45
17	A	824	CLA	CAA-C2A-C1A	-3.82	103.69	112.14
17	F	302	CLA	CHD-C1D-ND	-3.81	120.95	124.45
17	B	827	CLA	CHD-C1D-ND	-3.81	120.96	124.45
17	A	822	CLA	CHD-C1D-ND	-3.80	120.96	124.45
17	3	308	CLA	CHD-C1D-ND	-3.79	120.97	124.45
17	7	604	CLA	CHB-C1B-NB	-3.79	120.24	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	8	607	CLA	CHD-C1D-ND	-3.79	120.97	124.45
17	7	609	CLA	CHD-C1D-ND	-3.79	120.97	124.45
17	8	602	CLA	CHD-C1D-ND	-3.78	120.98	124.45
17	B	819	CLA	CHB-C1B-NB	-3.78	120.26	124.26
17	B	816	CLA	CHD-C1D-ND	-3.77	120.98	124.45
17	A	823	CLA	CAA-C2A-C1A	-3.77	103.79	112.14
17	7	608	CLA	CHB-C1B-NB	-3.77	120.26	124.26
17	A	829	CLA	CHD-C1D-ND	-3.77	120.99	124.45
17	J	101	CLA	CHD-C1D-ND	-3.77	120.99	124.45
17	8	609	CLA	CHD-C1D-ND	-3.77	120.99	124.45
17	B	813	CLA	CHB-C1B-NB	-3.76	120.27	124.26
17	5	315	CLA	CHD-C1D-ND	-3.76	121.00	124.45
17	4	601	CLA	CHD-C1D-ND	-3.76	121.00	124.45
17	B	809	CLA	CHD-C1D-ND	-3.75	121.01	124.45
17	A	806	CLA	CHD-C1D-ND	-3.74	121.02	124.45
17	B	814	CLA	CHD-C1D-ND	-3.74	121.02	124.45
17	B	839	CLA	CHD-C1D-ND	-3.73	121.02	124.45
20	6	607	CHL	CAA-C2A-C1A	3.73	120.40	112.14
17	A	823	CLA	CHD-C1D-ND	-3.73	121.03	124.45
17	7	611	CLA	C1D-ND-C4D	-3.72	103.69	106.33
17	6	602	CLA	CHD-C1D-ND	-3.72	121.03	124.45
17	A	820	CLA	CHD-C1D-ND	-3.72	121.03	124.45
17	A	816	CLA	C4A-NA-C1A	-3.72	105.03	106.71
17	3	310	CLA	C2A-C3A-C4A	-3.72	97.04	101.78
17	A	811	CLA	CHD-C1D-ND	-3.71	121.04	124.45
17	7	613	CLA	CHD-C1D-ND	-3.71	121.04	124.45
17	1	604	CLA	CHD-C1D-ND	-3.70	121.06	124.45
17	A	841	CLA	CHD-C1D-ND	-3.69	121.06	124.45
17	A	830	CLA	CAA-C2A-C1A	-3.69	103.96	112.14
16	A	801	CL0	CHC-C1C-NC	3.69	129.81	124.20
17	A	816	CLA	CHD-C1D-ND	-3.69	121.06	124.45
17	1	602	CLA	C1D-ND-C4D	-3.68	103.72	106.33
17	A	830	CLA	CHD-C1D-ND	-3.68	121.07	124.45
17	A	838	CLA	CHD-C1D-ND	-3.67	121.08	124.45
17	B	820	CLA	CHD-C1D-ND	-3.67	121.08	124.45
17	7	602	CLA	CHD-C1D-ND	-3.66	121.09	124.45
17	F	302	CLA	CHB-C1B-NB	-3.66	120.39	124.26
17	5	301	CLA	CHD-C1D-ND	-3.65	121.10	124.45
17	A	815	CLA	C1D-ND-C4D	-3.65	103.74	106.33
17	8	607	CLA	CHB-C1B-NB	-3.65	120.40	124.26
17	B	811	CLA	CHD-C1D-ND	-3.64	121.11	124.45
17	6	610	CLA	CHB-C1B-NB	-3.63	120.41	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	813	CLA	CHD-C1D-ND	-3.63	121.12	124.45
17	A	827	CLA	CHB-C1B-NB	-3.62	120.42	124.26
17	B	822	CLA	CHB-C1B-NB	-3.62	120.43	124.26
17	B	818	CLA	CHD-C1D-ND	-3.61	121.13	124.45
17	A	807	CLA	CHD-C1D-ND	-3.61	121.14	124.45
17	7	607	CLA	CHD-C1D-ND	-3.61	121.14	124.45
17	A	814	CLA	CHD-C1D-ND	-3.61	121.14	124.45
17	F	301	CLA	CHD-C1D-ND	-3.61	121.14	124.45
17	A	842	CLA	CHD-C1D-ND	-3.60	121.14	124.45
17	A	824	CLA	CHD-C1D-ND	-3.60	121.14	124.45
17	7	608	CLA	C1D-ND-C4D	-3.59	103.78	106.33
17	1	605	CLA	C2C-C1C-NC	3.59	113.33	109.97
17	8	610	CLA	C3B-C4B-NB	-3.59	107.19	110.52
17	B	802	CLA	C3A-C2A-C1A	-3.59	95.97	101.34
17	5	302	CLA	C2C-C1C-NC	3.58	113.33	109.97
17	A	810	CLA	CHD-C1D-ND	-3.58	121.16	124.45
17	8	603	CLA	C1D-ND-C4D	-3.58	103.79	106.33
17	A	826	CLA	CHD-C1D-ND	-3.58	121.16	124.45
17	8	604	CLA	CHD-C1D-ND	-3.58	121.17	124.45
17	A	803	CLA	CHD-C1D-ND	-3.57	121.17	124.45
17	A	833	CLA	C1D-ND-C4D	-3.57	103.80	106.33
17	B	834	CLA	CHD-C1D-ND	-3.56	121.18	124.45
17	3	310	CLA	C3B-C4B-NB	-3.56	107.21	110.52
17	A	835	CLA	C2C-C1C-NC	3.54	113.29	109.97
17	A	815	CLA	CHD-C1D-ND	-3.53	121.21	124.45
17	4	602	CLA	C1D-ND-C4D	-3.53	103.83	106.33
17	B	825	CLA	CHD-C1D-ND	-3.53	121.21	124.45
17	B	833	CLA	CHD-C1D-ND	-3.53	121.21	124.45
17	5	303	CLA	CHD-C1D-ND	-3.53	121.21	124.45
17	A	832	CLA	CHD-C1D-ND	-3.52	121.22	124.45
17	B	823	CLA	CHD-C1D-ND	-3.52	121.22	124.45
17	3	302	CLA	CHD-C1D-ND	-3.52	121.22	124.45
17	B	808	CLA	CHD-C1D-ND	-3.52	121.22	124.45
17	8	612	CLA	CHD-C1D-ND	-3.52	121.22	124.45
17	5	314	CLA	C3B-C4B-NB	-3.52	107.25	110.52
17	A	820	CLA	C1D-ND-C4D	-3.51	103.84	106.33
17	A	832	CLA	CHB-C1B-NB	-3.51	120.54	124.26
17	B	825	CLA	CHB-C1B-NB	-3.51	120.54	124.26
17	A	837	CLA	CHD-C1D-ND	-3.51	121.22	124.45
17	8	614	CLA	CHD-C1D-ND	-3.51	121.22	124.45
17	3	305	CLA	CHD-C1D-ND	-3.51	121.22	124.45
17	B	809	CLA	CHB-C1B-NB	-3.51	120.54	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	843	CLA	CHB-C1B-NB	-3.51	120.54	124.26
17	7	604	CLA	CHD-C1D-ND	-3.51	121.23	124.45
17	8	602	CLA	CHB-C1B-NB	-3.51	120.54	124.26
17	B	806	CLA	C1D-ND-C4D	-3.51	103.84	106.33
17	A	820	CLA	CHB-C1B-NB	-3.50	120.55	124.26
17	8	611	CLA	C1D-ND-C4D	-3.50	103.85	106.33
20	5	305	CHL	CHA-C1A-NA	-3.50	118.39	126.40
17	5	304	CLA	CHB-C1B-NB	-3.49	120.56	124.26
17	1	603	CLA	CHB-C1B-NB	-3.49	120.56	124.26
17	B	817	CLA	CHD-C1D-ND	-3.49	121.25	124.45
17	3	301	CLA	CHB-C1B-NB	-3.49	120.56	124.26
17	7	601	CLA	C2C-C1C-NC	3.48	113.23	109.97
17	6	602	CLA	C1D-ND-C4D	-3.48	103.87	106.33
17	7	607	CLA	CHB-C1B-NB	-3.48	120.58	124.26
17	6	609	CLA	CHB-C1B-NB	-3.47	120.58	124.26
17	A	811	CLA	CHB-C1B-NB	-3.47	120.58	124.26
17	6	603	CLA	C1D-ND-C4D	-3.47	103.87	106.33
17	8	601	CLA	C2C-C1C-NC	3.47	113.22	109.97
17	3	311	CLA	CHD-C1D-ND	-3.46	121.28	124.45
17	6	609	CLA	CHD-C1D-ND	-3.45	121.28	124.45
17	A	828	CLA	CHD-C1D-ND	-3.45	121.28	124.45
17	5	311	CLA	CHB-C1B-NB	-3.45	120.60	124.26
17	B	822	CLA	CHD-C1D-ND	-3.44	121.29	124.45
17	5	312	CLA	CHD-C1D-ND	-3.44	121.30	124.45
17	7	603	CLA	C1D-ND-C4D	-3.44	103.89	106.33
17	1	609	CLA	CHB-C1B-NB	-3.43	120.62	124.26
17	1	608	CLA	CHB-C1B-NB	-3.43	120.62	124.26
17	B	832	CLA	CHD-C1D-ND	-3.43	121.31	124.45
17	1	608	CLA	CHD-C1D-ND	-3.42	121.31	124.45
17	A	836	CLA	CHB-C1B-NB	-3.42	120.64	124.26
17	B	835	CLA	CHD-C1D-ND	-3.42	121.31	124.45
17	B	816	CLA	CHB-C1B-NB	-3.41	120.65	124.26
17	6	601	CLA	CHD-C1D-ND	-3.41	121.32	124.45
17	5	302	CLA	CHD-C1D-ND	-3.41	121.32	124.45
17	B	835	CLA	CHB-C1B-NB	-3.41	120.65	124.26
17	A	812	CLA	CHD-C1D-ND	-3.41	121.32	124.45
17	7	609	CLA	CAA-C2A-C1A	-3.40	104.62	112.14
17	6	603	CLA	CHB-C1B-NB	-3.39	120.66	124.26
17	B	802	CLA	C3B-C4B-NB	-3.39	107.37	110.52
17	A	808	CLA	CHD-C1D-ND	-3.39	121.34	124.45
17	5	314	CLA	CHB-C1B-NB	-3.39	120.67	124.26
17	B	807	CLA	CAA-C2A-C1A	-3.39	104.64	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	7	612	CLA	CHB-C1B-NB	-3.38	120.67	124.26
17	B	821	CLA	CHD-C1D-ND	-3.38	121.34	124.45
17	A	839	CLA	CHD-C1D-ND	-3.38	121.35	124.45
20	Z	601	CHL	CHD-C1D-ND	-3.38	121.35	124.45
17	7	609	CLA	CHB-C1B-NB	-3.38	120.68	124.26
17	6	604	CLA	CHD-C1D-ND	-3.38	121.35	124.45
20	7	606	CHL	CHD-C1D-ND	-3.38	121.35	124.45
17	A	828	CLA	CHB-C1B-NB	-3.38	120.68	124.26
17	3	309	CLA	CHB-C1B-NB	-3.38	120.68	124.26
20	1	601	CHL	CHD-C1D-ND	-3.38	121.35	124.45
17	B	832	CLA	CHB-C1B-NB	-3.36	120.70	124.26
17	A	815	CLA	CHB-C1B-NB	-3.36	120.70	124.26
17	1	603	CLA	CHD-C1D-ND	-3.36	121.36	124.45
17	B	828	CLA	CHB-C1B-NB	-3.36	120.70	124.26
17	5	306	CLA	CHB-C1B-NB	-3.35	120.71	124.26
17	8	608	CLA	C1D-ND-C4D	-3.35	103.95	106.33
17	A	803	CLA	C2C-C1C-NC	3.35	113.11	109.97
17	5	307	CLA	CHB-C1B-NB	-3.35	120.71	124.26
17	7	601	CLA	CHB-C1B-NB	-3.34	120.72	124.26
17	5	301	CLA	CHB-C1B-NB	-3.34	120.72	124.26
17	A	813	CLA	C1D-ND-C4D	-3.33	103.97	106.33
17	3	313	CLA	CHB-C1B-NB	-3.33	120.73	124.26
17	B	829	CLA	CHB-C1B-NB	-3.33	120.73	124.26
17	1	609	CLA	CHD-C1D-ND	-3.32	121.40	124.45
17	A	839	CLA	C2C-C1C-NC	3.32	113.08	109.97
17	5	311	CLA	CHD-C1D-ND	-3.32	121.40	124.45
17	8	612	CLA	CHB-C1B-NB	-3.31	120.75	124.26
17	B	807	CLA	C1D-ND-C4D	-3.31	103.98	106.33
17	A	829	CLA	C1D-ND-C4D	-3.31	103.98	106.33
17	3	306	CLA	CHB-C1B-NB	-3.31	120.75	124.26
17	8	613	CLA	CHB-C1B-NB	-3.31	120.75	124.26
17	A	805	CLA	C1D-ND-C4D	-3.31	103.98	106.33
17	J	101	CLA	C1D-ND-C4D	-3.31	103.99	106.33
17	B	814	CLA	C1D-ND-C4D	-3.30	103.99	106.33
17	B	821	CLA	C1D-ND-C4D	-3.30	103.99	106.33
17	A	842	CLA	CHB-C1B-NB	-3.30	120.76	124.26
17	B	810	CLA	C3B-C4B-NB	-3.30	107.45	110.52
17	8	610	CLA	CHB-C1B-NB	-3.30	120.76	124.26
17	5	309	CLA	C1D-ND-C4D	-3.30	103.99	106.33
17	B	836	CLA	C2C-C1C-NC	3.30	113.06	109.97
17	B	815	CLA	C3A-C2A-C1A	-3.30	96.40	101.34
17	8	601	CLA	CHD-C1D-ND	-3.29	121.43	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	810	CLA	CHB-C1B-NB	-3.29	120.78	124.26
17	B	801	CLA	C3B-C4B-NB	-3.28	107.47	110.52
17	B	805	CLA	CHB-C1B-NB	-3.28	120.78	124.26
17	7	605	CLA	CHD-C1D-ND	-3.28	121.44	124.45
17	1	606	CLA	CHB-C1B-NB	-3.28	120.79	124.26
17	8	601	CLA	CHB-C1B-NB	-3.28	120.79	124.26
17	3	301	CLA	C1D-ND-C4D	-3.27	104.01	106.33
17	3	302	CLA	C1D-ND-C4D	-3.27	104.01	106.33
17	A	823	CLA	CHB-C1B-NB	-3.27	120.79	124.26
17	3	302	CLA	CHB-C1B-NB	-3.27	120.80	124.26
17	7	614	CLA	C3A-C2A-C1A	-3.27	96.45	101.34
17	B	823	CLA	CHB-C1B-NB	-3.26	120.80	124.26
17	B	811	CLA	CAA-C2A-C1A	-3.26	104.92	112.14
17	1	610	CLA	CHB-C1B-NB	-3.26	120.80	124.26
17	5	308	CLA	CHB-C1B-NB	-3.26	120.81	124.26
17	A	843	CLA	CHD-C1D-ND	-3.26	121.46	124.45
17	7	602	CLA	CHB-C1B-NB	-3.26	120.81	124.26
17	4	601	CLA	C2C-C1C-NC	3.26	113.02	109.97
16	A	801	CL0	CHC-C1C-C2C	-3.25	117.69	126.73
17	8	605	CLA	C2C-C1C-NC	3.25	113.02	109.97
17	3	303	CLA	CHB-C1B-NB	-3.25	120.81	124.26
17	B	838	CLA	CHD-C1D-ND	-3.25	121.47	124.45
17	6	601	CLA	CHB-C1B-NB	-3.25	120.81	124.26
17	3	306	CLA	C3A-C2A-C1A	-3.25	96.47	101.34
17	A	825	CLA	C1D-ND-C4D	-3.25	104.03	106.33
17	5	310	CLA	CHD-C1D-ND	-3.25	121.47	124.45
17	8	613	CLA	CHD-C1D-ND	-3.25	121.47	124.45
17	6	604	CLA	CHB-C1B-NB	-3.24	120.82	124.26
17	A	812	CLA	CHB-C1B-NB	-3.24	120.82	124.26
17	1	610	CLA	CHD-C1D-ND	-3.24	121.47	124.45
20	6	606	CHL	CHD-C1D-ND	-3.24	121.47	124.45
17	A	826	CLA	CHB-C1B-NB	-3.24	120.83	124.26
17	5	306	CLA	C1D-ND-C4D	-3.23	104.04	106.33
17	A	834	CLA	CHB-C1B-NB	-3.23	120.84	124.26
17	B	836	CLA	CHB-C1B-NB	-3.23	120.84	124.26
17	B	806	CLA	C3A-C2A-C1A	-3.22	96.51	101.34
17	3	312	CLA	CAA-C2A-C1A	-3.22	105.00	112.14
17	5	302	CLA	CHB-C1B-NB	-3.22	120.84	124.26
17	A	814	CLA	CHB-C1B-NB	-3.22	120.85	124.26
20	5	313	CHL	CHD-C1D-ND	-3.22	121.50	124.45
20	6	605	CHL	CHD-C1D-ND	-3.22	121.50	124.45
17	A	827	CLA	CHD-C1D-ND	-3.21	121.50	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	802	CLA	CHB-C1B-NB	-3.21	120.86	124.26
17	B	815	CLA	CHB-C1B-NB	-3.21	120.86	124.26
17	4	602	CLA	CHB-C1B-NB	-3.21	120.86	124.26
17	A	817	CLA	CHB-C1B-NB	-3.20	120.87	124.26
17	7	611	CLA	CHB-C1B-NB	-3.20	120.87	124.26
17	B	831	CLA	CHB-C1B-NB	-3.20	120.87	124.26
17	B	827	CLA	CHB-C1B-NB	-3.20	120.87	124.26
17	8	602	CLA	C1D-ND-C4D	-3.20	104.06	106.33
17	7	601	CLA	CHD-C1D-ND	-3.19	121.52	124.45
17	1	605	CLA	CHB-C1B-NB	-3.19	120.88	124.26
17	3	306	CLA	CAA-C2A-C1A	-3.19	105.08	112.14
17	A	812	CLA	C2C-C1C-NC	3.19	112.96	109.97
17	4	604	CLA	CHD-C1D-ND	-3.19	121.53	124.45
17	1	602	CLA	CHB-C1B-NB	-3.19	120.88	124.26
17	8	613	CLA	C2C-C1C-NC	3.19	112.96	109.97
17	B	838	CLA	CHB-C1B-NB	-3.19	120.89	124.26
17	B	822	CLA	C2C-C1C-NC	3.18	112.95	109.97
17	B	839	CLA	CHB-C1B-NB	-3.18	120.89	124.26
17	B	817	CLA	C2C-C1C-NC	3.18	112.95	109.97
17	A	808	CLA	CHB-C1B-NB	-3.18	120.89	124.26
17	J	102	CLA	CHB-C1B-NB	-3.18	120.89	124.26
20	6	607	CHL	CHD-C1D-ND	-3.18	121.54	124.45
17	5	303	CLA	CHB-C1B-NB	-3.17	120.90	124.26
17	A	831	CLA	CHD-C1D-ND	-3.17	121.54	124.45
17	B	813	CLA	C1D-ND-C4D	-3.17	104.08	106.33
17	5	301	CLA	C1D-ND-C4D	-3.16	104.09	106.33
17	B	830	CLA	C1D-ND-C4D	-3.16	104.09	106.33
17	A	806	CLA	CHB-C1B-NB	-3.16	120.91	124.26
17	B	808	CLA	CHB-C1B-NB	-3.16	120.91	124.26
17	4	601	CLA	CHB-C1B-NB	-3.16	120.91	124.26
17	6	608	CLA	CHB-C1B-NB	-3.16	120.91	124.26
17	J	101	CLA	CAA-C2A-C1A	-3.16	105.15	112.14
17	A	806	CLA	C1D-ND-C4D	-3.16	104.09	106.33
17	1	608	CLA	C1D-ND-C4D	-3.16	104.09	106.33
17	6	602	CLA	CHB-C1B-NB	-3.15	120.92	124.26
17	1	604	CLA	CHB-C1B-NB	-3.15	120.92	124.26
17	7	612	CLA	CHD-C1D-ND	-3.15	121.56	124.45
17	B	821	CLA	CHB-C1B-NB	-3.15	120.93	124.26
20	3	307	CHL	CHA-C1A-NA	-3.15	119.19	126.40
17	3	311	CLA	CHB-C1B-NB	-3.15	120.93	124.26
20	6	607	CHL	CHA-C1A-NA	-3.14	119.20	126.40
17	B	825	CLA	C1D-ND-C4D	-3.14	104.10	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	825	CLA	CHB-C1B-NB	-3.14	120.93	124.26
17	7	609	CLA	C1D-ND-C4D	-3.14	104.10	106.33
17	8	602	CLA	C2C-C1C-NC	3.14	112.91	109.97
17	5	309	CLA	CHB-C1B-NB	-3.13	120.94	124.26
17	A	835	CLA	CHB-C1B-NB	-3.13	120.94	124.26
17	A	802	CLA	C1D-ND-C4D	-3.13	104.11	106.33
17	1	603	CLA	C1D-ND-C4D	-3.13	104.11	106.33
17	A	818	CLA	C2C-C1C-NC	3.13	112.90	109.97
17	4	605	CLA	C2C-C1C-NC	3.13	112.90	109.97
17	B	832	CLA	C1D-ND-C4D	-3.13	104.11	106.33
20	5	305	CHL	C2C-C3C-C4C	3.13	108.72	106.49
17	B	815	CLA	CAA-C2A-C1A	-3.13	101.73	111.97
17	8	609	CLA	CHB-C1B-NB	-3.12	120.96	124.26
17	A	835	CLA	CHD-C1D-ND	-3.12	121.59	124.45
17	7	605	CLA	C2C-C1C-NC	3.12	112.89	109.97
17	A	811	CLA	C1D-ND-C4D	-3.11	104.12	106.33
17	5	312	CLA	CHB-C1B-NB	-3.11	120.96	124.26
17	A	803	CLA	CHB-C1B-NB	-3.11	120.97	124.26
17	8	603	CLA	CHB-C1B-NB	-3.11	120.97	124.26
17	B	838	CLA	C2C-C1C-NC	3.11	112.88	109.97
17	B	824	CLA	CHB-C1B-NB	-3.11	120.97	124.26
17	B	818	CLA	C2C-C1C-NC	3.11	112.88	109.97
17	B	837	CLA	C1D-ND-C4D	-3.10	104.13	106.33
17	J	102	CLA	C1D-ND-C4D	-3.10	104.13	106.33
17	6	609	CLA	C2C-C1C-NC	3.10	112.88	109.97
17	A	829	CLA	CHB-C1B-NB	-3.10	120.98	124.26
17	8	607	CLA	C2C-C1C-NC	3.10	112.87	109.97
17	7	608	CLA	CHC-C1C-NC	3.09	128.90	124.20
17	5	314	CLA	C2B-C1B-NB	-3.09	108.16	110.23
17	J	102	CLA	CAA-C2A-C1A	-3.09	105.30	112.14
17	A	834	CLA	C1D-ND-C4D	-3.09	104.14	106.33
17	A	802	CLA	CHB-C1B-NB	-3.09	120.99	124.26
17	B	826	CLA	C1D-ND-C4D	-3.08	104.14	106.33
17	1	605	CLA	CHD-C1D-ND	-3.08	121.62	124.45
17	B	807	CLA	CHB-C1B-NB	-3.08	121.00	124.26
17	3	304	CLA	CHB-C1B-NB	-3.08	121.00	124.26
17	7	613	CLA	CHB-C1B-NB	-3.08	121.00	124.26
16	A	801	CL0	C1D-ND-C4D	-3.07	104.15	106.33
17	8	614	CLA	CHB-C1B-NB	-3.07	121.00	124.26
17	A	838	CLA	C1D-ND-C4D	-3.07	104.15	106.33
17	A	830	CLA	C1D-ND-C4D	-3.07	104.16	106.33
17	6	601	CLA	C2C-C1C-NC	3.07	112.84	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	5	303	CLA	C1D-ND-C4D	-3.06	104.16	106.33
17	A	805	CLA	CHB-C1B-NB	-3.06	121.02	124.26
17	A	827	CLA	C2C-C1C-NC	3.06	112.84	109.97
17	B	811	CLA	CHB-C1B-NB	-3.06	121.02	124.26
17	B	809	CLA	CHC-C1C-NC	3.05	128.84	124.20
17	A	829	CLA	C2C-C1C-NC	3.05	112.83	109.97
20	8	606	CHL	CHA-C1A-NA	-3.05	119.41	126.40
17	B	808	CLA	C2C-C1C-NC	3.05	112.83	109.97
17	A	813	CLA	CHB-C1B-NB	-3.05	121.03	124.26
17	A	833	CLA	C2C-C1C-NC	3.05	112.83	109.97
17	B	818	CLA	CHB-C1B-NB	-3.04	121.03	124.26
17	4	605	CLA	CHB-C1B-NB	-3.04	121.03	124.26
17	A	821	CLA	C3A-C2A-C1A	-3.04	96.78	101.34
17	A	830	CLA	CHB-C1B-NB	-3.04	121.04	124.26
17	A	818	CLA	CHB-C1B-NB	-3.04	121.04	124.26
17	A	808	CLA	C2C-C1C-NC	3.04	112.82	109.97
17	8	612	CLA	C1D-ND-C4D	-3.04	104.18	106.33
17	8	611	CLA	CHB-C1B-NB	-3.04	121.04	124.26
17	B	809	CLA	CHC-C1C-C2C	-3.04	118.30	126.73
17	1	607	CLA	CHB-C1B-NB	-3.04	121.04	124.26
17	8	605	CLA	CHB-C1B-NB	-3.03	121.04	124.26
17	5	310	CLA	CHB-C1B-NB	-3.03	121.05	124.26
17	A	833	CLA	CHB-C1B-NB	-3.03	121.05	124.26
17	F	302	CLA	C2C-C1C-NC	3.03	112.81	109.97
17	B	818	CLA	C1D-ND-C4D	-3.03	104.18	106.33
17	5	302	CLA	CHC-C1C-C2C	-3.03	118.32	126.73
17	B	817	CLA	CHB-C1B-NB	-3.03	121.05	124.26
17	4	604	CLA	CHB-C1B-NB	-3.02	121.06	124.26
17	7	602	CLA	C1D-ND-C4D	-3.02	104.19	106.33
17	A	839	CLA	CHB-C1B-NB	-3.02	121.06	124.26
17	B	831	CLA	C1D-ND-C4D	-3.02	104.19	106.33
17	8	607	CLA	C1D-ND-C4D	-3.02	104.19	106.33
17	B	834	CLA	CHB-C1B-NB	-3.02	121.06	124.26
20	5	305	CHL	CAA-C2A-C1A	3.01	121.84	111.97
17	8	605	CLA	CHD-C1D-ND	-3.01	121.69	124.45
17	1	604	CLA	CAA-C2A-C1A	-3.01	105.48	112.14
17	B	804	CLA	CHB-C1B-NB	-3.01	121.07	124.26
20	5	305	CHL	CHD-C1D-ND	-3.01	121.69	124.45
17	A	823	CLA	C2C-C1C-NC	3.00	112.79	109.97
17	A	837	CLA	CHB-C1B-NB	-3.00	121.08	124.26
17	7	601	CLA	CHC-C1C-C2C	-3.00	118.39	126.73
17	5	309	CLA	CAA-C2A-C1A	-3.00	105.50	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	817	CLA	C1D-ND-C4D	-3.00	104.20	106.33
17	3	310	CLA	CHB-C1B-NB	-3.00	121.08	124.26
17	B	827	CLA	C1D-ND-C4D	-2.99	104.21	106.33
17	A	839	CLA	CHC-C1C-C2C	-2.99	118.41	126.73
17	8	612	CLA	C2C-C1C-NC	2.99	112.77	109.97
20	7	606	CHL	CHA-C1A-NA	-2.99	119.55	126.40
17	B	816	CLA	C2C-C1C-NC	2.99	112.77	109.97
17	A	822	CLA	CHB-C1B-NB	-2.99	121.09	124.26
17	B	830	CLA	CHB-C1B-NB	-2.99	121.09	124.26
17	B	812	CLA	CHB-C1B-NB	-2.98	121.10	124.26
17	1	609	CLA	CHC-C1C-NC	2.98	128.73	124.20
17	A	810	CLA	C1D-ND-C4D	-2.98	104.22	106.33
17	5	315	CLA	CHB-C1B-NB	-2.98	121.10	124.26
17	A	813	CLA	C2C-C1C-NC	2.98	112.76	109.97
17	B	834	CLA	C2C-C1C-NC	2.98	112.76	109.97
17	A	821	CLA	C1-C2-C3	-2.98	120.89	126.04
17	A	814	CLA	C1D-ND-C4D	-2.98	104.22	106.33
17	3	312	CLA	C1D-ND-C4D	-2.98	104.22	106.33
17	8	601	CLA	CHC-C1C-C2C	-2.97	118.47	126.73
17	A	816	CLA	CHC-C1C-NC	2.97	128.70	124.20
17	3	305	CLA	C3B-C4B-NB	-2.96	107.77	110.52
17	J	101	CLA	CHB-C1B-NB	-2.96	121.12	124.26
17	A	825	CLA	CAA-C2A-C1A	-2.96	105.59	112.14
17	B	830	CLA	C2C-C1C-NC	2.96	112.74	109.97
17	4	601	CLA	CHC-C1C-C2C	-2.96	118.52	126.73
17	7	603	CLA	CHB-C1B-NB	-2.96	121.13	124.26
17	1	602	CLA	CAA-C2A-C1A	-2.96	105.60	112.14
17	A	835	CLA	CHC-C1C-C2C	-2.95	118.53	126.73
17	5	315	CLA	C1D-ND-C4D	-2.95	104.24	106.33
17	B	836	CLA	C1D-ND-C4D	-2.95	104.24	106.33
17	B	833	CLA	CHB-C1B-NB	-2.95	121.14	124.26
17	B	804	CLA	C3B-C4B-NB	-2.95	107.78	110.52
17	A	838	CLA	CHB-C1B-NB	-2.94	121.14	124.26
20	3	307	CHL	CAA-C2A-C1A	2.94	121.62	111.97
17	A	812	CLA	C1D-ND-C4D	-2.94	104.24	106.33
17	B	814	CLA	CHB-C1B-NB	-2.94	121.14	124.26
20	6	606	CHL	C2B-C1B-NB	2.94	112.20	110.23
17	7	611	CLA	C2C-C1C-NC	2.94	112.73	109.97
17	B	837	CLA	CHB-C1B-NB	-2.94	121.14	124.26
20	3	307	CHL	CHD-C1D-ND	-2.94	121.76	124.45
17	B	806	CLA	CHB-C1B-NB	-2.94	121.15	124.26
17	A	819	CLA	CHB-C1B-NB	-2.93	121.15	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	6	606	CHL	CHA-C1A-NA	-2.93	119.69	126.40
17	5	315	CLA	C2C-C1C-NC	2.93	112.72	109.97
17	7	613	CLA	C2C-C1C-NC	2.92	112.71	109.97
17	1	604	CLA	C1D-ND-C4D	-2.92	104.26	106.33
17	6	609	CLA	C1D-ND-C4D	-2.92	104.26	106.33
17	F	301	CLA	CHB-C1B-NB	-2.92	121.16	124.26
17	6	602	CLA	C2C-C1C-NC	2.92	112.71	109.97
17	7	604	CLA	CHA-C1A-NA	-2.92	119.72	126.40
17	A	824	CLA	CHB-C1B-NB	-2.92	121.17	124.26
17	7	613	CLA	C1D-ND-C4D	-2.92	104.26	106.33
17	8	603	CLA	CHC-C1C-NC	2.91	128.62	124.20
17	3	308	CLA	C3A-C2A-C1A	-2.91	96.98	101.34
17	1	607	CLA	C1D-ND-C4D	-2.91	104.27	106.33
17	6	609	CLA	CHC-C1C-C2C	-2.90	118.67	126.73
17	8	614	CLA	C1D-ND-C4D	-2.90	104.27	106.33
17	5	312	CLA	C2C-C1C-NC	2.90	112.69	109.97
17	1	603	CLA	C2C-C1C-NC	2.90	112.69	109.97
17	3	305	CLA	CAA-C2A-C1A	-2.90	105.72	112.14
17	A	838	CLA	C2C-C1C-NC	2.90	112.69	109.97
17	3	309	CLA	C1D-ND-C4D	-2.90	104.28	106.33
17	1	609	CLA	CHC-C1C-C2C	-2.90	118.69	126.73
17	A	823	CLA	CHC-C1C-C2C	-2.89	118.69	126.73
17	5	304	CLA	C2C-C1C-NC	2.89	112.68	109.97
17	B	817	CLA	C1D-ND-C4D	-2.89	104.28	106.33
17	B	801	CLA	CHB-C1B-NB	-2.89	121.20	124.26
17	B	816	CLA	CHC-C1C-C2C	-2.89	118.70	126.73
17	1	605	CLA	CHC-C1C-C2C	-2.89	118.71	126.73
17	6	610	CLA	C2C-C1C-NC	2.88	112.67	109.97
17	3	308	CLA	CHB-C1B-NB	-2.88	121.20	124.26
17	A	832	CLA	CHC-C1C-NC	2.88	128.58	124.20
17	6	608	CLA	C3B-C4B-NB	-2.88	107.84	110.52
17	7	610	CLA	CHB-C1B-NB	-2.88	121.21	124.26
17	1	610	CLA	C1D-ND-C4D	-2.88	104.29	106.33
17	A	804	CLA	C1D-ND-C4D	-2.88	104.29	106.33
17	B	839	CLA	C1D-ND-C4D	-2.87	104.29	106.33
17	A	837	CLA	C2C-C1C-NC	2.87	112.66	109.97
17	A	816	CLA	CHC-C1C-C2C	-2.87	118.75	126.73
17	A	827	CLA	CHC-C1C-C2C	-2.87	118.76	126.73
20	6	605	CHL	CAA-C2A-C1A	2.87	118.50	112.14
17	8	609	CLA	C1D-ND-C4D	-2.87	104.30	106.33
17	5	304	CLA	CHD-C1D-ND	-2.87	121.82	124.45
17	A	815	CLA	CGD-CBD-CAD	-2.87	101.44	110.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	4	601	CLA	C1D-ND-C4D	-2.87	104.30	106.33
17	A	818	CLA	C1D-ND-C4D	-2.87	104.30	106.33
17	A	821	CLA	CHB-C1B-NB	-2.86	121.23	124.26
17	7	614	CLA	CHB-C1B-NB	-2.86	121.23	124.26
17	4	604	CLA	C2C-C1C-NC	2.86	112.65	109.97
17	A	831	CLA	C1D-ND-C4D	-2.86	104.31	106.33
17	A	816	CLA	C1D-ND-C4D	-2.85	104.31	106.33
17	8	604	CLA	CHB-C1B-NB	-2.85	121.24	124.26
17	8	604	CLA	C1D-ND-C4D	-2.85	104.31	106.33
17	B	819	CLA	CHC-C1C-C2C	-2.85	118.81	126.73
17	A	804	CLA	C2A-C3A-C4A	-2.85	97.27	101.87
17	1	607	CLA	CHA-C1A-NA	-2.85	119.88	126.40
17	7	608	CLA	CHC-C1C-C2C	-2.85	118.82	126.73
17	8	607	CLA	CHC-C1C-C2C	-2.84	118.83	126.73
17	B	817	CLA	CHC-C1C-C2C	-2.84	118.83	126.73
17	8	602	CLA	CHC-C1C-C2C	-2.84	118.84	126.73
17	1	602	CLA	C2C-C1C-NC	2.84	112.63	109.97
17	B	837	CLA	CHC-C1C-C2C	-2.84	118.85	126.73
17	3	311	CLA	C1D-ND-C4D	-2.84	104.32	106.33
17	A	803	CLA	CHC-C1C-C2C	-2.83	118.86	126.73
17	3	305	CLA	C2C-C1C-NC	2.83	112.63	109.97
17	A	818	CLA	CHC-C1C-C2C	-2.83	118.86	126.73
17	3	303	CLA	C2C-C1C-NC	2.83	112.62	109.97
17	B	816	CLA	CHC-C1C-NC	2.83	128.50	124.20
17	F	302	CLA	C3B-C4B-NB	-2.83	107.89	110.52
17	6	604	CLA	C1D-ND-C4D	-2.83	104.33	106.33
17	B	837	CLA	C2C-C1C-NC	2.83	112.62	109.97
17	5	302	CLA	CHA-C1A-NA	-2.83	119.92	126.40
17	B	822	CLA	CHC-C1C-C2C	-2.82	118.88	126.73
17	B	836	CLA	CHC-C1C-C2C	-2.82	118.90	126.73
17	B	810	CLA	CHB-C1B-NB	-2.82	121.28	124.26
17	3	304	CLA	CHC-C1C-NC	2.82	128.48	124.20
17	A	815	CLA	CHC-C1C-NC	2.82	128.47	124.20
17	A	820	CLA	CHC-C1C-NC	2.82	128.47	124.20
17	B	823	CLA	C2C-C1C-NC	2.81	112.61	109.97
17	B	835	CLA	C2C-C1C-NC	2.81	112.61	109.97
17	A	809	CLA	CHB-C1B-NB	-2.81	121.28	124.26
17	J	101	CLA	CHC-C1C-C2C	-2.81	118.93	126.73
17	7	602	CLA	C2C-C1C-NC	2.81	112.60	109.97
17	7	611	CLA	CHC-C1C-C2C	-2.81	118.94	126.73
17	6	609	CLA	CHC-C1C-NC	2.80	128.46	124.20
17	A	834	CLA	CHC-C1C-NC	2.80	128.46	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	3	309	CLA	C2C-C1C-NC	2.80	112.60	109.97
17	A	808	CLA	CHC-C1C-C2C	-2.80	118.95	126.73
17	5	310	CLA	C1D-ND-C4D	-2.80	104.35	106.33
17	B	831	CLA	CHC-C1C-NC	2.80	128.45	124.20
17	5	314	CLA	C1D-ND-C4D	-2.80	104.35	106.33
17	4	601	CLA	CHC-C1C-NC	2.80	128.45	124.20
17	A	823	CLA	CHC-C1C-NC	2.80	128.45	124.20
17	8	612	CLA	CHC-C1C-C2C	-2.80	118.96	126.73
17	B	813	CLA	CHC-C1C-NC	2.80	128.44	124.20
17	3	304	CLA	CHC-C1C-C2C	-2.80	118.96	126.73
20	8	606	CHL	CHD-C1D-ND	-2.79	121.89	124.45
17	A	836	CLA	C1D-ND-C4D	-2.79	104.35	106.33
17	A	829	CLA	CHC-C1C-C2C	-2.79	118.98	126.73
17	A	834	CLA	CHC-C1C-C2C	-2.79	118.98	126.73
17	B	812	CLA	C3B-C4B-NB	-2.79	107.93	110.52
17	7	605	CLA	CHB-C1B-NB	-2.79	121.30	124.26
17	8	608	CLA	C2C-C1C-NC	2.79	112.58	109.97
20	6	607	CHL	C2B-C1B-NB	2.79	112.10	110.23
17	B	815	CLA	C1D-ND-C4D	-2.79	104.36	106.33
17	1	610	CLA	C2C-C1C-NC	2.79	112.58	109.97
20	8	606	CHL	CAA-C2A-C1A	2.79	118.31	112.14
17	B	801	CLA	C2C-C1C-NC	2.79	112.58	109.97
17	8	608	CLA	CHB-C1B-NB	-2.78	121.31	124.26
17	J	101	CLA	CHC-C1C-NC	2.78	128.43	124.20
17	3	301	CLA	CHC-C1C-NC	2.78	128.42	124.20
17	B	809	CLA	CAC-C3C-C4C	2.78	128.42	124.81
17	5	308	CLA	C2B-C1B-NB	-2.78	108.37	110.23
17	B	839	CLA	C2C-C1C-NC	2.78	112.58	109.97
17	8	603	CLA	CHC-C1C-C2C	-2.78	119.01	126.73
17	1	609	CLA	C1D-ND-C4D	-2.78	104.36	106.33
17	7	612	CLA	CHC-C1C-C2C	-2.78	119.02	126.73
17	8	613	CLA	CHC-C1C-C2C	-2.78	119.02	126.73
17	B	838	CLA	CHC-C1C-C2C	-2.78	119.02	126.73
17	6	610	CLA	CHA-C1A-NA	-2.77	120.05	126.40
17	7	610	CLA	CAA-C2A-C1A	-2.77	104.96	111.81
17	B	830	CLA	CAA-C2A-C1A	-2.77	106.00	112.14
17	7	607	CLA	C1D-ND-C4D	-2.77	104.37	106.33
17	J	101	CLA	C2C-C1C-NC	2.77	112.57	109.97
20	6	605	CHL	CHA-C1A-NA	-2.77	120.05	126.40
17	A	827	CLA	CHC-C1C-NC	2.77	128.40	124.20
17	A	836	CLA	C2C-C1C-NC	2.77	112.57	109.97
17	B	832	CLA	C2C-C1C-NC	2.77	112.57	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	828	CLA	C1D-ND-C4D	-2.77	104.37	106.33
17	3	308	CLA	C3B-C4B-NB	-2.77	107.95	110.52
17	6	601	CLA	CHC-C1C-C2C	-2.76	119.05	126.73
17	8	611	CLA	C2C-C1C-NC	2.76	112.56	109.97
17	7	603	CLA	CHC-C1C-NC	2.76	128.39	124.20
17	B	822	CLA	CAA-C2A-C1A	-2.76	106.04	112.14
17	1	610	CLA	CHC-C1C-C2C	-2.76	119.08	126.73
17	A	822	CLA	C1D-ND-C4D	-2.75	104.38	106.33
17	A	805	CLA	C2C-C1C-NC	2.75	112.55	109.97
17	6	610	CLA	CHC-C1C-C2C	-2.75	119.08	126.73
20	5	313	CHL	CHA-C1A-NA	-2.75	120.10	126.40
17	7	601	CLA	CHC-C1C-NC	2.75	128.38	124.20
17	4	605	CLA	CHD-C1D-ND	-2.75	121.93	124.45
17	A	803	CLA	C1D-ND-C4D	-2.75	104.38	106.33
17	1	606	CLA	C1D-ND-C4D	-2.75	104.38	106.33
17	A	817	CLA	C3A-C2A-C1A	-2.75	97.23	101.34
17	A	808	CLA	C1D-ND-C4D	-2.75	104.38	106.33
17	B	834	CLA	C1D-ND-C4D	-2.74	104.39	106.33
17	7	613	CLA	CHC-C1C-C2C	-2.74	119.11	126.73
17	B	808	CLA	CHC-C1C-C2C	-2.74	119.12	126.73
17	A	839	CLA	CHC-C1C-NC	2.74	128.36	124.20
17	6	603	CLA	C2C-C1C-NC	2.74	112.54	109.97
17	3	303	CLA	CHC-C1C-C2C	-2.74	119.13	126.73
17	3	311	CLA	C2C-C1C-NC	2.74	112.53	109.97
17	B	831	CLA	CHC-C1C-C2C	-2.73	119.13	126.73
17	A	811	CLA	C2C-C1C-NC	2.73	112.53	109.97
17	8	604	CLA	C2C-C1C-NC	2.73	112.53	109.97
17	B	837	CLA	CAA-C2A-C1A	-2.73	106.09	112.14
17	4	603	CLA	C1D-ND-C4D	-2.73	104.39	106.33
17	B	804	CLA	C3A-C2A-C1A	-2.73	97.25	101.34
17	A	816	CLA	C2C-C1C-NC	2.73	112.53	109.97
17	5	315	CLA	CHC-C1C-C2C	-2.73	119.15	126.73
17	7	604	CLA	C2C-C1C-NC	2.73	112.53	109.97
17	A	826	CLA	CHC-C1C-NC	2.73	128.34	124.20
17	B	824	CLA	CAA-C2A-C1A	-2.73	105.08	111.81
17	5	302	CLA	CHC-C1C-NC	2.73	128.34	124.20
17	B	816	CLA	C1D-ND-C4D	-2.73	104.40	106.33
17	A	809	CLA	C1D-ND-C4D	-2.72	104.40	106.33
17	3	311	CLA	CHC-C1C-C2C	-2.72	119.17	126.73
17	A	812	CLA	CHC-C1C-C2C	-2.72	119.17	126.73
17	7	602	CLA	CHC-C1C-C2C	-2.72	119.17	126.73
17	B	804	CLA	CHC-C1C-NC	2.72	128.33	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	809	CLA	C1D-ND-C4D	-2.72	104.40	106.33
17	4	604	CLA	CHC-C1C-C2C	-2.72	119.18	126.73
17	A	810	CLA	CHC-C1C-NC	2.72	128.32	124.20
17	7	612	CLA	CHC-C1C-NC	2.71	128.32	124.20
17	3	304	CLA	C1D-ND-C4D	-2.71	104.41	106.33
17	4	602	CLA	CHC-C1C-C2C	-2.71	119.19	126.73
17	A	821	CLA	C1D-ND-C4D	-2.71	104.41	106.33
17	7	611	CLA	CHC-C1C-NC	2.71	128.31	124.20
17	B	837	CLA	CHC-C1C-NC	2.71	128.31	124.20
17	5	304	CLA	CHC-C1C-C2C	-2.71	119.21	126.73
17	1	606	CLA	C2C-C1C-NC	2.70	112.50	109.97
17	B	829	CLA	CGD-CBD-CAD	-2.70	101.98	110.73
17	A	805	CLA	CHC-C1C-C2C	-2.70	119.22	126.73
17	A	839	CLA	C1D-ND-C4D	-2.70	104.42	106.33
17	F	302	CLA	CHC-C1C-C2C	-2.70	119.23	126.73
17	A	831	CLA	CHA-C1A-NA	-2.70	120.22	126.40
17	A	837	CLA	CHC-C1C-C2C	-2.70	119.24	126.73
17	4	605	CLA	CHC-C1C-C2C	-2.70	119.24	126.73
17	A	807	CLA	CHB-C1B-NB	-2.69	121.41	124.26
17	A	821	CLA	CHC-C1C-NC	2.69	128.29	124.20
17	8	601	CLA	CHC-C1C-NC	2.69	128.29	124.20
16	A	801	CL0	C2C-C1C-NC	2.69	112.49	109.97
17	4	602	CLA	CHC-C1C-NC	2.69	128.29	124.20
17	A	829	CLA	CAA-C2A-C1A	-2.69	106.18	112.14
17	6	604	CLA	CHC-C1C-C2C	-2.69	119.26	126.73
17	B	820	CLA	C1D-ND-C4D	-2.69	104.43	106.33
17	A	811	CLA	CHC-C1C-C2C	-2.69	119.27	126.73
17	A	820	CLA	CHC-C1C-C2C	-2.68	119.27	126.73
17	1	608	CLA	CHC-C1C-NC	2.68	128.27	124.20
17	3	308	CLA	CHC-C1C-NC	2.68	128.27	124.20
17	A	810	CLA	CHC-C1C-C2C	-2.68	119.28	126.73
17	B	834	CLA	CHC-C1C-C2C	-2.68	119.28	126.73
17	1	603	CLA	CHC-C1C-C2C	-2.68	119.28	126.73
17	A	819	CLA	CHC-C1C-C2C	-2.68	119.28	126.73
17	B	805	CLA	CAA-C2A-C1A	-2.68	106.21	112.14
17	A	842	CLA	C4A-NA-C1A	-2.68	105.50	106.71
17	1	608	CLA	CHC-C1C-C2C	-2.68	119.29	126.73
17	B	835	CLA	CHC-C1C-C2C	-2.68	119.29	126.73
17	6	603	CLA	CHC-C1C-C2C	-2.68	119.29	126.73
17	5	304	CLA	CHA-C1A-NA	-2.68	120.27	126.40
17	B	811	CLA	CHC-C1C-NC	2.67	128.26	124.20
17	5	307	CLA	C2C-C1C-NC	2.67	112.48	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	4	603	CLA	CHB-C1B-NB	-2.67	121.43	124.26
17	A	838	CLA	CHC-C1C-C2C	-2.67	119.31	126.73
17	6	604	CLA	CHC-C1C-NC	2.67	128.26	124.20
17	B	825	CLA	CHC-C1C-C2C	-2.67	119.31	126.73
17	B	825	CLA	CHC-C1C-NC	2.67	128.25	124.20
17	8	608	CLA	CAA-C2A-C1A	-2.67	106.24	112.14
17	8	602	CLA	CHC-C1C-NC	2.67	128.25	124.20
17	B	811	CLA	CHC-C1C-C2C	-2.67	119.32	126.73
17	8	608	CLA	CHC-C1C-C2C	-2.67	119.32	126.73
17	3	310	CLA	CAA-C2A-C1A	-2.66	105.23	111.81
17	A	804	CLA	CAA-C2A-C1A	-2.66	106.24	112.14
17	B	810	CLA	CHC-C1C-NC	2.66	128.24	124.20
17	J	102	CLA	CHC-C1C-C2C	-2.66	119.34	126.73
17	8	605	CLA	CHC-C1C-C2C	-2.66	119.34	126.73
17	B	823	CLA	CHC-C1C-C2C	-2.66	119.34	126.73
17	A	831	CLA	C2C-C1C-NC	2.66	112.46	109.97
17	A	814	CLA	CHC-C1C-C2C	-2.66	119.35	126.73
17	A	819	CLA	C2C-C1C-NC	2.66	112.46	109.97
17	6	610	CLA	CHC-C1C-NC	2.66	128.23	124.20
17	3	303	CLA	CHC-C1C-NC	2.66	128.23	124.20
17	B	838	CLA	CHA-C1A-NA	-2.65	120.32	126.40
17	8	613	CLA	C1D-ND-C4D	-2.65	104.45	106.33
17	3	301	CLA	CHC-C1C-C2C	-2.65	119.36	126.73
17	1	605	CLA	CHA-C1A-NA	-2.65	120.33	126.40
17	3	302	CLA	C2C-C1C-NC	2.65	112.45	109.97
17	5	301	CLA	CHC-C1C-NC	2.65	128.22	124.20
17	A	822	CLA	C2C-C1C-NC	2.65	112.45	109.97
17	8	611	CLA	CHC-C1C-C2C	-2.65	119.38	126.73
17	A	830	CLA	CHC-C1C-C2C	-2.65	119.38	126.73
17	7	604	CLA	C1D-ND-C4D	-2.65	104.45	106.33
17	6	610	CLA	CHD-C1D-ND	-2.65	122.02	124.45
17	A	834	CLA	C2C-C1C-NC	2.65	112.45	109.97
20	5	305	CHL	C4B-CHC-C1C	-2.65	120.06	126.34
17	A	831	CLA	CHC-C1C-C2C	-2.64	119.38	126.73
17	B	830	CLA	CHC-C1C-C2C	-2.64	119.38	126.73
17	1	610	CLA	CHC-C1C-NC	2.64	128.21	124.20
17	B	817	CLA	CHC-C1C-NC	2.64	128.21	124.20
17	J	102	CLA	CHC-C1C-NC	2.64	128.21	124.20
17	4	602	CLA	C2C-C1C-NC	2.64	112.44	109.97
17	8	614	CLA	C2C-C1C-NC	2.64	112.44	109.97
17	A	805	CLA	CHC-C1C-NC	2.64	128.21	124.20
17	A	837	CLA	C1D-ND-C4D	-2.64	104.46	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	7	602	CLA	CHC-C1C-NC	2.64	128.21	124.20
17	A	833	CLA	CHC-C1C-C2C	-2.64	119.40	126.73
17	8	607	CLA	CHC-C1C-NC	2.64	128.20	124.20
17	7	607	CLA	CHC-C1C-C2C	-2.64	119.41	126.73
17	A	823	CLA	C1D-ND-C4D	-2.64	104.46	106.33
17	F	302	CLA	C1D-ND-C4D	-2.63	104.46	106.33
17	A	842	CLA	C3B-C4B-NB	-2.63	108.07	110.52
17	3	306	CLA	CHC-C1C-NC	2.63	128.20	124.20
17	3	305	CLA	CHB-C1B-NB	-2.63	121.47	124.26
17	3	312	CLA	CHB-C1B-NB	-2.63	121.47	124.26
17	B	838	CLA	C1D-ND-C4D	-2.63	104.47	106.33
17	7	610	CLA	C1D-ND-C4D	-2.63	104.47	106.33
17	8	601	CLA	C1D-ND-C4D	-2.63	104.47	106.33
17	A	813	CLA	CHC-C1C-C2C	-2.63	119.42	126.73
17	A	804	CLA	CHB-C1B-NB	-2.63	121.47	124.26
17	B	818	CLA	CHC-C1C-C2C	-2.63	119.42	126.73
17	B	833	CLA	CHC-C1C-C2C	-2.63	119.42	126.73
17	B	839	CLA	CHC-C1C-C2C	-2.63	119.43	126.73
17	6	602	CLA	CHC-C1C-C2C	-2.63	119.43	126.73
17	B	826	CLA	CHB-C1B-NB	-2.63	121.48	124.26
17	A	819	CLA	CHC-C1C-NC	2.63	128.19	124.20
17	8	604	CLA	CHC-C1C-C2C	-2.62	119.44	126.73
17	5	311	CLA	C1D-ND-C4D	-2.62	104.47	106.33
17	A	826	CLA	CHC-C1C-C2C	-2.62	119.45	126.73
17	B	833	CLA	C2C-C1C-NC	2.62	112.43	109.97
17	5	301	CLA	CHC-C1C-C2C	-2.62	119.46	126.73
17	5	306	CLA	CHC-C1C-NC	2.62	128.17	124.20
17	7	605	CLA	CHC-C1C-C2C	-2.62	119.46	126.73
17	A	811	CLA	CHC-C1C-NC	2.62	128.17	124.20
17	3	313	CLA	C3A-C2A-C1A	-2.62	97.42	101.34
17	7	604	CLA	CHC-C1C-C2C	-2.62	119.46	126.73
17	7	614	CLA	CHA-C1A-NA	-2.62	120.41	126.40
17	1	606	CLA	CHC-C1C-C2C	-2.62	119.47	126.73
17	A	829	CLA	CHC-C1C-NC	2.61	128.17	124.20
17	B	824	CLA	C3B-C4B-NB	-2.61	108.09	110.52
17	6	603	CLA	CHC-C1C-NC	2.61	128.17	124.20
17	B	822	CLA	CHC-C1C-NC	2.61	128.16	124.20
17	A	814	CLA	CHC-C1C-NC	2.61	128.16	124.20
17	B	820	CLA	CHB-C1B-NB	-2.61	121.50	124.26
20	Z	601	CHL	CHA-C1A-NA	-2.61	120.43	126.40
17	A	808	CLA	CHC-C1C-NC	2.61	128.16	124.20
17	B	823	CLA	CHA-C1A-NA	-2.61	120.43	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	841	CLA	CHC-C1C-C2C	-2.61	119.49	126.73
17	A	836	CLA	CHC-C1C-C2C	-2.60	119.50	126.73
17	B	819	CLA	C2D-C1D-ND	-2.60	108.19	110.10
17	A	842	CLA	C2C-C1C-NC	2.60	112.41	109.97
17	5	314	CLA	CGD-CBD-CAD	-2.60	102.31	110.73
17	5	308	CLA	CHC-C1C-NC	2.60	128.15	124.20
17	5	311	CLA	CHC-C1C-NC	2.60	128.15	124.20
17	7	614	CLA	CHC-C1C-C2C	-2.60	119.52	126.73
17	A	835	CLA	CHC-C1C-NC	2.60	128.14	124.20
17	B	817	CLA	CAA-C2A-C1A	-2.60	106.39	112.14
17	6	608	CLA	CHC-C1C-C2C	-2.60	119.52	126.73
17	B	812	CLA	C1D-ND-C4D	-2.59	104.49	106.33
17	B	824	CLA	C2C-C1C-NC	2.59	112.40	109.97
17	7	603	CLA	CHC-C1C-C2C	-2.59	119.53	126.73
17	3	311	CLA	CHC-C1C-NC	2.59	128.13	124.20
17	B	825	CLA	C2C-C1C-NC	2.59	112.40	109.97
17	B	804	CLA	CHC-C4B-NB	-2.59	121.52	124.26
17	A	818	CLA	CHC-C1C-NC	2.59	128.13	124.20
17	A	830	CLA	CHC-C1C-NC	2.59	128.13	124.20
20	6	606	CHL	CHC-C1C-NC	2.59	128.13	124.20
17	B	813	CLA	CHC-C1C-C2C	-2.59	119.55	126.73
17	A	825	CLA	CHC-C1C-NC	2.58	128.12	124.20
20	1	601	CHL	CHC-C1C-NC	2.58	128.12	124.20
17	A	824	CLA	C1D-ND-C4D	-2.58	104.50	106.33
17	1	602	CLA	CHC-C1C-C2C	-2.58	119.56	126.73
17	7	604	CLA	CGD-CBD-CAD	-2.58	102.37	110.73
17	5	315	CLA	CHC-C1C-NC	2.58	128.12	124.20
17	A	828	CLA	CHC-C1C-C2C	-2.58	119.56	126.73
17	8	601	CLA	CHA-C1A-NA	-2.58	120.49	126.40
17	B	829	CLA	CHC-C1C-C2C	-2.58	119.57	126.73
17	3	302	CLA	CHC-C1C-C2C	-2.58	119.57	126.73
20	1	601	CHL	CHA-C1A-NA	-2.58	120.49	126.40
17	7	613	CLA	CHC-C1C-NC	2.58	128.11	124.20
17	8	614	CLA	CHC-C1C-C2C	-2.58	119.58	126.73
17	A	828	CLA	C2C-C1C-NC	2.58	112.39	109.97
17	6	608	CLA	C1D-ND-C4D	-2.57	104.51	106.33
17	B	810	CLA	CHC-C1C-C2C	-2.57	119.58	126.73
17	B	804	CLA	CHA-C1A-NA	-2.57	120.50	126.40
17	B	832	CLA	CHC-C1C-C2C	-2.57	119.58	126.73
17	5	311	CLA	CHC-C1C-C2C	-2.57	119.58	126.73
17	8	612	CLA	CHC-C1C-NC	2.57	128.11	124.20
17	B	801	CLA	C1D-ND-C4D	-2.57	104.51	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	5	307	CLA	CHC-C1C-C2C	-2.57	119.58	126.73
17	B	801	CLA	CHC-C1C-C2C	-2.57	119.59	126.73
17	B	833	CLA	CHC-C1C-NC	2.57	128.10	124.20
17	J	102	CLA	C2C-C1C-NC	2.57	112.38	109.97
17	A	828	CLA	C1D-ND-C4D	-2.57	104.51	106.33
17	A	822	CLA	CHC-C1C-C2C	-2.57	119.59	126.73
17	A	802	CLA	CHC-C1C-NC	2.57	128.10	124.20
17	A	808	CLA	CHA-C1A-NA	-2.57	120.52	126.40
17	F	301	CLA	C3B-C4B-NB	-2.57	108.13	110.52
17	7	602	CLA	CAA-C2A-C1A	-2.56	106.46	112.14
17	B	823	CLA	C1D-ND-C4D	-2.56	104.51	106.33
17	A	805	CLA	CAA-C2A-C1A	-2.56	106.47	112.14
17	B	809	CLA	C2C-C1C-NC	2.56	112.37	109.97
17	A	815	CLA	CHC-C1C-C2C	-2.56	119.61	126.73
17	B	829	CLA	CHC-C1C-NC	2.56	128.09	124.20
17	7	601	CLA	CHA-C1A-NA	-2.56	120.54	126.40
17	7	612	CLA	C2C-C1C-NC	2.56	112.37	109.97
17	7	614	CLA	CHC-C1C-NC	2.56	128.08	124.20
17	A	843	CLA	C1D-ND-C4D	-2.56	104.52	106.33
17	B	838	CLA	CHC-C1C-NC	2.56	128.08	124.20
17	A	831	CLA	CHC-C1C-NC	2.55	128.08	124.20
17	6	609	CLA	CHA-C1A-NA	-2.55	120.55	126.40
17	A	802	CLA	CHC-C1C-C2C	-2.55	119.64	126.73
20	7	606	CHL	C2C-C3C-C4C	2.55	108.31	106.49
17	A	830	CLA	C2C-C1C-NC	2.55	112.36	109.97
20	Z	601	CHL	CHC-C1C-NC	2.55	128.07	124.20
17	1	608	CLA	CHA-C1A-NA	-2.55	120.56	126.40
17	7	610	CLA	C3B-C4B-NB	-2.55	108.15	110.52
17	A	841	CLA	C1D-ND-C4D	-2.55	104.53	106.33
17	7	614	CLA	C1D-ND-C4D	-2.55	104.53	106.33
17	A	821	CLA	CHC-C1C-C2C	-2.54	119.67	126.73
17	5	309	CLA	CHC-C1C-C2C	-2.54	119.68	126.73
17	8	611	CLA	CHC-C1C-NC	2.54	128.06	124.20
17	A	843	CLA	CHC-C1C-C2C	-2.54	119.68	126.73
17	6	601	CLA	C1D-ND-C4D	-2.54	104.53	106.33
17	A	842	CLA	CHA-C1A-NA	-2.53	120.59	126.40
17	6	604	CLA	C2C-C1C-NC	2.53	112.35	109.97
17	A	816	CLA	CAA-C2A-C1A	-2.53	106.53	112.14
17	3	312	CLA	CHC-C1C-C2C	-2.53	119.69	126.73
17	B	829	CLA	C2C-C1C-NC	2.53	112.34	109.97
17	B	808	CLA	CHC-C1C-NC	2.53	128.04	124.20
20	3	307	CHL	C2A-C1A-CHA	2.53	128.28	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	3	310	CLA	C2B-C1B-NB	-2.53	108.54	110.23
17	A	843	CLA	CHC-C1C-NC	2.53	128.04	124.20
17	1	608	CLA	C2C-C1C-NC	2.53	112.34	109.97
17	B	835	CLA	CHC-C1C-NC	2.53	128.04	124.20
17	7	610	CLA	CHC-C1C-NC	2.53	128.04	124.20
17	4	604	CLA	C1D-ND-C4D	-2.53	104.54	106.33
17	6	601	CLA	CHC-C1C-NC	2.53	128.03	124.20
17	B	823	CLA	CHC-C1C-NC	2.53	128.03	124.20
17	A	814	CLA	C2C-C1C-NC	2.52	112.34	109.97
17	3	309	CLA	CHC-C1C-C2C	-2.52	119.72	126.73
17	B	836	CLA	CHC-C1C-NC	2.52	128.03	124.20
17	1	603	CLA	CHC-C1C-NC	2.52	128.03	124.20
17	5	302	CLA	C1D-ND-C4D	-2.52	104.55	106.33
17	5	309	CLA	CHC-C1C-NC	2.52	128.02	124.20
17	7	603	CLA	CAA-C2A-C1A	-2.52	106.57	112.14
17	3	313	CLA	CHC-C1C-NC	2.52	128.02	124.20
17	A	842	CLA	CHC-C1C-C2C	-2.51	119.75	126.73
17	B	828	CLA	CHC-C1C-C2C	-2.51	119.75	126.73
17	A	819	CLA	C1D-ND-C4D	-2.51	104.55	106.33
17	1	606	CLA	CHC-C1C-NC	2.51	128.02	124.20
17	B	828	CLA	CHC-C1C-NC	2.51	128.01	124.20
17	8	608	CLA	CHC-C1C-NC	2.51	128.01	124.20
17	5	312	CLA	CHC-C1C-C2C	-2.51	119.75	126.73
17	3	303	CLA	C1D-ND-C4D	-2.51	104.55	106.33
17	8	613	CLA	CHC-C1C-NC	2.51	128.01	124.20
17	A	834	CLA	C3B-C4B-NB	-2.51	108.19	110.52
17	3	313	CLA	CHC-C1C-C2C	-2.51	119.76	126.73
17	A	803	CLA	CHC-C1C-NC	2.51	128.01	124.20
17	A	841	CLA	CHC-C1C-NC	2.51	128.01	124.20
17	5	312	CLA	CHA-C1A-NA	-2.51	120.66	126.40
17	B	815	CLA	CHC-C1C-C2C	-2.51	119.77	126.73
17	B	815	CLA	CHC-C1C-NC	2.51	128.00	124.20
20	3	307	CHL	C2C-C3C-C4C	2.50	108.27	106.49
17	1	607	CLA	CHC-C1C-NC	2.50	128.00	124.20
20	5	313	CHL	C2C-C3C-C4C	2.50	108.27	106.49
17	3	306	CLA	C2A-C3A-C4A	-2.50	97.83	101.87
17	3	311	CLA	CHA-C1A-NA	-2.50	120.67	126.40
17	B	827	CLA	CHC-C1C-NC	2.50	127.99	124.20
17	3	306	CLA	C1D-ND-C4D	-2.50	104.56	106.33
17	B	802	CLA	CHC-C1C-NC	2.50	127.99	124.20
17	B	810	CLA	C3A-C2A-C1A	-2.50	97.60	101.34
17	4	605	CLA	C1D-ND-C4D	-2.50	104.56	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	814	CLA	CHC-C1C-NC	2.49	127.99	124.20
17	3	306	CLA	CHC-C1C-C2C	-2.49	119.80	126.73
17	5	304	CLA	CHC-C1C-NC	2.49	127.98	124.20
17	B	807	CLA	C2C-C1C-NC	2.49	112.31	109.97
17	6	610	CLA	C1D-ND-C4D	-2.49	104.57	106.33
17	B	839	CLA	CHC-C1C-NC	2.49	127.98	124.20
20	3	307	CHL	C4B-CHC-C1C	-2.48	120.44	126.34
17	4	604	CLA	CHC-C1C-NC	2.48	127.97	124.20
17	3	302	CLA	CAA-C2A-C1A	-2.48	106.65	112.14
17	7	607	CLA	CHC-C1C-NC	2.48	127.97	124.20
17	6	608	CLA	CHC-C1C-NC	2.48	127.97	124.20
17	5	314	CLA	CHC-C1C-C2C	-2.48	119.84	126.73
17	5	308	CLA	C1D-ND-C4D	-2.48	104.58	106.33
17	6	608	CLA	CAA-C2A-C1A	-2.48	106.66	112.14
17	3	308	CLA	CHC-C1C-C2C	-2.48	119.85	126.73
17	7	610	CLA	C2A-C3A-C4A	-2.48	98.63	101.78
17	7	604	CLA	CHC-C1C-NC	2.48	127.96	124.20
17	B	820	CLA	C3B-C4B-NB	-2.47	108.22	110.52
17	5	310	CLA	CHC-C1C-C2C	-2.47	119.86	126.73
20	6	605	CHL	CHB-C1B-NB	2.47	126.88	124.26
17	A	841	CLA	C3B-C4B-NB	-2.47	108.22	110.52
17	8	614	CLA	CHC-C1C-NC	2.47	127.96	124.20
17	6	608	CLA	C2C-C1C-NC	2.47	112.29	109.97
17	7	609	CLA	CHC-C1C-C2C	-2.47	119.86	126.73
17	A	825	CLA	CHC-C1C-C2C	-2.47	119.86	126.73
17	5	314	CLA	C2C-C1C-NC	2.47	112.29	109.97
17	F	301	CLA	CAA-C2A-C1A	-2.47	106.67	112.14
17	1	604	CLA	CHC-C1C-NC	2.47	127.95	124.20
17	5	306	CLA	CHC-C1C-C2C	-2.47	119.87	126.73
17	1	605	CLA	CHC-C1C-NC	2.47	127.94	124.20
17	8	607	CLA	CHA-C1A-NA	-2.47	120.75	126.40
17	7	607	CLA	C2C-C1C-NC	2.47	112.28	109.97
17	8	610	CLA	CHC-C1C-C2C	-2.47	119.88	126.73
17	B	814	CLA	CHC-C1C-C2C	-2.46	119.88	126.73
17	7	609	CLA	C2C-C1C-NC	2.46	112.28	109.97
17	A	838	CLA	CHC-C1C-NC	2.46	127.94	124.20
17	B	834	CLA	CHC-C1C-NC	2.46	127.94	124.20
17	F	302	CLA	CHC-C1C-NC	2.46	127.94	124.20
17	A	807	CLA	CHC-C1C-C2C	-2.46	119.89	126.73
17	5	307	CLA	CHC-C1C-NC	2.46	127.94	124.20
17	1	604	CLA	CHC-C1C-C2C	-2.46	119.89	126.73
17	B	827	CLA	CHC-C1C-C2C	-2.46	119.90	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	7	606	CHL	CHC-C1C-NC	2.46	127.93	124.20
17	8	604	CLA	CHC-C1C-NC	2.46	127.93	124.20
17	A	822	CLA	CHC-C1C-NC	2.46	127.93	124.20
17	A	836	CLA	CHC-C1C-NC	2.45	127.93	124.20
17	A	841	CLA	CHB-C1B-NB	-2.45	121.66	124.26
17	A	830	CLA	CGD-CBD-CAD	-2.45	102.79	110.73
20	6	607	CHL	CHC-C1C-NC	2.45	127.92	124.20
17	8	603	CLA	C2C-C1C-NC	2.45	112.27	109.97
17	B	826	CLA	CHC-C1C-NC	2.45	127.92	124.20
17	7	614	CLA	C2C-C1C-NC	2.45	112.27	109.97
17	B	822	CLA	CHA-C1A-NA	-2.45	120.79	126.40
17	B	820	CLA	CHC-C1C-NC	2.45	127.92	124.20
17	A	804	CLA	C3B-C4B-NB	-2.44	108.25	110.52
17	B	834	CLA	CHA-C1A-NA	-2.44	120.80	126.40
17	B	805	CLA	CHA-C1A-NA	-2.44	120.80	126.40
17	B	808	CLA	CHA-C1A-NA	-2.44	120.80	126.40
17	A	802	CLA	C2C-C1C-NC	2.44	112.26	109.97
17	4	603	CLA	CHC-C1C-NC	2.44	127.91	124.20
17	8	605	CLA	CHA-C1A-NA	-2.44	120.81	126.40
17	5	308	CLA	CHC-C1C-C2C	-2.44	119.95	126.73
17	A	837	CLA	CHC-C1C-NC	2.44	127.90	124.20
20	6	607	CHL	C4B-CHC-C1C	-2.44	120.55	126.34
17	A	807	CLA	C1D-ND-C4D	-2.44	104.60	106.33
17	A	832	CLA	C2C-C1C-NC	2.44	112.26	109.97
17	A	807	CLA	C2C-C1C-NC	2.44	112.25	109.97
17	5	307	CLA	C1D-ND-C4D	-2.43	104.61	106.33
17	A	828	CLA	CHC-C1C-NC	2.43	127.89	124.20
17	5	312	CLA	CAA-C2A-C1A	-2.43	106.76	112.14
17	7	601	CLA	C1D-ND-C4D	-2.42	104.61	106.33
17	B	819	CLA	CAA-C2A-C1A	-2.42	106.78	112.14
17	A	824	CLA	C2C-C1C-NC	2.42	112.24	109.97
17	8	610	CLA	C2C-C1C-NC	2.42	112.24	109.97
17	B	818	CLA	CGD-CBD-CAD	-2.42	102.89	110.73
20	1	601	CHL	C4B-CHC-C1C	-2.42	120.60	126.34
17	3	305	CLA	CHC-C1C-C2C	-2.42	120.01	126.73
17	B	805	CLA	C3B-C4B-NB	-2.42	108.27	110.52
17	3	304	CLA	C2C-C1C-NC	2.42	112.23	109.97
17	B	833	CLA	C1D-ND-C4D	-2.41	104.62	106.33
17	8	610	CLA	C1D-ND-C4D	-2.41	104.62	106.33
17	A	812	CLA	CHC-C1C-NC	2.41	127.86	124.20
17	3	302	CLA	CHC-C1C-NC	2.41	127.86	124.20
17	7	610	CLA	CHC-C1C-C2C	-2.41	120.04	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	4	605	CLA	CHC-C1C-NC	2.41	127.86	124.20
17	8	610	CLA	CHC-C1C-NC	2.41	127.86	124.20
17	B	829	CLA	C1D-ND-C4D	-2.41	104.62	106.33
17	7	609	CLA	CHC-C1C-NC	2.40	127.85	124.20
17	5	303	CLA	CHC-C1C-C2C	-2.40	120.05	126.73
17	B	832	CLA	CHC-C1C-NC	2.40	127.85	124.20
17	5	310	CLA	CHC-C1C-NC	2.40	127.85	124.20
17	B	826	CLA	C3B-C4B-NB	-2.40	108.29	110.52
17	A	841	CLA	CHA-C1A-NA	-2.40	120.90	126.40
17	B	824	CLA	CHC-C1C-C2C	-2.40	120.06	126.73
20	7	606	CHL	C4B-CHC-C1C	-2.40	120.64	126.34
17	B	805	CLA	CHC-C1C-NC	2.40	127.84	124.20
17	A	826	CLA	C3B-C4B-NB	-2.40	108.29	110.52
17	4	603	CLA	CHA-C1A-NA	-2.40	120.91	126.40
17	A	810	CLA	C2C-C1C-NC	2.40	112.22	109.97
20	Z	601	CHL	C4B-CHC-C1C	-2.40	120.66	126.34
17	A	842	CLA	CHC-C1C-NC	2.40	127.84	124.20
17	B	806	CLA	CHC-C1C-NC	2.40	127.84	124.20
17	B	802	CLA	CHA-C1A-NA	-2.39	120.92	126.40
17	3	310	CLA	CHA-C1A-NA	-2.39	120.92	126.40
17	3	308	CLA	C2B-C1B-NB	-2.39	108.63	110.23
17	5	311	CLA	C2C-C1C-NC	2.39	112.21	109.97
17	1	609	CLA	C2C-C1C-NC	2.39	112.21	109.97
17	B	829	CLA	CHA-C1A-NA	-2.39	120.93	126.40
17	3	313	CLA	C1D-ND-C4D	-2.39	104.64	106.33
20	3	307	CHL	CHC-C1C-NC	2.39	127.82	124.20
20	6	606	CHL	CHB-C1B-NB	2.38	126.78	124.26
20	8	606	CHL	CHC-C1C-NC	2.38	127.82	124.20
17	8	609	CLA	CAA-C2A-C1A	-2.38	106.87	112.14
17	6	610	CLA	C2A-C1A-CHA	2.38	128.02	123.86
17	4	601	CLA	CHA-C1A-NA	-2.38	120.95	126.40
17	B	820	CLA	CHC-C1C-C2C	-2.38	120.12	126.73
17	A	836	CLA	C3B-C4B-NB	-2.38	108.31	110.52
17	A	809	CLA	CAA-C2A-C1A	-2.38	106.88	112.14
17	A	841	CLA	C1-C2-C3	-2.38	121.94	126.04
17	B	807	CLA	CHC-C1C-C2C	-2.37	120.13	126.73
17	6	602	CLA	CHC-C1C-NC	2.37	127.81	124.20
17	A	817	CLA	CHC-C1C-NC	2.37	127.80	124.20
20	5	313	CHL	C2B-C1B-NB	2.37	111.82	110.23
17	1	602	CLA	CHC-C1C-NC	2.37	127.80	124.20
17	A	817	CLA	CHC-C1C-C2C	-2.37	120.14	126.73
17	7	612	CLA	CHA-C1A-NA	-2.37	120.97	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	820	CLA	C2C-C1C-NC	2.37	112.19	109.97
20	5	313	CHL	C4B-CHC-C1C	-2.37	120.71	126.34
17	B	830	CLA	CHC-C1C-NC	2.37	127.80	124.20
17	5	314	CLA	CHC-C1C-NC	2.37	127.80	124.20
17	5	314	CLA	C4B-CHC-C1C	-2.37	120.72	126.34
17	1	607	CLA	CBA-CAA-C2A	2.37	118.74	113.47
17	5	301	CLA	C2C-C1C-NC	2.37	112.19	109.97
17	1	605	CLA	C1D-ND-C4D	-2.37	104.65	106.33
17	B	813	CLA	C3B-C4B-NB	-2.37	108.64	110.23
17	B	815	CLA	C2A-C1A-CHA	2.37	128.00	123.86
17	A	814	CLA	CHA-C1A-NA	-2.37	120.98	126.40
20	5	313	CHL	CHC-C1C-NC	2.37	127.79	124.20
17	7	607	CLA	C3B-C4B-NB	-2.36	108.33	110.52
17	3	313	CLA	C2C-C1C-NC	2.36	112.18	109.97
17	A	826	CLA	C2C-C1C-NC	2.35	112.18	109.97
17	3	312	CLA	C2C-C1C-NC	2.35	112.18	109.97
17	A	821	CLA	CHA-C1A-NA	-2.35	121.01	126.40
17	A	806	CLA	CHC-C1C-C2C	-2.35	120.19	126.73
17	B	801	CLA	CHC-C1C-NC	2.35	127.77	124.20
17	B	815	CLA	C2C-C1C-NC	2.35	112.17	109.97
17	A	833	CLA	CHC-C1C-NC	2.35	127.77	124.20
17	B	824	CLA	C3A-C2A-C1A	-2.35	97.66	101.64
17	A	831	CLA	CGD-CBD-CAD	-2.35	103.12	110.73
17	A	813	CLA	CHC-C1C-NC	2.35	127.77	124.20
17	A	813	CLA	CAA-C2A-C1A	-2.35	106.94	112.14
17	F	301	CLA	CHC-C1C-C2C	-2.35	120.21	126.73
17	5	309	CLA	C3B-C4B-NB	-2.35	108.34	110.52
17	B	819	CLA	CHD-C1D-ND	-2.35	122.30	124.45
20	8	606	CHL	C4B-CHC-C1C	-2.34	120.78	126.34
17	7	608	CLA	C2C-C1C-NC	2.34	112.17	109.97
17	8	607	CLA	CAA-C2A-C3A	-2.34	108.40	114.26
17	3	312	CLA	CHC-C1C-NC	2.34	127.76	124.20
17	7	610	CLA	CHA-C1A-NA	-2.34	121.03	126.40
17	7	605	CLA	C1D-ND-C4D	-2.34	104.67	106.33
17	5	304	CLA	C1D-ND-C4D	-2.34	104.67	106.33
17	4	603	CLA	CHC-C1C-C2C	-2.34	120.23	126.73
17	A	839	CLA	CHA-C1A-NA	-2.34	121.04	126.40
17	B	804	CLA	CHC-C1C-C2C	-2.34	120.23	126.73
17	A	832	CLA	CHA-C1A-NA	-2.34	121.04	126.40
17	B	811	CLA	C2C-C1C-NC	2.34	112.16	109.97
17	B	802	CLA	CHC-C1C-C2C	-2.33	120.24	126.73
17	B	820	CLA	C3A-C2A-C1A	-2.33	97.84	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	808	CLA	C1D-ND-C4D	-2.33	104.68	106.33
17	B	805	CLA	CHC-C1C-C2C	-2.33	120.25	126.73
17	1	607	CLA	CHC-C1C-C2C	-2.33	120.25	126.73
17	A	841	CLA	C2C-C1C-NC	2.33	112.16	109.97
17	B	824	CLA	C1D-ND-C4D	-2.33	104.68	106.33
17	A	826	CLA	CHA-C1A-NA	-2.33	121.07	126.40
17	B	812	CLA	CHC-C1C-NC	2.33	127.73	124.20
17	A	806	CLA	CHC-C1C-NC	2.32	127.73	124.20
17	B	816	CLA	CAA-C2A-C1A	-2.32	107.00	112.14
17	F	301	CLA	C1D-ND-C4D	-2.32	104.69	106.33
17	1	609	CLA	CHA-C1A-NA	-2.32	121.08	126.40
17	5	303	CLA	C2C-C1C-NC	2.32	112.15	109.97
17	7	612	CLA	C1D-ND-C4D	-2.32	104.69	106.33
17	B	829	CLA	C3B-C4B-NB	-2.32	108.36	110.52
17	A	832	CLA	CAA-C2A-C1A	-2.32	107.01	112.14
20	7	606	CHL	CAA-C2A-C1A	2.32	117.27	112.14
17	A	807	CLA	CHC-C1C-NC	2.32	127.72	124.20
17	5	311	CLA	CAA-C2A-C1A	-2.32	107.02	112.14
17	6	601	CLA	CAA-C2A-C1A	-2.32	107.02	112.14
17	A	819	CLA	CHA-C1A-NA	-2.31	121.10	126.40
17	A	822	CLA	CHA-C1A-NA	-2.31	121.10	126.40
17	8	609	CLA	CHC-C1C-C2C	-2.31	120.31	126.73
17	A	803	CLA	CHA-C1A-NA	-2.31	121.11	126.40
17	B	833	CLA	C3B-C4B-NB	-2.31	108.38	110.52
17	A	831	CLA	CAA-C2A-C3A	-2.30	108.50	114.26
17	A	843	CLA	C2C-C1C-NC	2.30	112.13	109.97
17	F	301	CLA	CHC-C1C-NC	2.30	127.69	124.20
17	B	821	CLA	CHA-C1A-NA	-2.30	121.13	126.40
20	6	606	CHL	C4B-CHC-C1C	-2.30	120.89	126.34
17	A	824	CLA	CHC-C1C-C2C	-2.29	120.37	126.73
20	5	305	CHL	CHC-C1C-NC	2.29	127.68	124.20
17	A	843	CLA	CHA-C1A-NA	-2.29	121.15	126.40
20	3	307	CHL	C2B-C1B-NB	2.29	111.77	110.23
17	3	310	CLA	CHC-C1C-NC	2.29	127.68	124.20
17	3	310	CLA	CHC-C1C-C2C	-2.29	120.38	126.73
17	A	827	CLA	CHA-C1A-NA	-2.29	121.16	126.40
17	A	804	CLA	C3A-C2A-C1A	-2.28	97.92	101.34
17	B	818	CLA	CHC-C1C-NC	2.28	127.67	124.20
17	A	833	CLA	CHA-C1A-NA	-2.28	121.17	126.40
17	A	810	CLA	CAA-C2A-C1A	-2.28	107.09	112.14
17	3	309	CLA	CHC-C1C-NC	2.28	127.66	124.20
17	B	819	CLA	C3D-C2D-C1D	2.27	108.94	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	7	605	CLA	CHC-C1C-NC	2.27	127.65	124.20
17	A	832	CLA	C4C-C3C-C2C	-2.27	106.38	108.89
17	B	826	CLA	CHC-C1C-C2C	-2.27	120.43	126.73
17	3	306	CLA	C2A-C1A-CHA	2.27	127.83	123.86
17	8	609	CLA	CHC-C1C-NC	2.27	127.64	124.20
17	7	607	CLA	CHA-C1A-NA	-2.26	121.22	126.40
17	A	835	CLA	C1D-ND-C4D	-2.26	104.73	106.33
17	5	306	CLA	CGD-CBD-CAD	-2.26	103.41	110.73
17	5	309	CLA	C2C-C1C-NC	2.26	112.09	109.97
17	3	306	CLA	CHA-C1A-NA	-2.26	121.23	126.40
20	6	605	CHL	C2C-C3C-C4C	2.26	108.10	106.49
17	B	823	CLA	CAA-C2A-C3A	-2.25	108.63	114.26
17	A	838	CLA	CHA-C1A-NA	-2.25	121.24	126.40
17	8	605	CLA	CHC-C1C-NC	2.25	127.62	124.20
17	A	828	CLA	CHA-C1A-NA	-2.25	121.25	126.40
17	5	303	CLA	CHC-C1C-NC	2.25	127.62	124.20
17	A	832	CLA	C1D-ND-C4D	-2.25	104.74	106.33
17	B	827	CLA	C2C-C1C-NC	2.25	112.08	109.97
17	A	827	CLA	C1D-ND-C4D	-2.25	104.74	106.33
17	B	819	CLA	C1D-CHD-C4C	-2.24	121.22	126.06
17	B	812	CLA	CHA-C1A-NA	-2.24	121.26	126.40
17	F	301	CLA	C2C-C1C-NC	2.24	112.07	109.97
17	B	815	CLA	C3D-C4D-ND	2.24	113.86	110.24
20	6	605	CHL	C2B-C1B-NB	2.24	111.73	110.23
16	A	801	CL0	CGD-CBD-CAD	-2.24	103.48	110.73
17	A	836	CLA	CHC-C4B-NB	-2.24	121.89	124.26
17	B	812	CLA	CHC-C1C-C2C	-2.24	120.51	126.73
17	7	611	CLA	C3A-C2A-C1A	2.24	104.69	101.34
17	8	604	CLA	CHA-C1A-NA	-2.23	121.28	126.40
17	A	825	CLA	C3B-C4B-NB	-2.23	108.44	110.52
20	6	606	CHL	CHB-C1B-C2B	-2.23	120.93	127.24
17	A	821	CLA	C3B-C4B-NB	-2.23	108.44	110.52
17	B	815	CLA	CHA-C1A-NA	-2.23	121.29	126.40
17	B	812	CLA	C2A-C3A-C4A	-2.23	98.27	101.87
17	B	806	CLA	CGD-CBD-CAD	-2.23	103.52	110.73
17	B	835	CLA	C1D-ND-C4D	-2.23	104.75	106.33
17	3	310	CLA	C1D-ND-C4D	-2.23	104.75	106.33
17	B	831	CLA	C2C-C1C-NC	2.23	112.06	109.97
17	3	306	CLA	CGD-CBD-CAD	-2.22	103.53	110.73
17	A	809	CLA	CHC-C1C-C2C	-2.22	120.55	126.73
17	B	820	CLA	CHA-C1A-NA	-2.22	121.31	126.40
17	5	307	CLA	CHA-C1A-NA	-2.22	121.31	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	810	CLA	C1D-ND-C4D	-2.22	104.76	106.33
17	A	804	CLA	CHC-C1C-C2C	-2.22	120.56	126.73
17	7	603	CLA	C3A-C2A-C1A	-2.22	98.02	101.34
17	B	819	CLA	C3C-C4C-NC	-2.22	108.08	110.57
16	A	801	CL0	CHA-C1A-NA	-2.22	121.32	126.40
17	8	603	CLA	CHA-C1A-NA	-2.21	121.33	126.40
20	6	605	CHL	CHC-C1C-NC	2.21	127.56	124.20
17	8	608	CLA	CHA-C1A-NA	-2.21	121.33	126.40
17	B	807	CLA	CHC-C1C-NC	2.21	127.56	124.20
17	6	604	CLA	CHA-C1A-NA	-2.21	121.33	126.40
17	A	837	CLA	CHA-C1A-NA	-2.21	121.34	126.40
20	7	606	CHL	C2B-C1B-NB	2.21	111.71	110.23
17	1	604	CLA	CHA-C1A-NA	-2.21	121.34	126.40
17	A	828	CLA	CAA-C2A-C1A	-2.21	107.26	112.14
20	5	305	CHL	C2B-C1B-NB	2.21	111.71	110.23
17	B	806	CLA	C2A-C3A-C4A	-2.21	98.31	101.87
17	5	312	CLA	CHC-C1C-NC	2.20	127.55	124.20
17	8	605	CLA	C1D-ND-C4D	-2.20	104.77	106.33
17	3	306	CLA	C3B-C4B-NB	-2.20	108.47	110.52
20	7	606	CHL	CHB-C1B-NB	2.20	126.59	124.26
17	3	303	CLA	CHA-C1A-NA	-2.20	121.36	126.40
17	6	601	CLA	CHA-C1A-NA	-2.20	121.36	126.40
17	8	613	CLA	CHA-C1A-NA	-2.20	121.37	126.40
17	1	604	CLA	C2C-C1C-NC	2.20	112.03	109.97
17	8	610	CLA	CHA-C1A-NA	-2.20	121.37	126.40
17	B	801	CLA	C2B-C1B-NB	-2.19	108.76	110.23
17	B	811	CLA	C3B-C4B-NB	-2.19	108.48	110.52
17	A	809	CLA	CHA-C1A-NA	-2.19	121.38	126.40
17	B	836	CLA	CHA-C1A-NA	-2.19	121.38	126.40
17	7	613	CLA	CHA-C1A-NA	-2.19	121.39	126.40
17	B	839	CLA	CHA-C1A-NA	-2.18	121.40	126.40
17	A	818	CLA	CHA-C1A-NA	-2.18	121.41	126.40
17	A	806	CLA	CAA-C2A-C1A	-2.18	107.32	112.14
17	A	827	CLA	CAA-C2A-C1A	-2.18	107.32	112.14
17	5	301	CLA	CHA-C1A-NA	-2.18	121.41	126.40
17	A	804	CLA	CHC-C1C-NC	2.17	127.50	124.20
17	1	608	CLA	CAA-C2A-C3A	-2.17	108.83	114.26
17	1	610	CLA	CHA-C1A-NA	-2.17	121.42	126.40
17	7	608	CLA	CAA-C2A-C1A	-2.17	107.33	112.14
20	6	605	CHL	C4B-CHC-C1C	-2.17	121.19	126.34
17	A	817	CLA	C2C-C1C-NC	2.17	112.00	109.97
17	4	603	CLA	CBA-CAA-C2A	2.17	118.29	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	8	606	CHL	CHB-C1B-NB	2.16	126.55	124.26
17	1	603	CLA	CHA-C1A-NA	-2.16	121.44	126.40
17	B	817	CLA	CHA-C1A-NA	-2.16	121.45	126.40
17	A	825	CLA	C2C-C1C-NC	2.16	112.00	109.97
17	5	310	CLA	CHA-C1A-NA	-2.16	121.45	126.40
17	5	303	CLA	CHA-C1A-NA	-2.16	121.46	126.40
17	7	603	CLA	C2C-C1C-NC	2.16	111.99	109.97
17	B	821	CLA	CHC-C1C-NC	2.16	127.47	124.20
17	3	308	CLA	C1D-ND-C4D	-2.16	104.80	106.33
17	B	807	CLA	CHA-C1A-NA	-2.15	121.47	126.40
17	6	604	CLA	CAA-C2A-C1A	-2.15	107.37	112.14
17	B	821	CLA	CHC-C1C-C2C	-2.15	120.76	126.73
17	3	312	CLA	C3B-C4B-NB	-2.15	108.52	110.52
17	3	306	CLA	C2C-C1C-NC	2.15	111.98	109.97
17	5	308	CLA	C4B-CHC-C1C	-2.15	121.25	126.34
17	B	824	CLA	CHC-C1C-NC	2.15	127.46	124.20
20	5	313	CHL	CHB-C1B-NB	2.14	126.53	124.26
17	3	313	CLA	C3B-C4B-NB	-2.14	108.53	110.52
17	3	313	CLA	CHA-C1A-NA	-2.14	121.50	126.40
20	6	607	CHL	C2C-C3C-C4C	2.14	108.02	106.49
17	B	806	CLA	CHC-C1C-C2C	-2.14	120.79	126.73
17	A	809	CLA	CHC-C1C-NC	2.14	127.45	124.20
17	A	835	CLA	CHA-C1A-NA	-2.13	121.52	126.40
17	6	608	CLA	C4B-CHC-C1C	-2.13	121.30	126.34
17	B	813	CLA	CHA-C1A-NA	-2.13	121.53	126.40
17	B	811	CLA	CHA-C1A-NA	-2.12	121.53	126.40
17	A	829	CLA	CHA-C1A-NA	-2.12	121.54	126.40
17	B	814	CLA	C2C-C1C-NC	2.12	111.96	109.97
17	3	310	CLA	C2A-C1A-CHA	2.12	127.56	123.85
17	7	605	CLA	CHA-C1A-NA	-2.12	121.54	126.40
17	8	609	CLA	C2C-C1C-NC	2.12	111.96	109.97
17	5	310	CLA	C2C-C1C-NC	2.12	111.96	109.97
17	A	824	CLA	CHA-C1A-NA	-2.12	121.55	126.40
17	3	301	CLA	CAA-C2A-C1A	-2.11	107.47	112.14
17	3	305	CLA	C2B-C1B-NB	-2.11	108.82	110.23
17	A	838	CLA	CGD-CBD-CAD	-2.11	103.90	110.73
17	B	833	CLA	CHA-C1A-NA	-2.11	121.57	126.40
17	7	605	CLA	CAA-C2A-C1A	-2.11	107.47	112.14
17	B	802	CLA	C2B-C1B-NB	-2.10	108.82	110.23
17	8	608	CLA	CGD-CBD-CAD	-2.10	103.92	110.73
17	A	842	CLA	CAA-C2A-C1A	-2.10	107.49	112.14
17	5	315	CLA	CHA-C1A-NA	-2.10	121.59	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	835	CLA	CHA-C1A-NA	-2.10	121.59	126.40
17	B	825	CLA	CHA-C1A-NA	-2.10	121.59	126.40
17	6	602	CLA	CHA-C1A-NA	-2.10	121.60	126.40
17	B	839	CLA	C3B-C4B-NB	-2.10	108.57	110.52
17	A	825	CLA	CHA-C1A-NA	-2.10	121.60	126.40
17	A	810	CLA	CHA-C1A-NA	-2.09	121.61	126.40
17	3	310	CLA	C2C-C1C-NC	2.09	111.93	109.97
17	4	605	CLA	CHA-C1A-NA	-2.09	121.61	126.40
17	B	801	CLA	CHD-C1D-C2D	2.09	129.86	125.48
17	3	310	CLA	CHD-C1D-C2D	2.09	129.86	125.48
17	B	806	CLA	C3D-C4D-ND	2.08	113.61	110.24
17	7	603	CLA	C3D-C4D-ND	2.08	113.61	110.24
17	7	608	CLA	C3D-C4D-ND	2.08	113.61	110.24
17	A	807	CLA	C3B-C4B-NB	-2.08	108.58	110.52
17	A	813	CLA	CHA-C1A-NA	-2.08	121.63	126.40
17	7	614	CLA	C2A-C3A-C4A	-2.08	98.51	101.87
17	5	312	CLA	C1D-ND-C4D	-2.08	104.86	106.33
17	A	824	CLA	CHC-C1C-NC	2.08	127.35	124.20
17	B	831	CLA	CHA-C1A-NA	-2.08	121.64	126.40
17	A	815	CLA	CHA-C1A-NA	-2.07	121.65	126.40
17	A	819	CLA	C3B-C4B-NB	-2.07	108.59	110.52
17	A	804	CLA	C2C-C1C-NC	2.07	111.91	109.97
17	5	303	CLA	C3B-C4B-NB	-2.07	108.59	110.52
17	8	614	CLA	CHA-C1A-NA	-2.07	121.66	126.40
20	Z	601	CHL	CHB-C1B-NB	2.07	126.45	124.26
17	A	812	CLA	CHA-C1A-NA	-2.07	121.66	126.40
20	6	605	CHL	CHB-C1B-C2B	-2.07	121.39	127.24
17	3	301	CLA	C2C-C1C-NC	2.07	111.91	109.97
17	B	827	CLA	C3B-C4B-NB	-2.07	108.59	110.52
17	8	612	CLA	CHA-C1A-NA	-2.07	121.66	126.40
17	5	308	CLA	CHD-C1D-C2D	2.07	129.81	125.48
17	F	302	CLA	CHA-C1A-NA	-2.07	121.67	126.40
17	7	602	CLA	CHA-C1A-NA	-2.07	121.67	126.40
17	B	806	CLA	C2A-C1A-CHA	2.07	127.47	123.86
17	B	805	CLA	C2C-C1C-NC	2.06	111.90	109.97
17	6	608	CLA	CHA-C1A-NA	-2.06	121.68	126.40
17	A	805	CLA	CHA-C1A-NA	-2.06	121.68	126.40
17	6	603	CLA	CGD-CBD-CAD	-2.06	104.06	110.73
17	B	810	CLA	CHA-C1A-NA	-2.06	121.69	126.40
20	1	601	CHL	CHB-C1B-NB	2.05	126.43	124.26
20	Z	601	CHL	C2C-C3C-C4C	2.05	107.95	106.49
17	4	602	CLA	CHA-C1A-NA	-2.05	121.70	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	3	305	CLA	CHC-C1C-NC	2.05	127.31	124.20
17	B	819	CLA	CHC-C4B-NB	-2.05	122.09	124.26
17	B	832	CLA	CHA-C1A-NA	-2.05	121.71	126.40
17	A	823	CLA	CHA-C1A-NA	-2.05	121.71	126.40
17	8	602	CLA	CHA-C1A-NA	-2.05	121.71	126.40
17	3	305	CLA	C1D-ND-C4D	-2.05	104.88	106.33
20	1	601	CHL	C2C-C3C-C4C	2.05	107.95	106.49
17	1	606	CLA	CHD-C1D-C2D	2.04	129.77	125.48
17	3	302	CLA	CHA-C1A-NA	-2.04	121.72	126.40
17	A	824	CLA	C3B-C4B-NB	-2.04	108.62	110.52
17	A	836	CLA	CHA-C1A-NA	-2.04	121.73	126.40
17	A	839	CLA	CAA-C2A-C1A	-2.04	107.63	112.14
17	B	814	CLA	CHA-C1A-NA	-2.04	121.73	126.40
17	B	811	CLA	C1D-ND-C4D	-2.04	104.89	106.33
17	J	102	CLA	CHA-C1A-NA	-2.04	121.74	126.40
17	7	609	CLA	CGD-CBD-CAD	-2.03	104.14	110.73
20	Z	601	CHL	C2B-C1B-NB	2.03	111.60	110.23
17	A	821	CLA	C2C-C1C-NC	2.03	111.88	109.97
17	7	614	CLA	CHD-C1D-C2D	2.03	129.74	125.48
17	B	828	CLA	CHA-C1A-NA	-2.03	121.75	126.40
20	6	607	CHL	C2A-C1A-CHA	2.03	127.41	123.86
17	B	824	CLA	CHA-C1A-NA	-2.03	121.76	126.40
17	B	822	CLA	C1D-ND-C4D	-2.03	104.90	106.33
20	6	606	CHL	C2C-C3C-C4C	2.02	107.93	106.49
17	F	301	CLA	CHA-C1A-NA	-2.02	121.77	126.40
17	3	301	CLA	CHA-C1A-NA	-2.02	121.77	126.40
17	B	837	CLA	CHA-C1A-NA	-2.02	121.77	126.40
17	A	816	CLA	CHA-C1A-NA	-2.02	121.78	126.40
17	A	811	CLA	CAA-C2A-C1A	-2.02	107.68	112.14
17	A	817	CLA	CHA-C1A-NA	-2.01	121.78	126.40
17	3	304	CLA	CHA-C1A-NA	-2.01	121.79	126.40
17	A	807	CLA	CHA-C1A-NA	-2.01	121.79	126.40
17	A	802	CLA	CHC-C4B-NB	-2.01	122.13	124.26
17	A	830	CLA	CHA-C1A-NA	-2.01	121.80	126.40
17	B	815	CLA	C1-C2-C3	-2.01	122.57	126.04
17	7	604	CLA	C1D-CHD-C4C	-2.01	121.73	126.06
17	7	610	CLA	C2C-C1C-NC	2.00	111.85	109.97
17	B	820	CLA	C2C-C1C-NC	2.00	111.85	109.97

There are no chirality outliers.

All (609) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	A	802	CLA	C1A-C2A-CAA-CBA
17	A	802	CLA	CHA-CBD-CGD-O1D
17	A	802	CLA	CHA-CBD-CGD-O2D
17	A	803	CLA	C2B-C3B-CAB-CBB
17	A	803	CLA	C4B-C3B-CAB-CBB
17	A	803	CLA	CHA-CBD-CGD-O1D
17	A	803	CLA	CHA-CBD-CGD-O2D
17	A	805	CLA	C1A-C2A-CAA-CBA
17	A	805	CLA	C4B-C3B-CAB-CBB
17	A	806	CLA	C1A-C2A-CAA-CBA
17	A	807	CLA	CHA-CBD-CGD-O1D
17	A	807	CLA	CHA-CBD-CGD-O2D
17	A	809	CLA	C1A-C2A-CAA-CBA
17	A	811	CLA	C2B-C3B-CAB-CBB
17	A	811	CLA	C4B-C3B-CAB-CBB
17	A	812	CLA	C3A-C2A-CAA-CBA
17	A	814	CLA	C1A-C2A-CAA-CBA
17	A	814	CLA	C4B-C3B-CAB-CBB
17	A	816	CLA	C1A-C2A-CAA-CBA
17	A	816	CLA	C3A-C2A-CAA-CBA
17	A	817	CLA	C1A-C2A-CAA-CBA
17	A	817	CLA	C3A-C2A-CAA-CBA
17	A	817	CLA	C2B-C3B-CAB-CBB
17	A	817	CLA	C4B-C3B-CAB-CBB
17	A	819	CLA	CHA-CBD-CGD-O1D
17	A	819	CLA	CHA-CBD-CGD-O2D
17	A	820	CLA	C3A-C2A-CAA-CBA
17	A	821	CLA	C1A-C2A-CAA-CBA
17	A	821	CLA	C3A-C2A-CAA-CBA
17	A	821	CLA	C2B-C3B-CAB-CBB
17	A	821	CLA	C4B-C3B-CAB-CBB
17	A	821	CLA	C2-C3-C5-C6
17	A	822	CLA	C1A-C2A-CAA-CBA
17	A	824	CLA	C2B-C3B-CAB-CBB
17	A	824	CLA	C4B-C3B-CAB-CBB
17	A	827	CLA	C2B-C3B-CAB-CBB
17	A	827	CLA	C4B-C3B-CAB-CBB
17	A	828	CLA	C2B-C3B-CAB-CBB
17	A	828	CLA	C4B-C3B-CAB-CBB
17	A	829	CLA	C1A-C2A-CAA-CBA
17	A	829	CLA	C2B-C3B-CAB-CBB
17	A	829	CLA	C4B-C3B-CAB-CBB
17	A	830	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
17	A	831	CLA	C1A-C2A-CAA-CBA
17	A	832	CLA	C1A-C2A-CAA-CBA
17	A	832	CLA	CHA-CBD-CGD-O1D
17	A	833	CLA	C2B-C3B-CAB-CBB
17	A	833	CLA	C4B-C3B-CAB-CBB
17	A	837	CLA	CHA-CBD-CGD-O1D
17	A	837	CLA	CHA-CBD-CGD-O2D
17	A	838	CLA	C1A-C2A-CAA-CBA
17	A	843	CLA	C4B-C3B-CAB-CBB
17	A	843	CLA	CHA-CBD-CGD-O1D
17	A	843	CLA	CHA-CBD-CGD-O2D
17	B	801	CLA	C1A-C2A-CAA-CBA
17	B	801	CLA	C3A-C2A-CAA-CBA
17	B	802	CLA	CHA-CBD-CGD-O1D
17	B	802	CLA	CHA-CBD-CGD-O2D
17	B	804	CLA	C1A-C2A-CAA-CBA
17	B	807	CLA	CAD-CBD-CGD-O1D
17	B	807	CLA	CAD-CBD-CGD-O2D
17	B	808	CLA	C2B-C3B-CAB-CBB
17	B	808	CLA	C4B-C3B-CAB-CBB
17	B	812	CLA	C1A-C2A-CAA-CBA
17	B	812	CLA	C2B-C3B-CAB-CBB
17	B	812	CLA	C4B-C3B-CAB-CBB
17	B	812	CLA	CHA-CBD-CGD-O1D
17	B	812	CLA	CHA-CBD-CGD-O2D
17	B	813	CLA	C1A-C2A-CAA-CBA
17	B	815	CLA	C1A-C2A-CAA-CBA
17	B	815	CLA	CHA-CBD-CGD-O1D
17	B	815	CLA	CHA-CBD-CGD-O2D
17	B	815	CLA	CAD-CBD-CGD-O1D
17	B	815	CLA	CAD-CBD-CGD-O2D
17	B	816	CLA	C3A-C2A-CAA-CBA
17	B	816	CLA	C2B-C3B-CAB-CBB
17	B	816	CLA	C4B-C3B-CAB-CBB
17	B	817	CLA	C1A-C2A-CAA-CBA
17	B	818	CLA	C1A-C2A-CAA-CBA
17	B	818	CLA	C3A-C2A-CAA-CBA
17	B	819	CLA	C1A-C2A-CAA-CBA
17	B	819	CLA	C3A-C2A-CAA-CBA
17	B	820	CLA	C1A-C2A-CAA-CBA
17	B	822	CLA	C1A-C2A-CAA-CBA
17	B	823	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
17	B	823	CLA	CHA-CBD-CGD-O2D
17	B	823	CLA	CAD-CBD-CGD-O1D
17	B	824	CLA	C4B-C3B-CAB-CBB
17	B	825	CLA	C1A-C2A-CAA-CBA
17	B	825	CLA	C3A-C2A-CAA-CBA
17	B	825	CLA	CAD-CBD-CGD-O1D
17	B	825	CLA	CAD-CBD-CGD-O2D
17	B	826	CLA	C1A-C2A-CAA-CBA
17	B	826	CLA	C3A-C2A-CAA-CBA
17	B	827	CLA	C3A-C2A-CAA-CBA
17	B	827	CLA	C2B-C3B-CAB-CBB
17	B	830	CLA	C1A-C2A-CAA-CBA
17	B	832	CLA	C1A-C2A-CAA-CBA
17	B	836	CLA	C1A-C2A-CAA-CBA
17	B	837	CLA	C1A-C2A-CAA-CBA
17	B	838	CLA	C1A-C2A-CAA-CBA
17	B	838	CLA	C2B-C3B-CAB-CBB
17	B	838	CLA	C4B-C3B-CAB-CBB
17	B	839	CLA	C2B-C3B-CAB-CBB
17	B	839	CLA	C4B-C3B-CAB-CBB
17	F	301	CLA	C3A-C2A-CAA-CBA
17	F	302	CLA	C2-C3-C5-C6
17	F	302	CLA	C4-C3-C5-C6
17	J	101	CLA	C1A-C2A-CAA-CBA
17	J	101	CLA	C3A-C2A-CAA-CBA
17	J	102	CLA	C2B-C3B-CAB-CBB
17	J	102	CLA	C4B-C3B-CAB-CBB
17	J	102	CLA	CAD-CBD-CGD-O1D
17	J	102	CLA	CAD-CBD-CGD-O2D
17	1	602	CLA	C1A-C2A-CAA-CBA
17	1	607	CLA	C1A-C2A-CAA-CBA
17	1	607	CLA	CHA-CBD-CGD-O1D
17	1	607	CLA	CHA-CBD-CGD-O2D
17	1	608	CLA	C1A-C2A-CAA-CBA
17	1	609	CLA	CHA-CBD-CGD-O1D
17	1	609	CLA	CHA-CBD-CGD-O2D
17	1	610	CLA	C3A-C2A-CAA-CBA
17	1	610	CLA	CHA-CBD-CGD-O1D
17	1	610	CLA	CHA-CBD-CGD-O2D
17	3	301	CLA	C1A-C2A-CAA-CBA
17	3	301	CLA	C3A-C2A-CAA-CBA
17	3	302	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
17	3	302	CLA	C4B-C3B-CAB-CBB
17	3	304	CLA	C2B-C3B-CAB-CBB
17	3	304	CLA	C4B-C3B-CAB-CBB
17	3	306	CLA	C3A-C2A-CAA-CBA
17	3	306	CLA	C2B-C3B-CAB-CBB
17	3	306	CLA	C4B-C3B-CAB-CBB
17	3	310	CLA	CHA-CBD-CGD-O1D
17	3	310	CLA	CHA-CBD-CGD-O2D
17	3	313	CLA	C2B-C3B-CAB-CBB
17	3	313	CLA	C4B-C3B-CAB-CBB
17	7	603	CLA	CHA-CBD-CGD-O1D
17	7	603	CLA	CHA-CBD-CGD-O2D
17	7	611	CLA	C1A-C2A-CAA-CBA
17	7	611	CLA	C3A-C2A-CAA-CBA
17	7	614	CLA	CHA-CBD-CGD-O1D
17	7	614	CLA	CHA-CBD-CGD-O2D
17	8	601	CLA	C2B-C3B-CAB-CBB
17	8	601	CLA	C4B-C3B-CAB-CBB
17	8	602	CLA	C1A-C2A-CAA-CBA
17	8	602	CLA	C2B-C3B-CAB-CBB
17	8	602	CLA	C4B-C3B-CAB-CBB
17	8	607	CLA	C2B-C3B-CAB-CBB
17	8	607	CLA	C4B-C3B-CAB-CBB
17	8	609	CLA	C1A-C2A-CAA-CBA
17	8	610	CLA	C1A-C2A-CAA-CBA
17	8	610	CLA	CHA-CBD-CGD-O1D
17	8	610	CLA	CHA-CBD-CGD-O2D
17	8	611	CLA	C1A-C2A-CAA-CBA
17	8	611	CLA	C4B-C3B-CAB-CBB
17	4	603	CLA	C1A-C2A-CAA-CBA
17	4	603	CLA	CHA-CBD-CGD-O1D
17	4	603	CLA	CHA-CBD-CGD-O2D
17	5	301	CLA	CHA-CBD-CGD-O1D
17	5	301	CLA	CHA-CBD-CGD-O2D
17	5	302	CLA	C1A-C2A-CAA-CBA
17	5	303	CLA	C4B-C3B-CAB-CBB
17	5	307	CLA	C1A-C2A-CAA-CBA
17	5	307	CLA	C2B-C3B-CAB-CBB
17	5	307	CLA	C4B-C3B-CAB-CBB
17	5	307	CLA	CHA-CBD-CGD-O1D
17	5	307	CLA	CHA-CBD-CGD-O2D
17	5	308	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
17	5	308	CLA	CHA-CBD-CGD-O2D
17	5	309	CLA	C1A-C2A-CAA-CBA
17	5	309	CLA	C3A-C2A-CAA-CBA
17	5	312	CLA	C2B-C3B-CAB-CBB
17	5	312	CLA	C4B-C3B-CAB-CBB
17	6	601	CLA	CHA-CBD-CGD-O1D
17	6	602	CLA	CHA-CBD-CGD-O1D
17	6	602	CLA	CHA-CBD-CGD-O2D
17	6	604	CLA	C2B-C3B-CAB-CBB
17	6	604	CLA	C4B-C3B-CAB-CBB
17	6	609	CLA	C2B-C3B-CAB-CBB
17	6	609	CLA	C4B-C3B-CAB-CBB
17	6	610	CLA	C2B-C3B-CAB-CBB
17	6	610	CLA	C4B-C3B-CAB-CBB
20	3	307	CHL	C1A-C2A-CAA-CBA
20	3	307	CHL	C2B-C3B-CAB-CBB
20	3	307	CHL	C4B-C3B-CAB-CBB
20	7	606	CHL	C4B-C3B-CAB-CBB
20	8	606	CHL	C2B-C3B-CAB-CBB
20	8	606	CHL	C4B-C3B-CAB-CBB
20	5	305	CHL	C1A-C2A-CAA-CBA
20	5	305	CHL	C3A-C2A-CAA-CBA
20	5	313	CHL	CHA-CBD-CGD-O1D
20	5	313	CHL	CHA-CBD-CGD-O2D
20	6	606	CHL	C2B-C3B-CAB-CBB
20	6	606	CHL	C4B-C3B-CAB-CBB
20	6	607	CHL	C3A-C2A-CAA-CBA
17	B	809	CLA	C2C-C3C-CAC-CBC
17	6	609	CLA	C2A-CAA-CBA-CGA
17	B	829	CLA	C2A-CAA-CBA-CGA
17	B	809	CLA	C4C-C3C-CAC-CBC
18	A	840	PQN	C19-C18-C20-C21
17	A	806	CLA	C4B-C3B-CAB-CBB
17	A	809	CLA	C4B-C3B-CAB-CBB
17	A	819	CLA	C4B-C3B-CAB-CBB
17	A	826	CLA	C4B-C3B-CAB-CBB
17	A	835	CLA	C4B-C3B-CAB-CBB
17	B	806	CLA	C4B-C3B-CAB-CBB
17	B	817	CLA	C4B-C3B-CAB-CBB
17	B	818	CLA	C4B-C3B-CAB-CBB
17	B	820	CLA	C4B-C3B-CAB-CBB
17	B	827	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
17	B	831	CLA	C4B-C3B-CAB-CBB
17	7	602	CLA	C4B-C3B-CAB-CBB
17	7	609	CLA	C4B-C3B-CAB-CBB
17	7	614	CLA	C4B-C3B-CAB-CBB
17	8	605	CLA	C4B-C3B-CAB-CBB
17	5	301	CLA	C4B-C3B-CAB-CBB
17	5	302	CLA	C4B-C3B-CAB-CBB
17	5	314	CLA	C4B-C3B-CAB-CBB
20	5	305	CHL	C4B-C3B-CAB-CBB
20	3	307	CHL	C3A-C2A-CAA-CBA
17	F	302	CLA	O2A-C1-C2-C3
17	A	805	CLA	C2B-C3B-CAB-CBB
17	A	806	CLA	C2B-C3B-CAB-CBB
17	A	809	CLA	C2B-C3B-CAB-CBB
17	A	814	CLA	C2B-C3B-CAB-CBB
17	A	819	CLA	C2B-C3B-CAB-CBB
17	A	822	CLA	C2B-C3B-CAB-CBB
17	A	826	CLA	C2B-C3B-CAB-CBB
17	A	835	CLA	C2B-C3B-CAB-CBB
17	A	843	CLA	C2B-C3B-CAB-CBB
17	B	806	CLA	C2B-C3B-CAB-CBB
17	B	817	CLA	C2B-C3B-CAB-CBB
17	B	818	CLA	C2B-C3B-CAB-CBB
17	B	820	CLA	C2B-C3B-CAB-CBB
17	B	824	CLA	C2B-C3B-CAB-CBB
17	B	831	CLA	C2B-C3B-CAB-CBB
17	7	602	CLA	C2B-C3B-CAB-CBB
17	7	609	CLA	C2B-C3B-CAB-CBB
17	7	614	CLA	C2B-C3B-CAB-CBB
17	8	605	CLA	C2B-C3B-CAB-CBB
17	8	611	CLA	C2B-C3B-CAB-CBB
17	5	301	CLA	C2B-C3B-CAB-CBB
17	5	302	CLA	C2B-C3B-CAB-CBB
17	5	303	CLA	C2B-C3B-CAB-CBB
17	5	308	CLA	C2B-C3B-CAB-CBB
17	5	311	CLA	C2B-C3B-CAB-CBB
17	5	314	CLA	C2B-C3B-CAB-CBB
20	7	606	CHL	C2B-C3B-CAB-CBB
20	5	305	CHL	C2B-C3B-CAB-CBB
18	B	840	PQN	C18-C20-C21-C22
17	B	815	CLA	C11-C10-C8-C7
17	A	841	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
17	5	314	CLA	C2C-C3C-CAC-CBC
17	B	815	CLA	C11-C10-C8-C9
17	B	828	CLA	C2C-C3C-CAC-CBC
17	B	802	CLA	C1A-C2A-CAA-CBA
17	B	810	CLA	C1A-C2A-CAA-CBA
17	B	829	CLA	C1A-C2A-CAA-CBA
17	4	605	CLA	C1A-C2A-CAA-CBA
17	A	802	CLA	C3A-C2A-CAA-CBA
17	A	805	CLA	C3A-C2A-CAA-CBA
17	A	831	CLA	C3A-C2A-CAA-CBA
17	B	838	CLA	C3A-C2A-CAA-CBA
17	1	608	CLA	C3A-C2A-CAA-CBA
17	8	611	CLA	C3A-C2A-CAA-CBA
17	4	603	CLA	C3A-C2A-CAA-CBA
17	4	604	CLA	C3A-C2A-CAA-CBA
17	5	302	CLA	C3A-C2A-CAA-CBA
17	5	303	CLA	O2A-C1-C2-C3
17	F	302	CLA	C6-C7-C8-C10
17	F	302	CLA	C6-C7-C8-C9
17	A	821	CLA	C2A-CAA-CBA-CGA
16	A	801	CL0	C4B-C3B-CAB-CBB
17	A	820	CLA	C4B-C3B-CAB-CBB
17	A	822	CLA	C4B-C3B-CAB-CBB
17	B	829	CLA	C4B-C3B-CAB-CBB
17	B	830	CLA	C4B-C3B-CAB-CBB
17	B	834	CLA	C4B-C3B-CAB-CBB
17	1	602	CLA	C4B-C3B-CAB-CBB
17	1	604	CLA	C4B-C3B-CAB-CBB
17	8	609	CLA	C4B-C3B-CAB-CBB
17	4	604	CLA	C4B-C3B-CAB-CBB
17	5	304	CLA	C4B-C3B-CAB-CBB
17	5	308	CLA	C4B-C3B-CAB-CBB
17	5	311	CLA	C4B-C3B-CAB-CBB
20	1	601	CHL	O2A-C1-C2-C3
17	A	841	CLA	C4-C3-C5-C6
17	5	315	CLA	C2A-CAA-CBA-CGA
17	A	820	CLA	C2B-C3B-CAB-CBB
17	B	830	CLA	C2B-C3B-CAB-CBB
17	B	834	CLA	C2B-C3B-CAB-CBB
17	B	835	CLA	C2B-C3B-CAB-CBB
17	1	602	CLA	C2B-C3B-CAB-CBB
17	8	609	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
17	4	604	CLA	C2B-C3B-CAB-CBB
17	5	304	CLA	C2B-C3B-CAB-CBB
17	A	841	CLA	C2-C3-C5-C6
18	A	840	PQN	C24-C23-C25-C26
17	A	821	CLA	C4-C3-C5-C6
20	3	307	CHL	C2A-CAA-CBA-CGA
17	A	828	CLA	C1A-C2A-CAA-CBA
17	A	833	CLA	C1A-C2A-CAA-CBA
17	B	816	CLA	C1A-C2A-CAA-CBA
17	B	827	CLA	C1A-C2A-CAA-CBA
17	F	301	CLA	C1A-C2A-CAA-CBA
17	3	302	CLA	C1A-C2A-CAA-CBA
17	3	306	CLA	C1A-C2A-CAA-CBA
17	3	313	CLA	C1A-C2A-CAA-CBA
17	7	602	CLA	C1A-C2A-CAA-CBA
17	7	607	CLA	C1A-C2A-CAA-CBA
17	7	609	CLA	C1A-C2A-CAA-CBA
17	5	312	CLA	C1A-C2A-CAA-CBA
17	6	602	CLA	C1A-C2A-CAA-CBA
17	6	608	CLA	C1A-C2A-CAA-CBA
20	6	606	CHL	C1A-C2A-CAA-CBA
20	6	607	CHL	C1A-C2A-CAA-CBA
17	A	822	CLA	CAD-CBD-CGD-O2D
17	B	808	CLA	CAD-CBD-CGD-O2D
17	B	820	CLA	CAD-CBD-CGD-O2D
17	B	823	CLA	CAD-CBD-CGD-O2D
17	B	832	CLA	CAD-CBD-CGD-O2D
17	B	836	CLA	CAD-CBD-CGD-O2D
17	3	301	CLA	CAD-CBD-CGD-O2D
17	3	305	CLA	CAD-CBD-CGD-O2D
17	7	608	CLA	CAD-CBD-CGD-O2D
17	7	611	CLA	CAD-CBD-CGD-O2D
17	8	607	CLA	CAD-CBD-CGD-O2D
17	8	611	CLA	CAD-CBD-CGD-O2D
17	8	614	CLA	CAD-CBD-CGD-O2D
17	5	306	CLA	CAD-CBD-CGD-O2D
17	5	309	CLA	CAD-CBD-CGD-O2D
17	6	608	CLA	CAD-CBD-CGD-O2D
16	A	801	CL0	CHA-CBD-CGD-O1D
16	A	801	CL0	CHA-CBD-CGD-O2D
17	A	804	CLA	CHA-CBD-CGD-O1D
17	A	811	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
17	A	811	CLA	CHA-CBD-CGD-O2D
17	A	813	CLA	CHA-CBD-CGD-O1D
17	A	813	CLA	CHA-CBD-CGD-O2D
17	A	818	CLA	CHA-CBD-CGD-O1D
17	A	818	CLA	CHA-CBD-CGD-O2D
17	A	823	CLA	CHA-CBD-CGD-O1D
17	A	823	CLA	CHA-CBD-CGD-O2D
17	A	829	CLA	CHA-CBD-CGD-O1D
17	A	829	CLA	CHA-CBD-CGD-O2D
17	A	832	CLA	CHA-CBD-CGD-O2D
17	A	835	CLA	CHA-CBD-CGD-O1D
17	A	841	CLA	CHA-CBD-CGD-O1D
17	A	842	CLA	CHA-CBD-CGD-O1D
17	A	842	CLA	CHA-CBD-CGD-O2D
17	B	821	CLA	CHA-CBD-CGD-O1D
17	B	821	CLA	CHA-CBD-CGD-O2D
17	B	829	CLA	CHA-CBD-CGD-O1D
17	B	829	CLA	CHA-CBD-CGD-O2D
17	B	834	CLA	CHA-CBD-CGD-O1D
17	B	834	CLA	CHA-CBD-CGD-O2D
17	B	835	CLA	CHA-CBD-CGD-O1D
17	B	835	CLA	CHA-CBD-CGD-O2D
17	J	101	CLA	CHA-CBD-CGD-O1D
17	7	601	CLA	CHA-CBD-CGD-O1D
17	7	601	CLA	CHA-CBD-CGD-O2D
17	7	602	CLA	CHA-CBD-CGD-O1D
17	7	602	CLA	CHA-CBD-CGD-O2D
17	7	605	CLA	CHA-CBD-CGD-O1D
17	7	610	CLA	CHA-CBD-CGD-O1D
17	8	602	CLA	CHA-CBD-CGD-O1D
17	8	602	CLA	CHA-CBD-CGD-O2D
17	8	613	CLA	CHA-CBD-CGD-O2D
17	4	601	CLA	CHA-CBD-CGD-O1D
17	4	601	CLA	CHA-CBD-CGD-O2D
17	5	304	CLA	CHA-CBD-CGD-O1D
17	5	304	CLA	CHA-CBD-CGD-O2D
17	5	311	CLA	CHA-CBD-CGD-O1D
17	5	311	CLA	CHA-CBD-CGD-O2D
17	6	601	CLA	CHA-CBD-CGD-O2D
20	1	601	CHL	CHA-CBD-CGD-O1D
20	Z	601	CHL	CHA-CBD-CGD-O1D
17	4	602	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
17	5	315	CLA	C1A-C2A-CAA-CBA
17	A	807	CLA	C4B-C3B-CAB-CBB
17	A	808	CLA	C4B-C3B-CAB-CBB
17	A	810	CLA	C4B-C3B-CAB-CBB
17	A	818	CLA	C4B-C3B-CAB-CBB
17	A	837	CLA	C4B-C3B-CAB-CBB
17	A	839	CLA	C4B-C3B-CAB-CBB
17	B	809	CLA	C4B-C3B-CAB-CBB
17	B	835	CLA	C4B-C3B-CAB-CBB
17	1	603	CLA	C4B-C3B-CAB-CBB
17	1	607	CLA	C4B-C3B-CAB-CBB
17	3	305	CLA	C4B-C3B-CAB-CBB
17	3	312	CLA	C4B-C3B-CAB-CBB
17	7	603	CLA	C4B-C3B-CAB-CBB
17	7	613	CLA	C4B-C3B-CAB-CBB
17	8	613	CLA	C4B-C3B-CAB-CBB
17	4	603	CLA	C4B-C3B-CAB-CBB
17	4	605	CLA	C4B-C3B-CAB-CBB
17	5	315	CLA	C4B-C3B-CAB-CBB
17	6	601	CLA	C4B-C3B-CAB-CBB
17	6	602	CLA	C4B-C3B-CAB-CBB
20	6	605	CHL	C4B-C3B-CAB-CBB
17	A	804	CLA	CAD-CBD-CGD-O1D
17	A	813	CLA	CAD-CBD-CGD-O1D
17	A	818	CLA	CAD-CBD-CGD-O1D
17	A	832	CLA	CAD-CBD-CGD-O1D
17	A	835	CLA	CAD-CBD-CGD-O1D
17	A	836	CLA	CAD-CBD-CGD-O1D
17	A	841	CLA	CAD-CBD-CGD-O1D
17	A	842	CLA	CAD-CBD-CGD-O1D
17	B	834	CLA	CAD-CBD-CGD-O1D
17	B	835	CLA	CAD-CBD-CGD-O1D
17	J	101	CLA	CAD-CBD-CGD-O1D
17	1	603	CLA	CAD-CBD-CGD-O1D
17	7	601	CLA	CAD-CBD-CGD-O1D
17	7	605	CLA	CAD-CBD-CGD-O1D
17	6	601	CLA	CAD-CBD-CGD-O1D
20	1	601	CHL	CAD-CBD-CGD-O1D
20	Z	601	CHL	CAD-CBD-CGD-O1D
17	B	834	CLA	C4C-C3C-CAC-CBC
17	A	837	CLA	C3A-C2A-CAA-CBA
17	5	308	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	6	606	CHL	C4C-C3C-CAC-CBC
17	5	314	CLA	C2A-CAA-CBA-CGA
16	A	801	CL0	C2B-C3B-CAB-CBB
17	A	818	CLA	C2B-C3B-CAB-CBB
17	A	837	CLA	C2B-C3B-CAB-CBB
17	B	802	CLA	C2B-C3B-CAB-CBB
17	B	811	CLA	C2B-C3B-CAB-CBB
17	B	829	CLA	C2B-C3B-CAB-CBB
17	1	604	CLA	C2B-C3B-CAB-CBB
17	1	607	CLA	C2B-C3B-CAB-CBB
17	3	312	CLA	C2B-C3B-CAB-CBB
17	7	610	CLA	C2B-C3B-CAB-CBB
17	8	613	CLA	C2B-C3B-CAB-CBB
17	4	603	CLA	C2B-C3B-CAB-CBB
17	4	605	CLA	C2B-C3B-CAB-CBB
17	6	602	CLA	C2B-C3B-CAB-CBB
20	6	607	CHL	C2B-C3B-CAB-CBB
17	3	312	CLA	C2C-C3C-CAC-CBC
17	B	834	CLA	C2C-C3C-CAC-CBC
17	5	306	CLA	C2-C1-O2A-CGA
17	A	823	CLA	C2C-C3C-CAC-CBC
17	B	821	CLA	C2C-C3C-CAC-CBC
18	A	840	PQN	C17-C18-C20-C21
18	A	840	PQN	C22-C23-C25-C26
18	B	840	PQN	C17-C18-C20-C21
20	6	606	CHL	C2C-C3C-CAC-CBC
20	1	601	CHL	C4-C3-C5-C6
17	5	315	CLA	CAA-CBA-CGA-O2A
17	B	802	CLA	C4B-C3B-CAB-CBB
17	B	811	CLA	C4B-C3B-CAB-CBB
17	7	610	CLA	C4B-C3B-CAB-CBB
17	5	306	CLA	C4B-C3B-CAB-CBB
20	6	607	CHL	C4B-C3B-CAB-CBB
17	B	815	CLA	C4-C3-C5-C6
17	B	815	CLA	C2-C1-O2A-CGA
17	B	815	CLA	C3A-C2A-CAA-CBA
17	5	315	CLA	CAA-CBA-CGA-O1A
17	4	602	CLA	CAA-CBA-CGA-O1A
17	A	841	CLA	C2C-C3C-CAC-CBC
17	A	841	CLA	C1A-C2A-CAA-CBA
17	A	807	CLA	C2B-C3B-CAB-CBB
17	A	808	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
17	A	810	CLA	C2B-C3B-CAB-CBB
17	A	815	CLA	C2B-C3B-CAB-CBB
17	A	816	CLA	C2B-C3B-CAB-CBB
17	A	839	CLA	C2B-C3B-CAB-CBB
17	B	809	CLA	C2B-C3B-CAB-CBB
17	B	815	CLA	C2B-C3B-CAB-CBB
17	B	825	CLA	C2B-C3B-CAB-CBB
17	1	603	CLA	C2B-C3B-CAB-CBB
17	3	305	CLA	C2B-C3B-CAB-CBB
17	7	601	CLA	C2B-C3B-CAB-CBB
17	7	603	CLA	C2B-C3B-CAB-CBB
17	7	613	CLA	C2B-C3B-CAB-CBB
17	5	310	CLA	C2B-C3B-CAB-CBB
17	5	315	CLA	C2B-C3B-CAB-CBB
17	6	601	CLA	C2B-C3B-CAB-CBB
20	6	605	CHL	C2B-C3B-CAB-CBB
17	B	812	CLA	C3A-C2A-CAA-CBA
17	1	605	CLA	C3A-C2A-CAA-CBA
17	4	602	CLA	CAA-CBA-CGA-O2A
17	7	612	CLA	CAA-CBA-CGA-O2A
18	B	840	PQN	C14-C13-C15-C16
17	A	820	CLA	C1A-C2A-CAA-CBA
17	8	613	CLA	C1A-C2A-CAA-CBA
20	6	605	CHL	C1A-C2A-CAA-CBA
17	B	802	CLA	CAA-CBA-CGA-O2A
17	A	816	CLA	C4B-C3B-CAB-CBB
17	A	832	CLA	C4B-C3B-CAB-CBB
17	B	815	CLA	C4B-C3B-CAB-CBB
17	B	825	CLA	C4B-C3B-CAB-CBB
17	3	308	CLA	C4B-C3B-CAB-CBB
17	7	601	CLA	C4B-C3B-CAB-CBB
17	B	810	CLA	CAA-CBA-CGA-O2A
17	6	610	CLA	CAA-CBA-CGA-O2A
17	8	607	CLA	C2C-C3C-CAC-CBC
17	7	612	CLA	CAA-CBA-CGA-O1A
16	A	801	CL0	CAD-CBD-CGD-O2D
17	A	810	CLA	CAD-CBD-CGD-O2D
17	A	816	CLA	CAD-CBD-CGD-O2D
17	A	831	CLA	CAD-CBD-CGD-O2D
17	A	838	CLA	CAD-CBD-CGD-O2D
17	A	839	CLA	CAD-CBD-CGD-O2D
17	B	816	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
17	B	818	CLA	CAD-CBD-CGD-O2D
17	B	819	CLA	CAD-CBD-CGD-O2D
17	B	824	CLA	CAD-CBD-CGD-O2D
17	B	829	CLA	CAD-CBD-CGD-O2D
17	B	830	CLA	CAD-CBD-CGD-O2D
17	B	833	CLA	CAD-CBD-CGD-O2D
17	1	604	CLA	CAD-CBD-CGD-O2D
17	1	605	CLA	CAD-CBD-CGD-O2D
17	1	608	CLA	CAD-CBD-CGD-O2D
17	3	304	CLA	CAD-CBD-CGD-O2D
17	3	308	CLA	CAD-CBD-CGD-O2D
17	7	607	CLA	CAD-CBD-CGD-O2D
17	7	610	CLA	CAD-CBD-CGD-O2D
17	8	601	CLA	CAD-CBD-CGD-O2D
17	5	311	CLA	CAD-CBD-CGD-O2D
17	6	603	CLA	CAD-CBD-CGD-O2D
20	5	305	CHL	CAD-CBD-CGD-O2D
18	B	840	PQN	C12-C13-C15-C16
17	8	603	CLA	CAA-CBA-CGA-O1A
17	5	306	CLA	O2A-C1-C2-C3
17	5	303	CLA	CAA-CBA-CGA-O2A
17	B	802	CLA	CAA-CBA-CGA-O1A
17	8	603	CLA	CAA-CBA-CGA-O2A
17	A	804	CLA	CHA-CBD-CGD-O2D
17	A	812	CLA	CHA-CBD-CGD-O2D
17	A	820	CLA	CHA-CBD-CGD-O1D
17	A	820	CLA	CHA-CBD-CGD-O2D
17	A	825	CLA	CHA-CBD-CGD-O1D
17	A	825	CLA	CHA-CBD-CGD-O2D
17	A	835	CLA	CHA-CBD-CGD-O2D
17	A	836	CLA	CHA-CBD-CGD-O1D
17	A	841	CLA	CHA-CBD-CGD-O2D
17	B	806	CLA	CHA-CBD-CGD-O1D
17	B	806	CLA	CHA-CBD-CGD-O2D
17	B	807	CLA	CHA-CBD-CGD-O1D
17	B	807	CLA	CHA-CBD-CGD-O2D
17	B	809	CLA	CHA-CBD-CGD-O1D
17	B	809	CLA	CHA-CBD-CGD-O2D
17	B	810	CLA	CHA-CBD-CGD-O1D
17	B	810	CLA	CHA-CBD-CGD-O2D
17	B	817	CLA	CHA-CBD-CGD-O1D
17	B	817	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
17	B	822	CLA	CHA-CBD-CGD-O1D
17	B	822	CLA	CHA-CBD-CGD-O2D
17	B	827	CLA	CHA-CBD-CGD-O2D
17	F	302	CLA	CHA-CBD-CGD-O1D
17	F	302	CLA	CHA-CBD-CGD-O2D
17	1	602	CLA	CHA-CBD-CGD-O1D
17	1	602	CLA	CHA-CBD-CGD-O2D
17	1	603	CLA	CHA-CBD-CGD-O1D
17	3	302	CLA	CHA-CBD-CGD-O2D
17	3	311	CLA	CHA-CBD-CGD-O1D
17	3	311	CLA	CHA-CBD-CGD-O2D
17	7	605	CLA	CHA-CBD-CGD-O2D
17	7	610	CLA	CHA-CBD-CGD-O2D
17	7	612	CLA	CHA-CBD-CGD-O1D
17	7	612	CLA	CHA-CBD-CGD-O2D
17	7	613	CLA	CHA-CBD-CGD-O1D
17	8	605	CLA	CHA-CBD-CGD-O1D
17	8	605	CLA	CHA-CBD-CGD-O2D
17	8	613	CLA	CHA-CBD-CGD-O1D
17	4	602	CLA	CHA-CBD-CGD-O2D
17	5	303	CLA	CHA-CBD-CGD-O1D
17	5	303	CLA	CHA-CBD-CGD-O2D
17	5	314	CLA	CHA-CBD-CGD-O1D
17	5	314	CLA	CHA-CBD-CGD-O2D
17	6	603	CLA	CHA-CBD-CGD-O1D
17	6	603	CLA	CHA-CBD-CGD-O2D
20	1	601	CHL	CHA-CBD-CGD-O2D
20	Z	601	CHL	CHA-CBD-CGD-O2D
17	B	810	CLA	CAA-CBA-CGA-O1A
17	A	835	CLA	C4C-C3C-CAC-CBC
17	5	314	CLA	CAA-CBA-CGA-O2A
17	1	605	CLA	C2B-C3B-CAB-CBB
17	3	308	CLA	C2B-C3B-CAB-CBB
17	A	841	CLA	C4C-C3C-CAC-CBC
17	F	302	CLA	C2C-C3C-CAC-CBC
17	6	610	CLA	CAA-CBA-CGA-O1A
20	3	307	CHL	CAA-CBA-CGA-O2A
20	1	601	CHL	C2-C3-C5-C6
17	A	815	CLA	C4B-C3B-CAB-CBB
17	A	830	CLA	C4B-C3B-CAB-CBB
17	B	819	CLA	C4B-C3B-CAB-CBB
17	B	832	CLA	C4B-C3B-CAB-CBB

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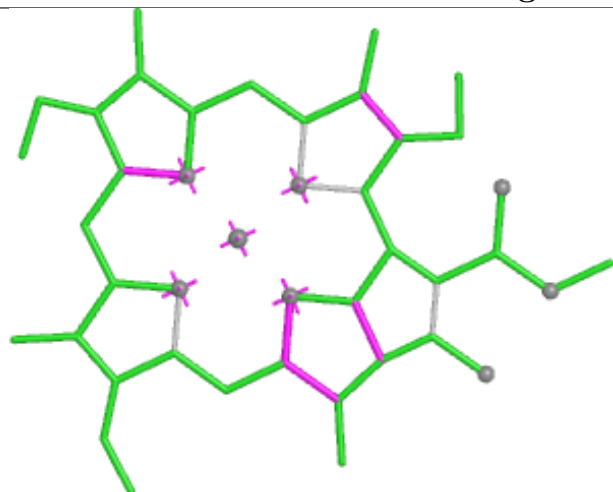
Mol	Chain	Res	Type	Atoms
17	B	837	CLA	C4B-C3B-CAB-CBB
17	F	301	CLA	C4B-C3B-CAB-CBB
17	7	604	CLA	C4B-C3B-CAB-CBB
17	8	614	CLA	C4B-C3B-CAB-CBB
17	5	310	CLA	C4B-C3B-CAB-CBB
17	6	603	CLA	C4B-C3B-CAB-CBB
17	7	607	CLA	C4C-C3C-CAC-CBC
17	5	303	CLA	CAA-CBA-CGA-O1A
17	3	304	CLA	CAA-CBA-CGA-O2A
17	A	809	CLA	CAD-CBD-CGD-O1D
17	B	801	CLA	CAD-CBD-CGD-O1D
17	B	827	CLA	CAD-CBD-CGD-O1D
17	B	839	CLA	CAD-CBD-CGD-O1D
17	3	311	CLA	CAD-CBD-CGD-O1D
17	5	314	CLA	CAD-CBD-CGD-O1D
17	6	610	CLA	CAD-CBD-CGD-O1D
17	B	820	CLA	C3A-C2A-CAA-CBA
20	3	307	CHL	CAA-CBA-CGA-O1A
18	A	840	PQN	C23-C25-C26-C27
17	5	314	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

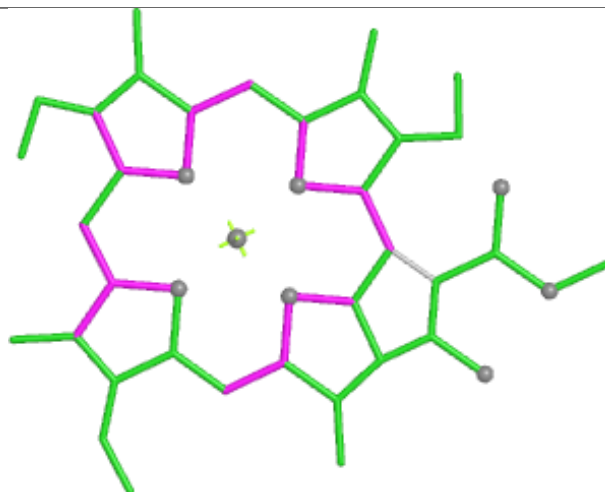
No monomer is involved in short contacts.

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.

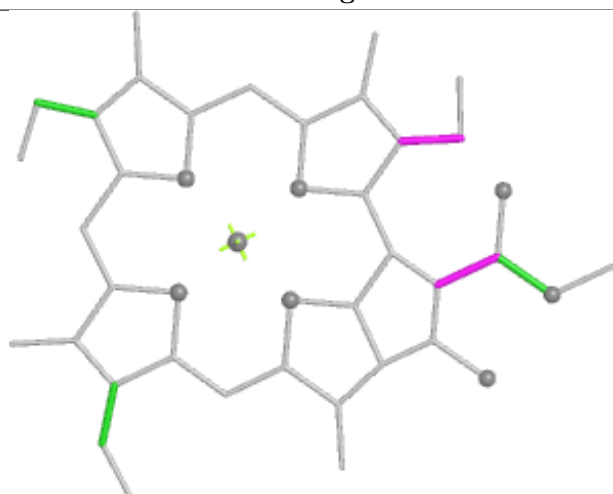
Ligand CLA 8 610



Bond lengths



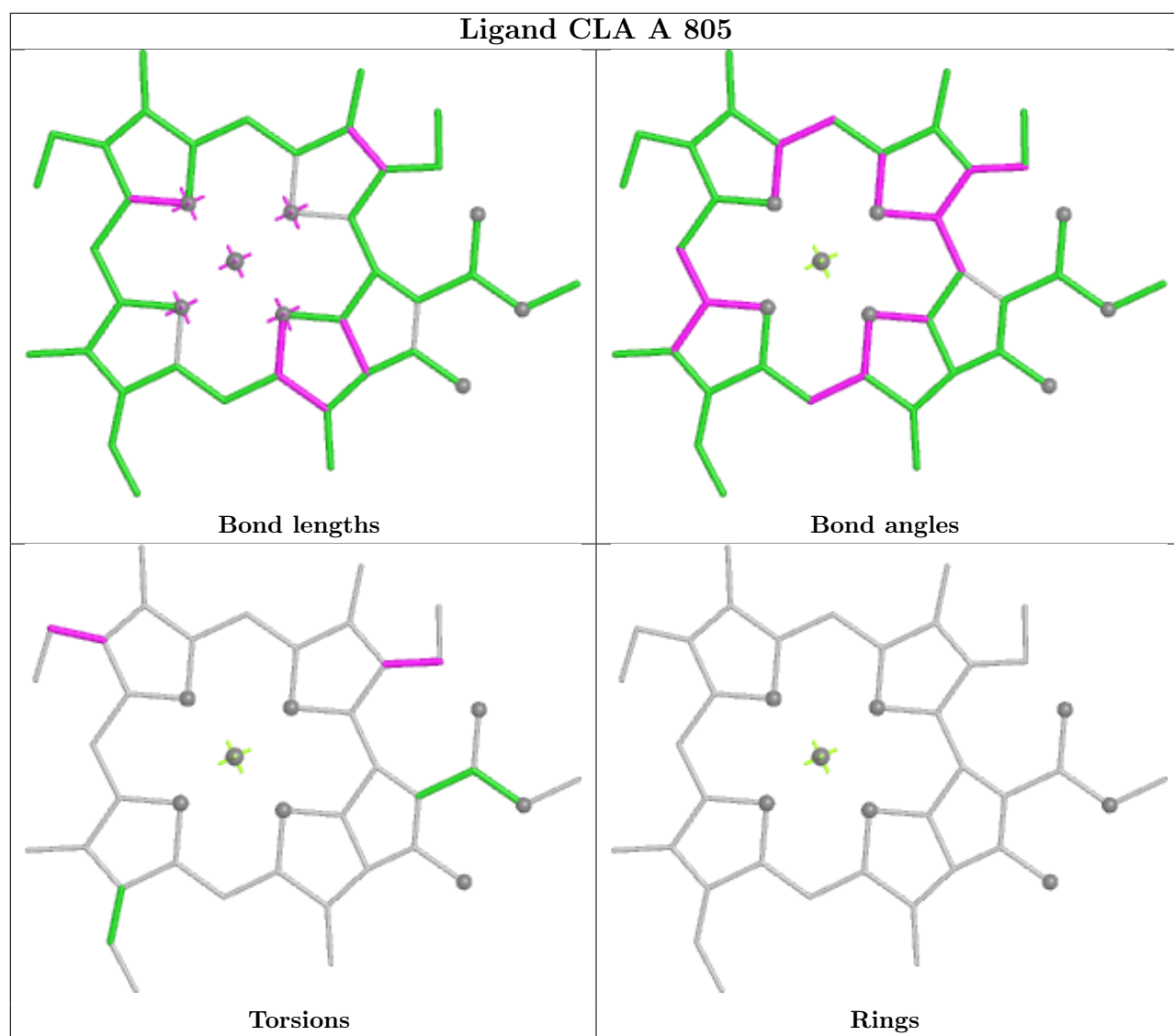
Bond angles



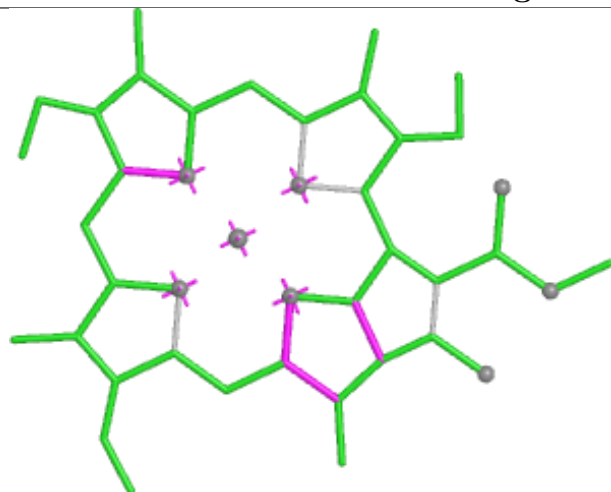
Torsions



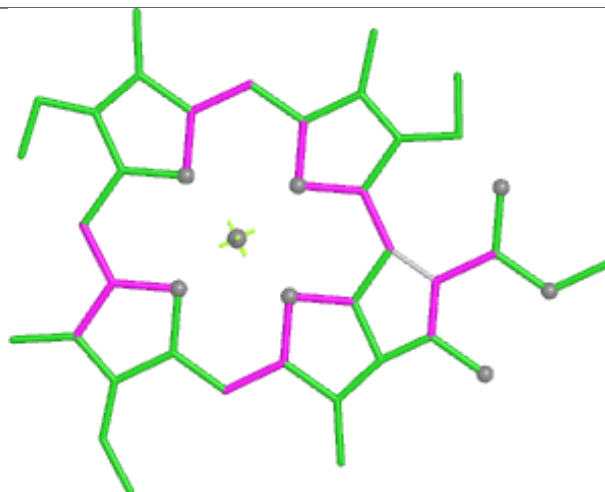
Rings



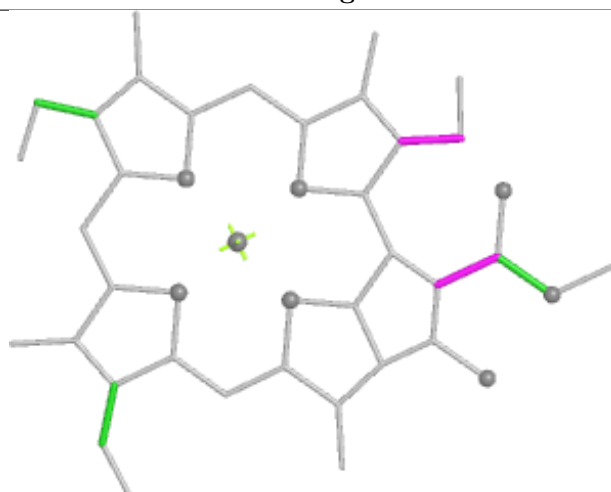
Ligand CLA A 838



Bond lengths



Bond angles

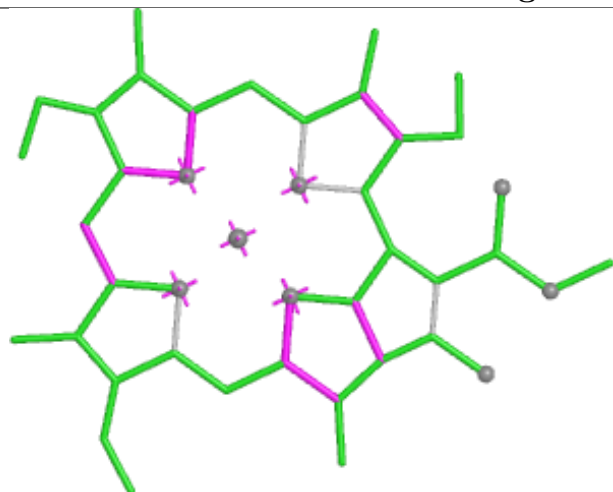


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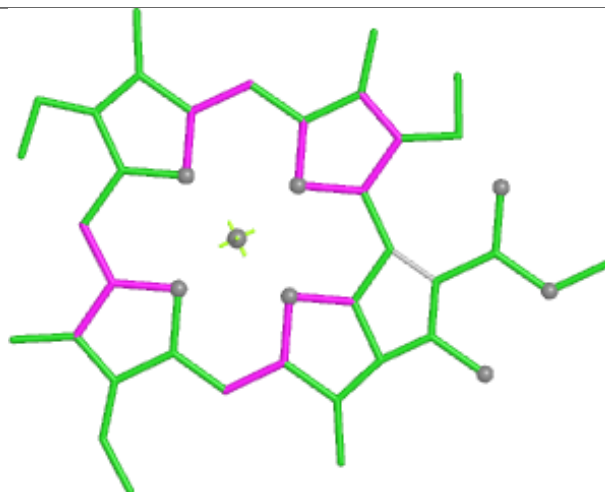


Rings

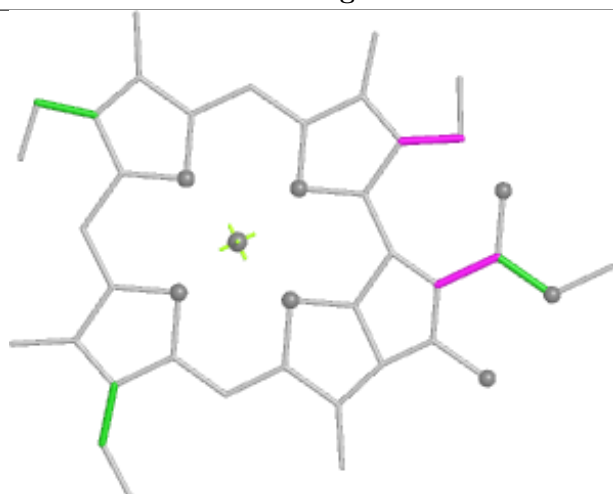
Ligand CLA 7 611



Bond lengths



Bond angles

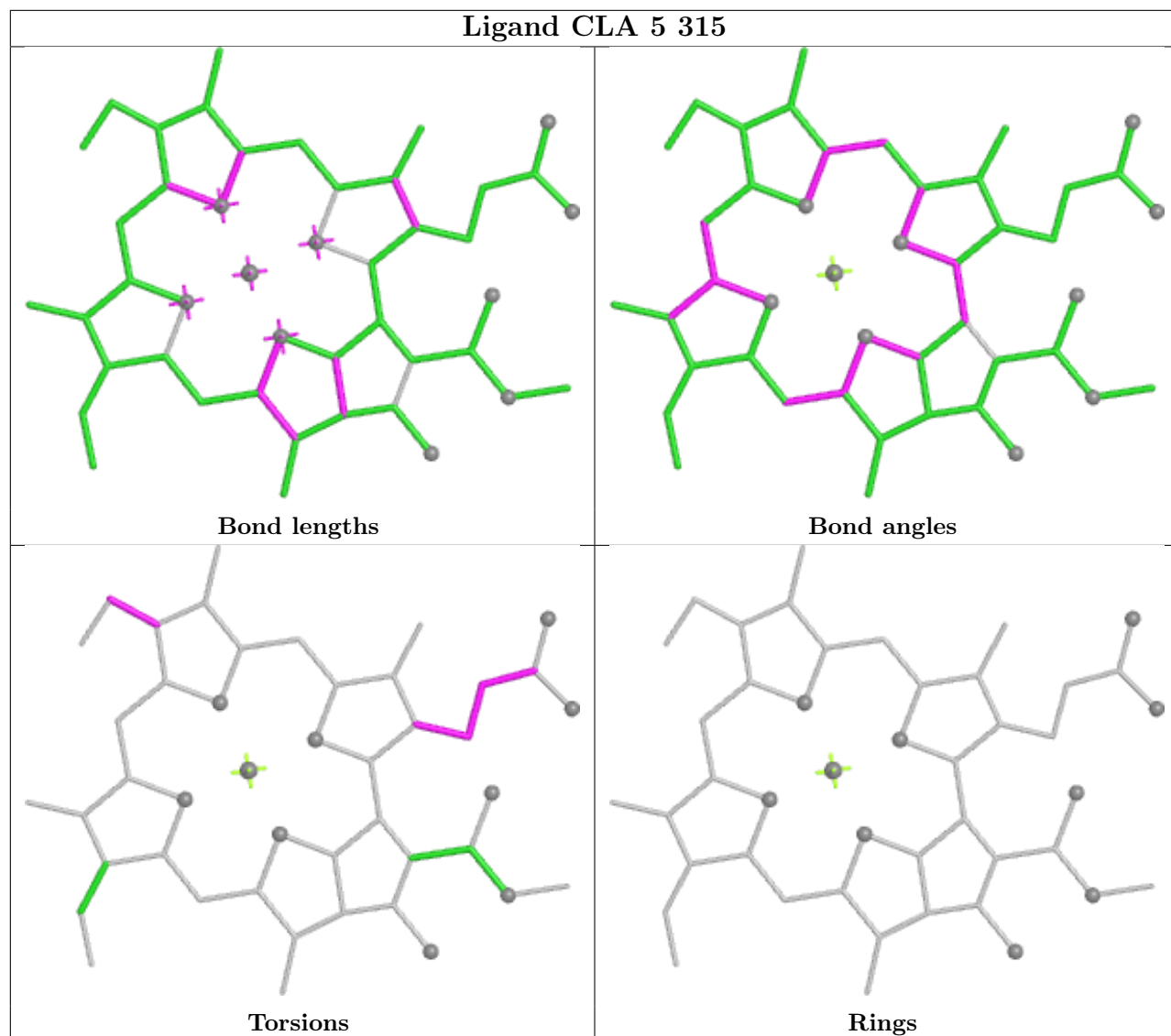


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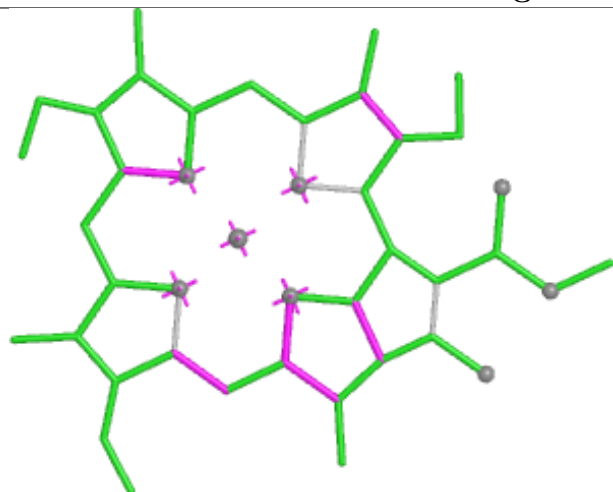


Rings

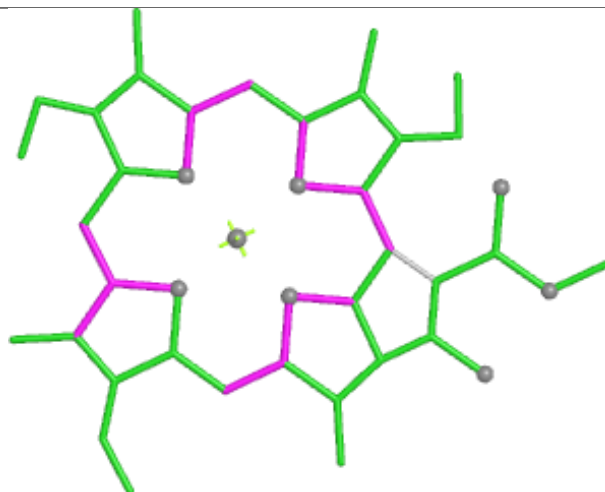
Ligand CLA 5 315



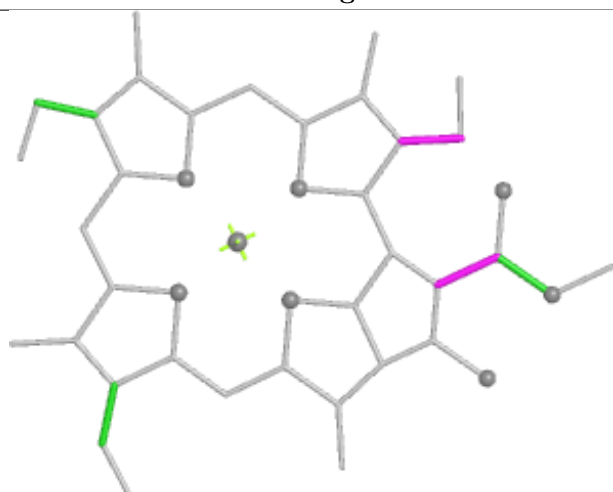
Ligand CLA A 812



Bond lengths



Bond angles

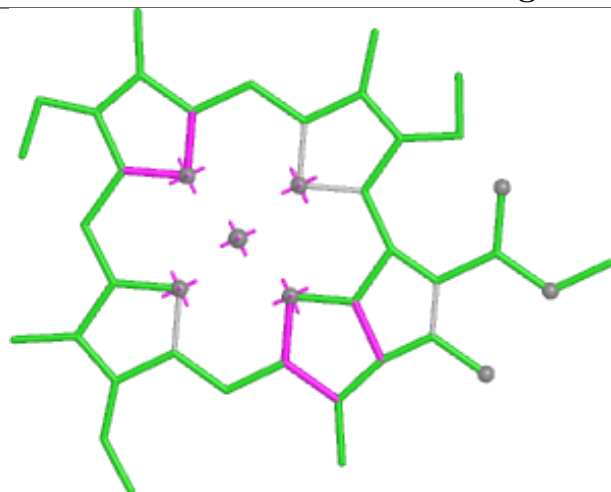


Torsions

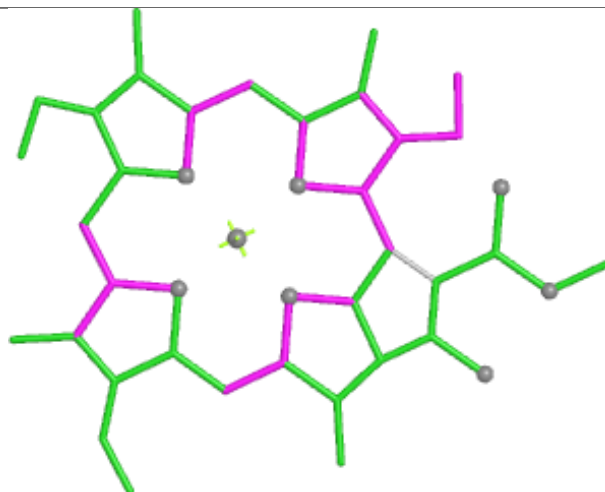


Rings

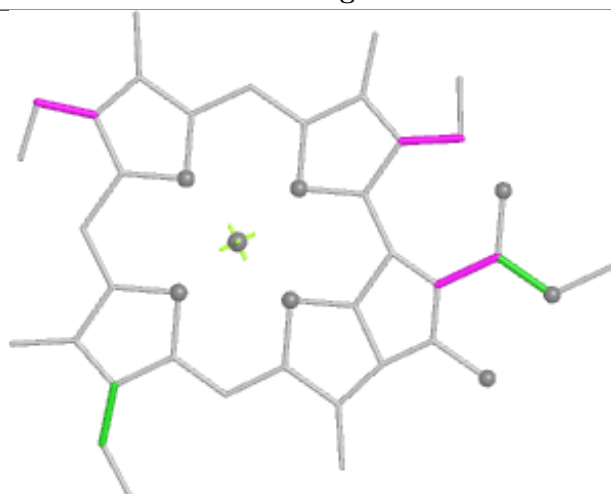
Ligand CLA 4 603



Bond lengths



Bond angles

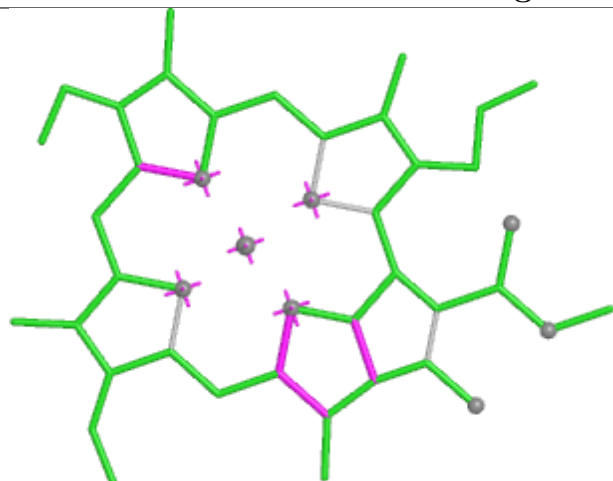


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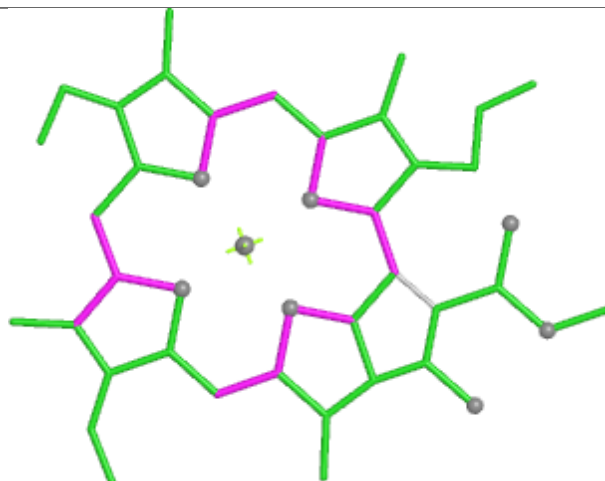


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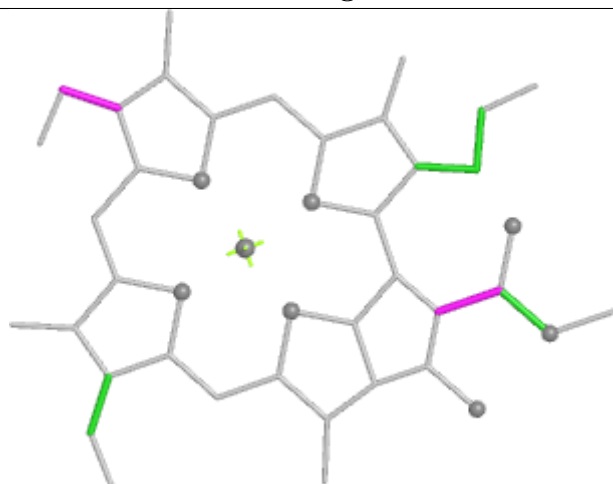
Ligand CLA B 835



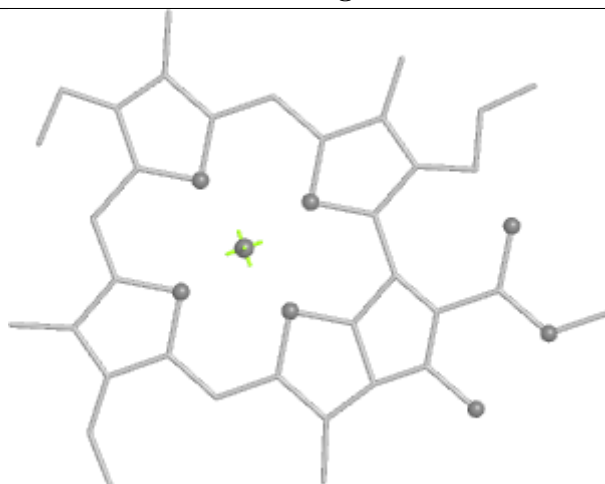
Bond lengths



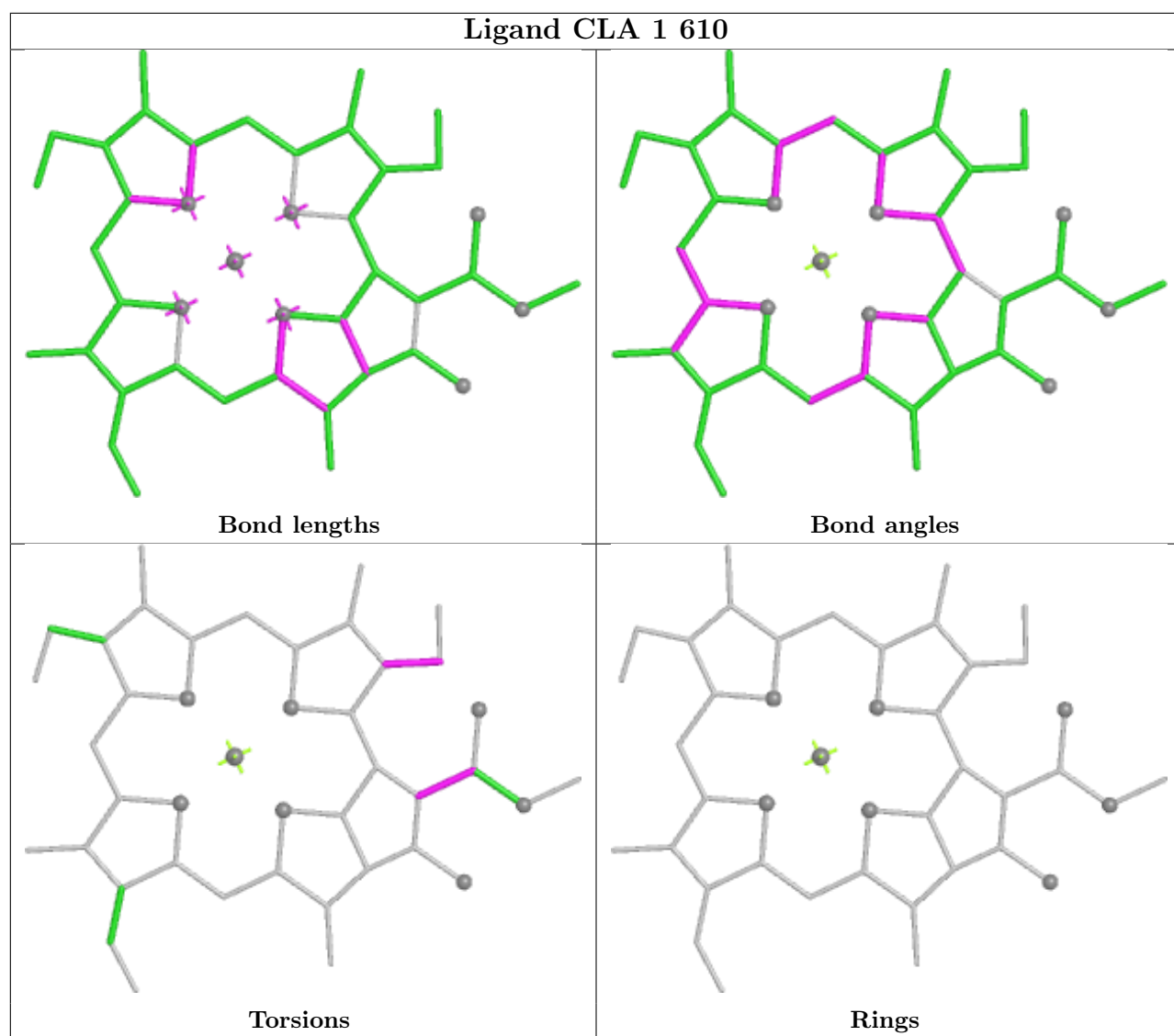
Bond angles



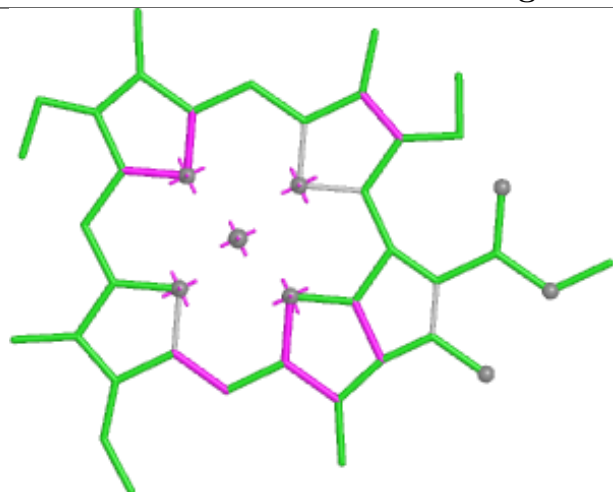
Torsions



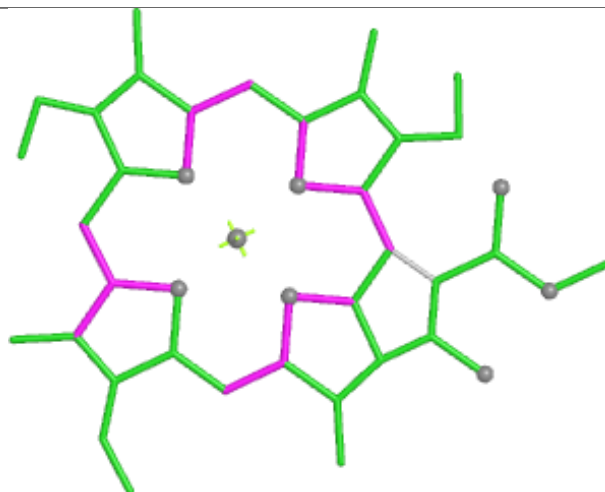
Rings



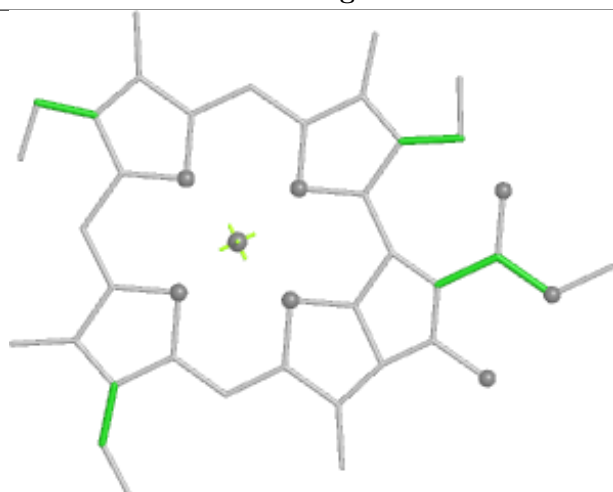
Ligand CLA 8 604



Bond lengths



Bond angles

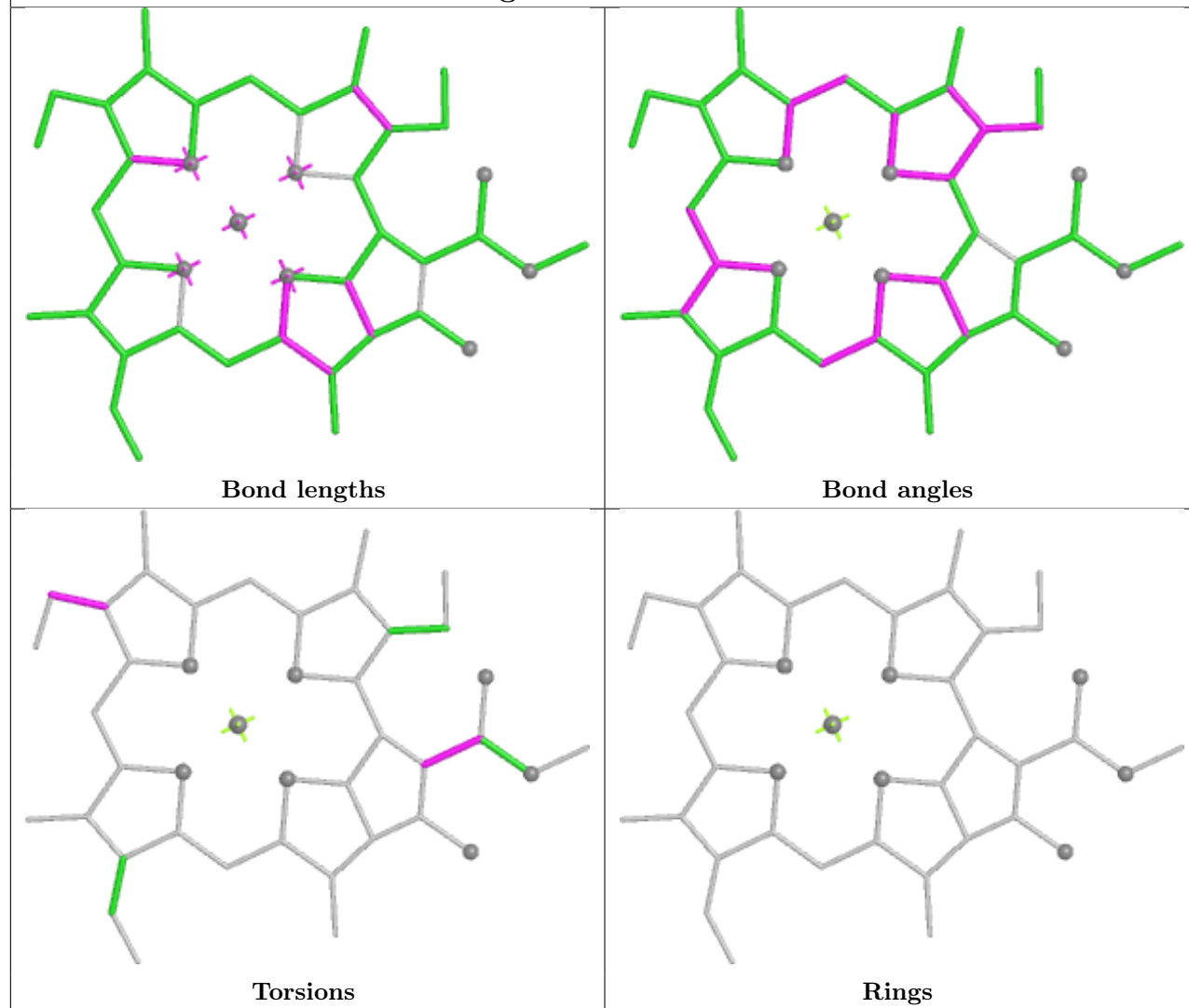


Torsions

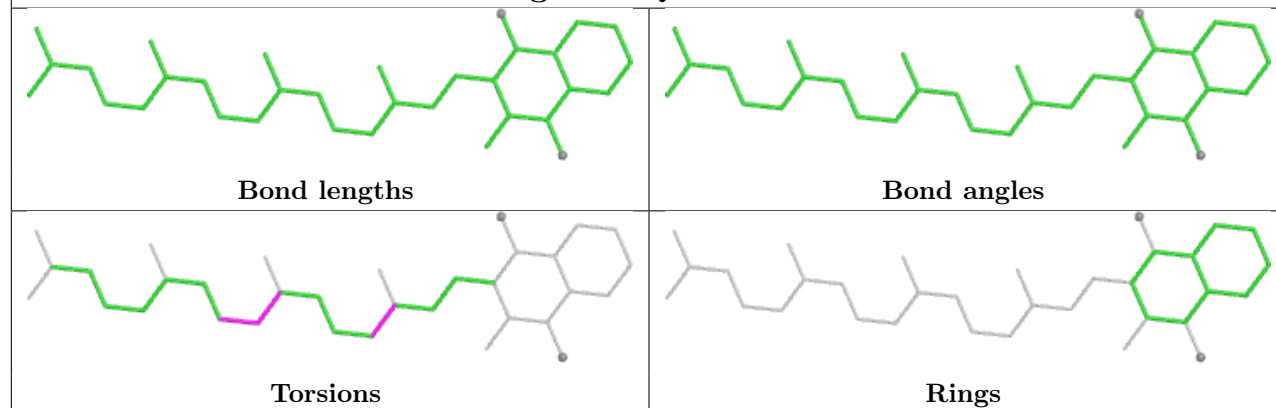


Rings

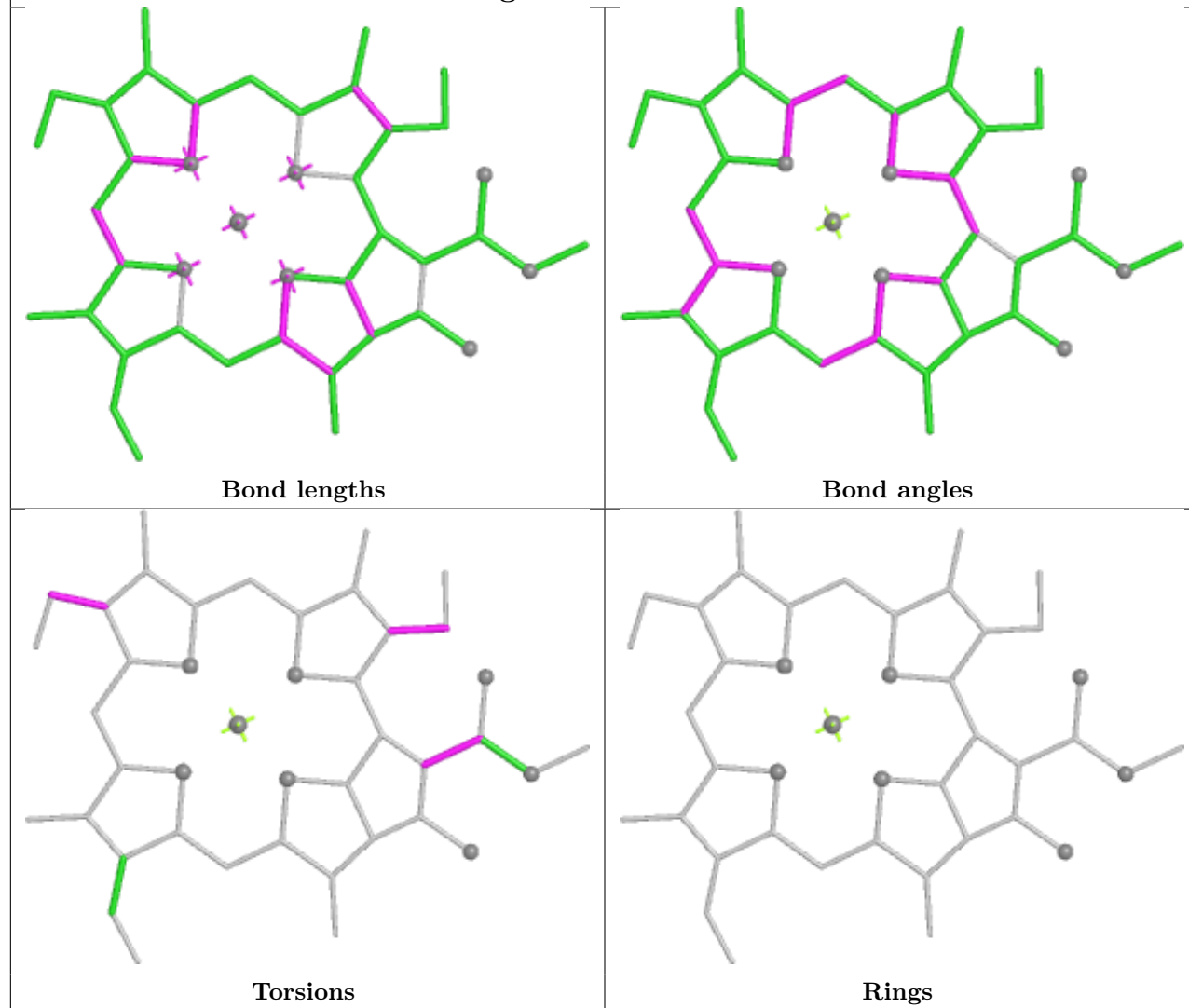
Ligand CLA 7 603



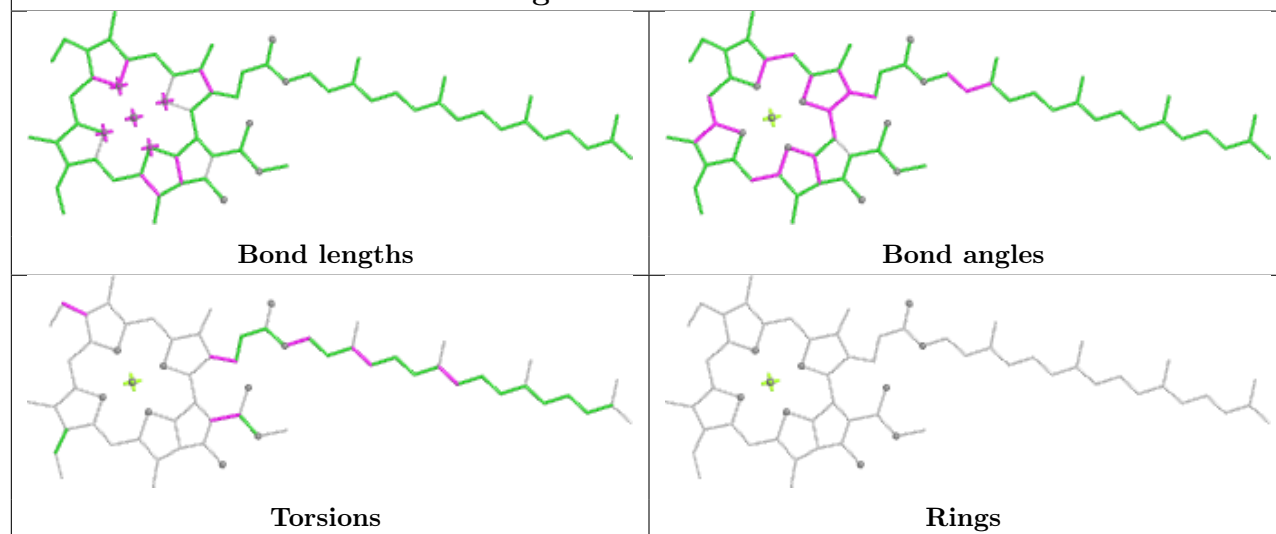
Ligand PQN B 840

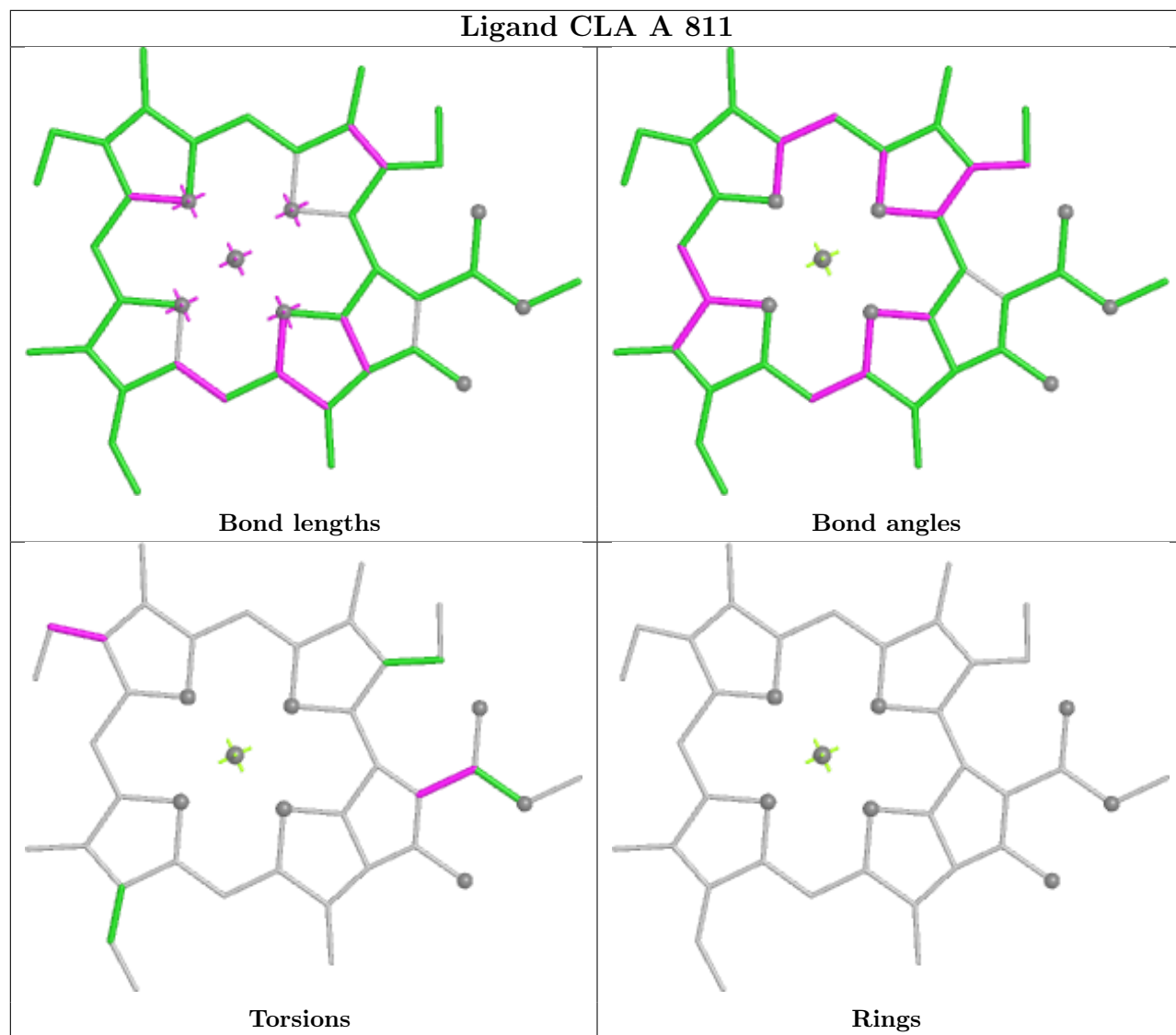


Ligand CLA 1 605

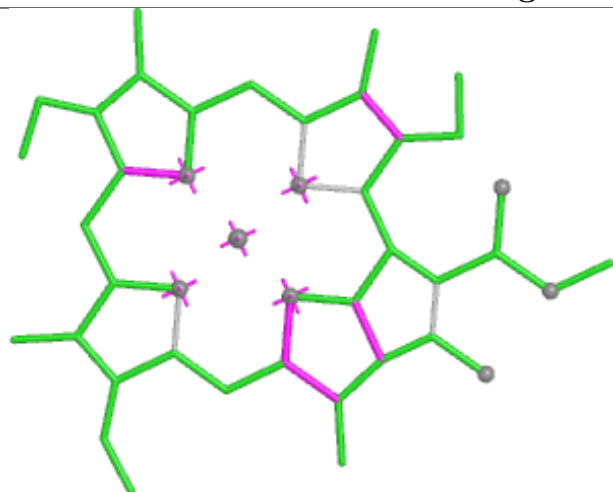


Ligand CLA B 815

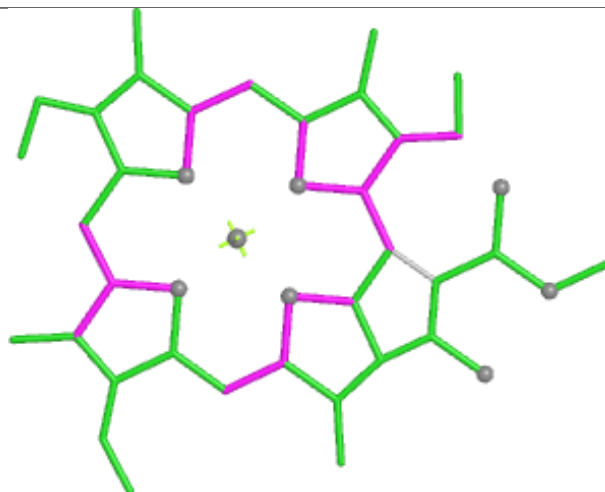




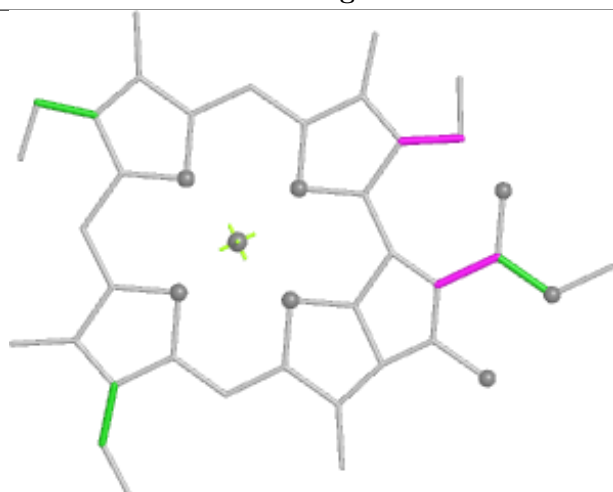
Ligand CLA 3 301



Bond lengths



Bond angles

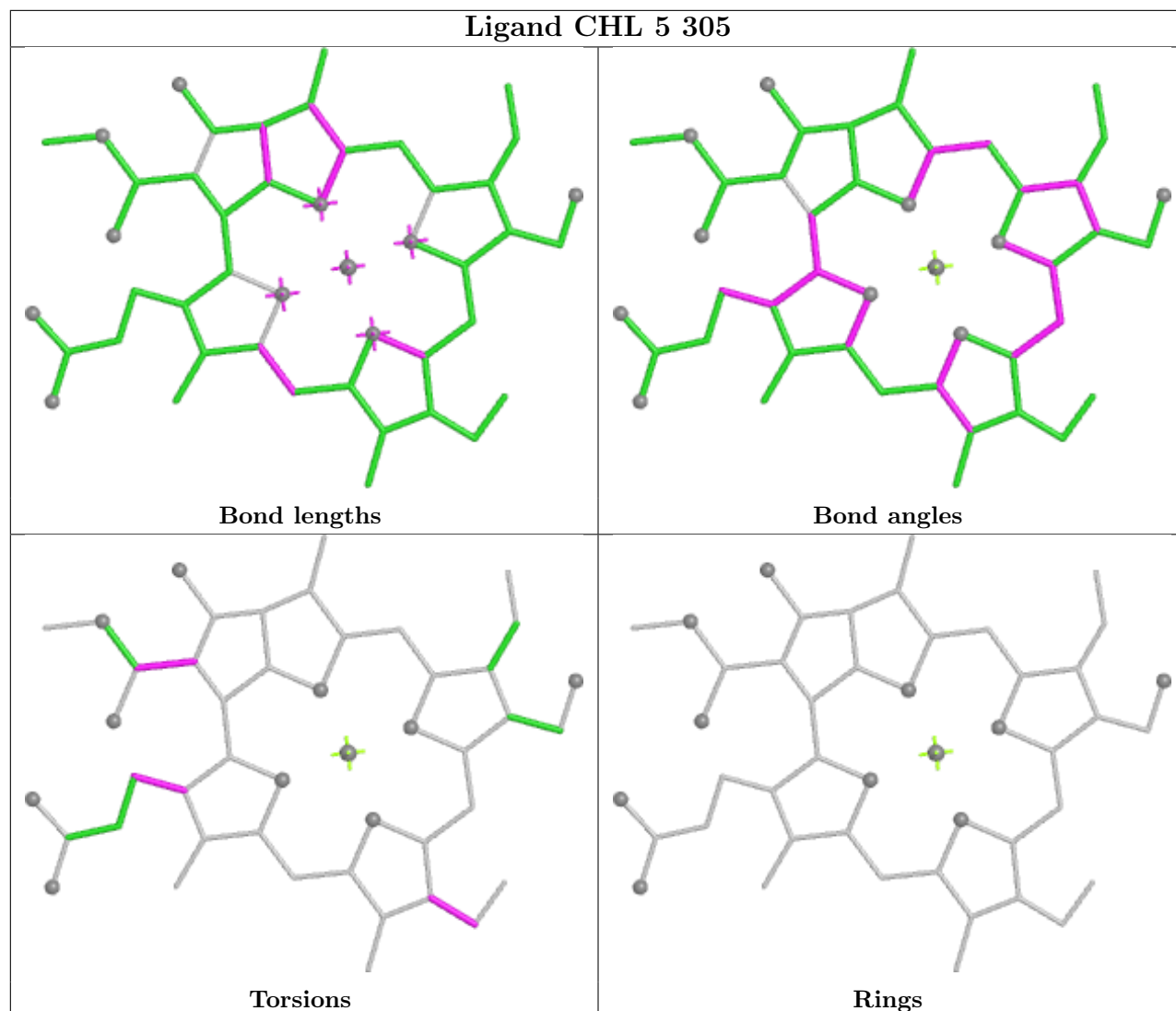


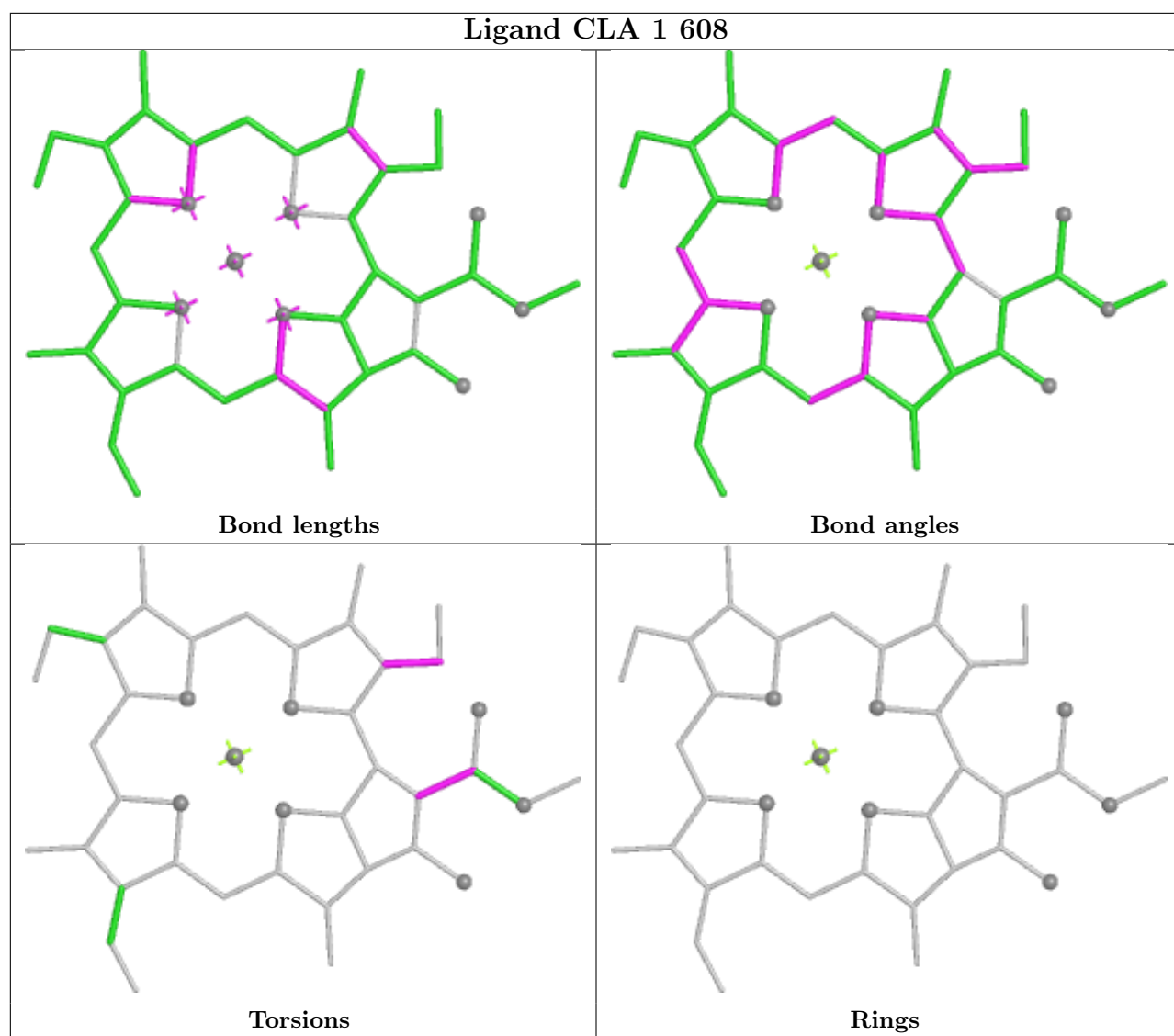
Torsions



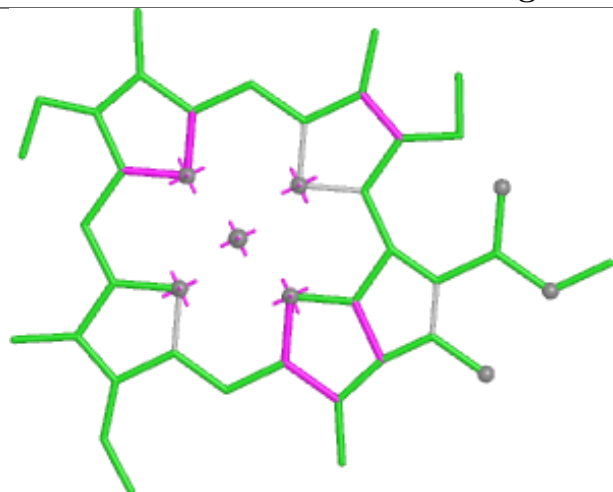
Rings

Ligand CHL 5 305

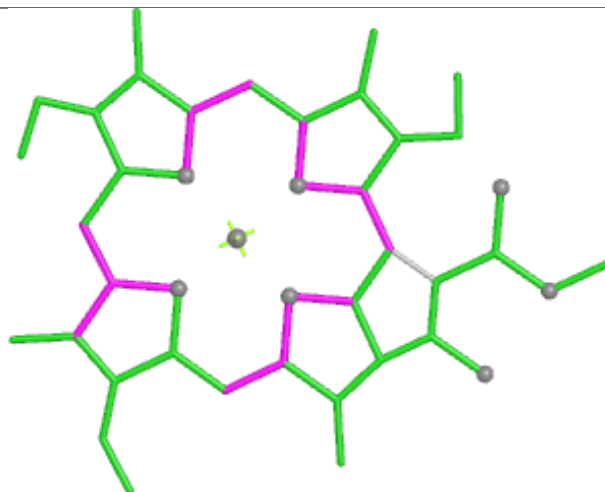




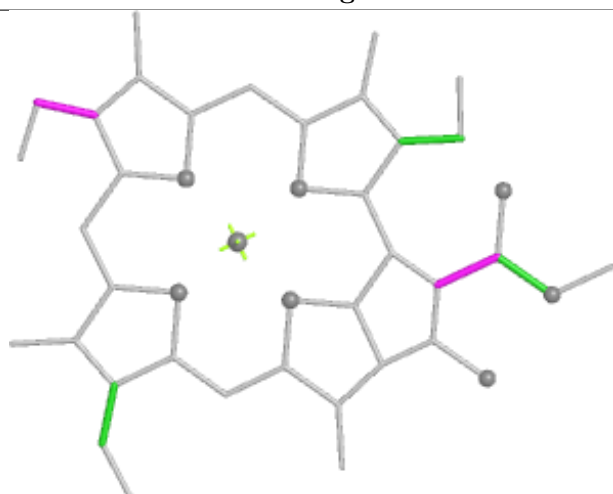
Ligand CLA 8 605



Bond lengths



Bond angles

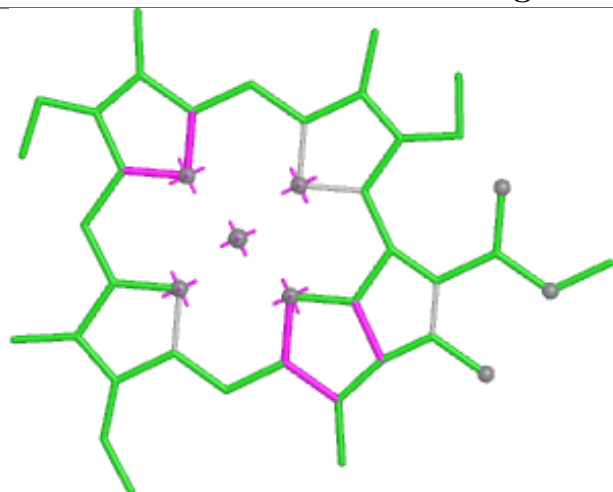


Torsions

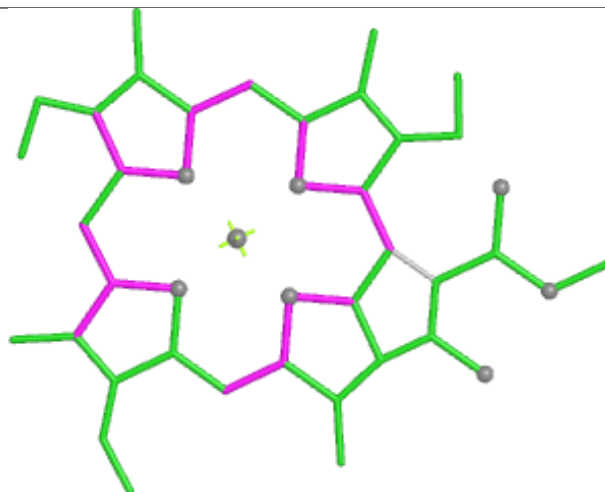


Rings

Ligand CLA A 819



Bond lengths



Bond angles

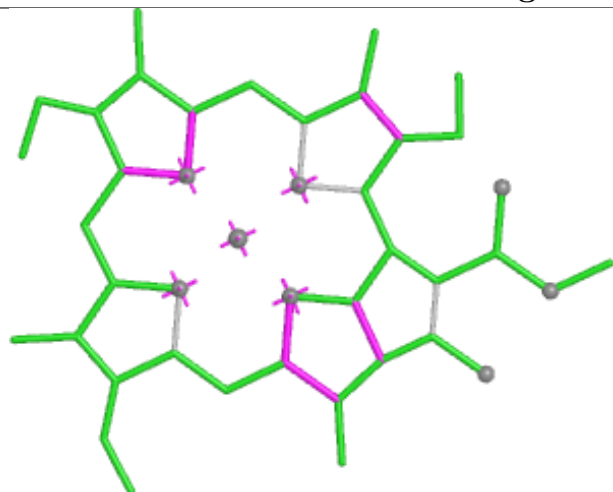


Torsions

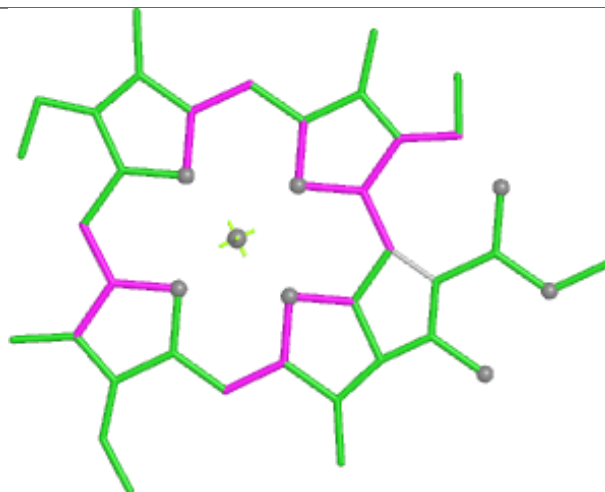


Rings

Ligand CLA 6 604



Bond lengths



Bond angles

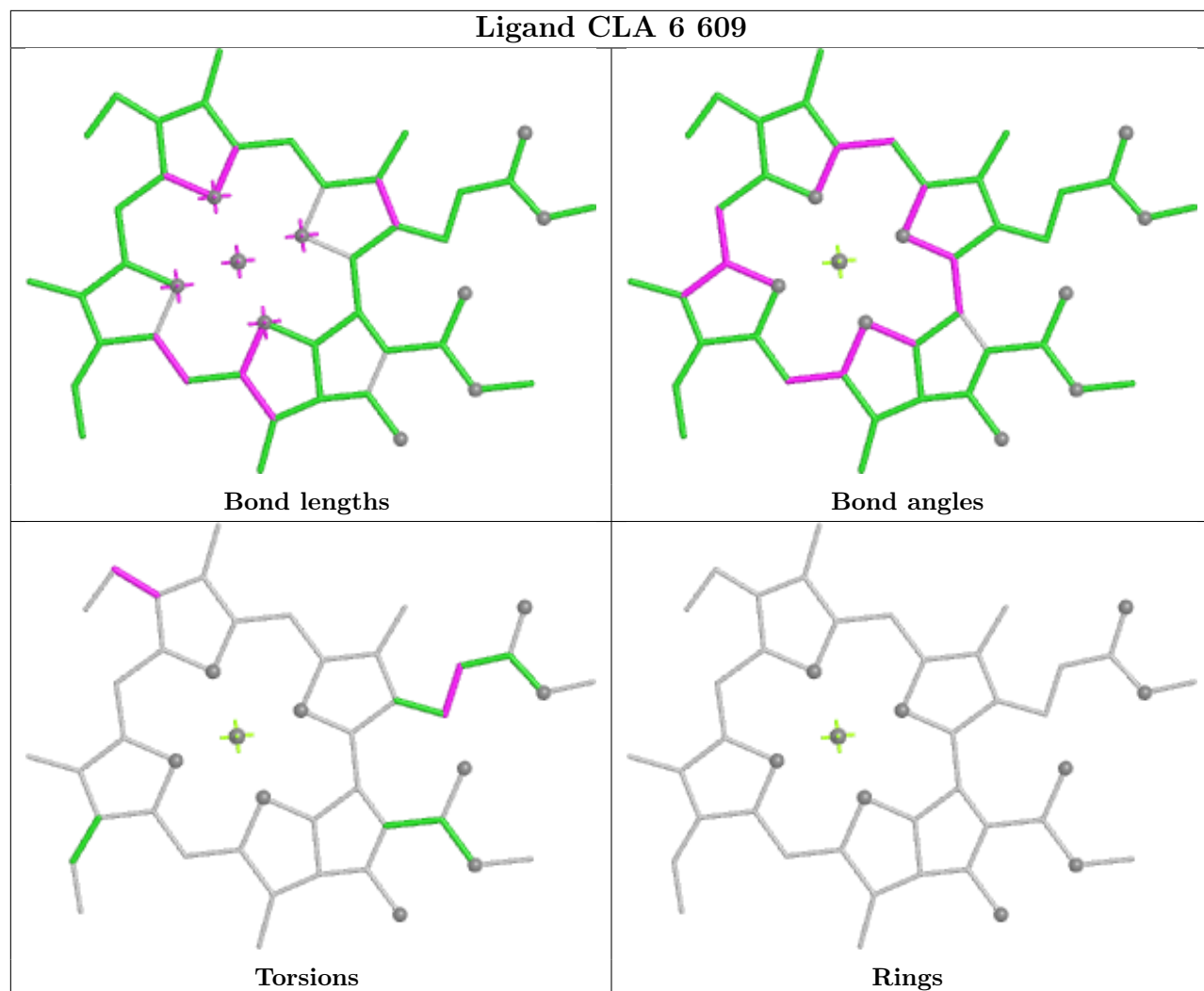


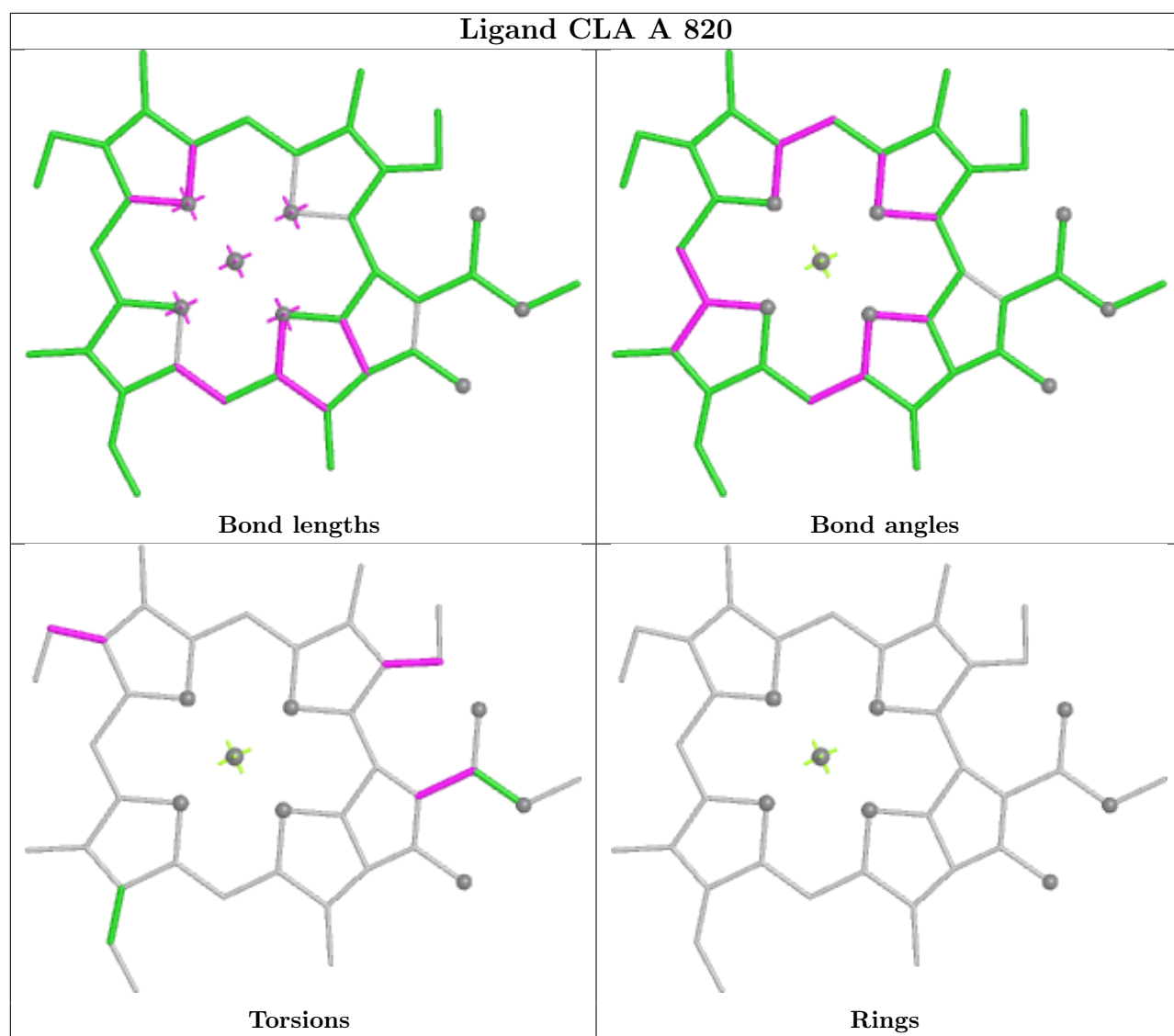
Torsions

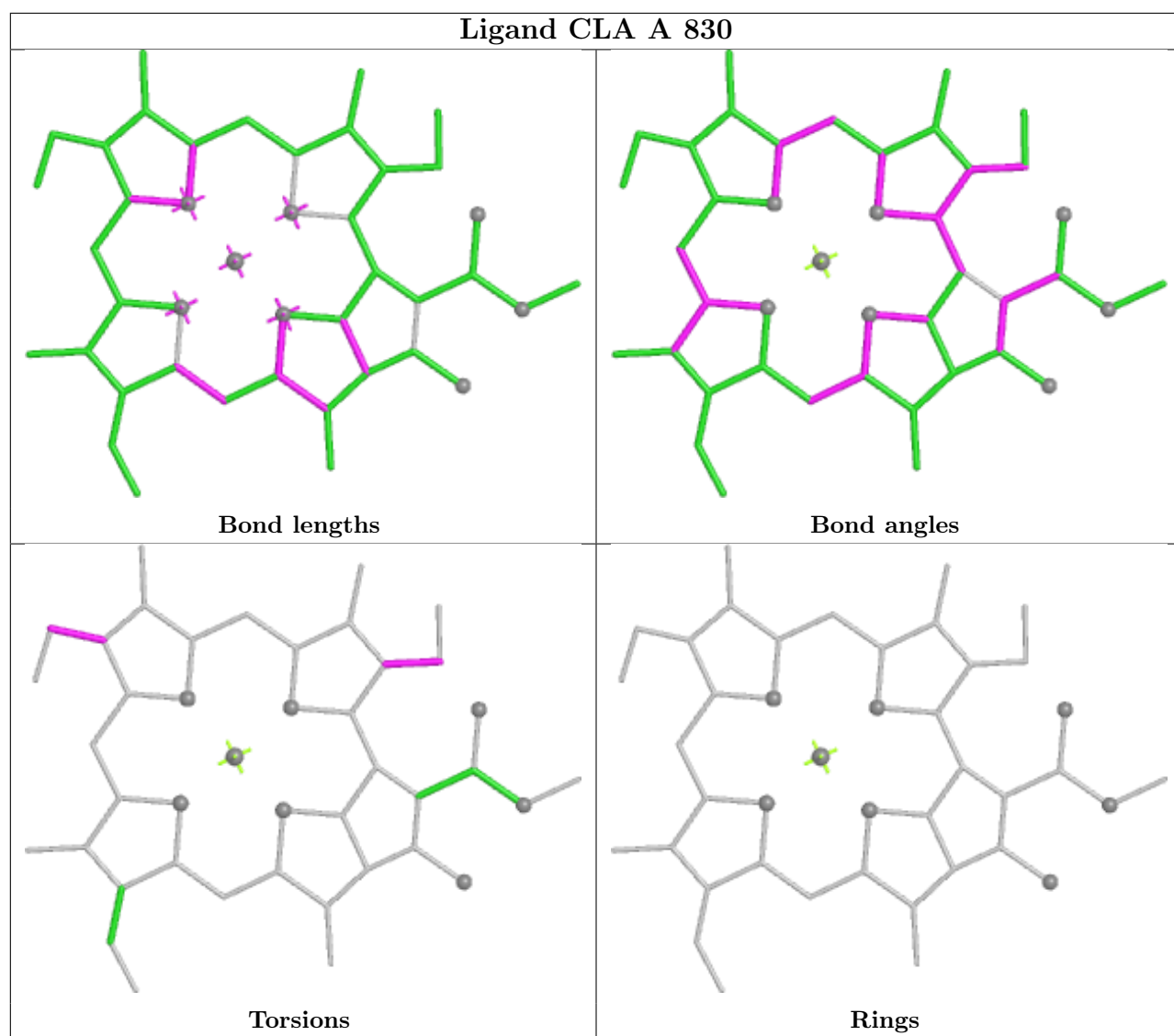


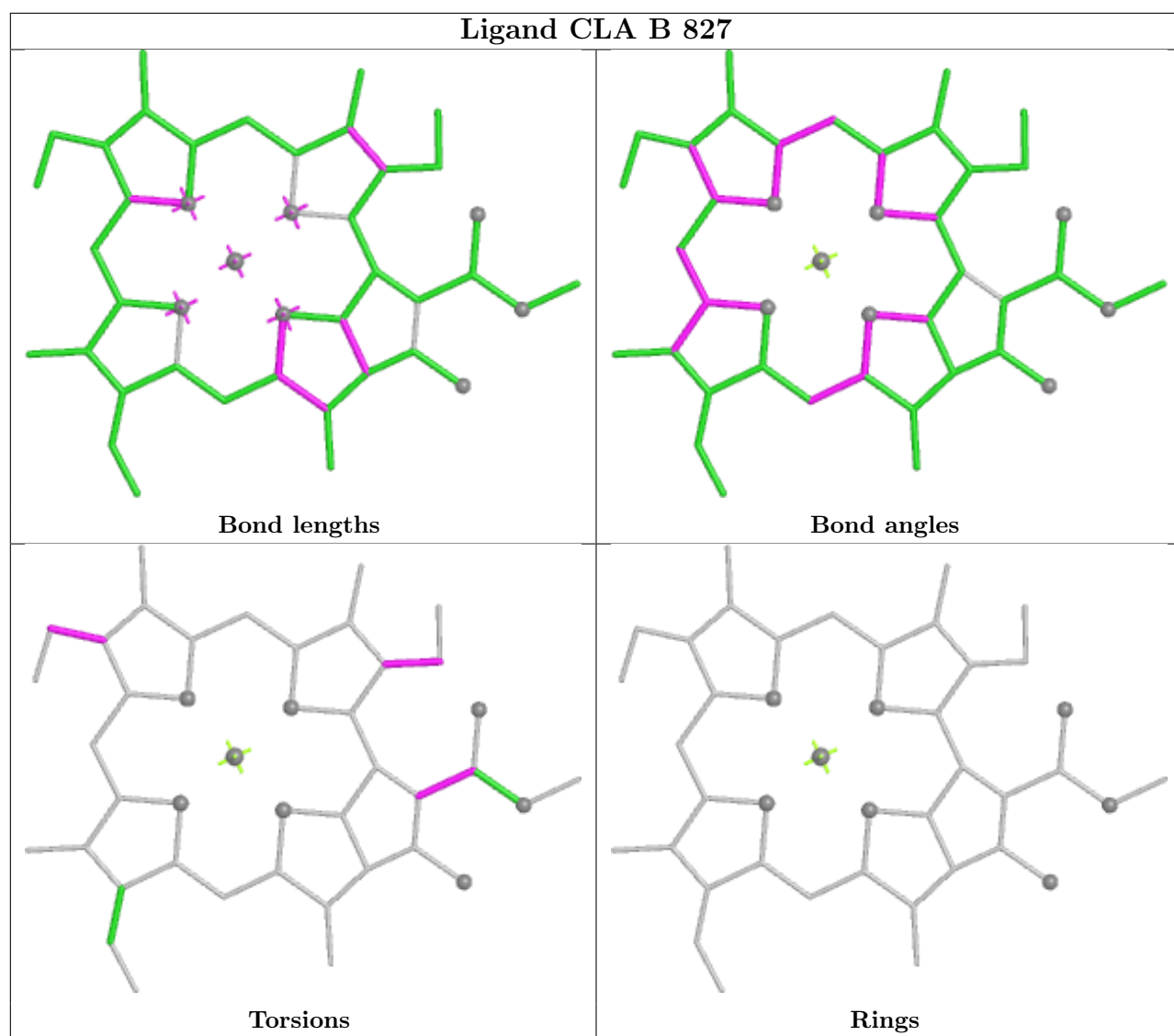
Rings

Ligand CLA 6 609

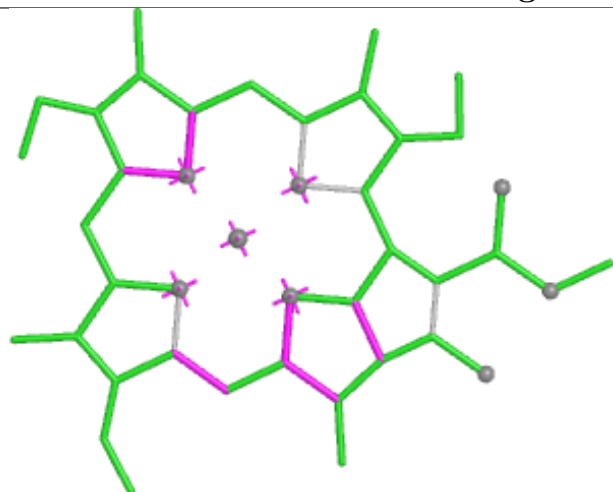




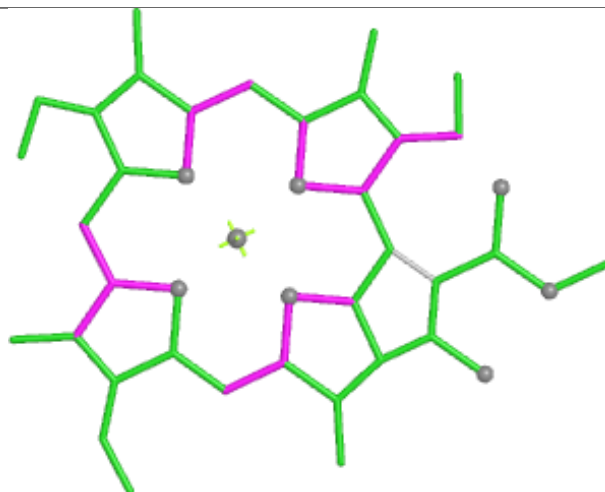




Ligand CLA 5 311



Bond lengths



Bond angles

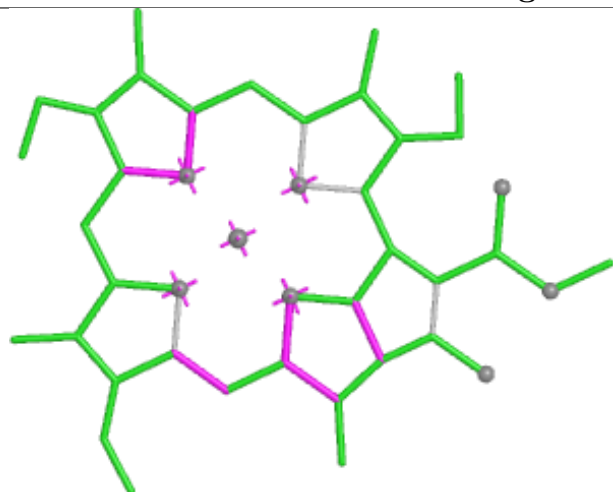


Torsions

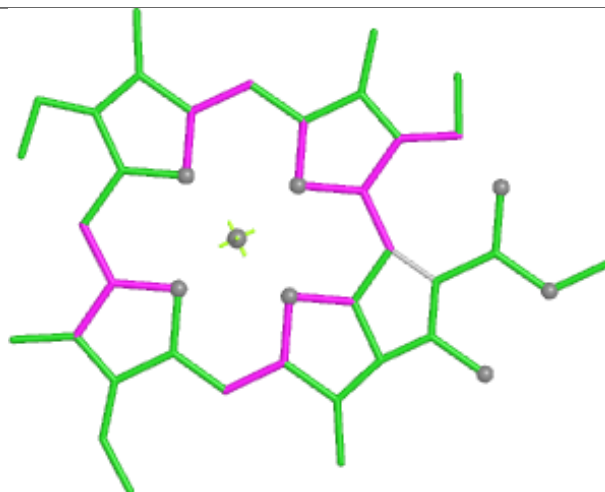


Rings

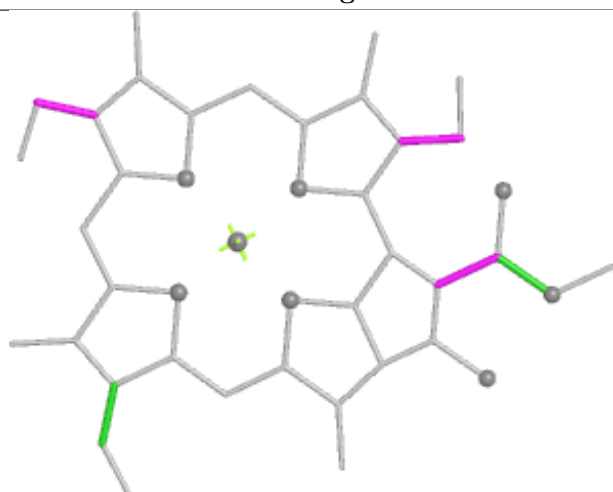
Ligand CLA 3 302



Bond lengths



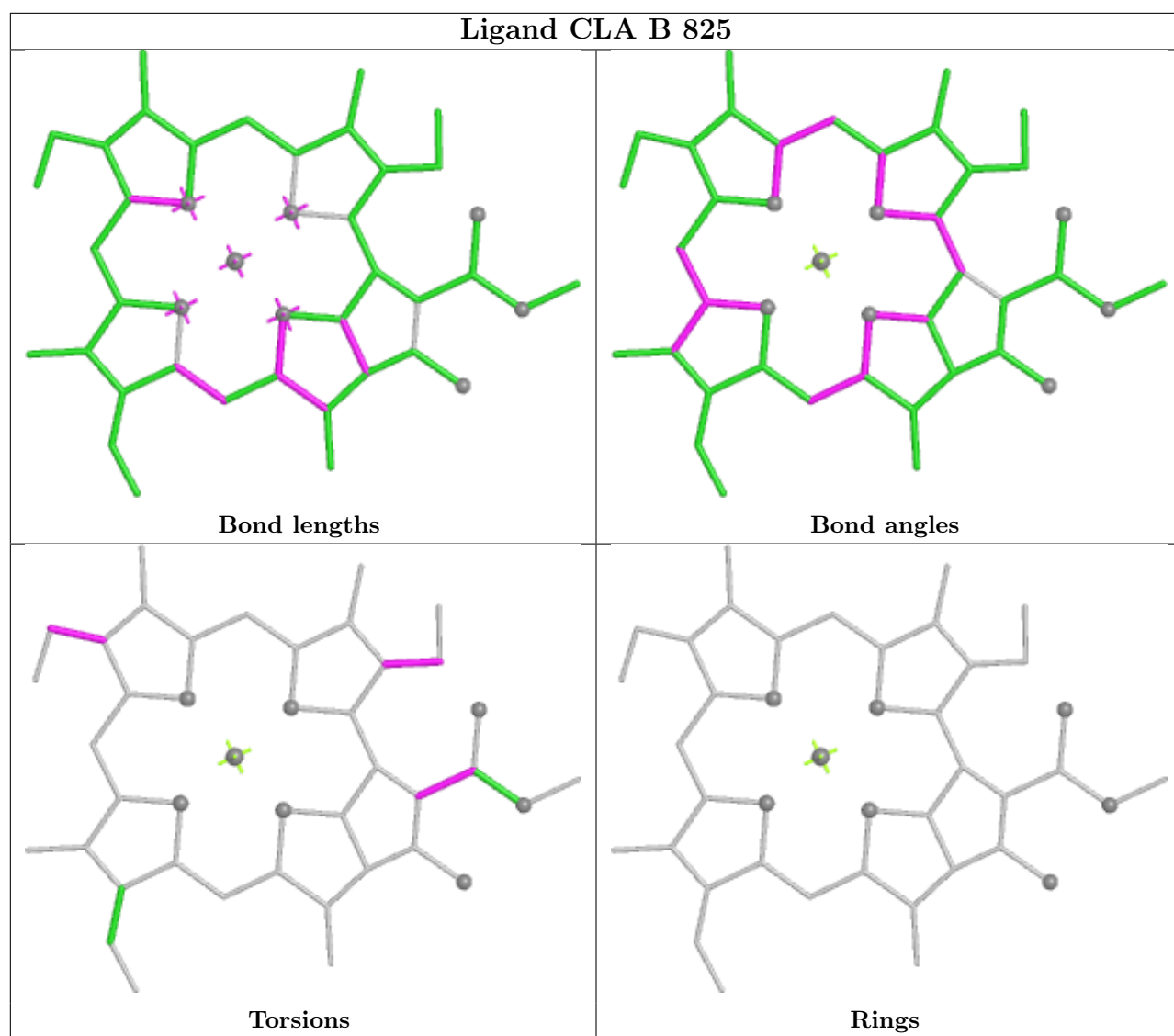
Bond angles



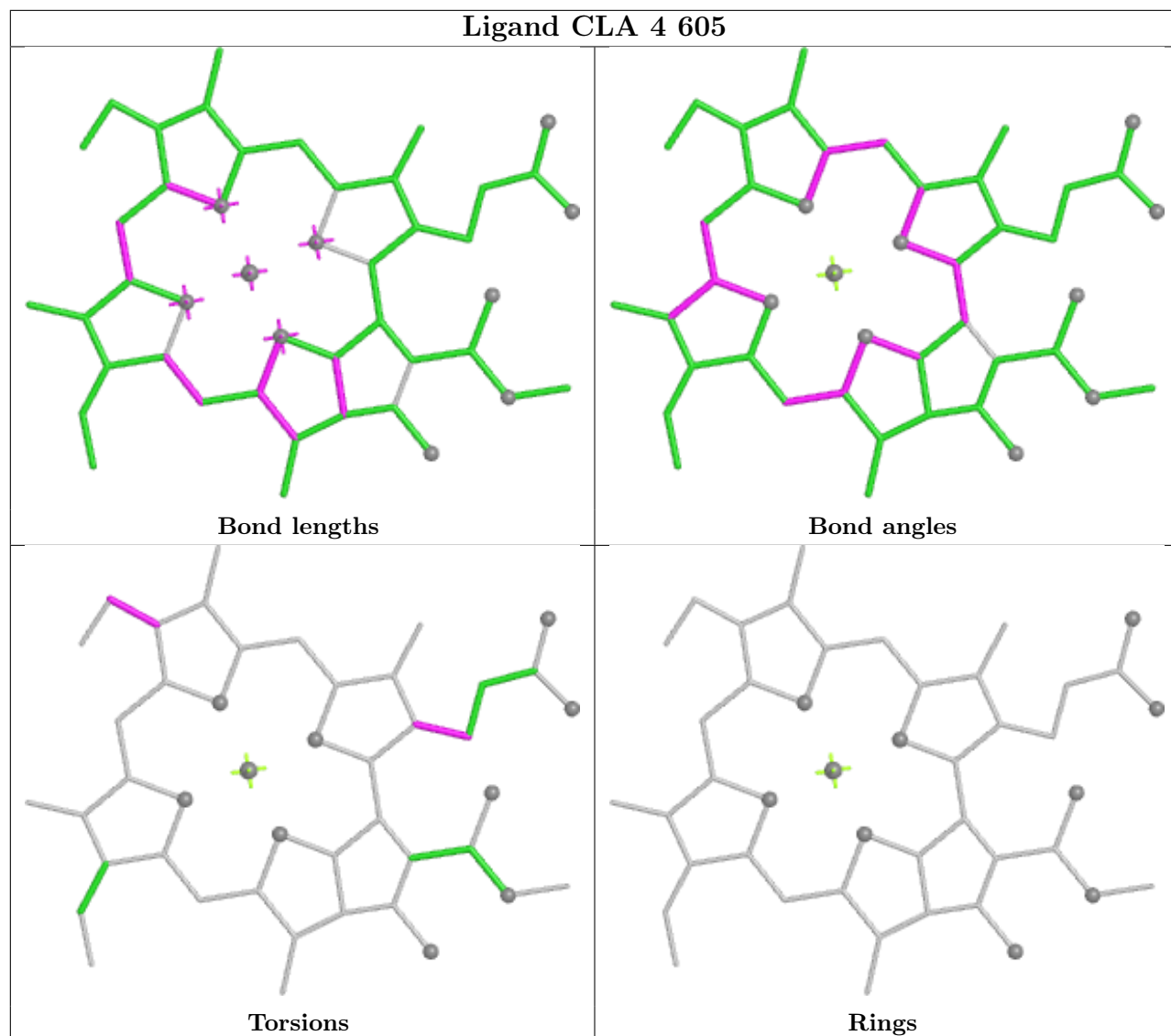
Torsions

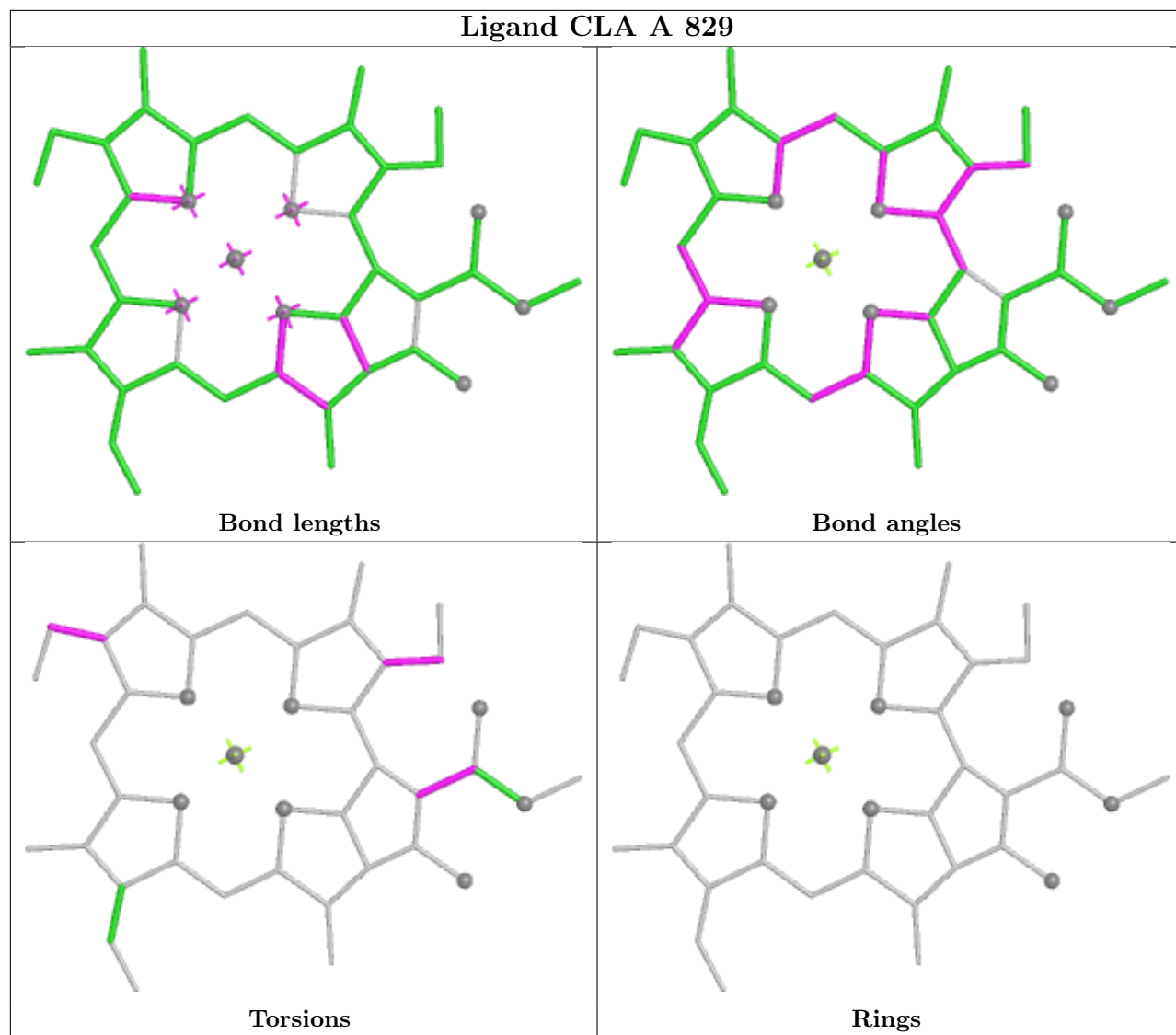


Rings

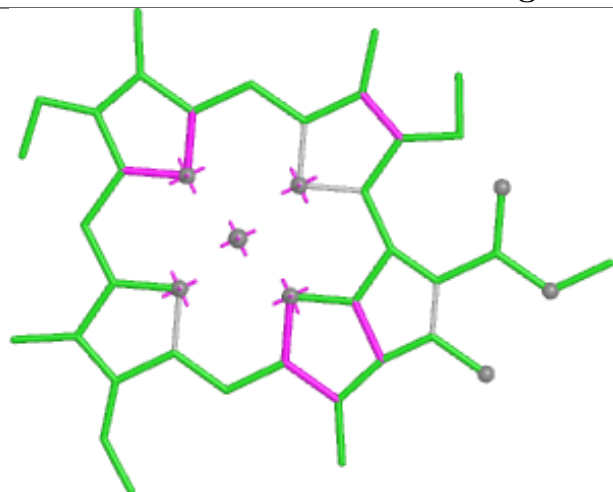


Ligand CLA 4 605

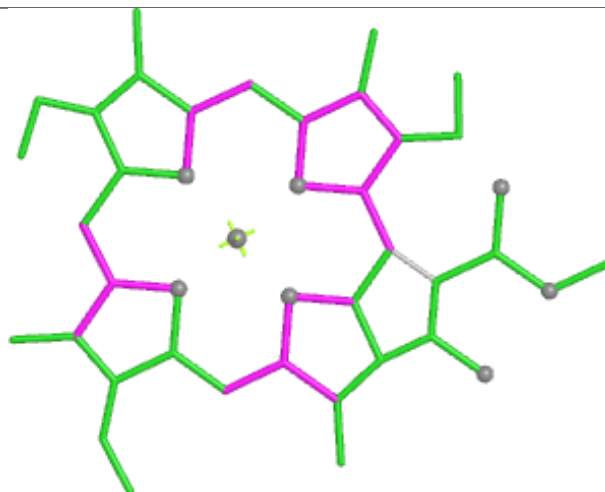




Ligand CLA 7 614



Bond lengths



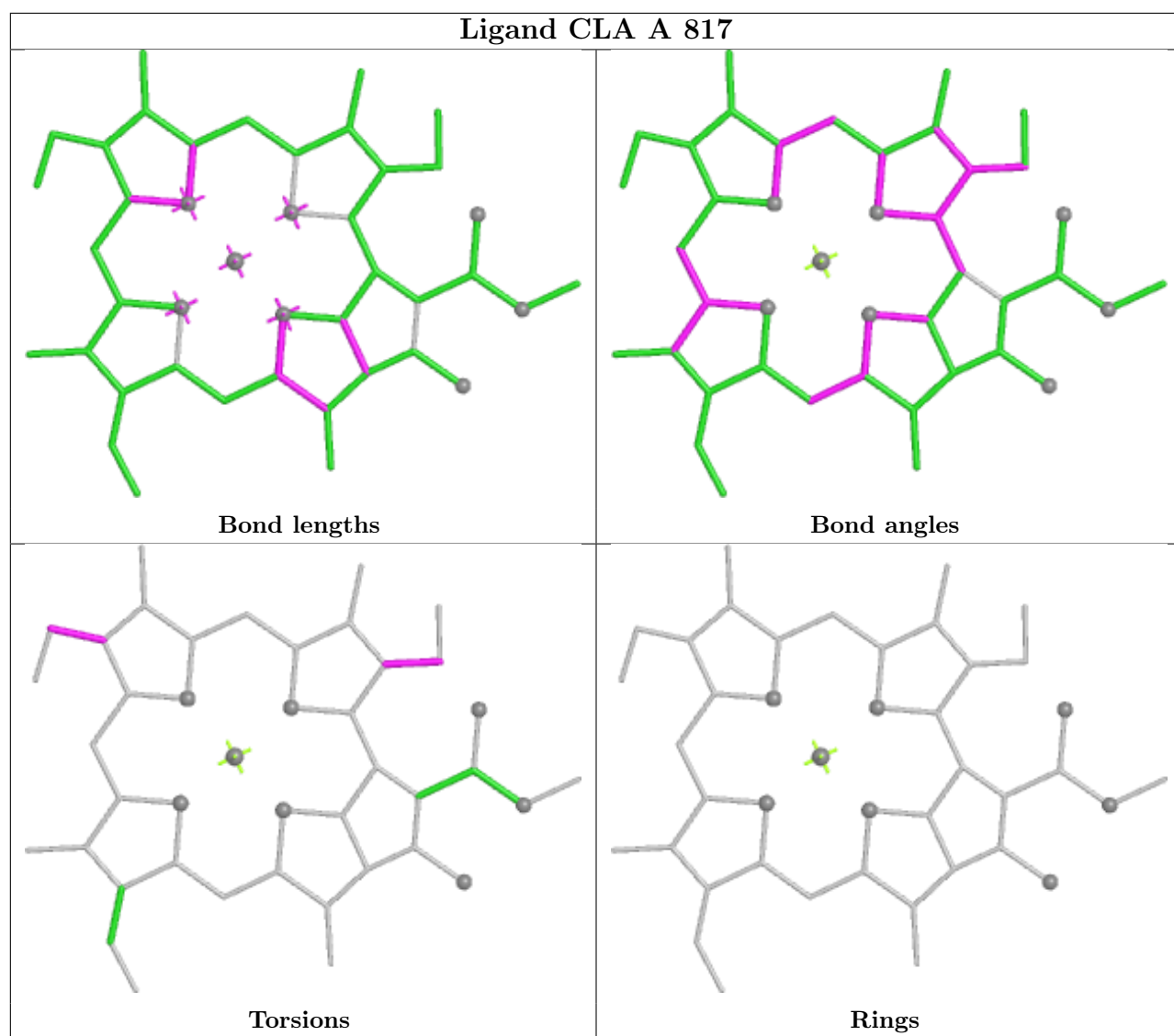
Bond angles



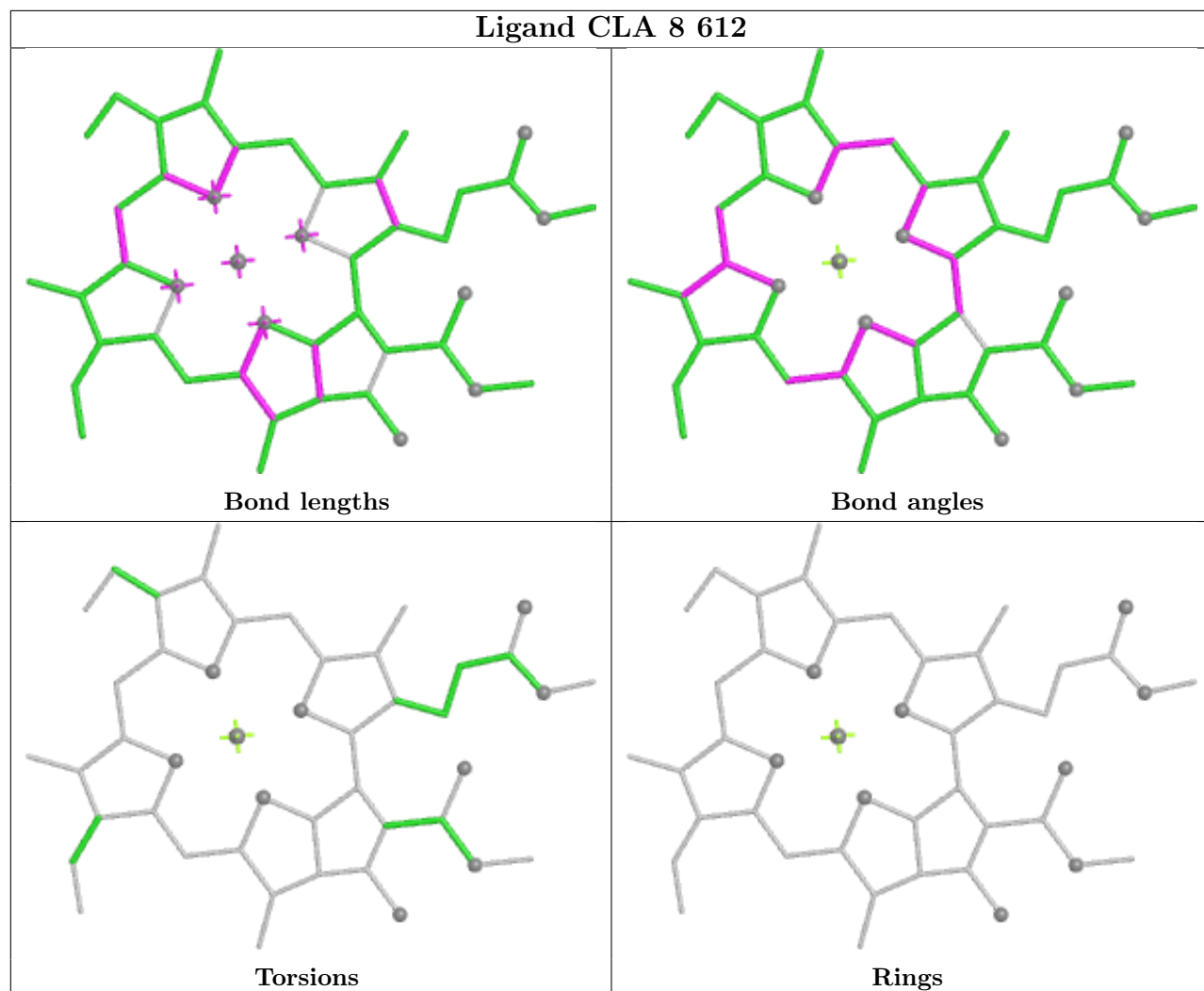
Torsions

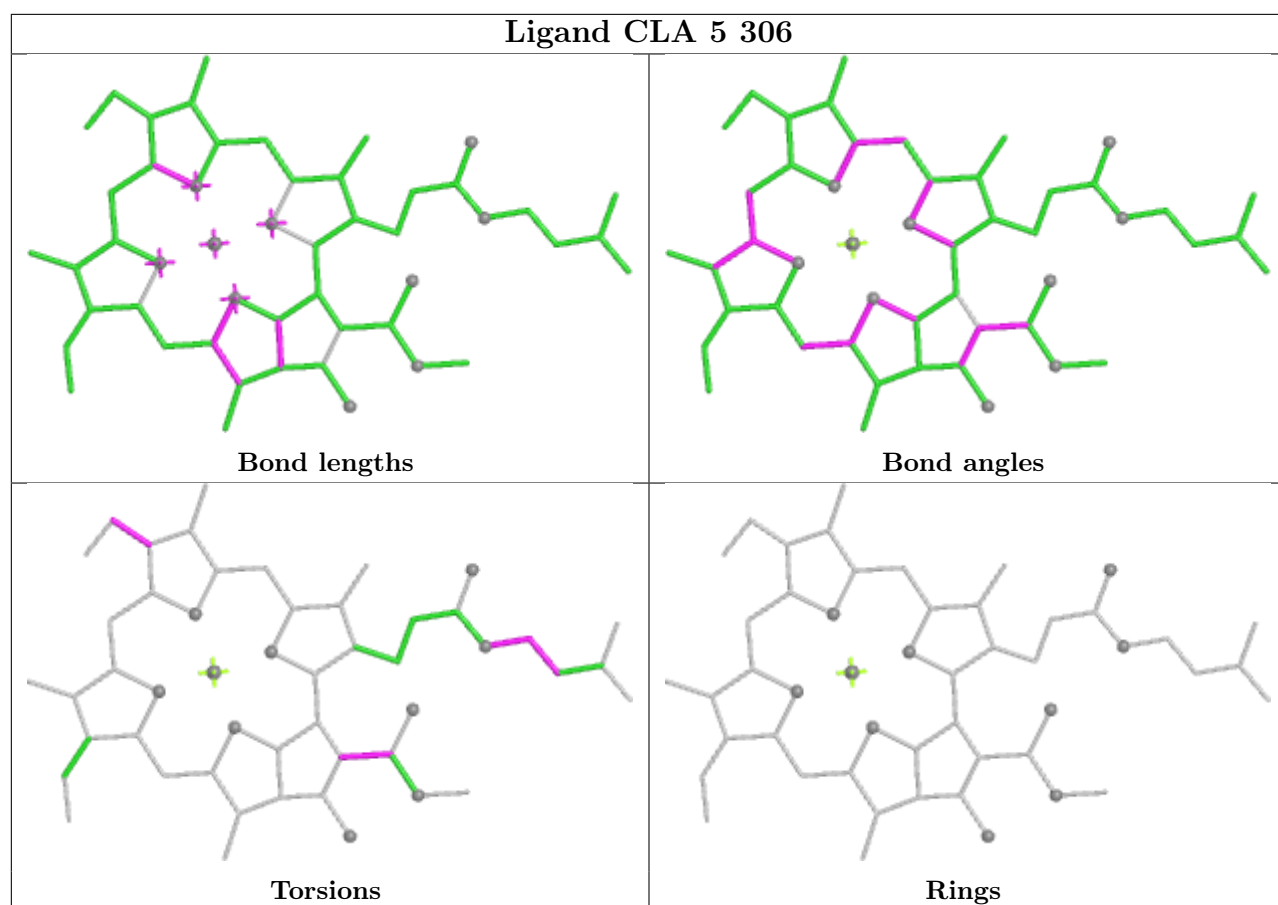


Rings

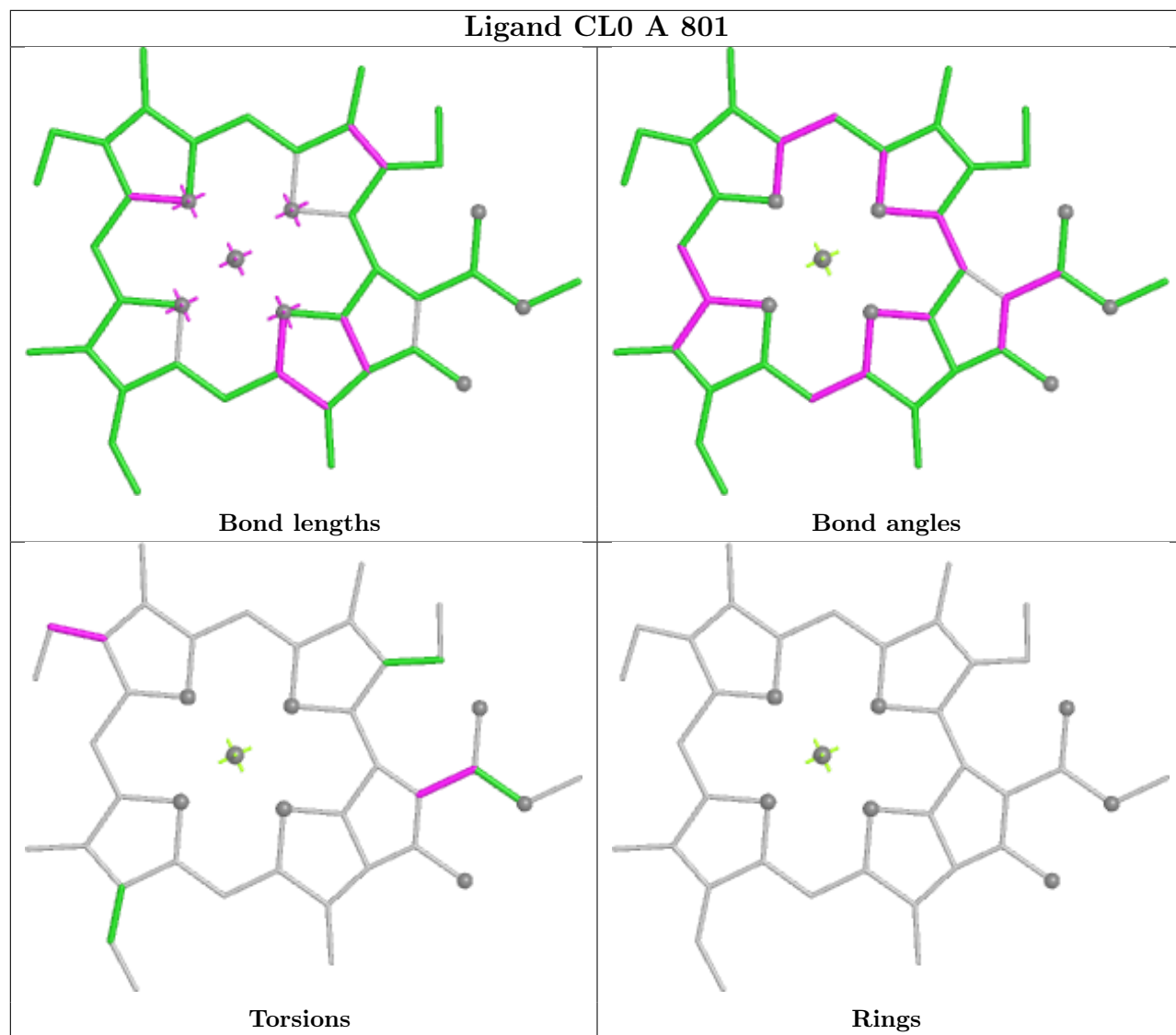


Ligand CLA 8 612

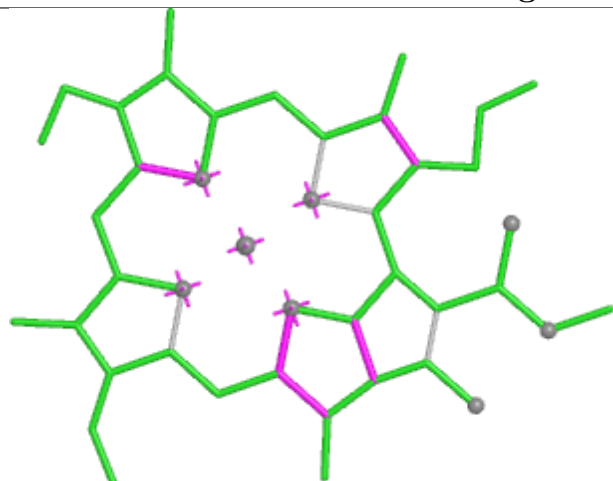




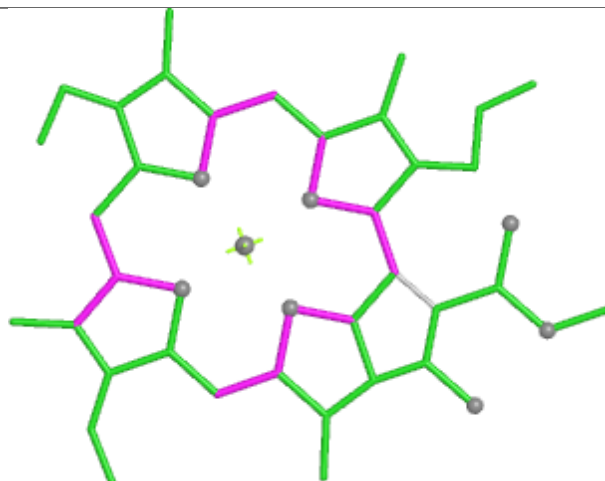
Ligand CL0 A 801



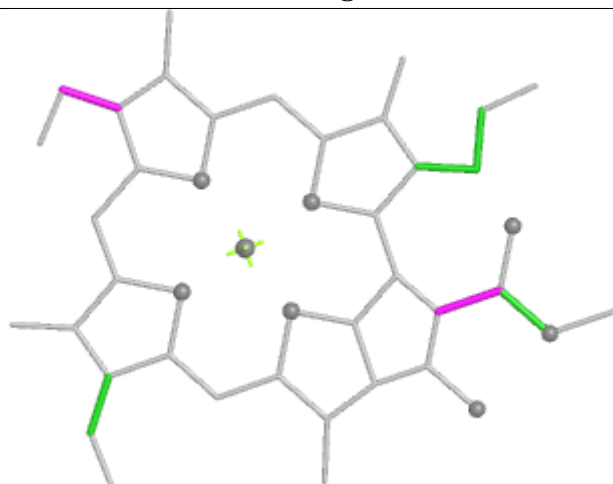
Ligand CLA 7 613



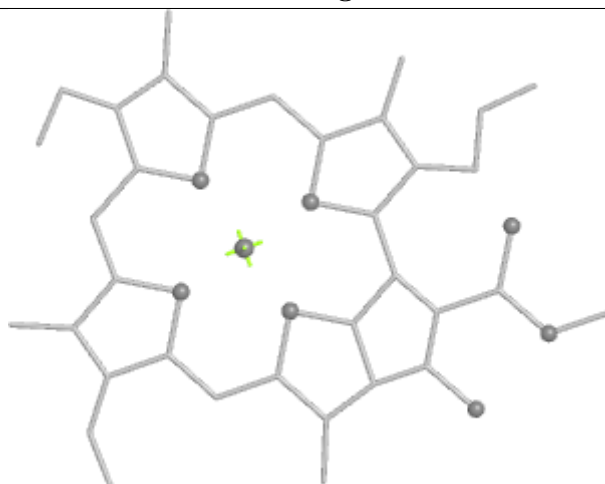
Bond lengths



Bond angles

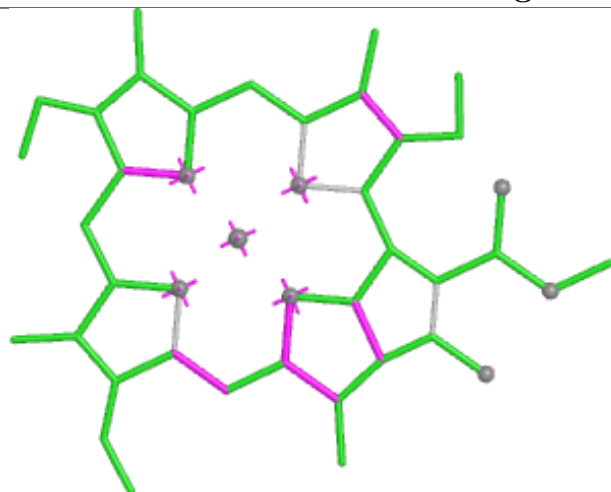


Torsions

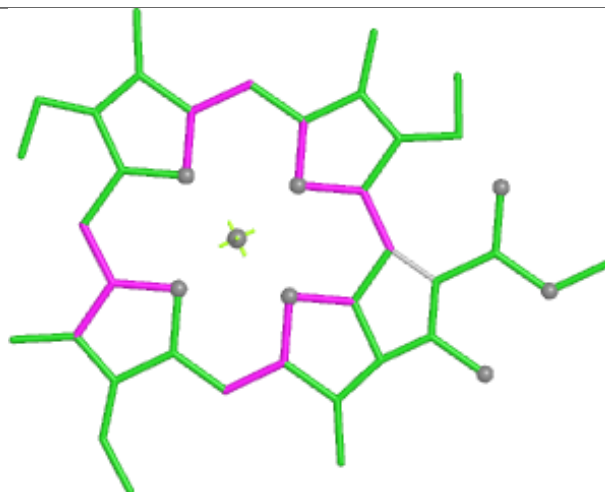


Rings

Ligand CLA B 832



Bond lengths



Bond angles

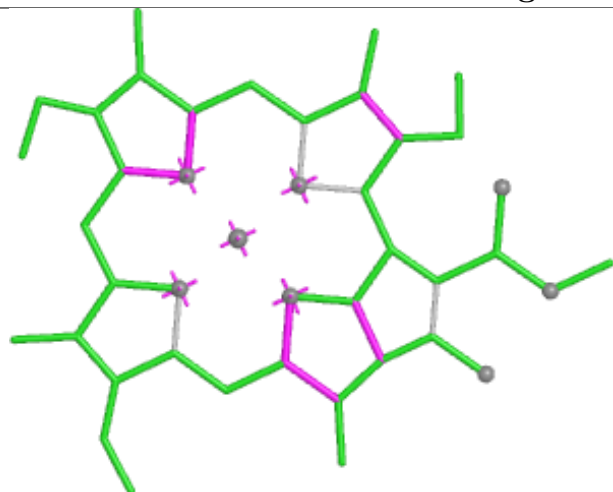


Torsions

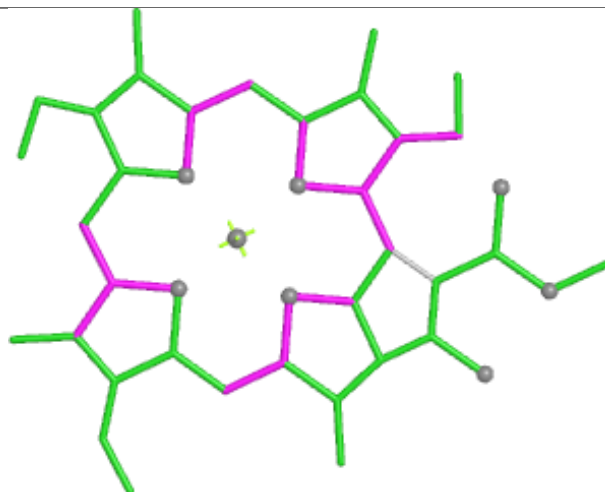


Rings

Ligand CLA J 102



Bond lengths



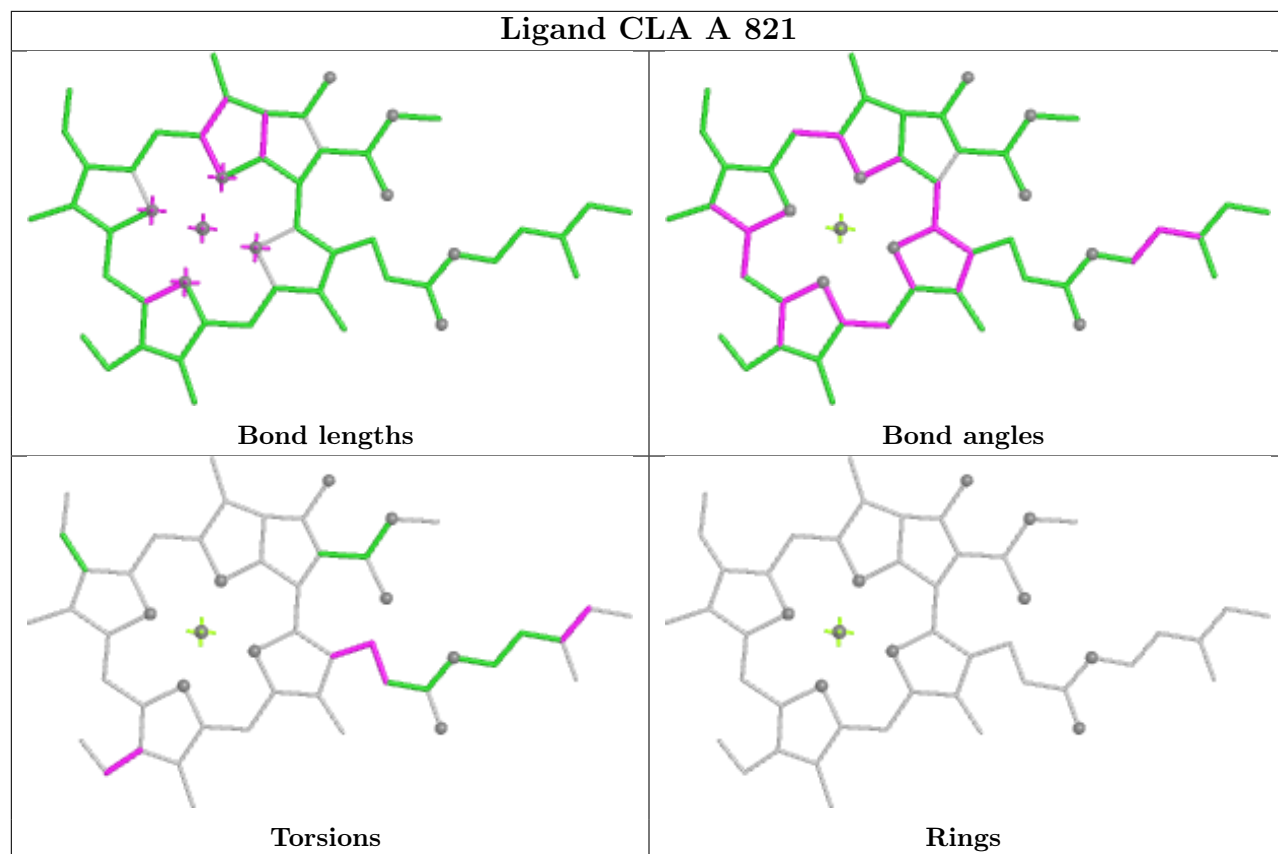
Bond angles

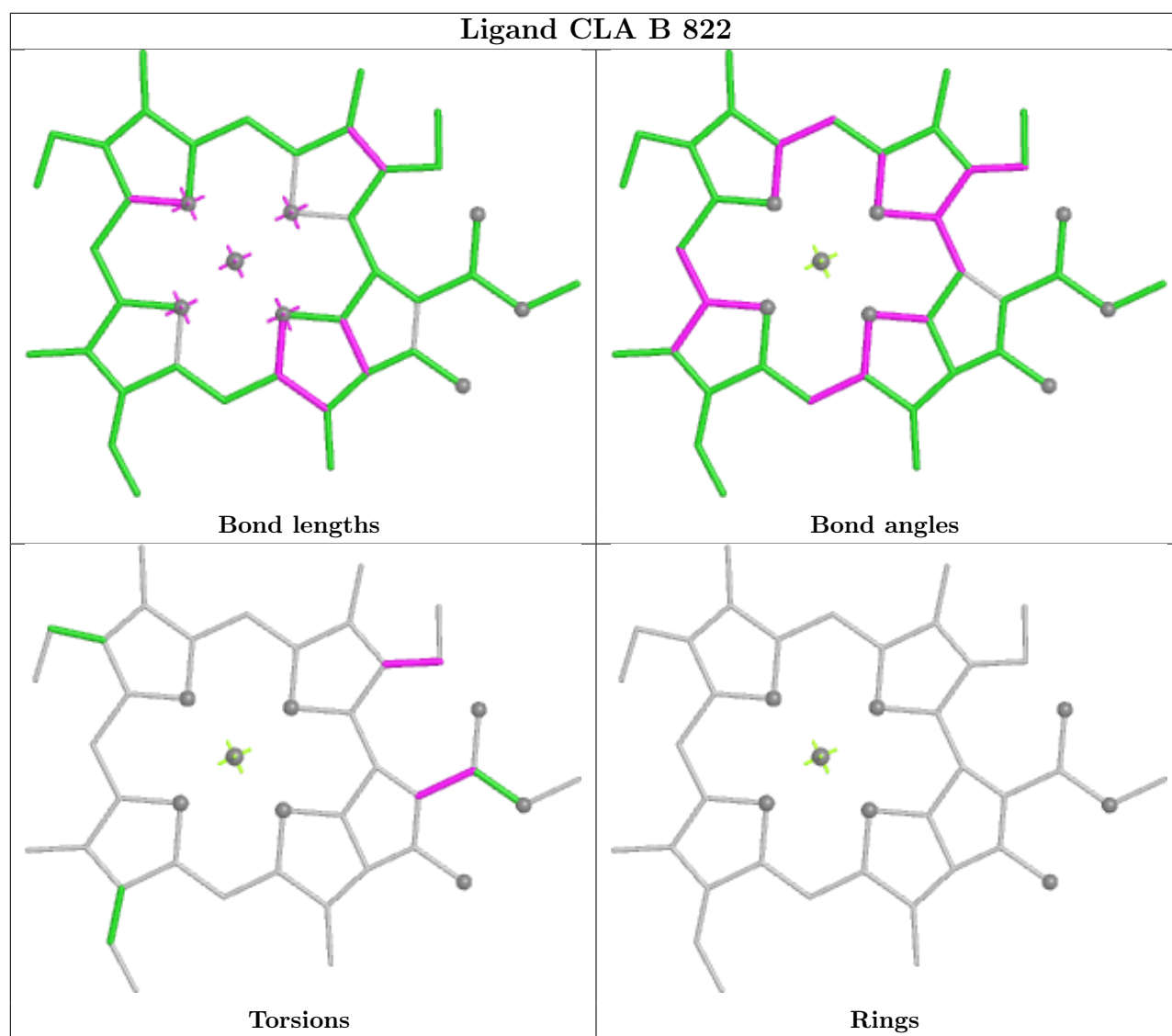


Torsions

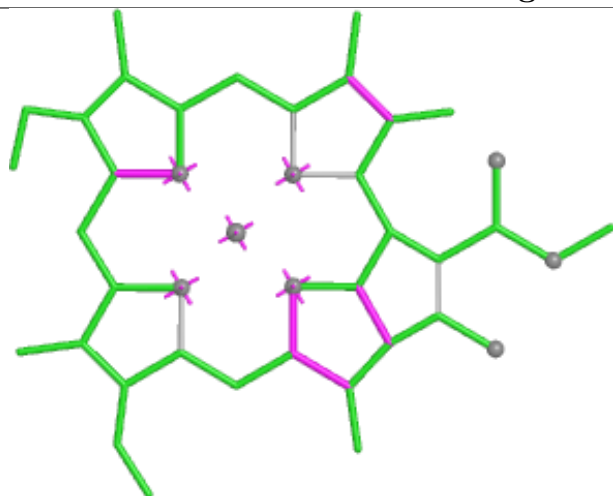


Rings





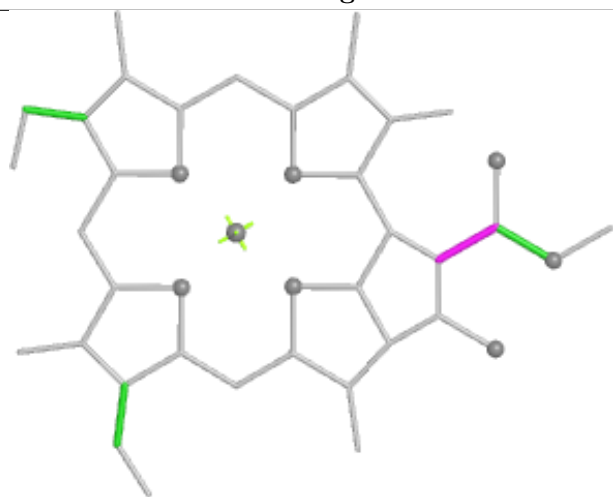
Ligand CLA 3 310



Bond lengths



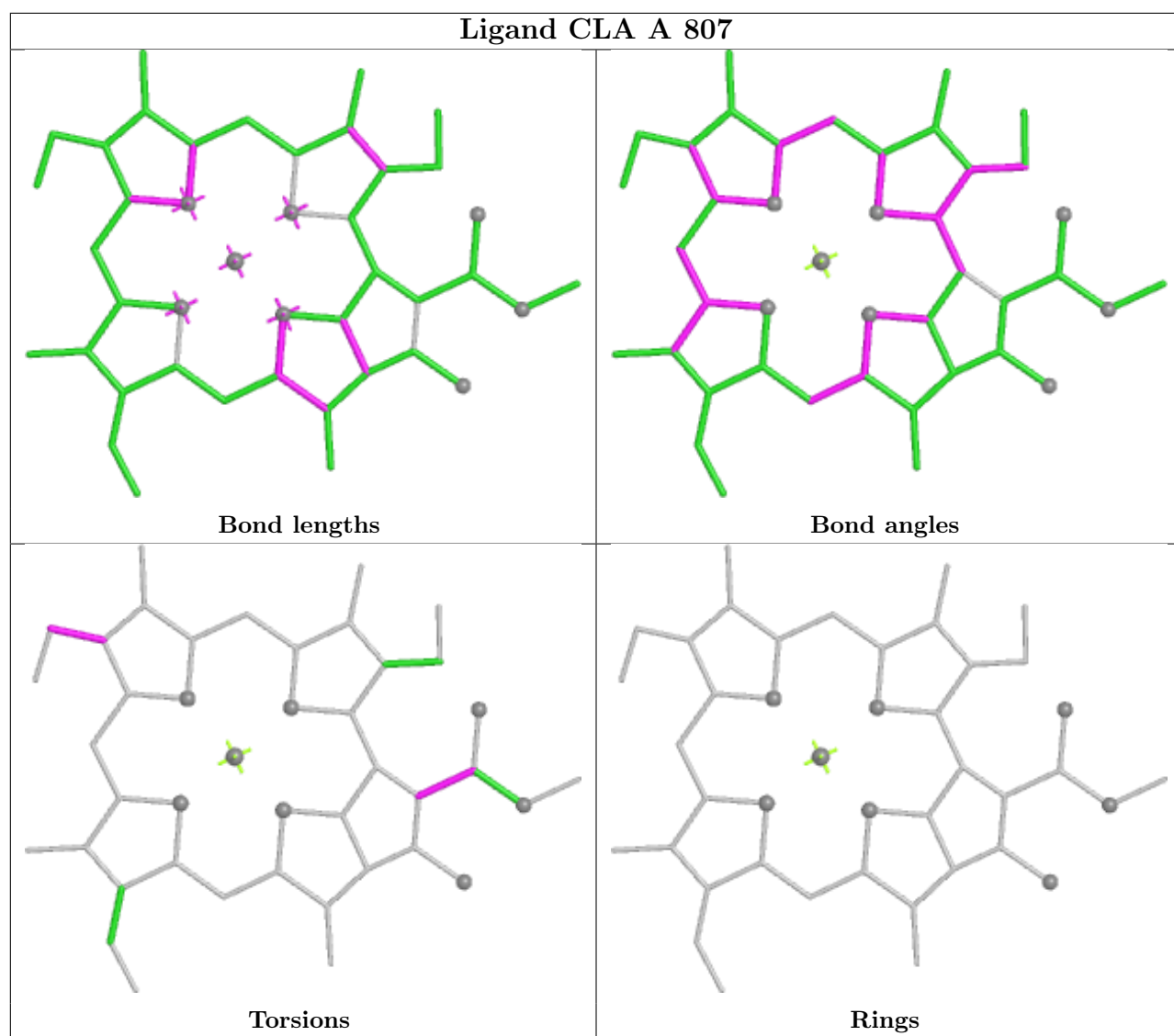
Bond angles

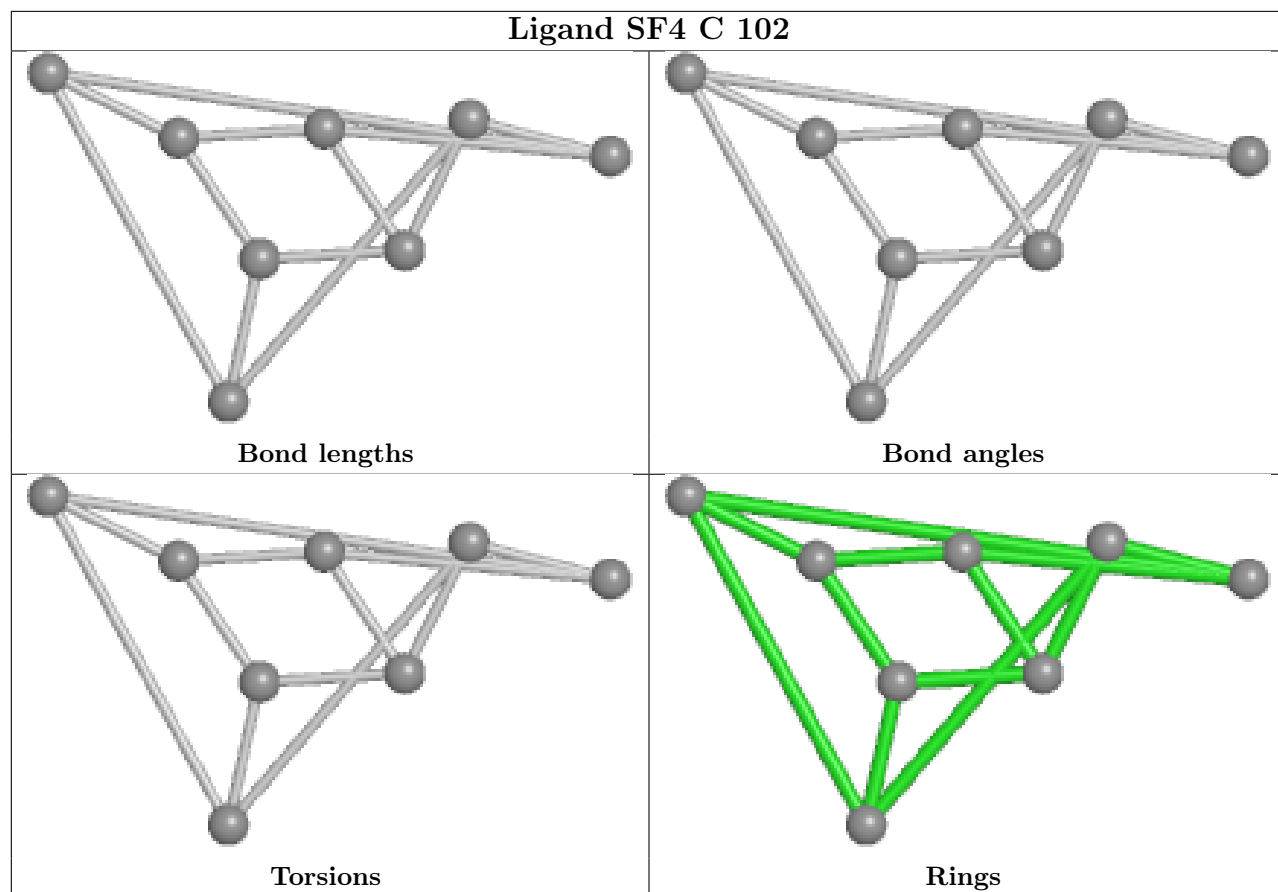


Torsions

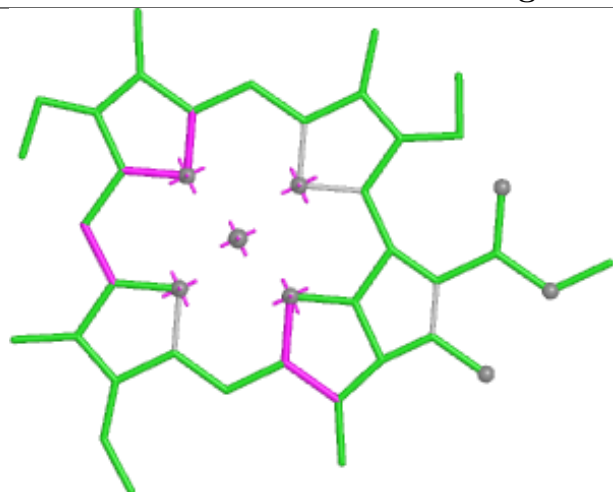


Rings

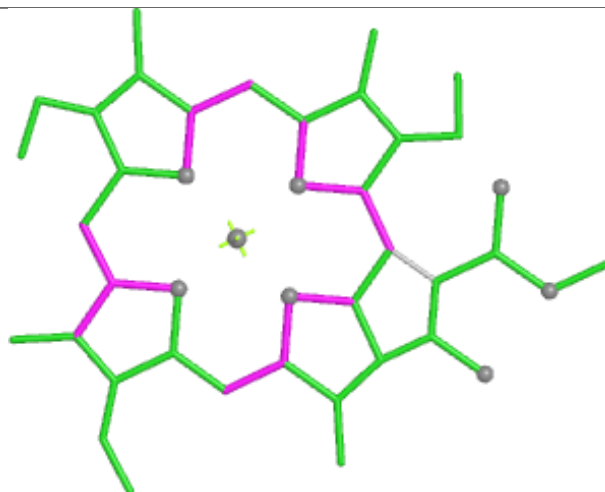




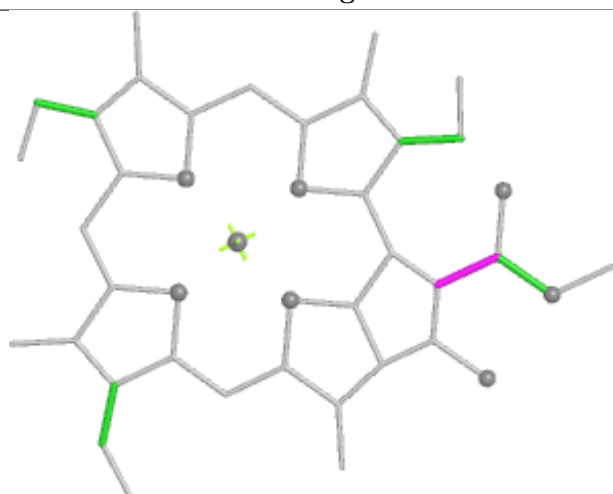
Ligand CLA 1 609



Bond lengths



Bond angles

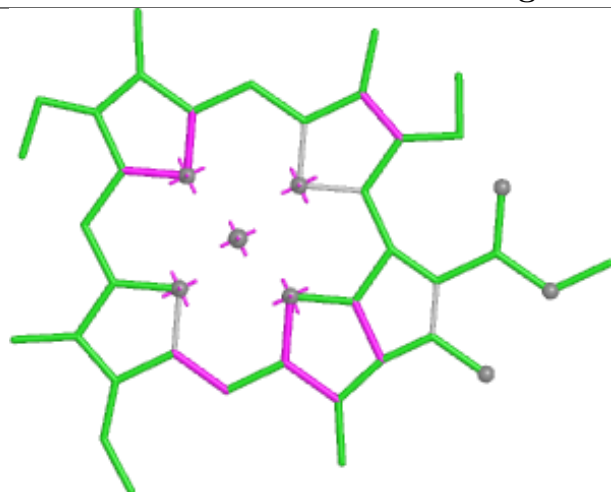


Torsions

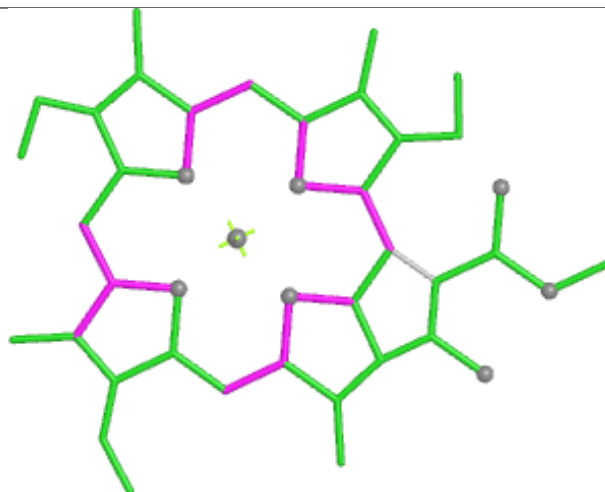


Rings

Ligand CLA 1 603



Bond lengths



Bond angles

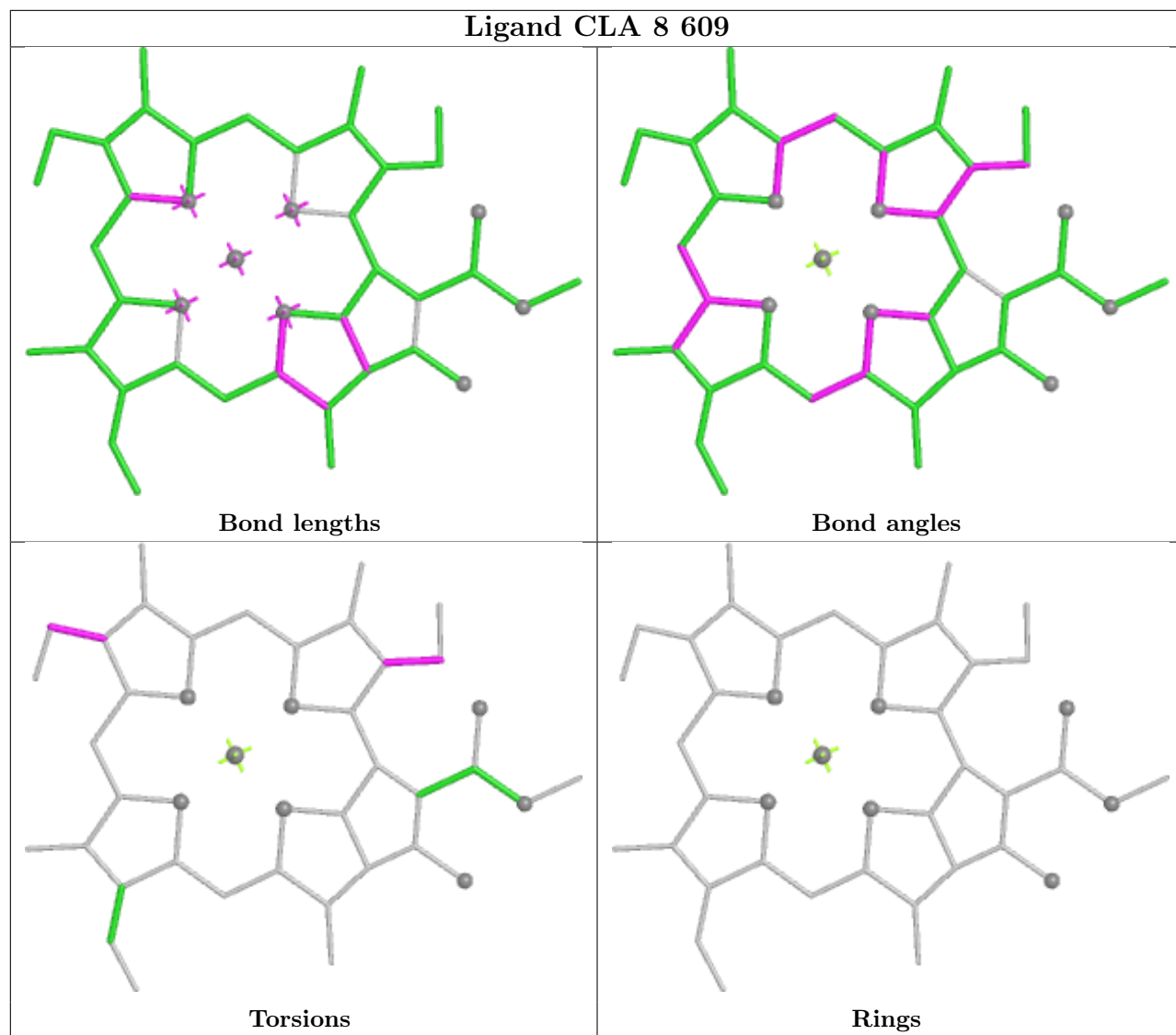


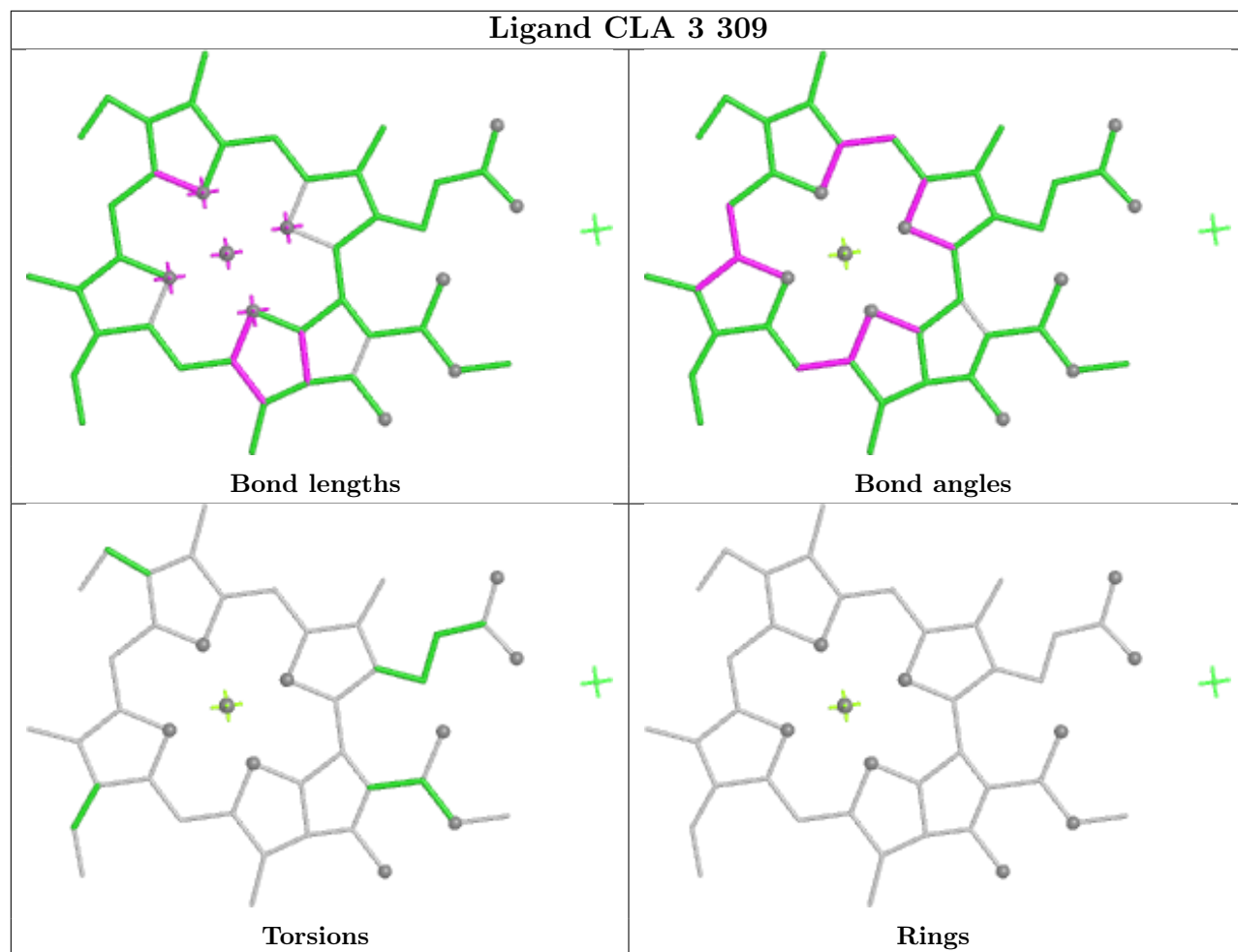
Torsions

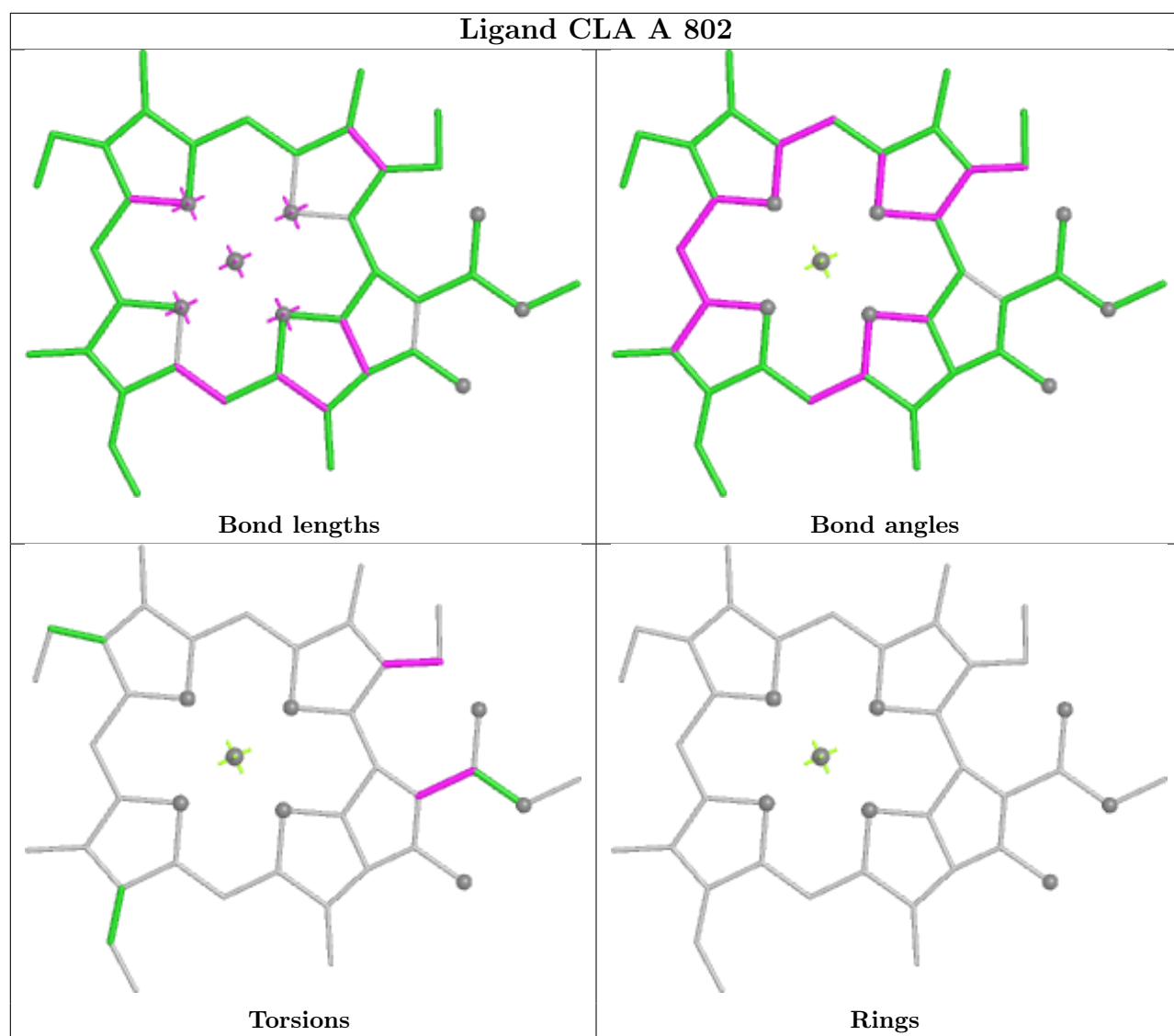


Rings

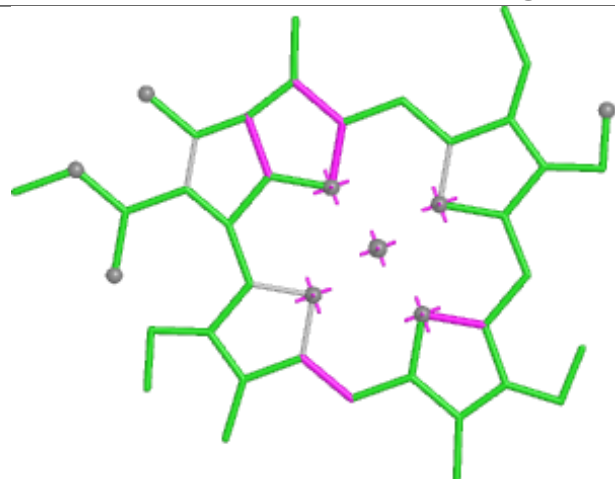
Ligand CLA 8 609



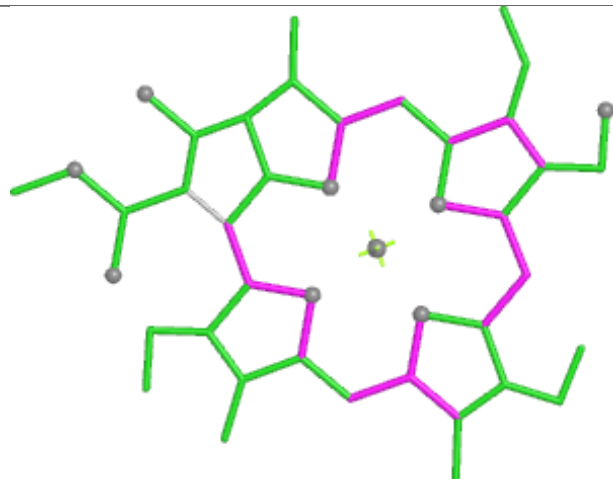




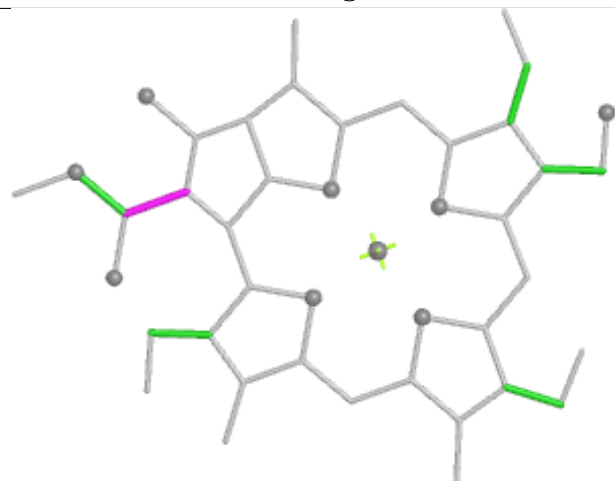
Ligand CHL 5 313



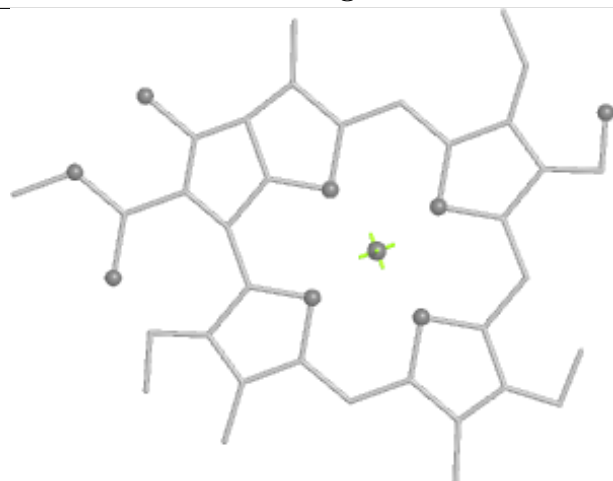
Bond lengths



Bond angles

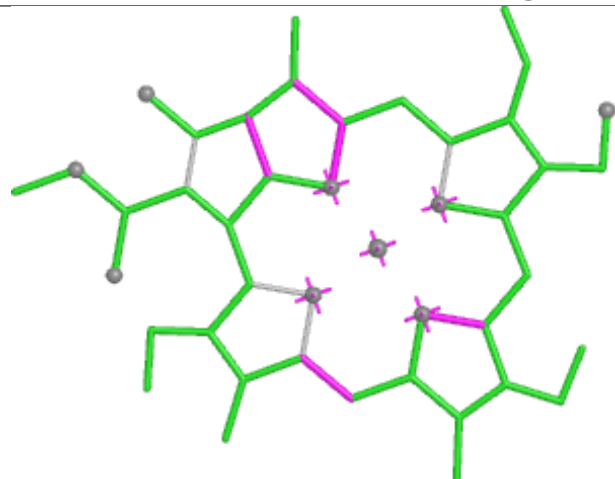


Torsions

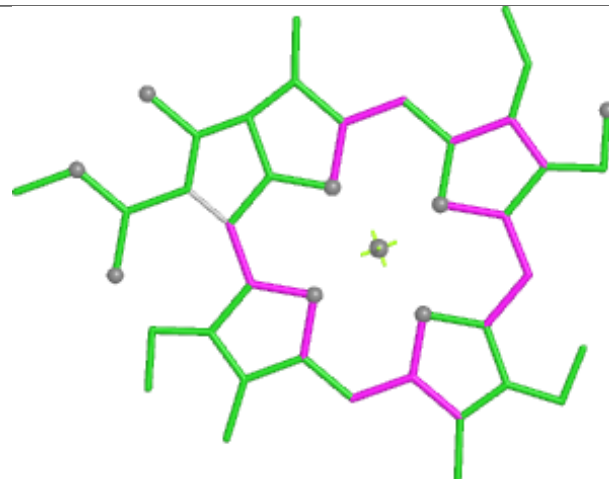


Rings

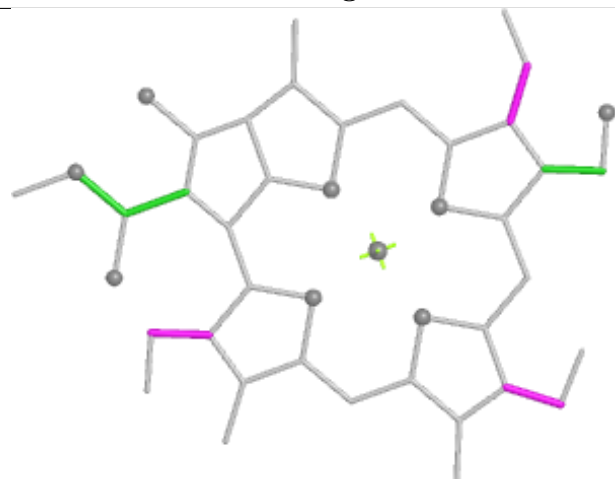
Ligand CHL 6 606



Bond lengths



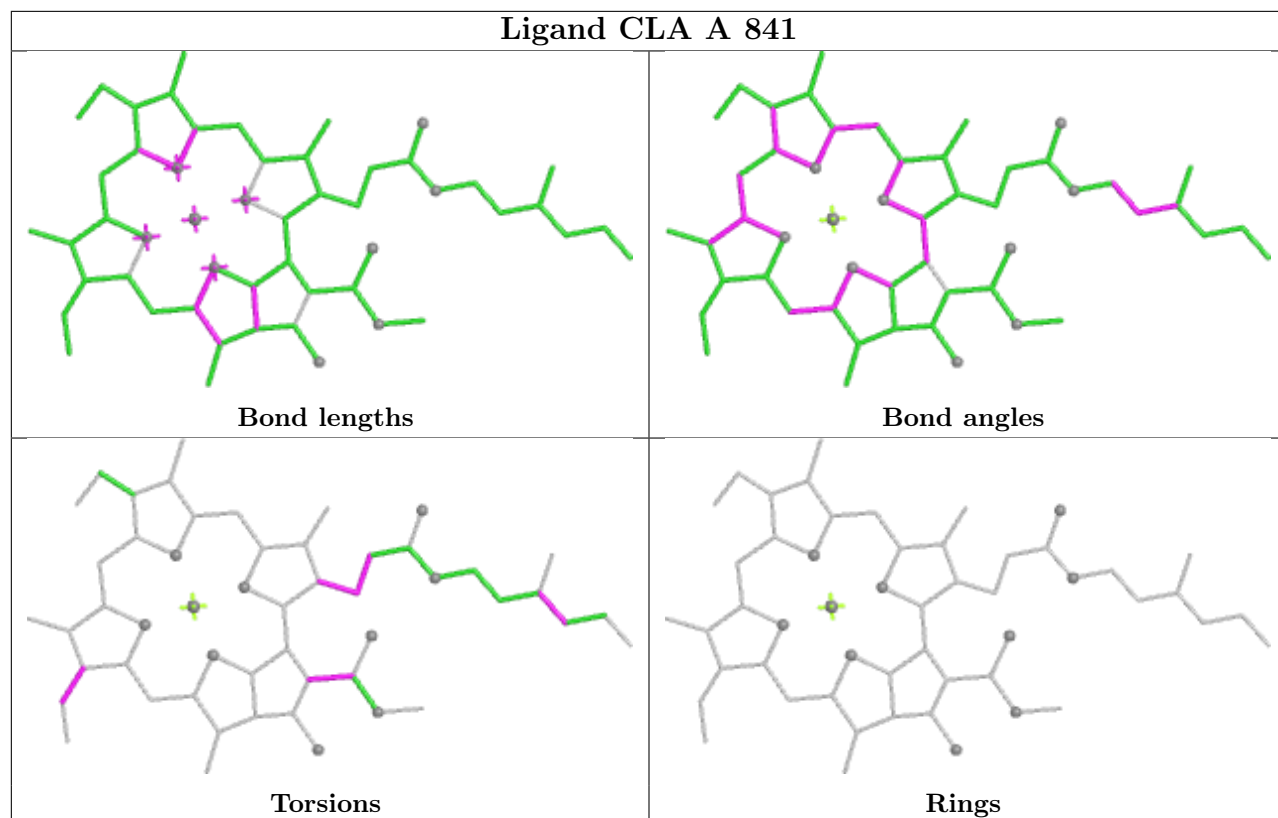
Bond angles

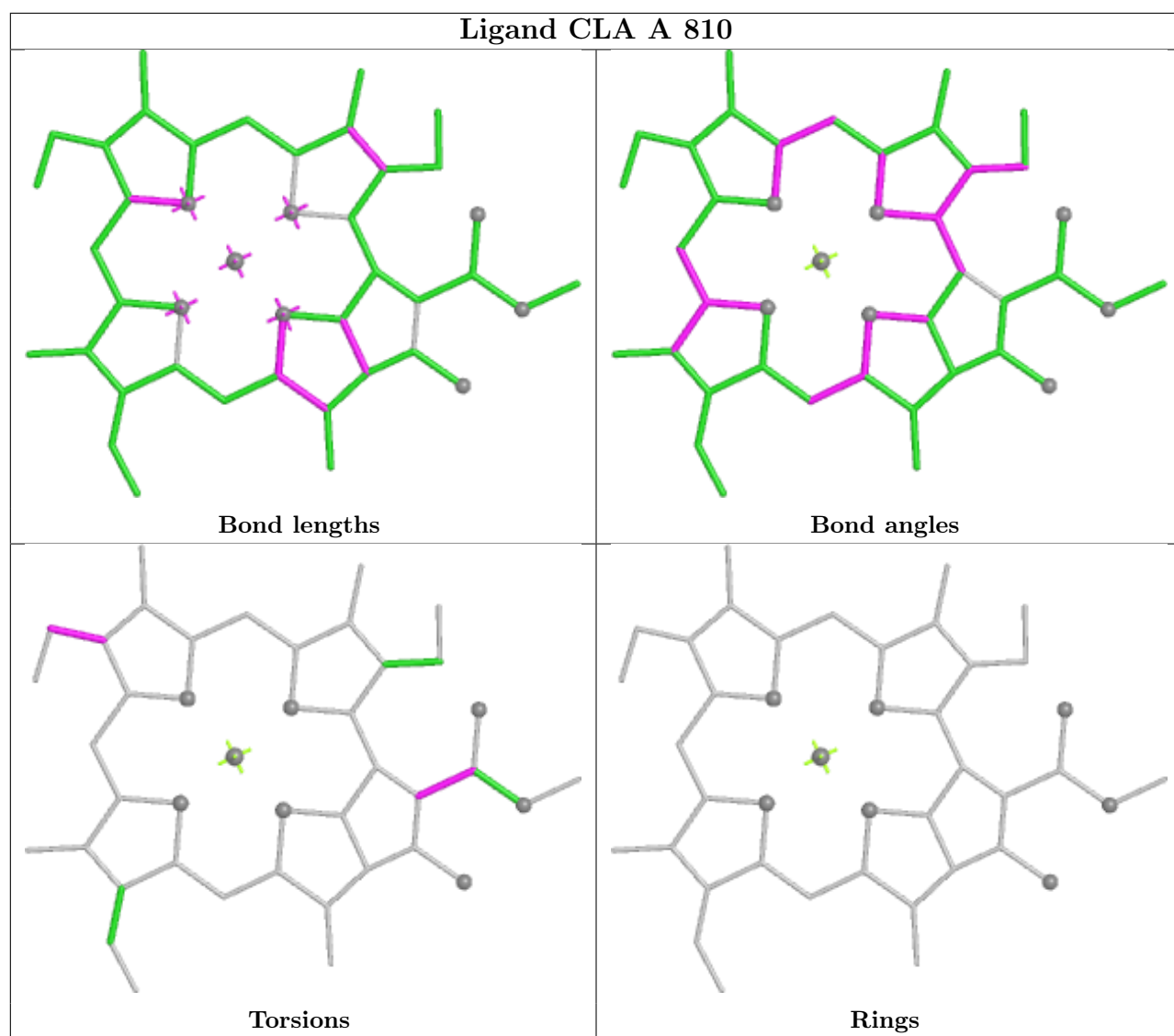


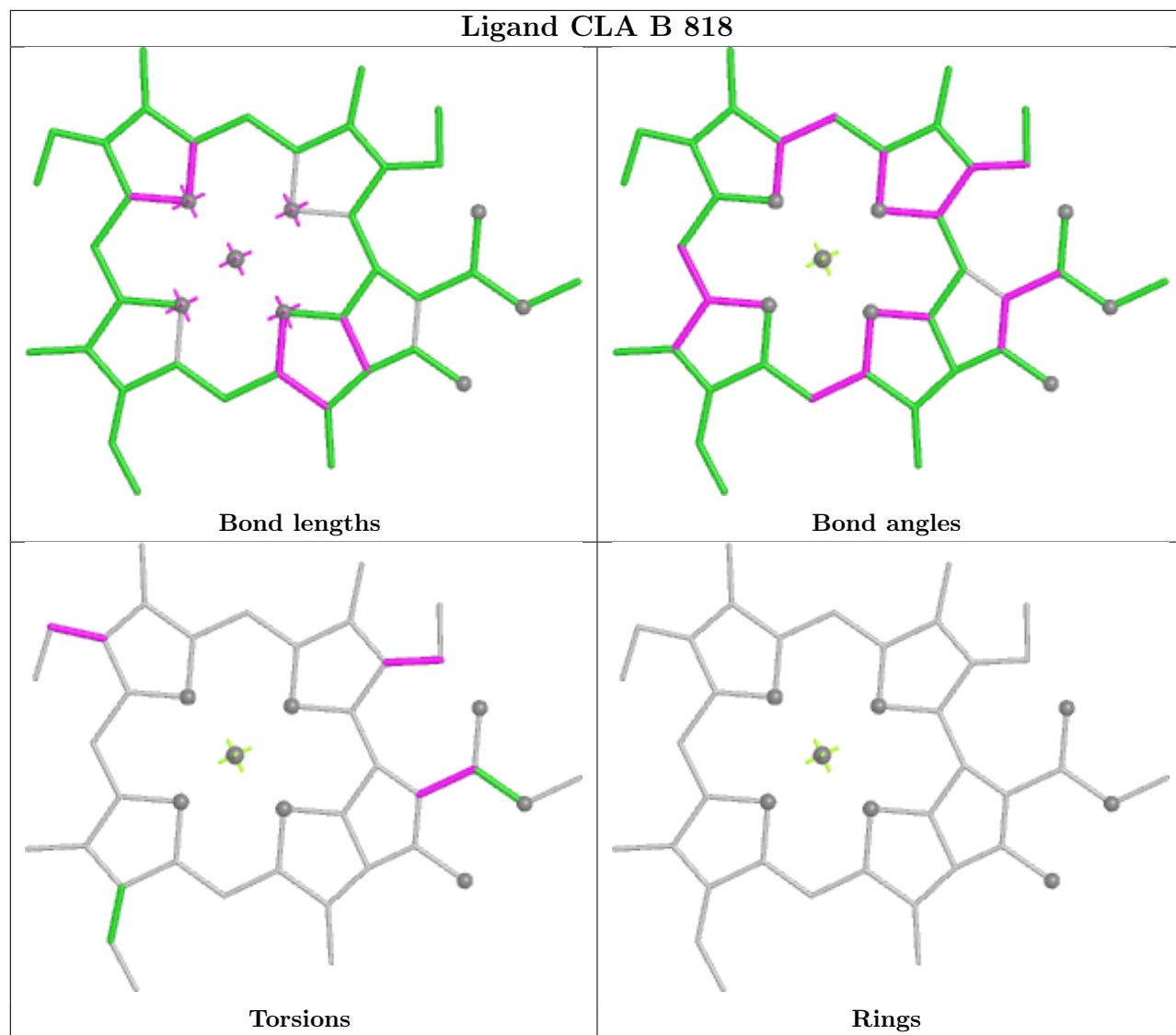
Torsions



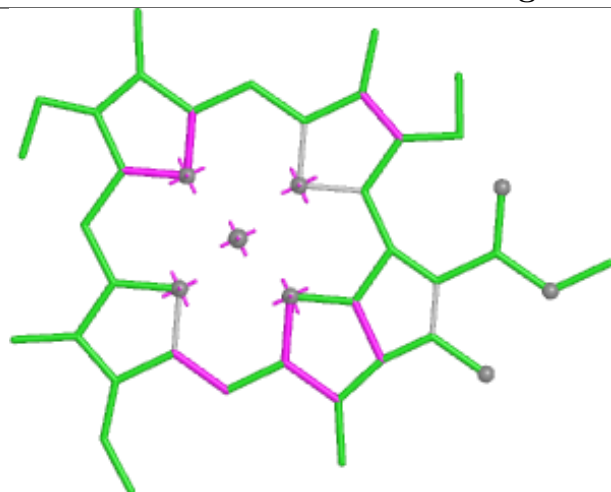
Rings



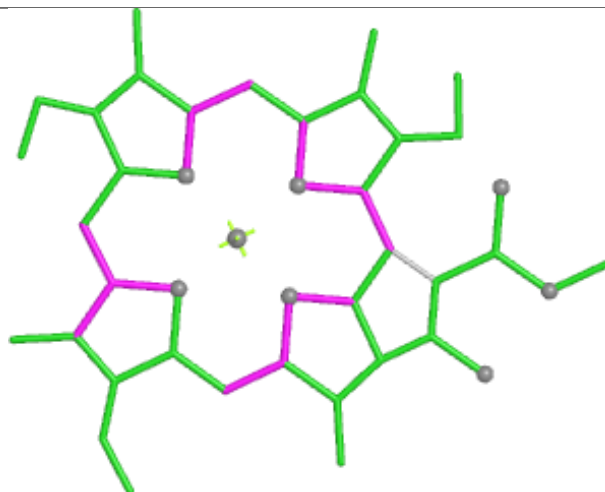




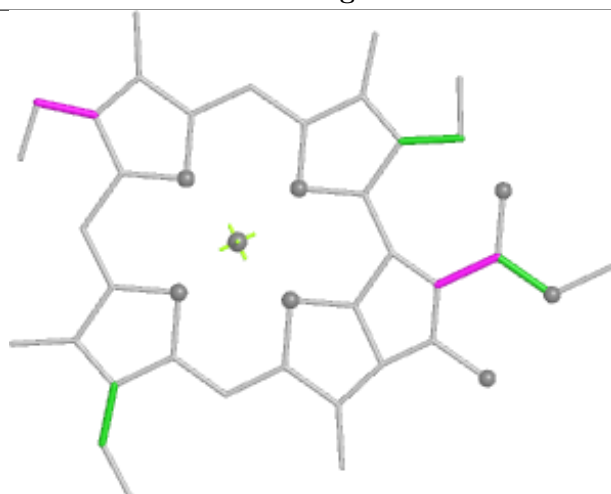
Ligand CLA 8 614



Bond lengths



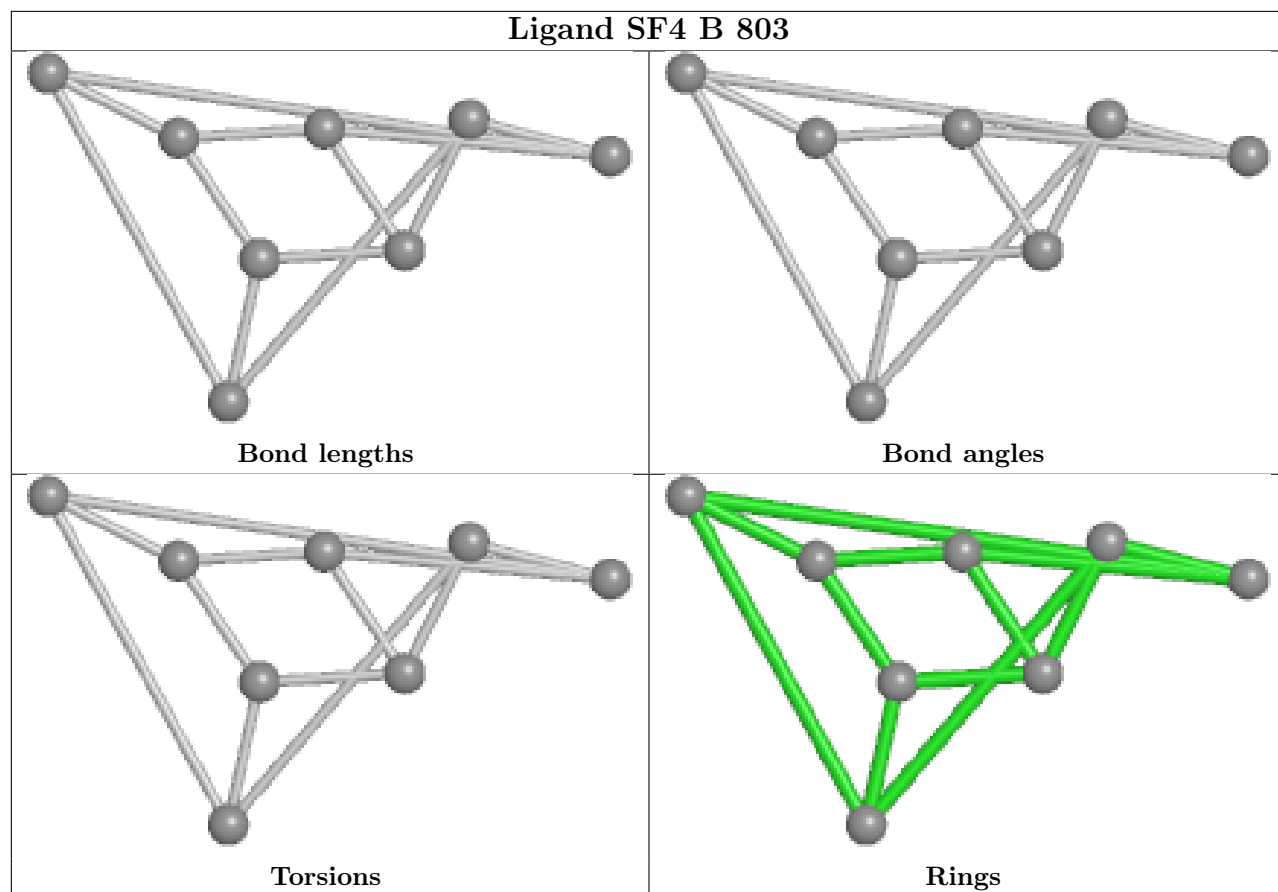
Bond angles



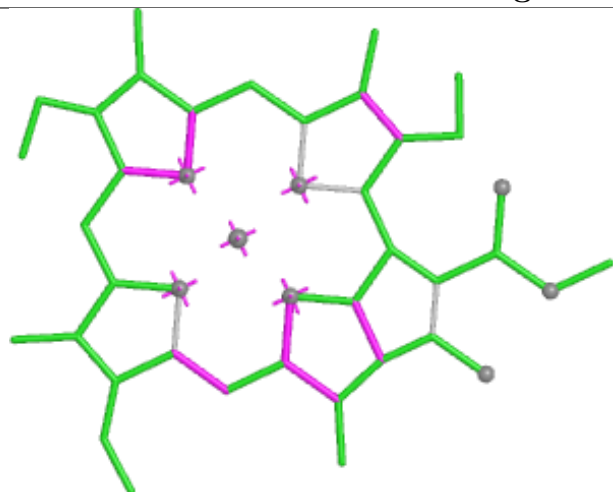
Torsions



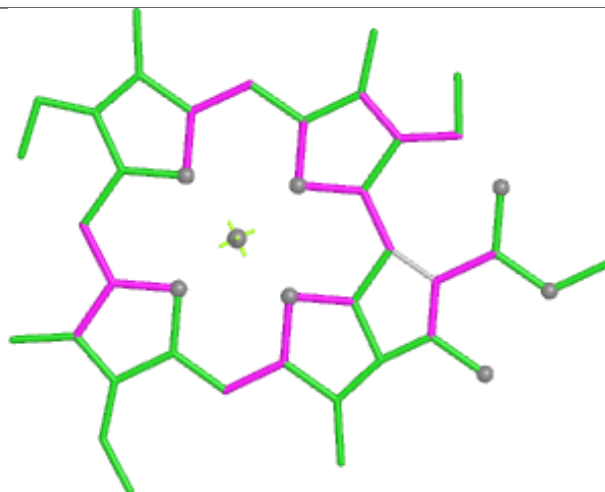
Rings



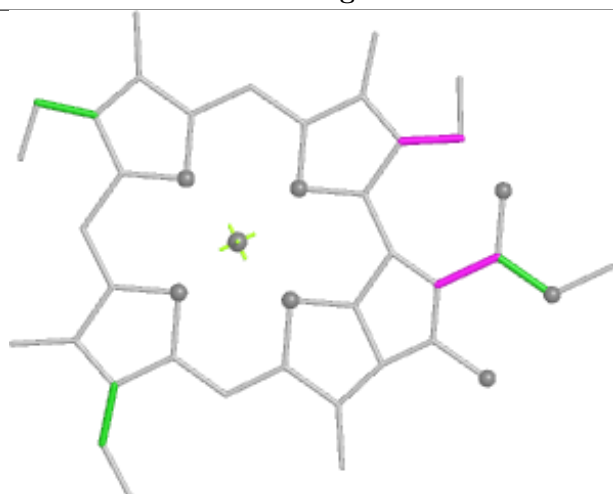
Ligand CLA A 831



Bond lengths



Bond angles

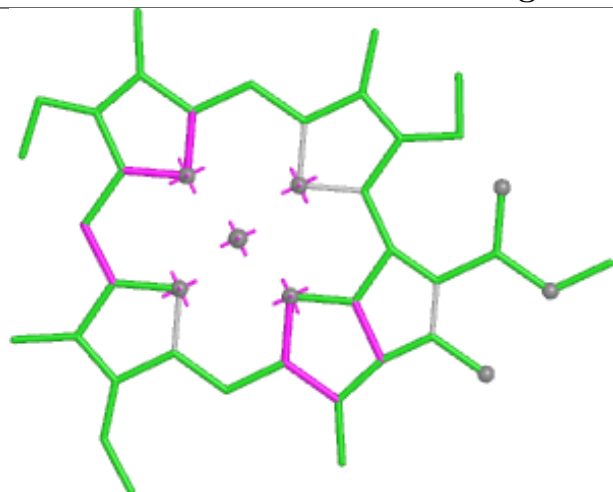


Torsions

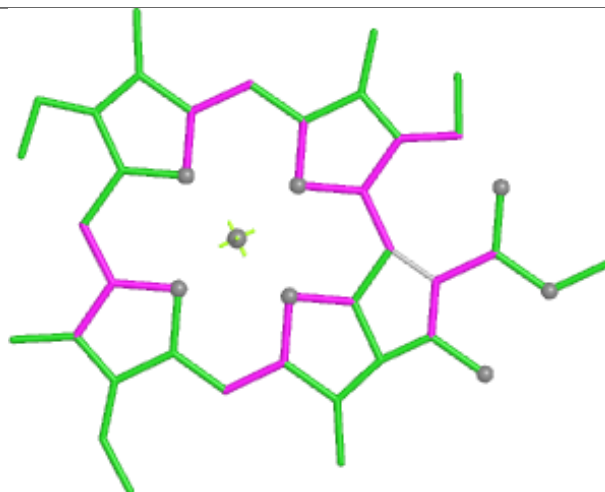


Rings

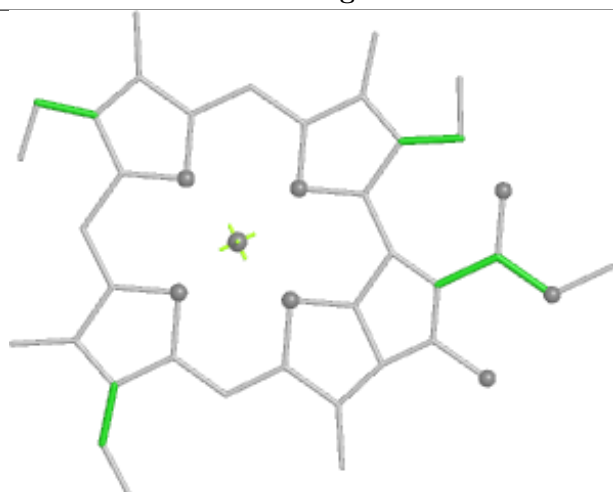
Ligand CLA 8 608



Bond lengths



Bond angles

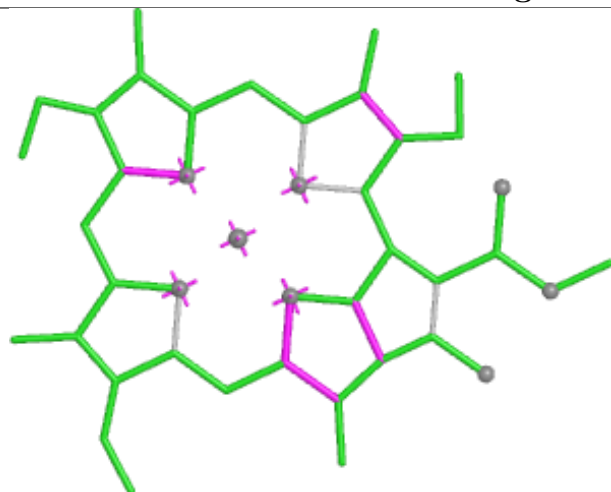


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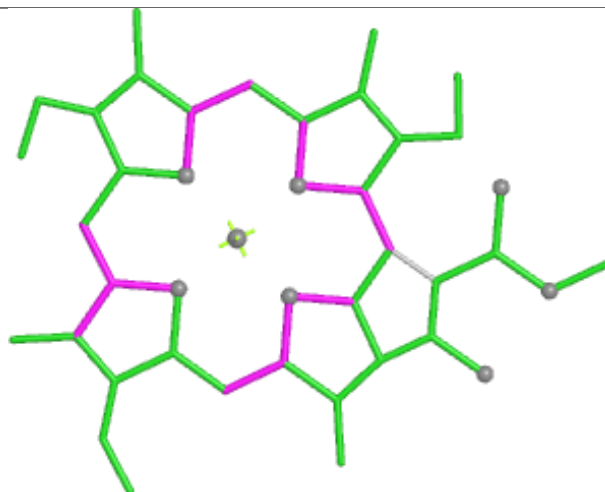


Rings

Ligand CLA B 834



Bond lengths



Bond angles

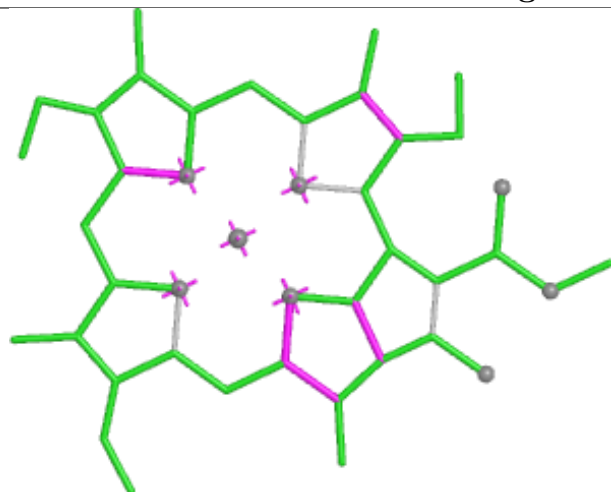


Torsions

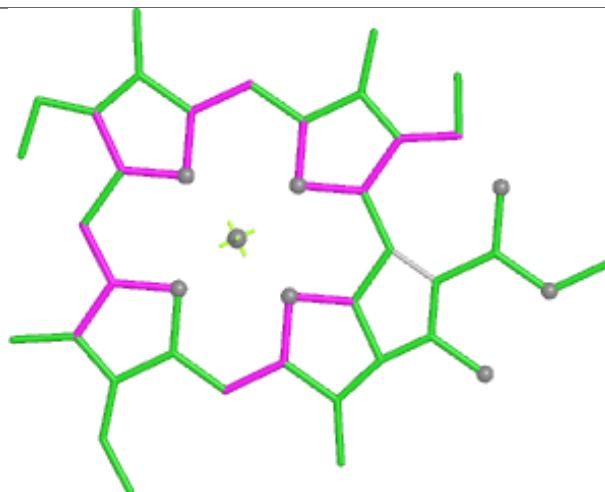


Rings

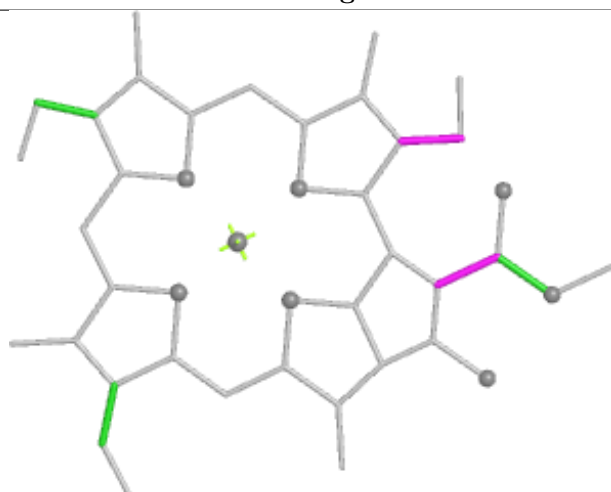
Ligand CLA 5 309



Bond lengths



Bond angles

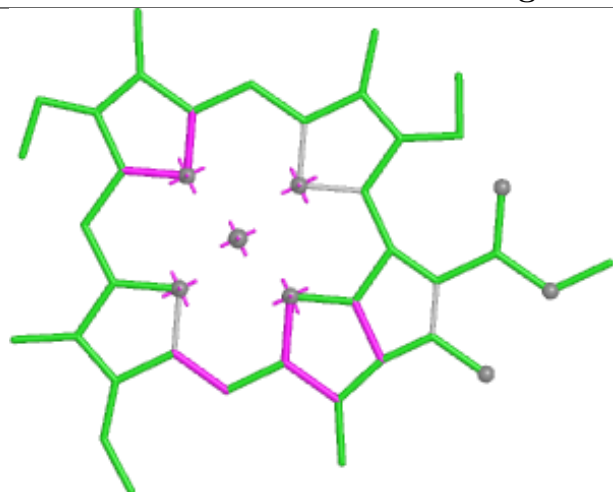


Torsions

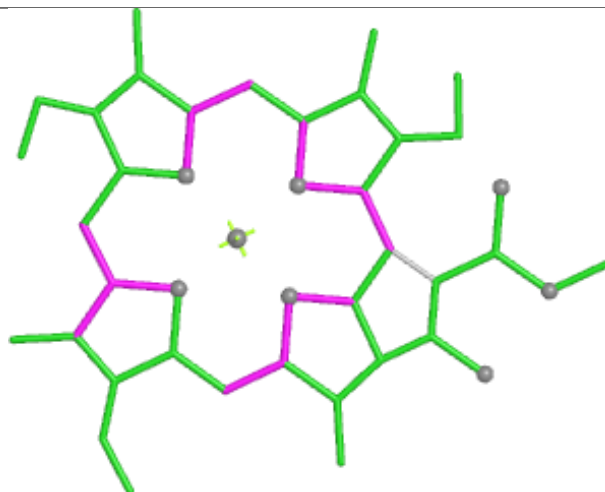


Rings

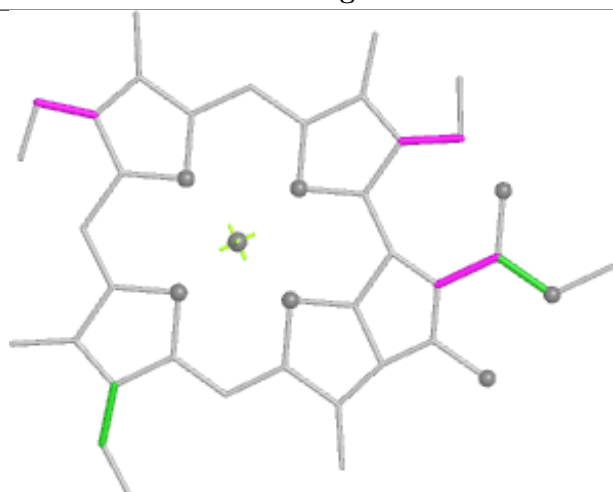
Ligand CLA 6 602



Bond lengths



Bond angles

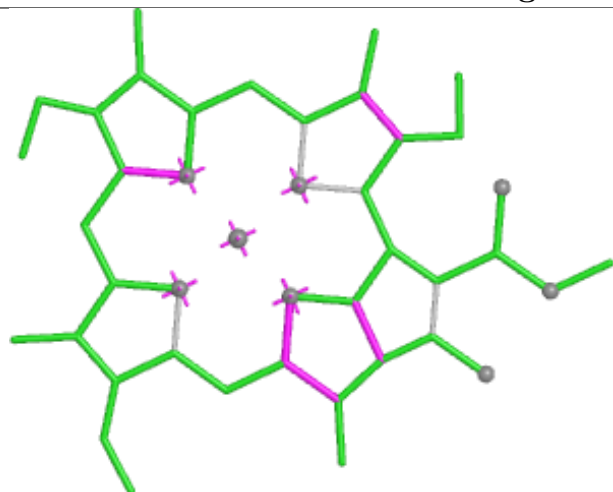


Torsions

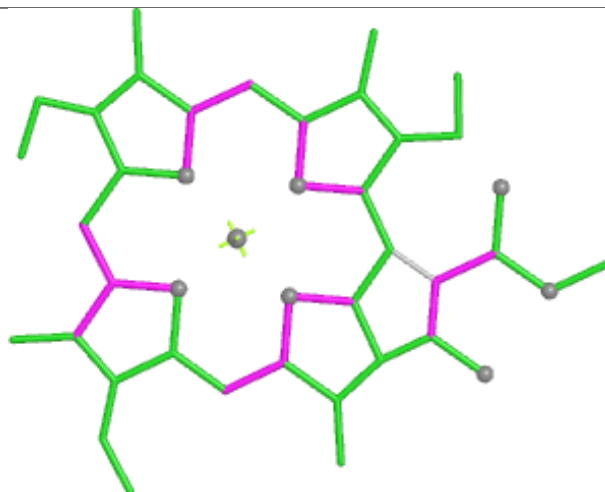


Rings

Ligand CLA 6 603



Bond lengths



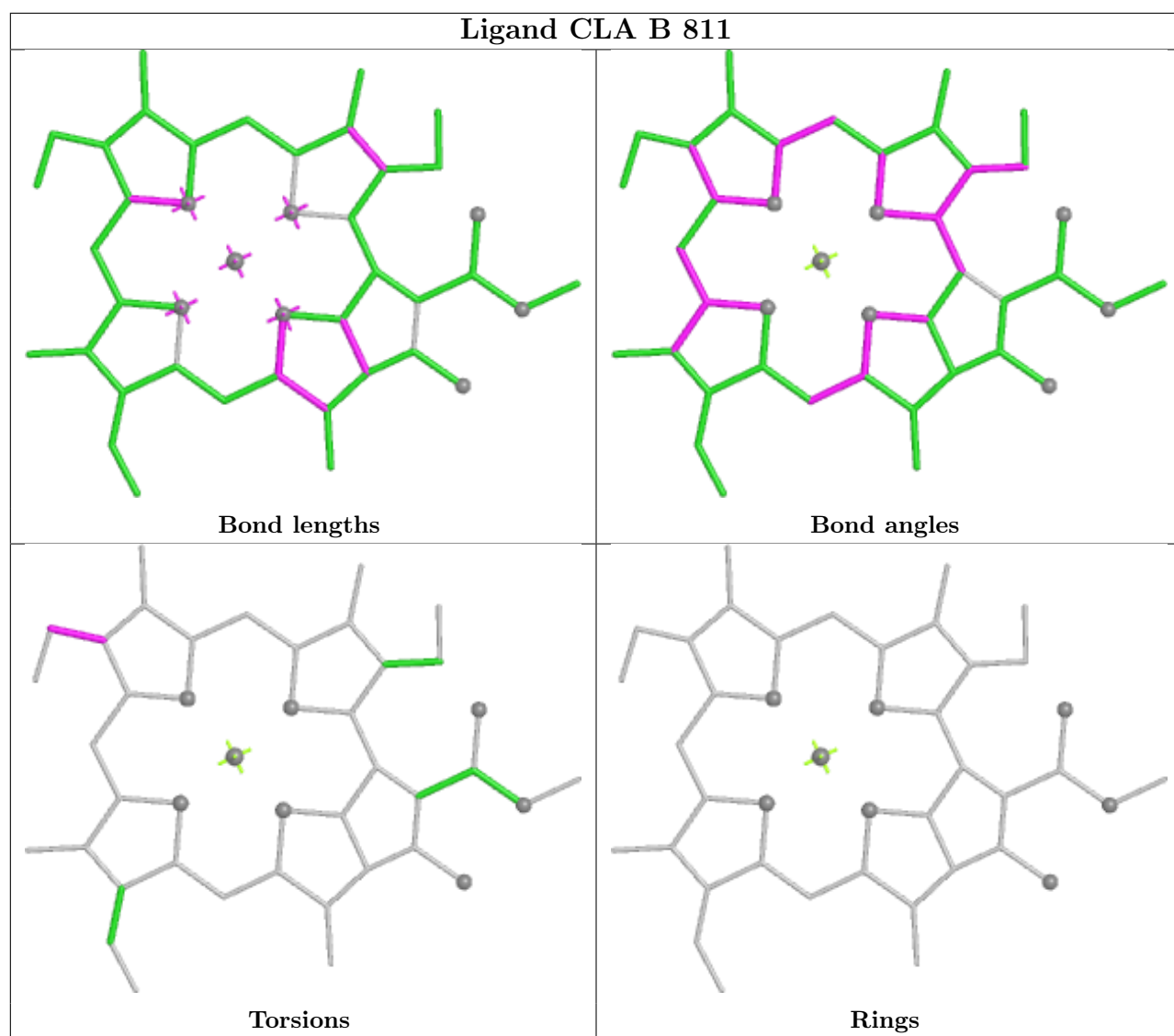
Bond angles



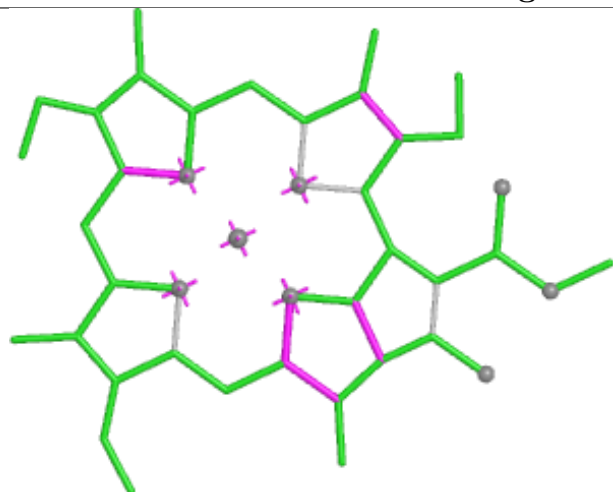
Torsions



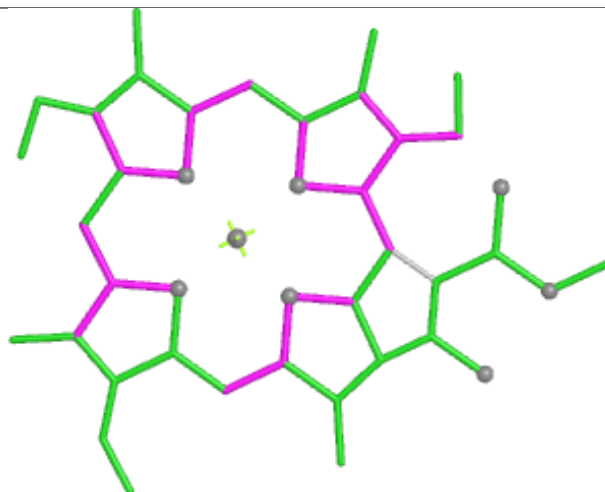
Rings



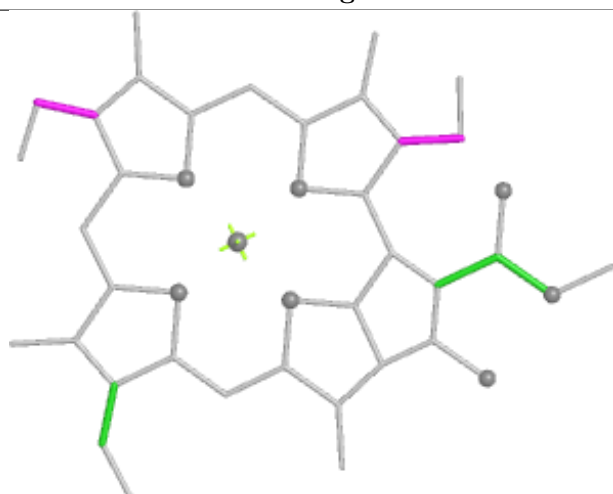
Ligand CLA 3 313



Bond lengths



Bond angles

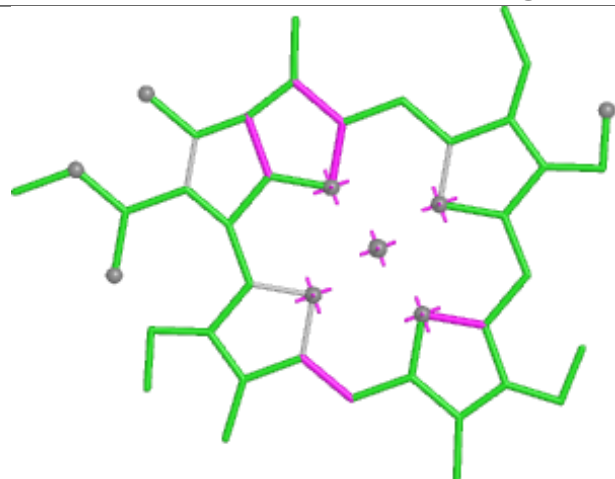


Torsions

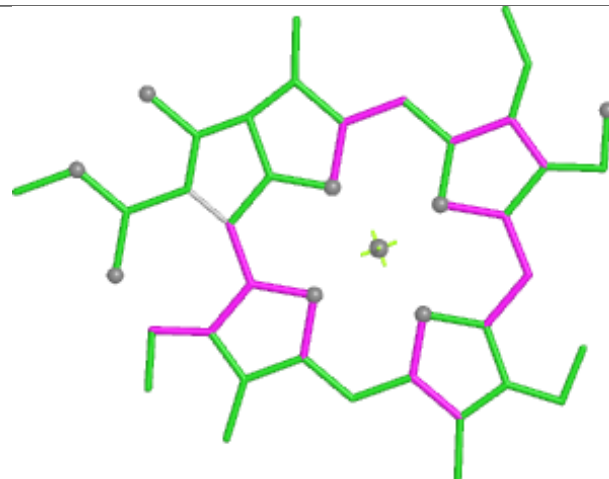


Rings

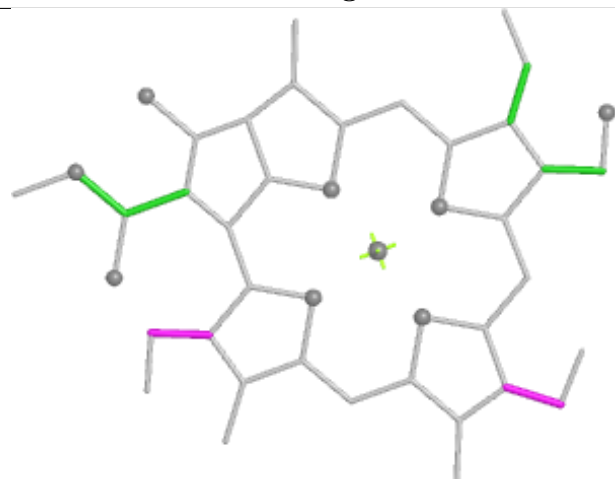
Ligand CHL 6 607



Bond lengths



Bond angles

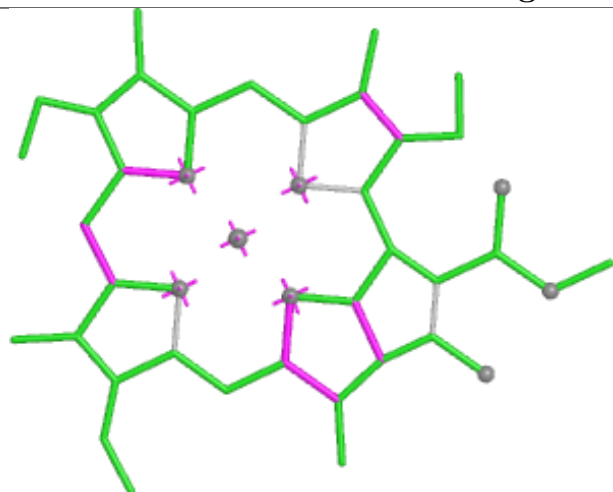


Torsions

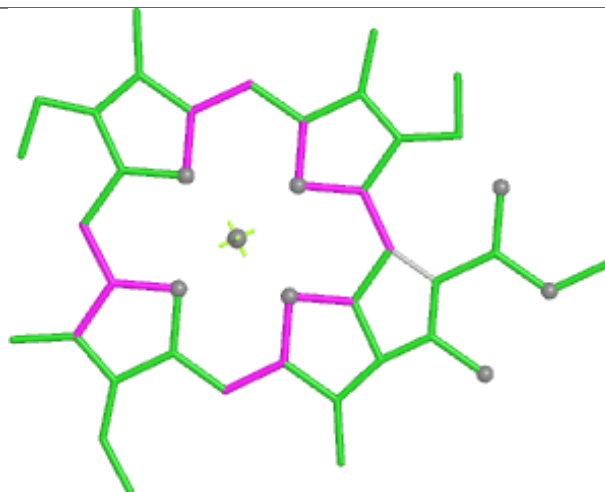


Rings

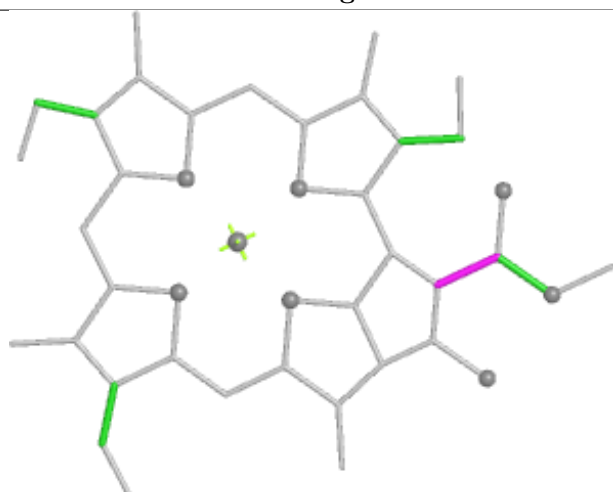
Ligand CLA 3 311



Bond lengths



Bond angles

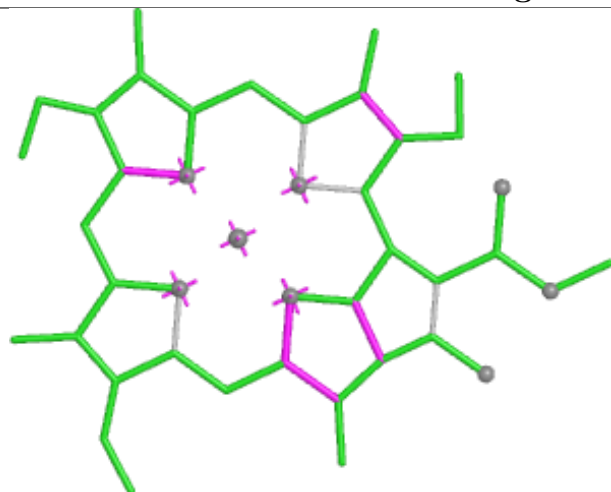


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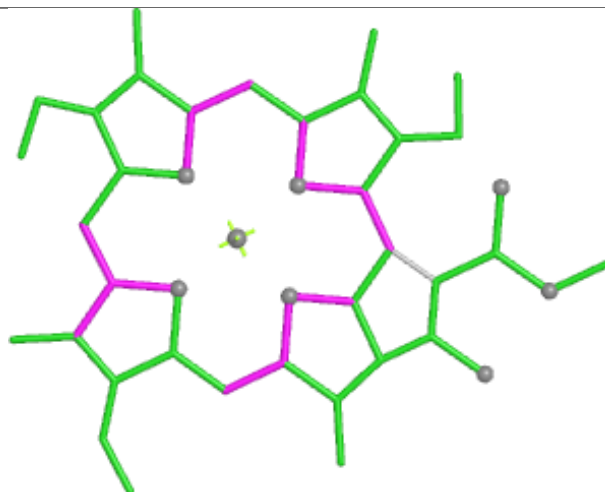


Rings

Ligand CLA B 808



Bond lengths



Bond angles

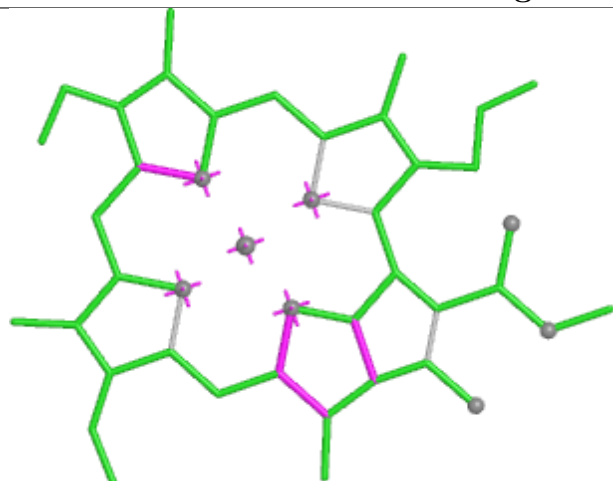


Torsions

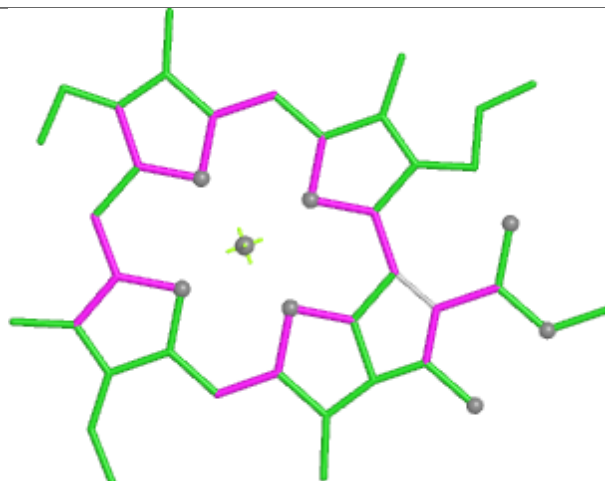


Rings

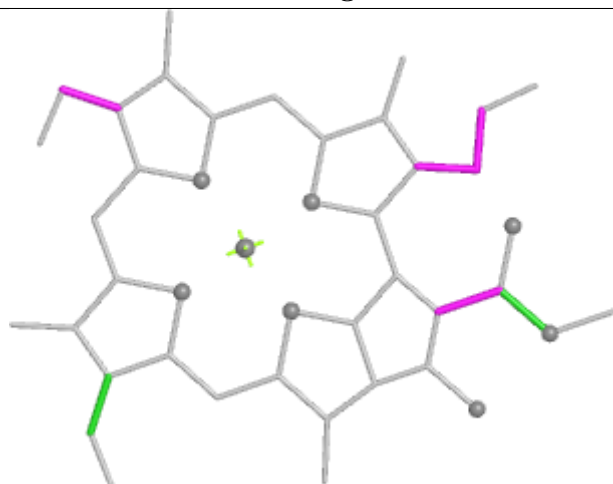
Ligand CLA B 829



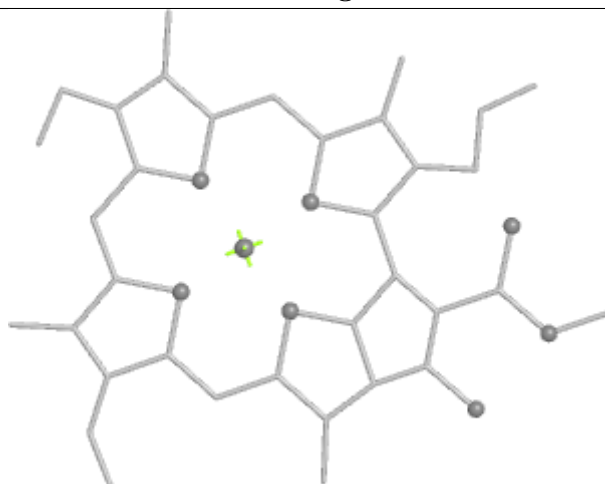
Bond lengths



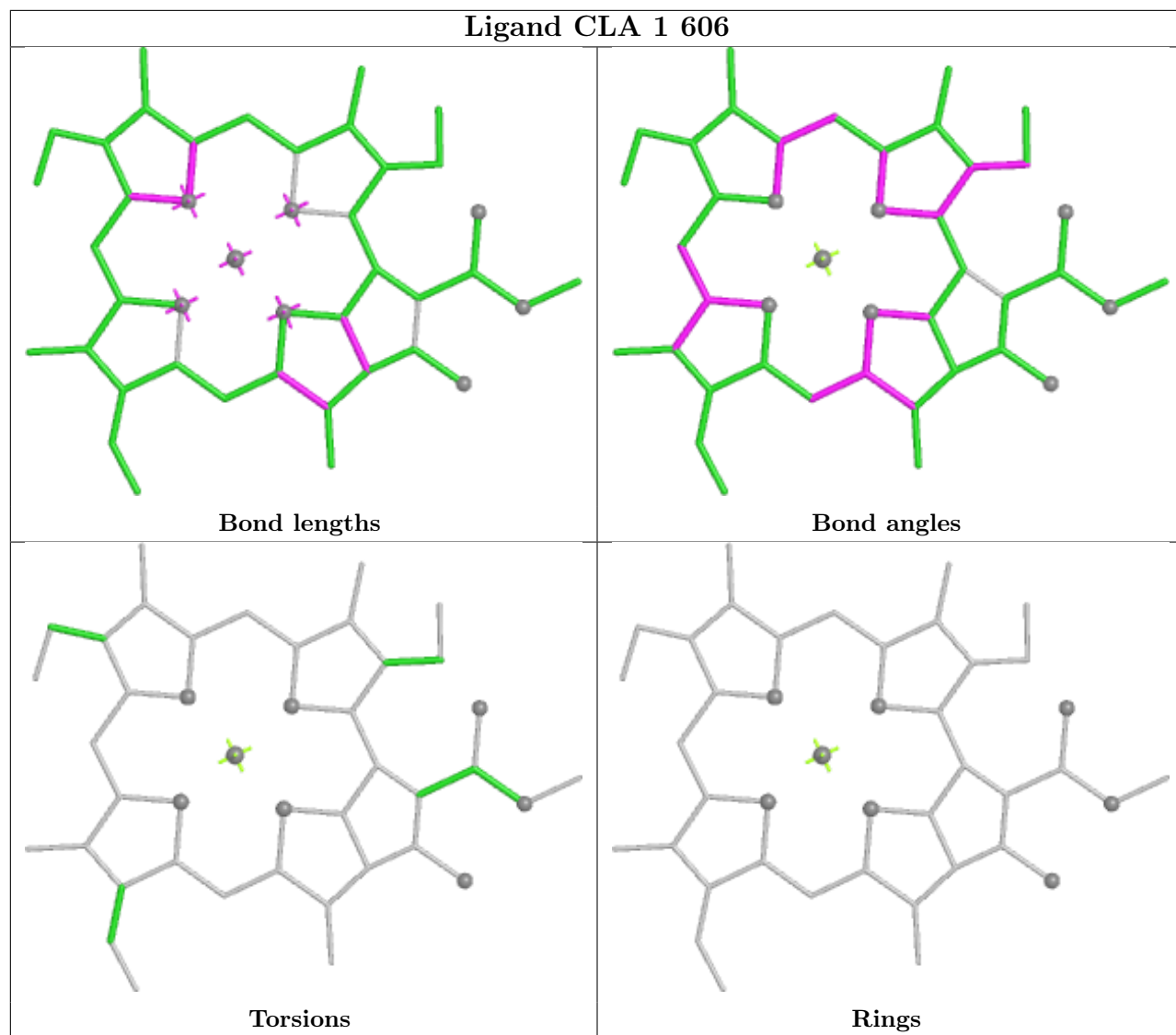
Bond angles

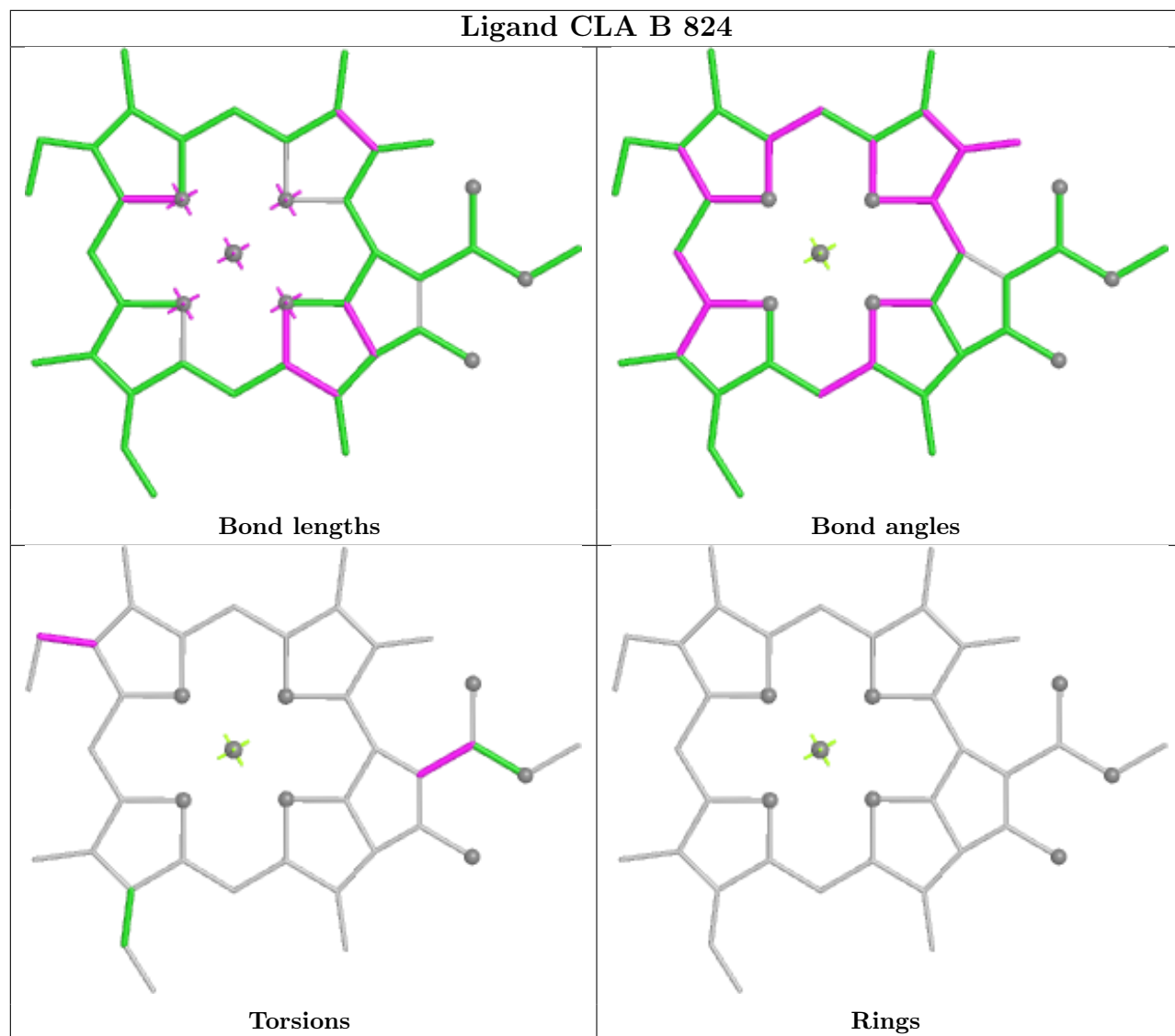


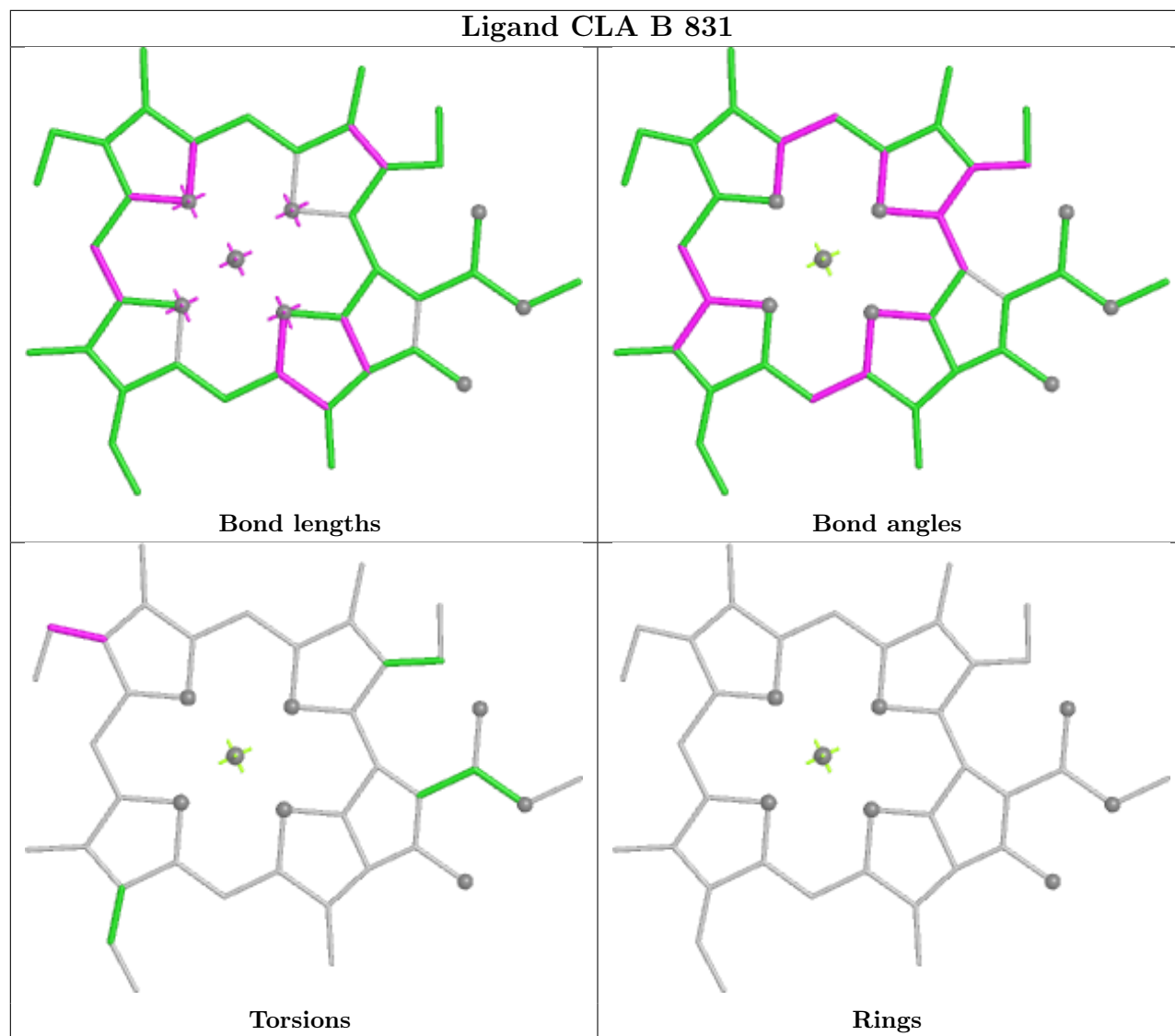
Torsions

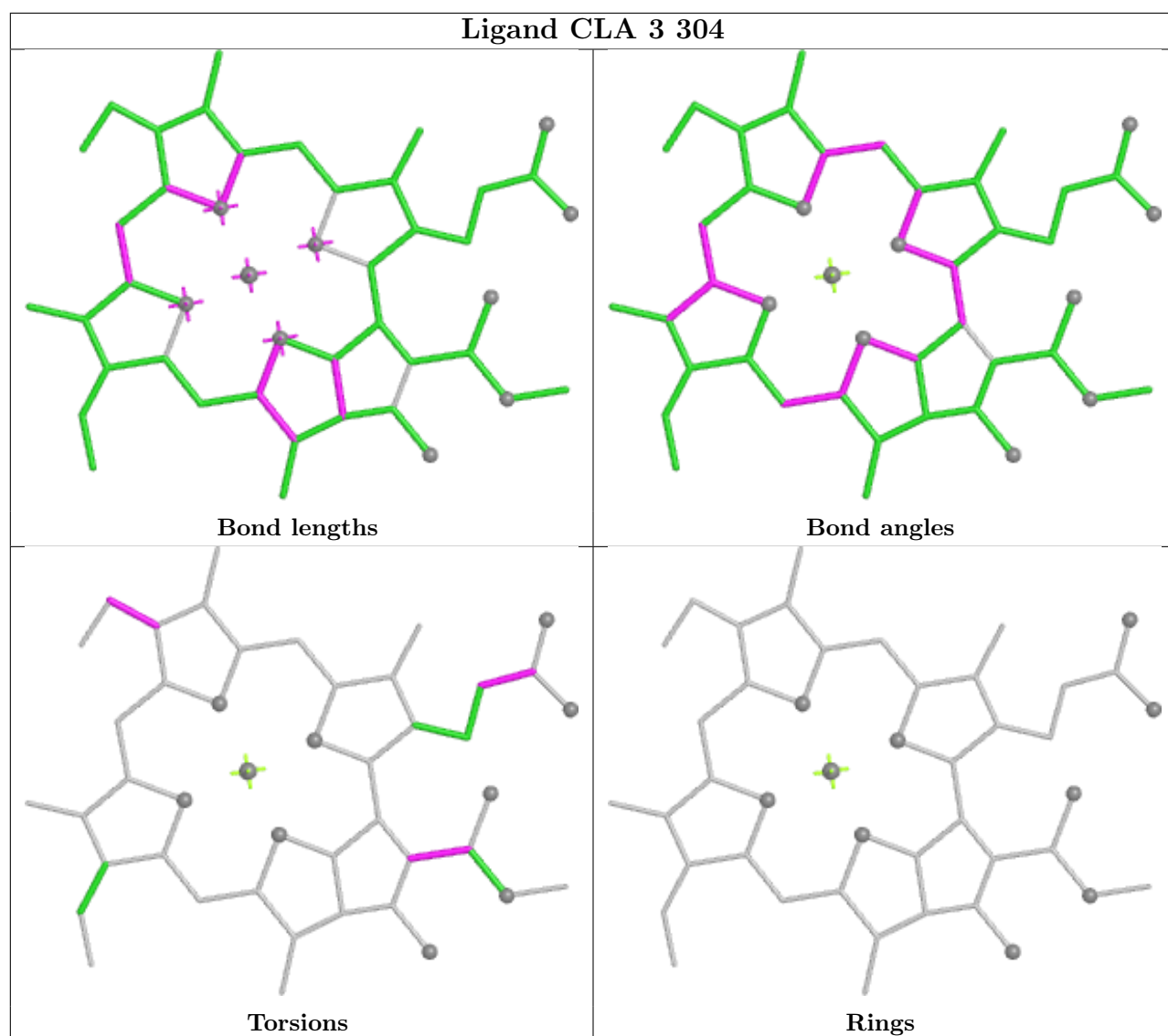


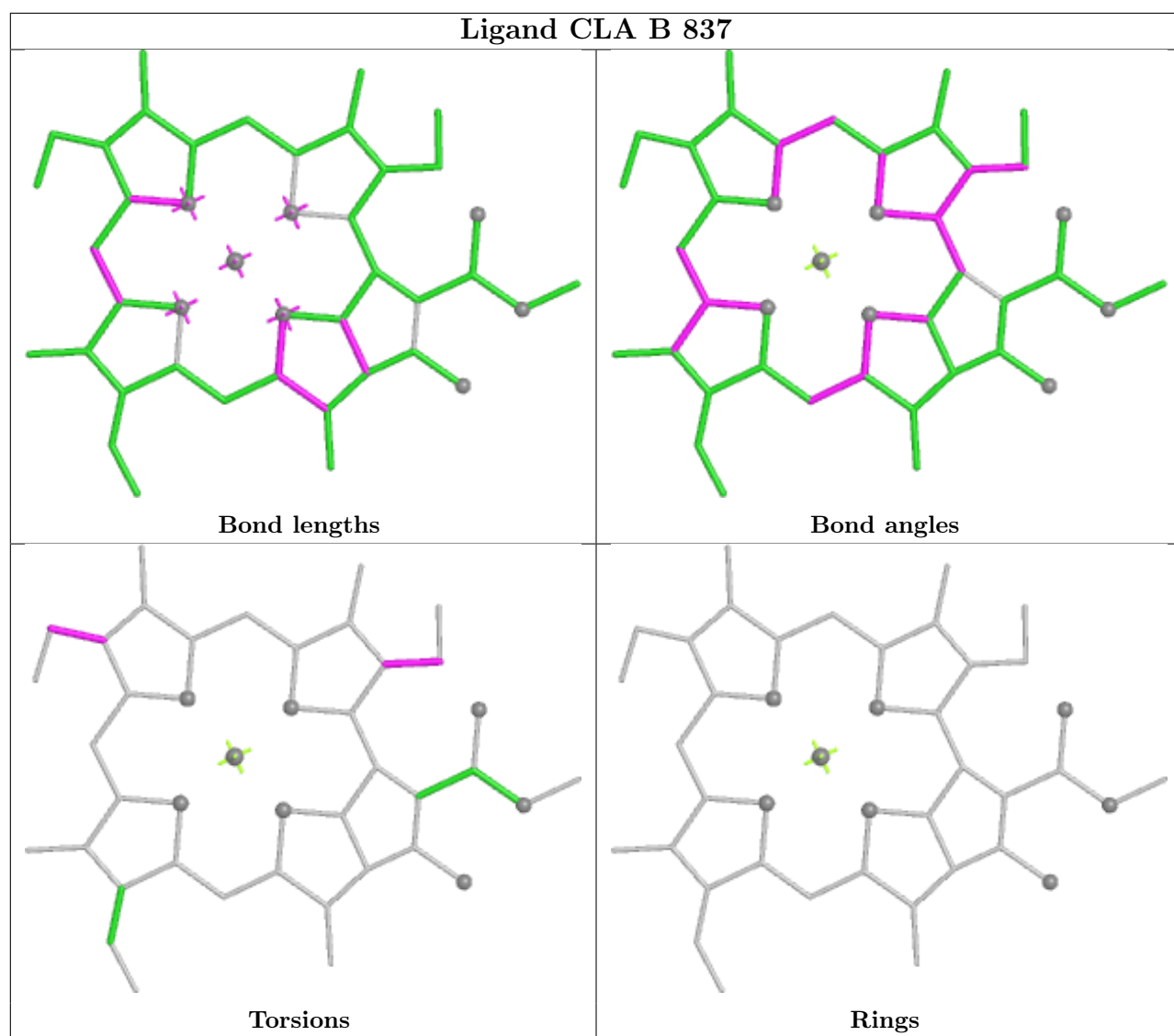
Rings

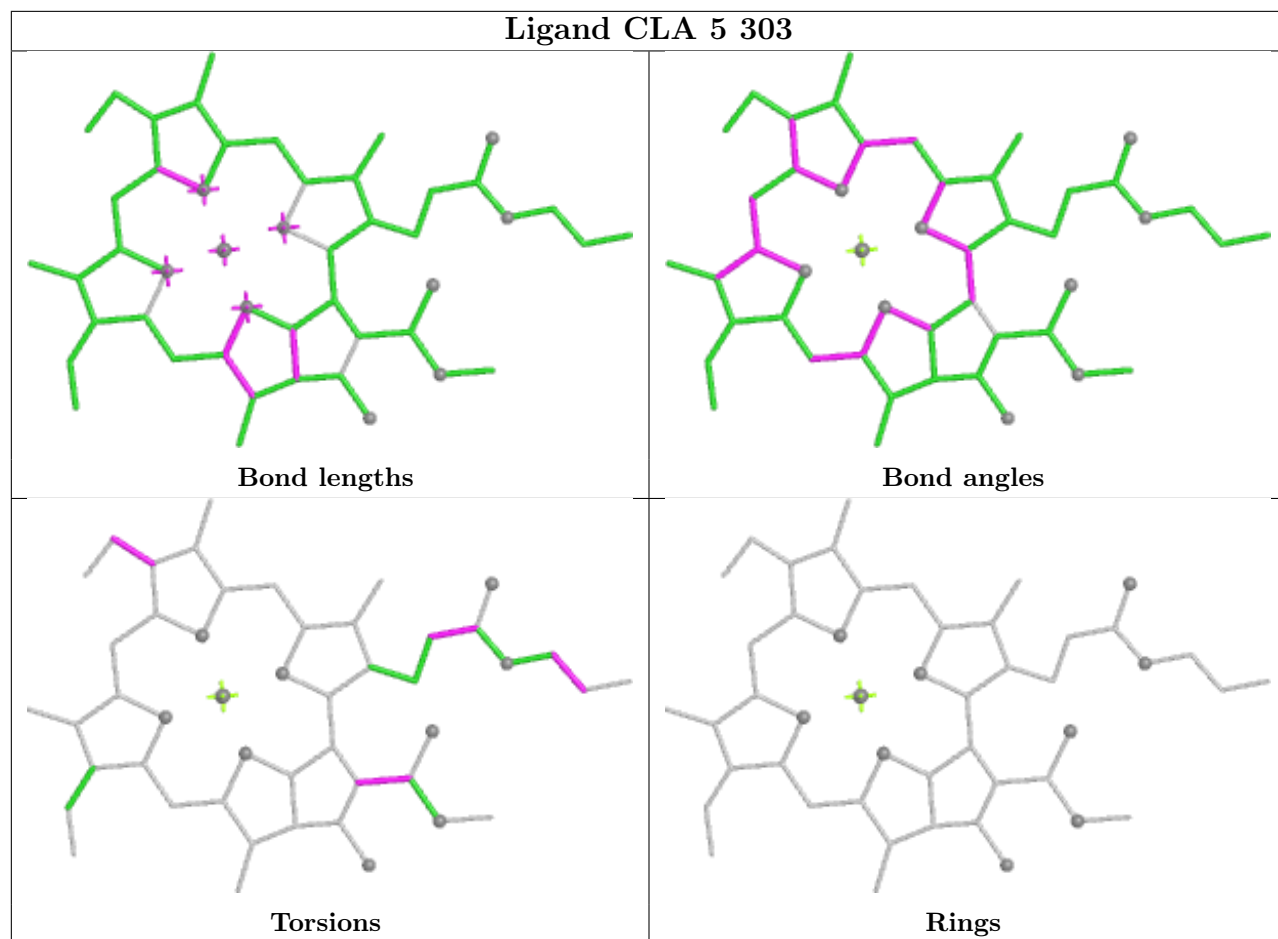




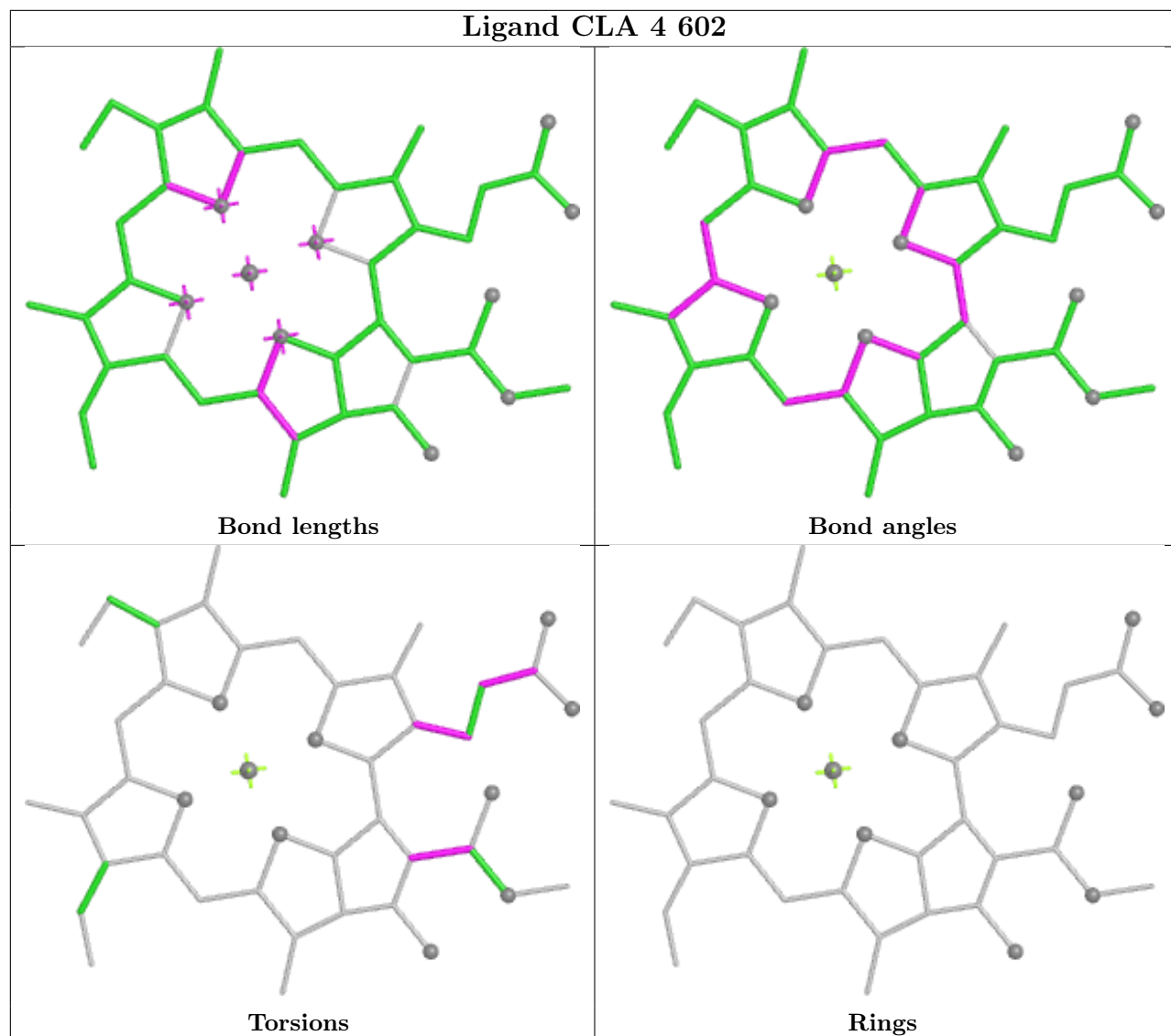




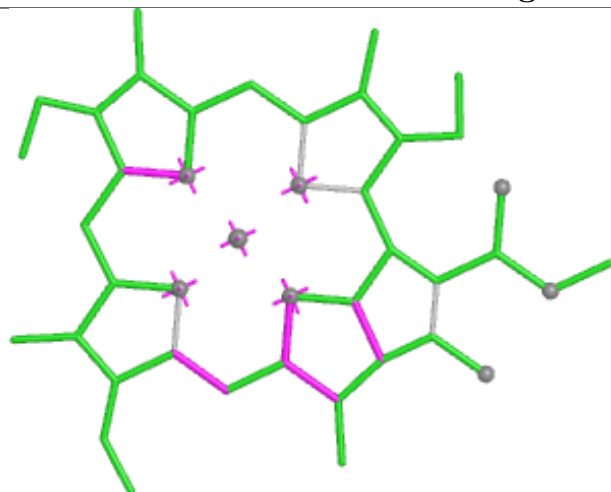




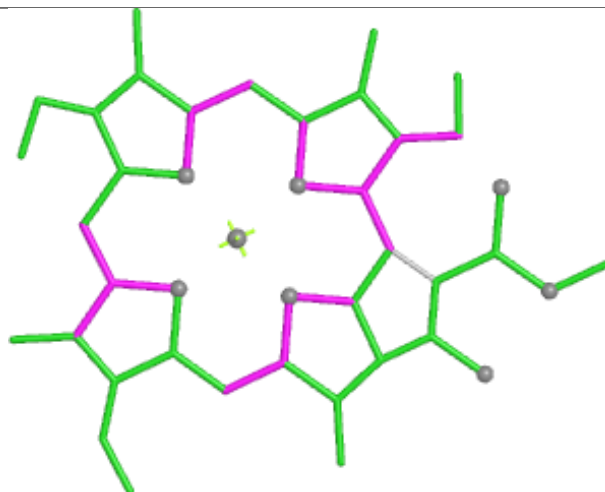
Ligand CLA 4 602



Ligand CLA 7 602



Bond lengths



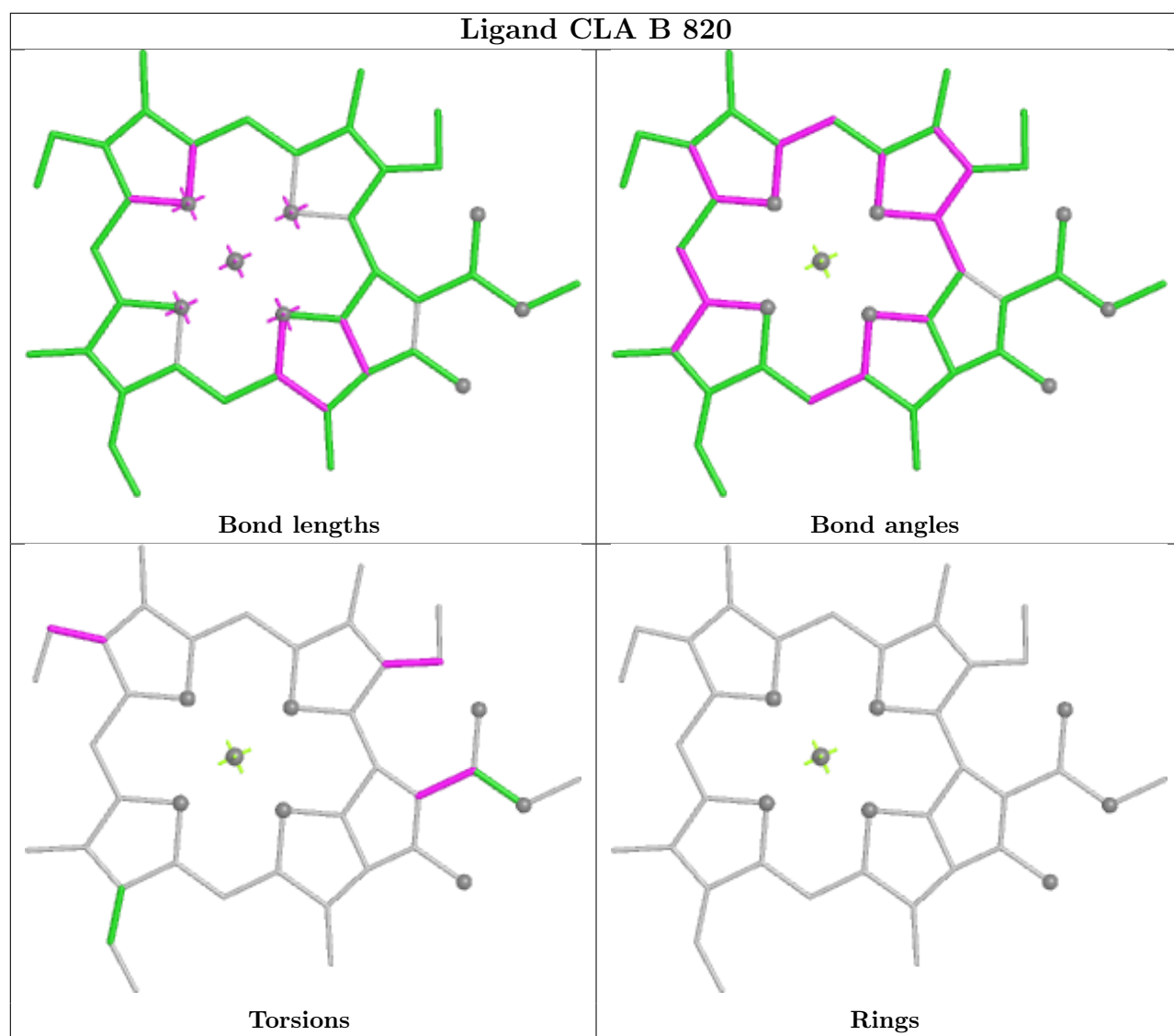
Bond angles



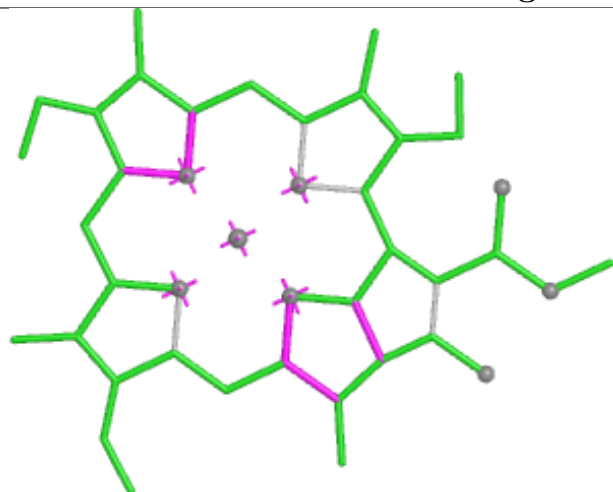
Torsions



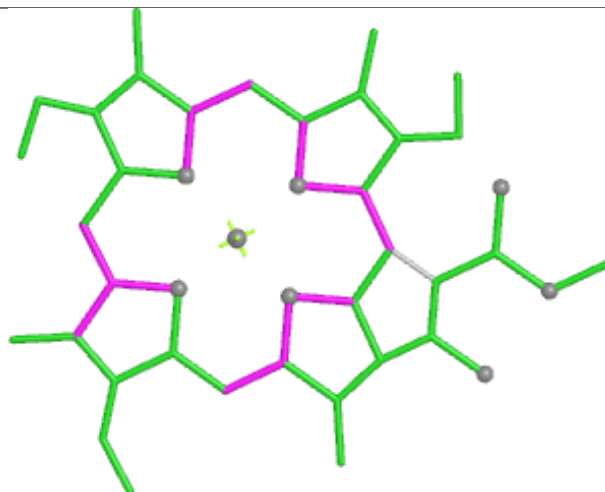
Rings



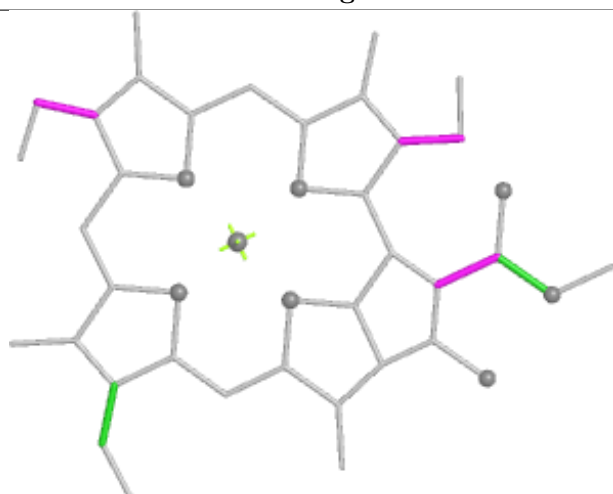
Ligand CLA 8 602



Bond lengths



Bond angles

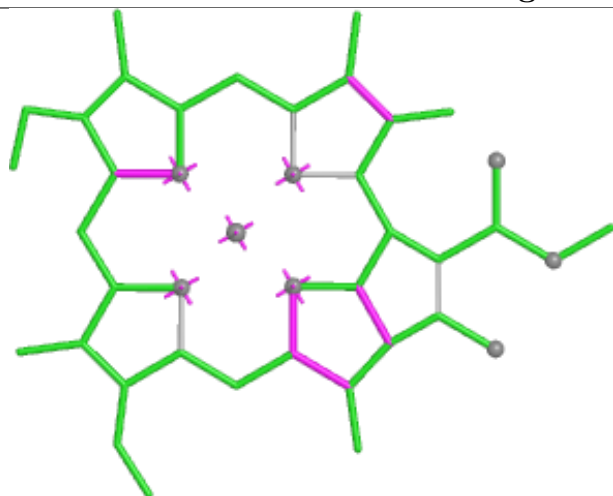


Torsions



Rings

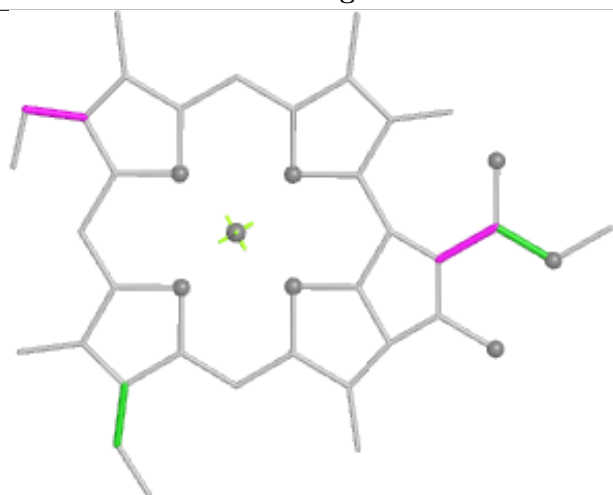
Ligand CLA 7 610



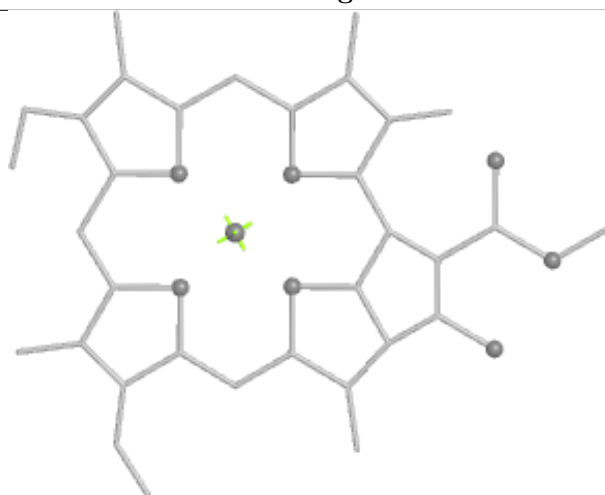
Bond lengths



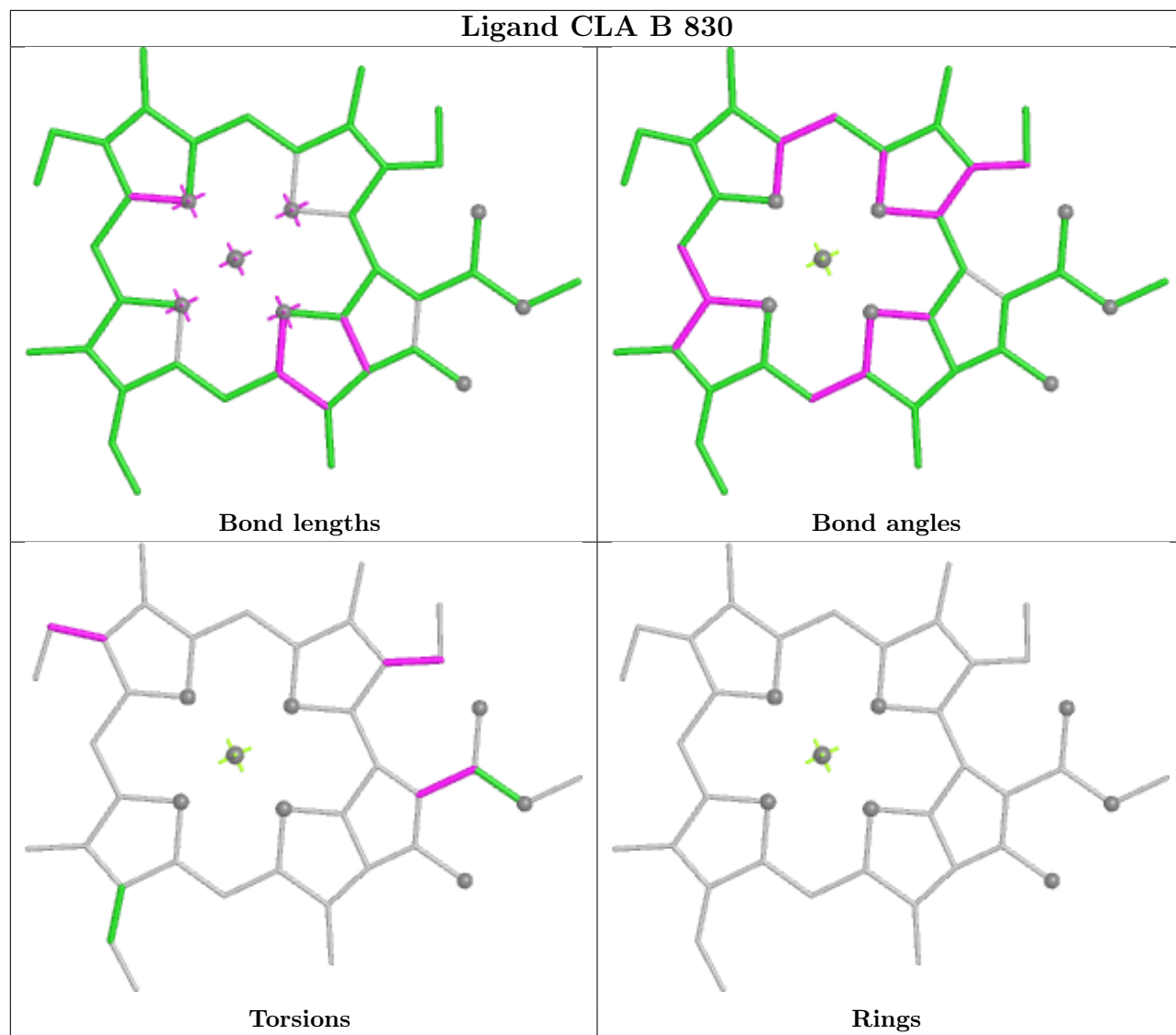
Bond angles



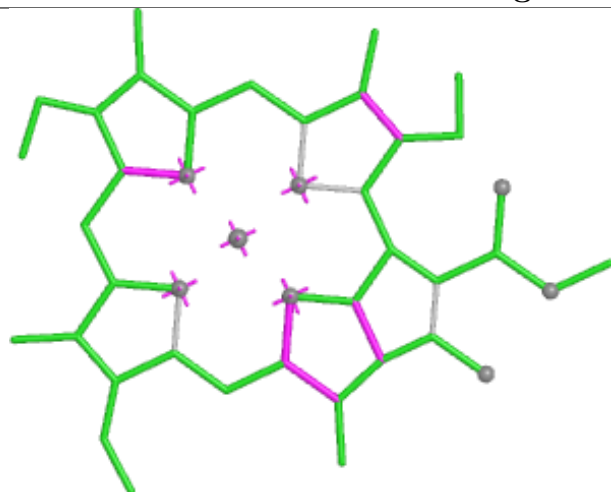
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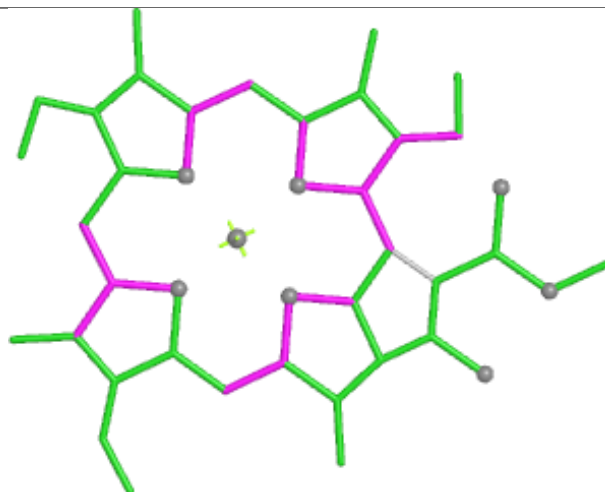
Rings



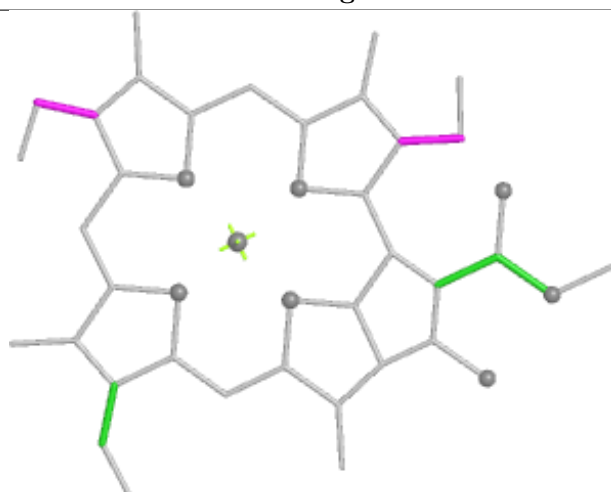
Ligand CLA A 828



Bond lengths



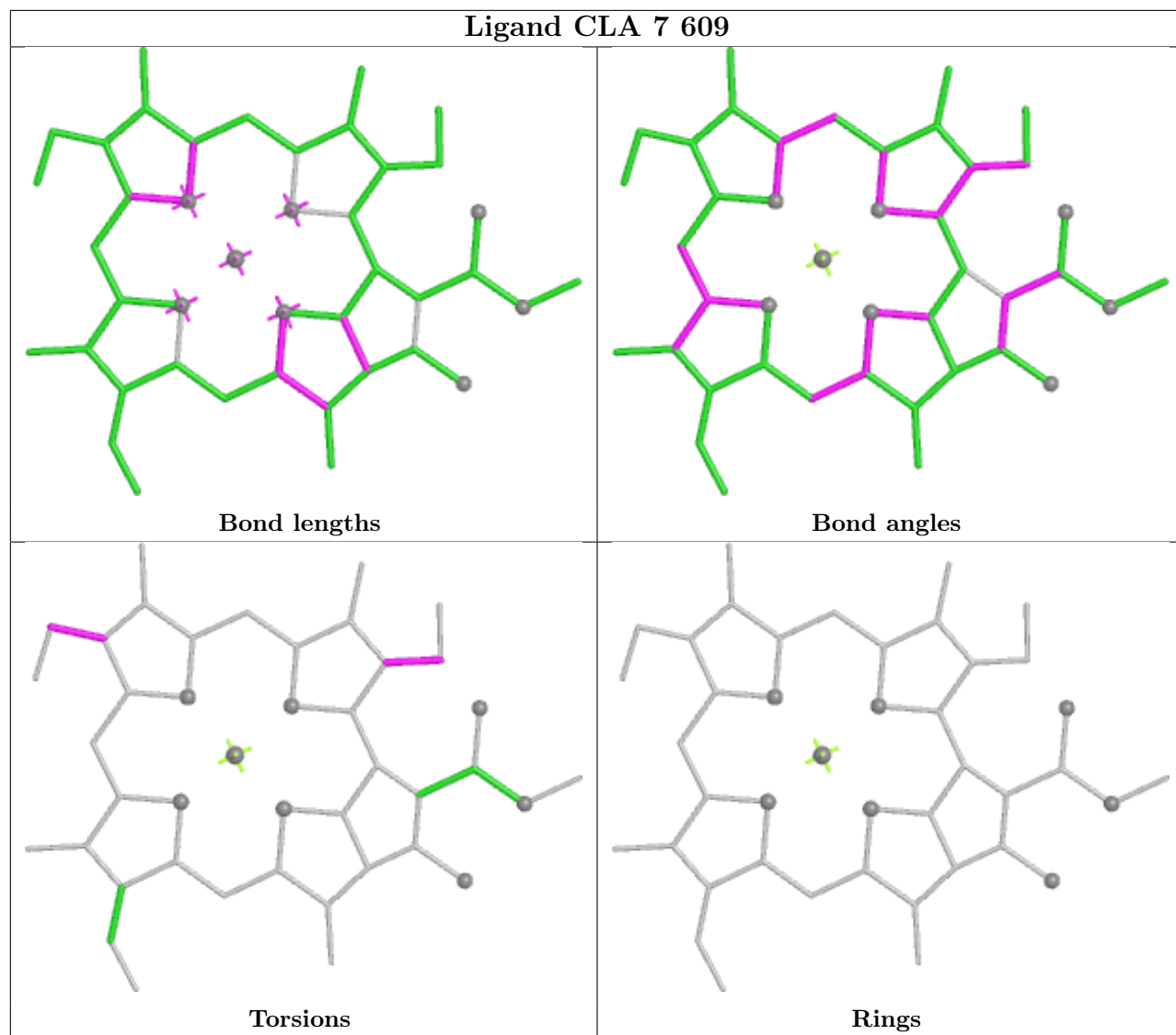
Bond angles

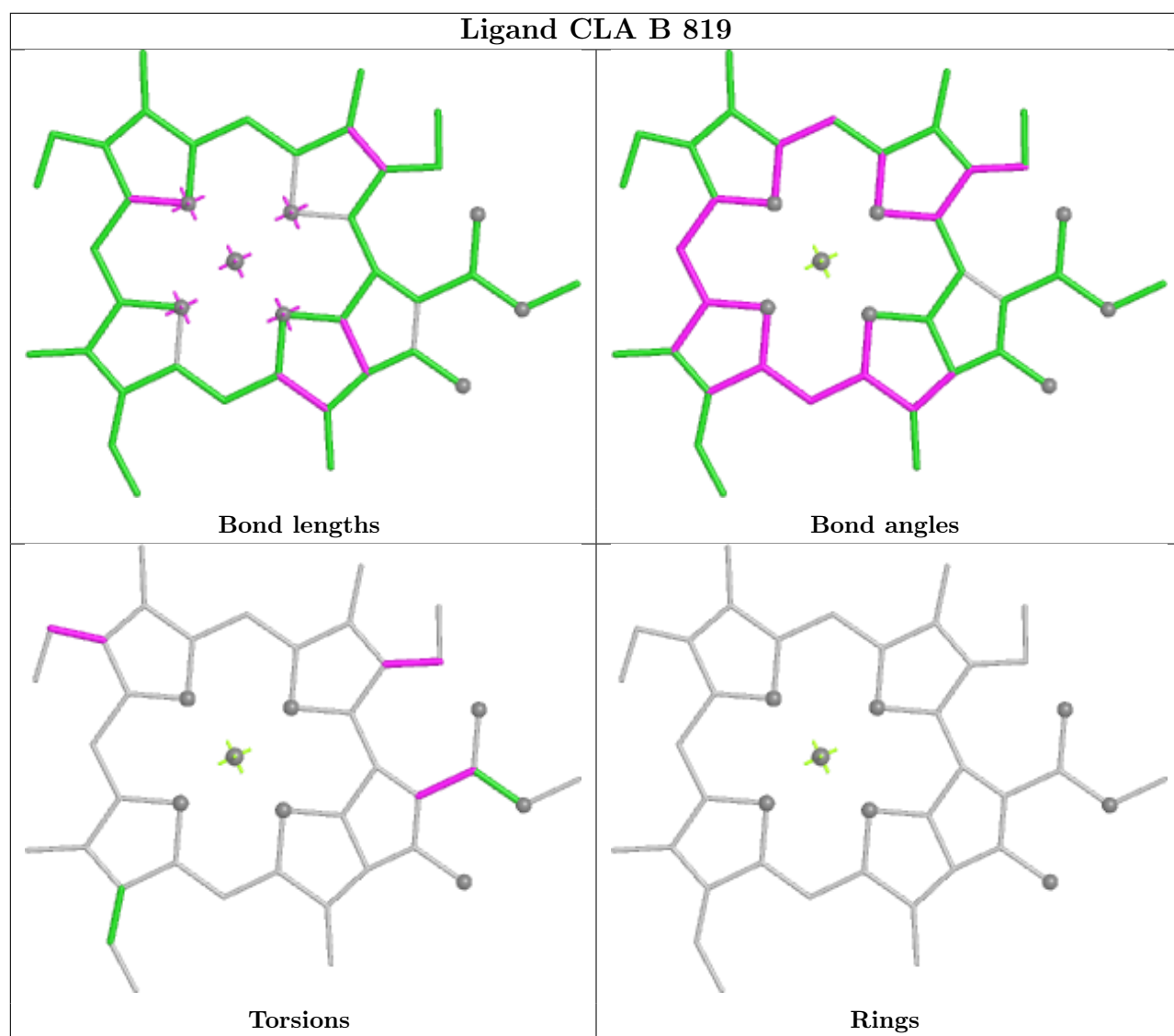


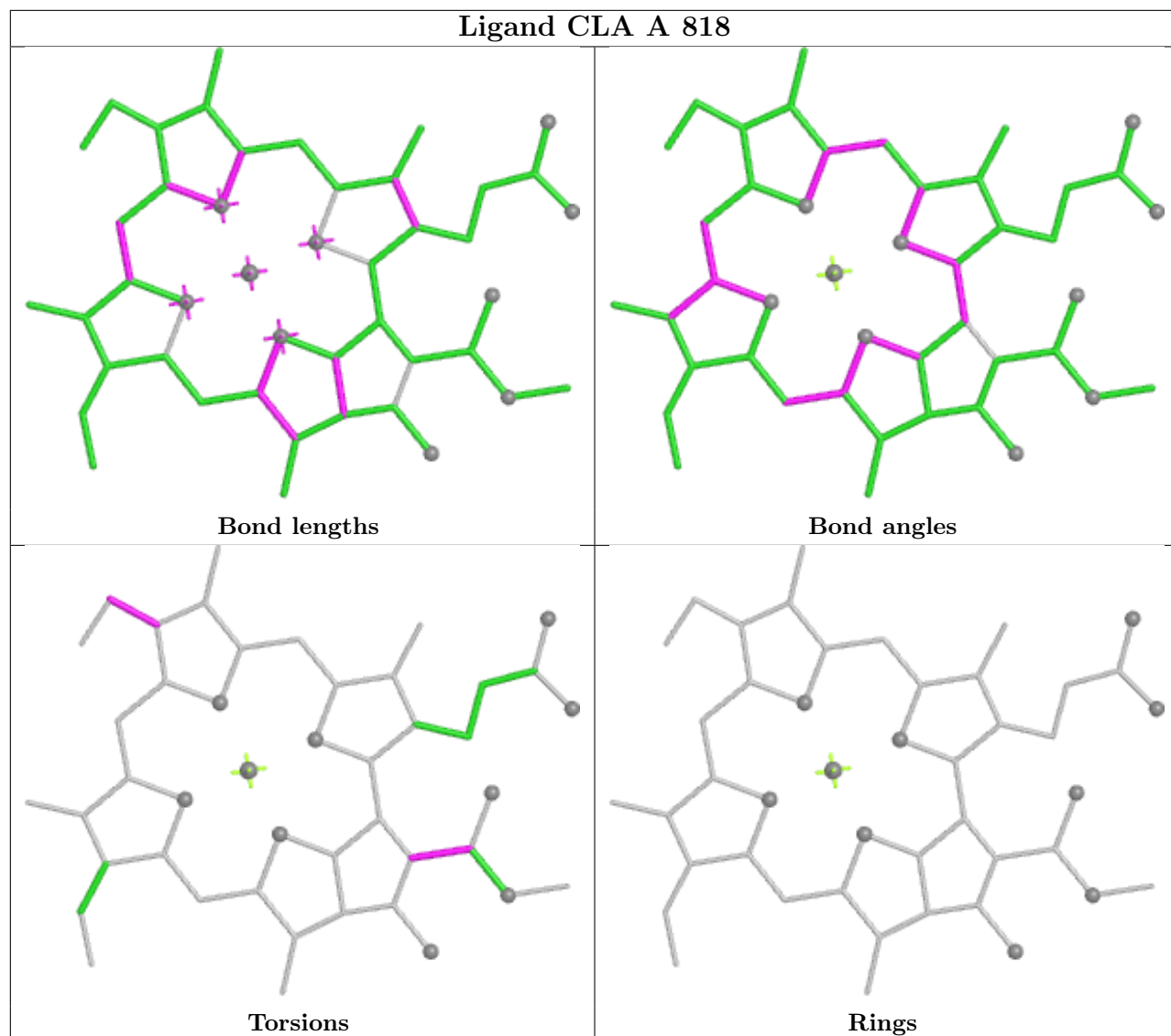
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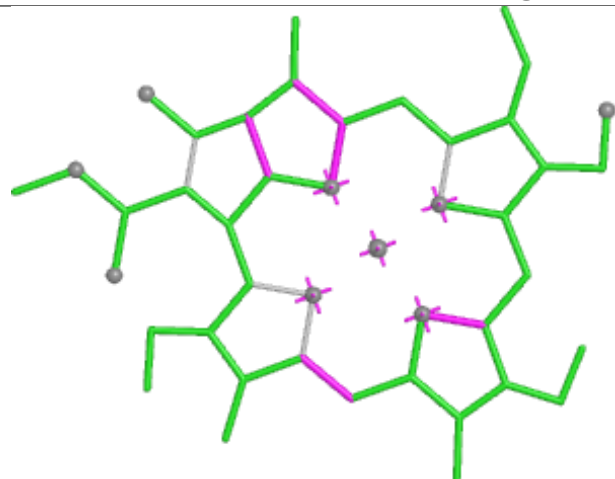
Rings



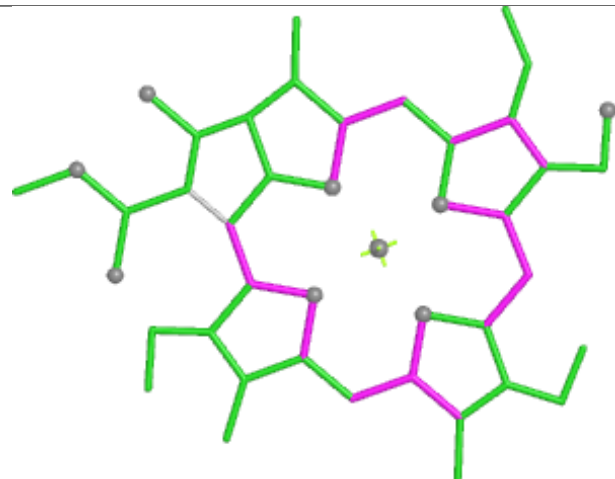




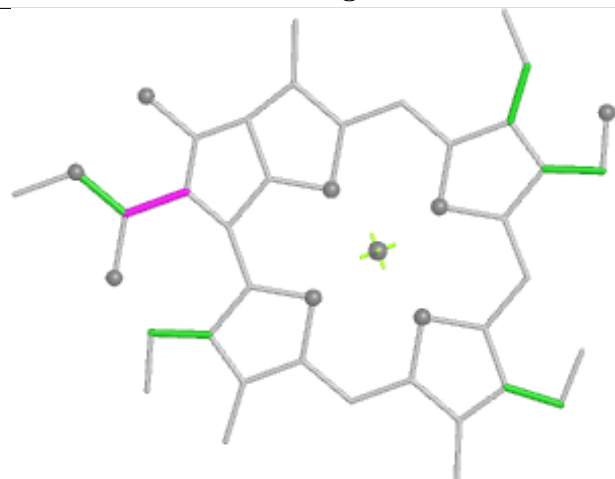
Ligand CHL Z 601



Bond lengths



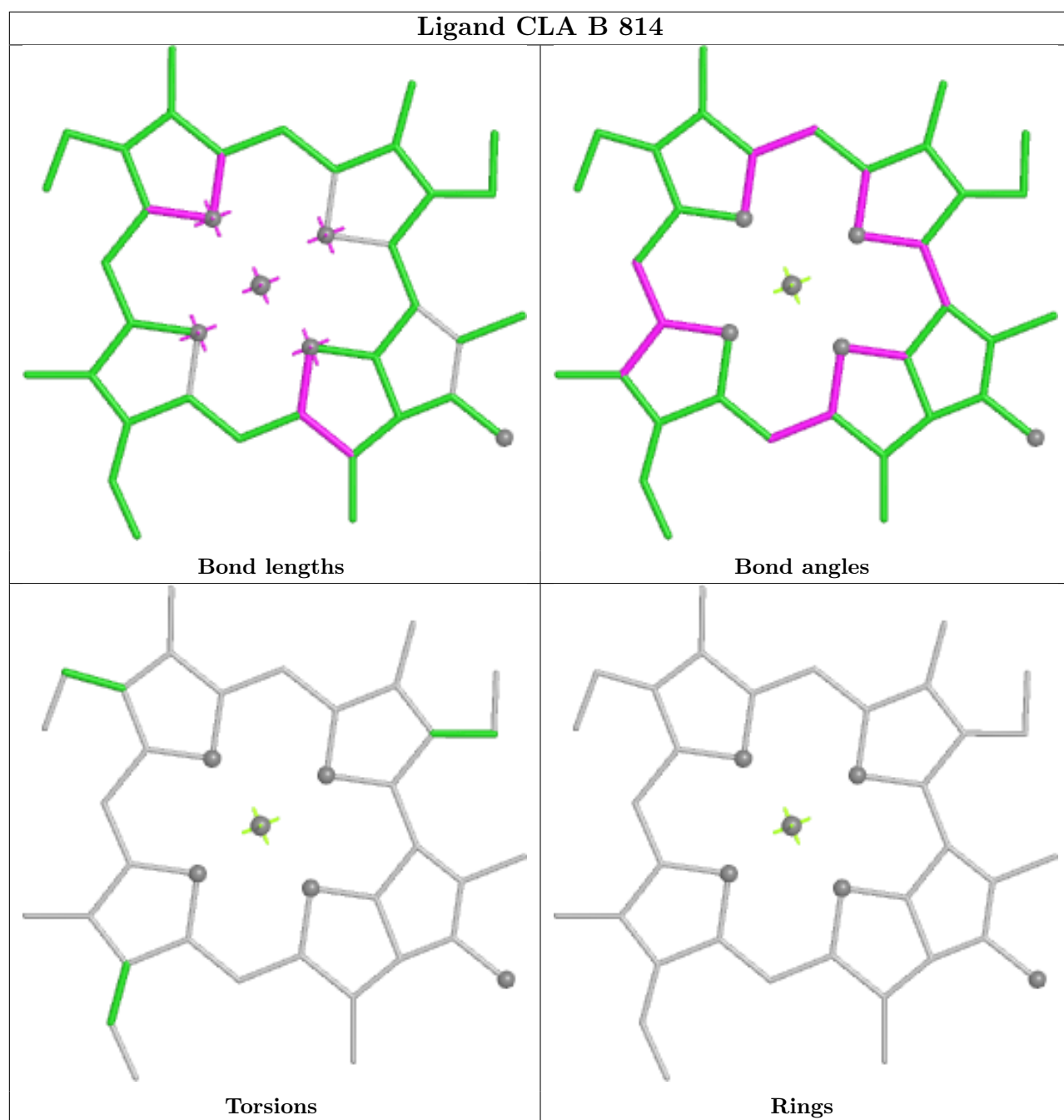
Bond angles



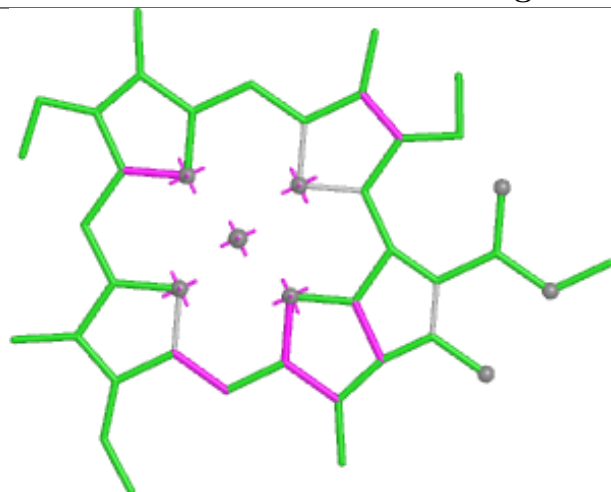
Torsions



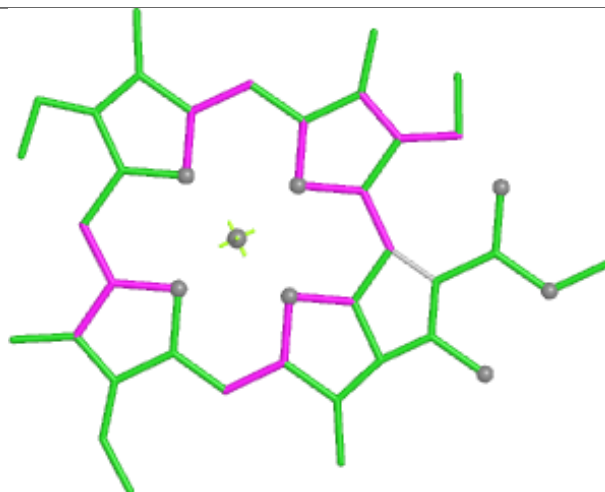
Rings



Ligand CLA B 823



Bond lengths



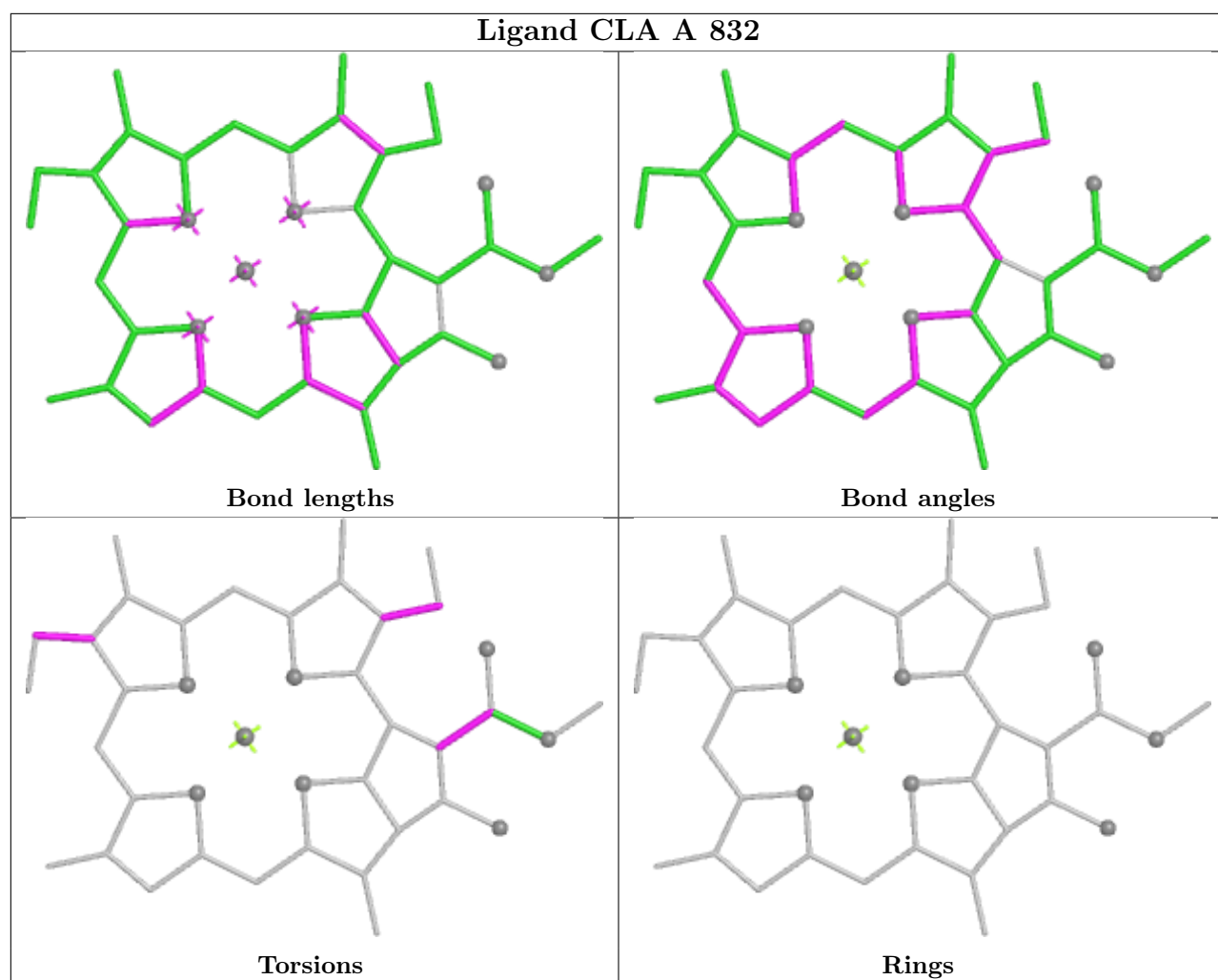
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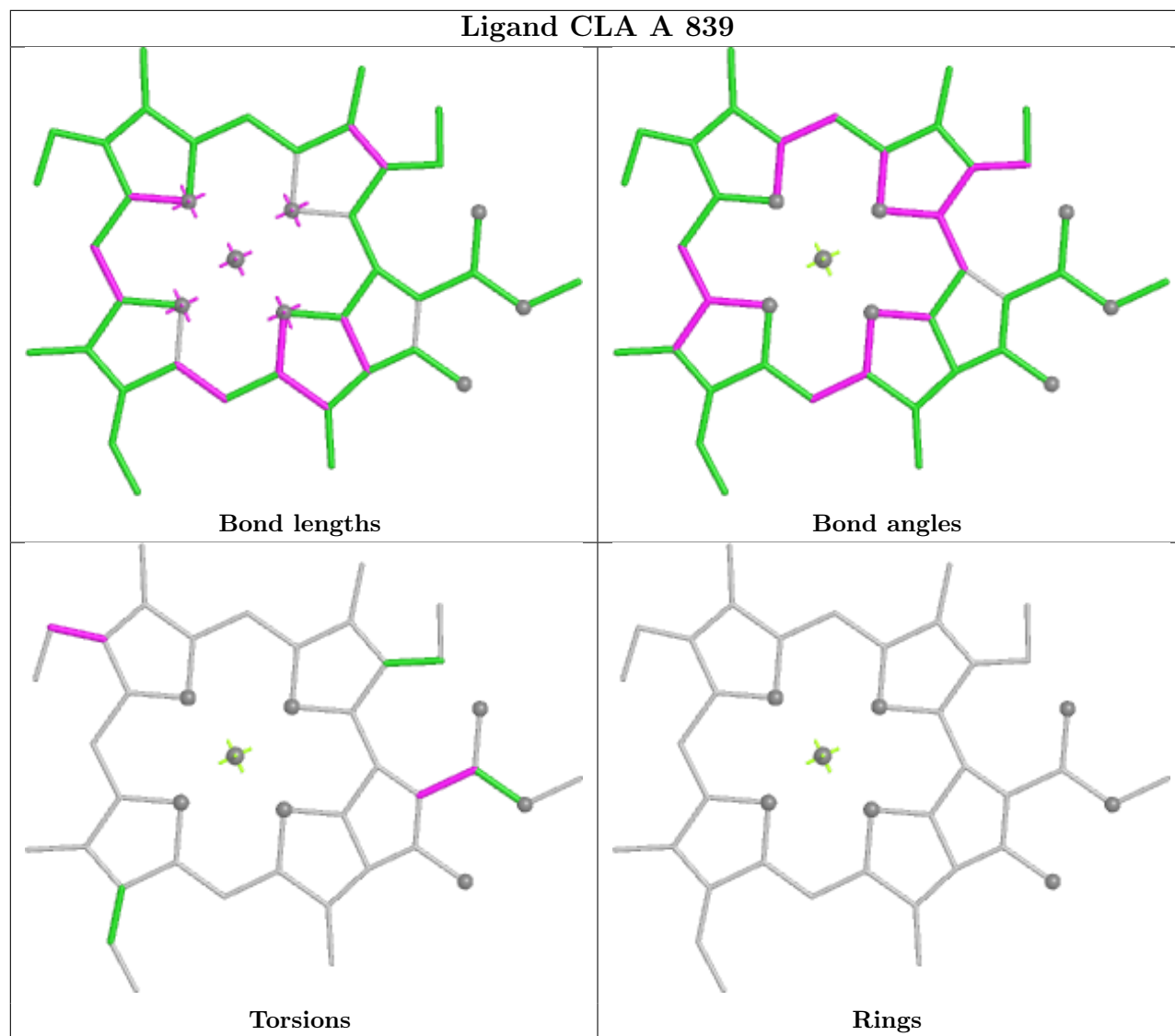


Torsions

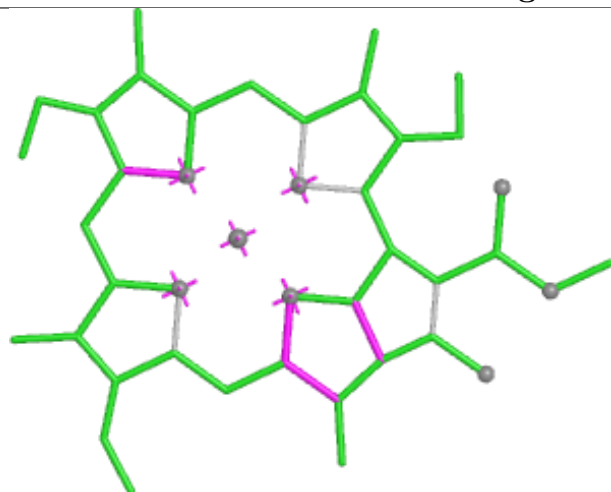


Rings

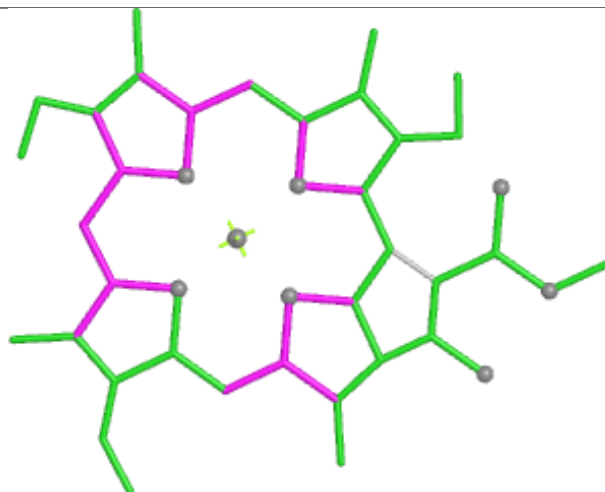




Ligand CLA 5 308



Bond lengths



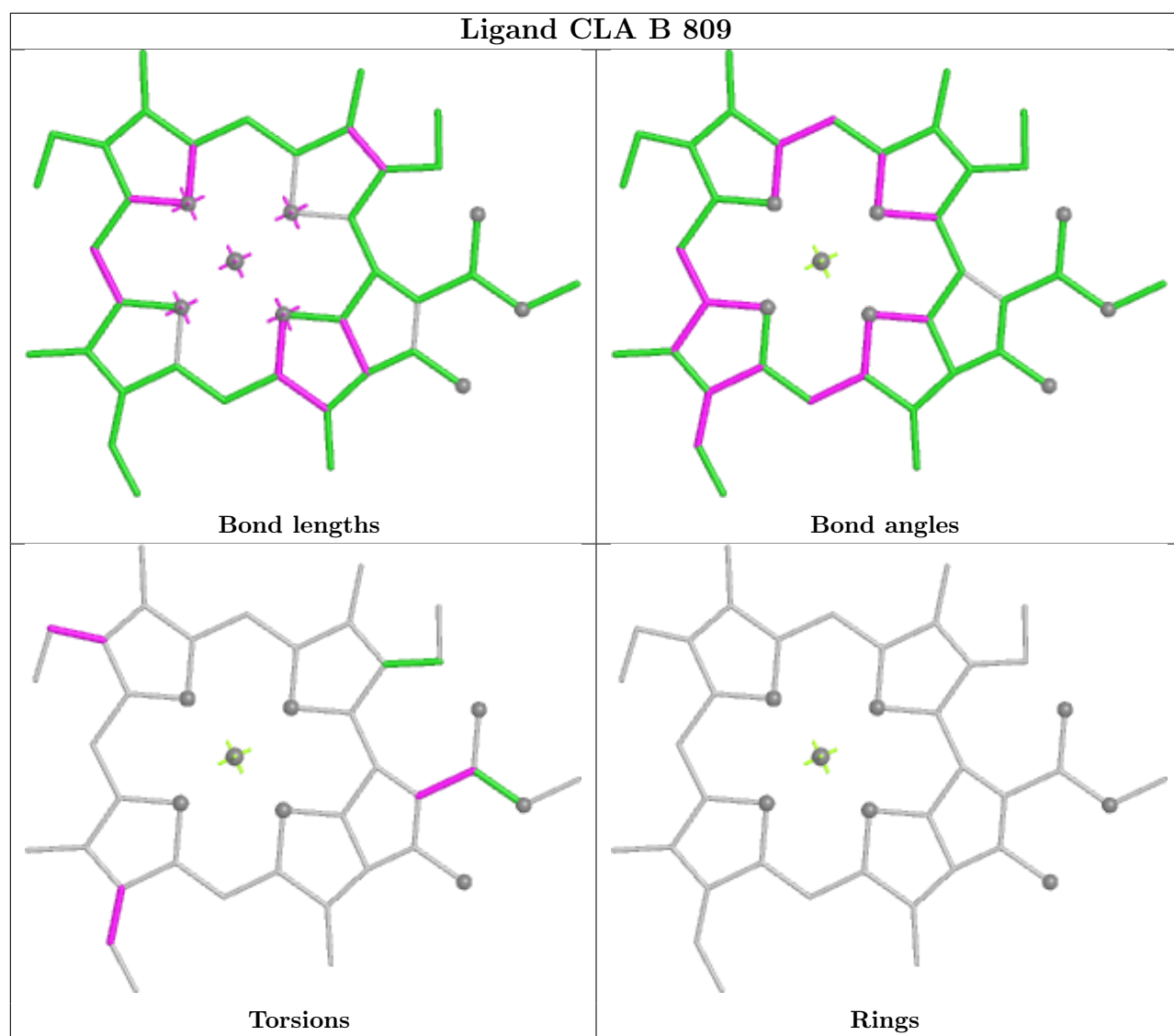
Bond angles



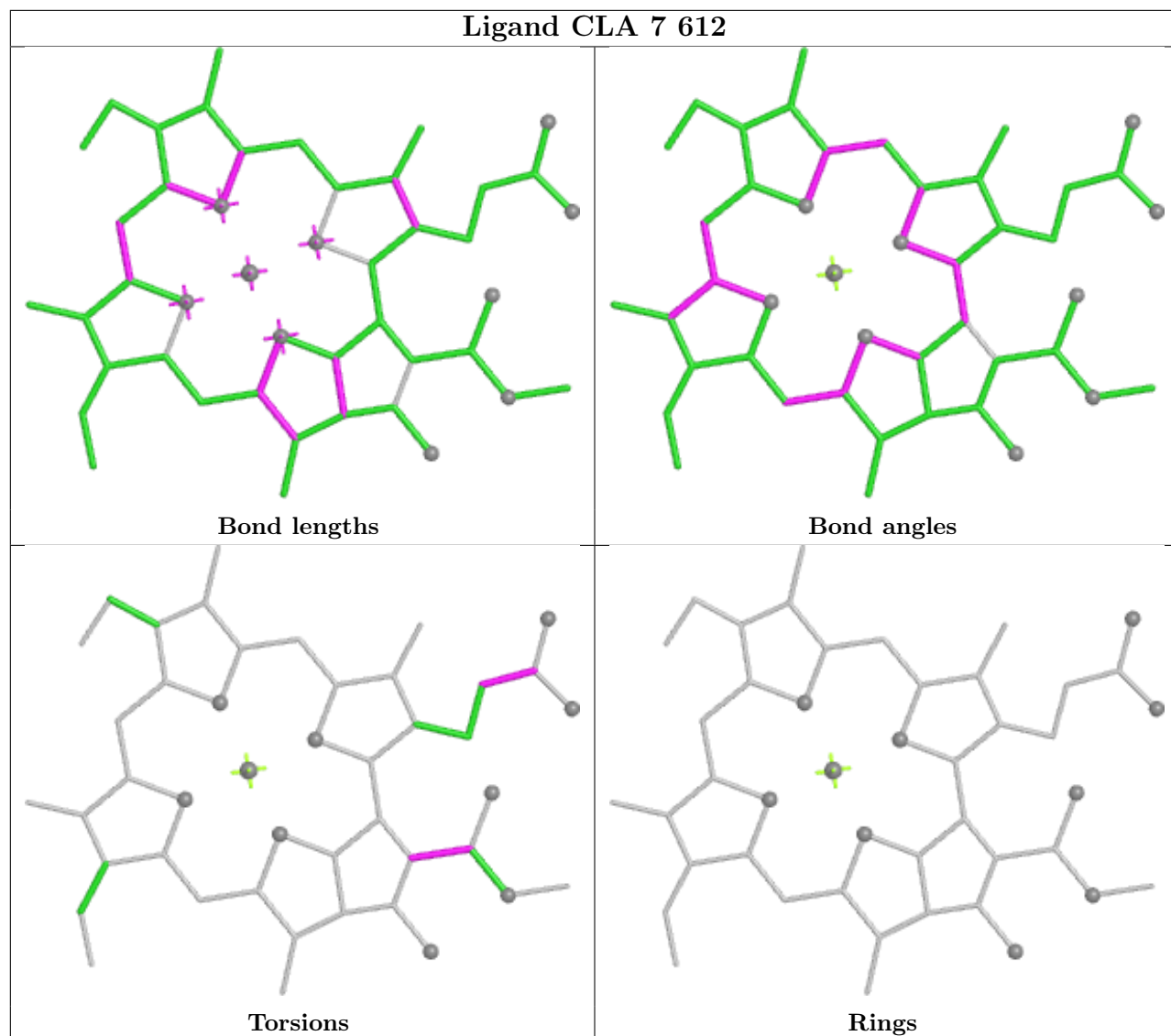
Torsions

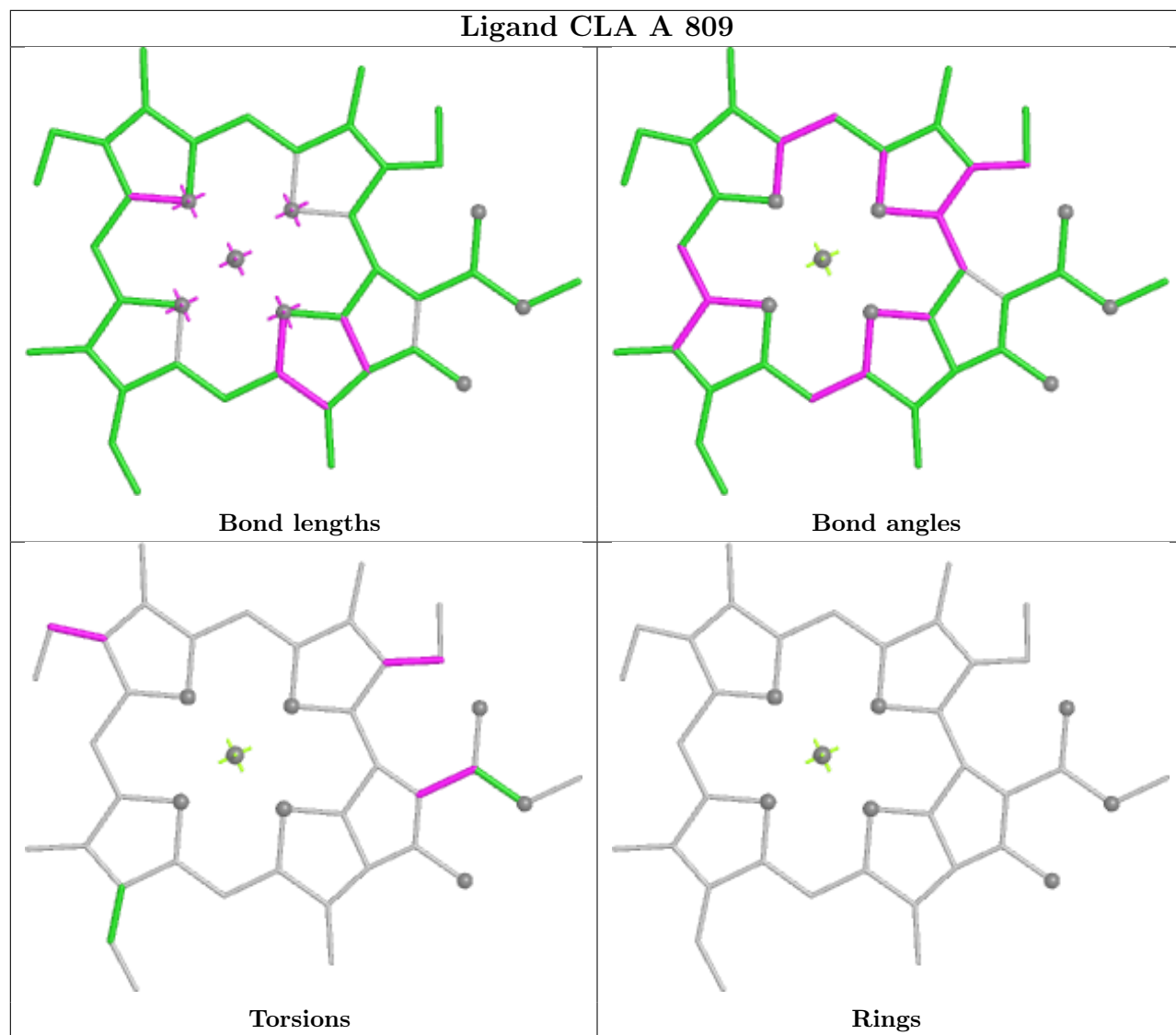


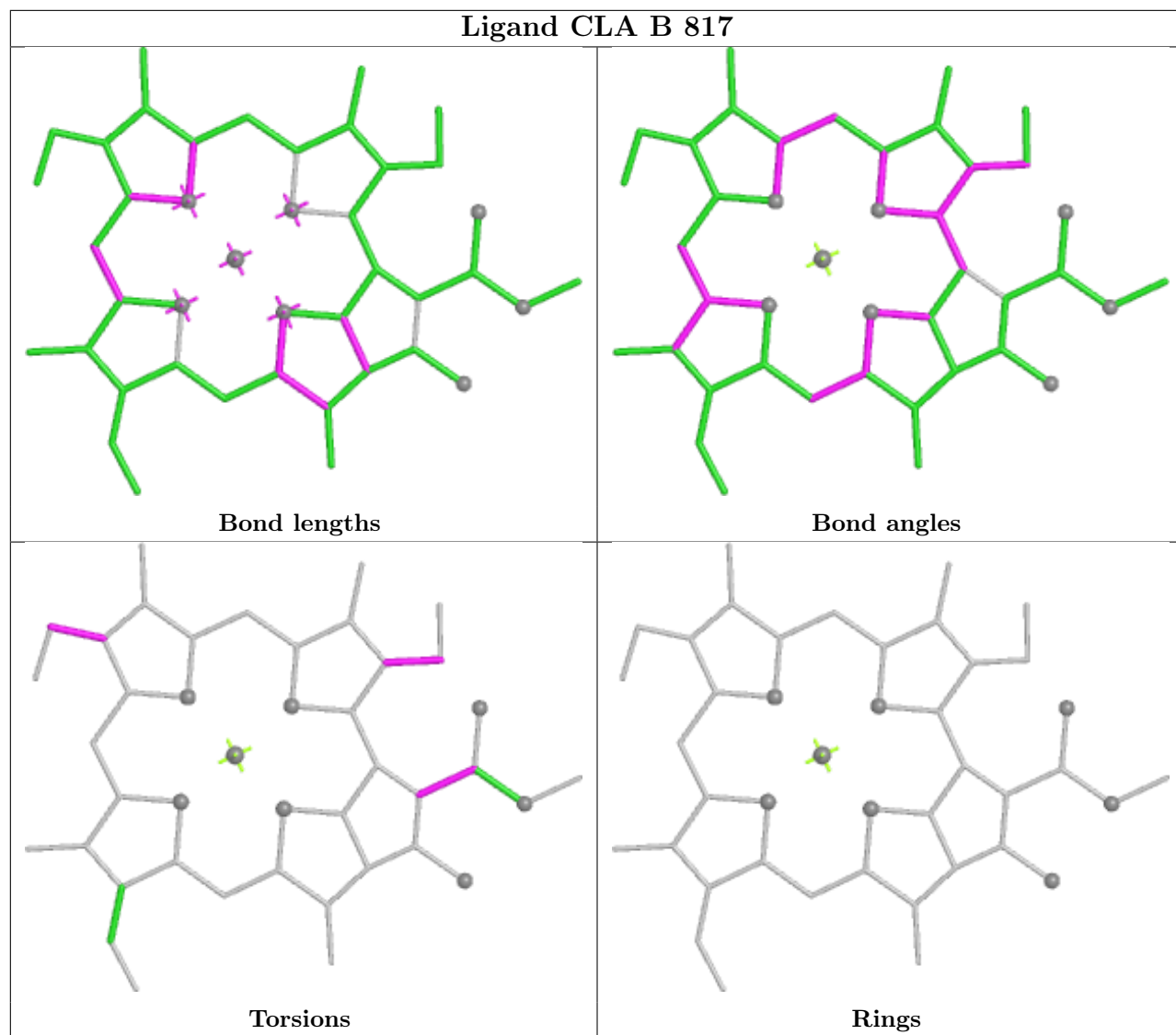
Rings

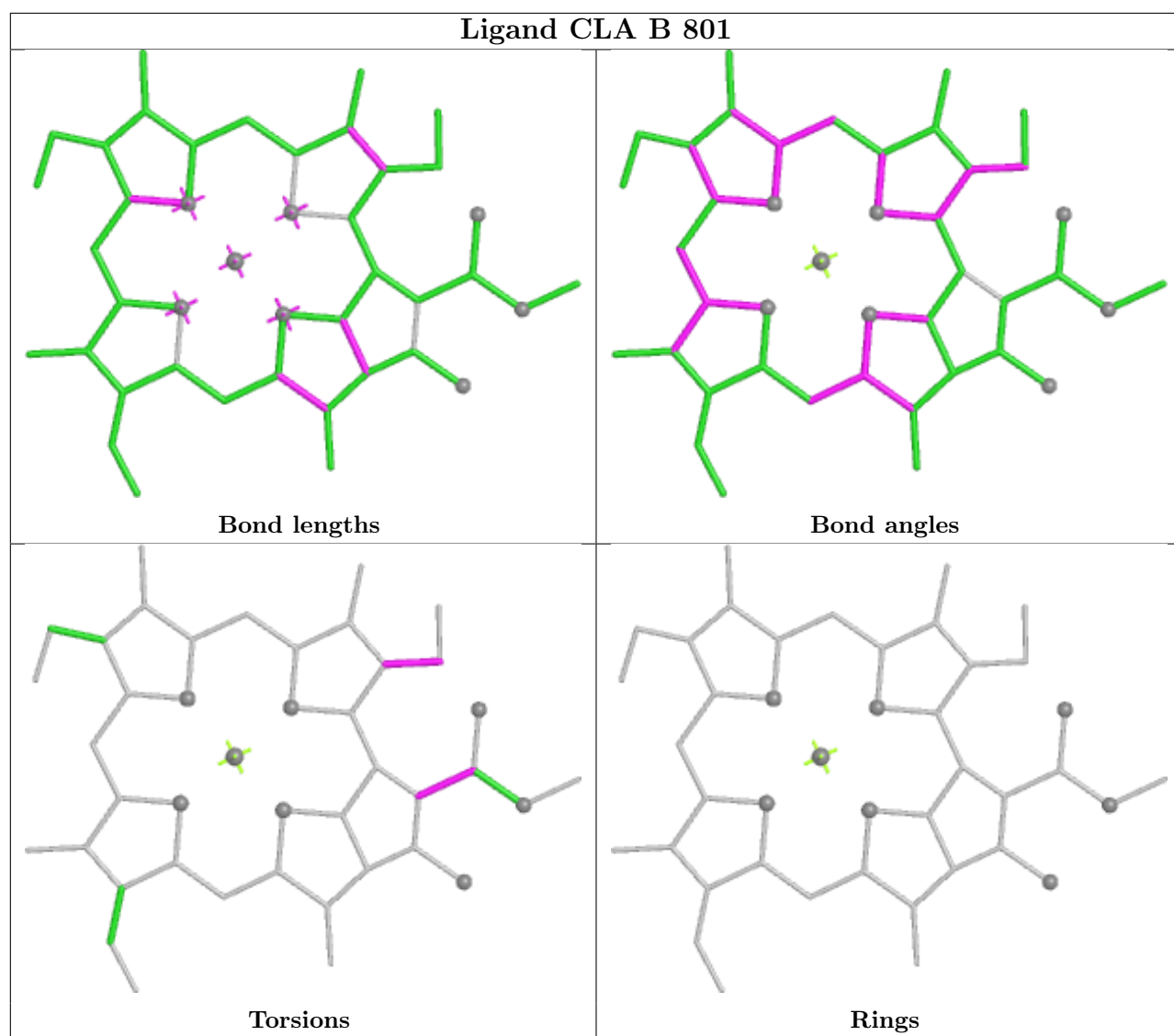


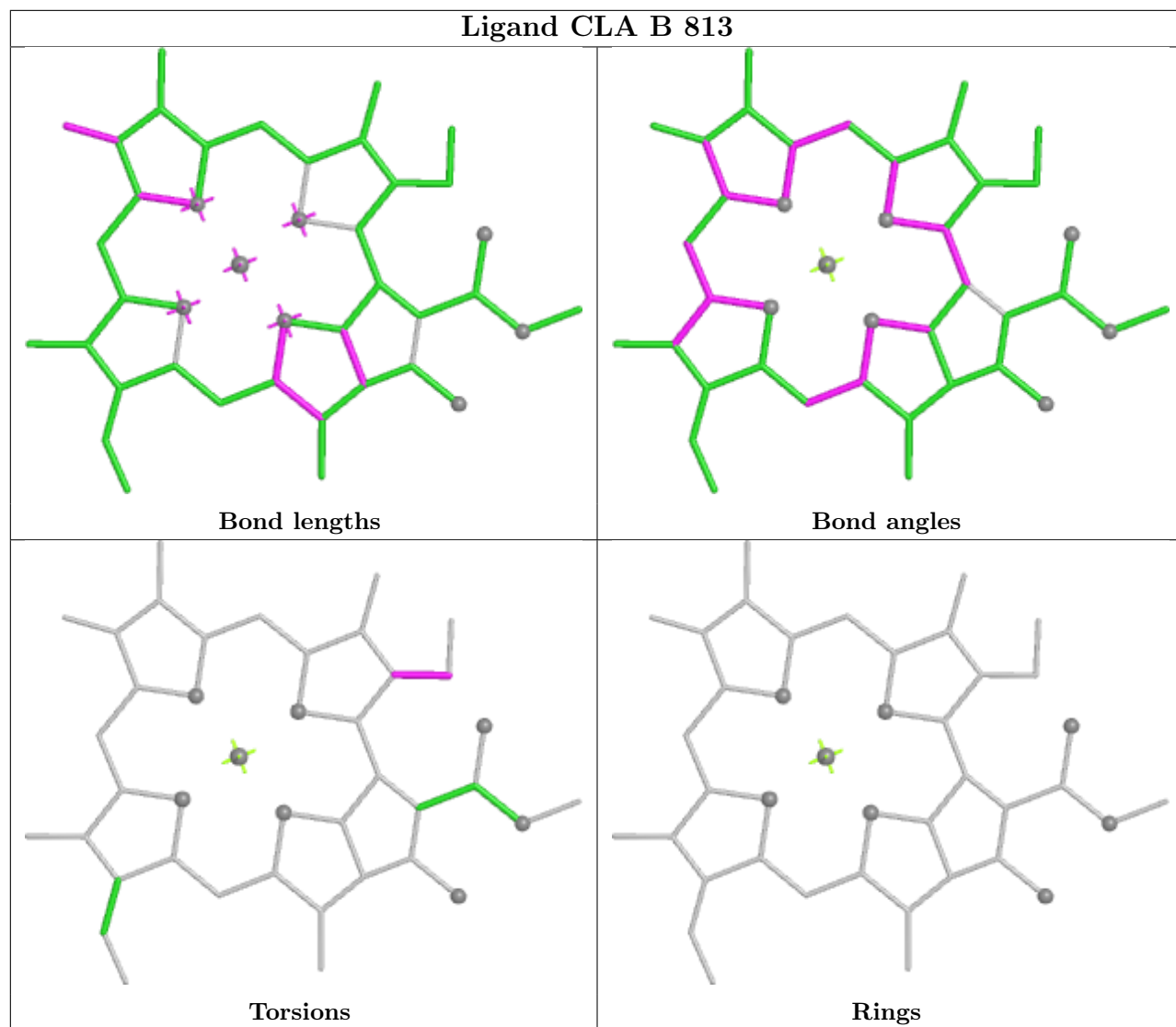
Ligand CLA 7 612



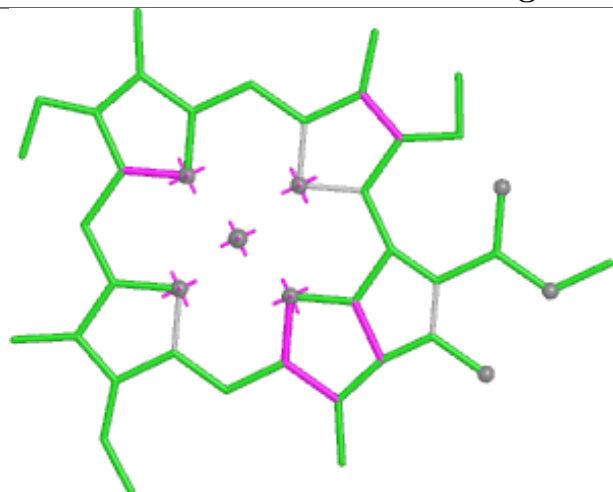




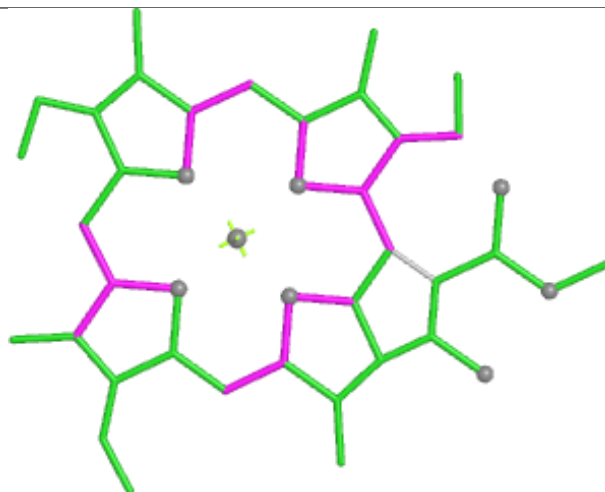




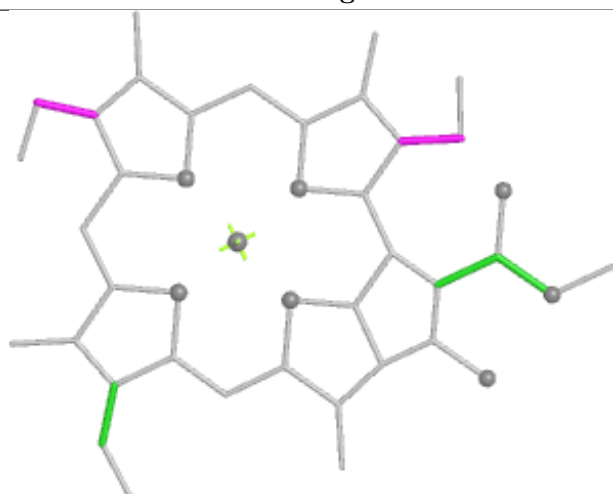
Ligand CLA 5 312



Bond lengths



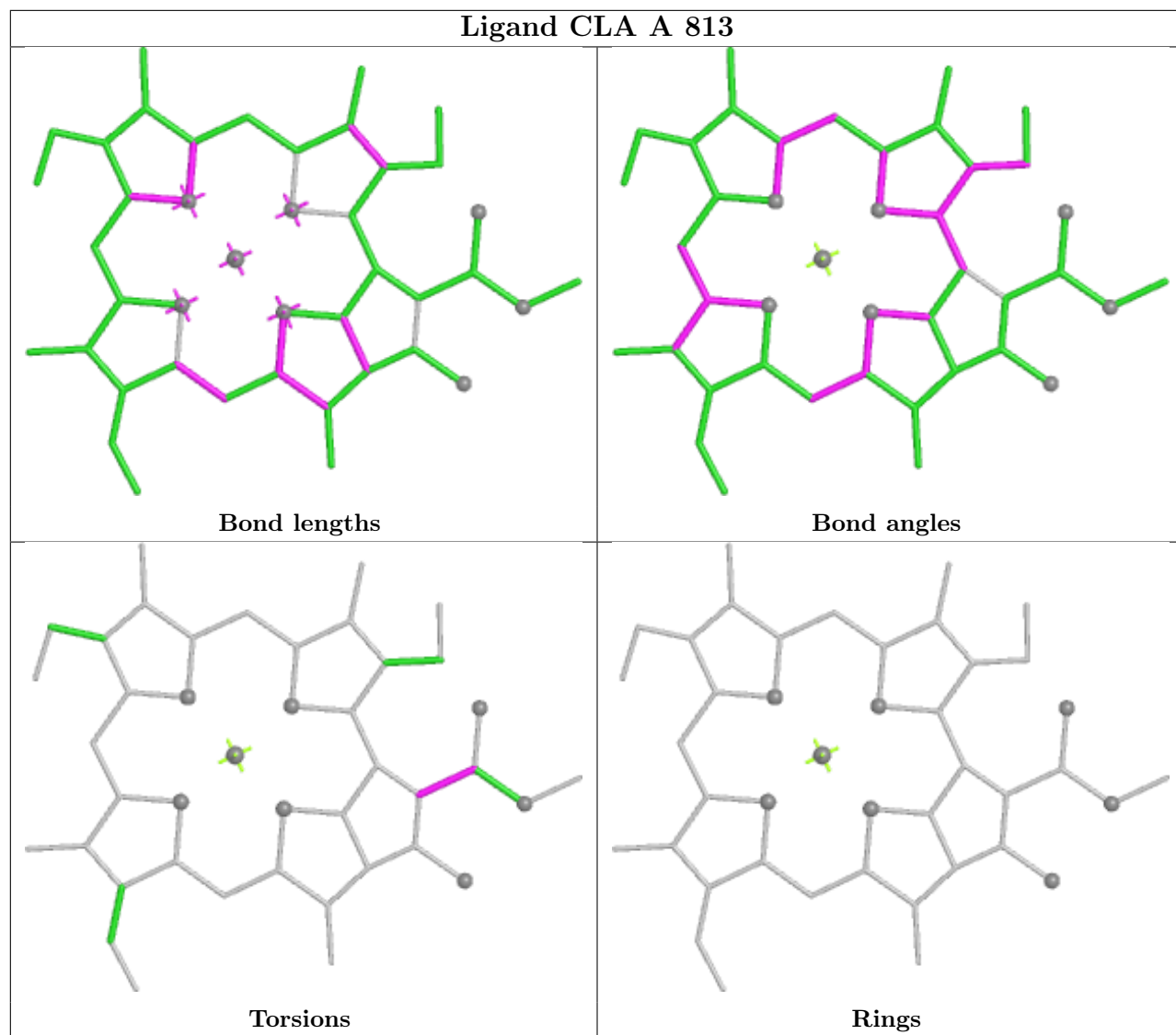
Bond angles



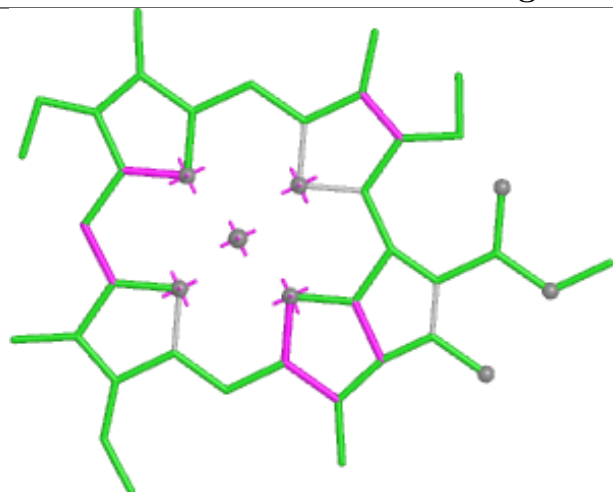
Torsions



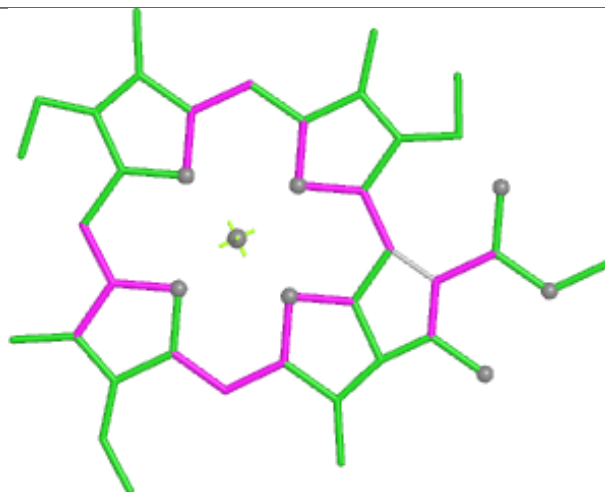
Rings



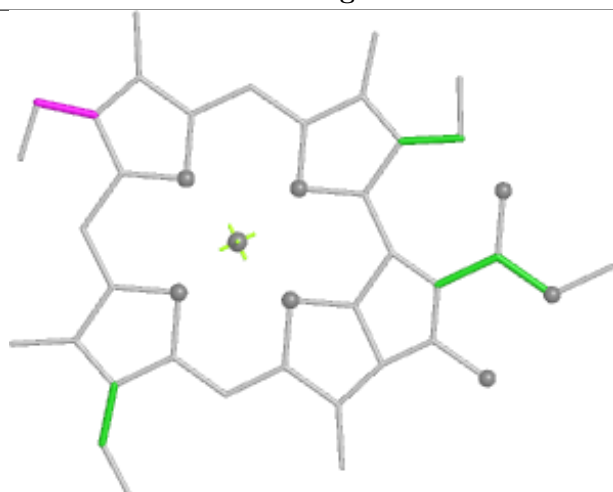
Ligand CLA 7 604



Bond lengths



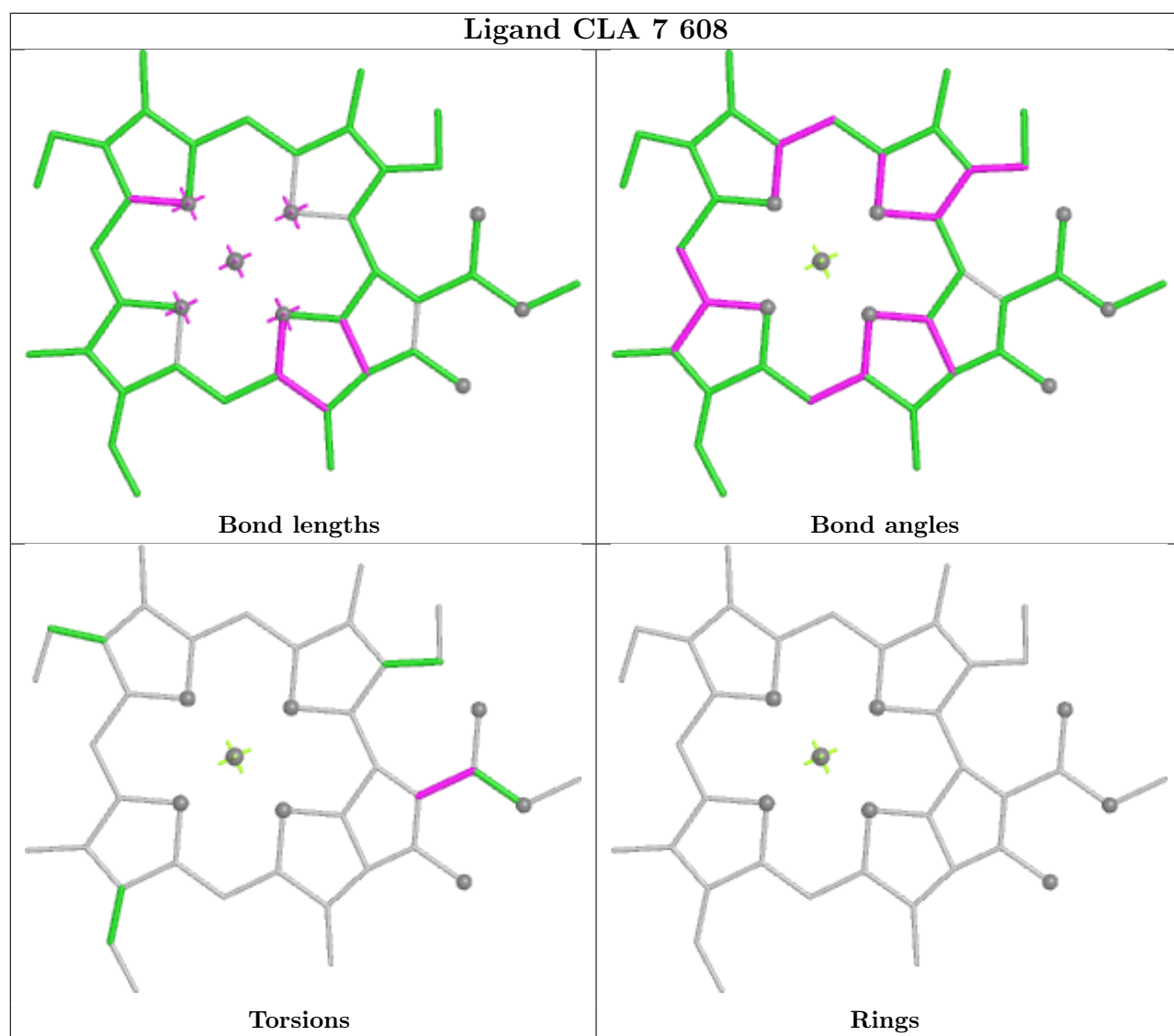
Bond angles

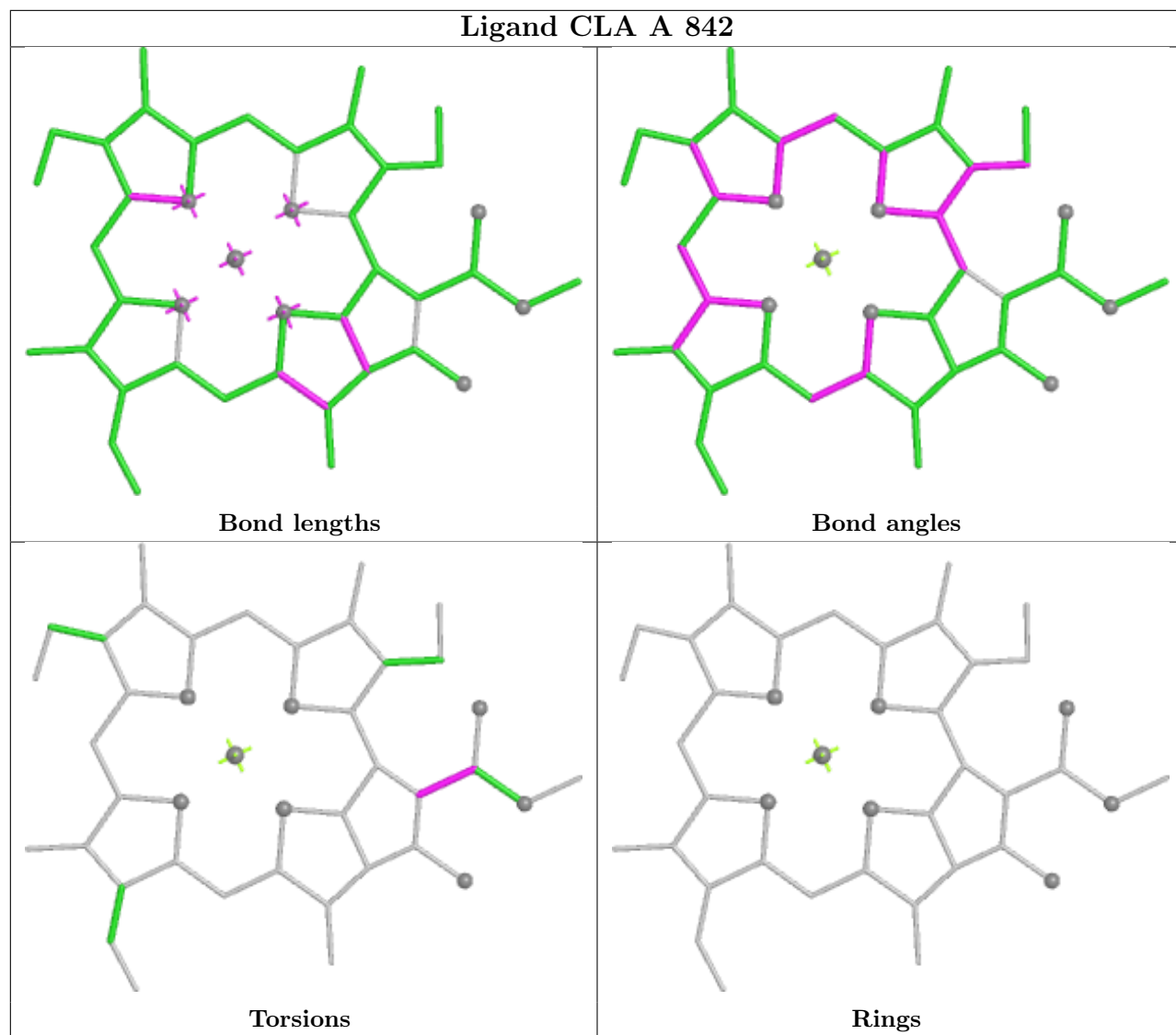


Torsions

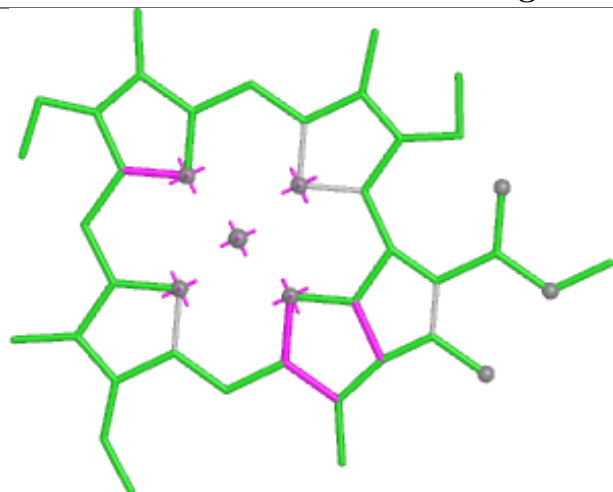


Rings

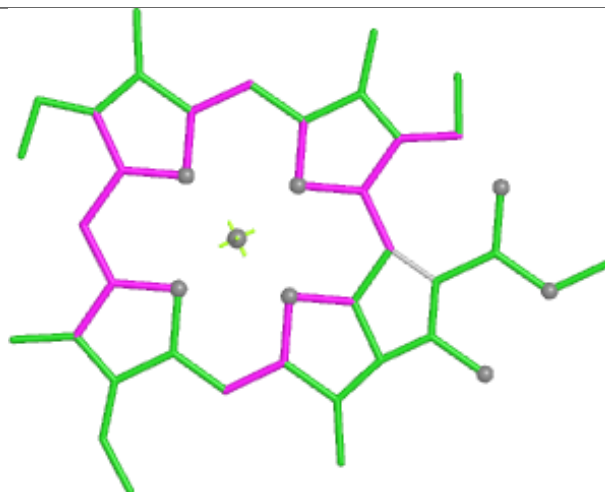




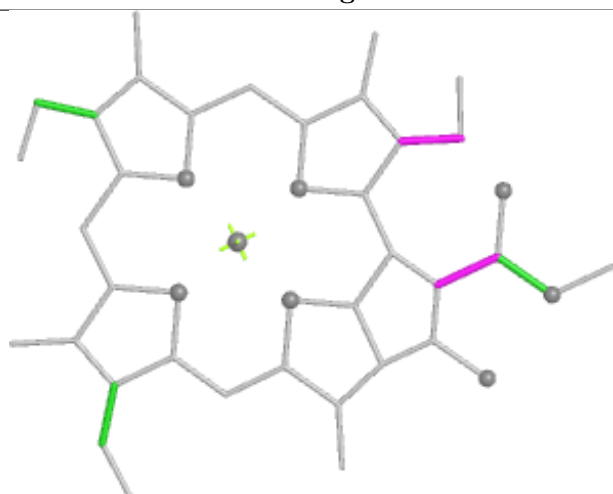
Ligand CLA 6 608



Bond lengths



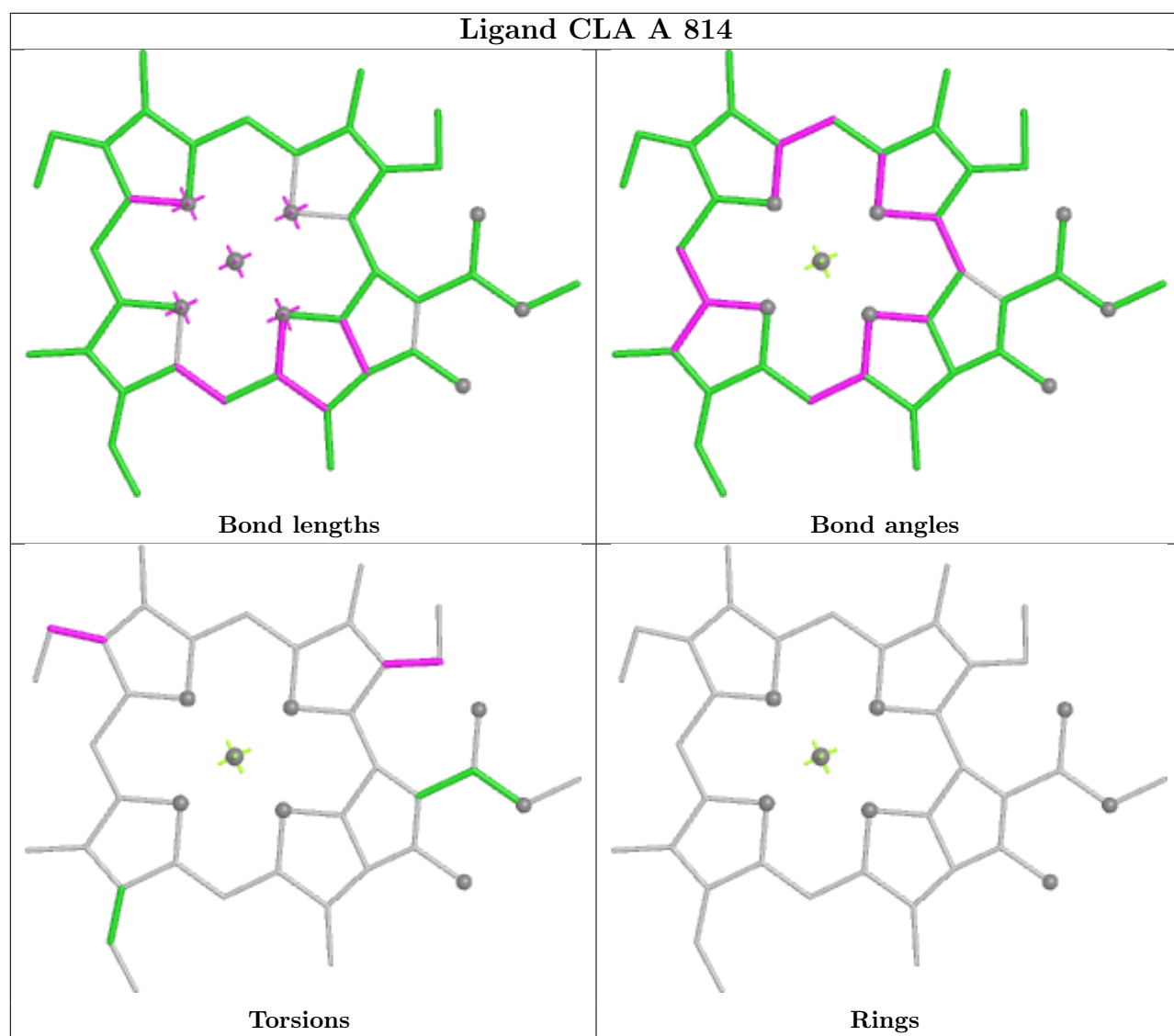
Bond angles

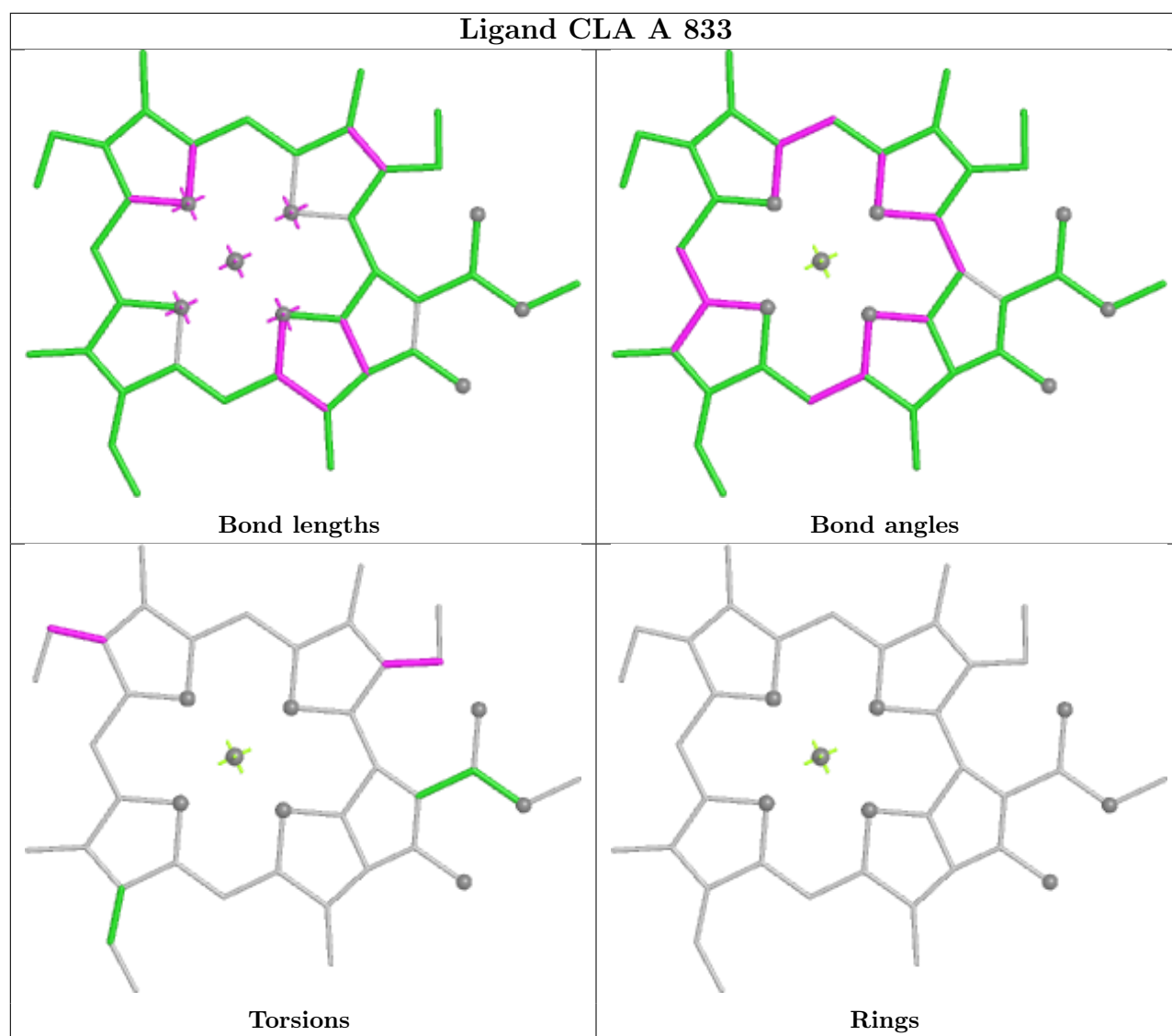


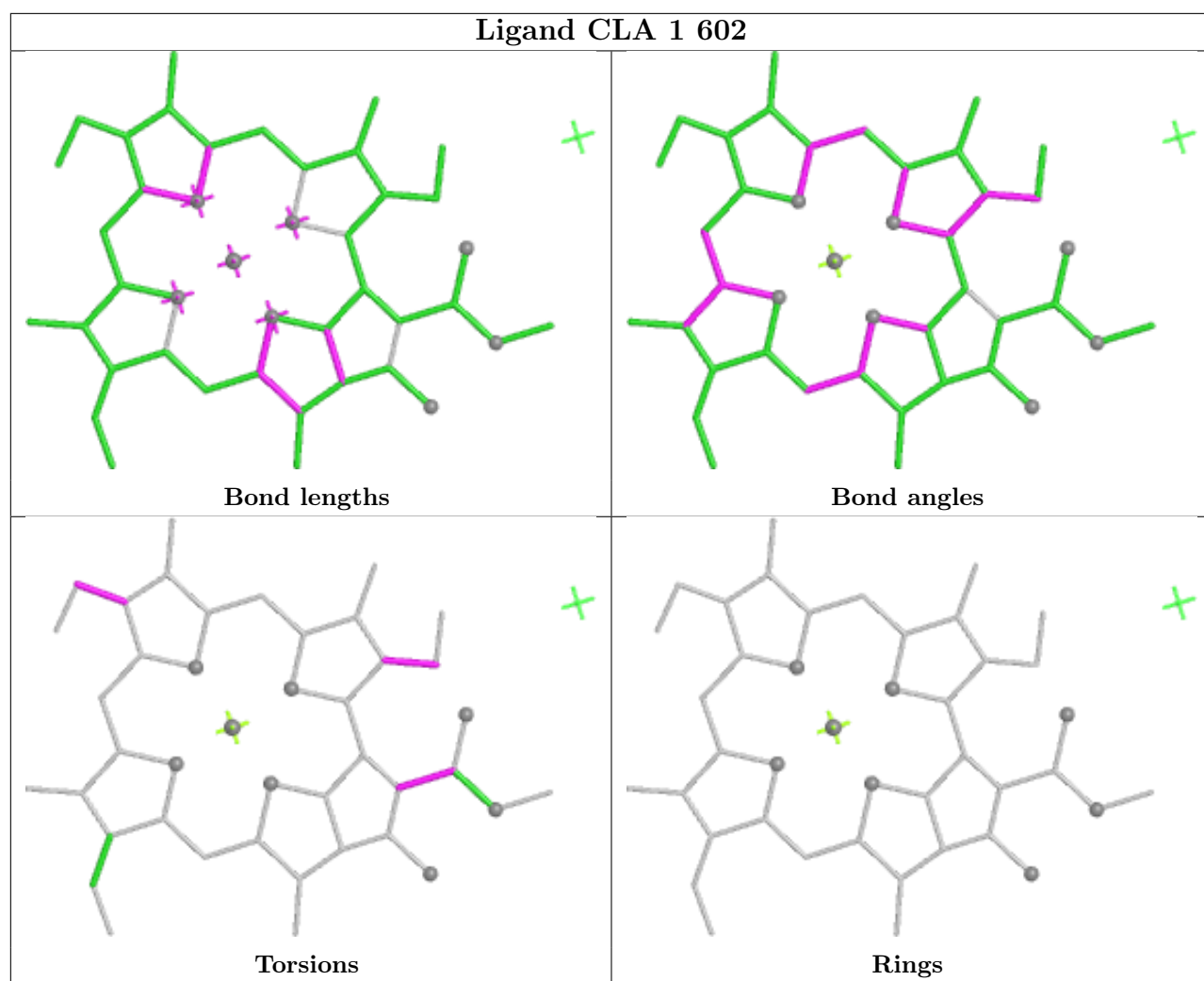
Torsions



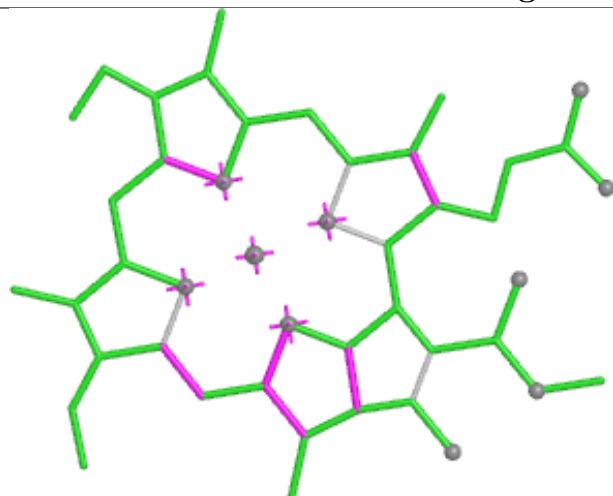
Rings



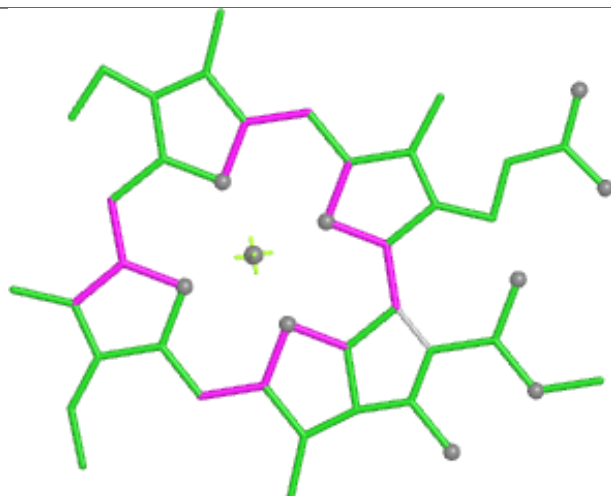




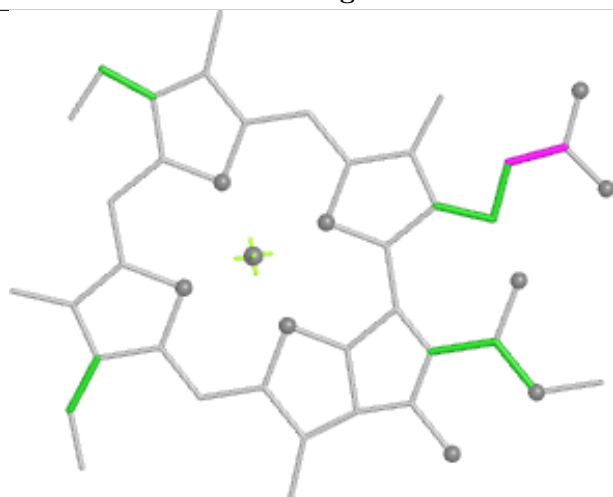
Ligand CLA 8 603



Bond lengths



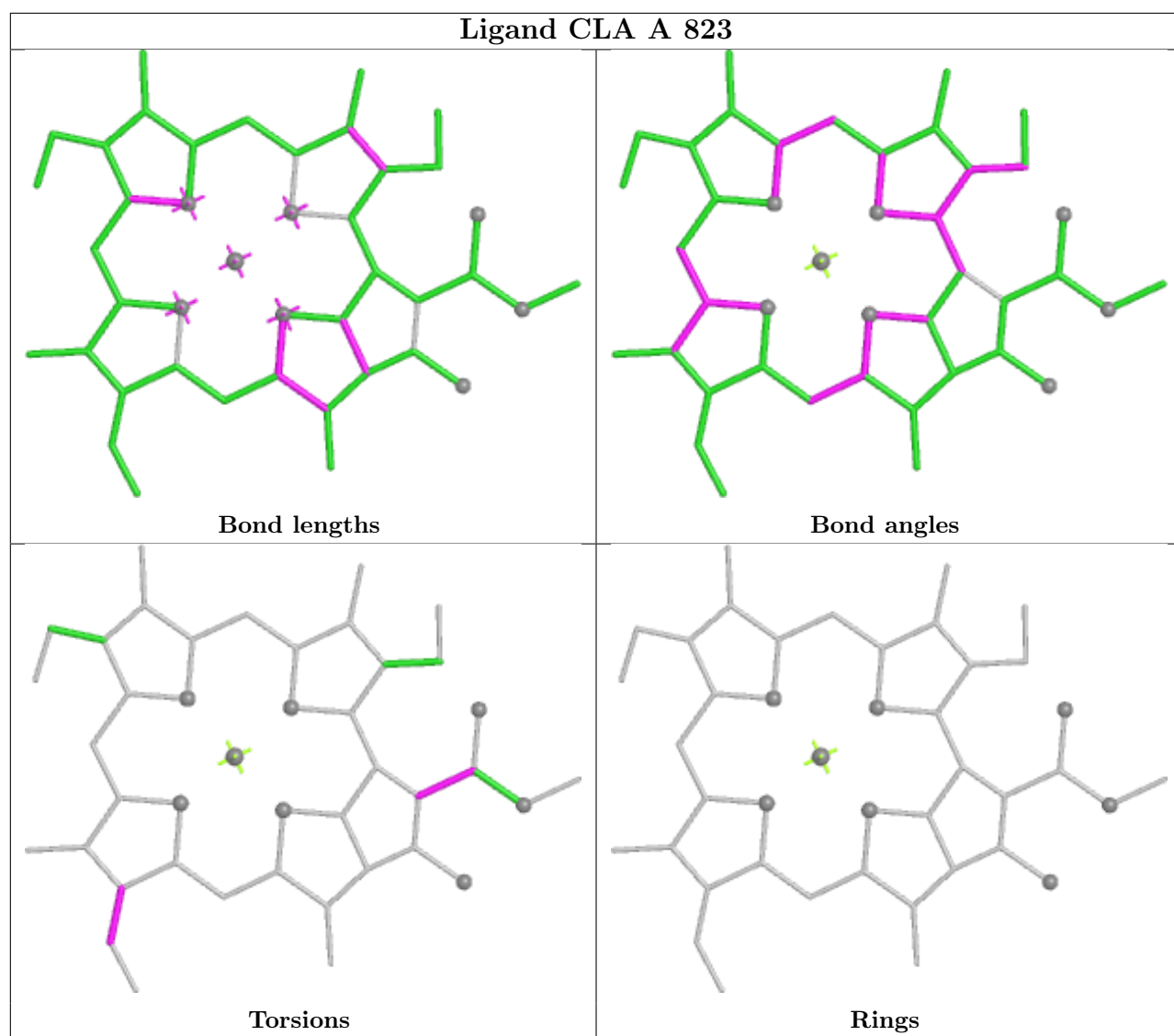
Bond angles

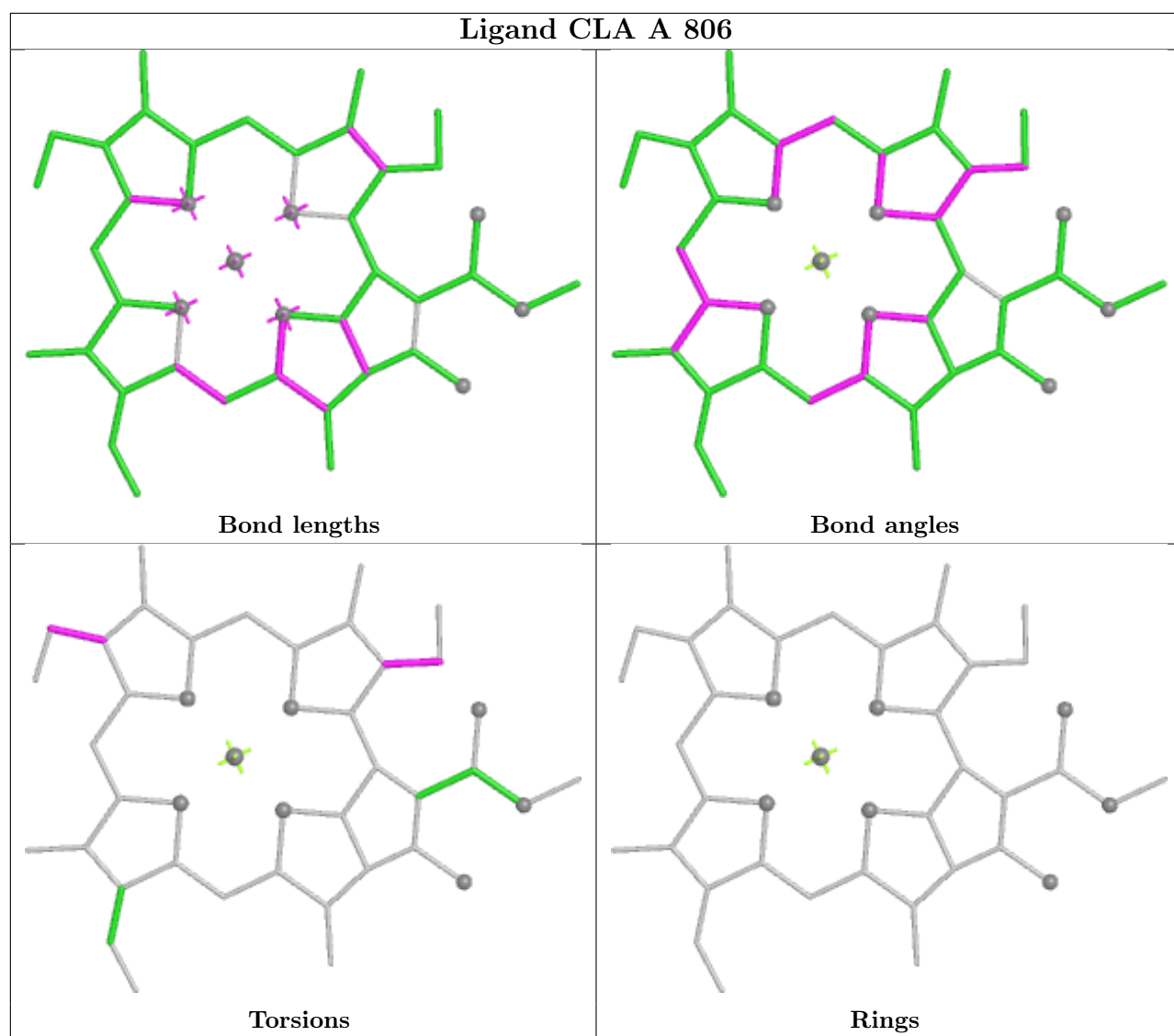


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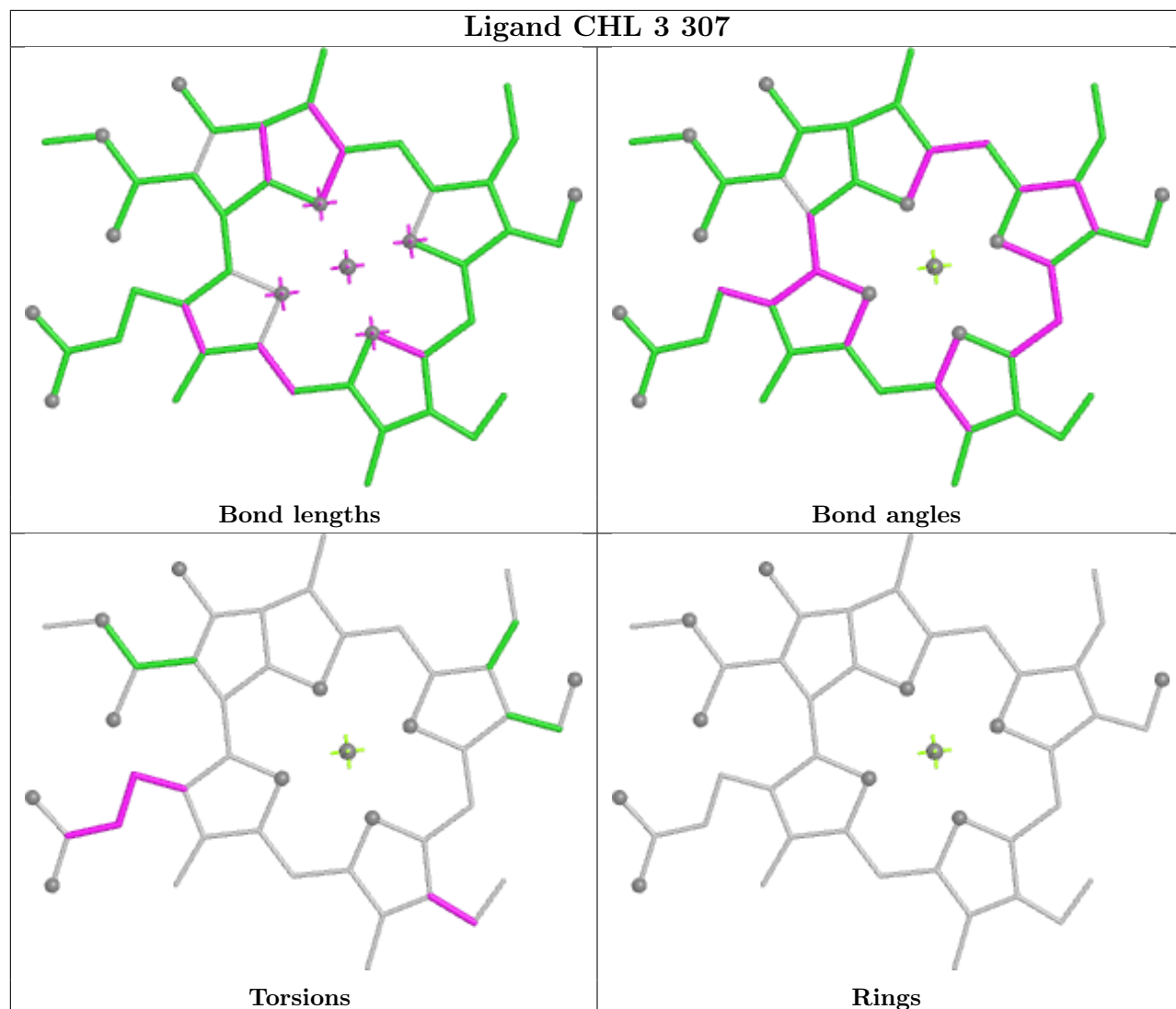


Rings

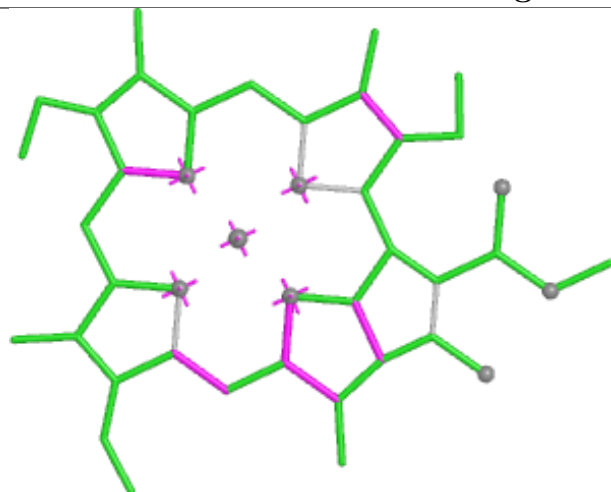




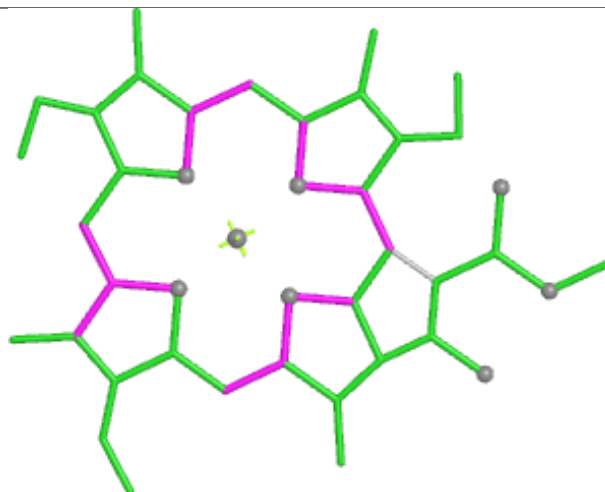
Ligand CHL 3 307



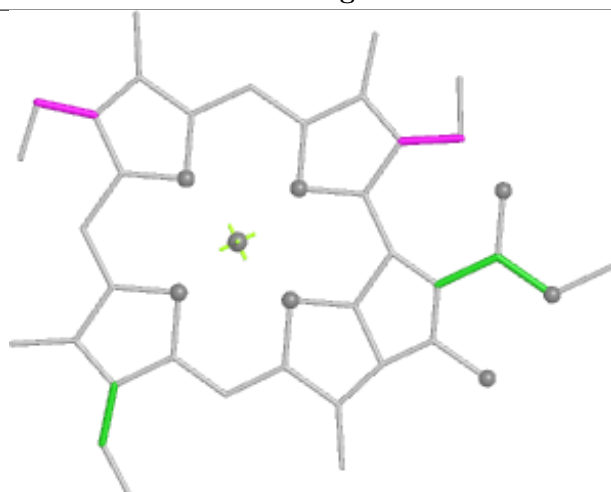
Ligand CLA B 838



Bond lengths



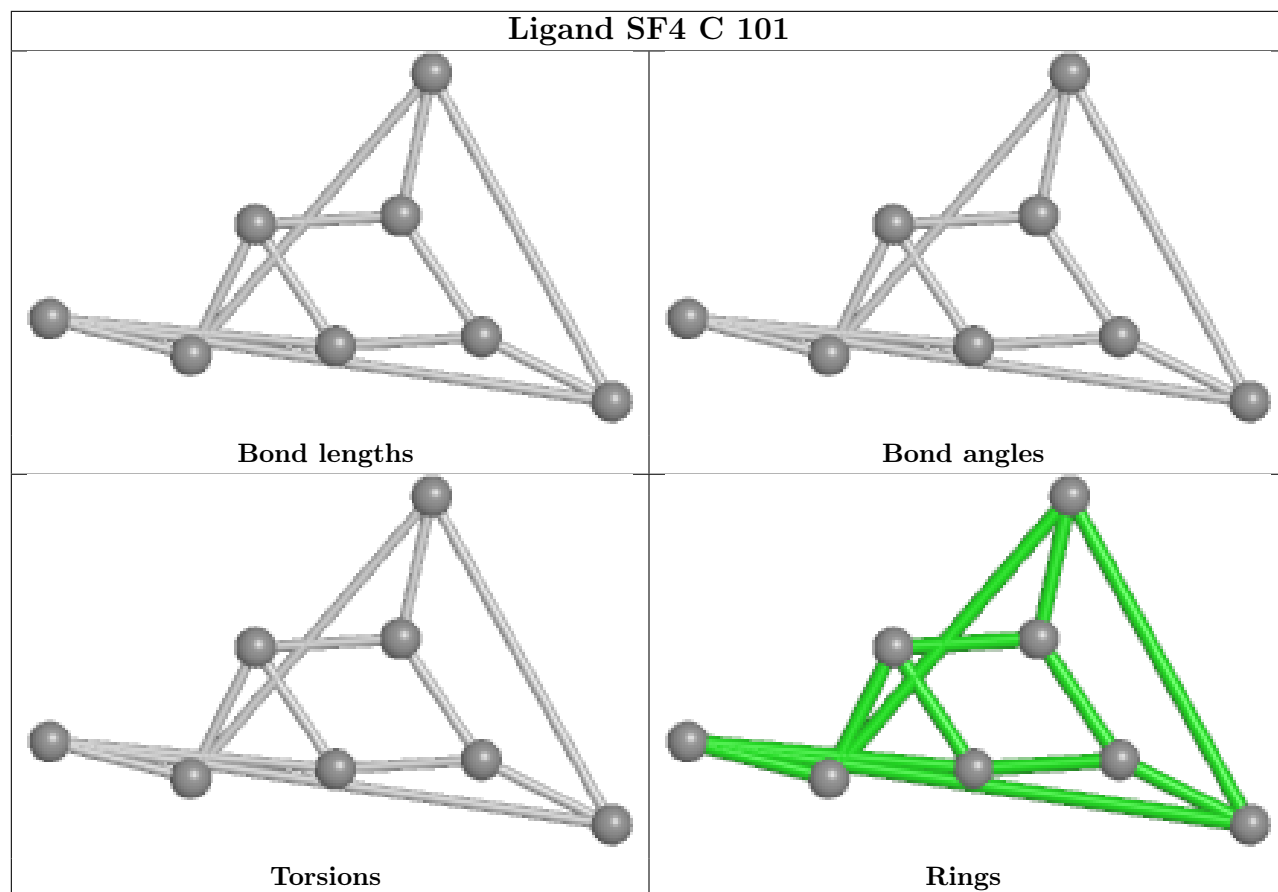
Bond angles



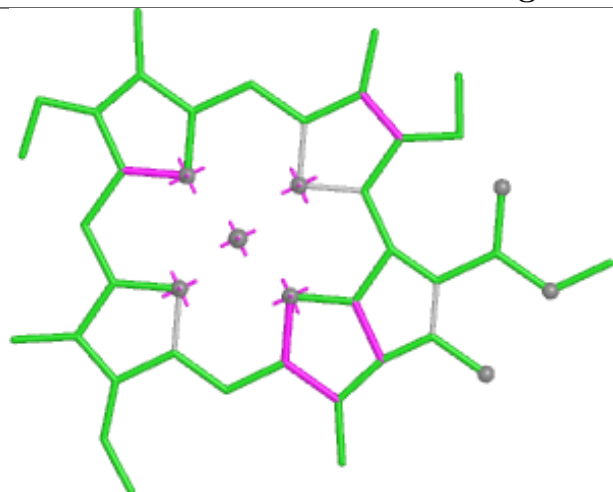
Torsions



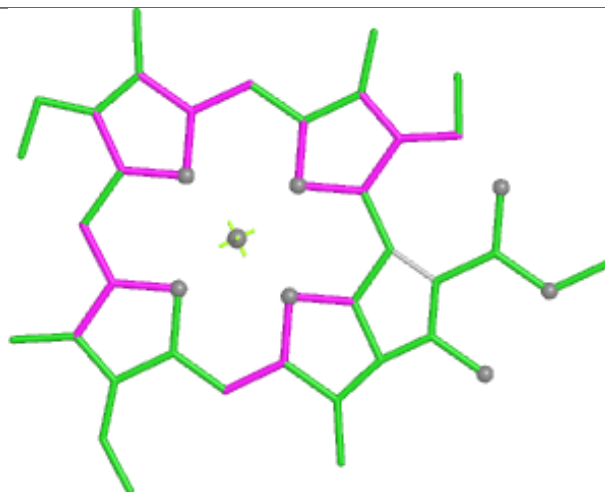
Rings



Ligand CLA 3 308



Bond lengths



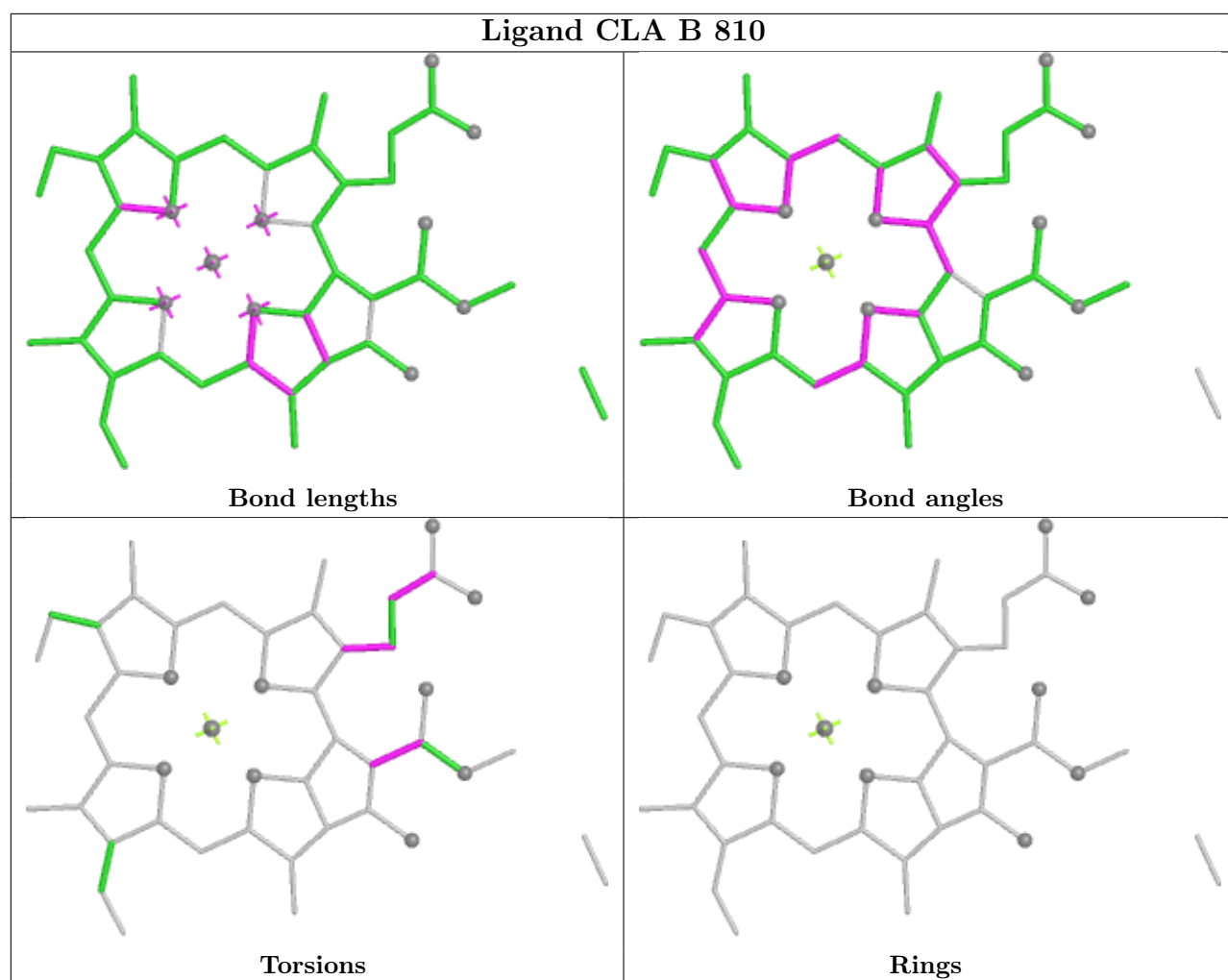
Bond angles



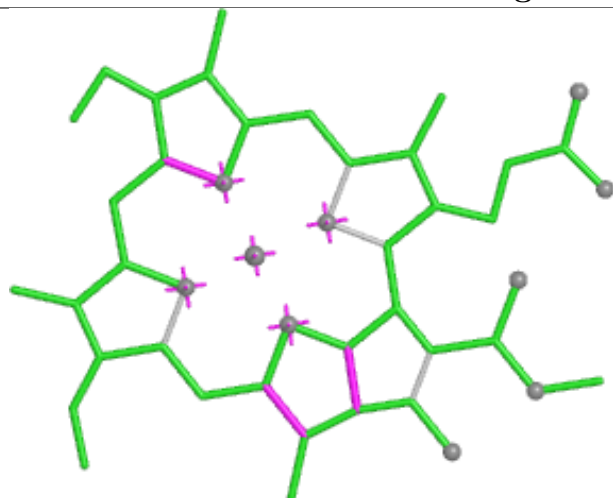
Torsions



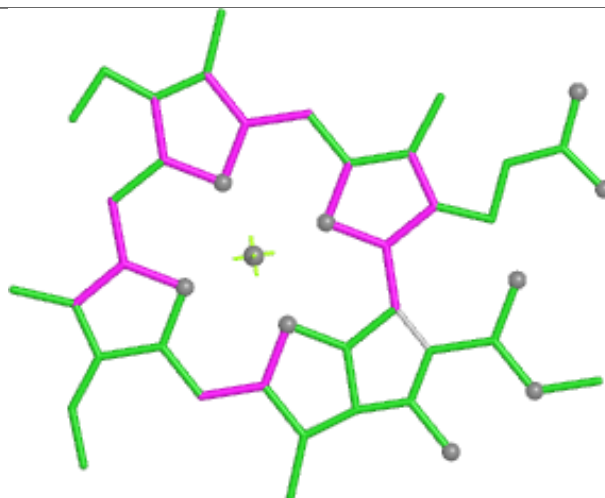
Rings



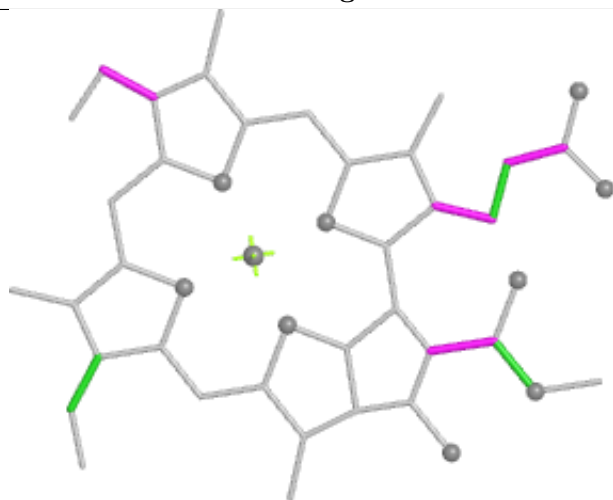
Ligand CLA B 802



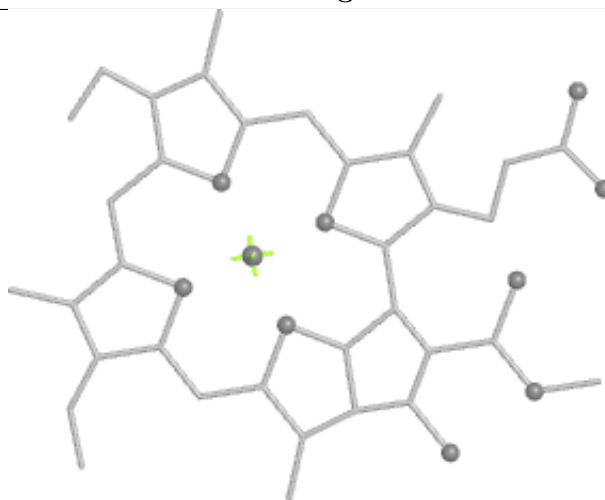
Bond lengths



Bond angles

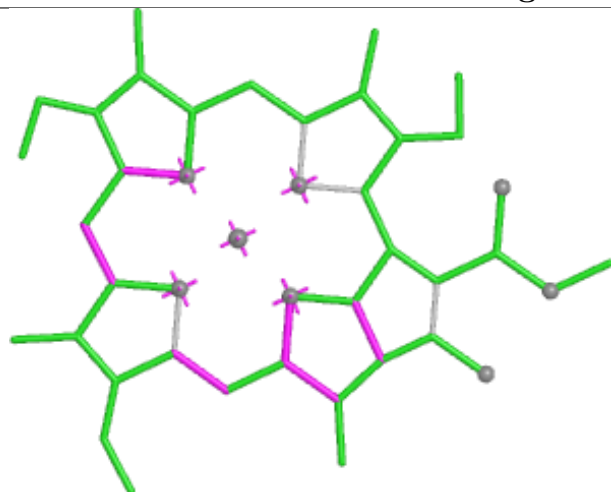


Torsions

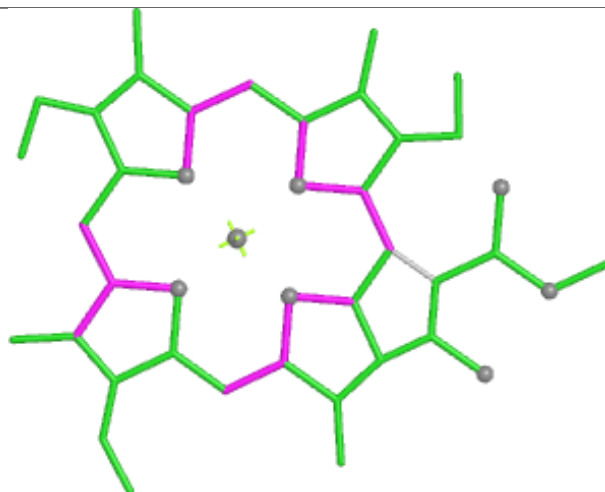


Rings

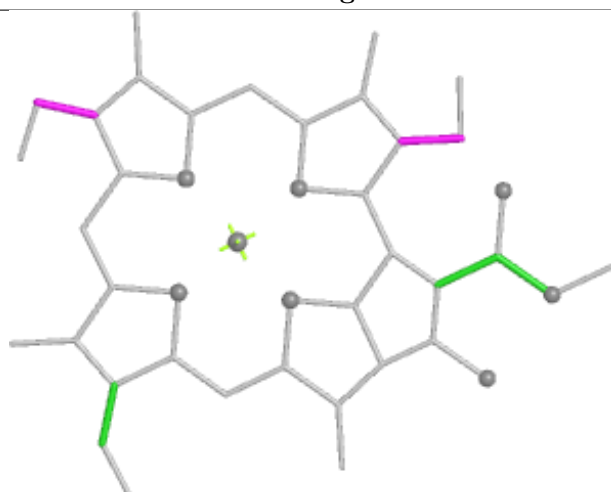
Ligand CLA 5 302



Bond lengths



Bond angles

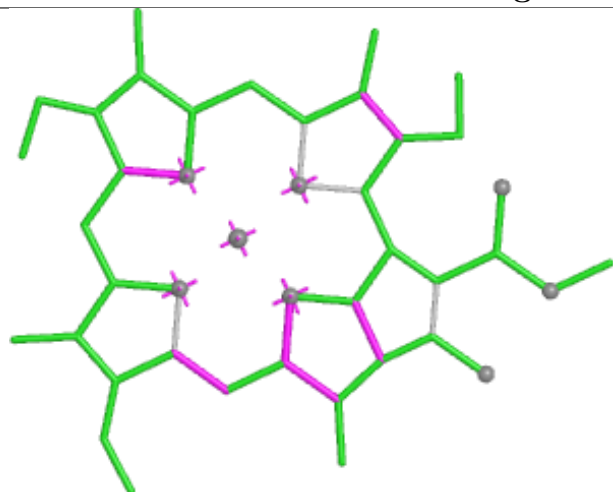


Torsions

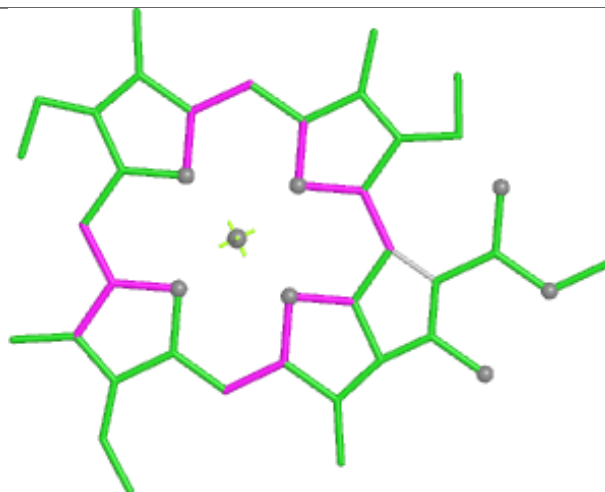


Rings

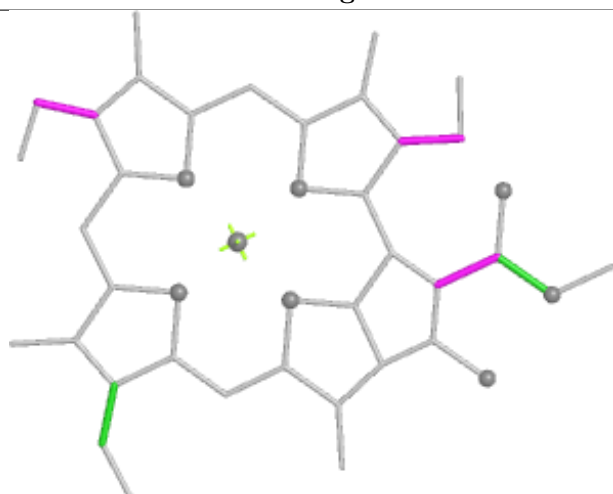
Ligand CLA A 837



Bond lengths



Bond angles

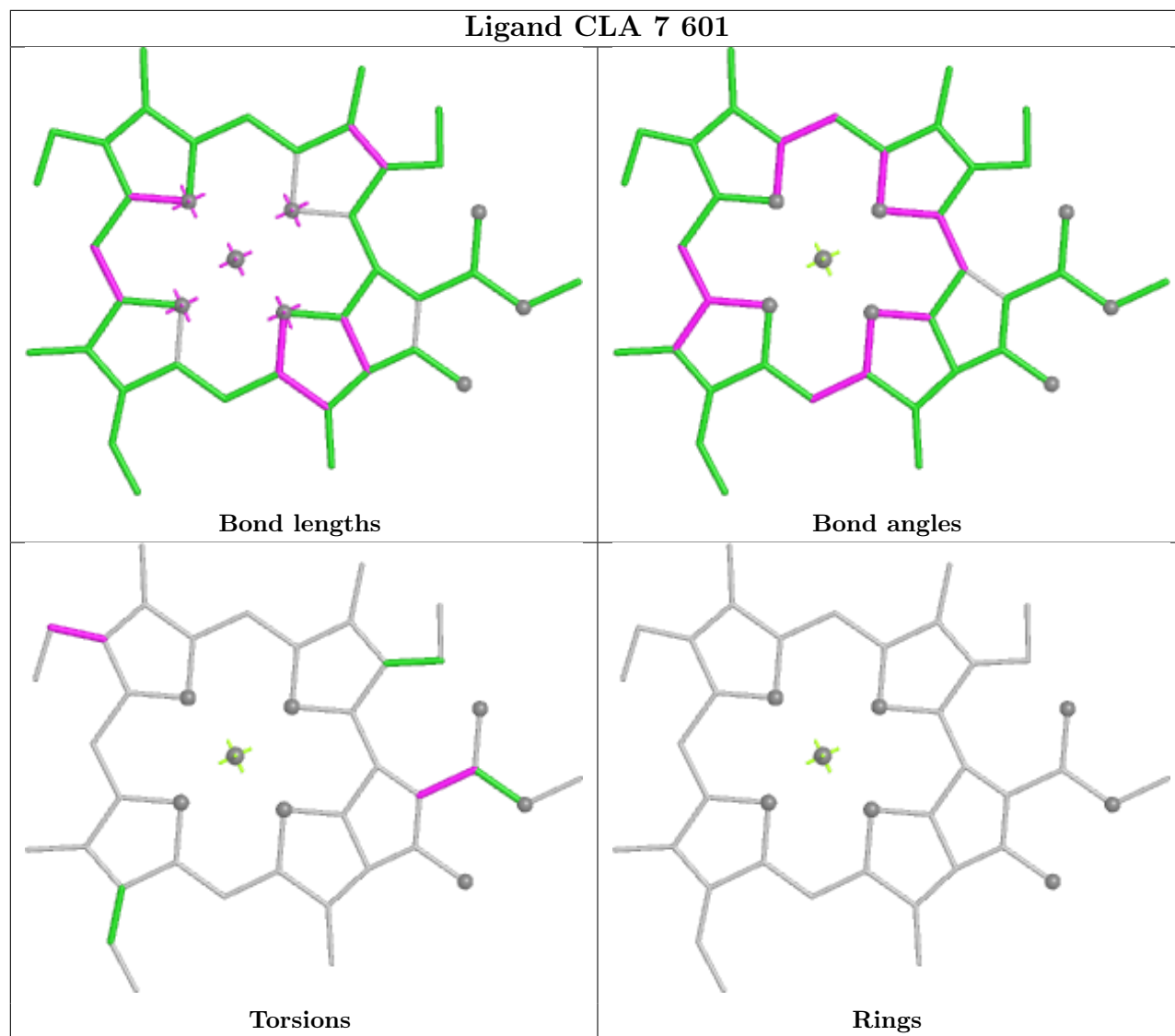


Torsions

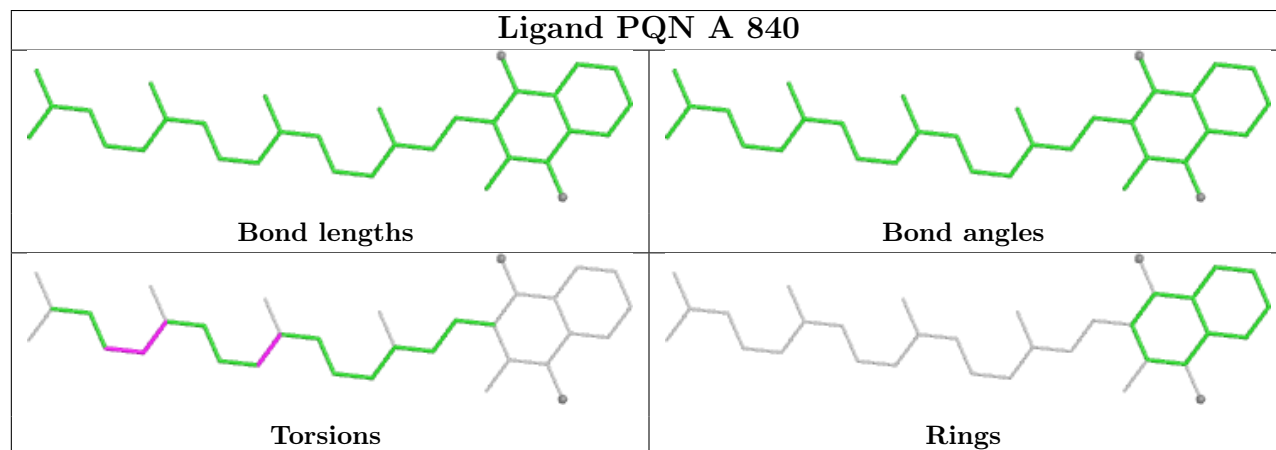


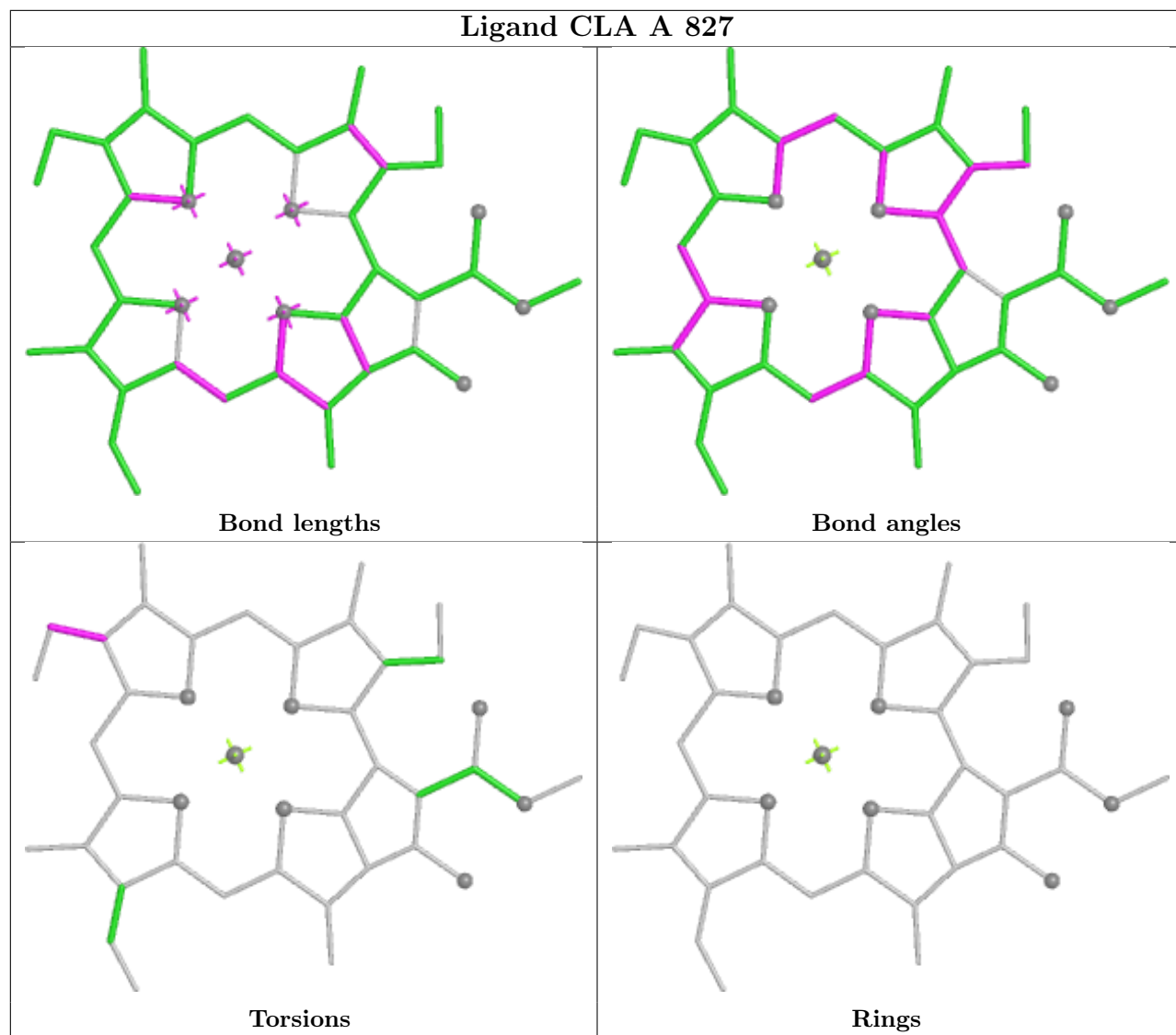
Rings

Ligand CLA 7 601

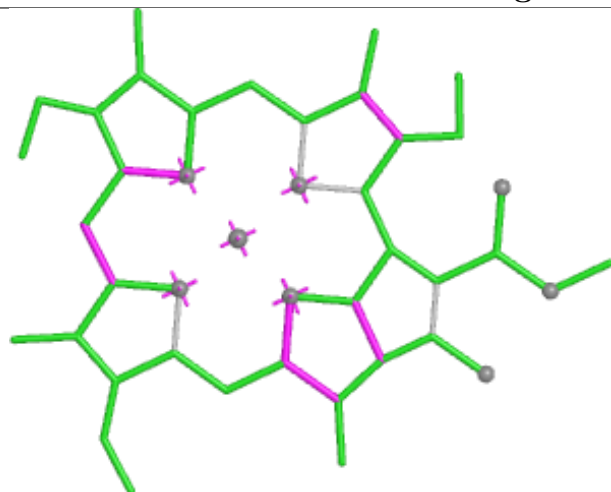


Ligand PQN A 840

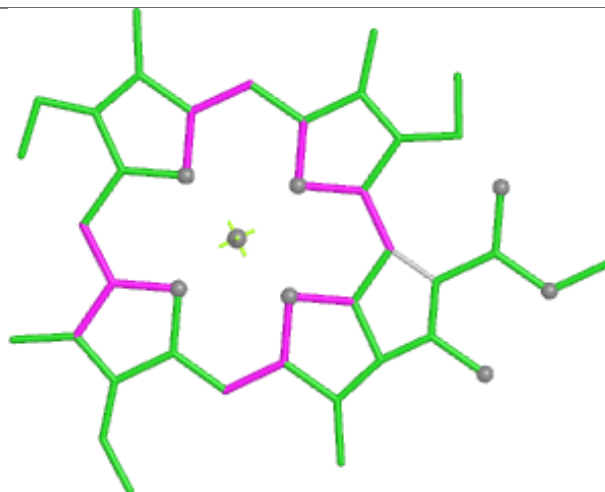




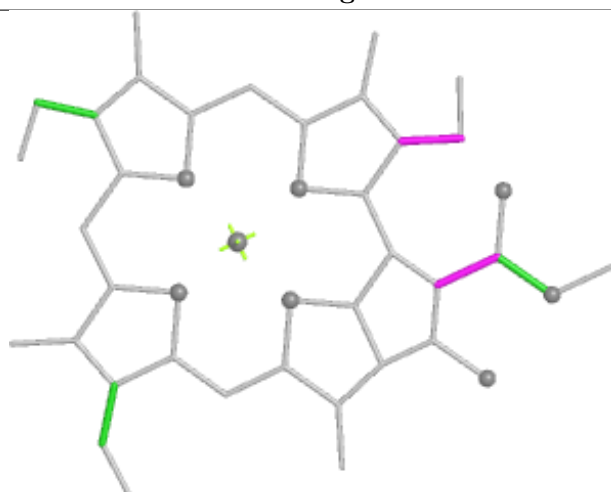
Ligand CLA B 836



Bond lengths



Bond angles

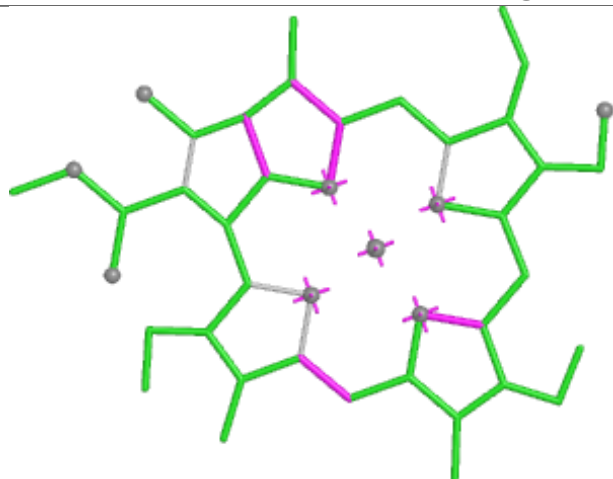


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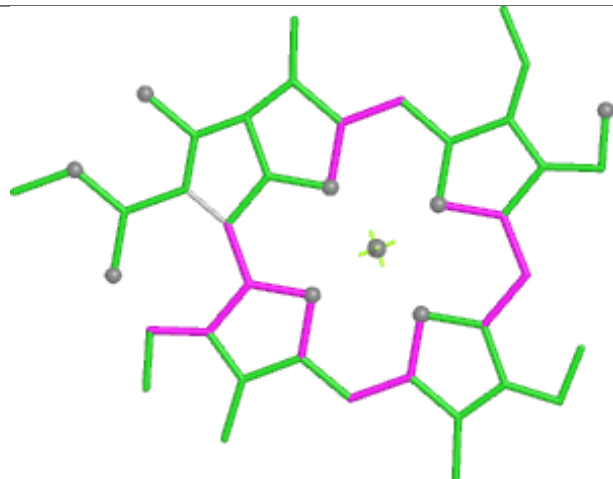


Rings

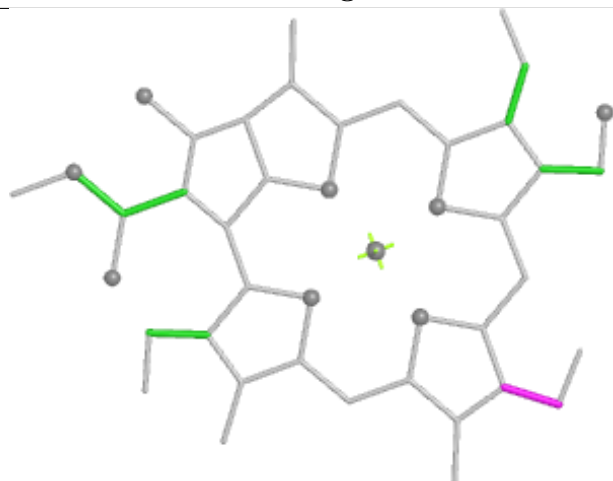
Ligand CHL 8 606



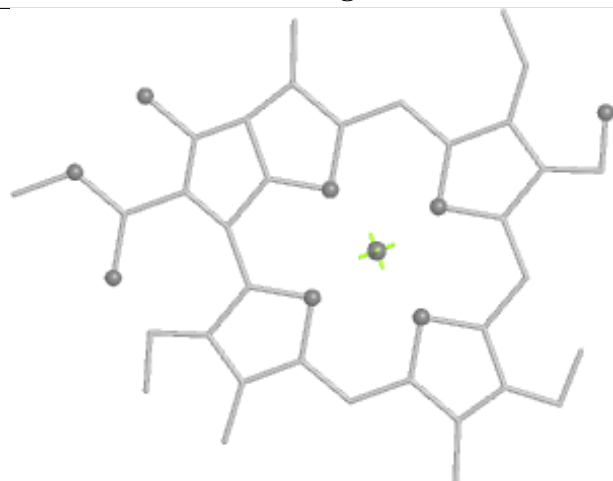
Bond lengths



Bond angles

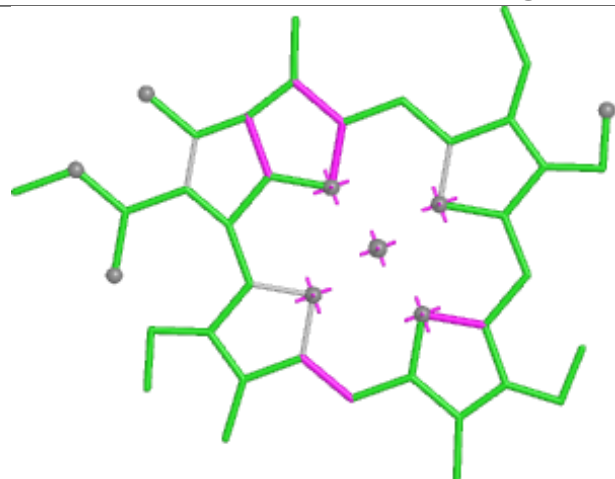


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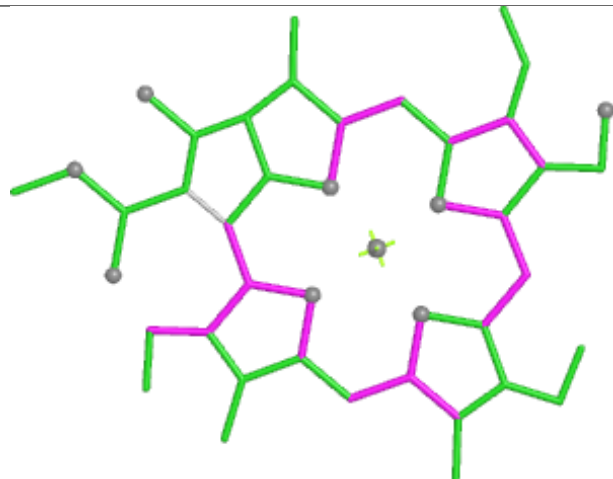


Rings

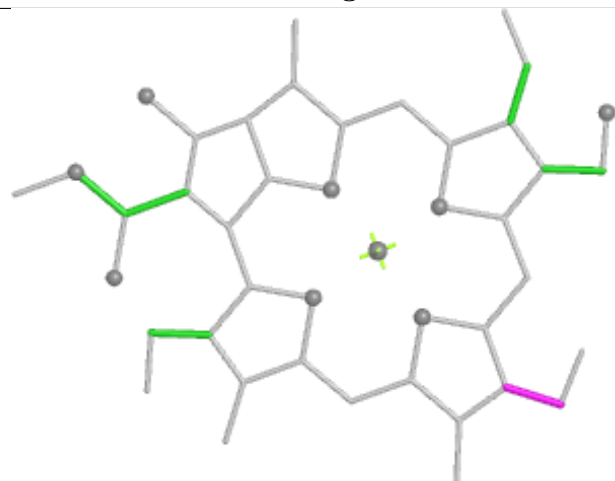
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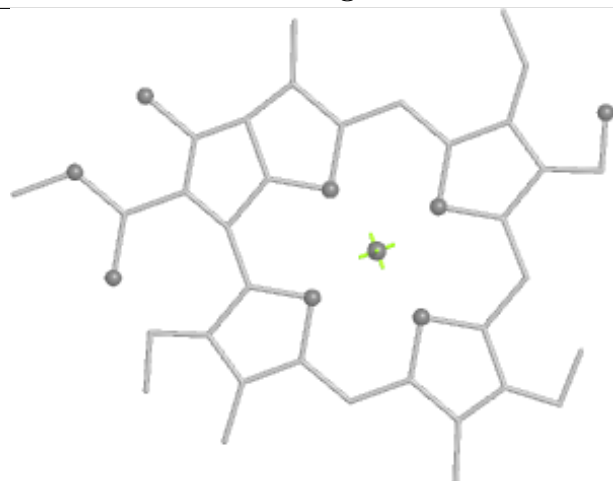
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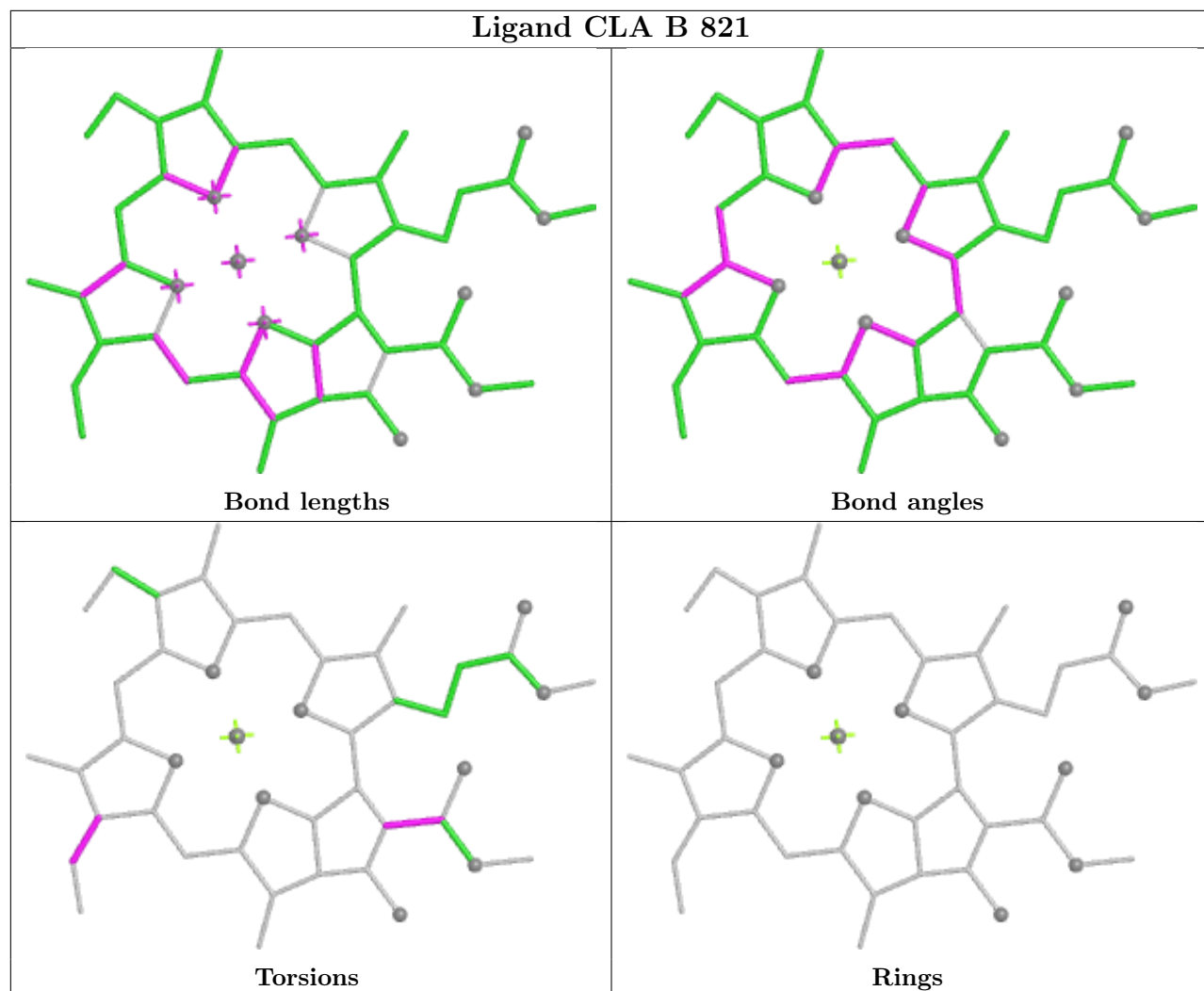
Bond angles



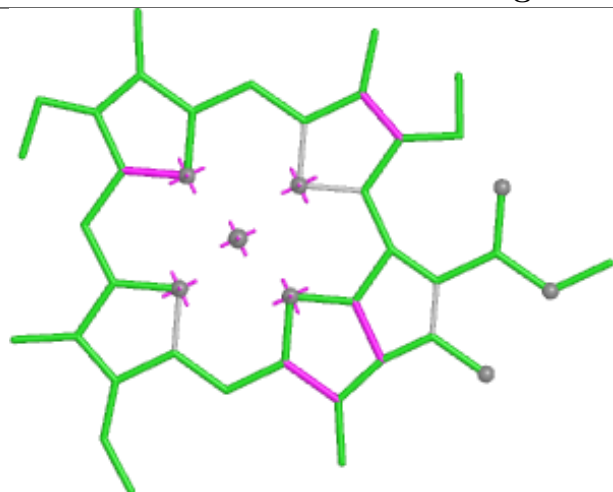
Torsions



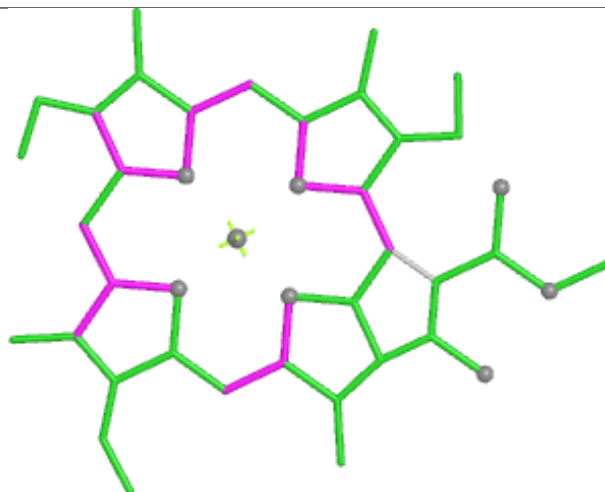
Rings



Ligand CLA A 826



Bond lengths



Bond angles

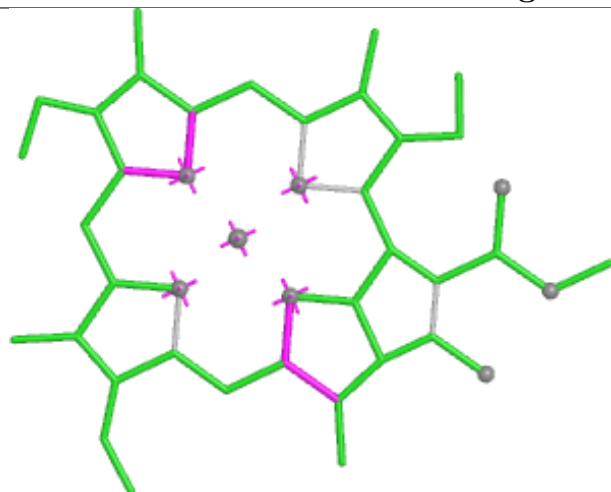


Torsions

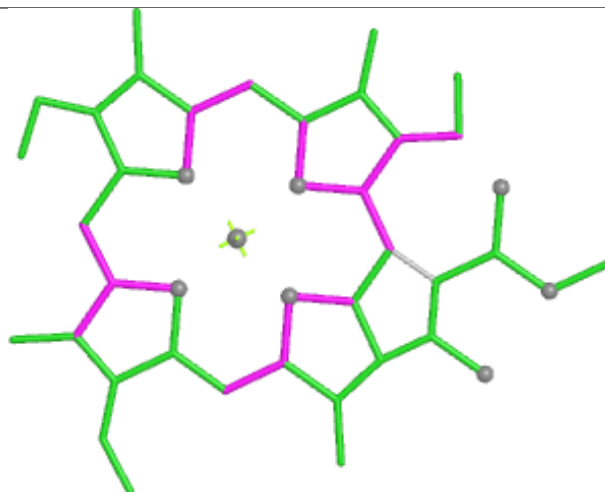


Rings

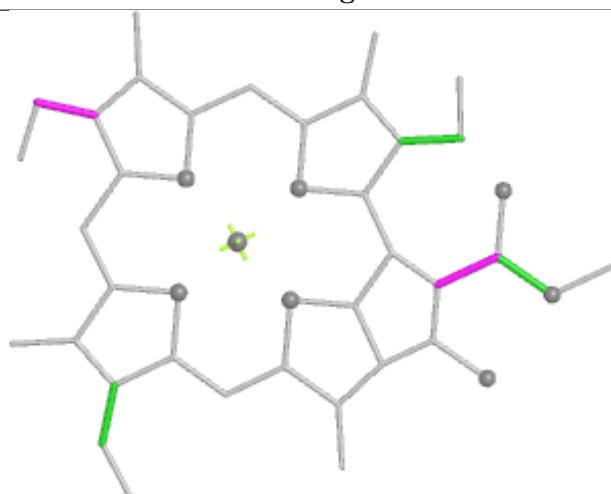
Ligand CLA 1 604



Bond lengths



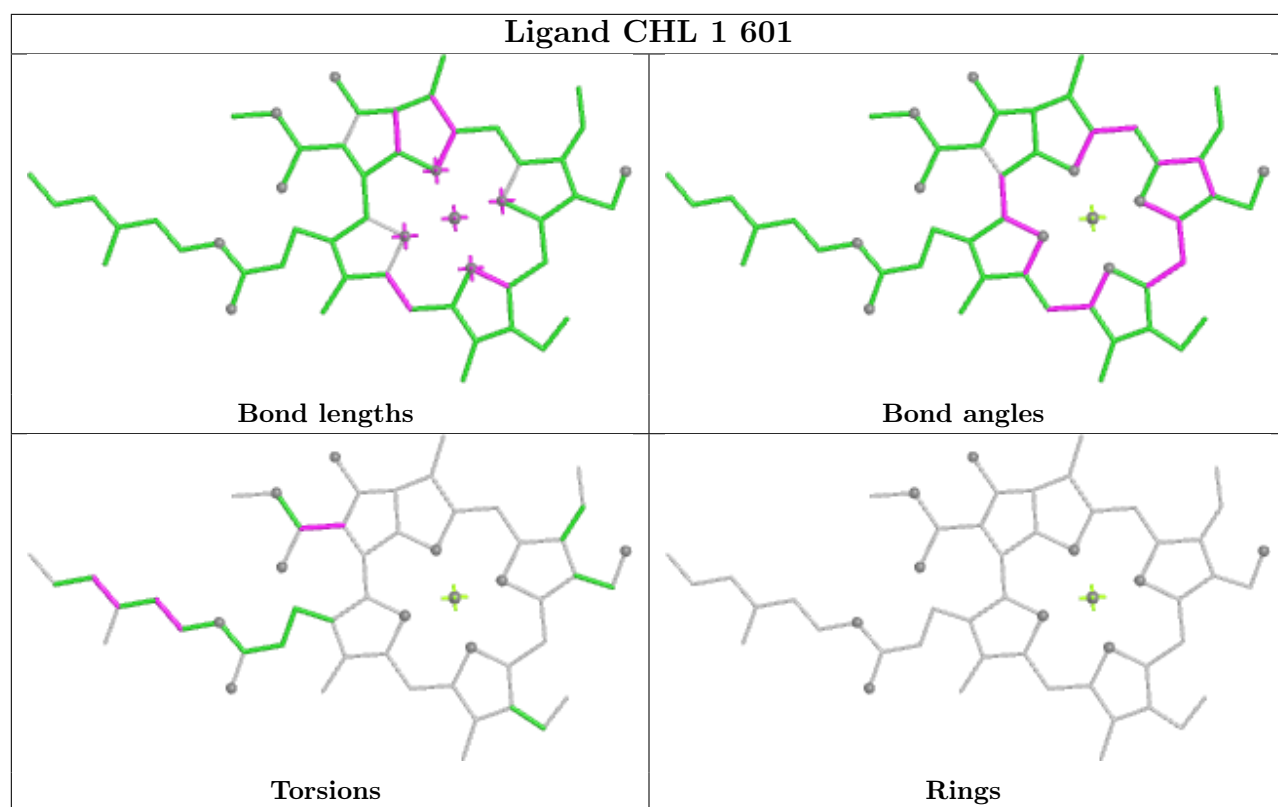
Bond angles



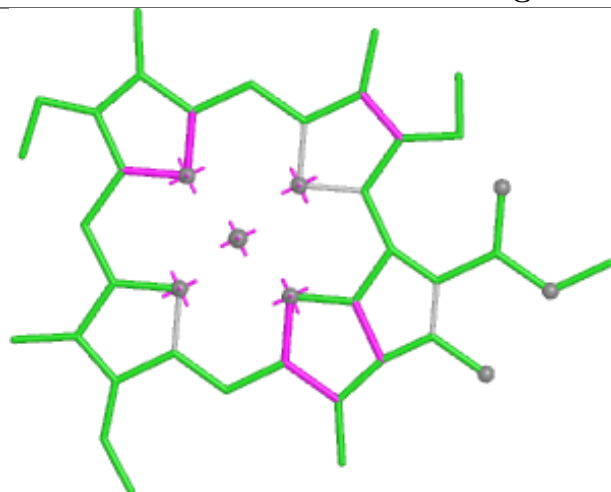
Torsions



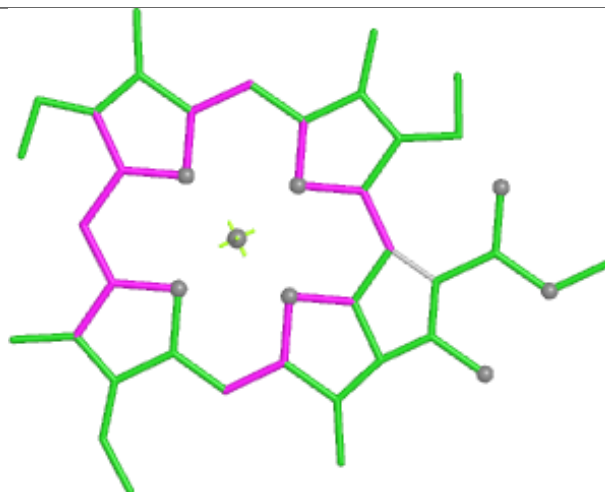
Rings



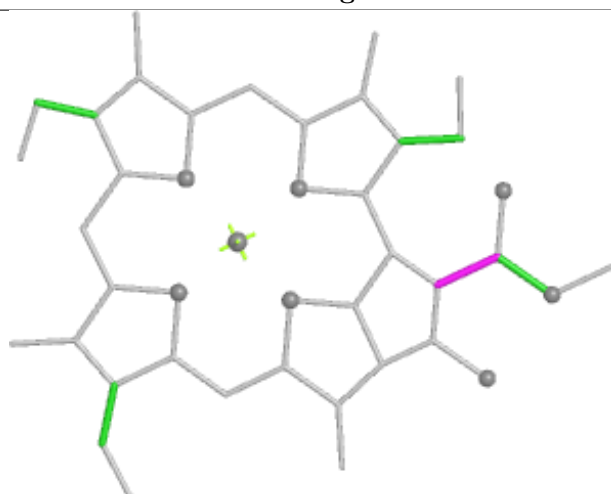
Ligand CLA A 836



Bond lengths



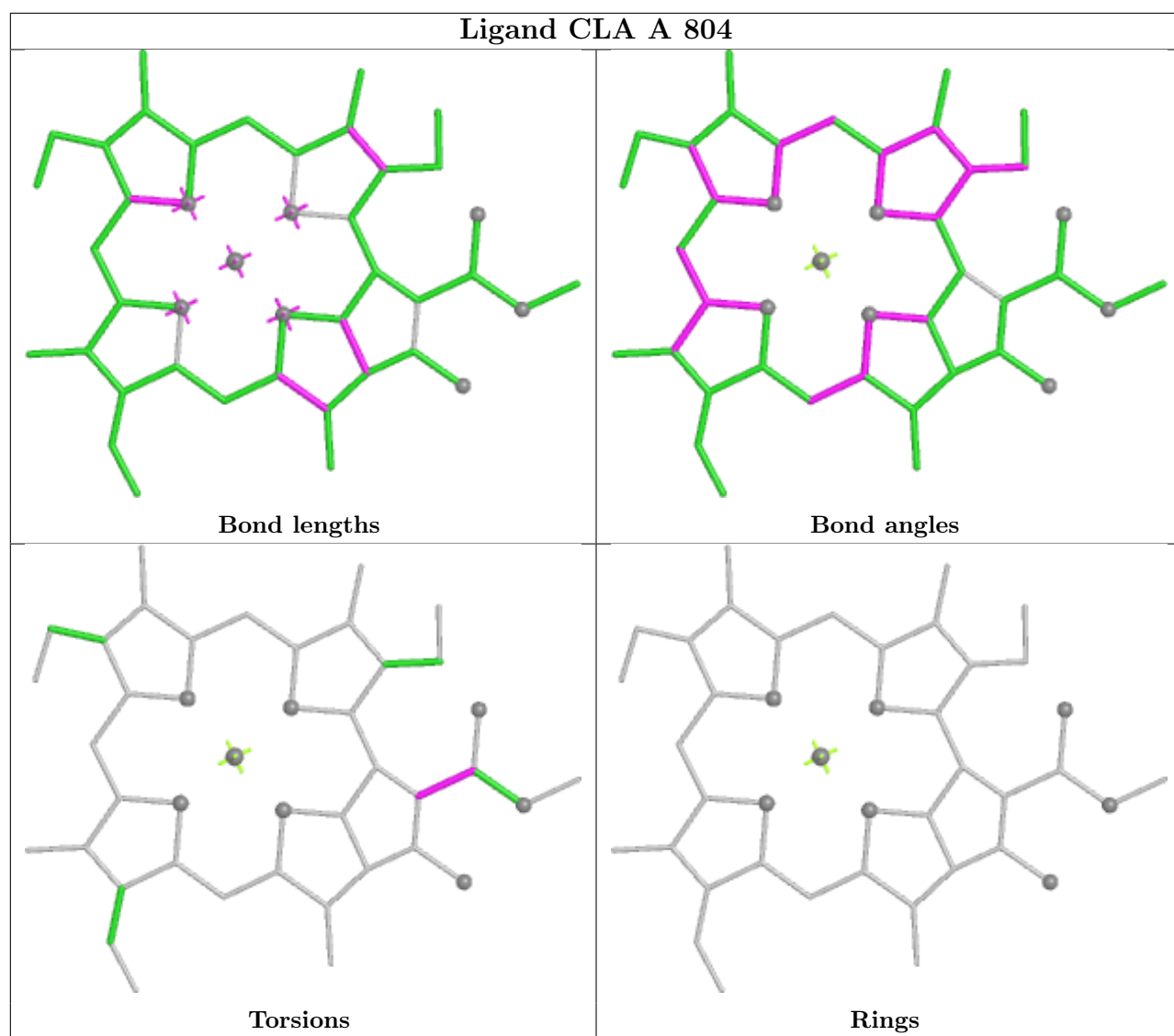
Bond angles

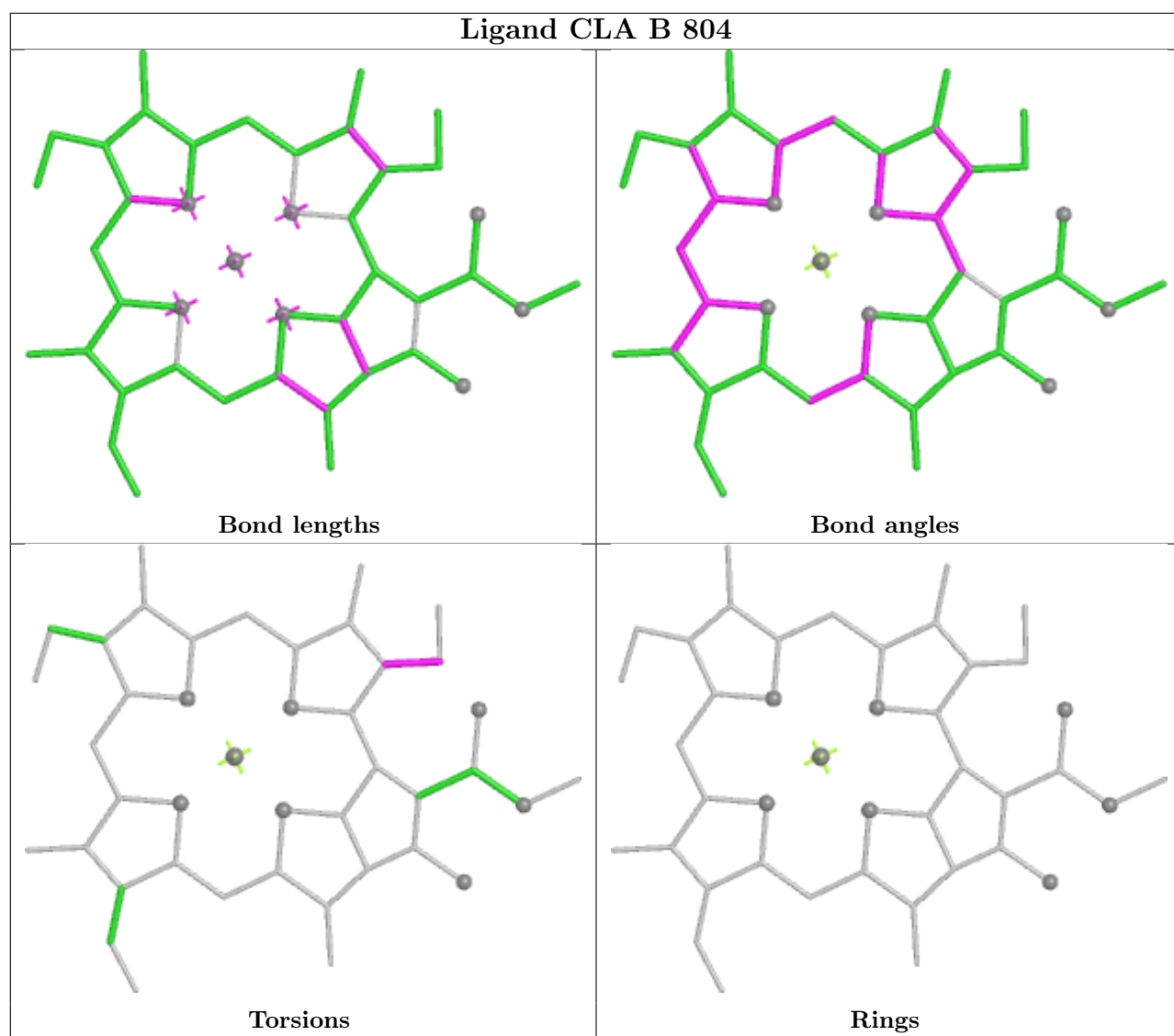


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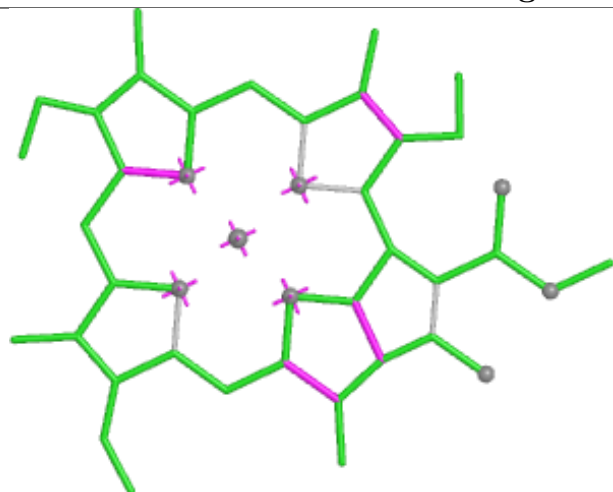


Rings

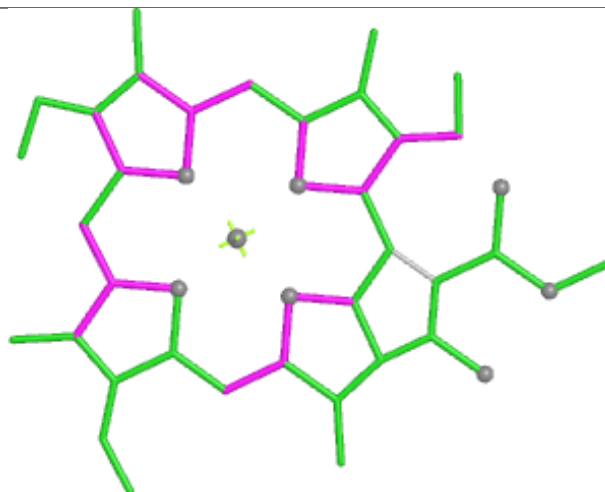




Ligand CLA 3 305



Bond lengths



Bond angles

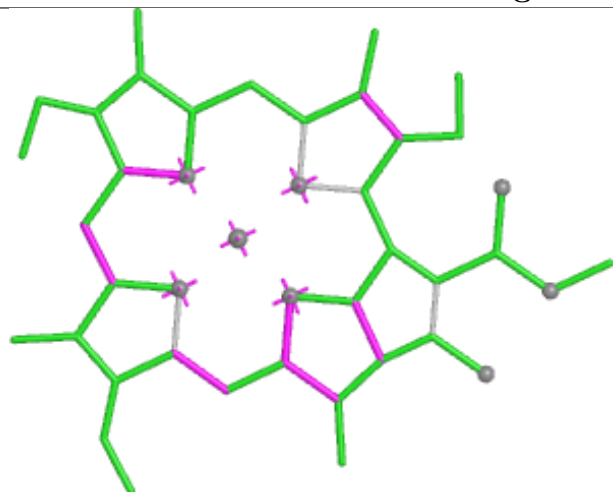


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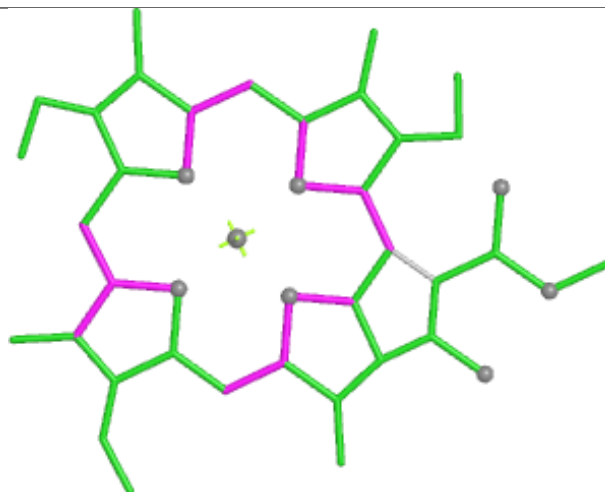


Rings

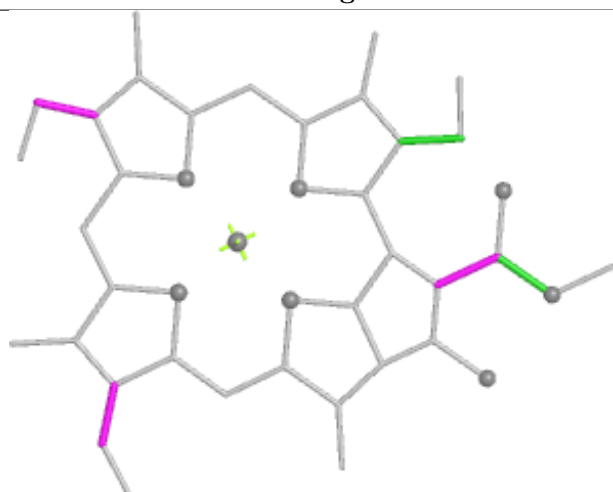
Ligand CLA A 835



Bond lengths



Bond angles

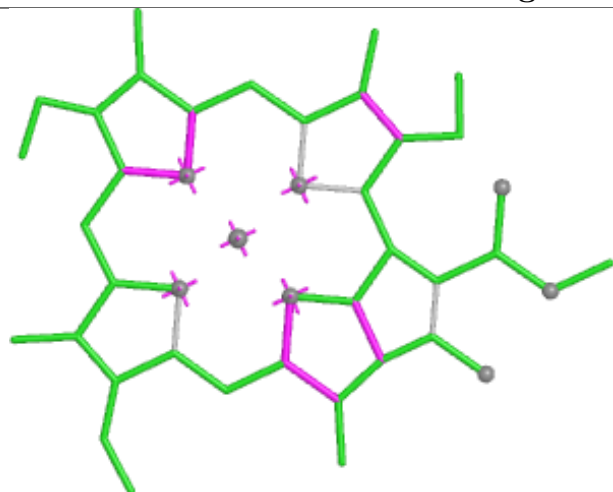


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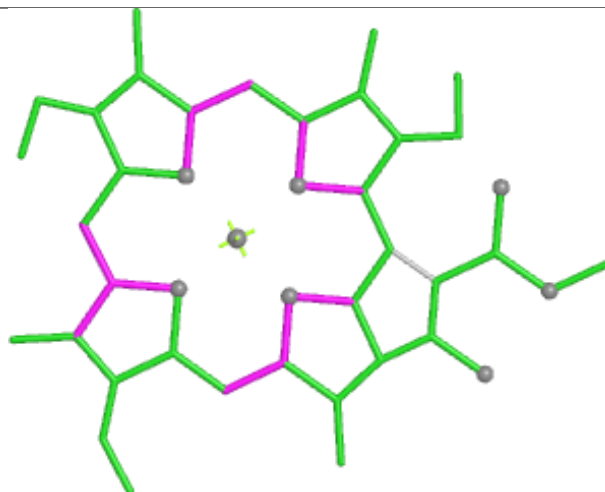


Rings

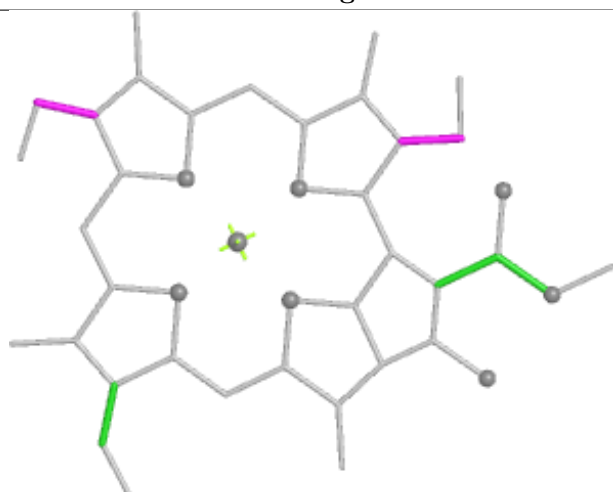
Ligand CLA 4 604



Bond lengths



Bond angles

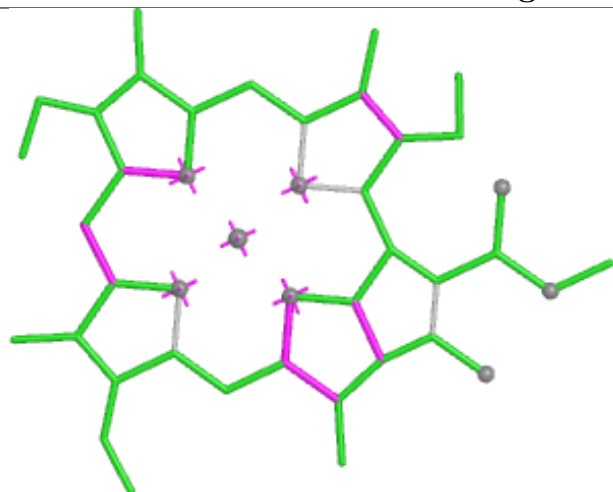


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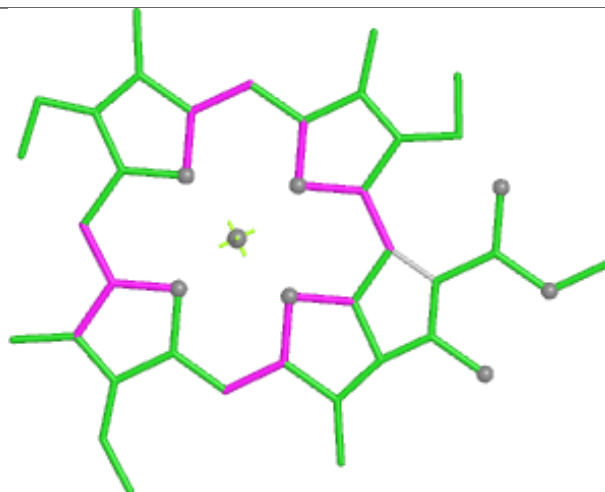


Rings

Ligand CLA 3 303



Bond lengths



Bond angles

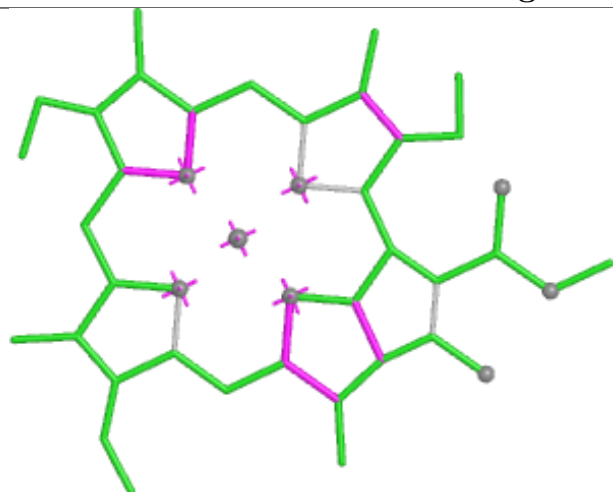


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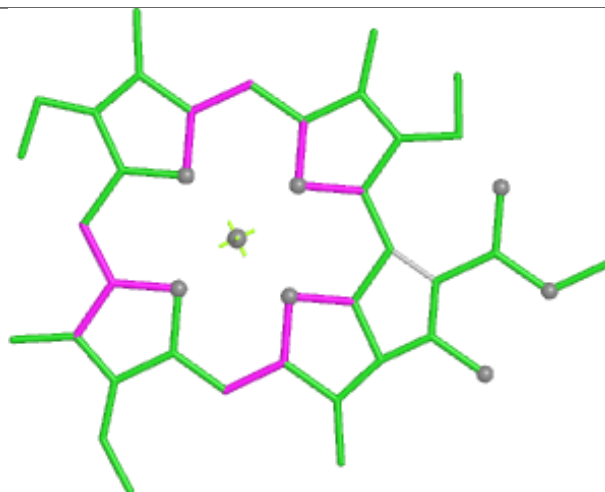


Rings

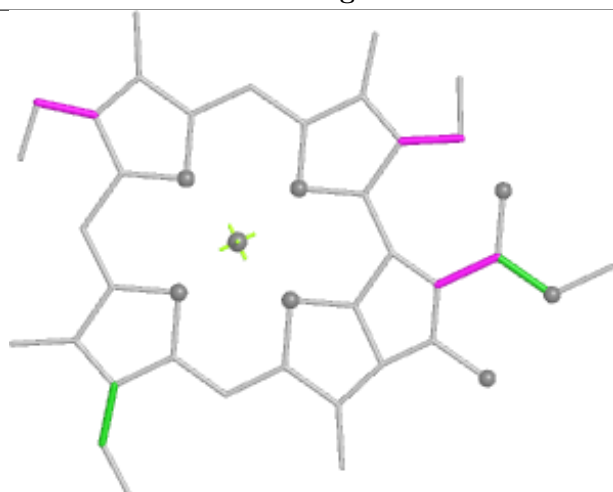
Ligand CLA 8 611



Bond lengths



Bond angles

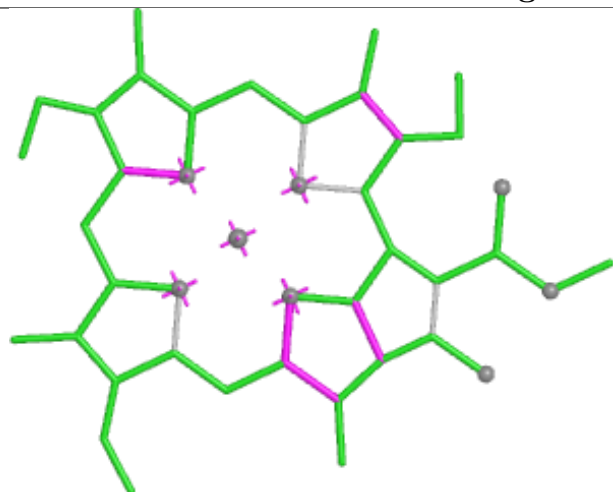


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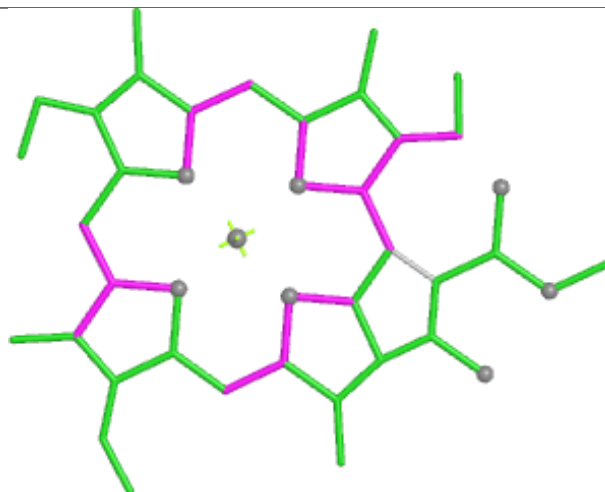


Rings

Ligand CLA 6 601



Bond lengths



Bond angles

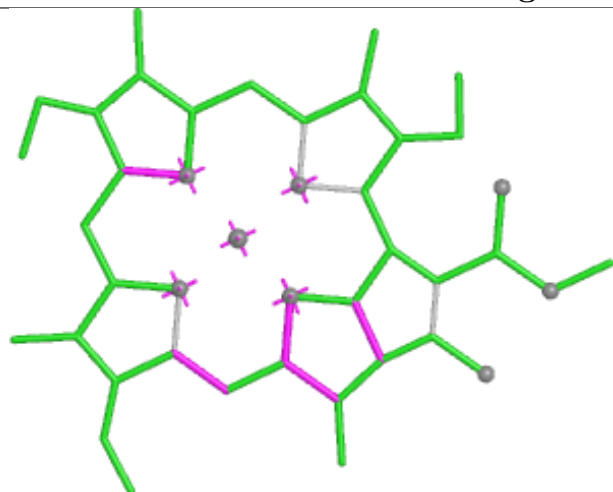


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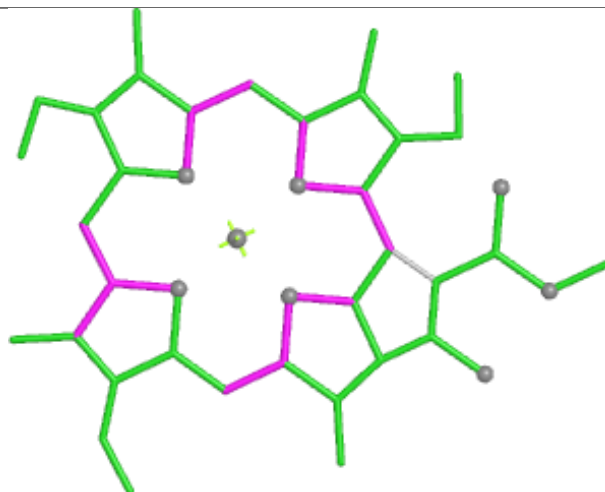


Rings

Ligand CLA 5 301



Bond lengths



Bond angles

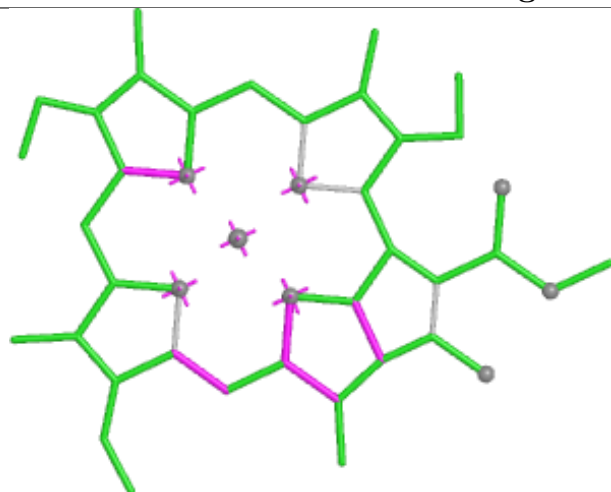


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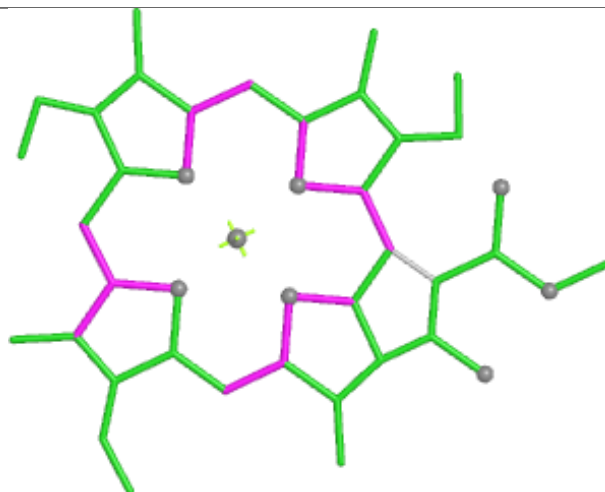


Rings

Ligand CLA 5 304



Bond lengths



Bond angles

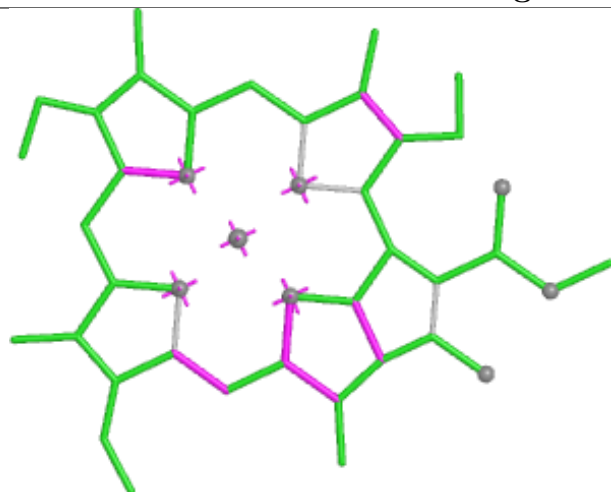


Torsions

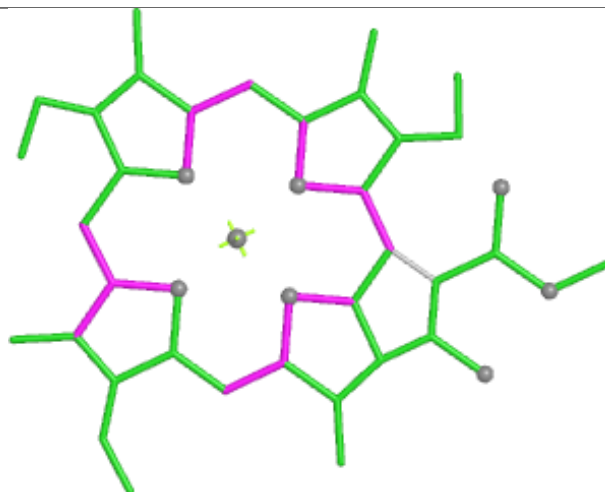


Rings

Ligand CLA A 843



Bond lengths



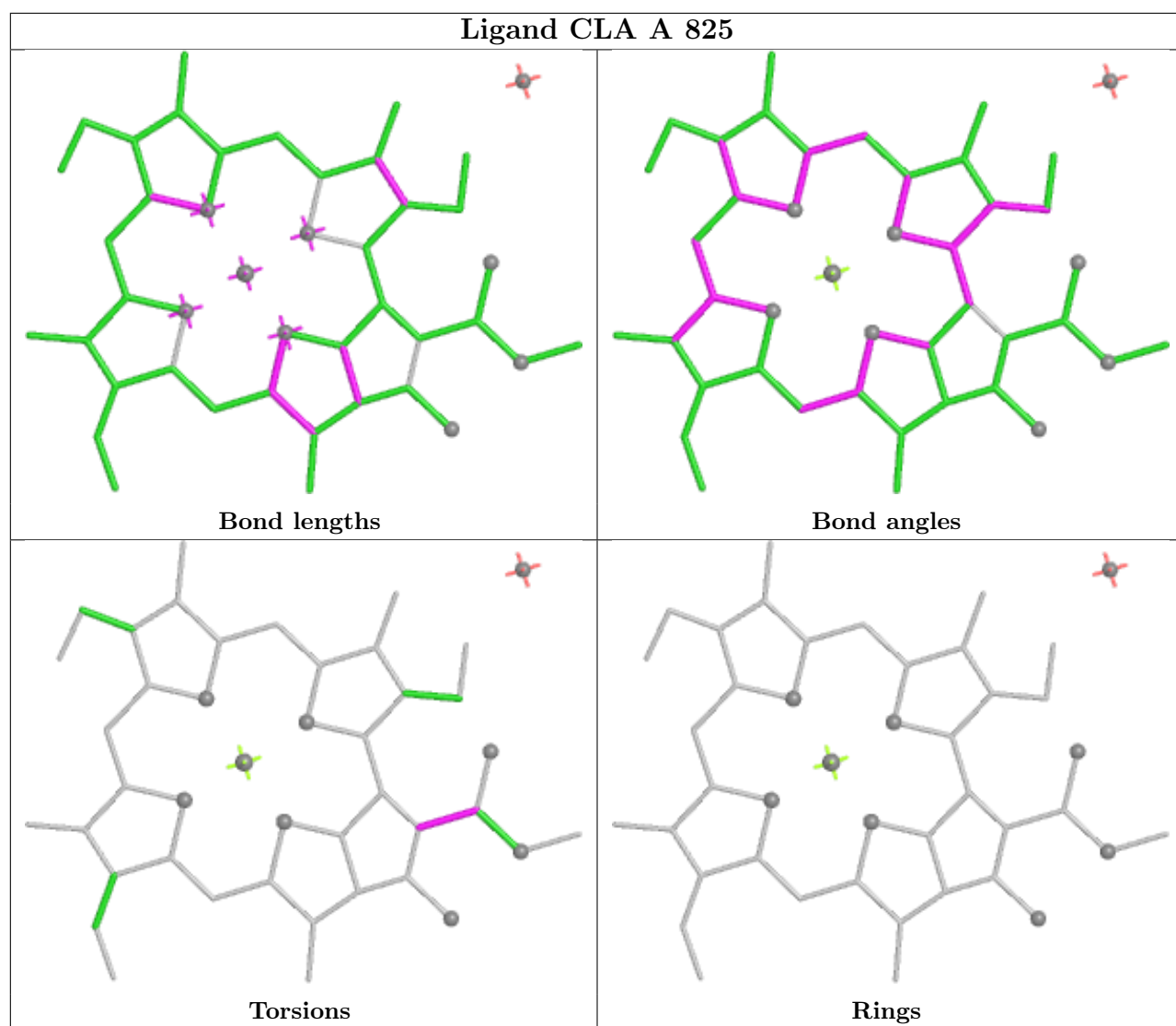
Bond angles

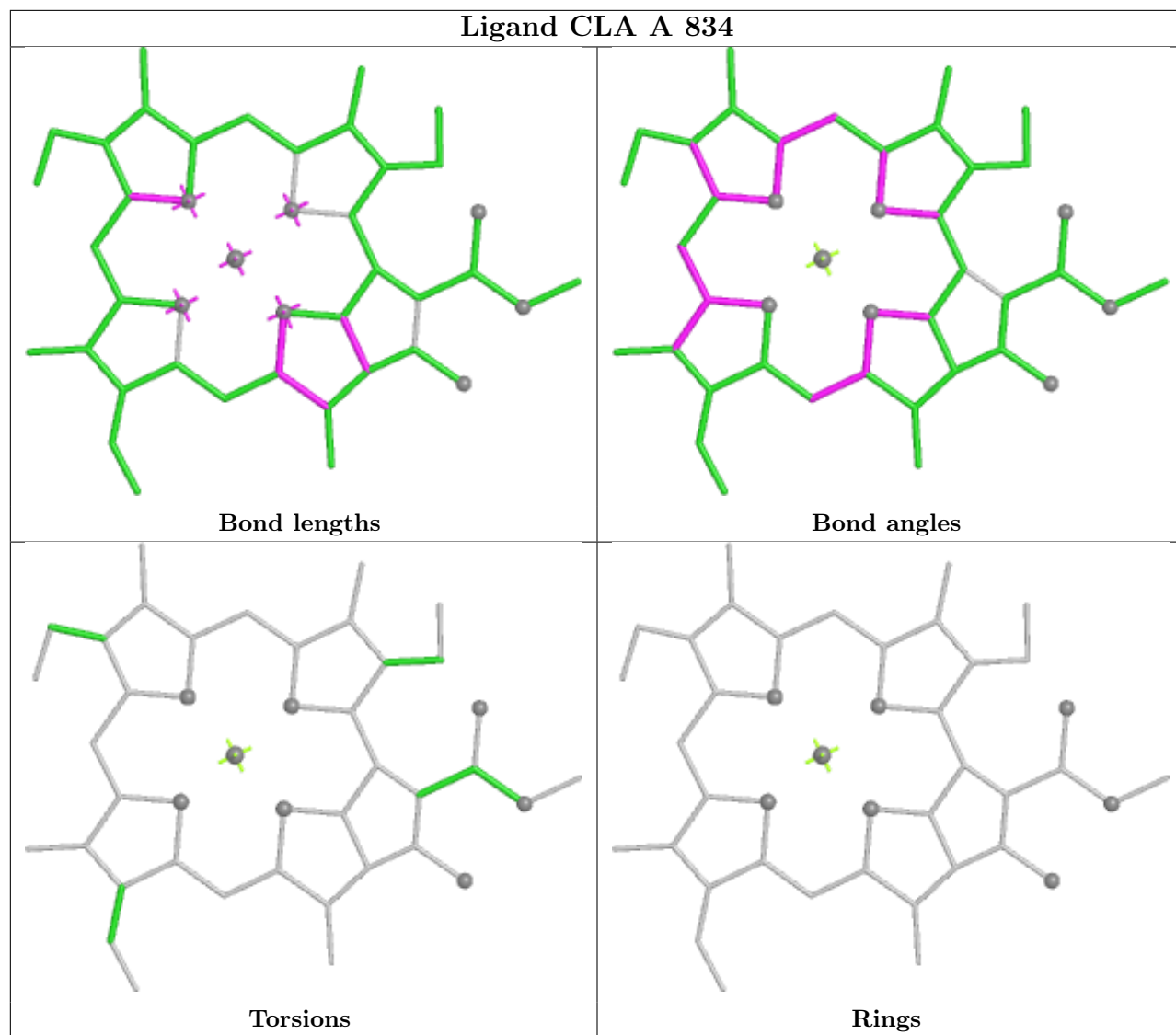


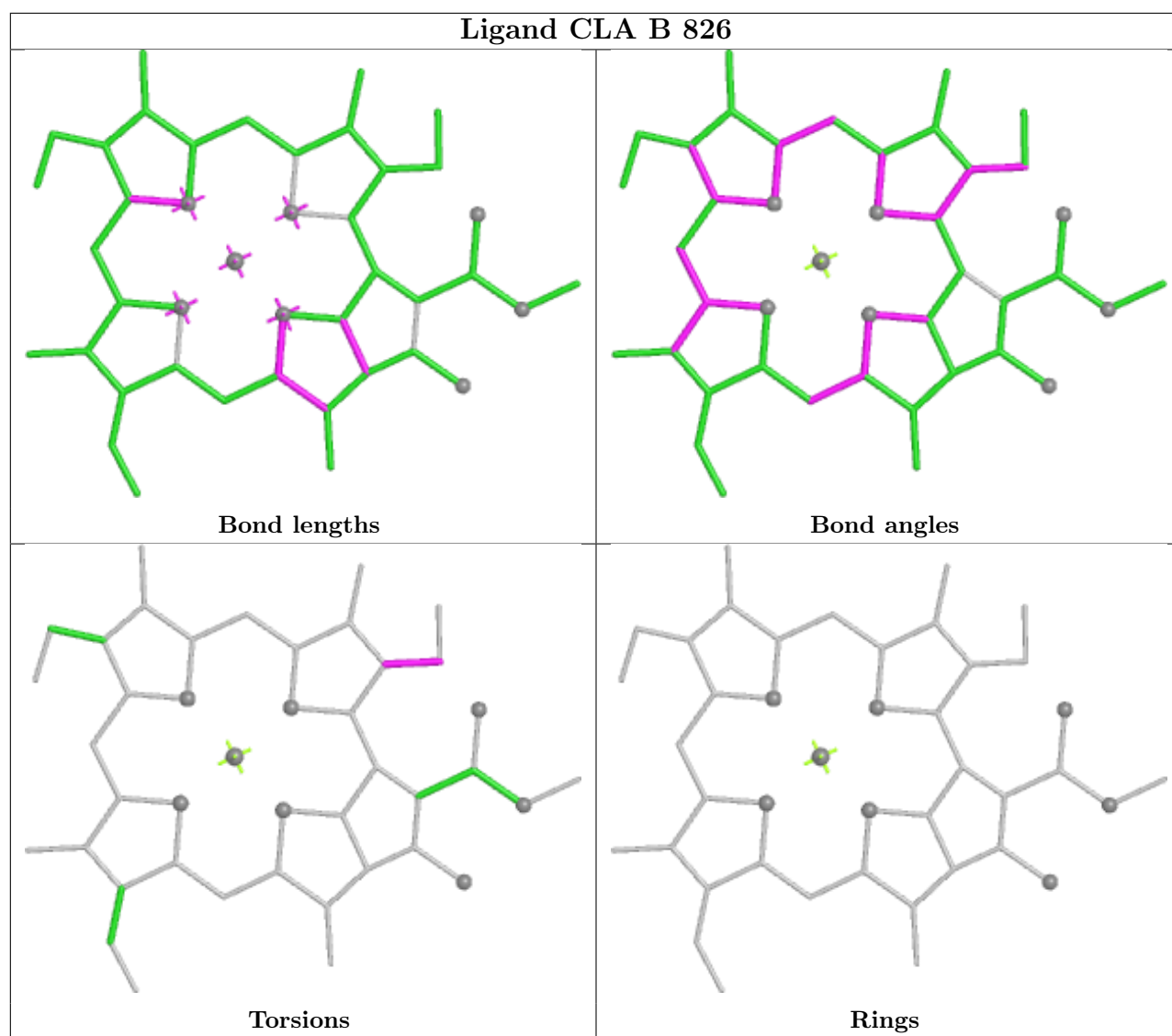
Torsions



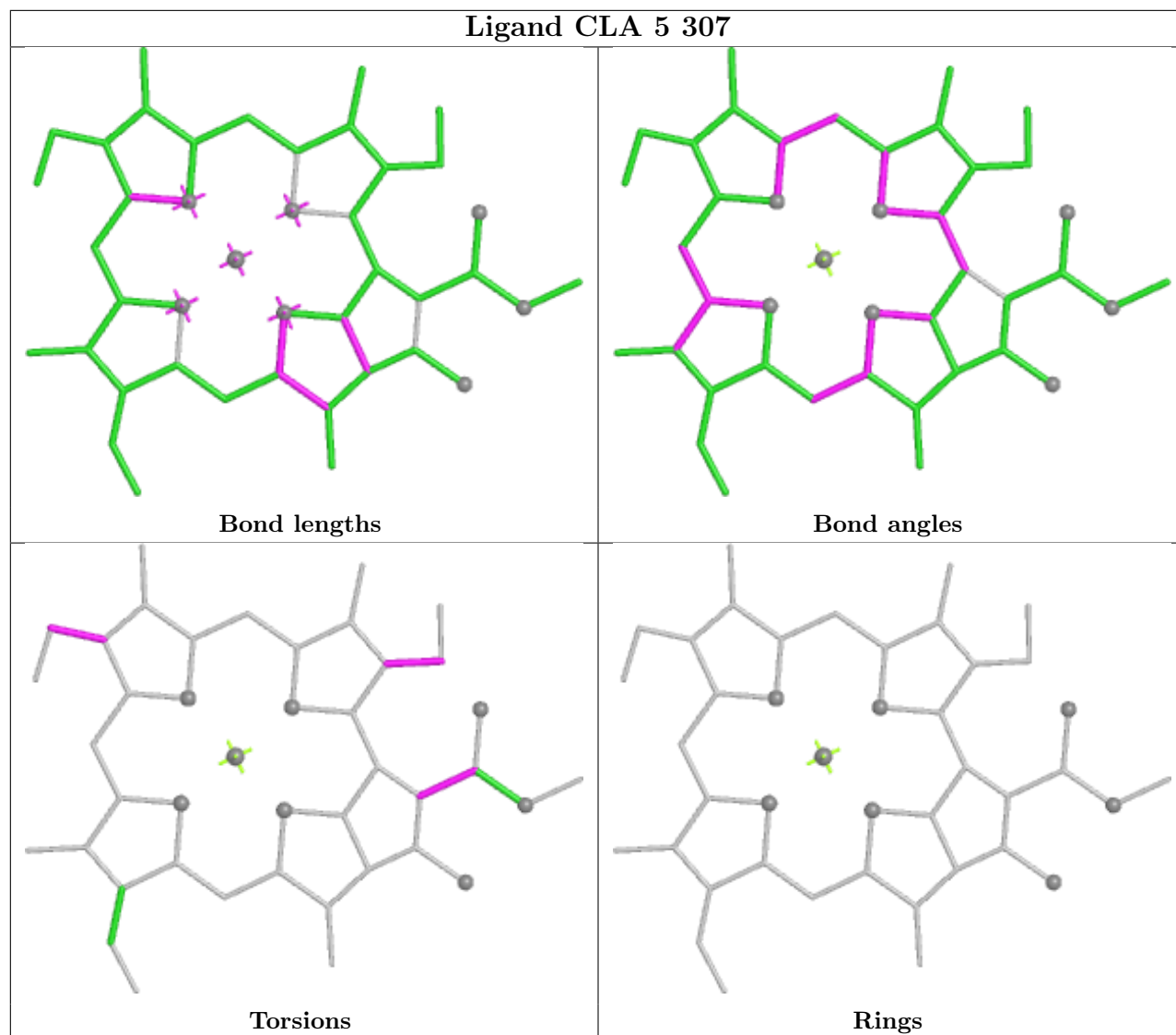
Rings



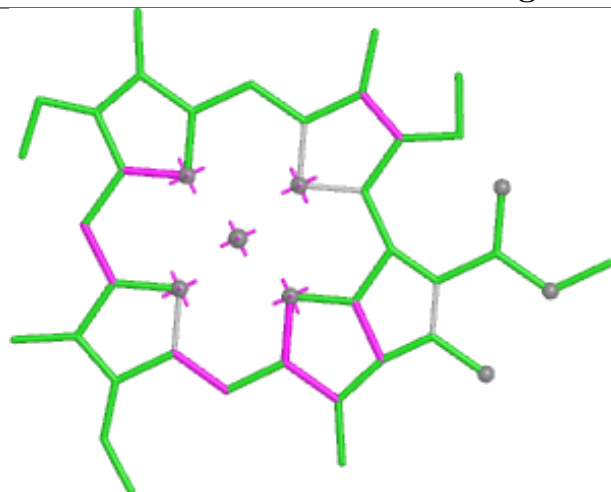




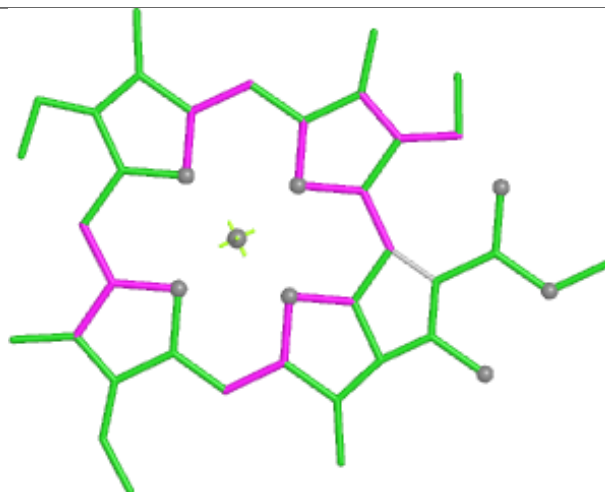
Ligand CLA 5 307



Ligand CLA 8 607



Bond lengths



Bond angles

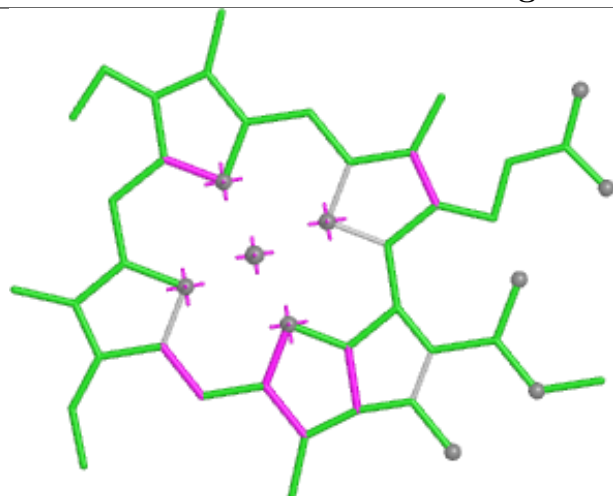


Torsions

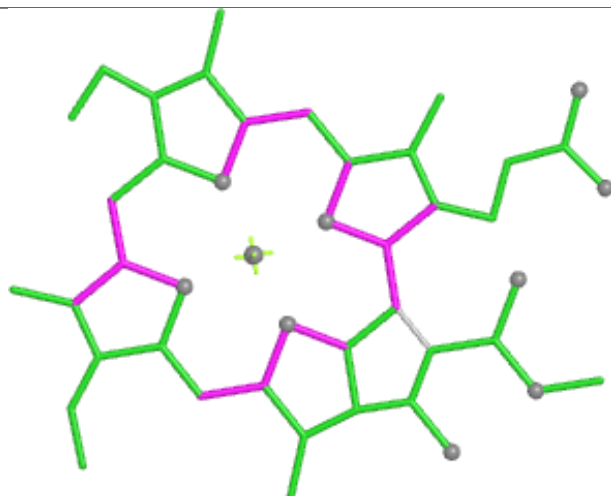


Rings

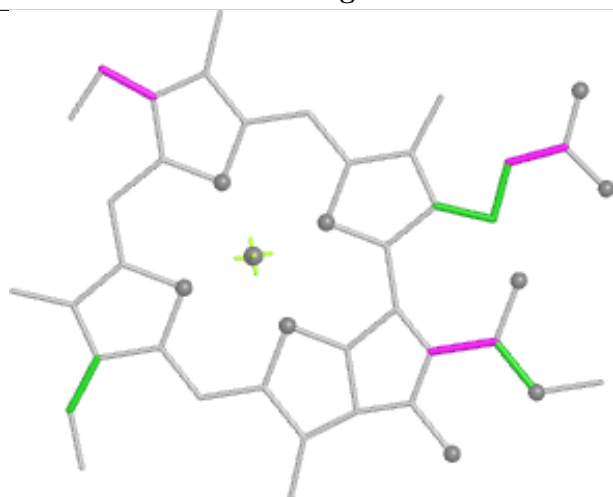
Ligand CLA 6 610



Bond lengths



Bond angles

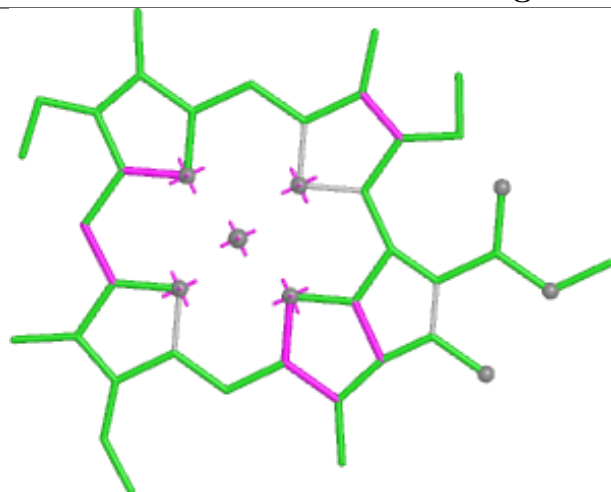


Torsions

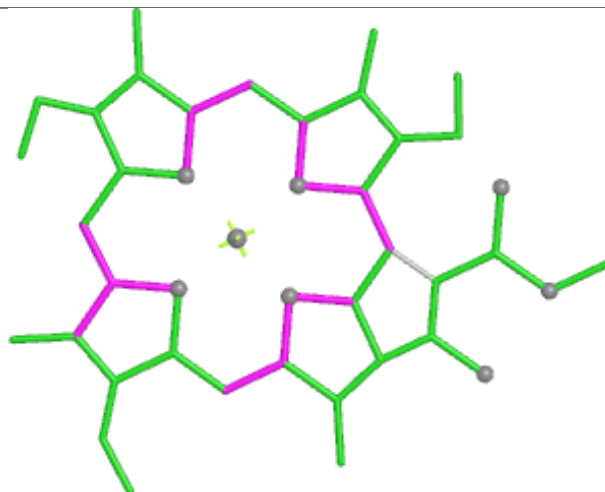


Rings

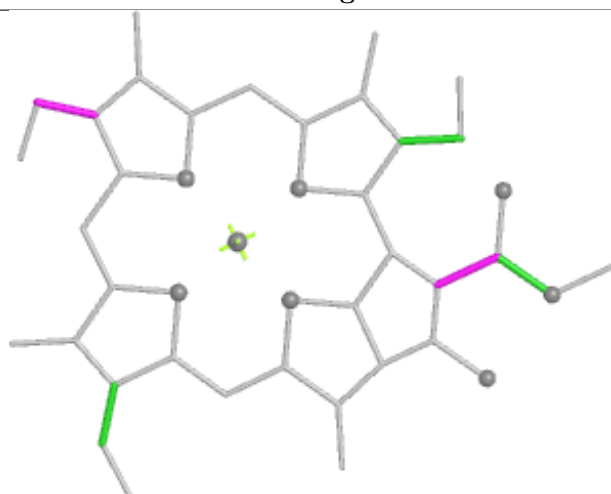
Ligand CLA A 803



Bond lengths



Bond angles

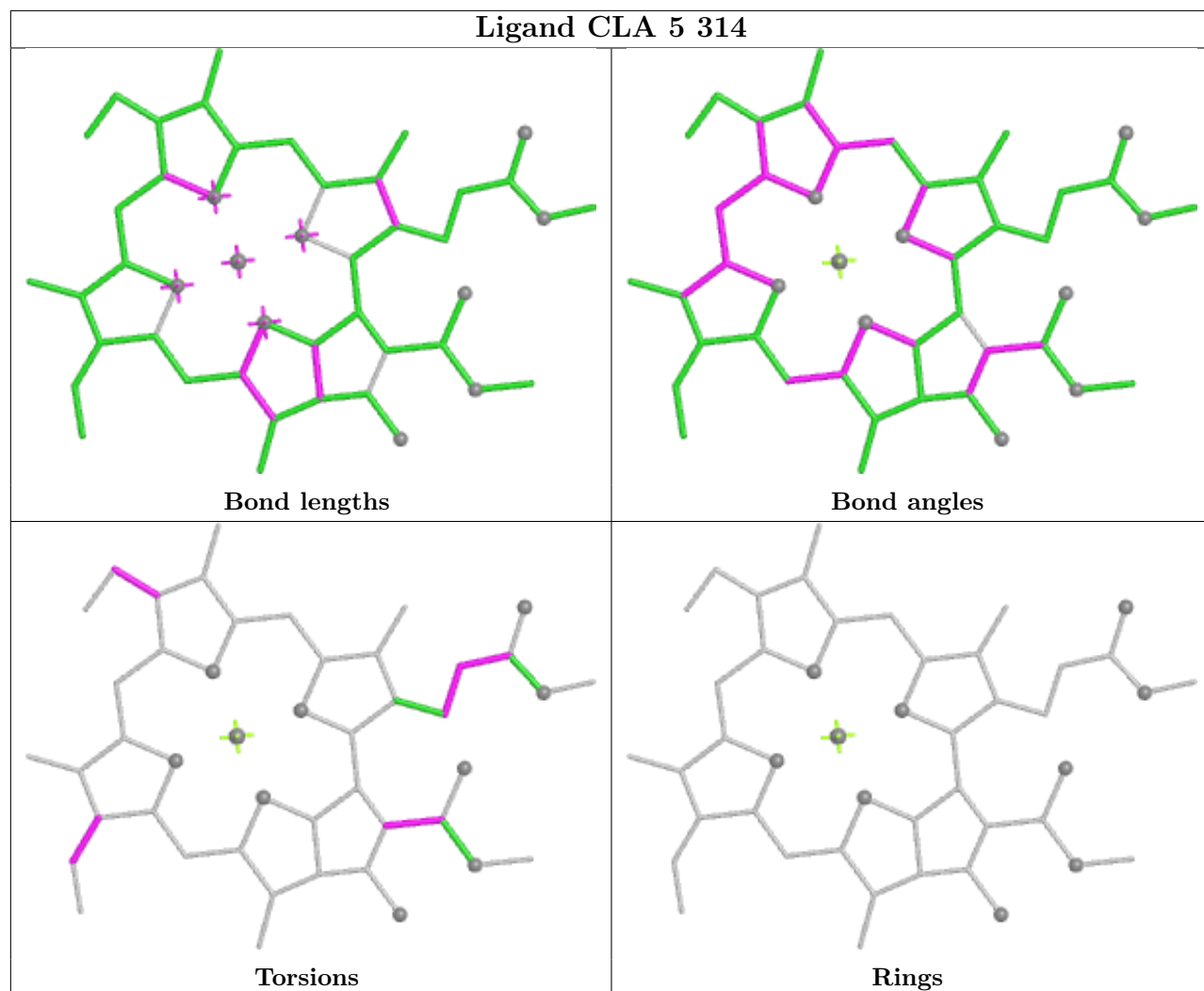


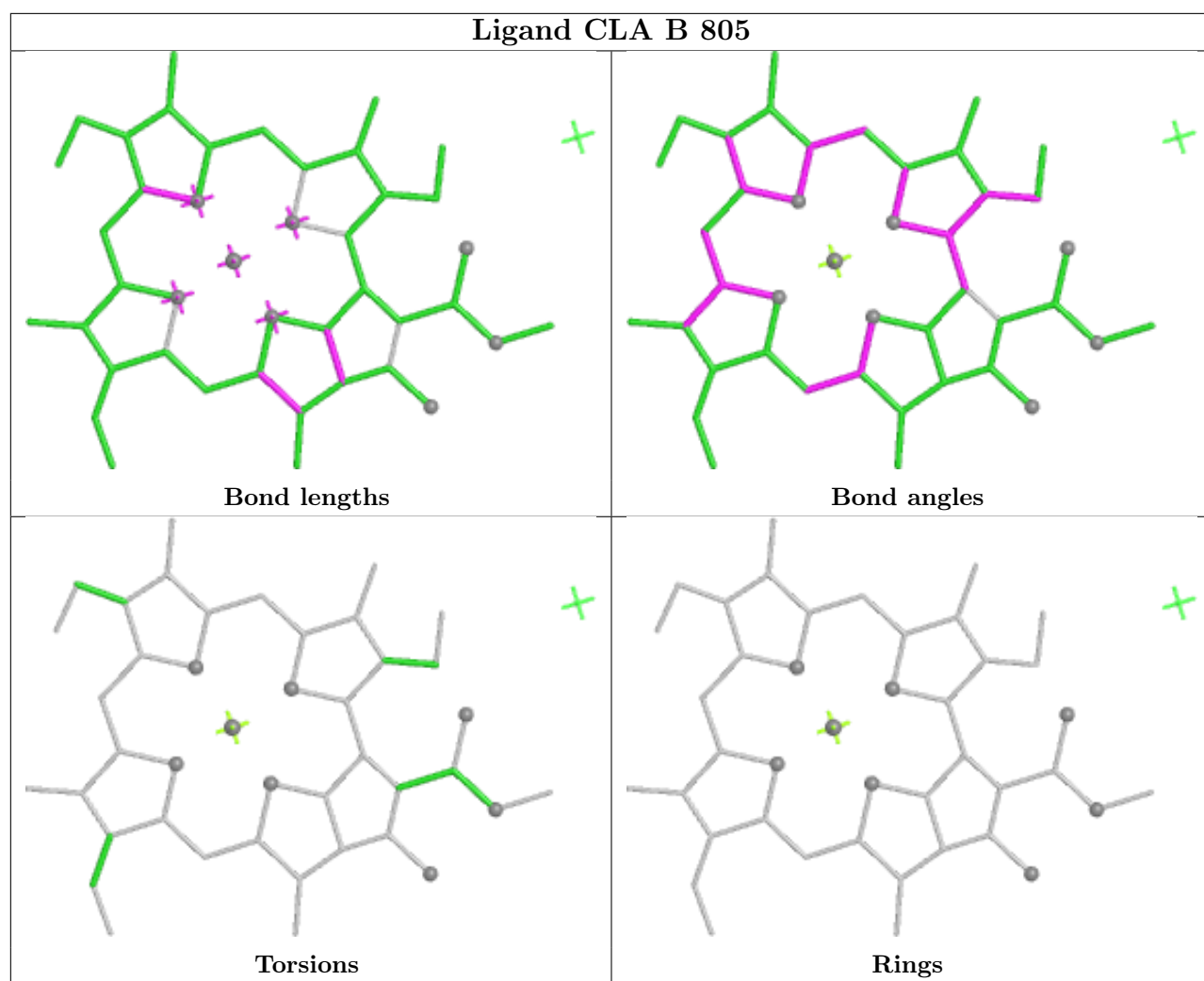
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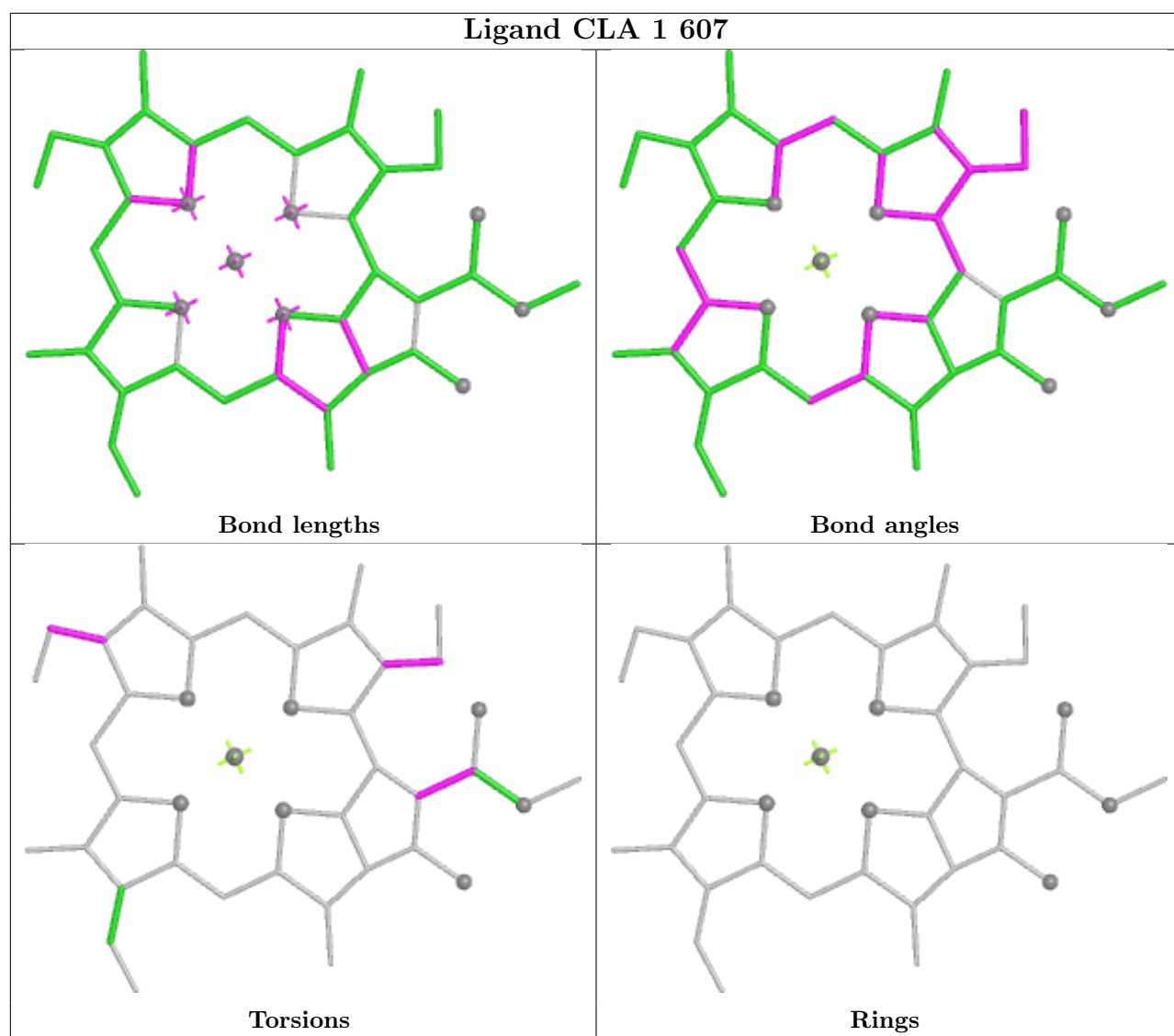


Rings

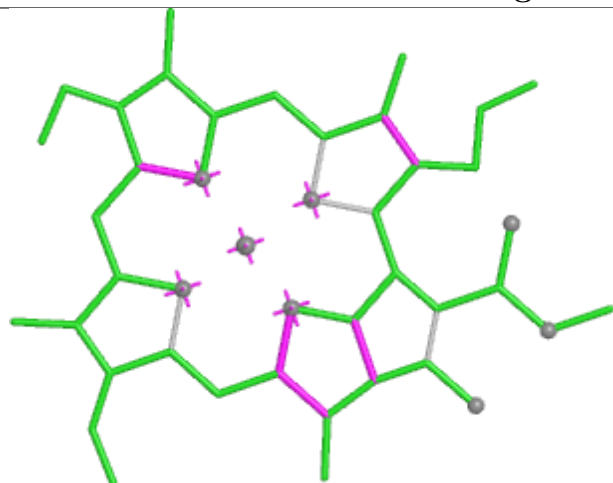
Ligand CLA 5 314



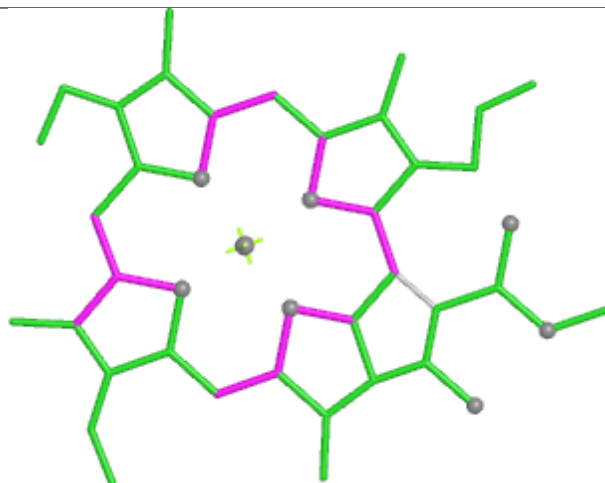




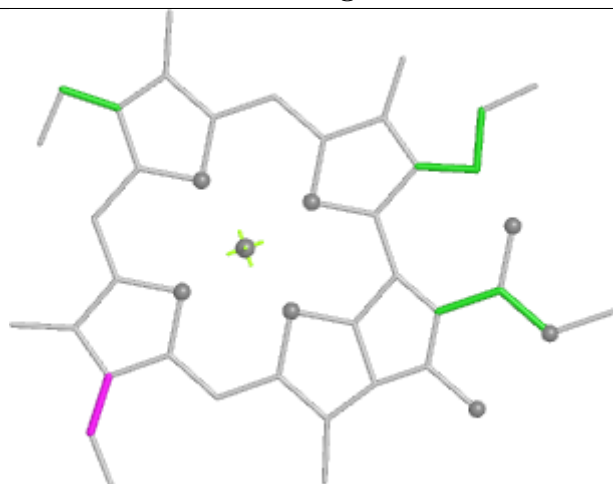
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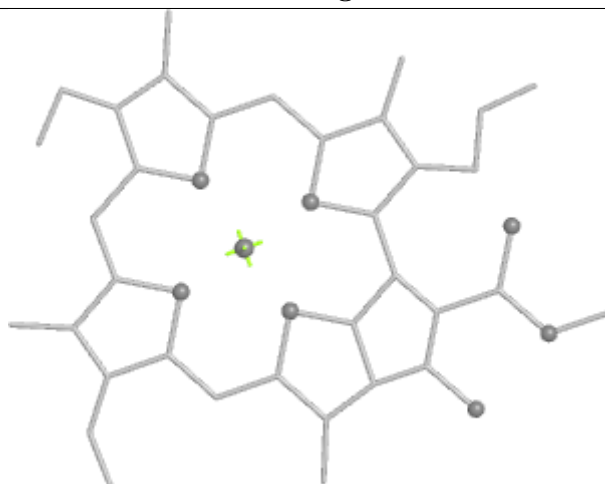
Bond lengths



Bond angles

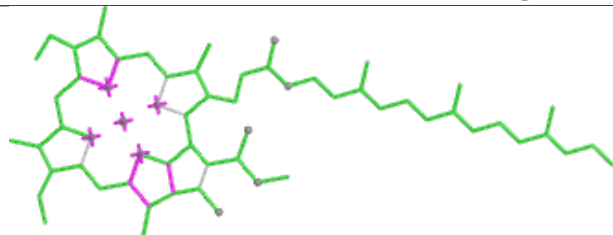


Torsions

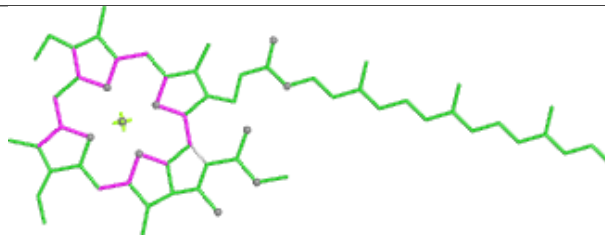


Rings

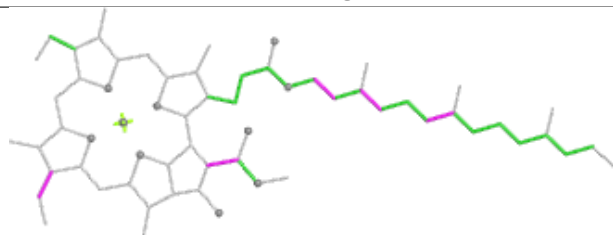
Ligand CLA F 302



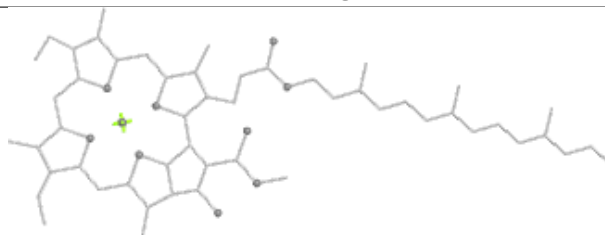
Bond lengths



Bond angles

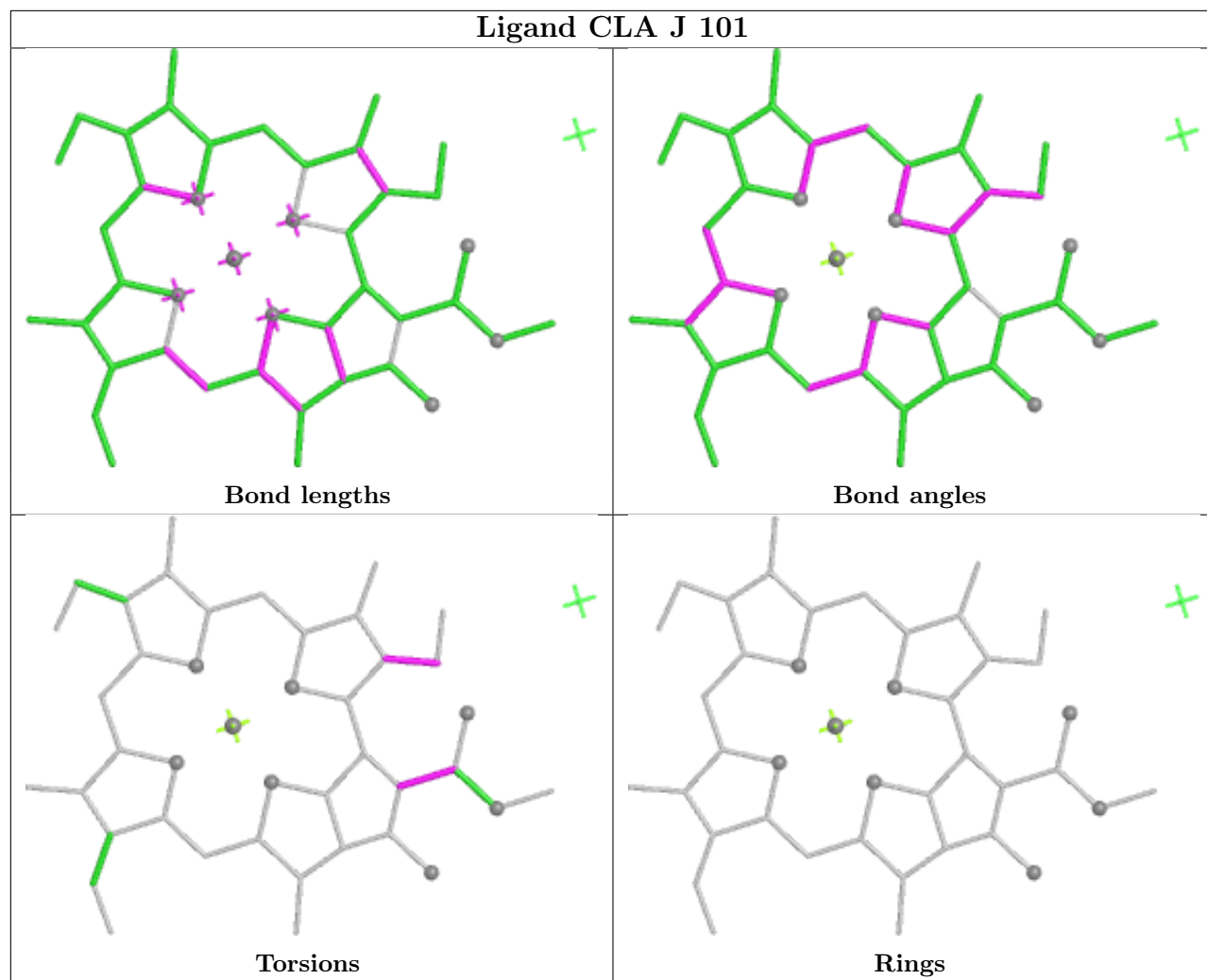


Torsions

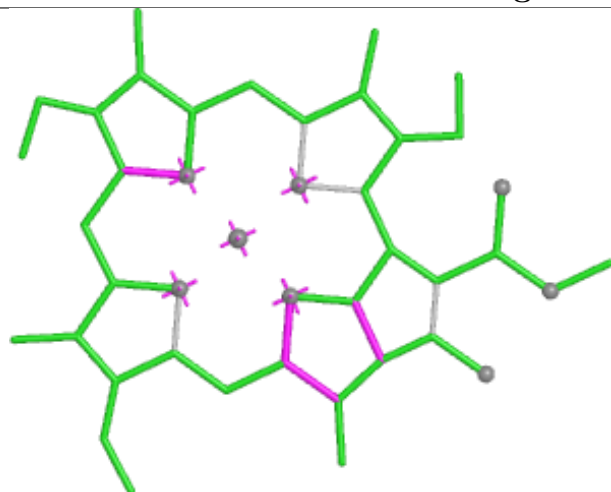


Rings

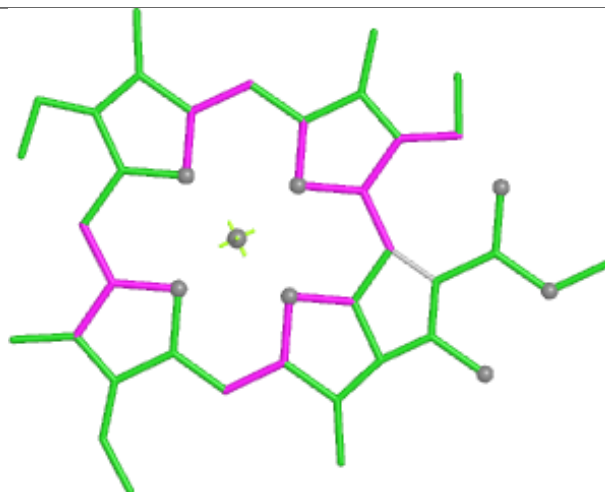
Ligand CLA J 101



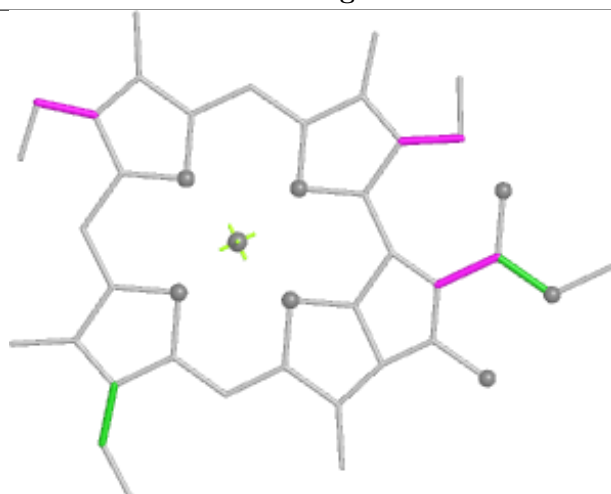
Ligand CLA A 816



Bond lengths



Bond angles

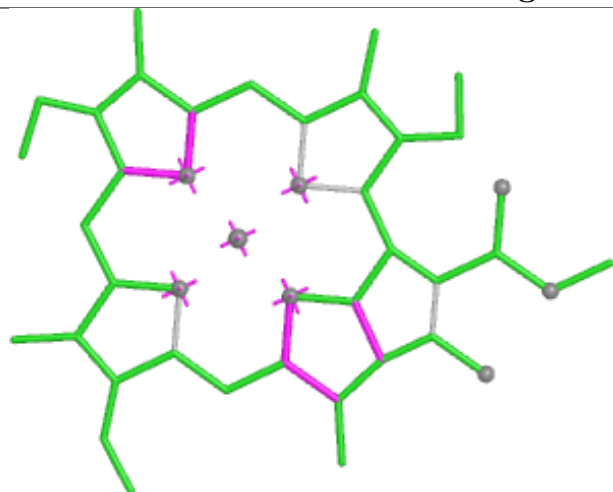


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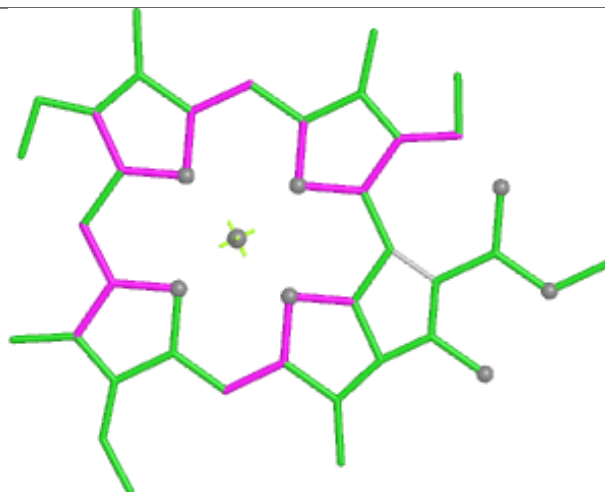


Rings

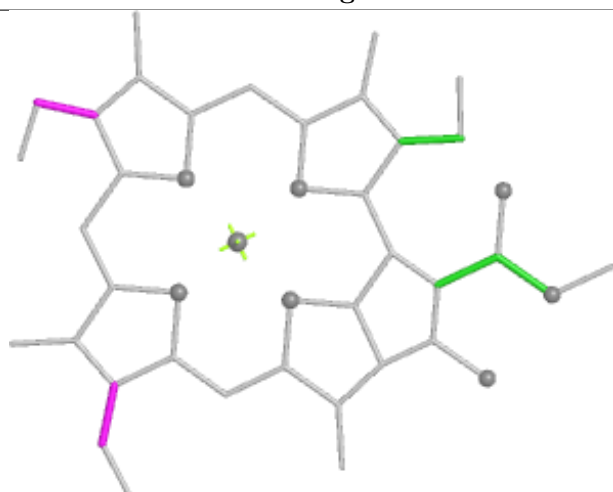
Ligand CLA 3 312



Bond lengths



Bond angles

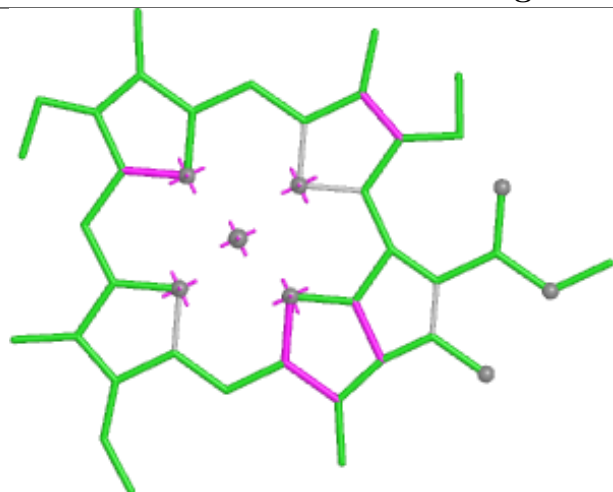


Torsions

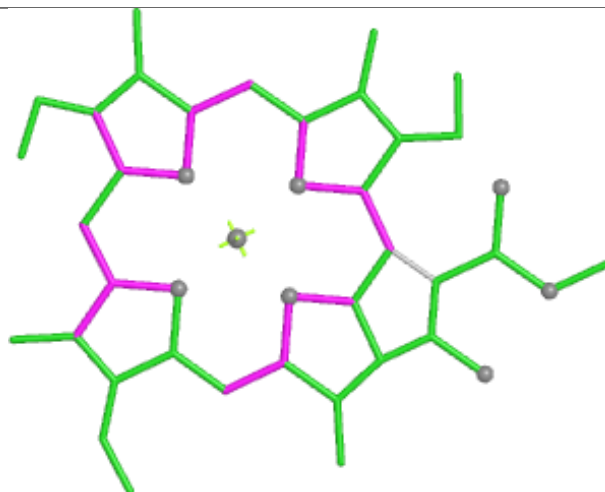


Rings

Ligand CLA B 839



Bond lengths



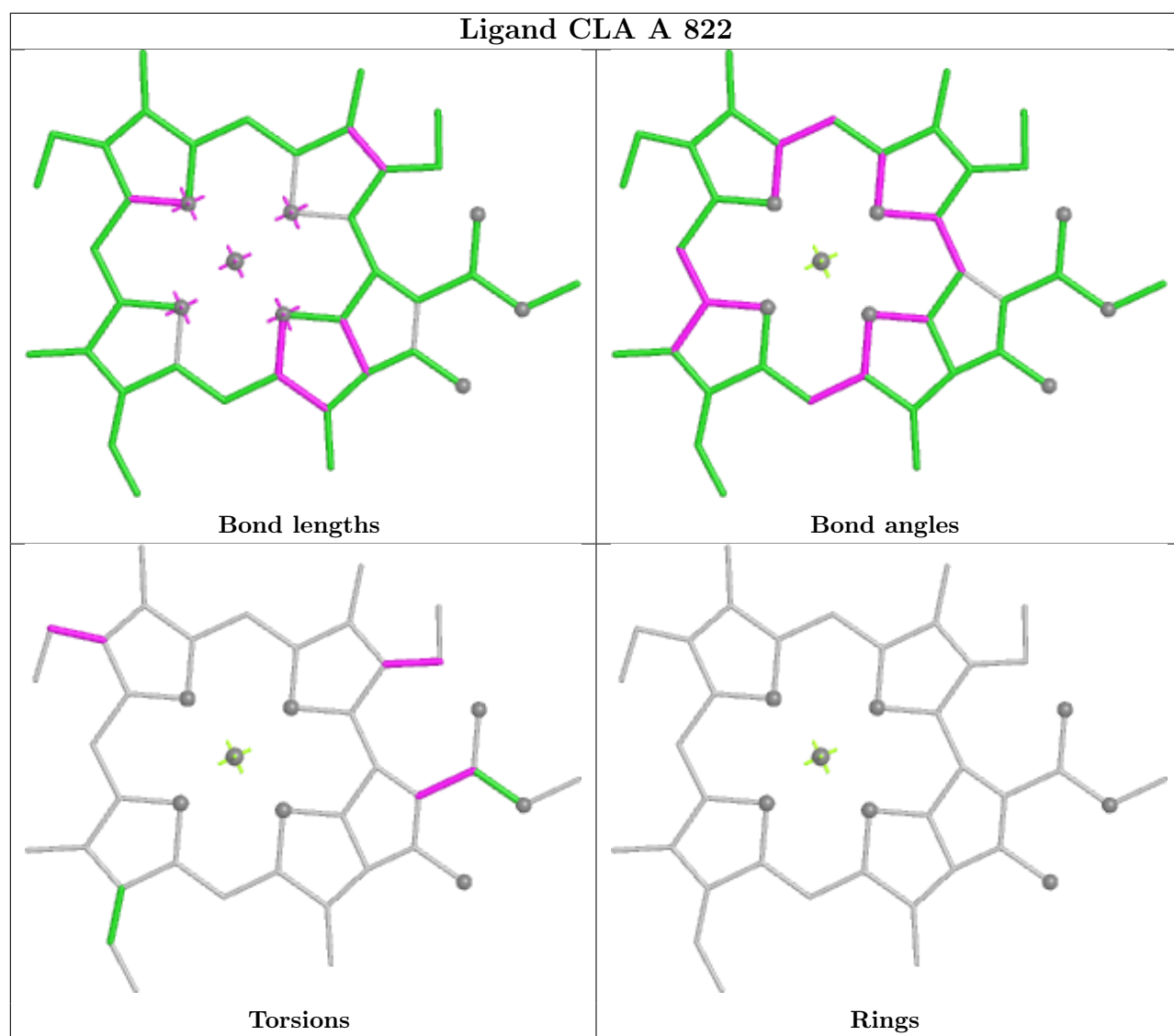
Bond angles



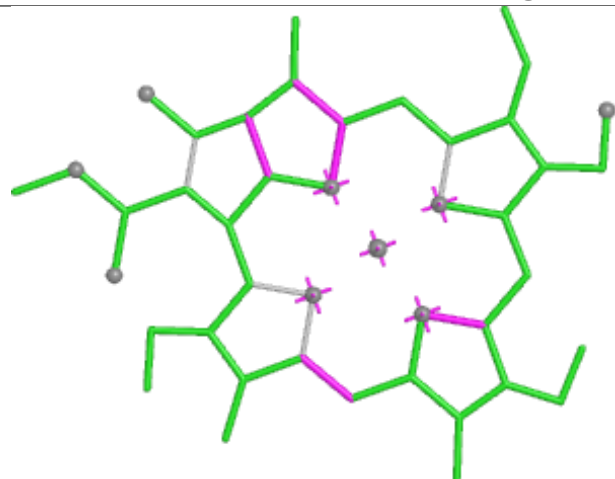
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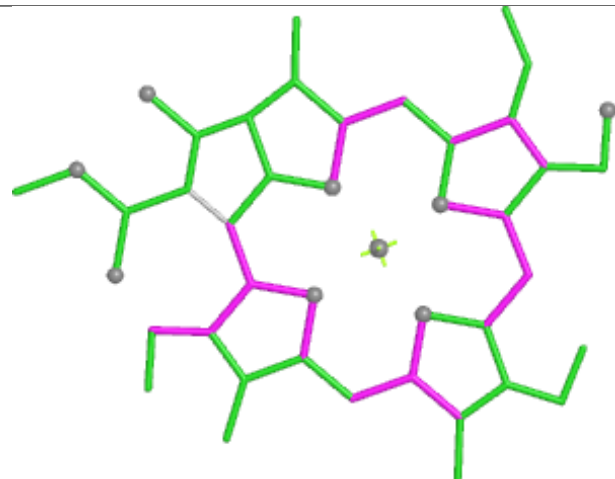
Rings



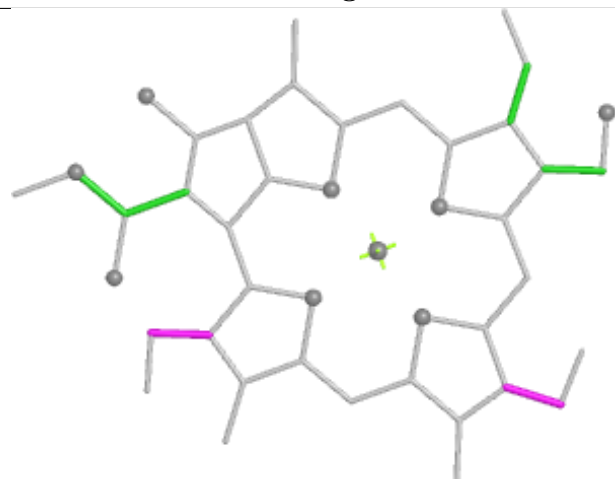
Ligand CHL 6 605



Bond lengths



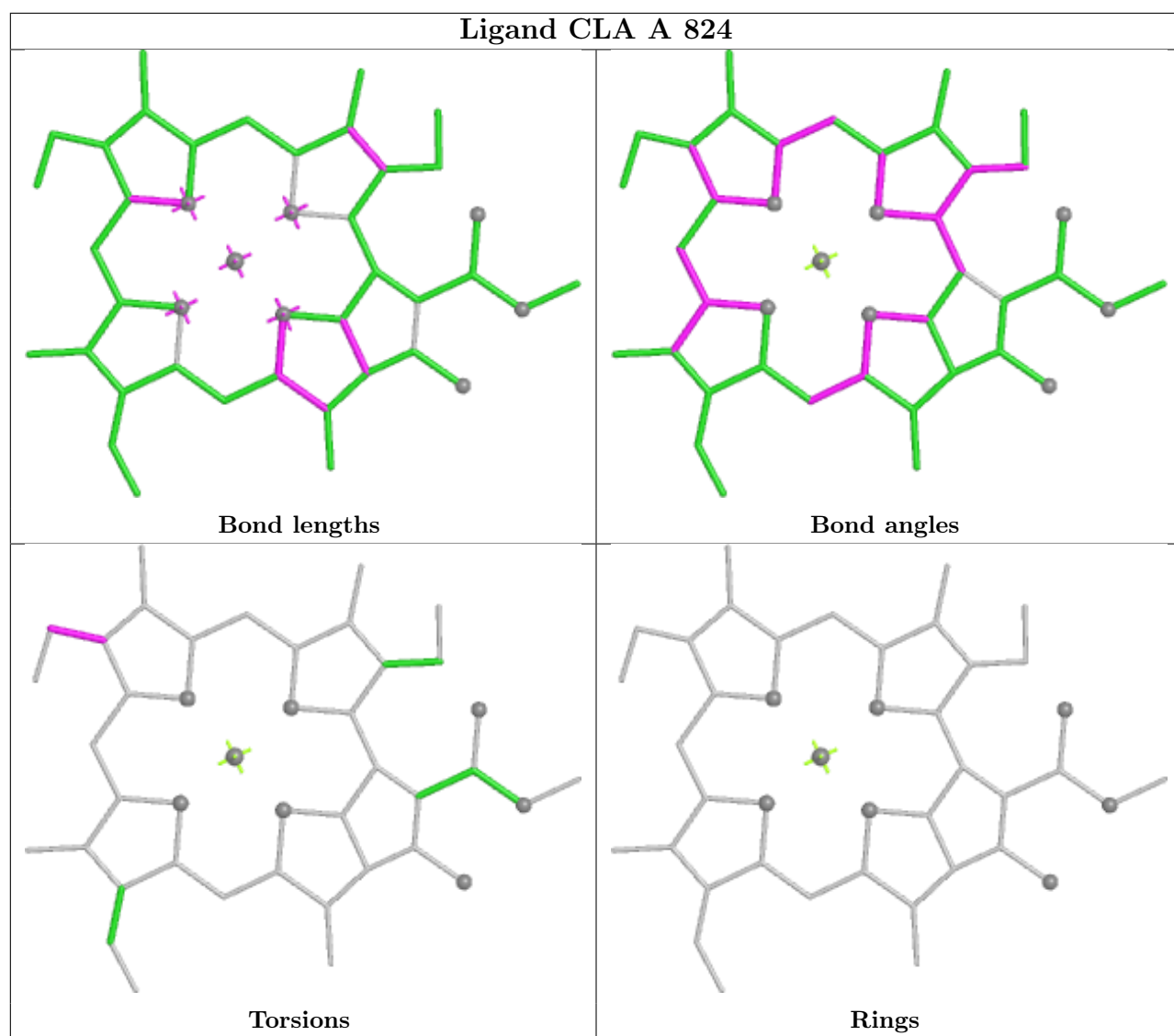
Bond angles

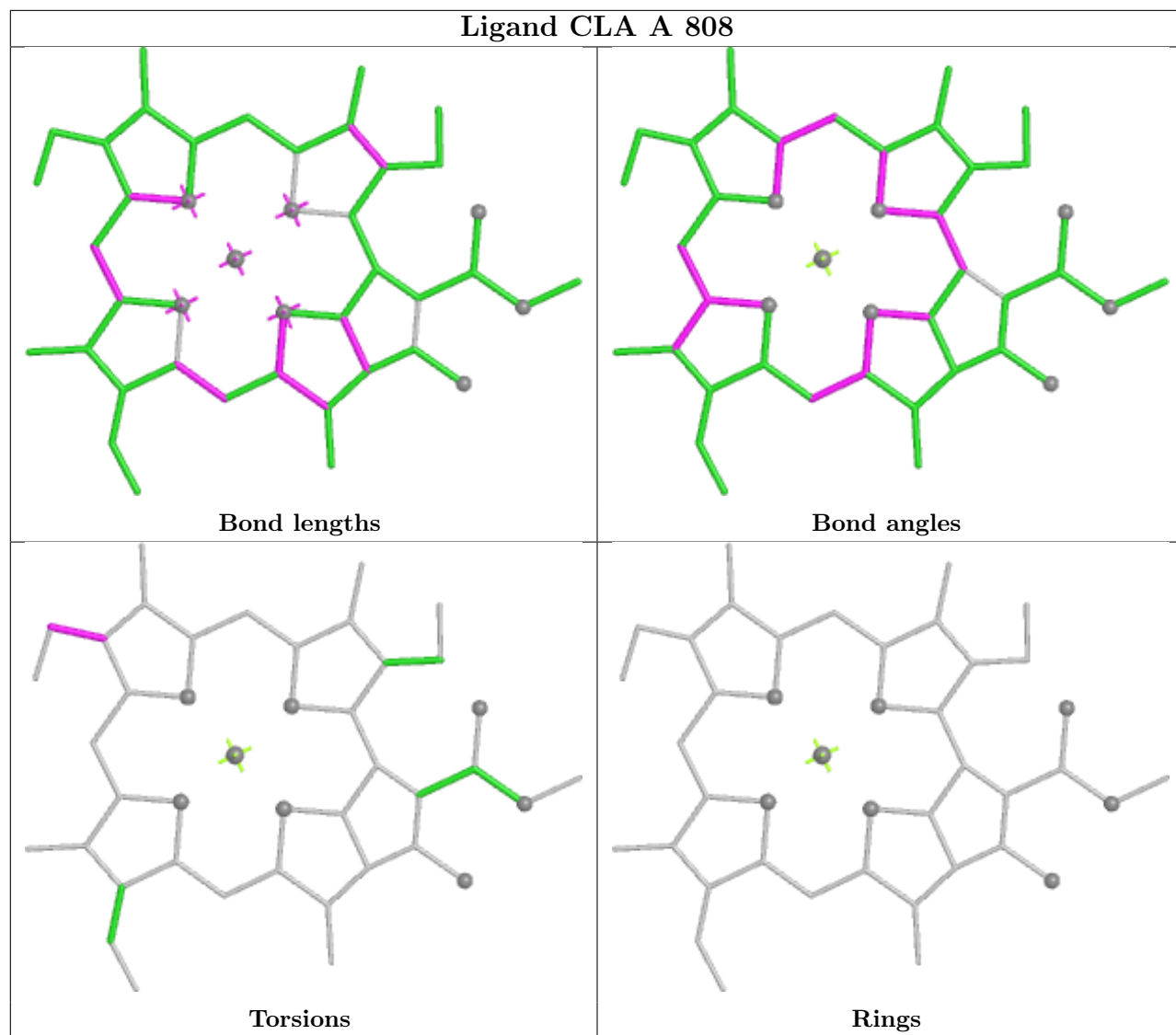


Torsions

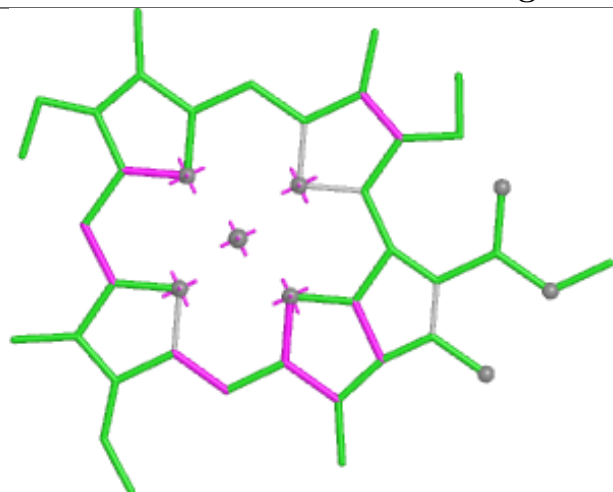


Rings

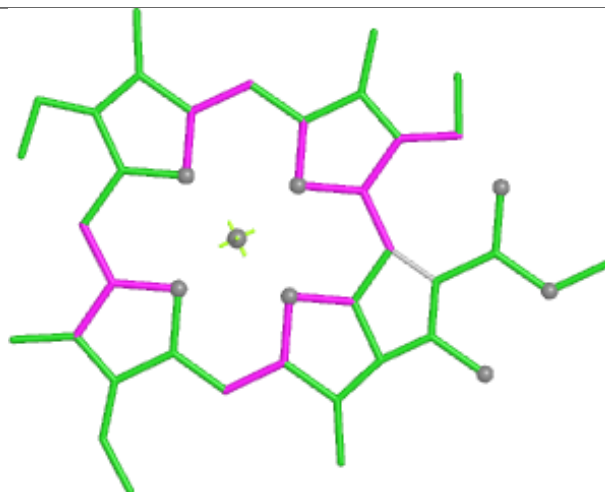




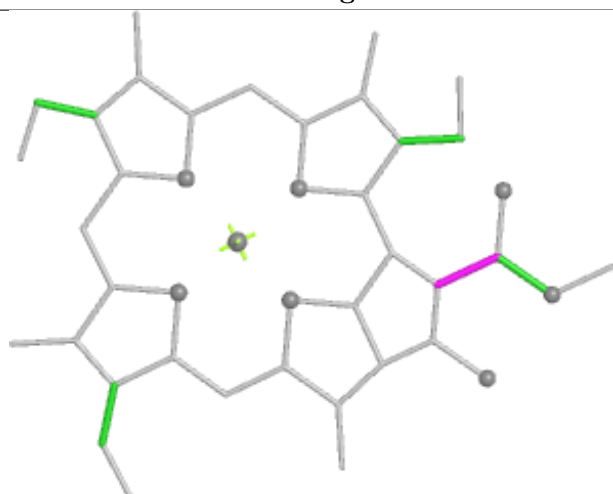
Ligand CLA 7 605



Bond lengths



Bond angles

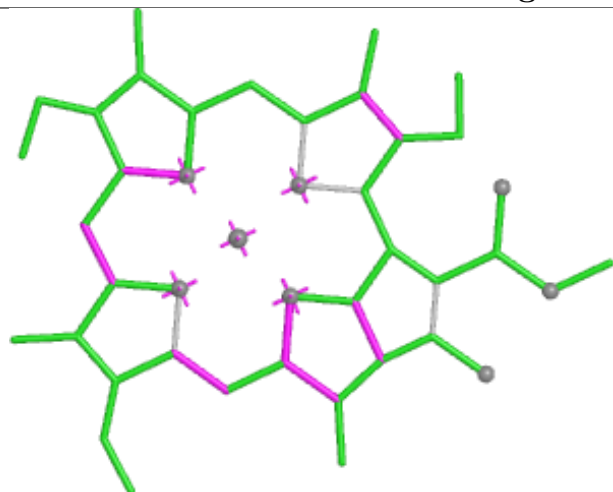


Torsions

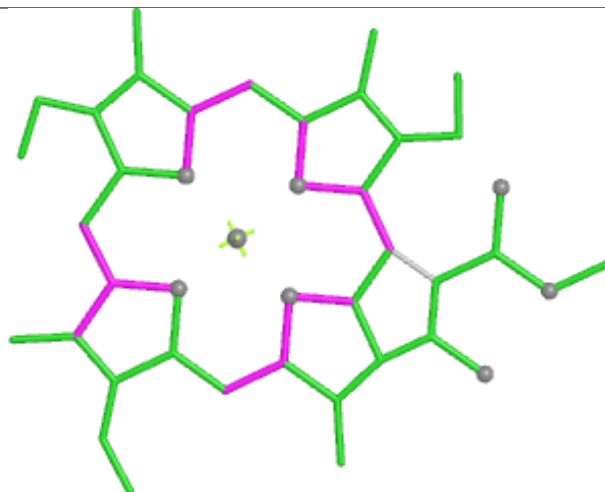


Rings

Ligand CLA 8 601



Bond lengths



Bond angles

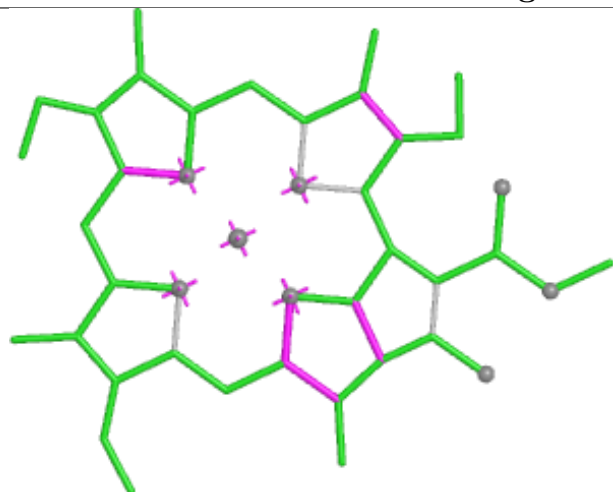


Torsions

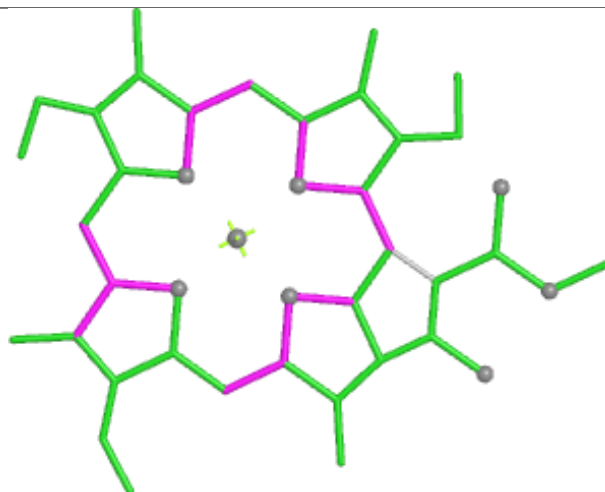


Rings

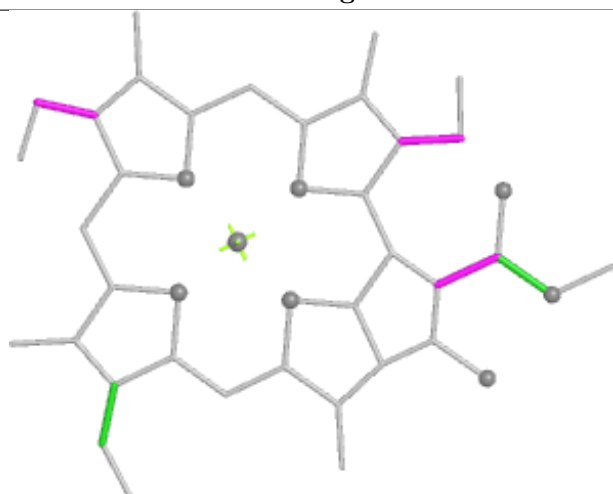
Ligand CLA 8 613



Bond lengths



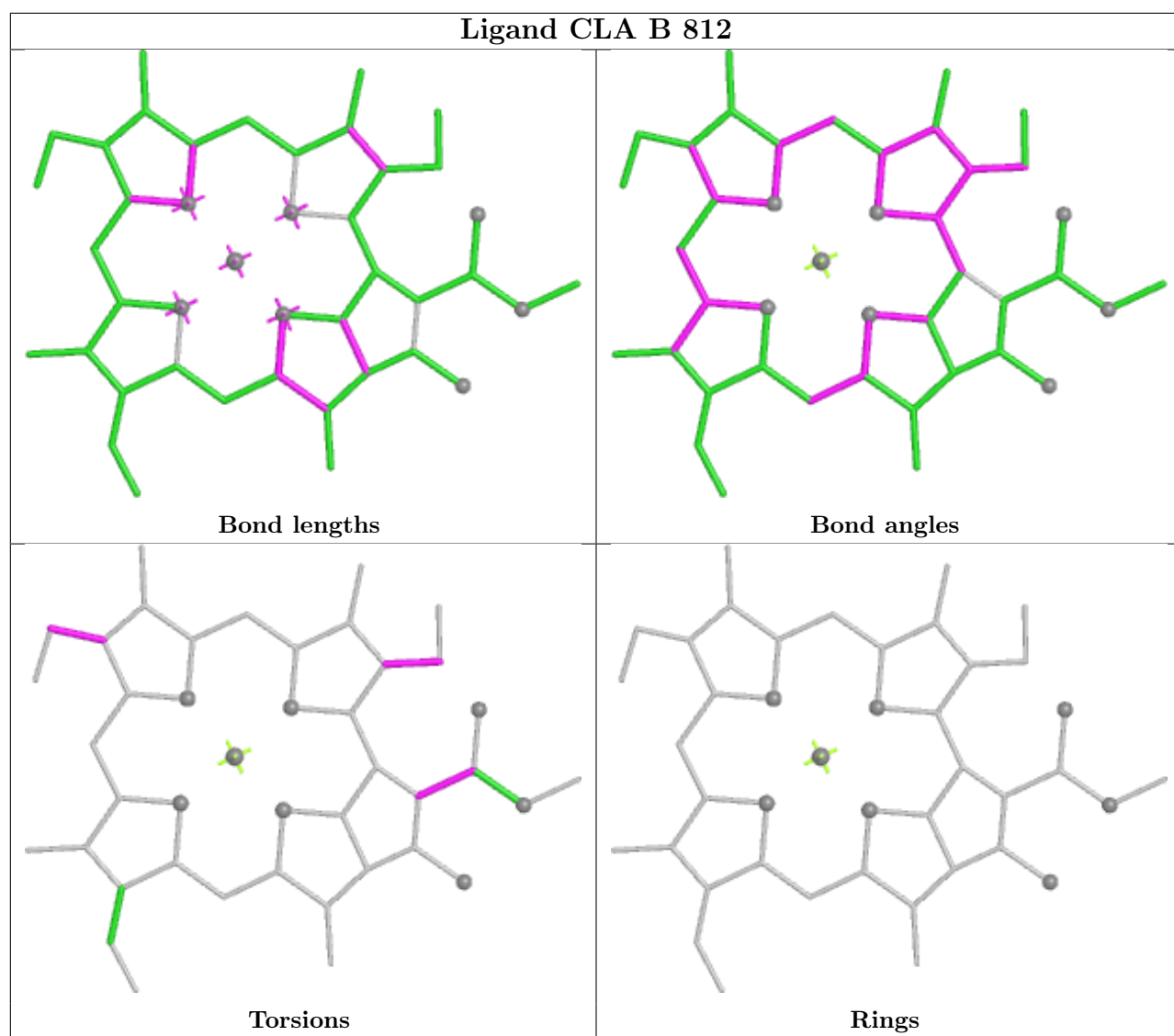
Bond angles

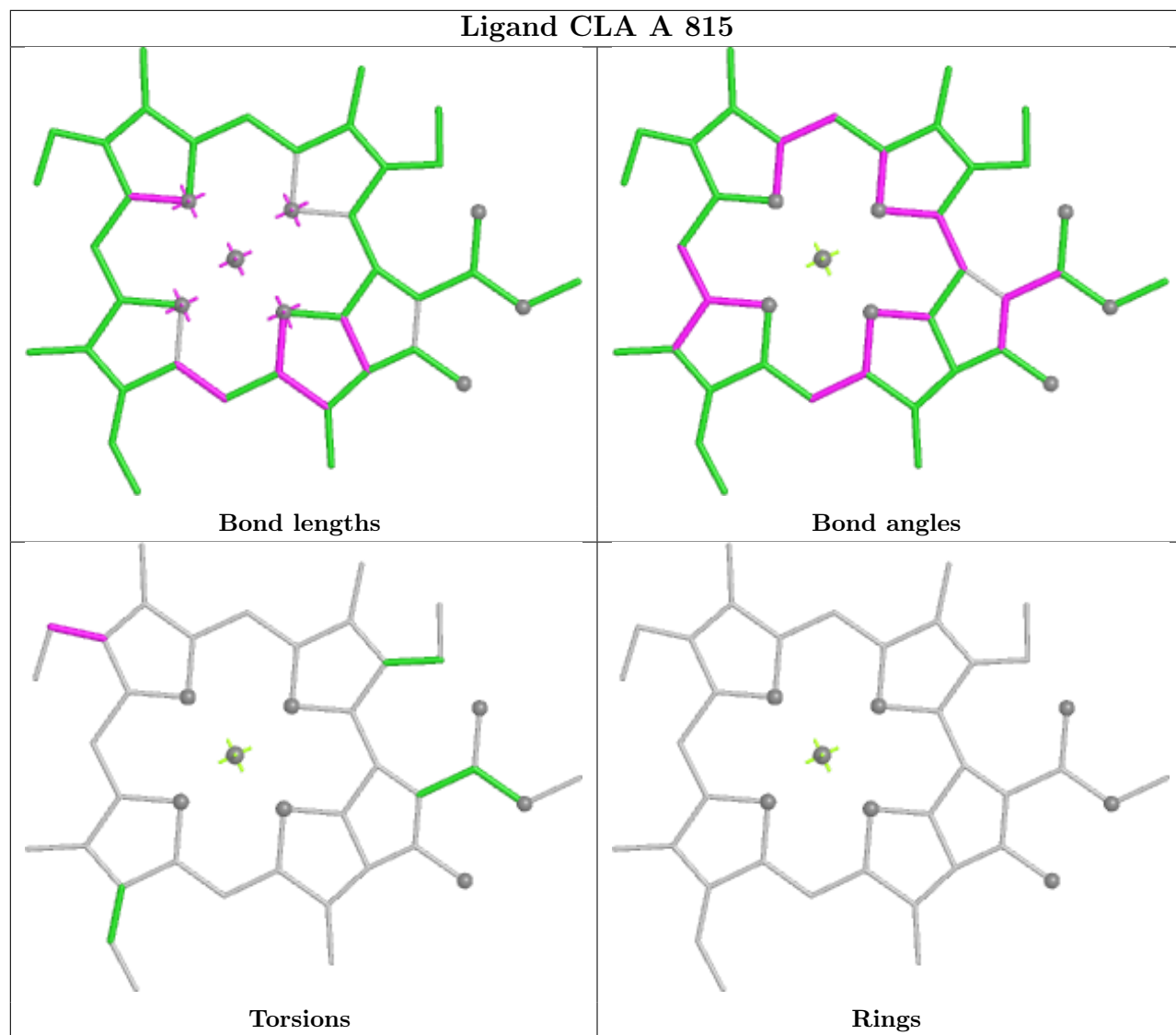


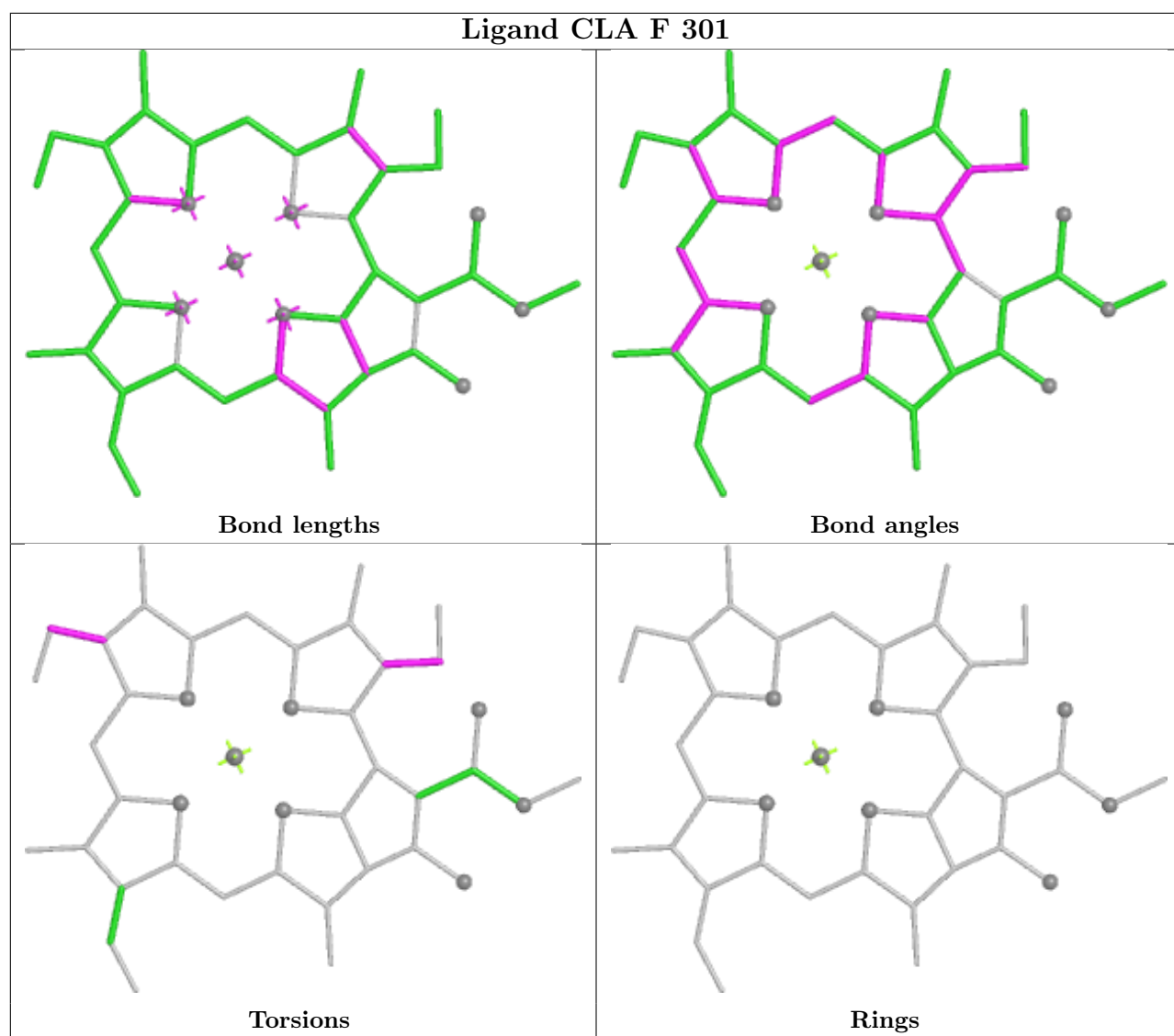
Torsions



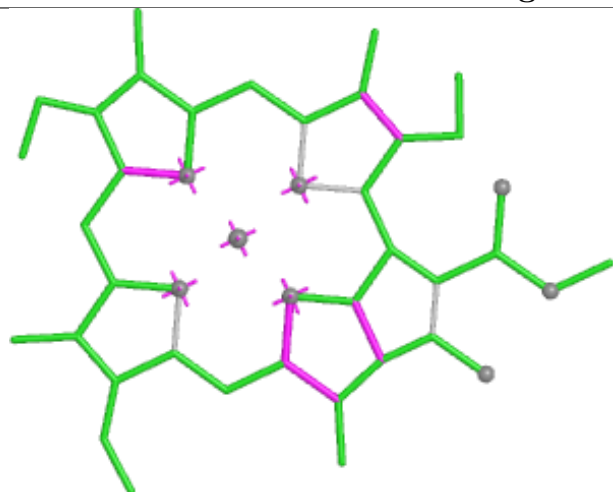
Rings



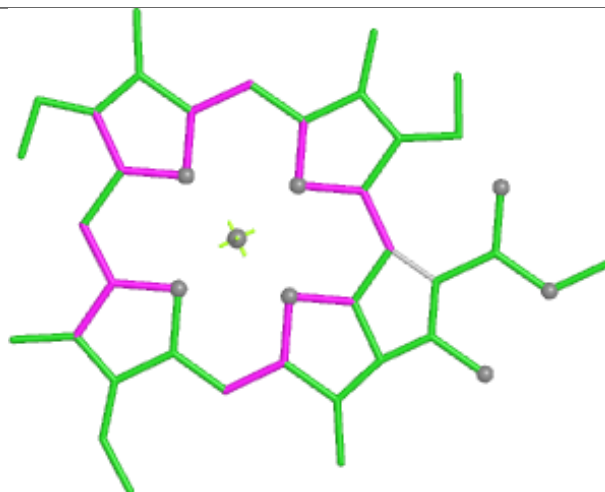




Ligand CLA 7 607



Bond lengths



Bond angles

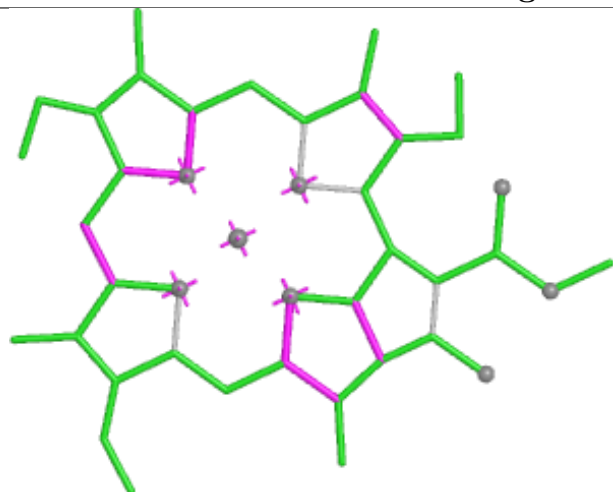


Torsions

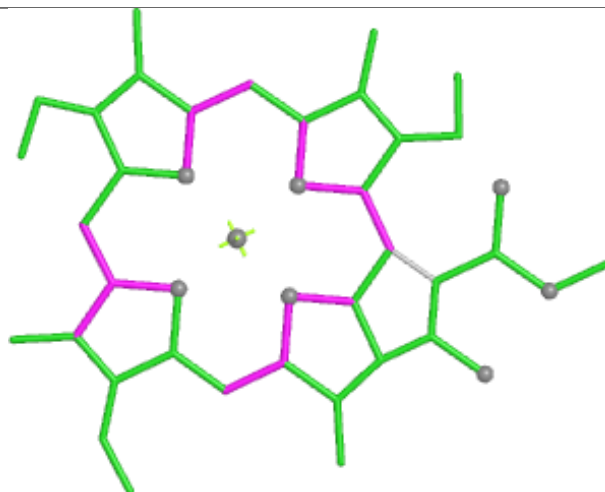


Rings

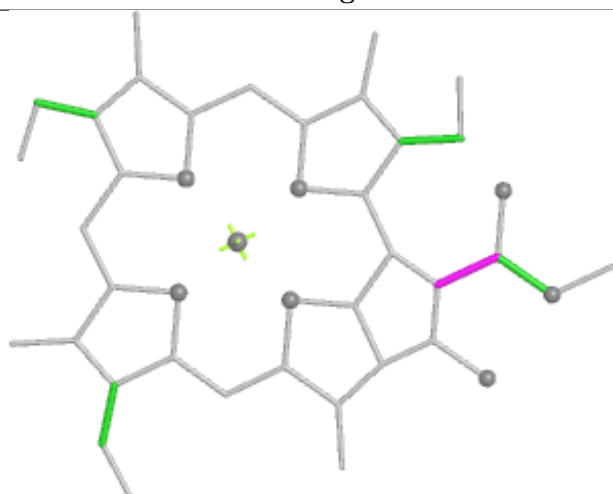
Ligand CLA 4 601



Bond lengths



Bond angles

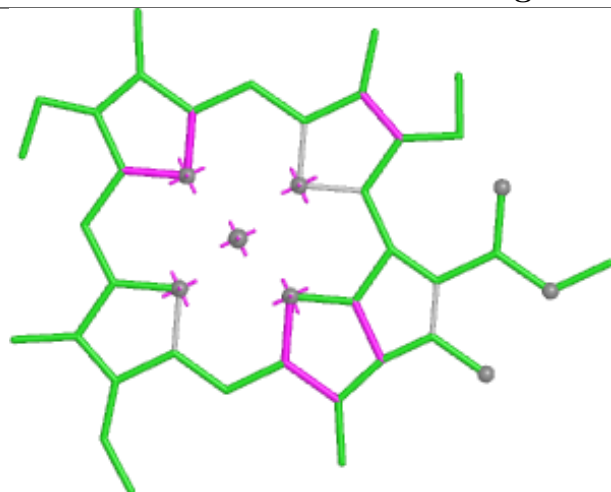


Torsions

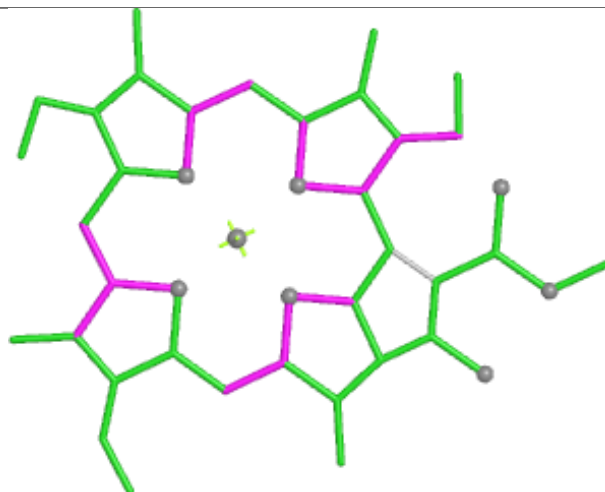


Rings

Ligand CLA B 816



Bond lengths



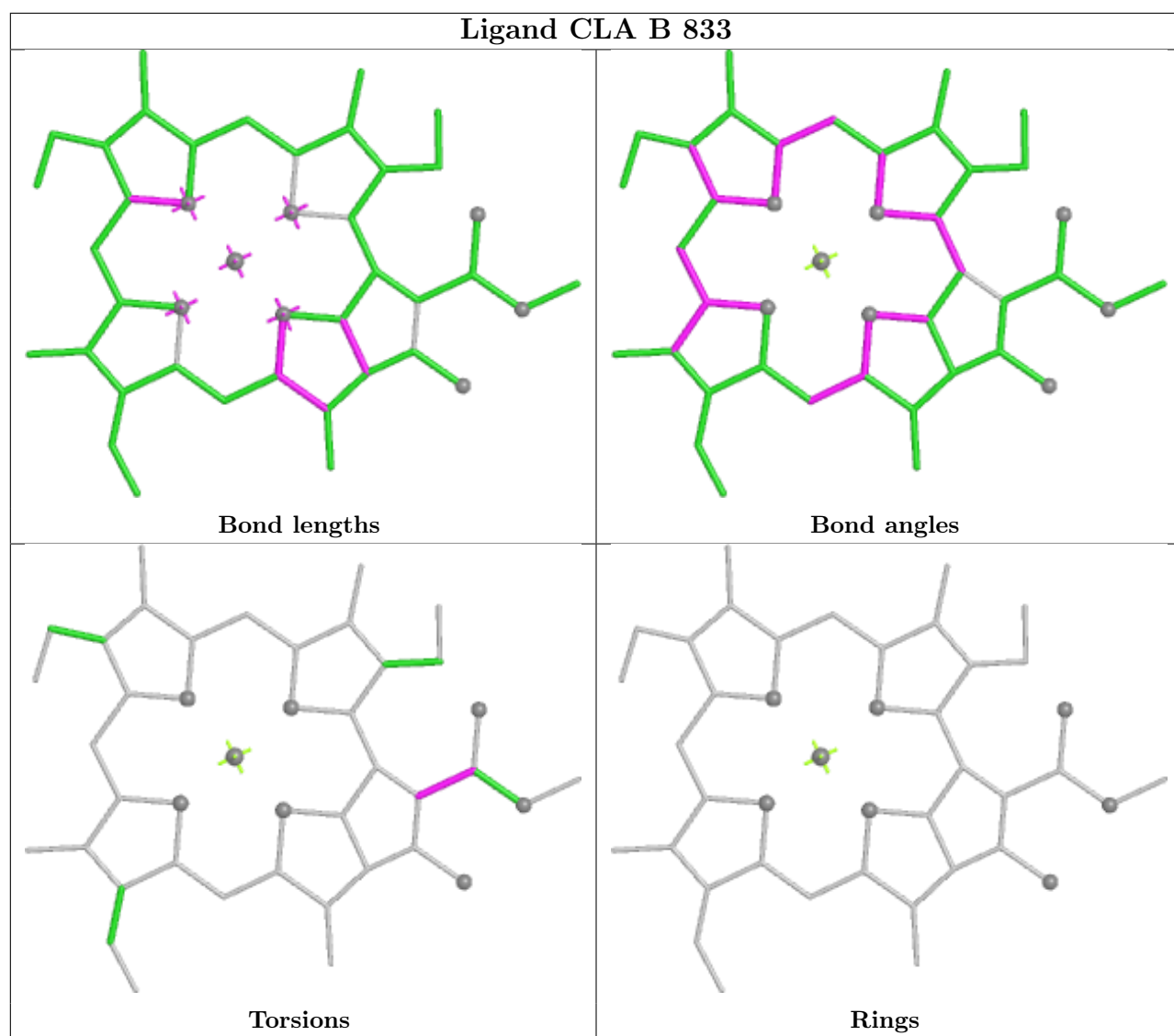
Bond angles



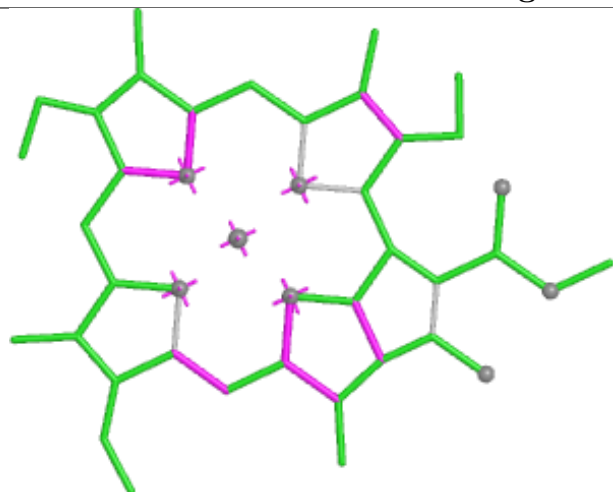
Torsions



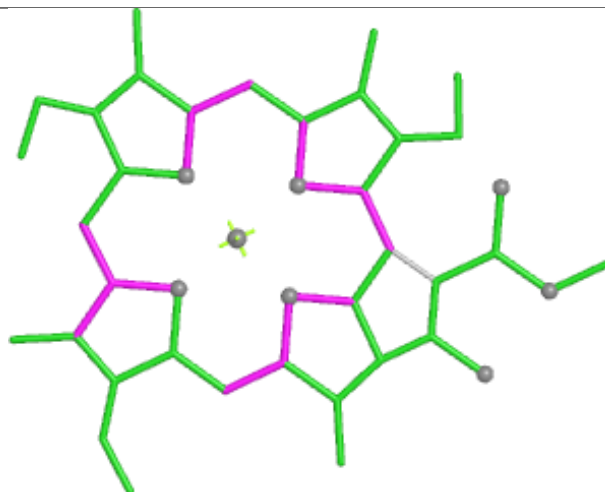
Rings



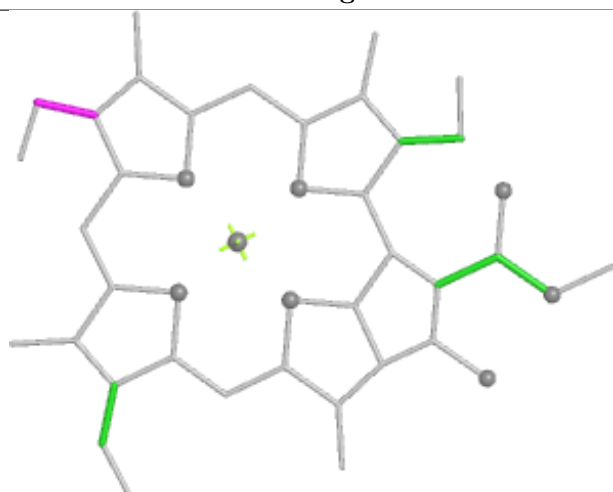
Ligand CLA 5 310



Bond lengths



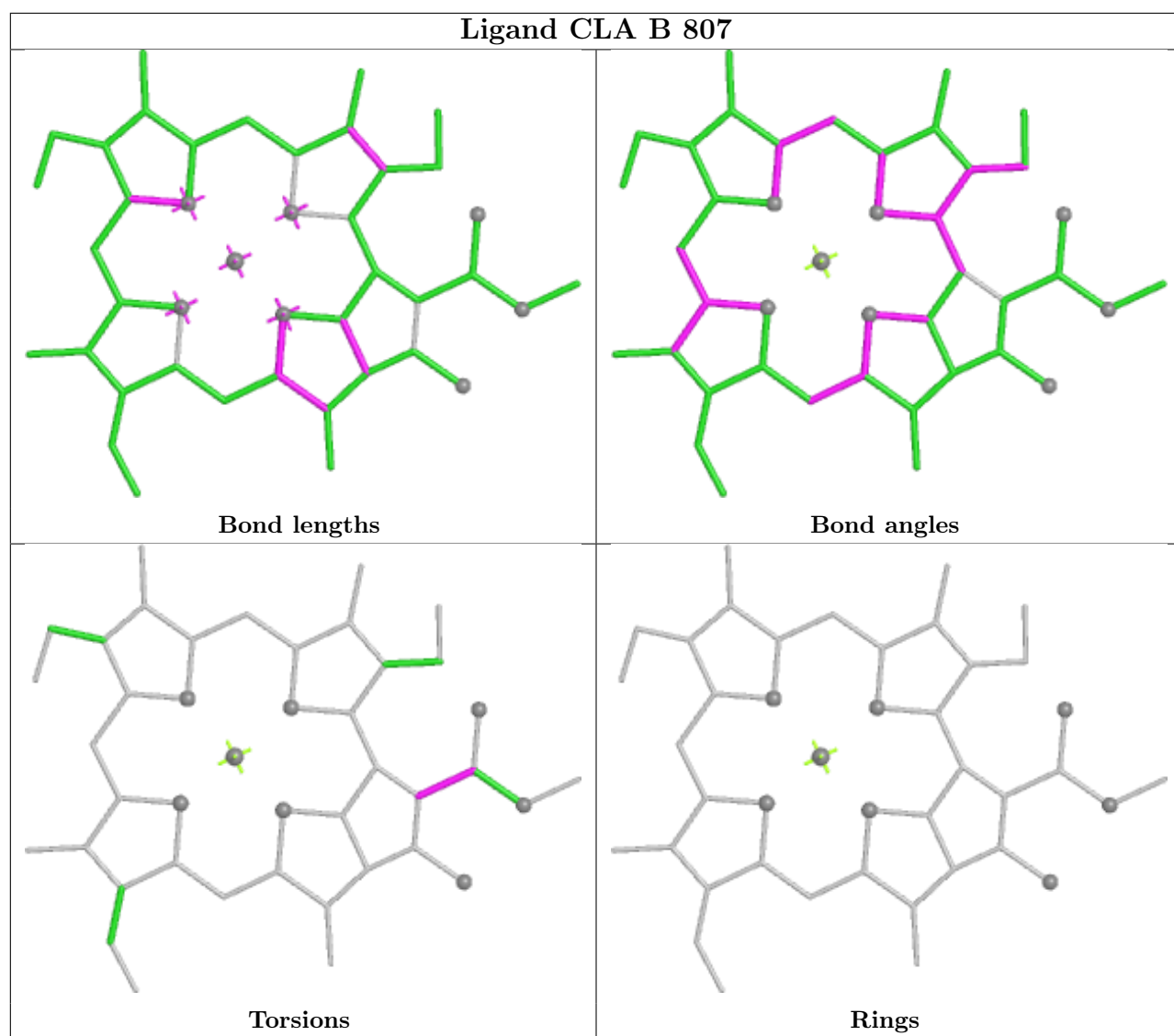
Bond angles

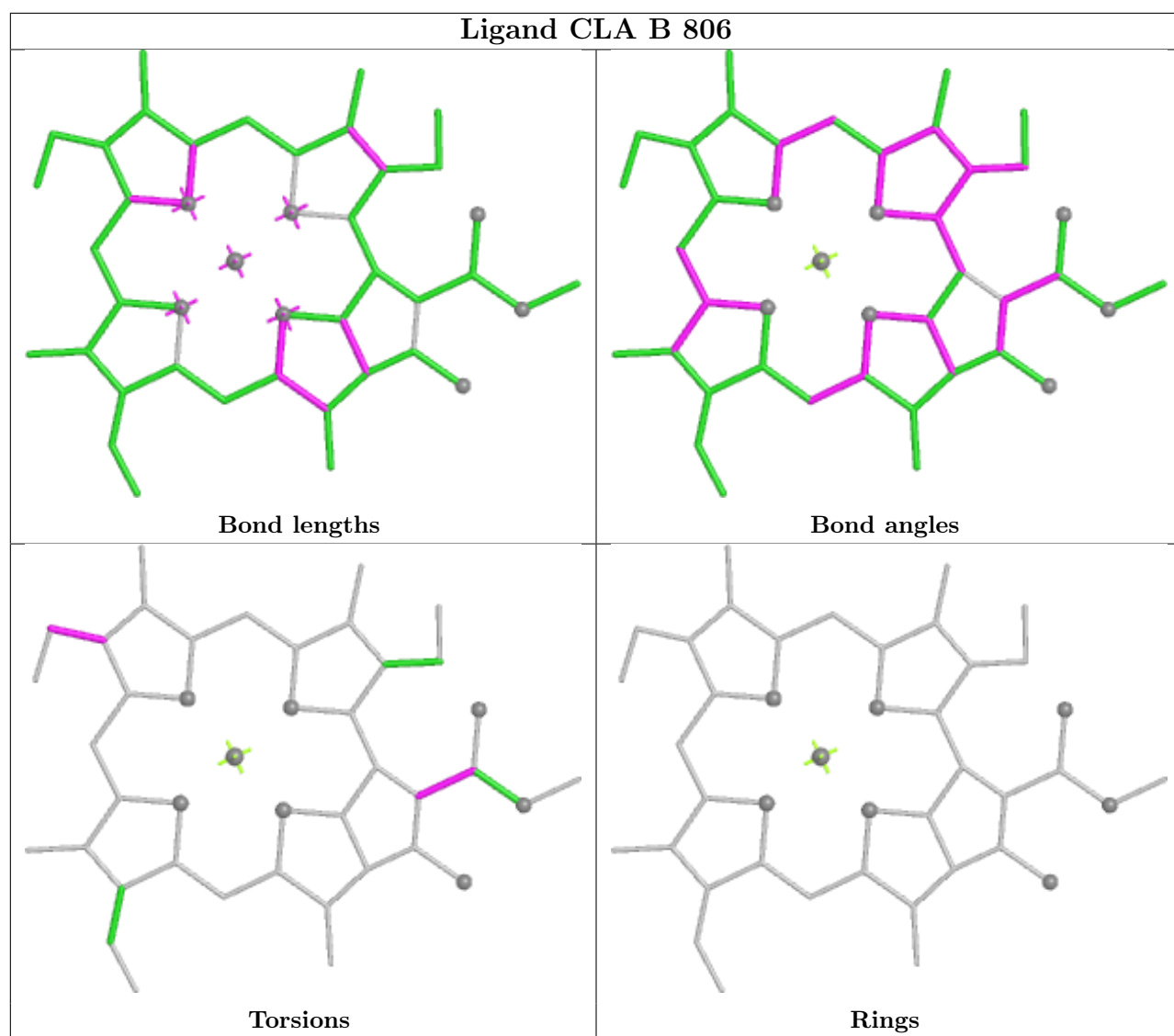


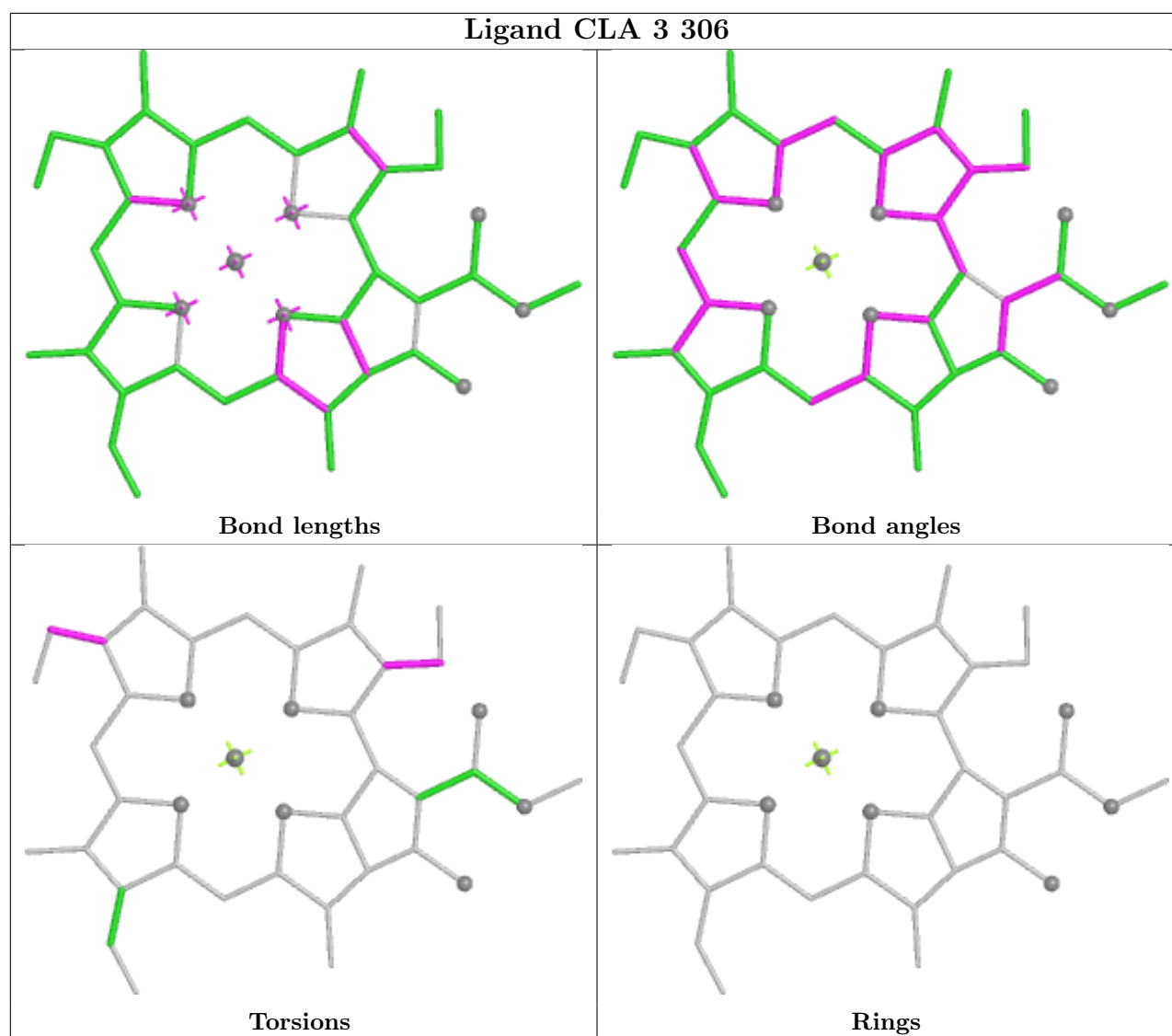
Torsions



Rings







4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

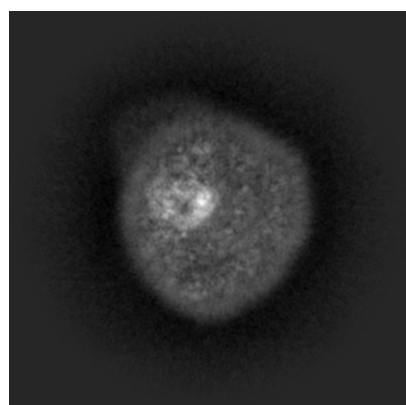
5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32892. These allow visual inspection of the internal detail of the map and identification of artifacts.

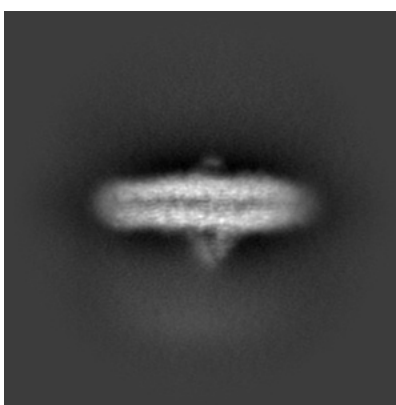
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

5.1 Orthogonal projections [i](#)

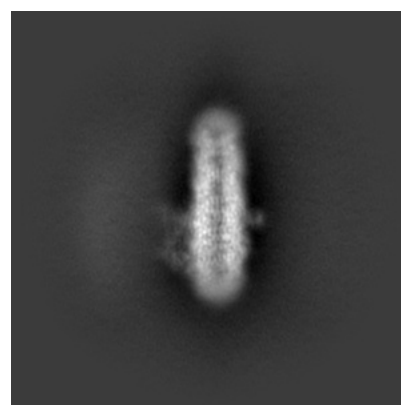
5.1.1 Primary map



X



Y

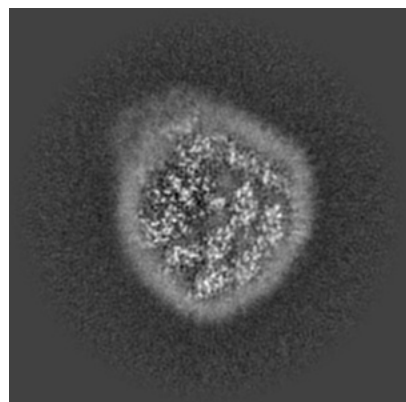


Z

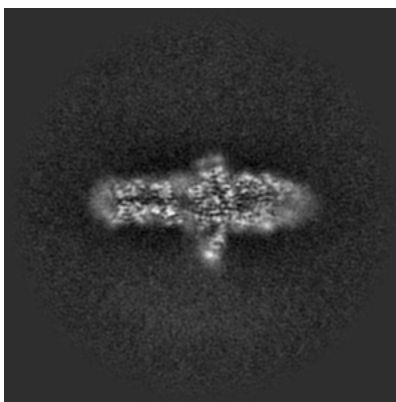
The images above show the map projected in three orthogonal directions.

5.2 Central slices [i](#)

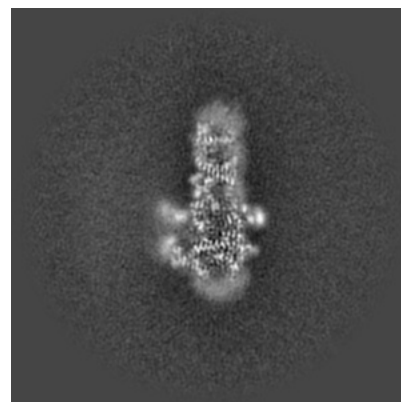
5.2.1 Primary map



X Index: 196



Y Index: 196

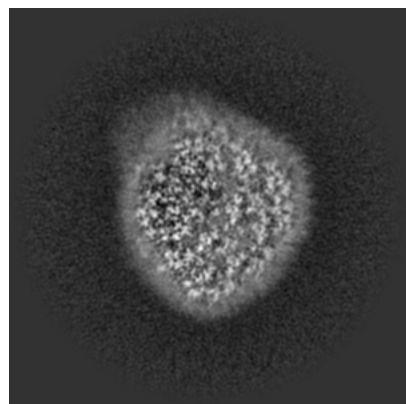


Z Index: 196

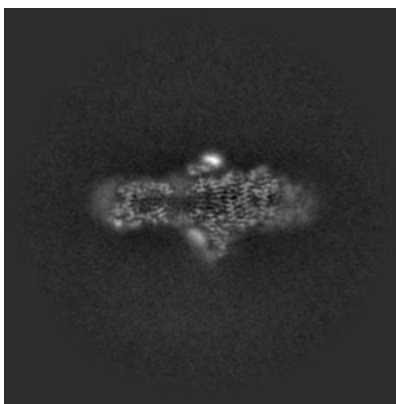
The images above show central slices of the map in three orthogonal directions.

5.3 Largest variance slices [i](#)

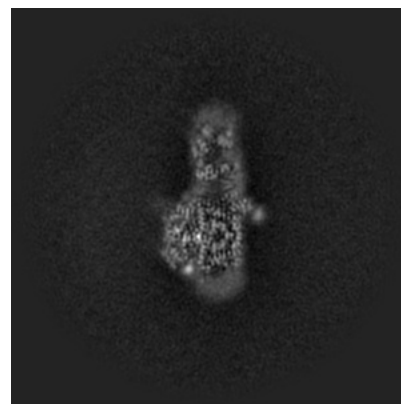
5.3.1 Primary map



X Index: 190



Y Index: 185

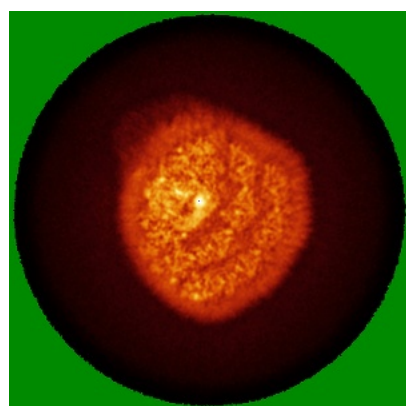


Z Index: 213

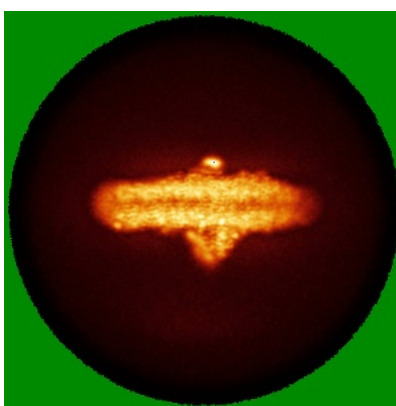
The images above show the largest variance slices of the map in three orthogonal directions.

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

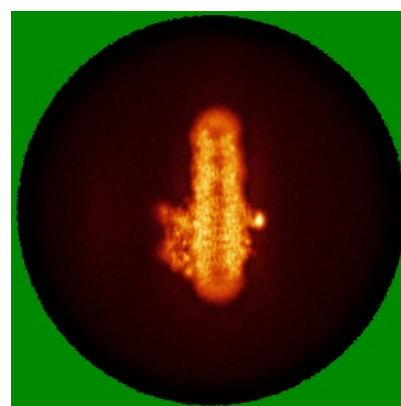
5.4.1 Primary map



X



Y

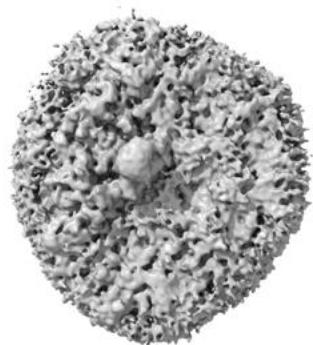


Z

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.

5.5 Orthogonal surface views [i](#)

5.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

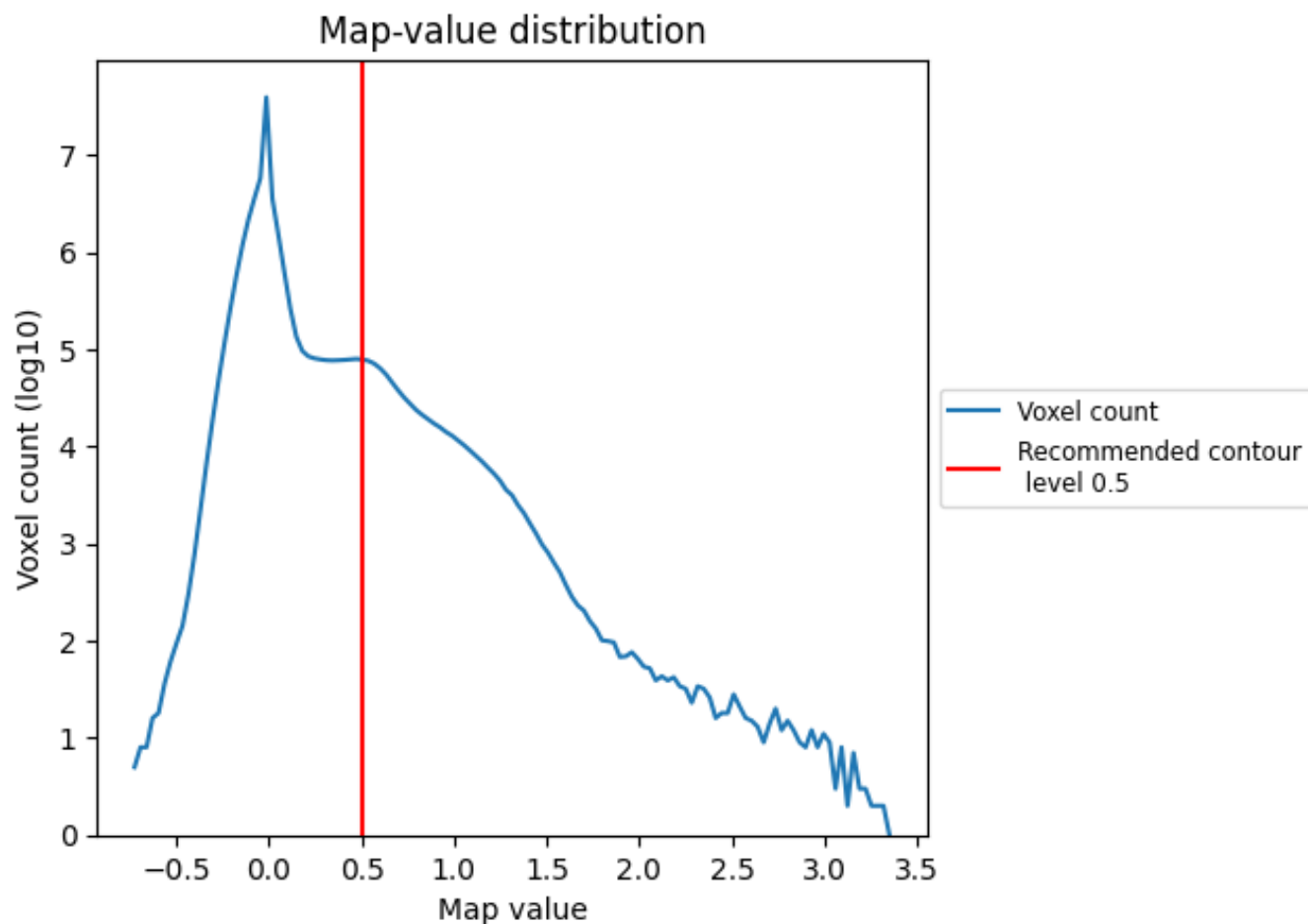
5.6 Mask visualisation [i](#)

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

6 Map analysis [i](#)

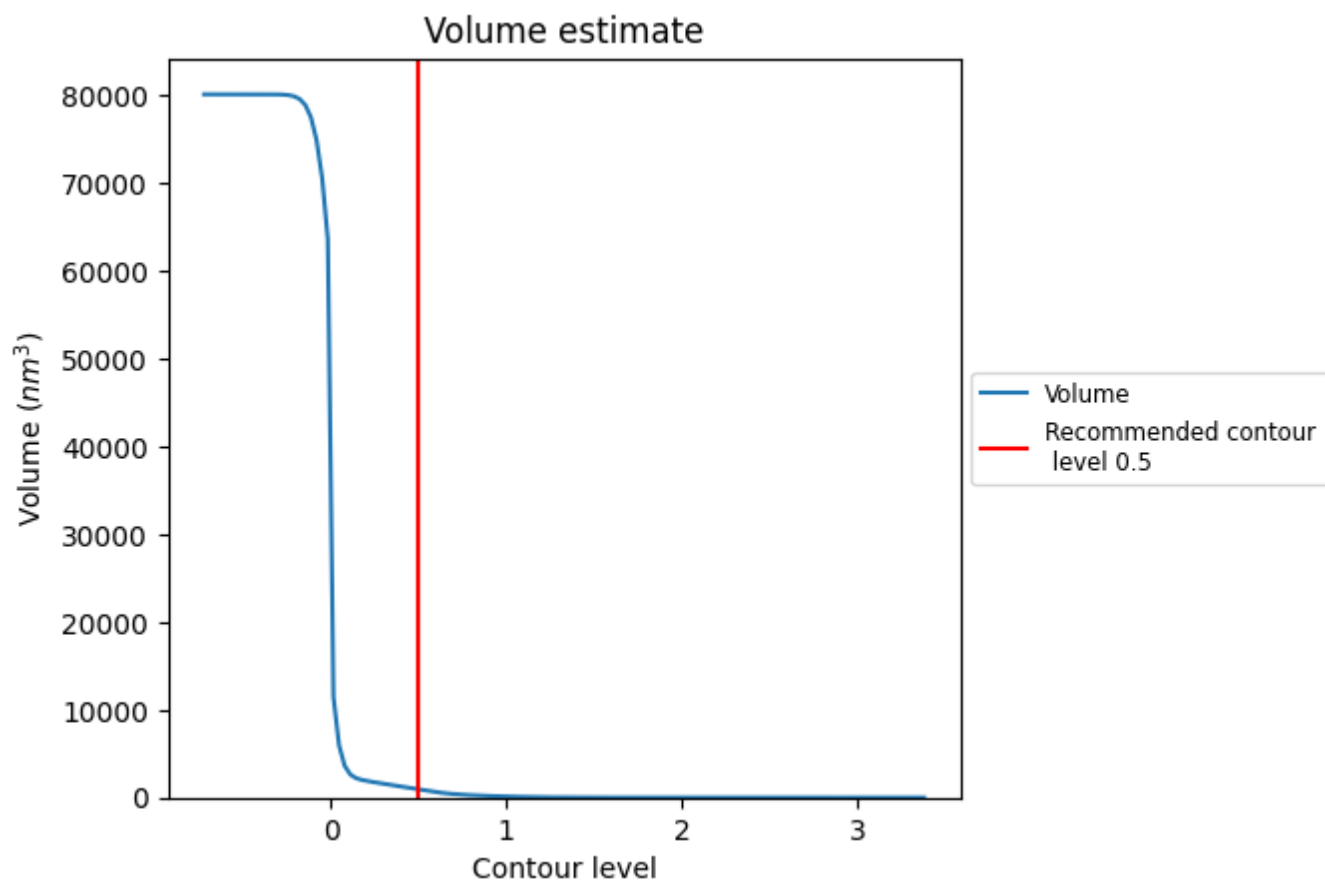
This section contains the results of statistical analysis of the map.

6.1 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.

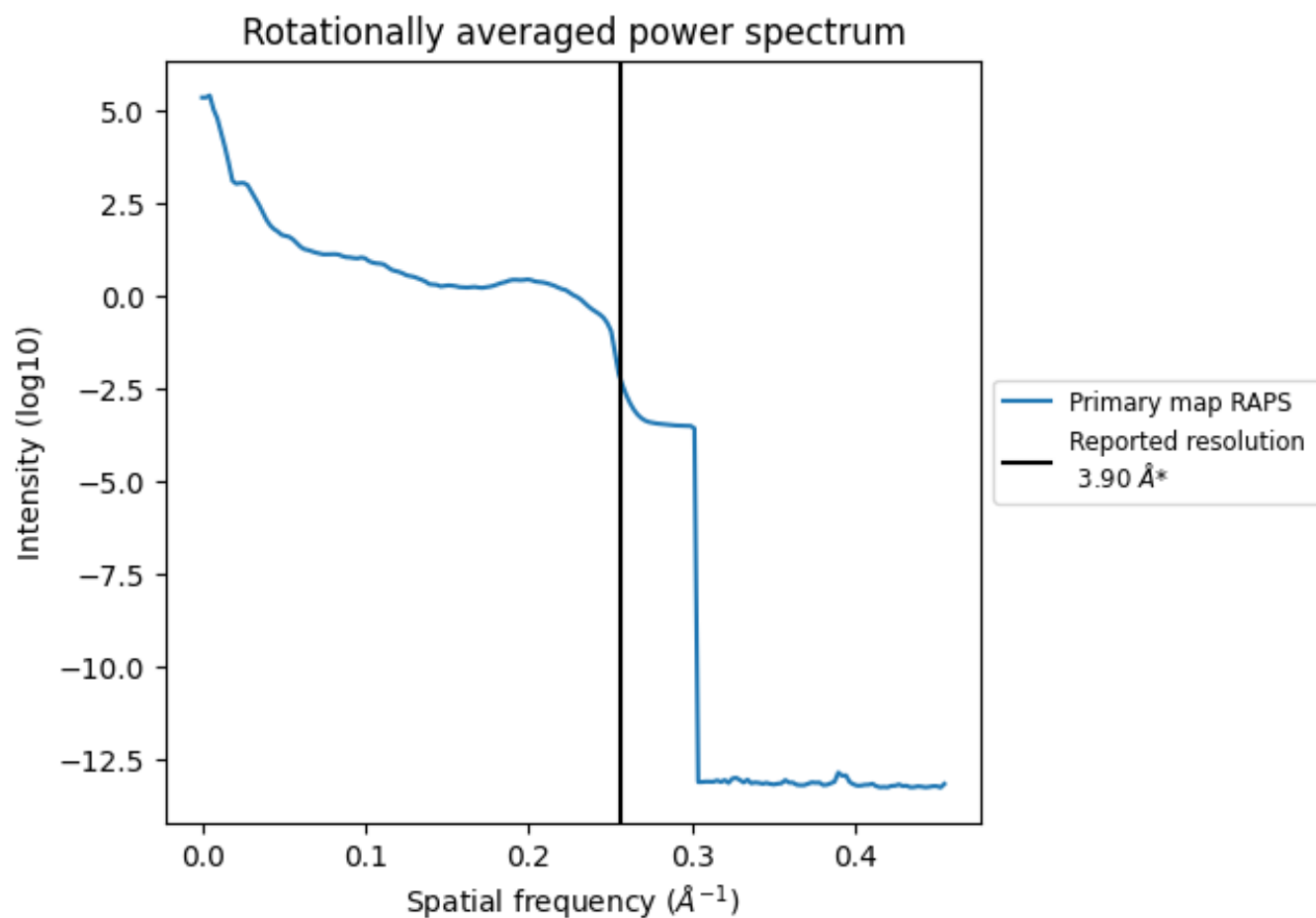
6.2 Volume estimate [i](#)



The volume at the recommended contour level is 932 nm³; this corresponds to an approximate mass of 842 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.

6.3 Rotationally averaged power spectrum ⓘ

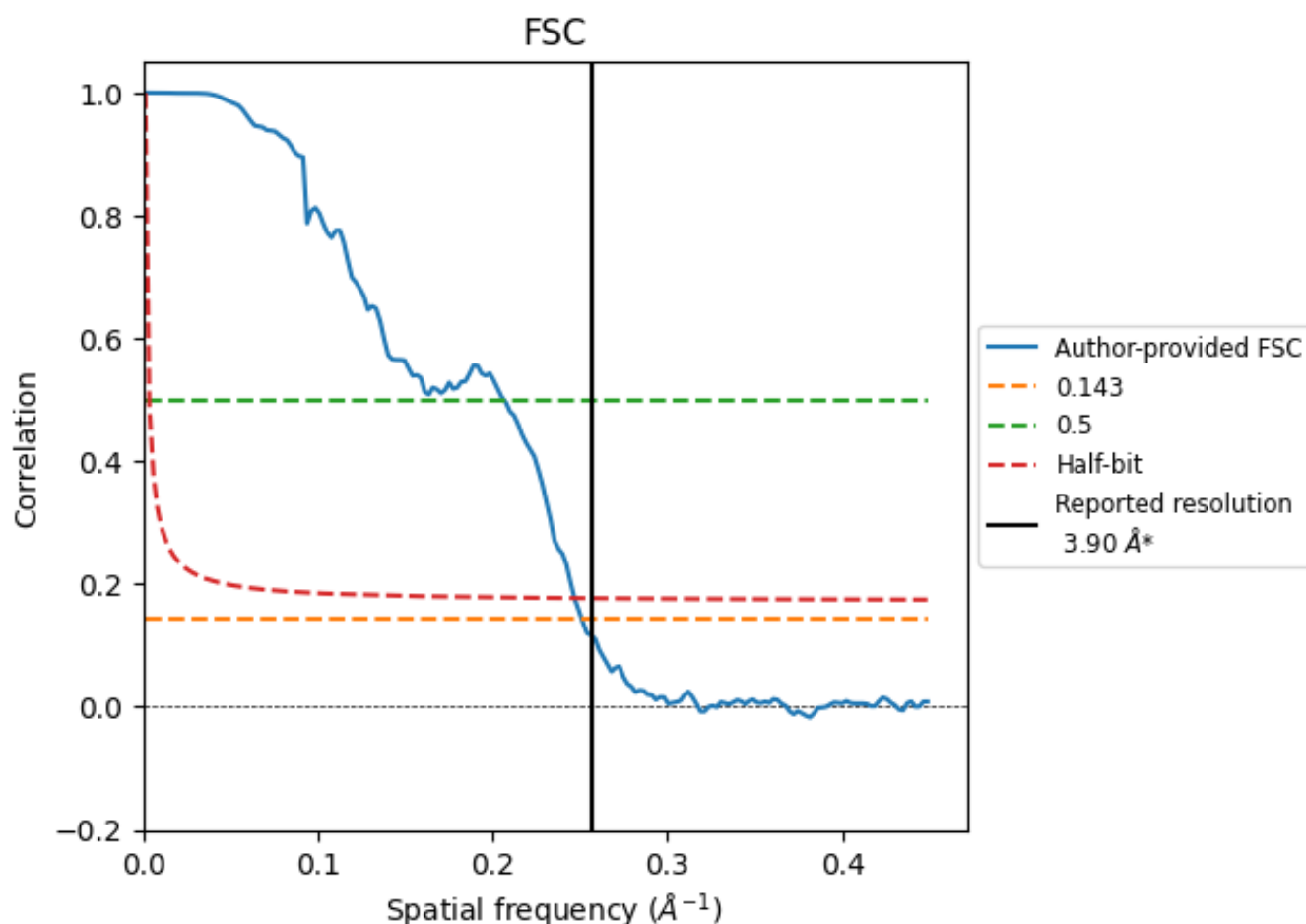


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

7 Fourier-Shell correlation [i](#)

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

7.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.256 $\text{\AA}^{-1}$

7.2 Resolution estimates [i](#)

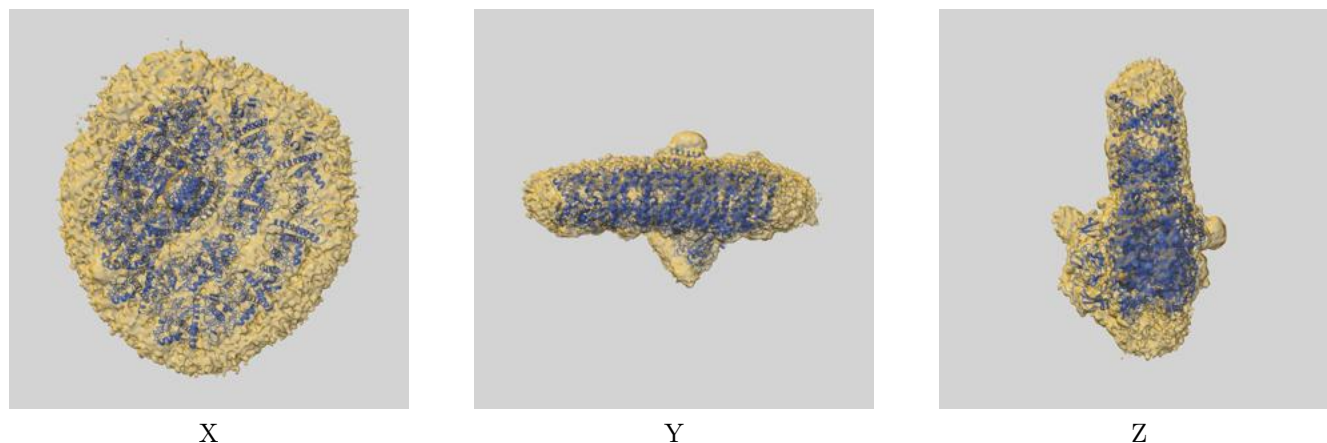
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.98	4.84	4.05
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

8 Map-model fit [i](#)

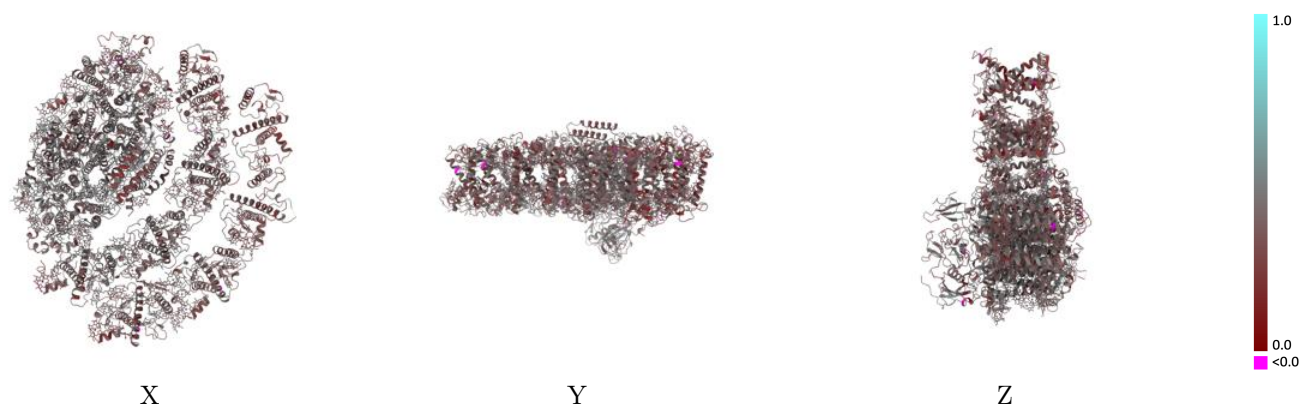
This section contains information regarding the fit between EMDB map EMD-32892 and PDB model 7WYI. Per-residue inclusion information can be found in section ?? on page ??.

8.1 Map-model overlay [i](#)



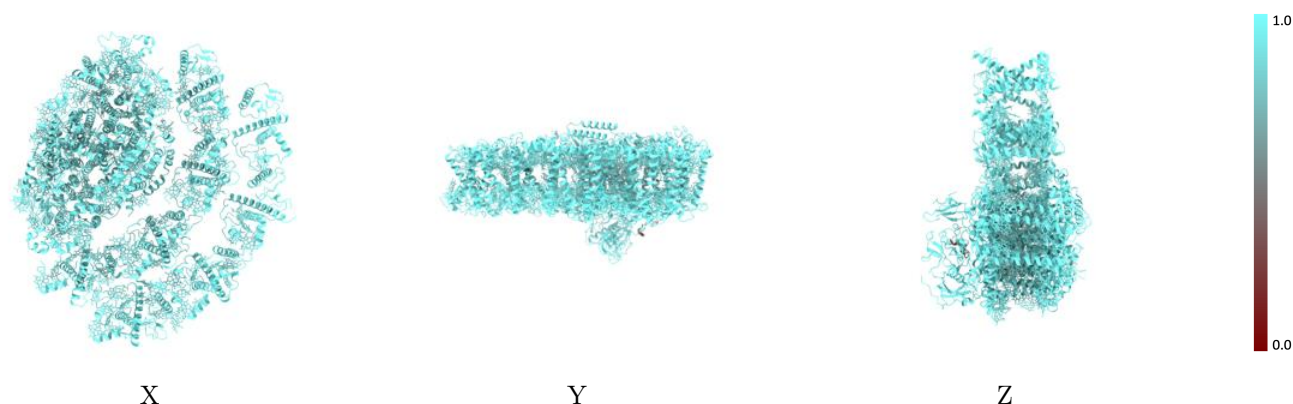
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



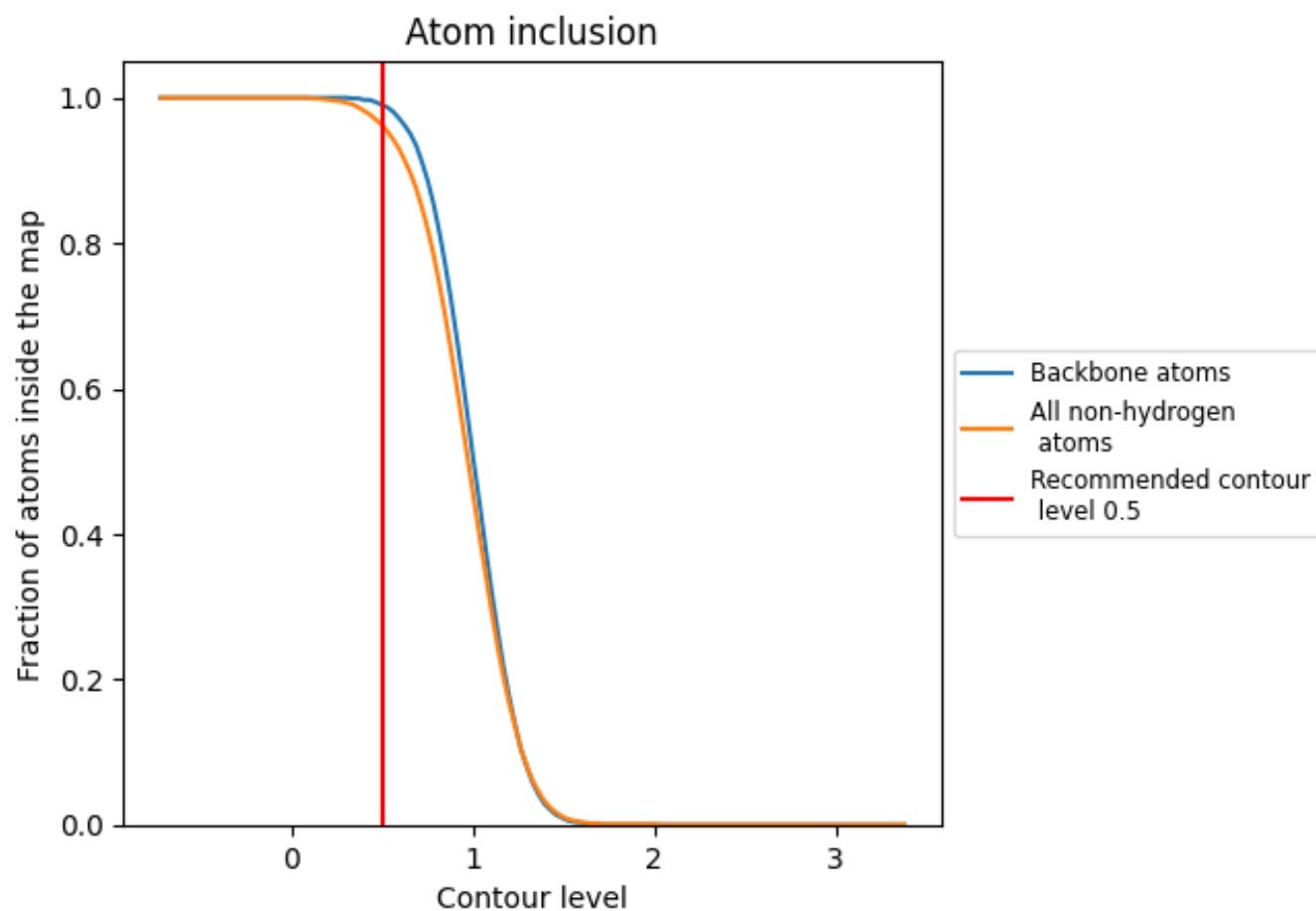
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

8.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).

8.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9620	0.3900
1	0.9600	0.3350
3	0.9640	0.3910
4	0.9760	0.3530
5	0.9670	0.3710
6	0.9670	0.3750
7	0.9710	0.4090
8	0.9670	0.3910
A	0.9600	0.4250
B	0.9480	0.3920
C	0.9900	0.4060
D	0.9320	0.3800
E	0.9970	0.4360
F	0.9670	0.3800
J	0.9590	0.4200
Z	0.9850	0.3180

1.0

0.0

<0.0