



wwPDB EM Validation Summary Report ⓘ

Mar 29, 2026 – 10:15 AM UTC

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 wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : **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) : 2.49

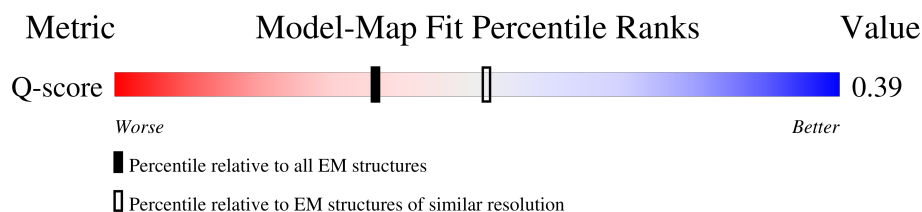
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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 [i](#)

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		

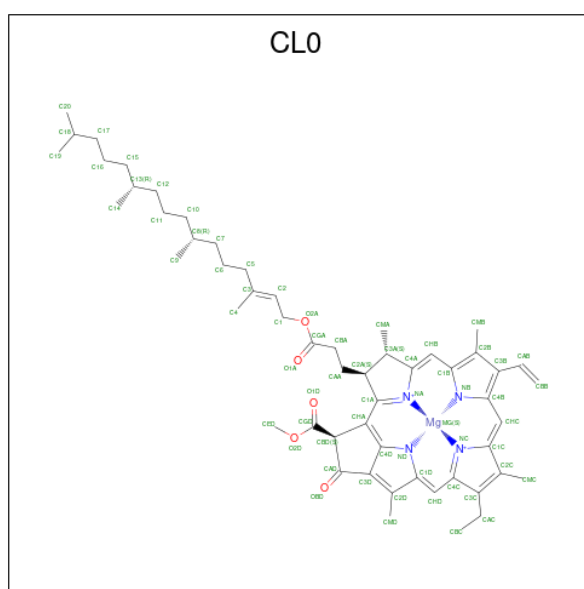
- Molecule 14 is a protein called Chlorophyll a-b binding protein, chloroplastic.

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.

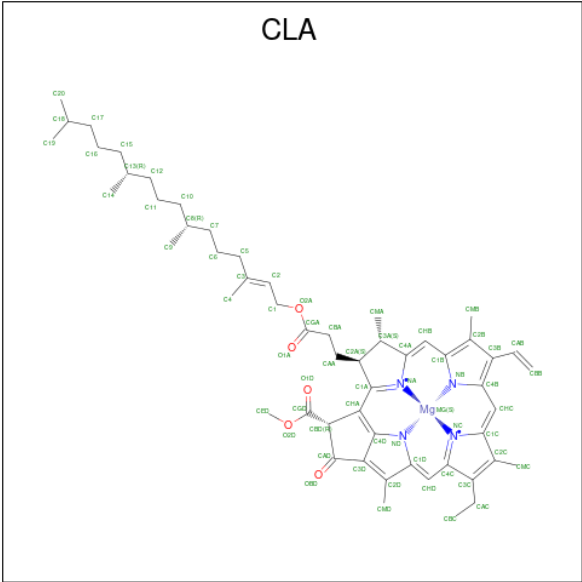
Mol	Chain	Residues	Atoms				AltConf	Trace
15	6	229	Total	C	N	O	0	0
			1122	664	229	229		

- 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

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

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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 42	C 34	Mg 1	N 4	O 3	0
17	3	1	Total 46	C 36	Mg 1	N 4	O 5	0
17	3	1	Total 41	C 33	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	7	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	7	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	7	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	7	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	7	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	7	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	7	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	7	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	7	1	Total 41	C 33	Mg 1	N 4	O 3	0
17	7	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	7	1	Total 43	C 35	Mg 1	N 4	O 3	0
17	7	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

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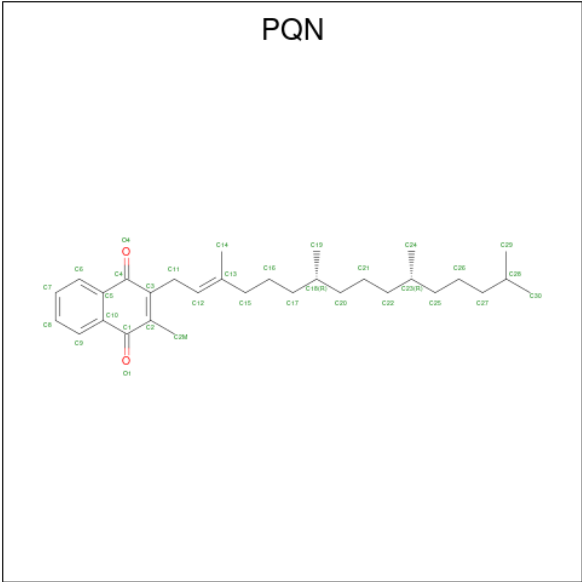
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17	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	8	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	8	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	8	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	8	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	8	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	8	1	Total 42	C 34	Mg 1	N 4	O 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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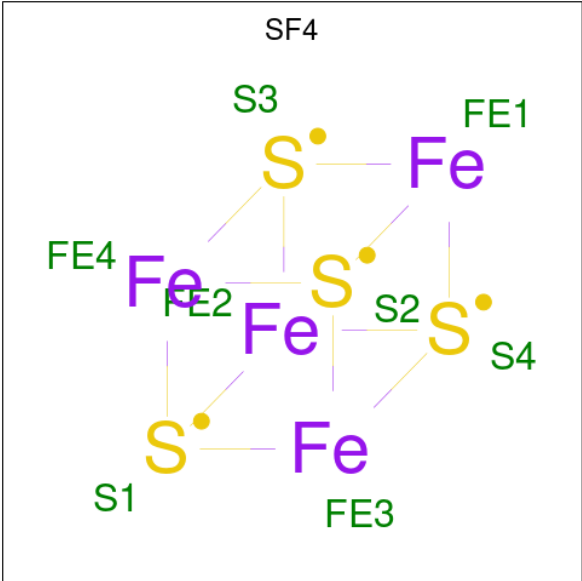
Mol	Chain	Residues	Atoms					AltConf
17	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	5	1	Total	C	Mg	N	O	0
			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: C₃₁H₄₆O₂) (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).



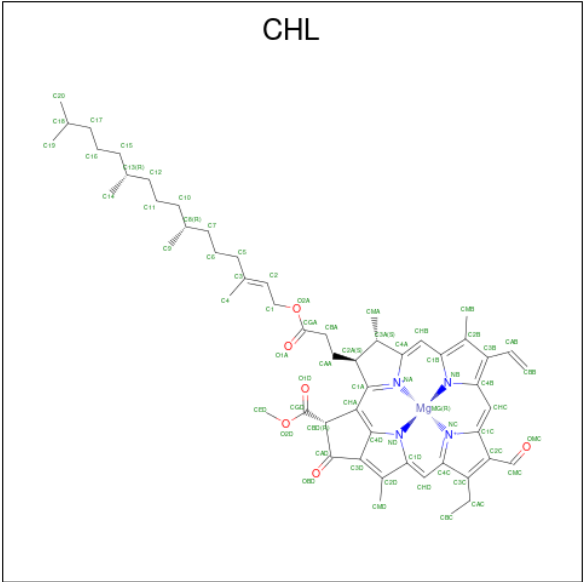
Mol	Chain	Residues	Atoms			AltConf
19	B	1	Total	Fe	S	0
			8	4	4	

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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).



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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	6	608	-	46,50,73	2.03	8 (17%)	53,85,113	1.44	11 (20%)
17	CLA	B	837	-	46,50,73	2.19	9 (19%)	53,85,113	1.47	9 (16%)
17	CLA	7	604	-	46,50,73	2.24	11 (23%)	53,85,113	1.45	10 (18%)
17	CLA	A	809	-	46,50,73	2.14	8 (17%)	53,85,113	1.42	7 (13%)
17	CLA	B	816	-	46,50,73	2.10	10 (21%)	53,85,113	1.40	8 (15%)
17	CLA	B	813	-	45,49,73	2.03	9 (20%)	54,84,113	1.38	7 (12%)
17	CLA	B	839	-	46,50,73	2.06	9 (19%)	53,85,113	1.37	9 (16%)
17	CLA	5	314	-	50,54,73	2.03	8 (16%)	59,90,113	1.50	11 (18%)
17	CLA	1	607	-	46,50,73	2.20	9 (19%)	53,85,113	1.77	10 (18%)
17	CLA	6	604	-	46,50,73	2.03	9 (19%)	53,85,113	1.31	9 (16%)
17	CLA	7	611	-	46,50,73	2.10	11 (23%)	53,85,113	1.39	8 (15%)
17	CLA	5	307	-	46,50,73	2.09	8 (17%)	53,85,113	1.36	8 (15%)
17	CLA	8	603	-	49,53,73	2.11	10 (20%)	58,89,113	1.36	8 (13%)
17	CLA	4	602	-	49,53,73	2.00	9 (18%)	58,89,113	1.31	9 (15%)
17	CLA	A	825	-	46,50,73	2.00	9 (19%)	53,85,113	1.52	9 (16%)
17	CLA	B	811	-	46,50,73	2.07	10 (21%)	53,85,113	1.38	10 (18%)
17	CLA	3	301	-	46,50,73	2.17	8 (17%)	53,85,113	1.46	9 (16%)
17	CLA	6	609	15	50,54,73	2.02	10 (20%)	59,90,113	1.31	8 (13%)
17	CLA	F	301	-	46,50,73	2.10	9 (19%)	53,85,113	1.49	8 (15%)
17	CLA	B	828	-	47,51,73	2.11	9 (19%)	55,86,113	1.34	7 (12%)
17	CLA	B	807	-	46,50,73	2.16	9 (19%)	53,85,113	1.72	10 (18%)
17	CLA	A	822	-	46,50,73	2.17	8 (17%)	53,85,113	1.49	7 (13%)
17	CLA	B	820	-	46,50,73	2.02	8 (17%)	53,85,113	1.48	8 (15%)
17	CLA	A	808	-	46,50,73	2.13	12 (26%)	53,85,113	1.34	8 (15%)
17	CLA	A	823	-	46,50,73	2.13	9 (19%)	53,85,113	1.46	9 (16%)
17	CLA	3	312	-	46,50,73	2.07	8 (17%)	53,85,113	1.50	8 (15%)
16	CL0	A	801	-	35,50,73	2.17	7 (20%)	32,85,113	1.85	3 (9%)
19	SF4	B	803	-	0,12,12	-	-	-	-	-
17	CLA	A	835	-	46,50,73	2.10	12 (26%)	53,85,113	1.33	8 (15%)
17	CLA	5	312	-	46,50,73	2.08	9 (19%)	53,85,113	1.33	9 (16%)
17	CLA	6	601	15	46,50,73	2.10	10 (21%)	53,85,113	1.34	9 (16%)
17	CLA	1	609	-	46,50,73	2.12	10 (21%)	53,85,113	1.29	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	A	830	-	46,50,73	2.10	10 (21%)	53,85,113	1.47	10 (18%)
17	CLA	A	836	-	46,50,73	2.07	9 (19%)	53,85,113	1.43	9 (16%)
17	CLA	B	826	-	46,50,73	2.16	8 (17%)	53,85,113	1.64	8 (15%)
17	CLA	5	315	-	49,53,73	2.03	10 (20%)	58,89,113	1.38	7 (12%)
17	CLA	B	825	-	46,50,73	2.09	10 (21%)	53,85,113	1.30	8 (15%)
17	CLA	3	309	-	49,53,73	1.98	8 (16%)	58,89,113	1.32	7 (12%)
17	CLA	3	313	-	46,50,73	2.16	8 (17%)	53,85,113	1.62	11 (20%)
17	CLA	B	817	-	46,50,73	2.11	11 (23%)	53,85,113	1.43	8 (15%)
17	CLA	A	827	-	46,50,73	2.04	9 (19%)	53,85,113	1.36	9 (16%)
20	CHL	8	606	-	37,51,74	2.37	9 (24%)	30,86,114	1.38	6 (20%)
17	CLA	1	603	-	46,50,73	2.07	10 (21%)	53,85,113	1.32	8 (15%)
17	CLA	J	102	-	46,50,73	2.12	10 (21%)	53,85,113	1.47	9 (16%)
17	CLA	A	841	-	56,60,73	1.97	8 (14%)	65,97,113	1.38	9 (13%)
17	CLA	3	310	-	45,49,73	2.25	9 (20%)	54,84,113	1.95	12 (22%)
17	CLA	5	306	-	54,58,73	1.97	9 (16%)	64,95,113	1.25	7 (10%)
17	CLA	A	805	-	46,50,73	2.17	9 (19%)	53,85,113	1.55	10 (18%)
17	CLA	A	838	-	46,50,73	2.17	9 (19%)	53,85,113	1.54	9 (16%)
17	CLA	J	101	-	46,50,73	2.17	9 (19%)	53,85,113	1.50	7 (13%)
17	CLA	A	807	-	46,50,73	2.18	10 (21%)	53,85,113	1.63	9 (16%)
20	CHL	6	606	-	37,51,74	2.58	9 (24%)	30,86,114	1.41	6 (20%)
17	CLA	B	835	-	47,51,73	2.04	9 (19%)	55,86,113	1.34	8 (14%)
20	CHL	6	605	-	37,51,74	2.54	9 (24%)	30,86,114	1.40	6 (20%)
17	CLA	A	829	-	46,50,73	2.08	9 (19%)	53,85,113	1.44	10 (18%)
17	CLA	A	806	-	46,50,73	2.15	10 (21%)	53,85,113	1.37	8 (15%)
17	CLA	5	302	14	46,50,73	2.13	10 (21%)	53,85,113	1.35	8 (15%)
17	CLA	7	609	-	46,50,73	2.04	8 (17%)	53,85,113	1.39	9 (16%)
17	CLA	B	836	-	46,50,73	2.10	10 (21%)	53,85,113	1.48	9 (16%)
17	CLA	B	833	-	46,50,73	2.06	8 (17%)	53,85,113	1.42	8 (15%)
17	CLA	7	601	10	46,50,73	2.09	10 (21%)	53,85,113	1.41	8 (15%)
17	CLA	8	608	-	46,50,73	2.18	11 (23%)	53,85,113	1.49	10 (18%)
17	CLA	A	819	-	46,50,73	2.04	8 (17%)	53,85,113	1.32	8 (15%)
17	CLA	B	819	-	46,50,73	2.10	9 (19%)	53,85,113	1.59	7 (13%)
17	CLA	A	812	-	46,50,73	2.12	10 (21%)	53,85,113	1.37	8 (15%)
17	CLA	A	831	-	46,50,73	2.08	12 (26%)	53,85,113	1.34	9 (16%)
17	CLA	7	602	-	46,50,73	2.06	10 (21%)	53,85,113	1.39	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	8	604	-	46,50,73	2.12	10 (21%)	53,85,113	1.34	7 (13%)
17	CLA	B	832	-	46,50,73	2.14	10 (21%)	53,85,113	1.39	8 (15%)
17	CLA	A	815	-	46,50,73	2.23	10 (21%)	53,85,113	1.41	9 (16%)
17	CLA	1	602	-	46,50,73	2.00	9 (19%)	53,85,113	1.41	9 (16%)
17	CLA	B	823	-	46,50,73	2.14	9 (19%)	53,85,113	1.40	8 (15%)
17	CLA	6	602	-	46,50,73	2.08	11 (23%)	53,85,113	1.38	8 (15%)
17	CLA	B	821	-	50,54,73	1.97	13 (26%)	59,90,113	1.25	7 (11%)
17	CLA	3	304	-	49,53,73	2.00	9 (18%)	58,89,113	1.25	8 (13%)
20	CHL	5	313	-	37,51,74	2.47	9 (24%)	30,86,114	1.37	5 (16%)
17	CLA	7	605	-	46,50,73	2.12	11 (23%)	53,85,113	1.35	8 (15%)
17	CLA	3	308	-	46,50,73	2.16	9 (19%)	53,85,113	1.77	8 (15%)
17	CLA	8	612	-	50,54,73	2.03	10 (20%)	59,90,113	1.28	8 (13%)
17	CLA	B	801	-	46,50,73	2.10	8 (17%)	53,85,113	1.60	10 (18%)
17	CLA	B	830	-	46,50,73	2.09	9 (19%)	53,85,113	1.44	7 (13%)
17	CLA	B	827	-	46,50,73	2.07	9 (19%)	53,85,113	1.34	8 (15%)
17	CLA	A	813	-	46,50,73	2.11	10 (21%)	53,85,113	1.40	9 (16%)
17	CLA	A	814	-	46,50,73	2.12	10 (21%)	53,85,113	1.34	8 (15%)
17	CLA	8	607	-	46,50,73	2.08	11 (23%)	53,85,113	1.39	8 (15%)
17	CLA	8	601	11	46,50,73	2.12	12 (26%)	53,85,113	1.38	8 (15%)
17	CLA	B	812	-	46,50,73	2.19	9 (19%)	53,85,113	1.88	10 (18%)
17	CLA	B	831	-	46,50,73	2.23	11 (23%)	53,85,113	1.64	8 (15%)
17	CLA	4	605	-	49,53,73	2.03	9 (18%)	58,89,113	1.26	8 (13%)
17	CLA	3	306	-	46,50,73	2.12	9 (19%)	53,85,113	1.80	13 (24%)
17	CLA	B	806	-	46,50,73	2.21	10 (21%)	53,85,113	1.84	11 (20%)
19	SF4	C	101	-	0,12,12	-	-	-	-	-
17	CLA	6	610	-	49,53,73	2.07	10 (20%)	58,89,113	1.33	8 (13%)
17	CLA	7	614	10	46,50,73	2.14	10 (21%)	53,85,113	1.70	10 (18%)
17	CLA	B	838	-	46,50,73	2.05	11 (23%)	53,85,113	1.41	8 (15%)
17	CLA	A	843	-	46,50,73	2.09	11 (23%)	53,85,113	1.28	8 (15%)
17	CLA	A	804	-	46,50,73	2.17	8 (17%)	53,85,113	1.83	11 (20%)
17	CLA	4	601	-	46,50,73	2.12	10 (21%)	53,85,113	1.37	8 (15%)
17	CLA	8	613	-	46,50,73	2.10	10 (21%)	53,85,113	1.38	8 (15%)
17	CLA	5	301	-	46,50,73	2.06	10 (21%)	53,85,113	1.33	8 (15%)
17	CLA	A	810	-	46,50,73	2.12	10 (21%)	53,85,113	1.40	9 (16%)
17	CLA	5	303	-	52,56,73	1.92	9 (17%)	61,92,113	1.24	9 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CHL	1	601	8	47,61,74	2.24	9 (19%)	41,98,114	1.16	5 (12%)
17	CLA	B	810	-	50,54,73	2.05	8 (16%)	58,89,113	1.41	8 (13%)
17	CLA	3	302	-	46,50,73	2.11	9 (19%)	53,85,113	1.34	9 (16%)
17	CLA	8	605	-	46,50,73	2.03	9 (19%)	53,85,113	1.30	8 (15%)
17	CLA	A	834	1	46,50,73	2.08	8 (17%)	53,85,113	1.44	8 (15%)
20	CHL	7	606	-	37,51,74	2.59	9 (24%)	30,86,114	1.42	6 (20%)
17	CLA	7	612	-	49,53,73	2.03	10 (20%)	58,89,113	1.26	8 (13%)
17	CLA	3	311	-	46,50,73	2.12	10 (21%)	53,85,113	1.32	8 (15%)
17	CLA	A	821	-	55,59,73	1.97	8 (14%)	64,96,113	1.48	9 (14%)
17	CLA	A	832	-	45,48,73	2.25	11 (24%)	51,82,113	1.97	10 (19%)
20	CHL	5	305	-	40,54,74	2.40	9 (22%)	34,90,114	1.24	5 (14%)
20	CHL	3	307	-	40,54,74	2.65	9 (22%)	34,90,114	1.31	6 (17%)
17	CLA	8	609	-	46,50,73	2.04	8 (17%)	53,85,113	1.33	8 (15%)
17	CLA	7	607	-	46,50,73	2.09	9 (19%)	53,85,113	1.37	9 (16%)
18	PQN	A	840	-	34,34,34	0.22	0	43,45,45	0.50	1 (2%)
17	CLA	A	820	-	46,50,73	2.11	11 (23%)	53,85,113	1.38	7 (13%)
17	CLA	A	842	-	46,50,73	2.11	7 (15%)	53,85,113	1.27	9 (16%)
17	CLA	B	808	-	46,50,73	2.05	9 (19%)	53,85,113	1.40	8 (15%)
17	CLA	8	610	-	46,50,73	2.07	8 (17%)	53,85,113	1.46	9 (16%)
17	CLA	B	809	-	46,50,73	2.13	10 (21%)	53,85,113	1.48	8 (15%)
17	CLA	3	305	-	46,50,73	2.05	8 (17%)	53,85,113	1.50	7 (13%)
17	CLA	4	603	-	46,50,73	2.18	9 (19%)	53,85,113	1.75	10 (18%)
17	CLA	A	811	-	46,50,73	2.08	11 (23%)	53,85,113	1.37	8 (15%)
17	CLA	5	310	-	46,50,73	2.16	10 (21%)	53,85,113	1.29	7 (13%)
17	CLA	6	603	-	46,50,73	2.08	10 (21%)	53,85,113	1.45	9 (16%)
17	CLA	1	605	-	46,50,73	2.10	11 (23%)	53,85,113	1.37	8 (15%)
17	CLA	A	824	-	46,50,73	2.09	9 (19%)	53,85,113	1.60	9 (16%)
17	CLA	B	818	-	46,50,73	2.06	8 (17%)	53,85,113	1.52	9 (16%)
17	CLA	4	604	-	46,50,73	2.11	10 (21%)	53,85,113	1.35	6 (11%)
17	CLA	8	611	-	46,50,73	2.12	10 (21%)	53,85,113	1.44	7 (13%)
17	CLA	A	837	-	46,50,73	2.12	10 (21%)	53,85,113	1.37	7 (13%)
17	CLA	A	802	-	46,50,73	2.21	9 (19%)	53,85,113	1.60	8 (15%)
17	CLA	8	602	-	46,50,73	2.05	9 (19%)	53,85,113	1.36	8 (15%)
17	CLA	5	308	-	46,50,73	1.95	8 (17%)	53,85,113	1.41	9 (16%)
17	CLA	1	604	-	46,50,73	2.10	8 (17%)	53,85,113	1.29	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	A	817	-	46,50,73	2.14	8 (17%)	53,85,113	1.59	10 (18%)
17	CLA	A	816	-	46,50,73	2.00	8 (17%)	53,85,113	1.33	9 (16%)
17	CLA	B	814	-	41,47,73	2.16	7 (17%)	51,81,113	1.37	6 (11%)
17	CLA	A	839	-	46,50,73	2.19	12 (26%)	53,85,113	1.40	8 (15%)
17	CLA	A	818	-	49,53,73	2.07	10 (20%)	58,89,113	1.33	8 (13%)
17	CLA	B	805	-	46,50,73	2.19	7 (15%)	53,85,113	1.41	8 (15%)
17	CLA	1	606	-	46,50,73	2.08	8 (17%)	53,85,113	1.59	10 (18%)
17	CLA	B	822	-	46,50,73	2.04	9 (19%)	53,85,113	1.38	10 (18%)
19	SF4	C	102	-	0,12,12	-	-	-	-	-
17	CLA	B	804	-	46,50,73	2.17	9 (19%)	53,85,113	1.57	8 (15%)
17	CLA	7	610	-	45,49,73	2.39	9 (20%)	54,84,113	1.82	11 (20%)
17	CLA	5	311	-	46,50,73	2.04	9 (19%)	53,85,113	1.40	8 (15%)
17	CLA	5	304	-	46,50,73	2.10	10 (21%)	53,85,113	1.28	8 (15%)
17	CLA	7	603	-	46,50,73	2.19	9 (19%)	53,85,113	1.58	9 (16%)
17	CLA	5	309	-	46,50,73	2.10	9 (19%)	53,85,113	1.51	10 (18%)
17	CLA	A	833	-	46,50,73	2.10	10 (21%)	53,85,113	1.45	8 (15%)
17	CLA	A	803	-	46,50,73	2.12	10 (21%)	53,85,113	1.47	8 (15%)
17	CLA	B	834	-	46,50,73	2.10	9 (19%)	53,85,113	1.47	7 (13%)
17	CLA	B	829	-	47,51,73	2.06	8 (17%)	55,86,113	1.45	10 (18%)
17	CLA	B	815	-	69,73,73	1.80	9 (13%)	82,113,113	1.50	13 (15%)
17	CLA	B	802	-	49,53,73	2.09	8 (16%)	58,89,113	1.58	8 (13%)
17	CLA	7	608	-	46,50,73	2.05	8 (17%)	53,85,113	1.46	9 (16%)
20	CHL	Z	601	12	37,51,74	2.51	9 (24%)	30,86,114	1.34	5 (16%)
17	CLA	B	824	-	45,49,73	2.29	8 (17%)	54,84,113	1.60	11 (20%)
18	PQN	B	840	-	34,34,34	0.22	0	43,45,45	0.48	1 (2%)
17	CLA	1	608	-	46,50,73	2.09	10 (21%)	53,85,113	1.36	8 (15%)
17	CLA	7	613	-	47,51,73	2.10	10 (21%)	55,86,113	1.31	8 (14%)
17	CLA	8	614	11	46,50,73	2.17	10 (21%)	53,85,113	1.52	8 (15%)
20	CHL	6	607	-	37,51,74	2.54	9 (24%)	30,86,114	1.55	7 (23%)
17	CLA	A	826	-	46,50,73	2.04	8 (17%)	53,85,113	1.34	8 (15%)
17	CLA	F	302	-	66,70,73	1.73	9 (13%)	78,109,113	1.16	9 (11%)
17	CLA	1	610	-	46,50,73	2.07	9 (19%)	53,85,113	1.31	8 (15%)
17	CLA	3	303	-	46,50,73	2.17	10 (21%)	53,85,113	1.37	8 (15%)
17	CLA	A	828	-	46,50,73	2.06	9 (19%)	53,85,113	1.30	9 (16%)

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	6	608	-	1/1/10/20	2/12/88/115	-
17	CLA	B	837	-	1/1/10/20	2/12/88/115	-
17	CLA	7	604	-	1/1/10/20	1/12/88/115	-
17	CLA	A	809	-	1/1/10/20	3/12/88/115	-
17	CLA	B	816	-	1/1/10/20	4/12/88/115	-
17	CLA	B	813	-	1/1/10/20	1/10/86/115	-
17	CLA	B	839	-	1/1/10/20	2/12/88/115	-
17	CLA	5	314	-	1/1/11/20	7/17/93/115	-
17	CLA	1	607	-	1/1/10/20	3/12/88/115	-
17	CLA	6	604	-	1/1/10/20	2/12/88/115	-
17	CLA	7	611	-	1/1/10/20	2/12/88/115	-
17	CLA	5	307	-	1/1/10/20	3/12/88/115	-
17	CLA	8	603	-	1/1/11/20	2/15/91/115	-
17	CLA	4	602	-	1/1/11/20	5/15/91/115	-
17	CLA	A	825	-	1/1/10/20	2/12/88/115	-
17	CLA	B	811	-	1/1/10/20	2/12/88/115	-
17	CLA	3	301	-	1/1/10/20	2/12/88/115	-
17	CLA	6	609	15	1/1/11/20	3/17/93/115	-
17	CLA	F	301	-	1/1/10/20	3/12/88/115	-
17	CLA	B	828	-	1/1/10/20	1/13/89/115	-
17	CLA	B	807	-	1/1/10/20	2/12/88/115	-
17	CLA	A	822	-	1/1/10/20	3/12/88/115	-
17	CLA	B	820	-	1/1/10/20	6/12/88/115	-
17	CLA	A	808	-	1/1/10/20	2/12/88/115	-
17	CLA	A	823	-	1/1/10/20	3/12/88/115	-
17	CLA	3	312	-	1/1/10/20	3/12/88/115	-
16	CL0	A	801	-	3/3/15/25	0/10/108/135	-
19	SF4	B	803	-	-	-	0/6/5/5
17	CLA	A	835	-	1/1/10/20	5/12/88/115	-
17	CLA	5	312	-	1/1/10/20	3/12/88/115	-
17	CLA	6	601	15	1/1/10/20	4/12/88/115	-
17	CLA	1	609	-	1/1/10/20	0/12/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	A	830	-	1/1/10/20	2/12/88/115	-
17	CLA	A	836	-	1/1/10/20	2/12/88/115	-
17	CLA	B	826	-	1/1/10/20	2/12/88/115	-
17	CLA	5	315	-	1/1/11/20	6/15/91/115	-
17	CLA	B	825	-	1/1/10/20	5/12/88/115	-
17	CLA	3	309	-	1/1/11/20	1/15/91/115	-
17	CLA	3	313	-	1/1/10/20	3/12/88/115	-
17	CLA	B	817	-	1/1/10/20	5/12/88/115	-
17	CLA	A	827	-	1/1/10/20	2/12/88/115	-
20	CHL	8	606	-	3/3/15/26	2/12/110/137	-
17	CLA	1	603	-	1/1/10/20	4/12/88/115	-
17	CLA	J	102	-	1/1/10/20	4/12/88/115	-
17	CLA	A	841	-	1/1/12/20	8/24/100/115	-
17	CLA	3	310	-	1/1/10/20	0/10/86/115	-
17	CLA	5	306	-	1/1/12/20	2/21/97/115	-
17	CLA	A	805	-	1/1/10/20	4/12/88/115	-
17	CLA	A	838	-	1/1/10/20	1/12/88/115	-
17	CLA	J	101	-	1/1/10/20	4/12/88/115	-
17	CLA	A	807	-	1/1/10/20	4/12/88/115	-
20	CHL	6	606	-	3/3/15/26	5/12/110/137	-
17	CLA	B	835	-	1/1/10/20	4/13/89/115	-
20	CHL	6	605	-	3/3/15/26	1/12/110/137	-
17	CLA	A	829	-	1/1/10/20	5/12/88/115	-
17	CLA	A	806	-	1/1/10/20	3/12/88/115	-
17	CLA	5	302	14	1/1/10/20	4/12/88/115	-
17	CLA	7	609	-	1/1/10/20	3/12/88/115	-
17	CLA	B	836	-	1/1/10/20	2/12/88/115	-
17	CLA	B	833	-	1/1/10/20	0/12/88/115	-
17	CLA	7	601	10	1/1/10/20	4/12/88/115	-
17	CLA	8	608	-	1/1/10/20	0/12/88/115	-
17	CLA	A	819	-	1/1/10/20	2/12/88/115	-
17	CLA	B	819	-	1/1/10/20	3/12/88/115	-
17	CLA	A	812	-	1/1/10/20	3/12/88/115	-
17	CLA	A	831	-	1/1/10/20	2/12/88/115	-
17	CLA	7	602	-	1/1/10/20	5/12/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	8	604	-	1/1/10/20	0/12/88/115	-
17	CLA	B	832	-	1/1/10/20	3/12/88/115	-
17	CLA	A	815	-	1/1/10/20	2/12/88/115	-
17	CLA	1	602	-	1/1/10/20	5/12/88/115	-
17	CLA	B	823	-	1/1/10/20	2/12/88/115	-
17	CLA	6	602	-	1/1/10/20	3/12/88/115	-
17	CLA	B	821	-	1/1/11/20	3/17/93/115	-
17	CLA	3	304	-	1/1/11/20	3/15/91/115	-
20	CHL	5	313	-	3/3/15/26	0/12/110/137	-
17	CLA	7	605	-	1/1/10/20	2/12/88/115	-
17	CLA	3	308	-	1/1/10/20	0/12/88/115	-
17	CLA	8	612	-	1/1/11/20	0/17/93/115	-
17	CLA	B	801	-	1/1/10/20	2/12/88/115	-
17	CLA	B	830	-	1/1/10/20	3/12/88/115	-
17	CLA	B	827	-	1/1/10/20	4/12/88/115	-
17	CLA	A	813	-	1/1/10/20	2/12/88/115	-
17	CLA	A	814	-	1/1/10/20	3/12/88/115	-
17	CLA	8	607	-	1/1/10/20	3/12/88/115	-
17	CLA	8	601	11	1/1/10/20	2/12/88/115	-
17	CLA	B	812	-	1/1/10/20	4/12/88/115	-
17	CLA	B	831	-	1/1/10/20	4/12/88/115	-
17	CLA	4	605	-	1/1/11/20	3/15/91/115	-
17	CLA	3	306	-	1/1/10/20	4/12/88/115	-
17	CLA	B	806	-	1/1/10/20	2/12/88/115	-
19	SF4	C	101	-	-	-	0/6/5/5
17	CLA	6	610	-	1/1/11/20	4/15/91/115	-
17	CLA	7	614	10	1/1/10/20	2/12/88/115	-
17	CLA	B	838	-	1/1/10/20	4/12/88/115	-
17	CLA	A	843	-	1/1/10/20	2/12/88/115	-
17	CLA	A	804	-	1/1/10/20	2/12/88/115	-
17	CLA	4	601	-	1/1/10/20	2/12/88/115	-
17	CLA	8	613	-	1/1/10/20	3/12/88/115	-
17	CLA	5	301	-	1/1/10/20	2/12/88/115	-
17	CLA	A	810	-	1/1/10/20	2/12/88/115	-
17	CLA	5	303	-	1/1/11/20	5/19/95/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CHL	1	601	8	3/3/17/26	5/24/122/137	-
17	CLA	B	810	-	1/1/11/20	5/15/91/115	-
17	CLA	3	302	-	1/1/10/20	5/12/88/115	-
17	CLA	8	605	-	1/1/10/20	4/12/88/115	-
17	CLA	A	834	1	1/1/10/20	0/12/88/115	-
20	CHL	7	606	-	3/3/15/26	0/12/110/137	-
17	CLA	7	612	-	1/1/11/20	2/15/91/115	-
17	CLA	3	311	-	1/1/10/20	0/12/88/115	-
17	CLA	A	821	-	1/1/12/20	7/23/99/115	-
17	CLA	A	832	-	1/1/10/20	4/10/86/115	-
20	CHL	5	305	-	3/3/16/26	1/15/113/137	-
20	CHL	3	307	-	3/3/16/26	6/15/113/137	-
17	CLA	8	609	-	1/1/10/20	3/12/88/115	-
17	CLA	7	607	-	1/1/10/20	2/12/88/115	-
18	PQN	A	840	-	-	3/23/43/43	0/2/2/2
17	CLA	A	820	-	1/1/10/20	6/12/88/115	-
17	CLA	A	842	-	1/1/10/20	2/12/88/115	-
17	CLA	B	808	-	1/1/10/20	3/12/88/115	-
17	CLA	8	610	-	1/1/10/20	1/12/88/115	-
17	CLA	B	809	-	1/1/10/20	4/12/88/115	-
17	CLA	3	305	-	1/1/10/20	2/12/88/115	-
17	CLA	4	603	-	1/1/10/20	4/12/88/115	-
17	CLA	A	811	-	1/1/10/20	4/12/88/115	-
17	CLA	5	310	-	1/1/10/20	2/12/88/115	-
17	CLA	6	603	-	1/1/10/20	2/12/88/115	-
17	CLA	1	605	-	1/1/10/20	1/12/88/115	-
17	CLA	A	824	-	1/1/10/20	2/12/88/115	-
17	CLA	B	818	-	1/1/10/20	4/12/88/115	-
17	CLA	4	604	-	1/1/10/20	5/12/88/115	-
17	CLA	8	611	-	1/1/10/20	4/12/88/115	-
17	CLA	A	837	-	1/1/10/20	3/12/88/115	-
17	CLA	A	802	-	1/1/10/20	2/12/88/115	-
17	CLA	8	602	-	1/1/10/20	5/12/88/115	-
17	CLA	5	308	-	1/1/10/20	3/12/88/115	-
17	CLA	1	604	-	1/1/10/20	2/12/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	A	817	-	1/1/10/20	4/12/88/115	-
17	CLA	A	816	-	1/1/10/20	3/12/88/115	-
17	CLA	B	814	-	1/1/9/20	0/6/82/115	-
17	CLA	A	839	-	1/1/10/20	2/12/88/115	-
17	CLA	A	818	-	1/1/11/20	4/15/91/115	-
17	CLA	B	805	-	1/1/10/20	0/12/88/115	-
17	CLA	1	606	-	1/1/10/20	0/12/88/115	-
17	CLA	B	822	-	1/1/10/20	1/12/88/115	-
19	SF4	C	102	-	-	-	0/6/5/5
17	CLA	B	804	-	1/1/10/20	1/12/88/115	-
17	CLA	7	610	-	1/1/10/20	2/10/86/115	-
17	CLA	5	311	-	1/1/10/20	2/12/88/115	-
17	CLA	5	304	-	1/1/10/20	4/12/88/115	-
17	CLA	7	603	-	1/1/10/20	2/12/88/115	-
17	CLA	5	309	-	1/1/10/20	2/12/88/115	-
17	CLA	A	833	-	1/1/10/20	3/12/88/115	-
17	CLA	A	803	-	1/1/10/20	2/12/88/115	-
17	CLA	B	834	-	1/1/10/20	6/12/88/115	-
17	CLA	B	829	-	1/1/10/20	4/13/89/115	-
17	CLA	B	815	-	1/1/15/20	10/39/115/115	-
17	CLA	B	802	-	1/1/11/20	5/15/91/115	-
17	CLA	7	608	-	1/1/10/20	0/12/88/115	-
20	CHL	Z	601	12	3/3/15/26	2/12/110/137	-
17	CLA	B	824	-	1/1/10/20	2/10/86/115	-
18	PQN	B	840	-	-	4/23/43/43	0/2/2/2
17	CLA	1	608	-	1/1/10/20	2/12/88/115	-
17	CLA	7	613	-	1/1/10/20	4/13/89/115	-
17	CLA	8	614	11	1/1/10/20	2/12/88/115	-
20	CHL	6	607	-	3/3/15/26	1/12/110/137	-
17	CLA	A	826	-	1/1/10/20	2/12/88/115	-
17	CLA	F	302	-	1/1/14/20	6/36/112/115	-
17	CLA	1	610	-	1/1/10/20	1/12/88/115	-
17	CLA	3	303	-	1/1/10/20	0/12/88/115	-
17	CLA	A	828	-	1/1/10/20	3/12/88/115	-

The worst 5 of 1546 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	3	307	CHL	C3A-C2A	-8.14	1.47	1.54
17	1	608	CLA	C4B-NB	8.10	1.48	1.37
17	7	604	CLA	C4B-NB	7.81	1.48	1.37
17	B	821	CLA	C4B-NB	7.70	1.48	1.37
17	B	814	CLA	C4B-NB	7.69	1.48	1.37

The worst 5 of 1389 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	804	CLA	C4A-NA-C1A	-9.53	102.33	106.68
17	3	310	CLA	C4A-NA-C1A	-9.12	102.52	106.68
17	A	832	CLA	C1C-NC-C4C	-8.81	102.66	106.68
17	B	815	CLA	C4A-NA-C1A	-8.74	102.69	106.68
17	B	812	CLA	C4A-NA-C1A	-8.67	102.72	106.68

5 of 188 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
16	A	801	CL0	NC
16	A	801	CL0	ND
16	A	801	CL0	NA
17	A	802	CLA	ND
17	A	803	CLA	ND

5 of 471 torsion outliers are listed below:

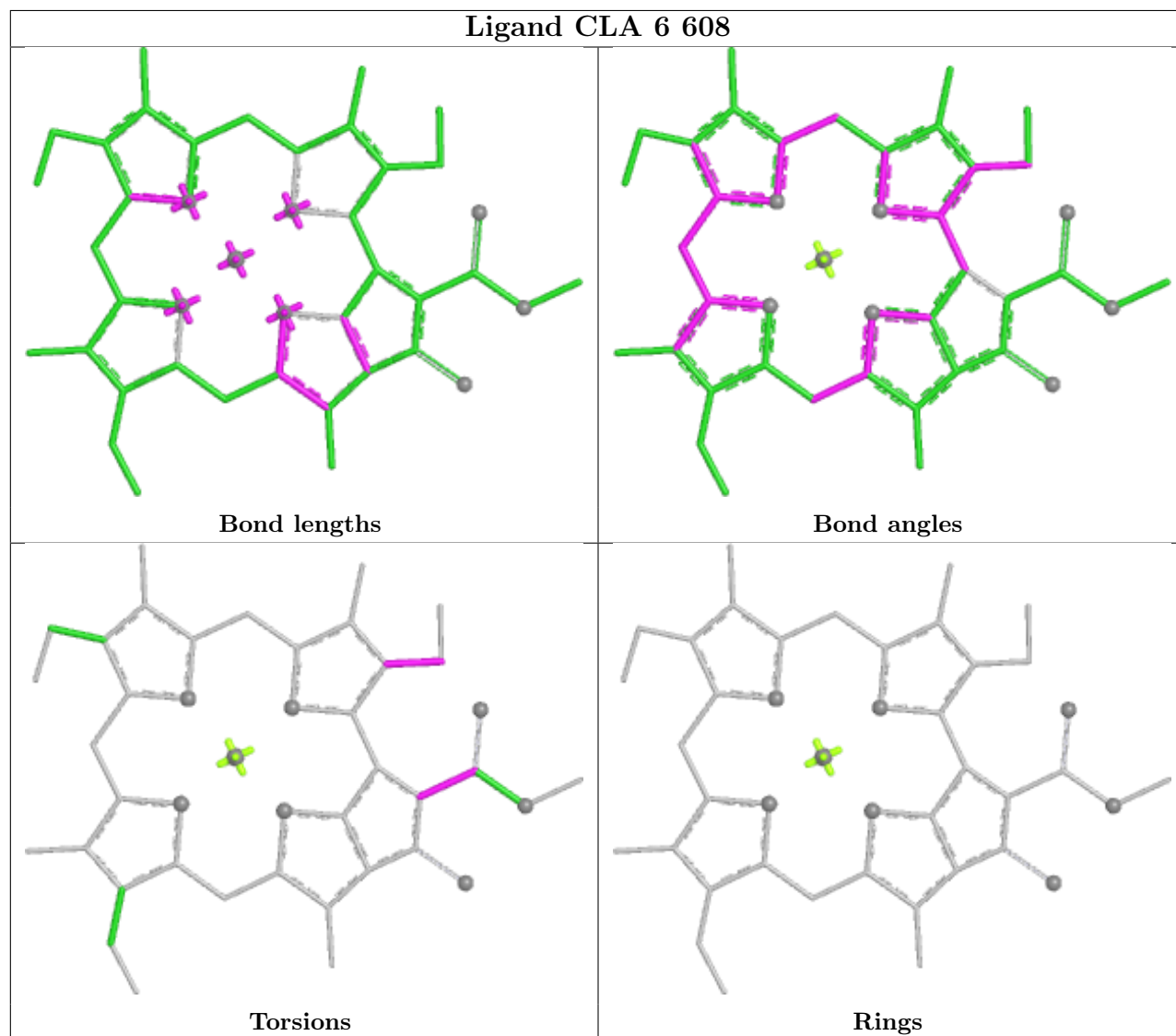
Mol	Chain	Res	Type	Atoms
17	A	802	CLA	C1A-C2A-CAA-CBA
17	A	803	CLA	C2B-C3B-CAB-CBB
17	A	803	CLA	C4B-C3B-CAB-CBB
17	A	805	CLA	C1A-C2A-CAA-CBA
17	A	805	CLA	C4B-C3B-CAB-CBB

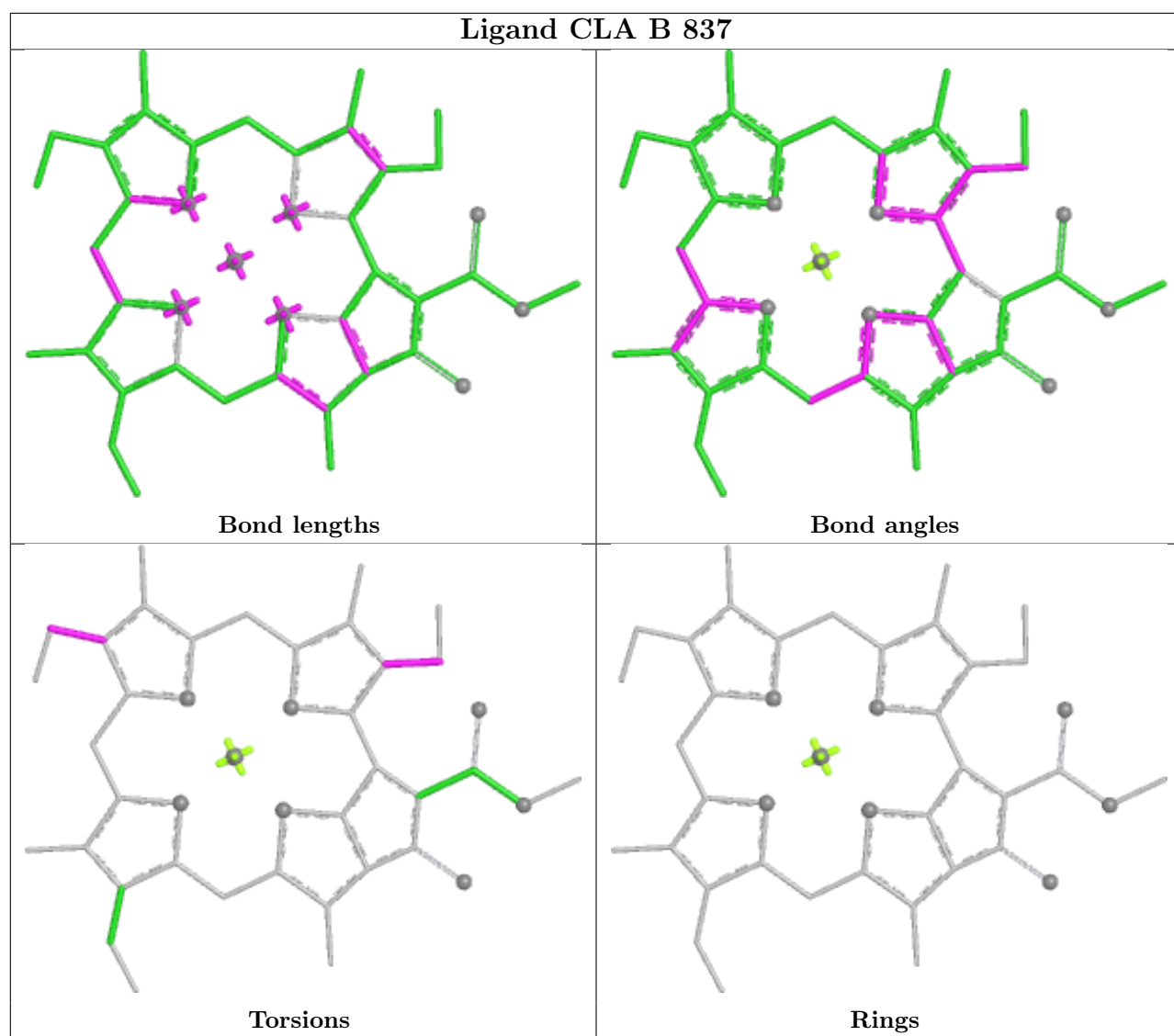
There are no ring outliers.

No monomer is involved in short contacts.

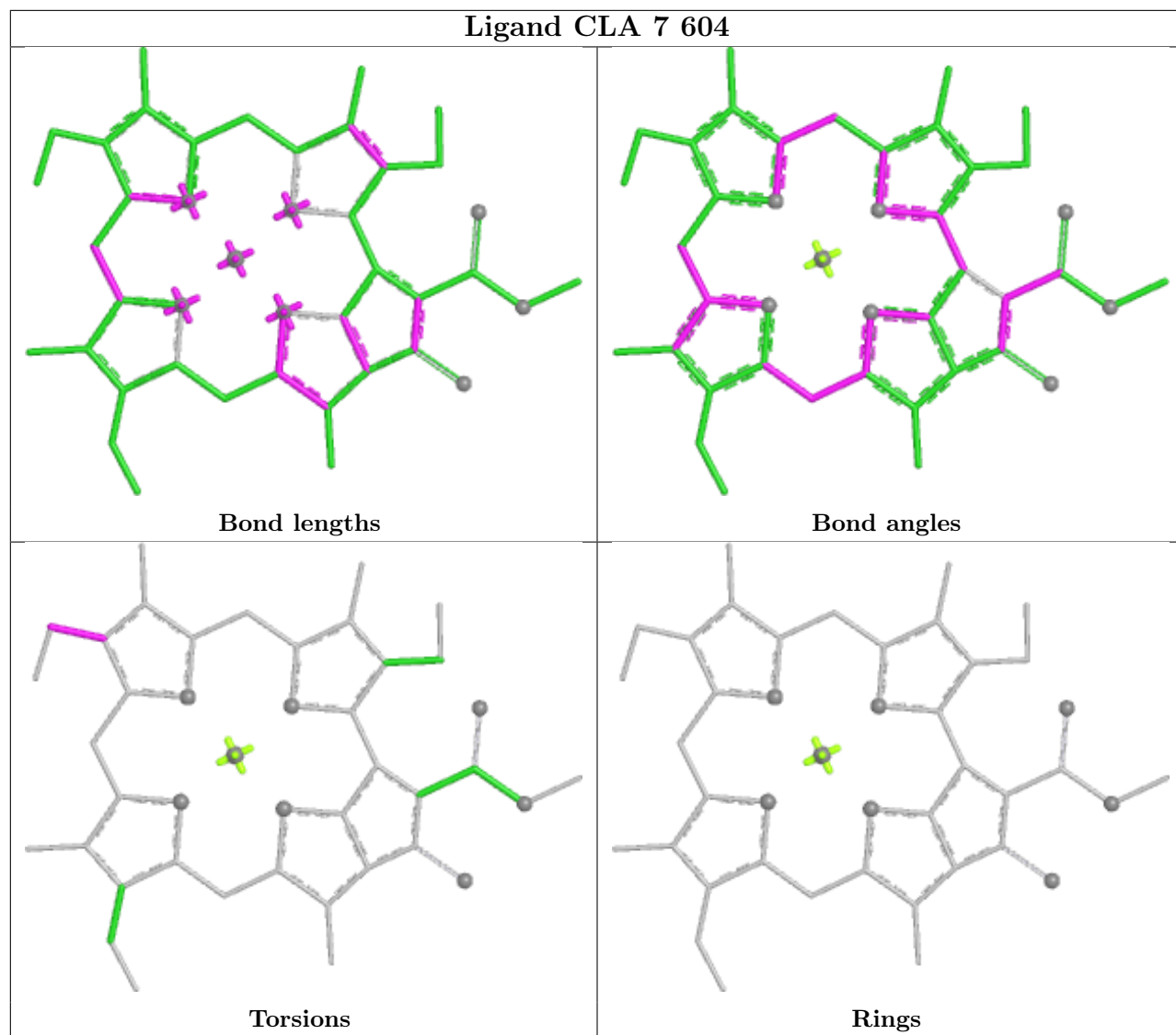
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

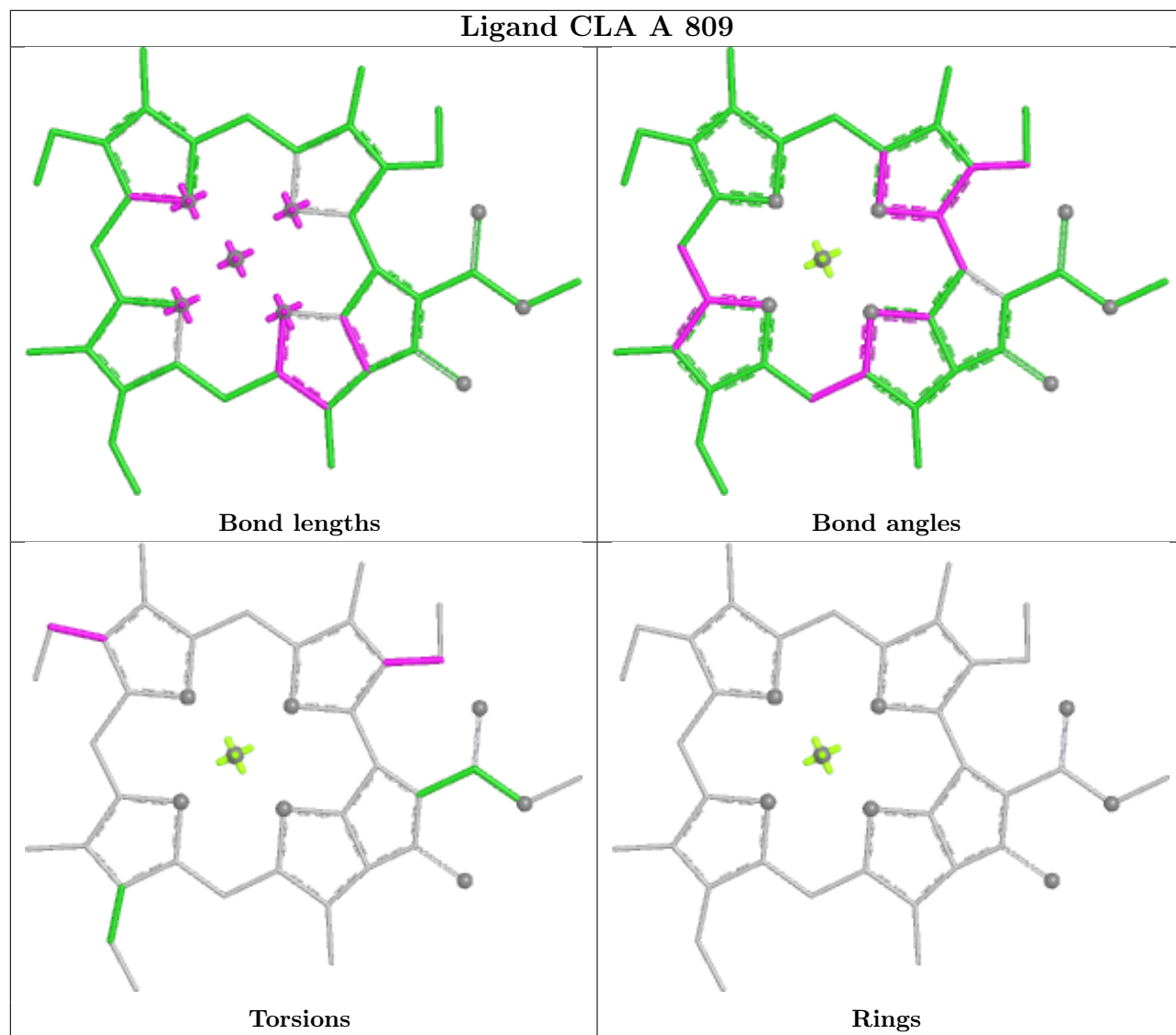




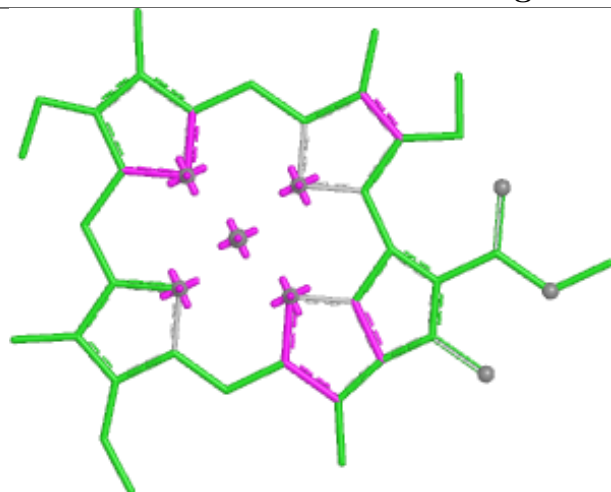
Ligand CLA 7 604



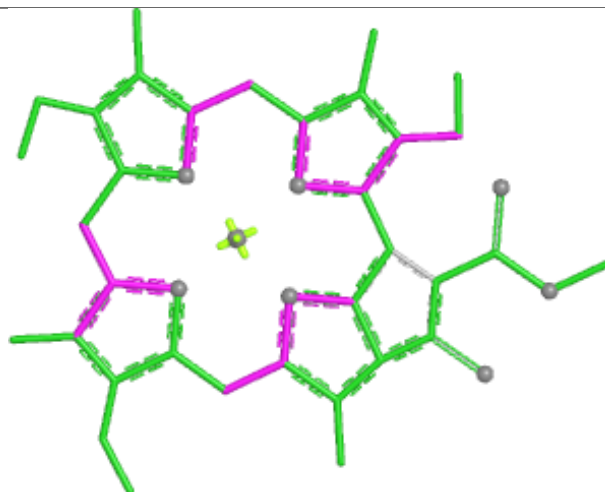
Ligand CLA A 809



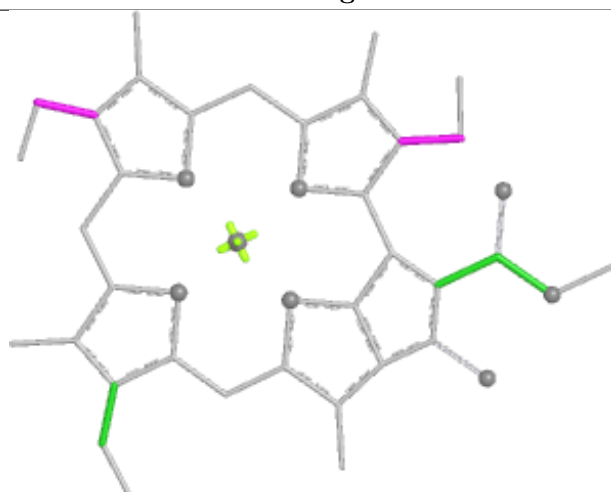
Ligand CLA B 816



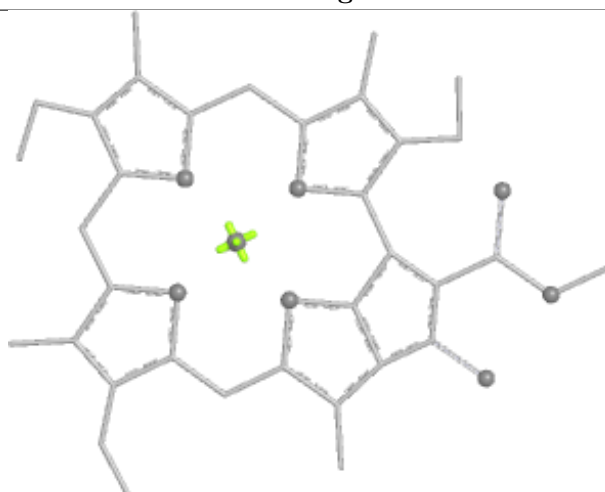
Bond lengths



Bond angles

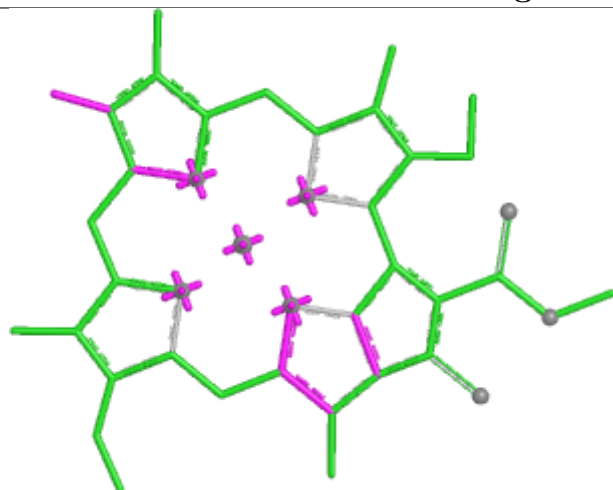


Torsions

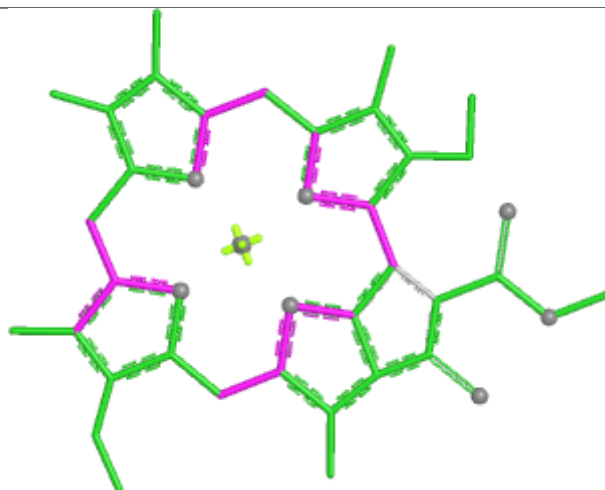


Rings

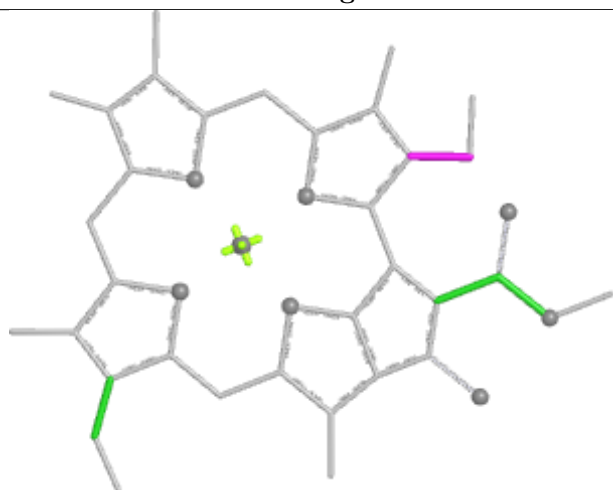
Ligand CLA B 813



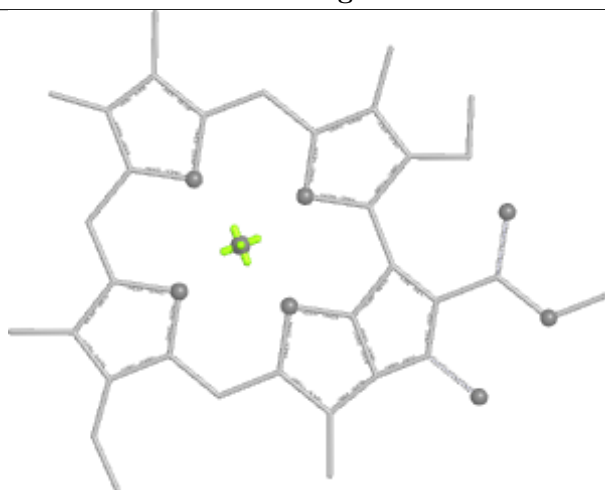
Bond lengths



Bond angles

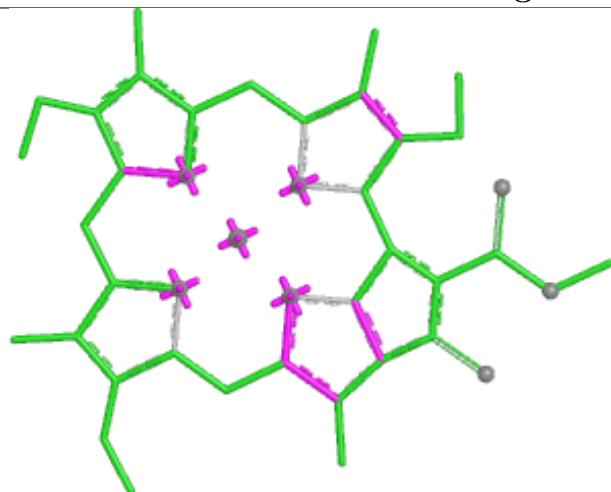


Torsions

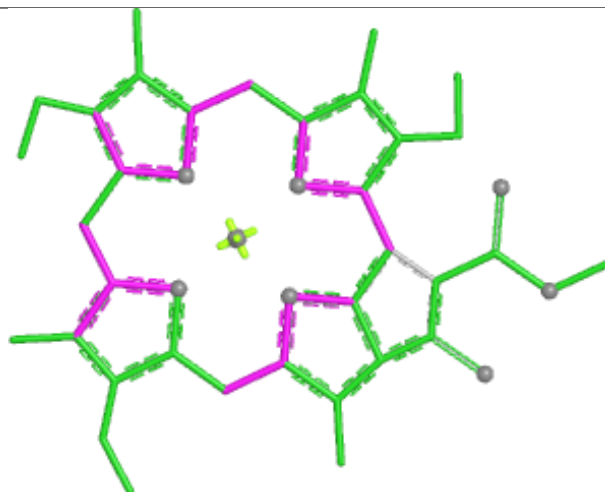


Rings

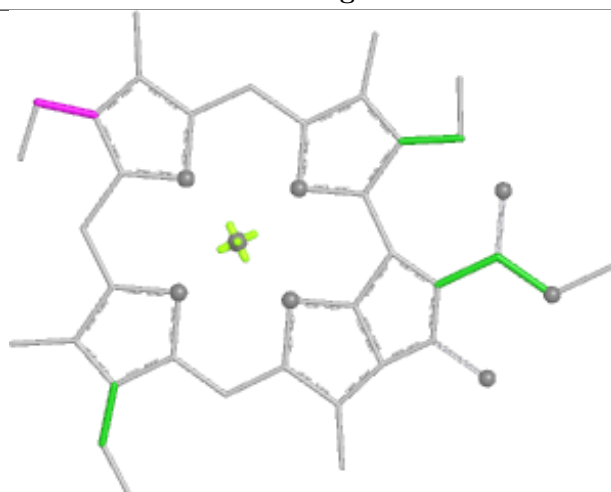
Ligand CLA B 839



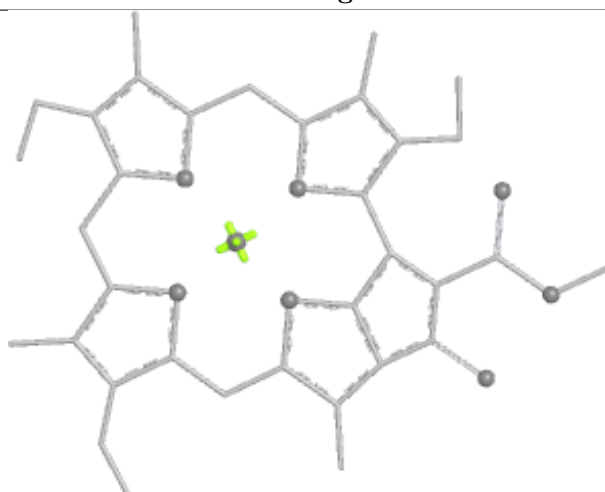
Bond lengths



Bond angles

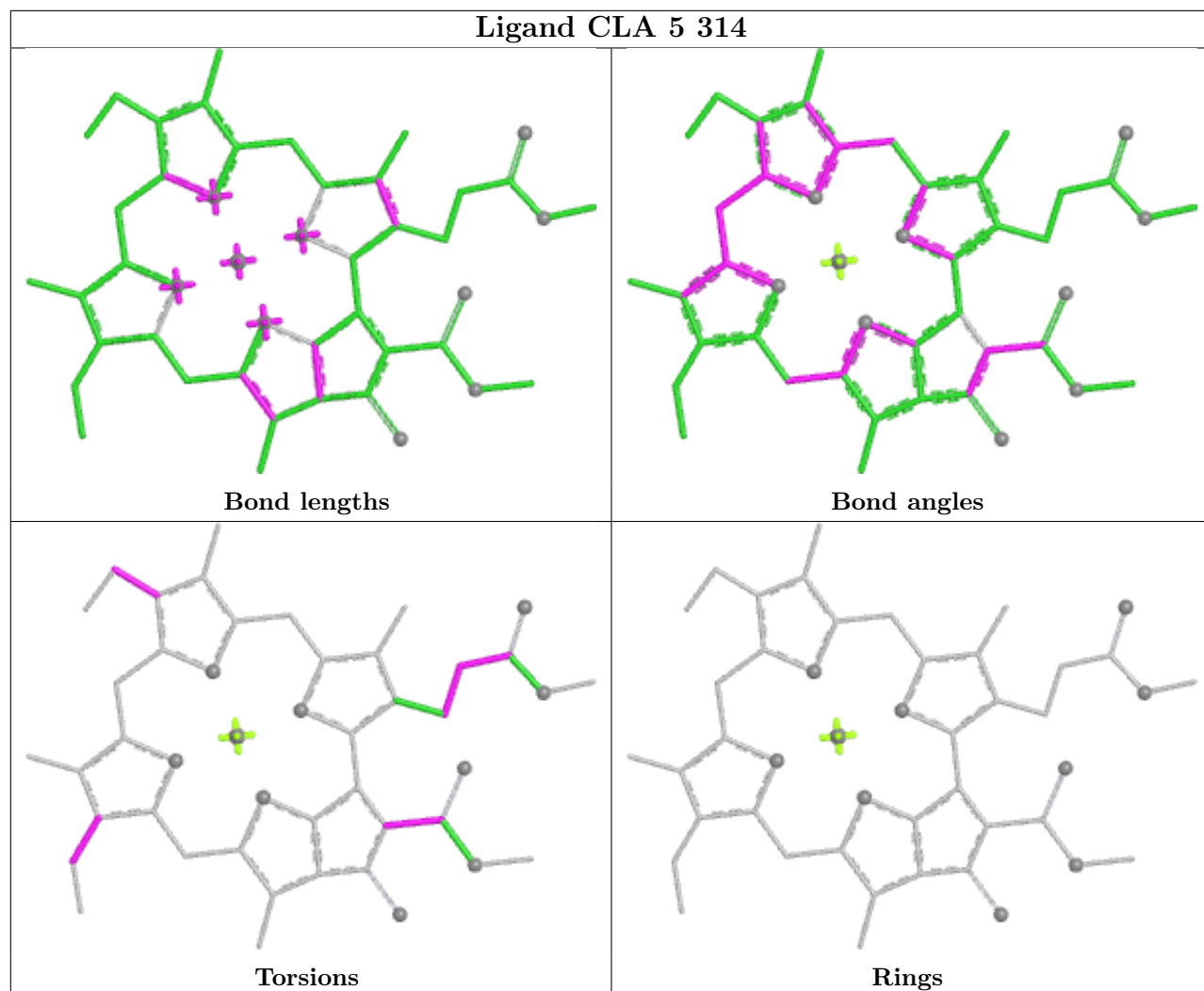


Torsions

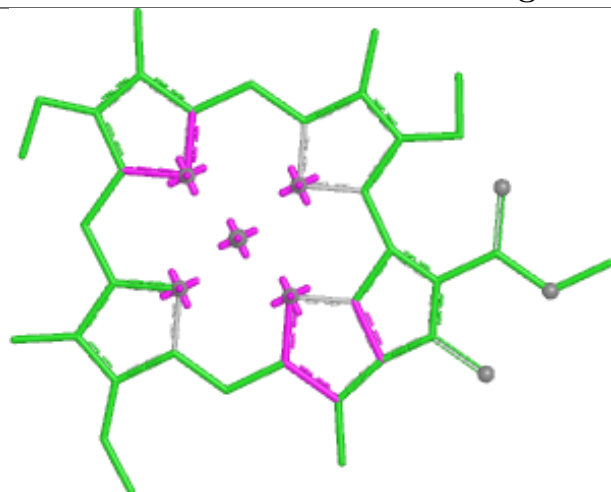


Rings

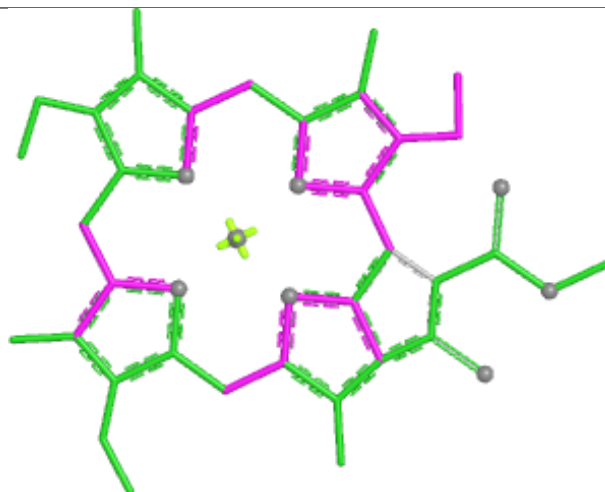
Ligand CLA 5 314



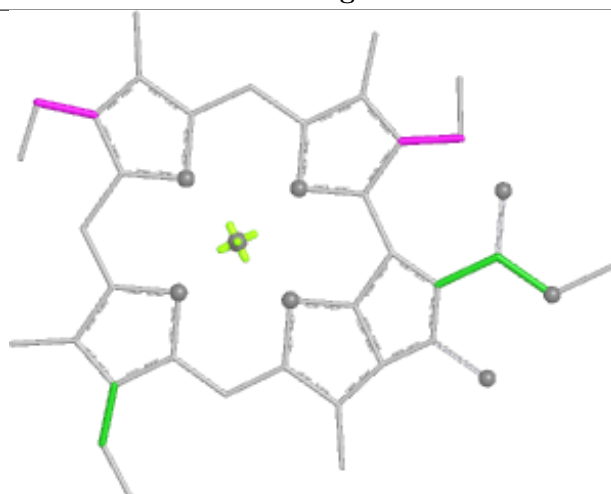
Ligand CLA 1 607



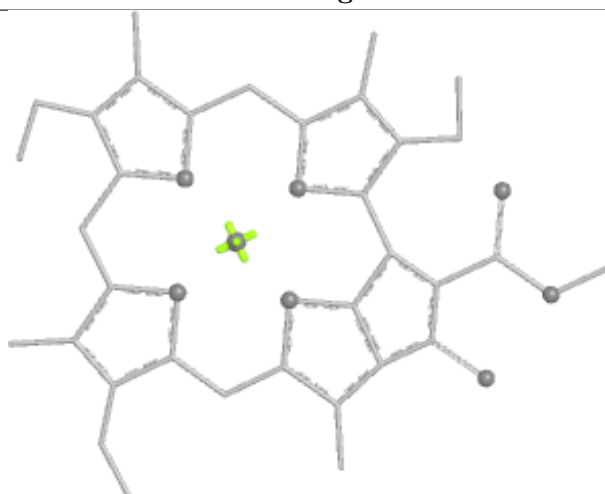
Bond lengths



Bond angles

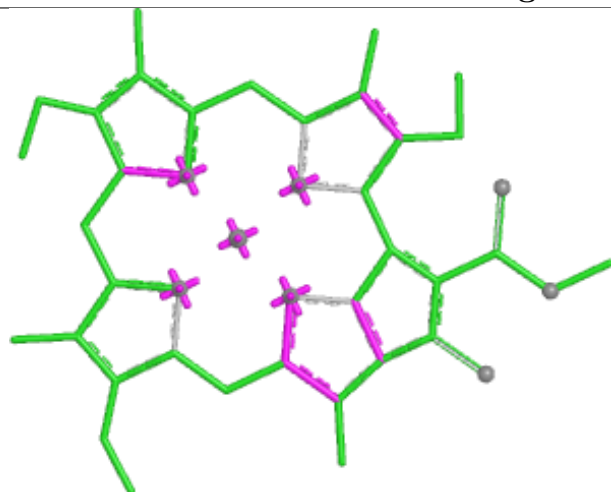


Torsions

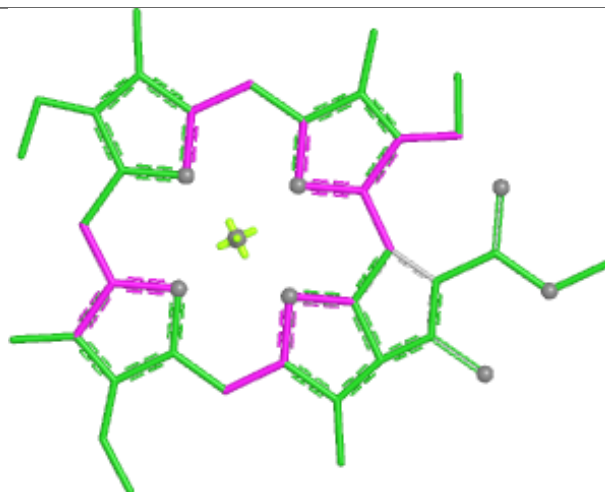


Rings

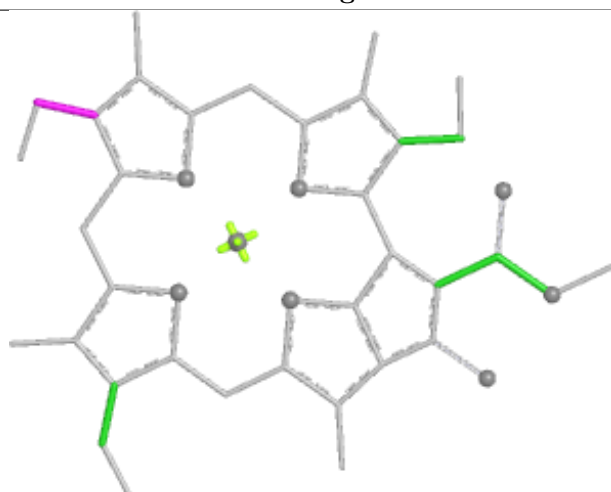
Ligand CLA 6 604



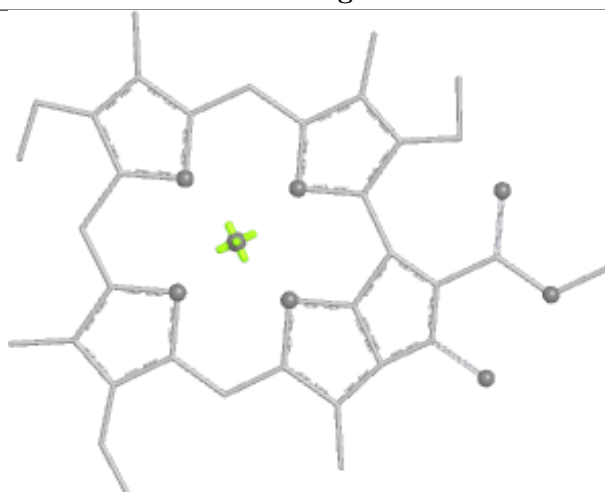
Bond lengths



Bond angles

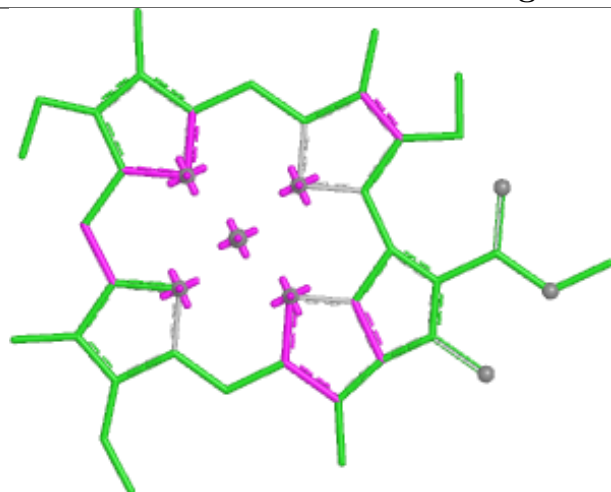


Torsions

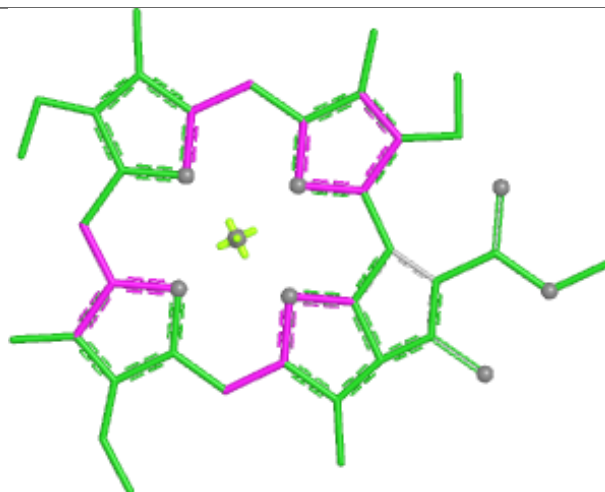


Rings

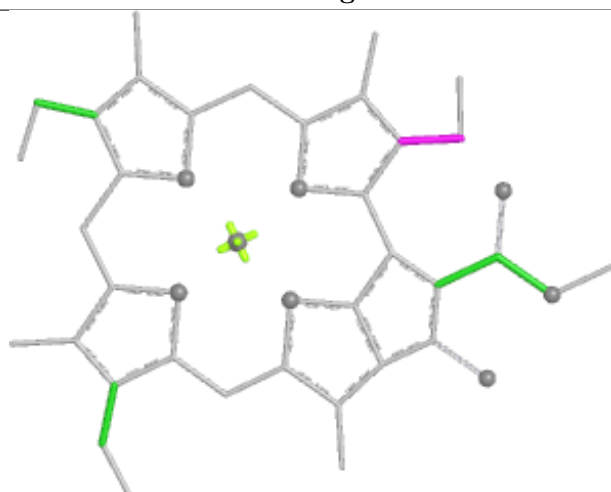
Ligand CLA 7 611



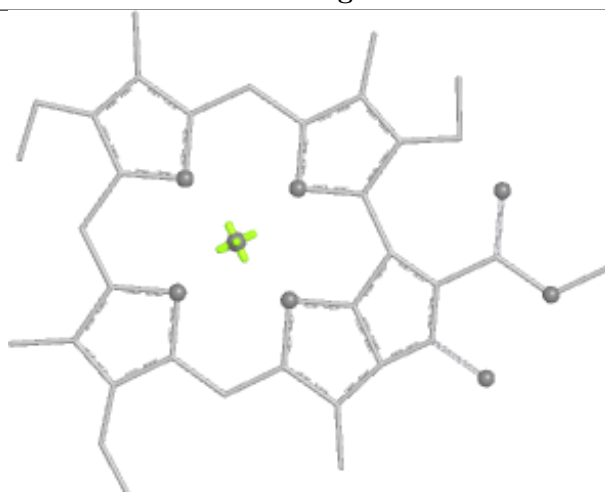
Bond lengths



Bond angles

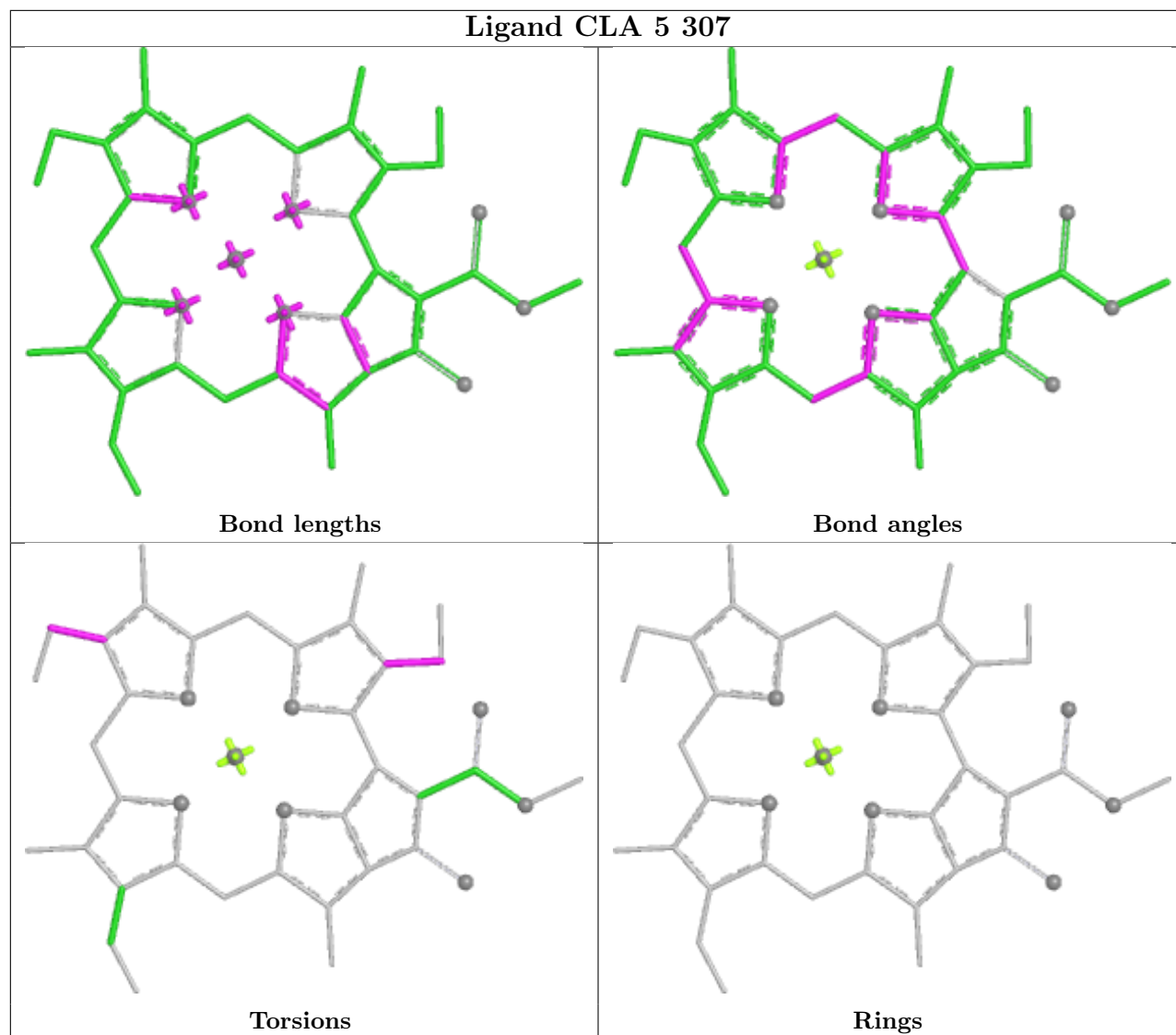


Torsions

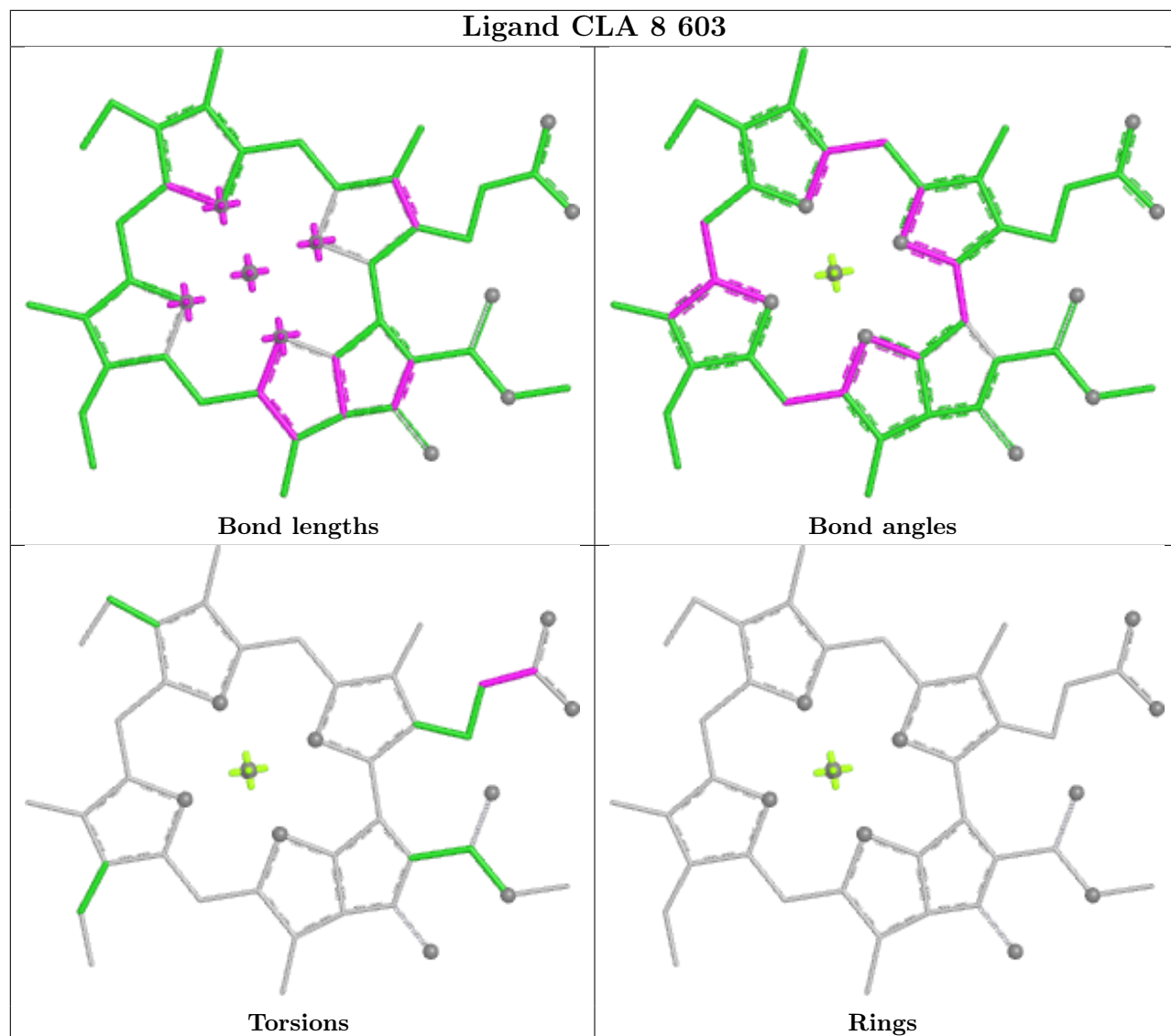


Rings

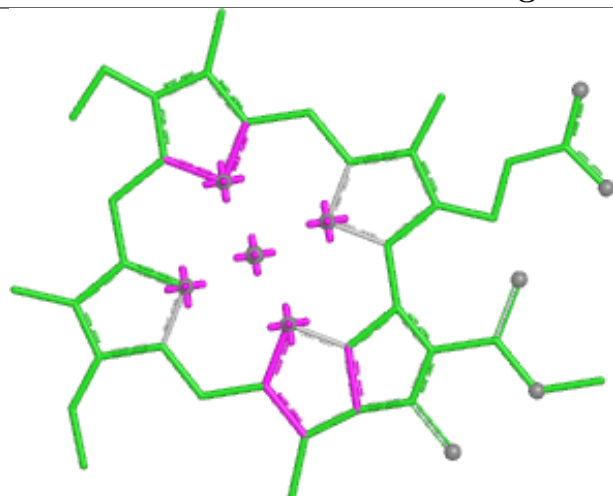
Ligand CLA 5 307



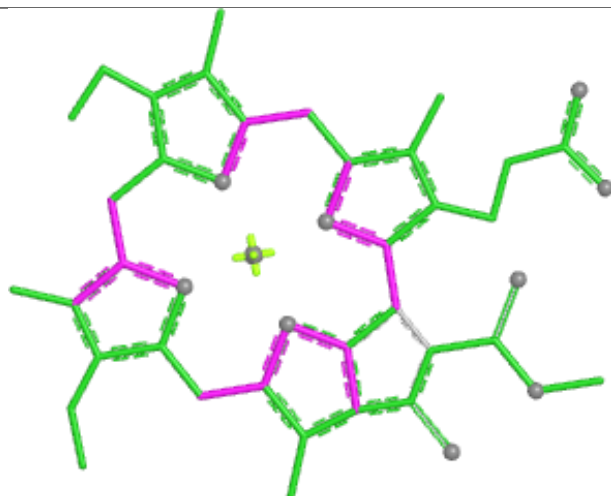
Ligand CLA 8 603



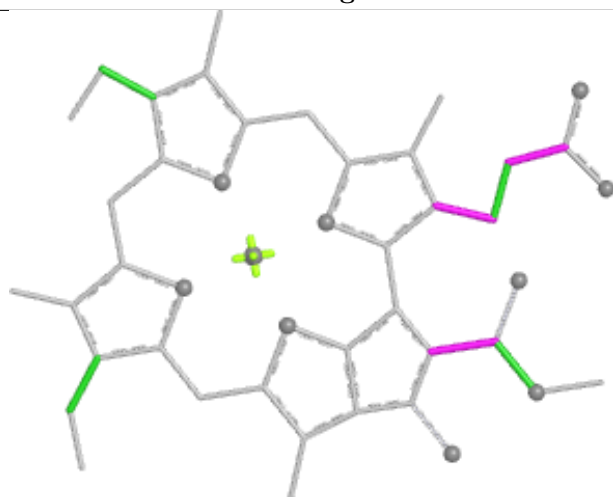
Ligand CLA 4 602



Bond lengths



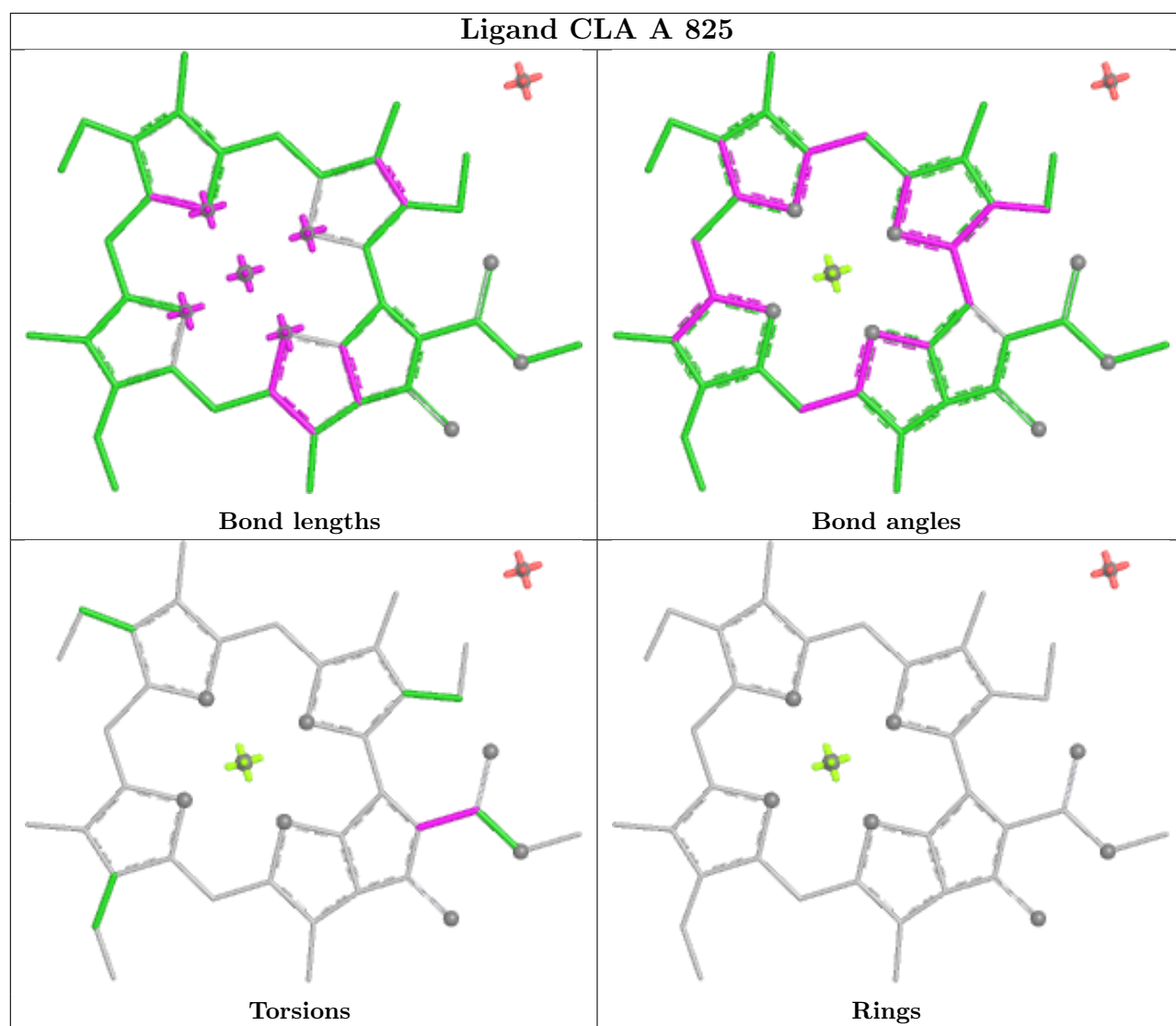
Bond angles



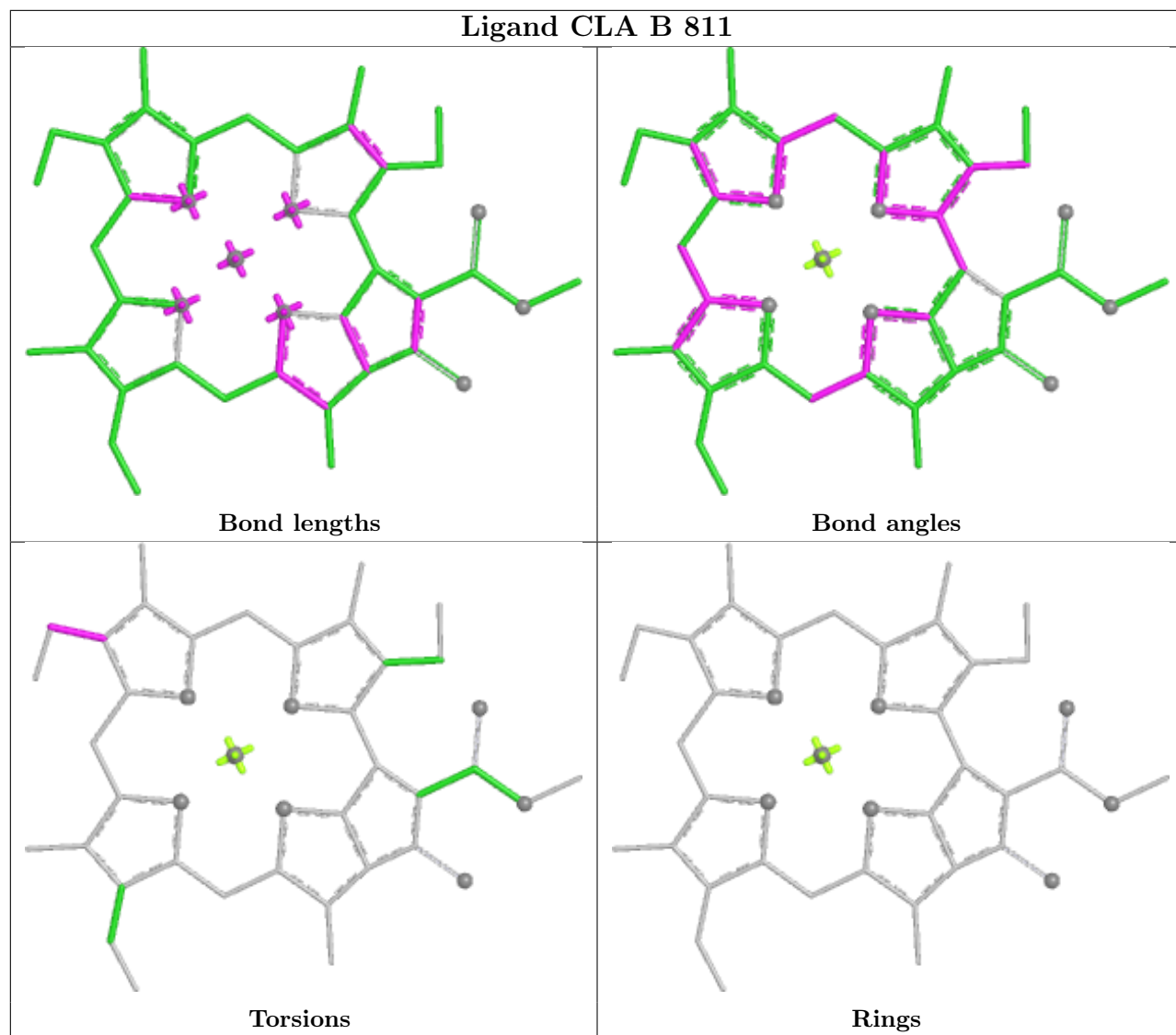
Torsions



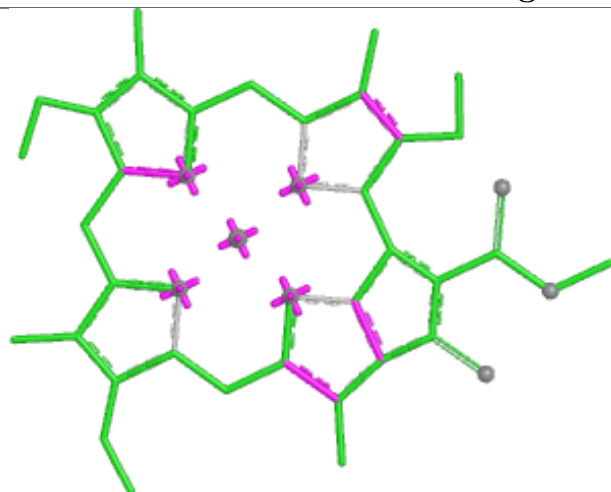
Rings



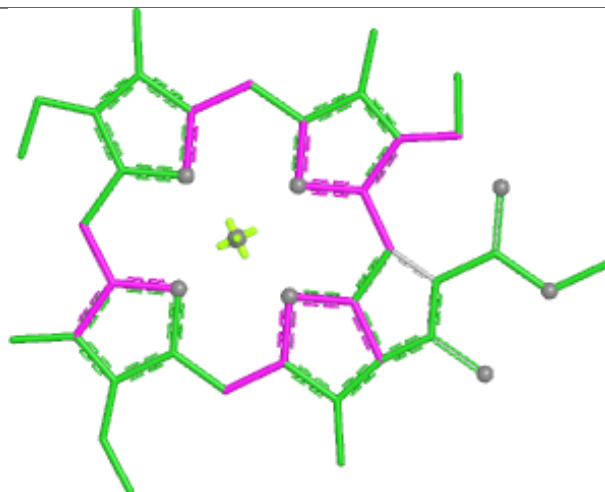
Ligand CLA B 811



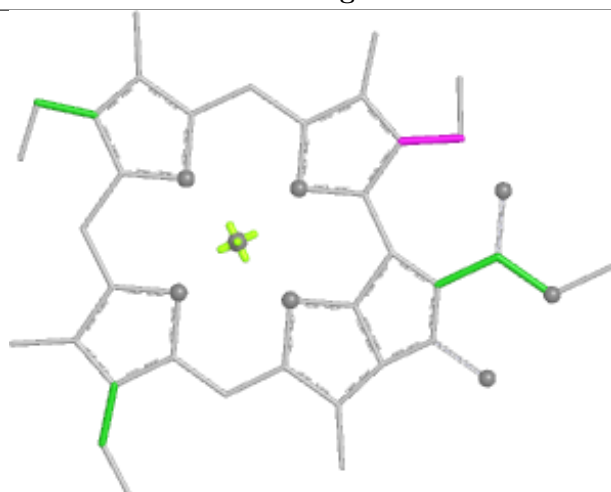
Ligand CLA 3 301



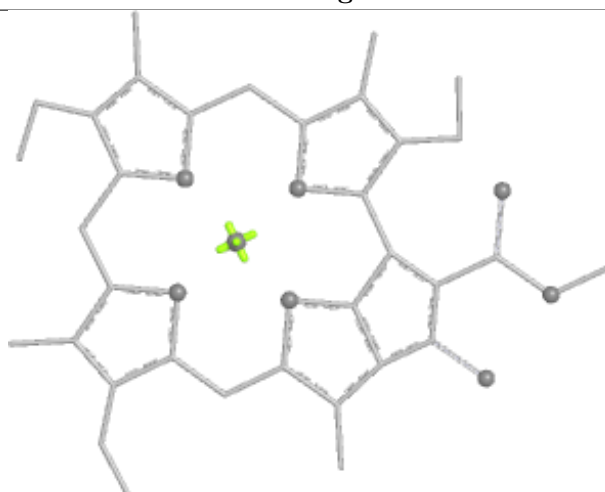
Bond lengths



Bond angles

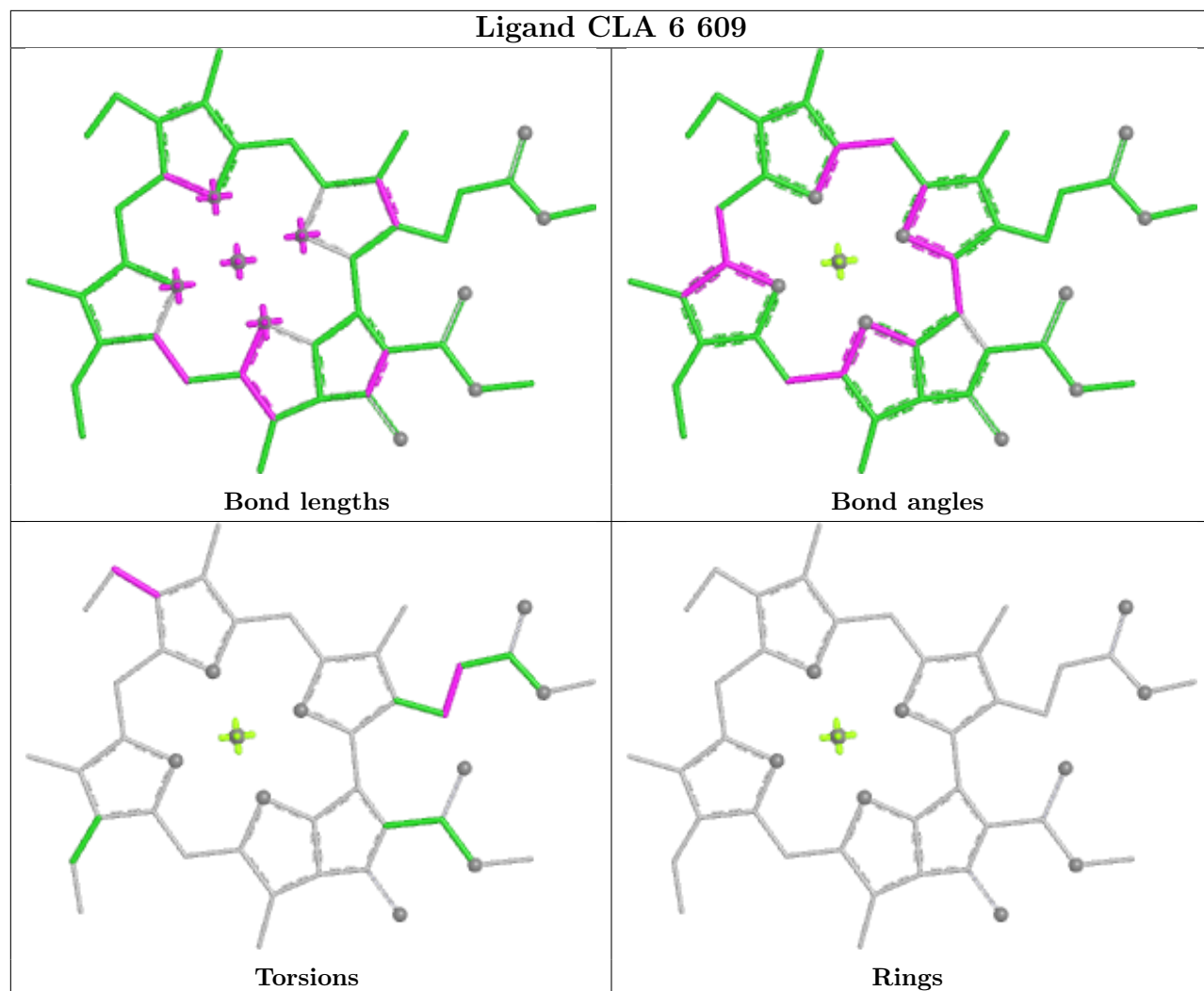


Torsions

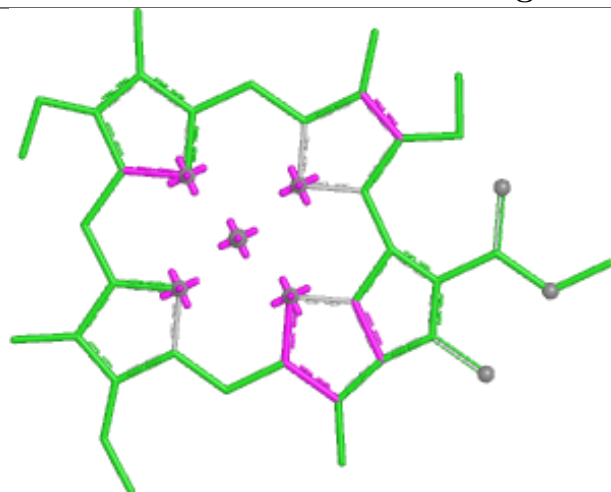


Rings

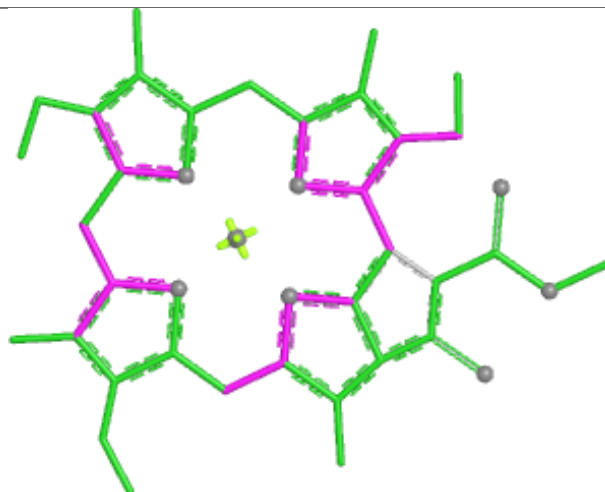
Ligand CLA 6 609



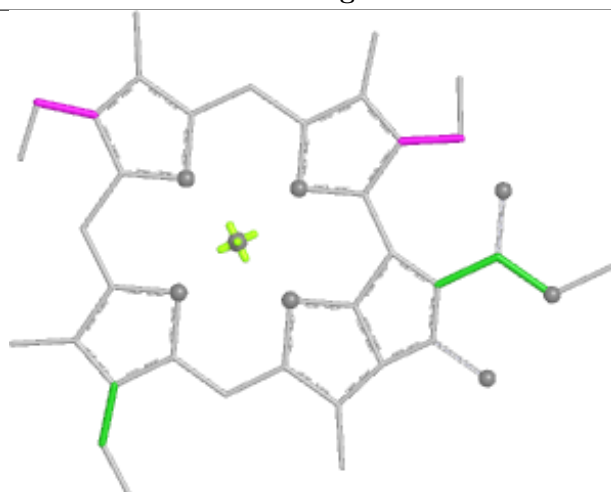
Ligand CLA F 301



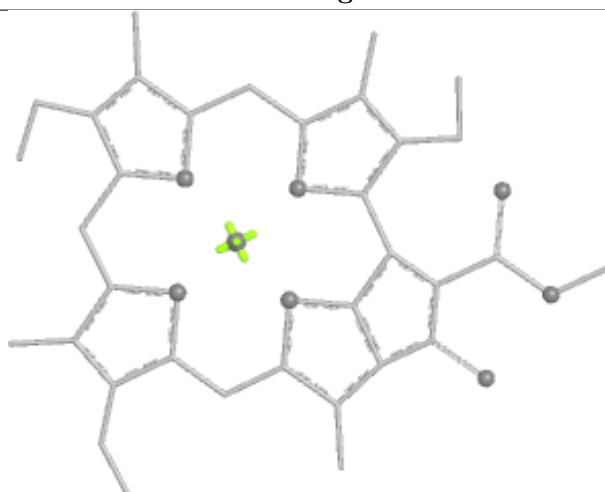
Bond lengths



Bond angles

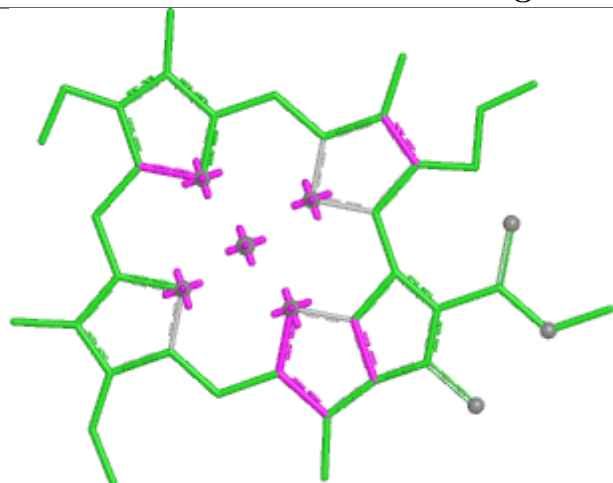


Torsions

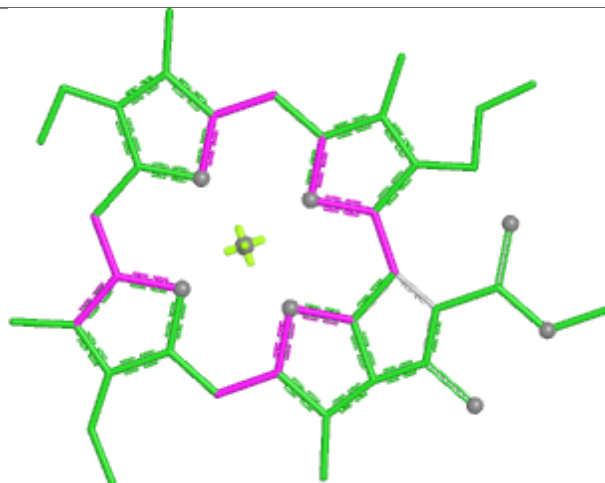


Rings

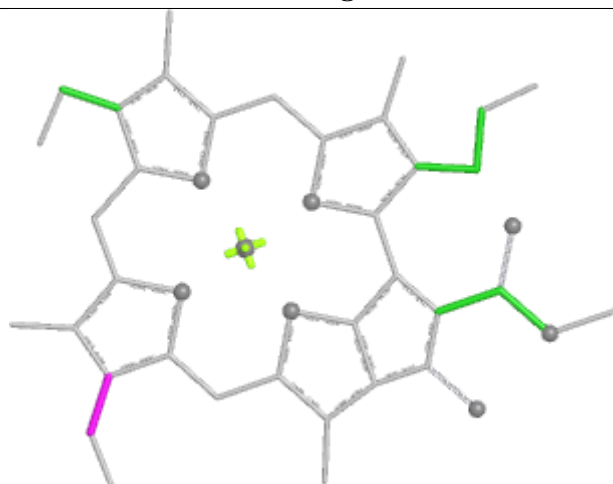
Ligand CLA B 828



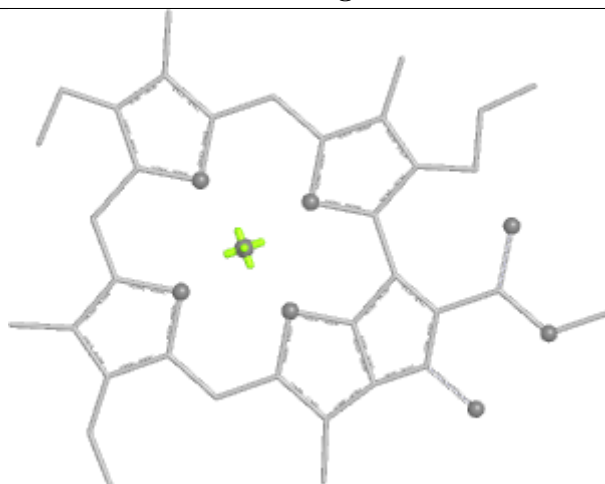
Bond lengths



Bond angles

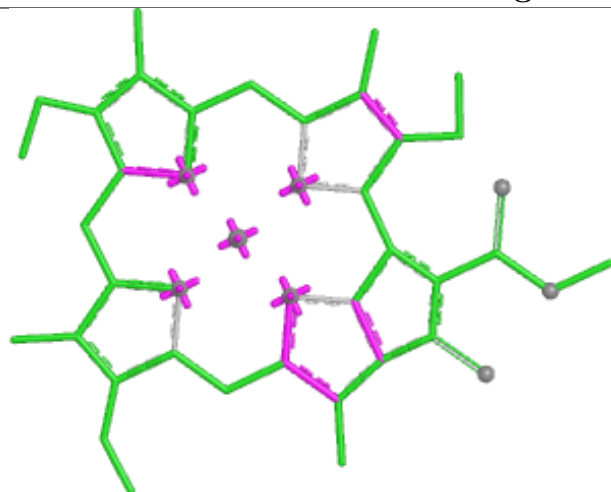


Torsions

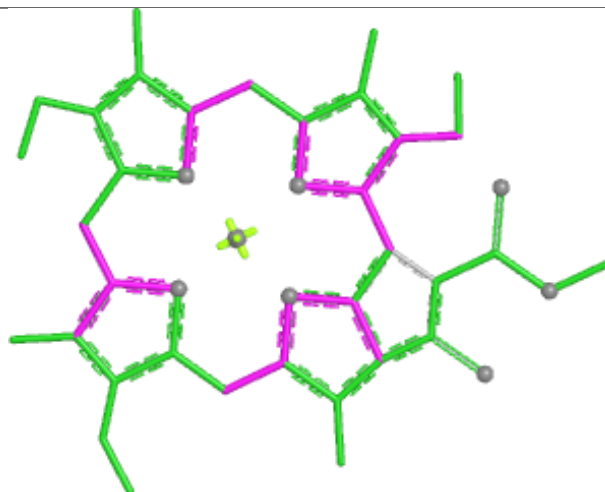


Rings

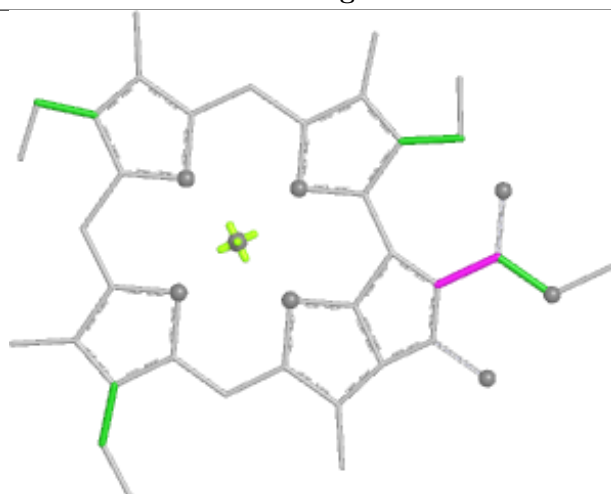
Ligand CLA B 807



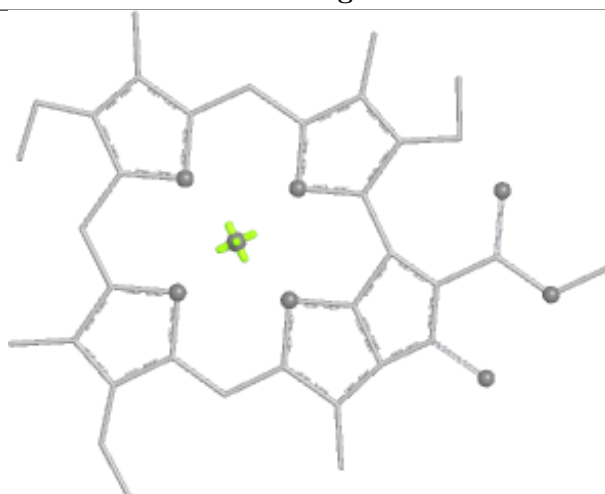
Bond lengths



Bond angles

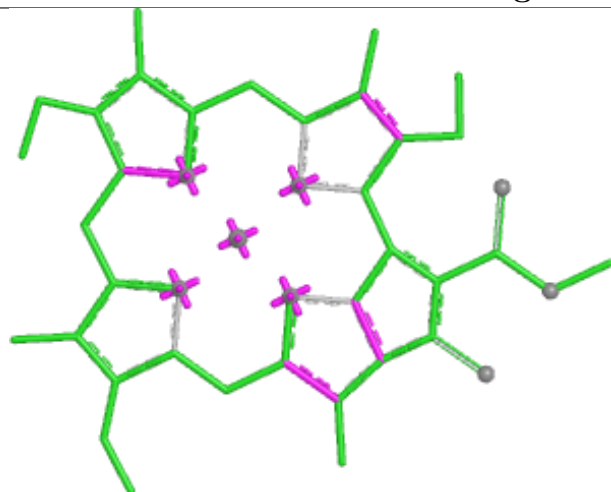


Torsions

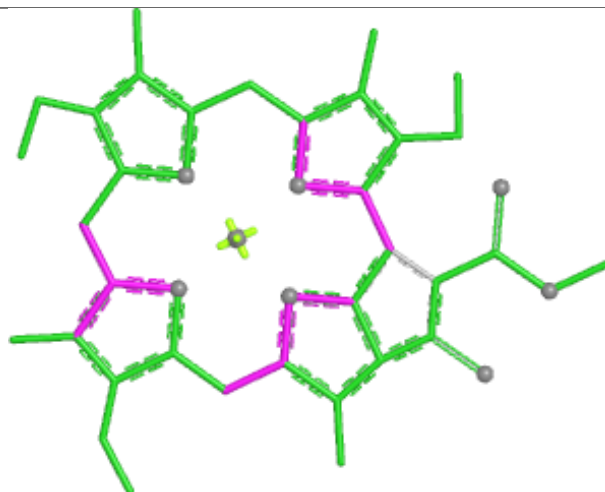


Rings

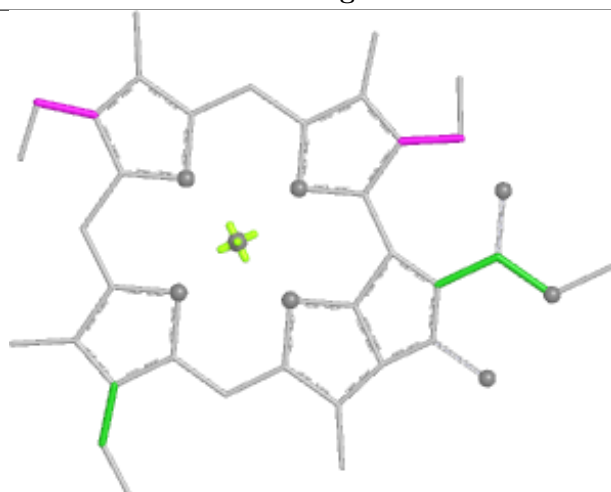
Ligand CLA A 822



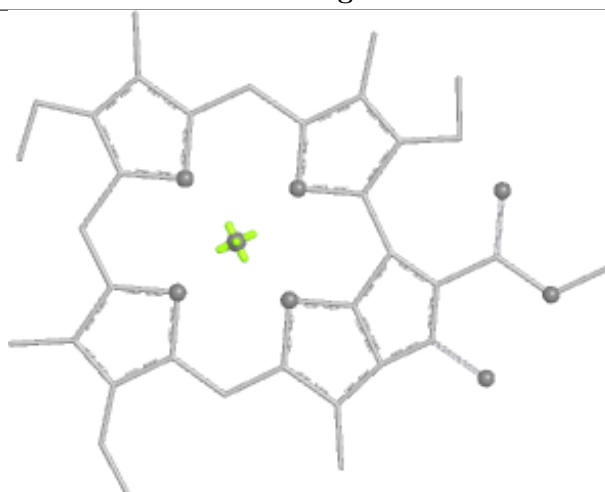
Bond lengths



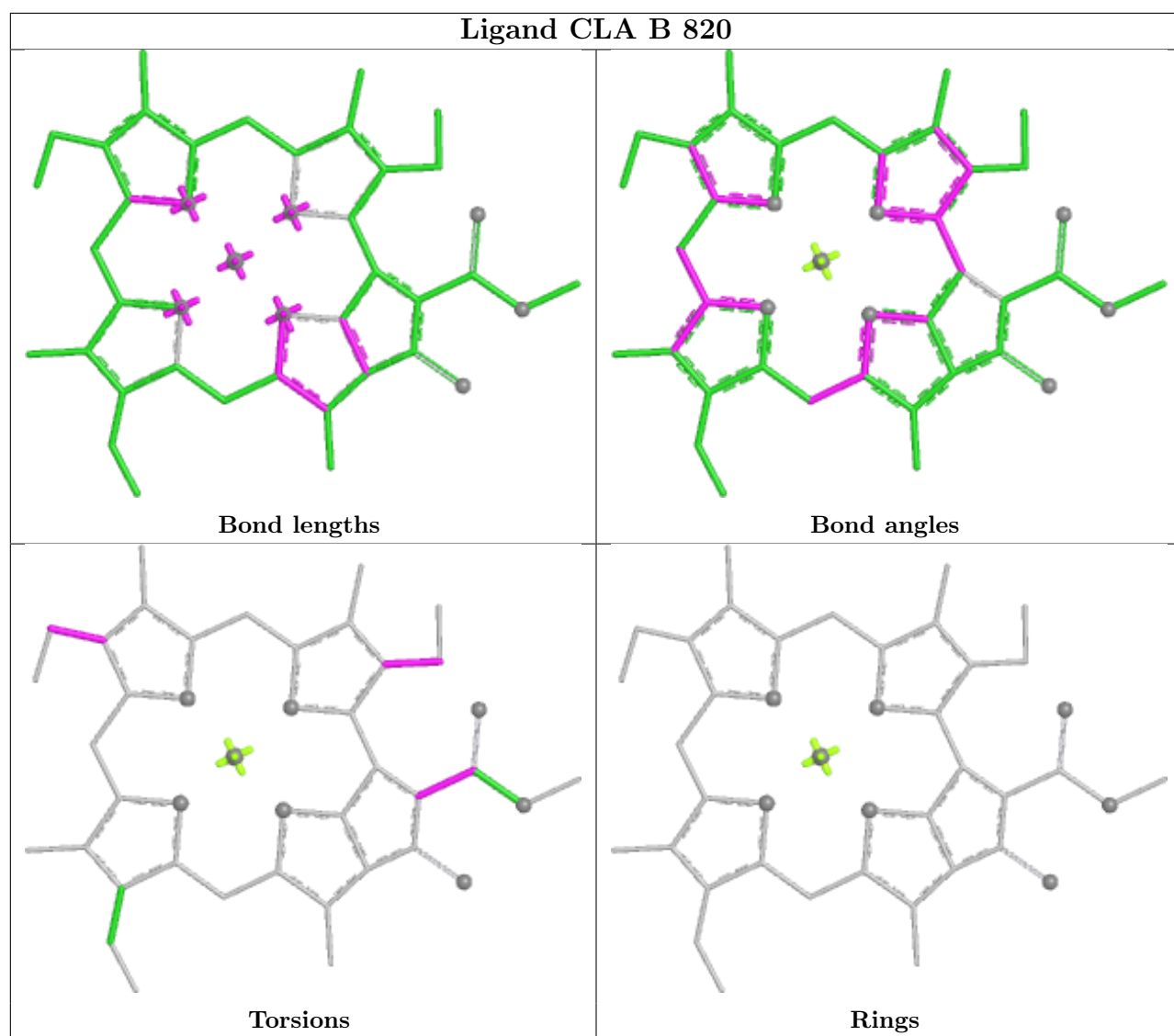
Bond angles



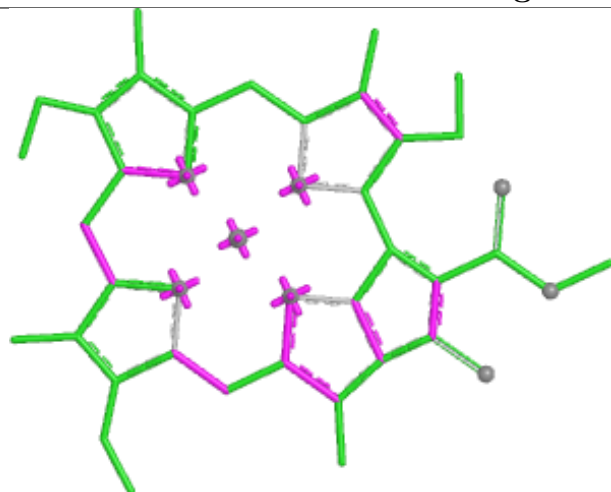
Torsions



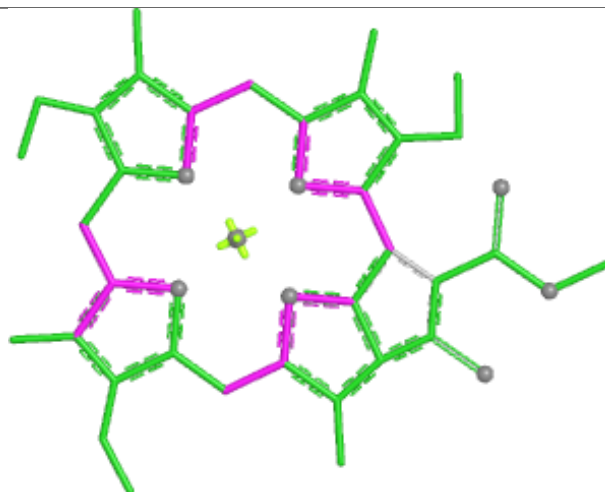
Rings



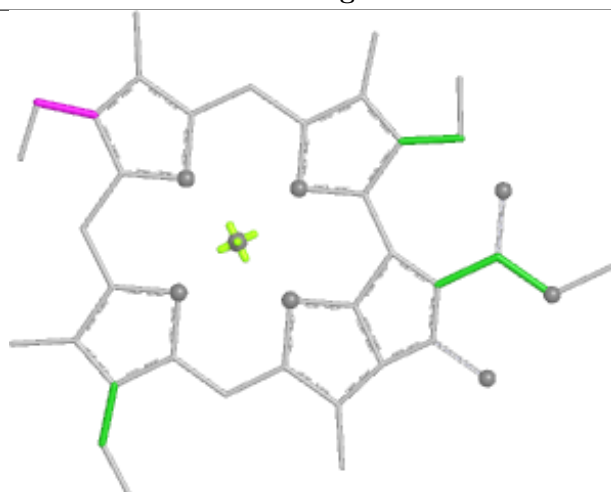
Ligand CLA A 808



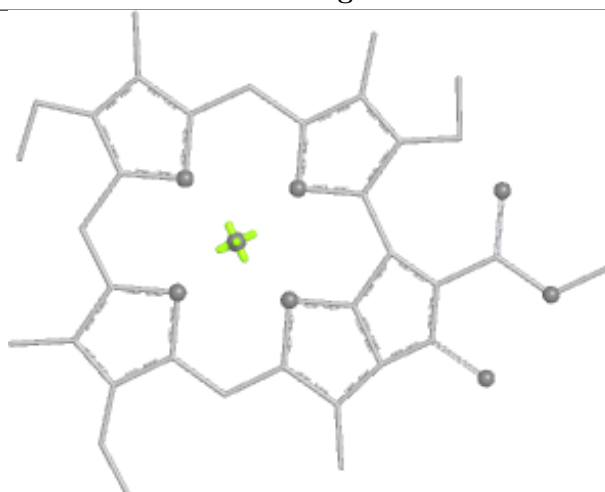
Bond lengths



Bond angles

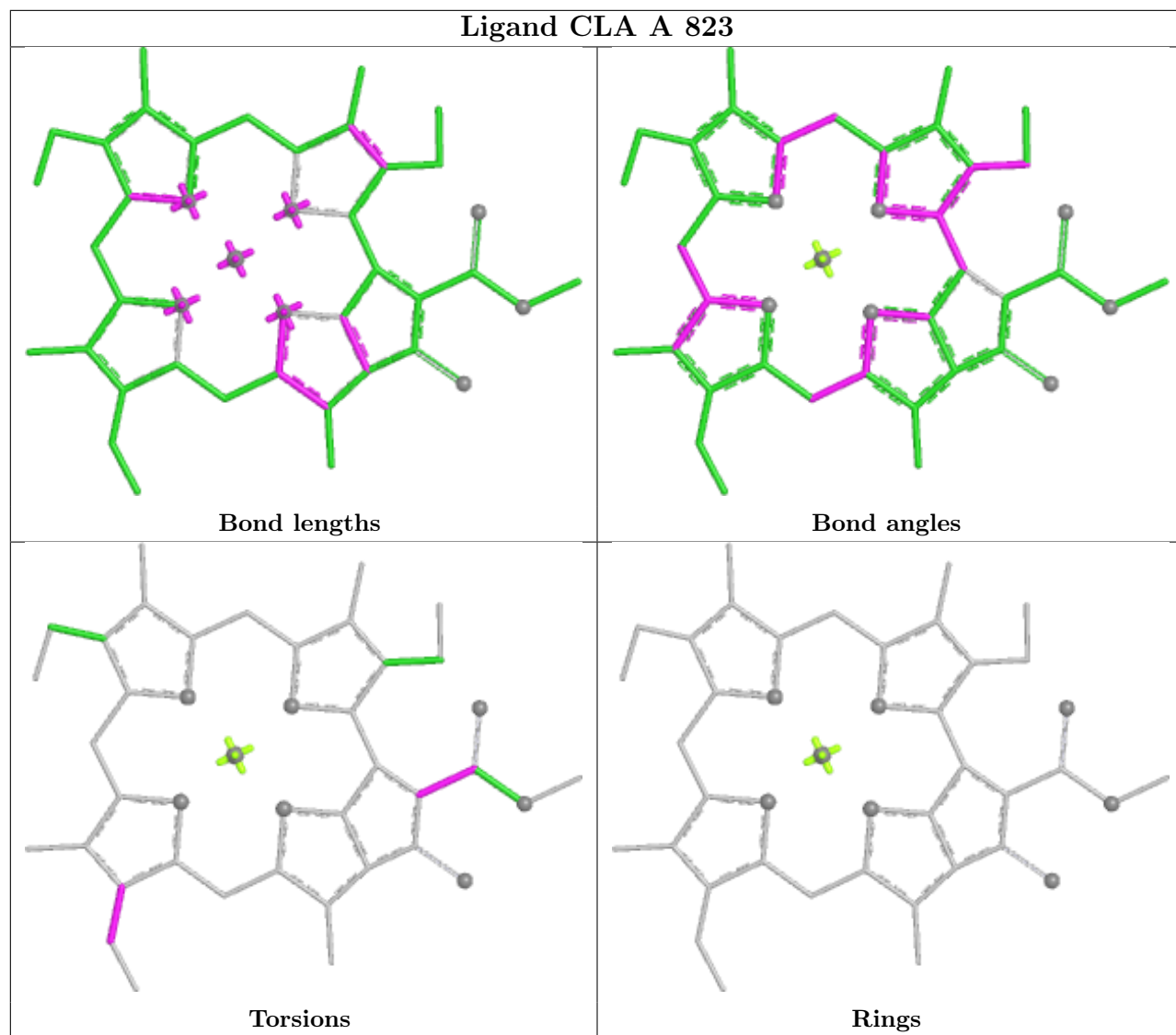


Torsions

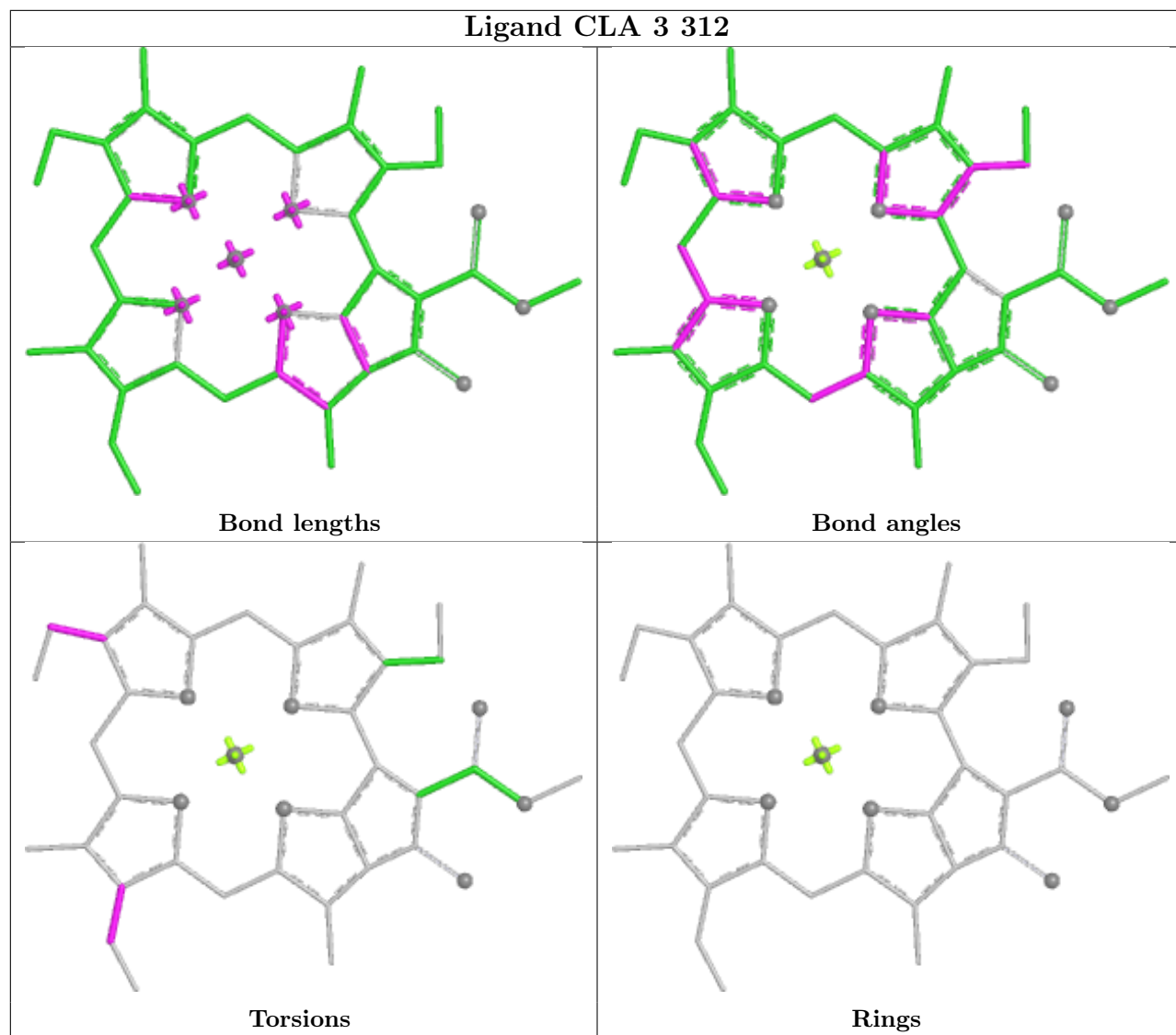


Rings

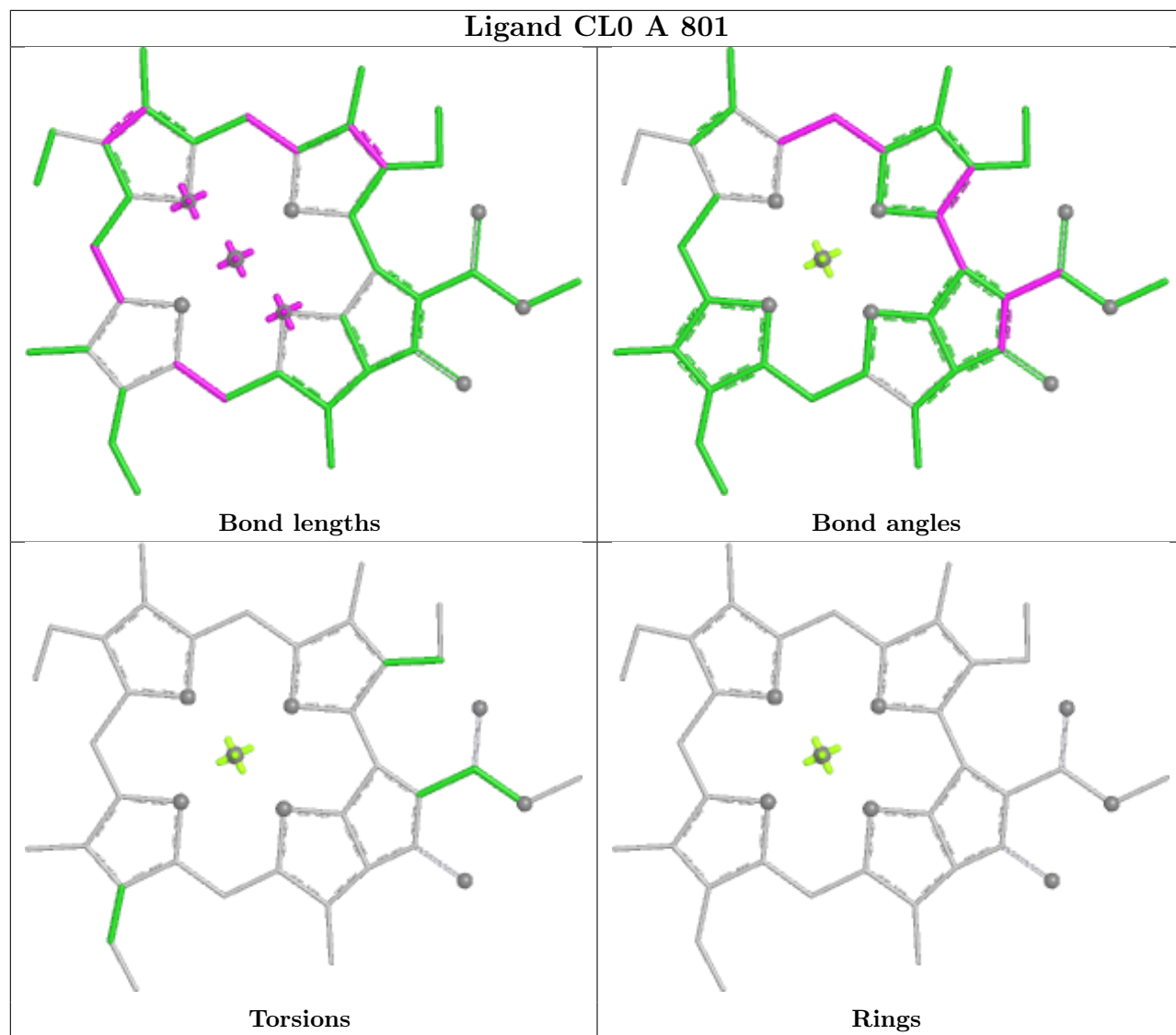
Ligand CLA A 823

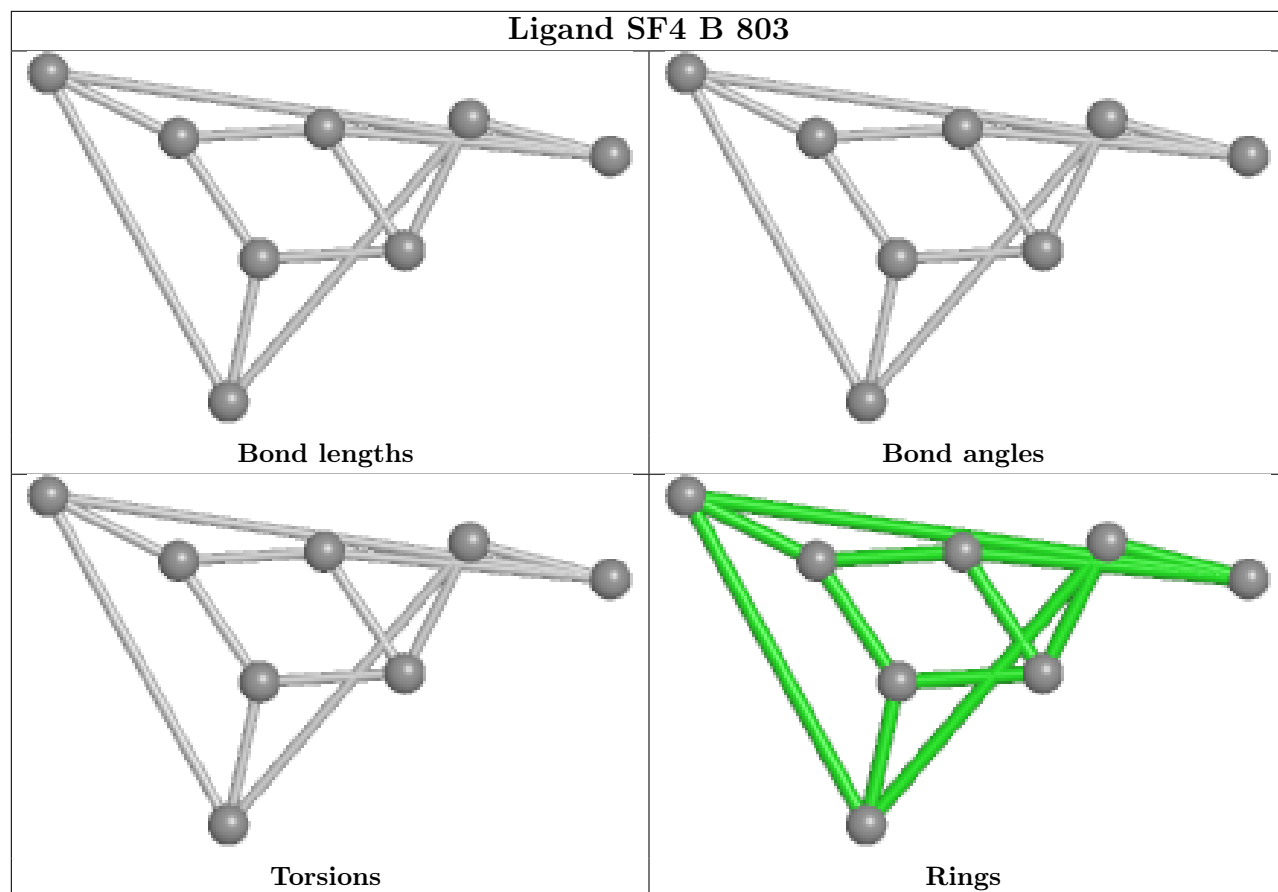


Ligand CLA 3 312

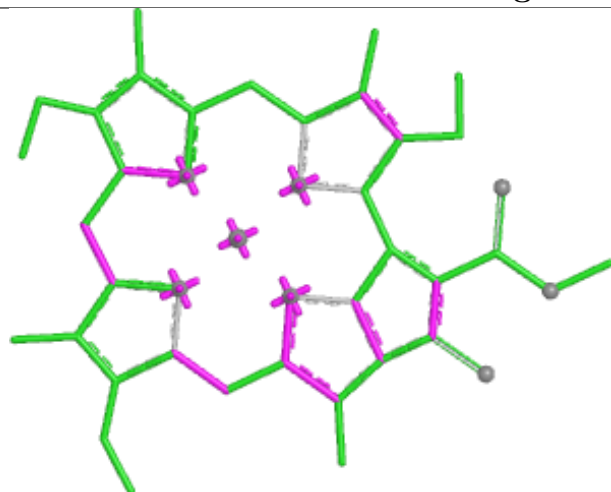


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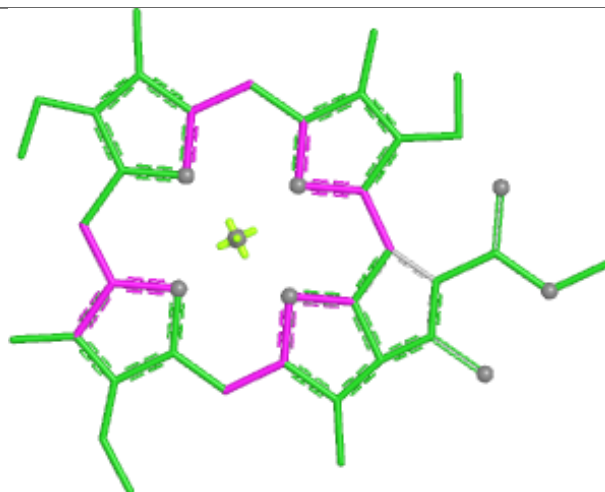




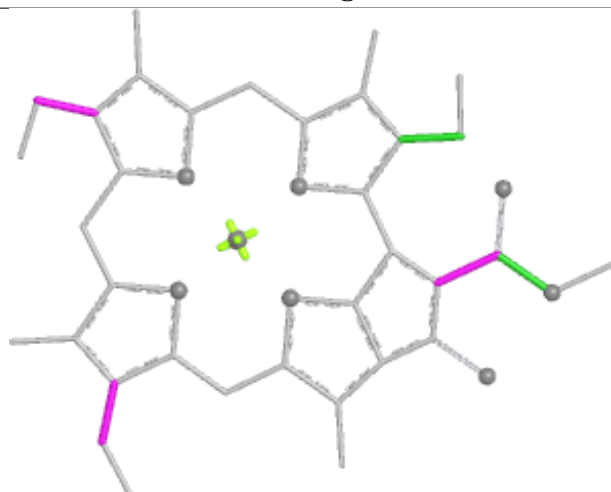
Ligand CLA A 835



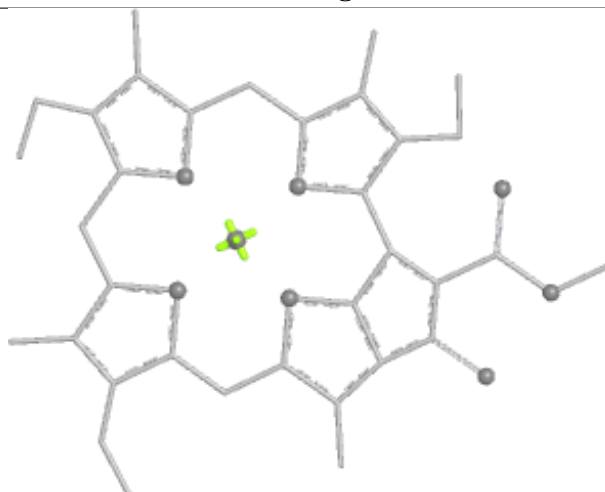
Bond lengths



Bond angles

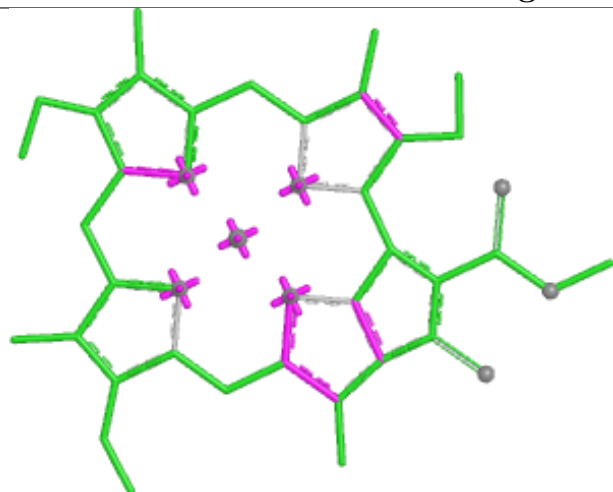


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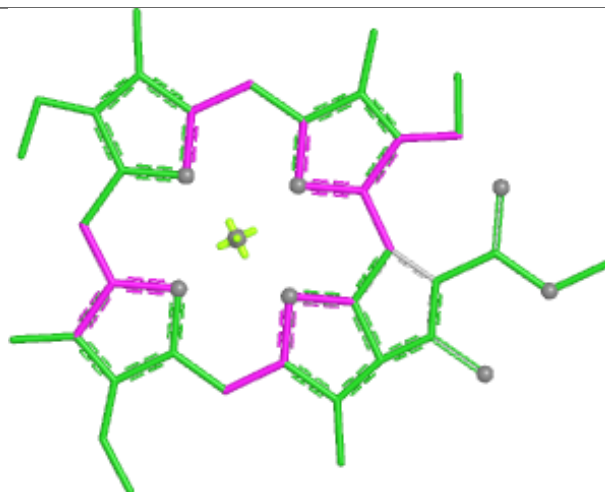


Rings

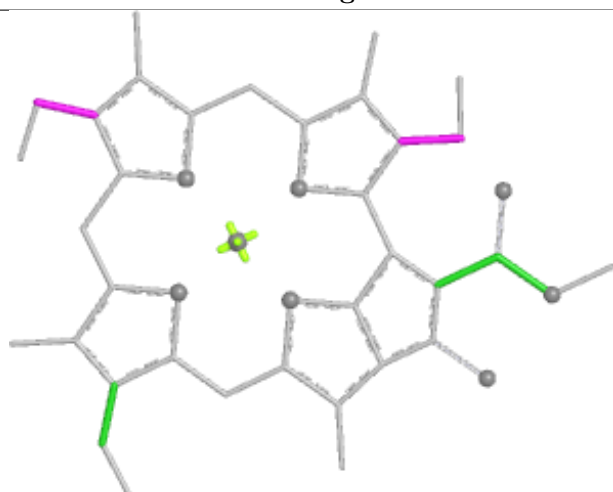
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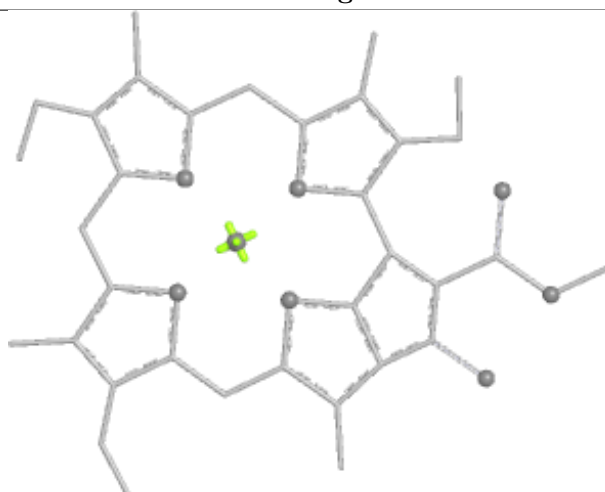
Bond lengths



Bond angles

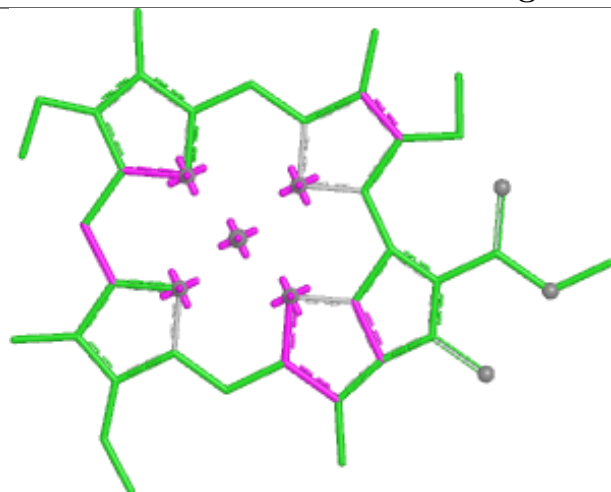


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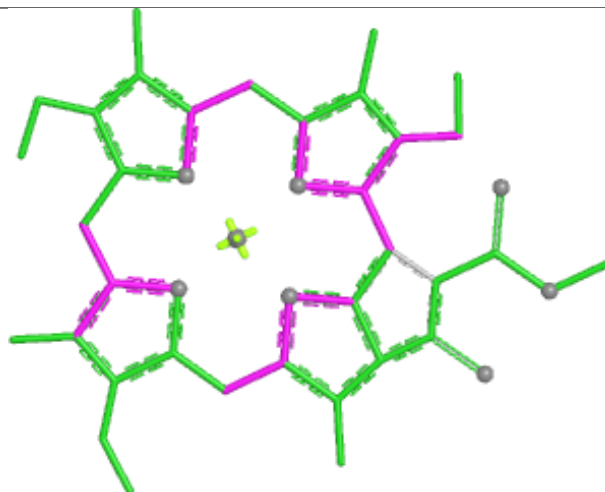


Rings

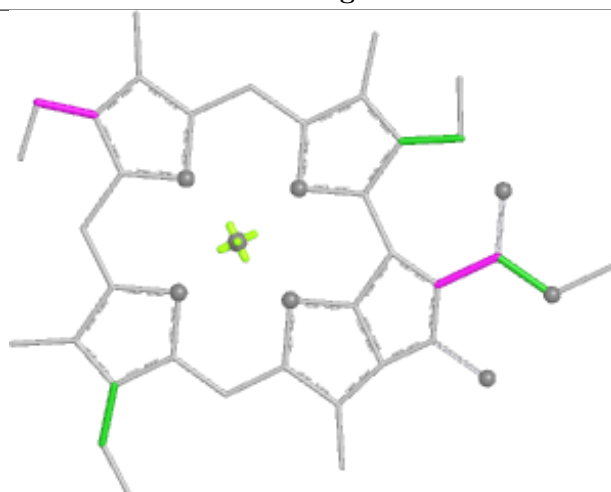
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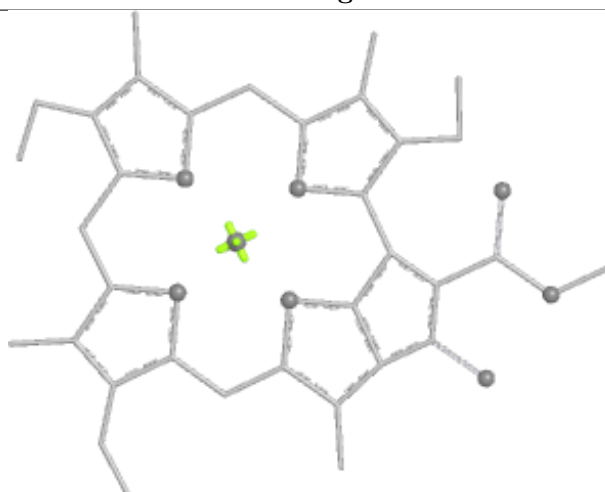
Bond lengths



Bond angles

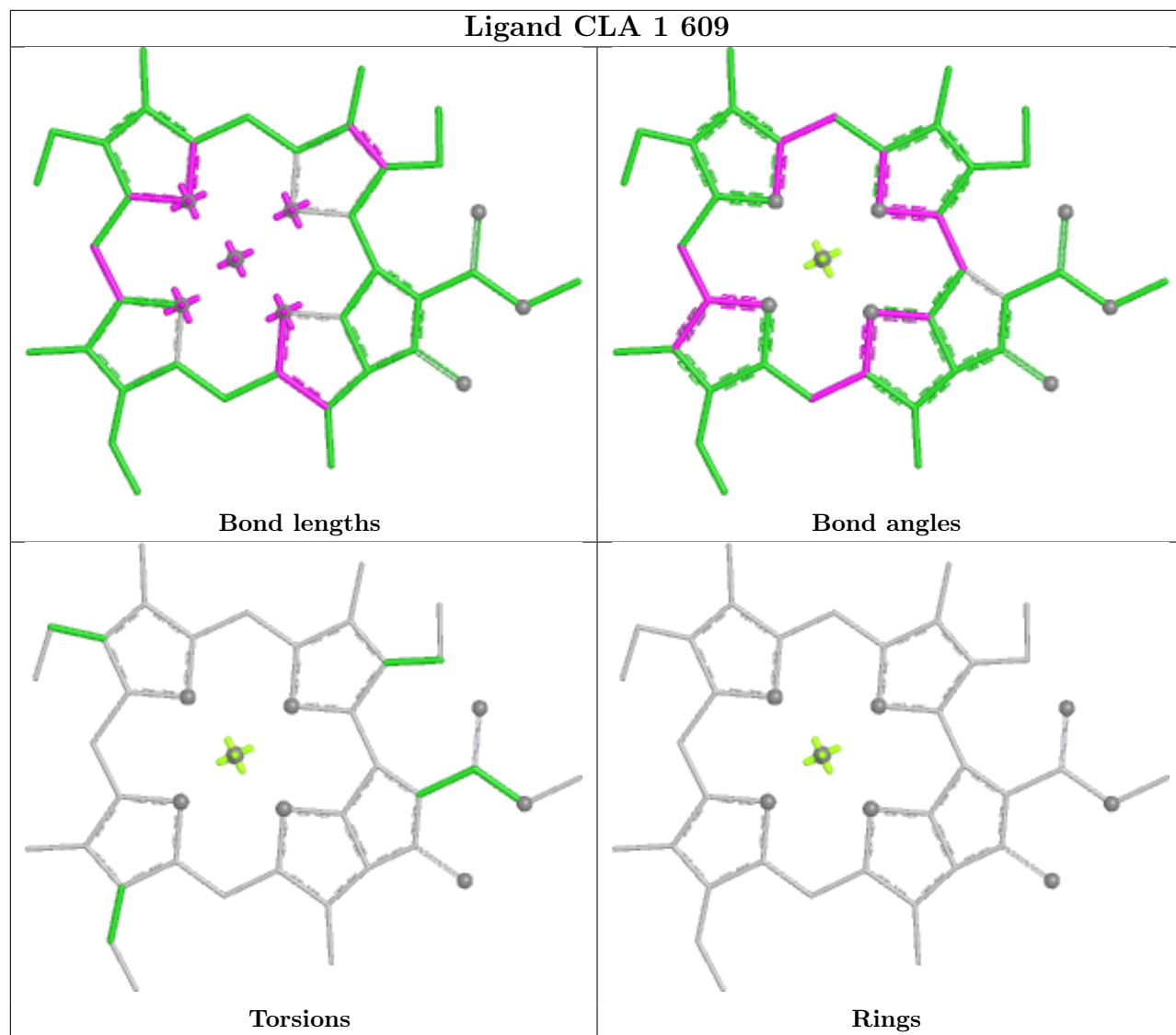


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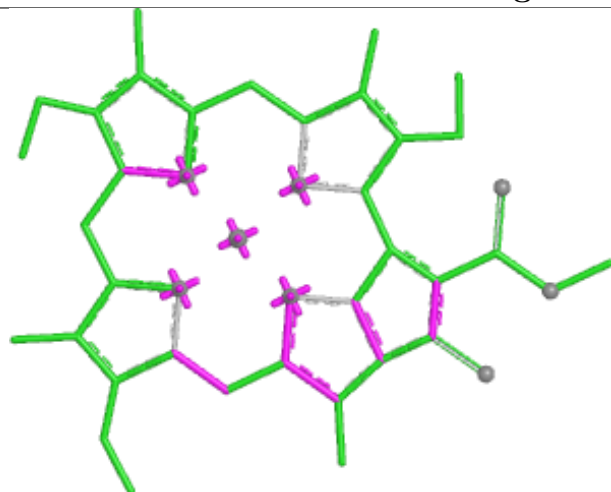


Rings

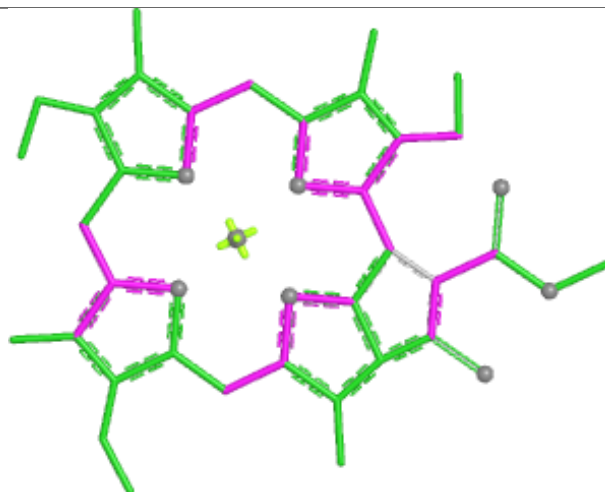
Ligand CLA 1 609



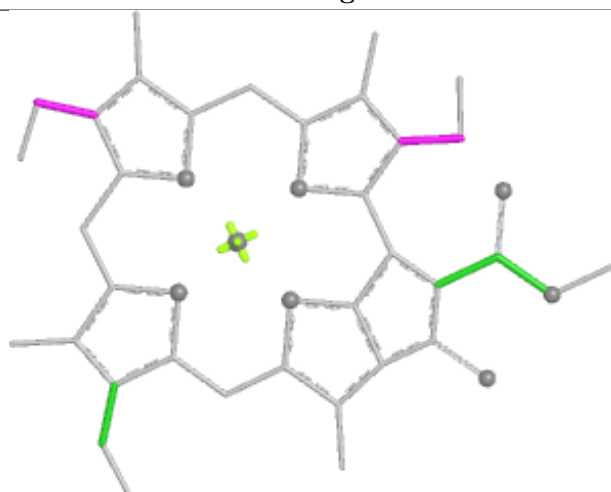
Ligand CLA A 830



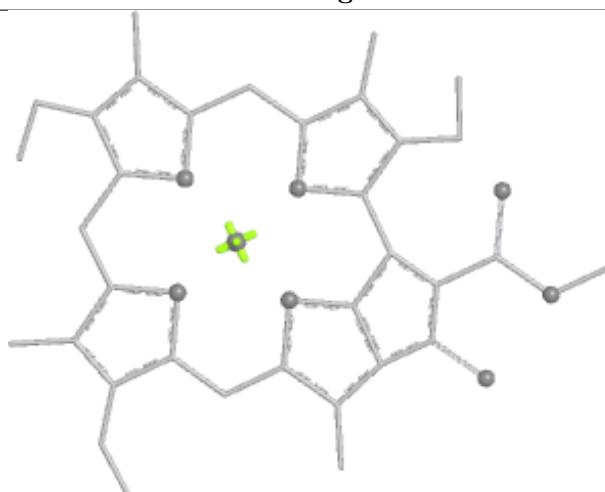
Bond lengths



Bond angles

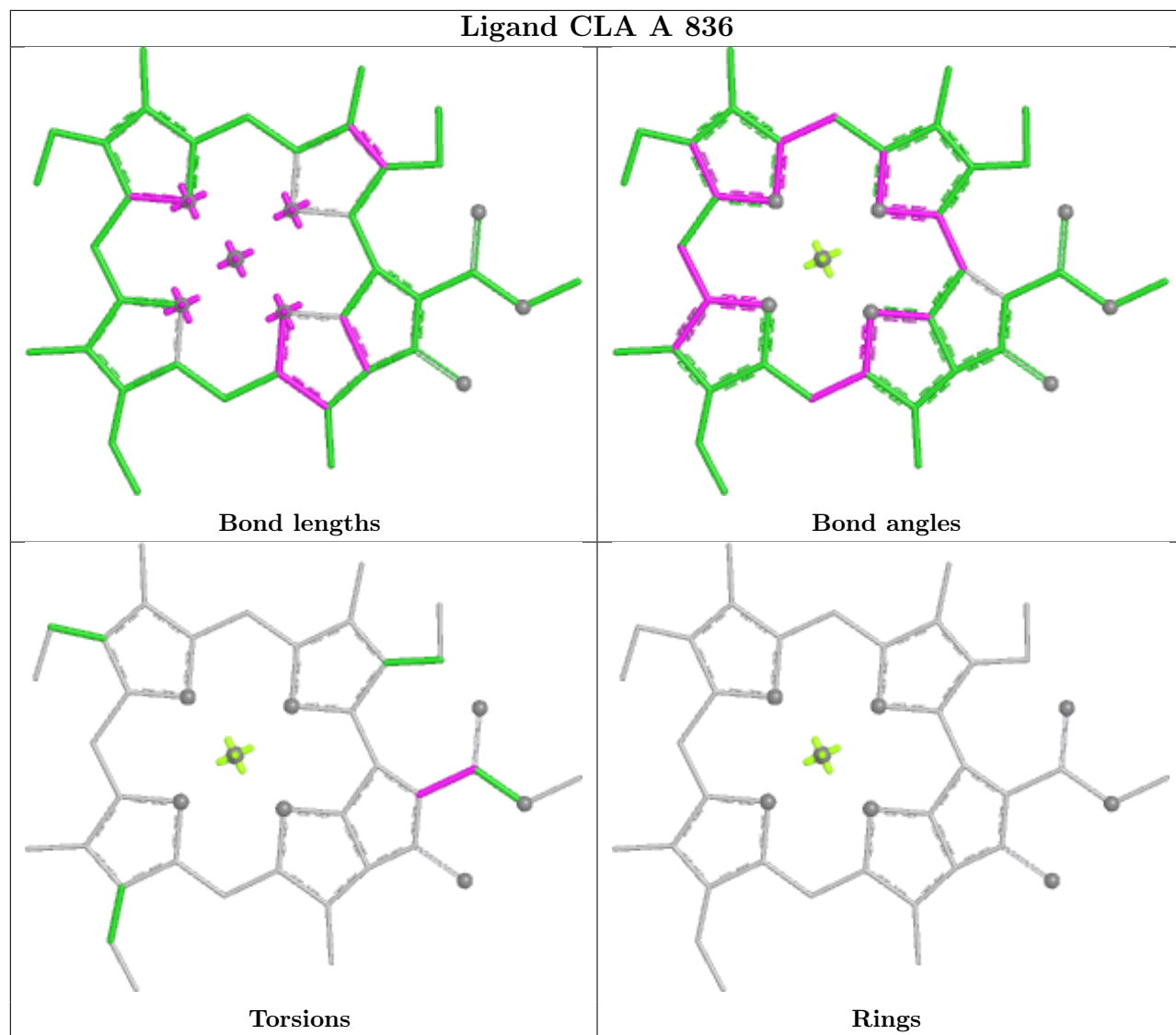


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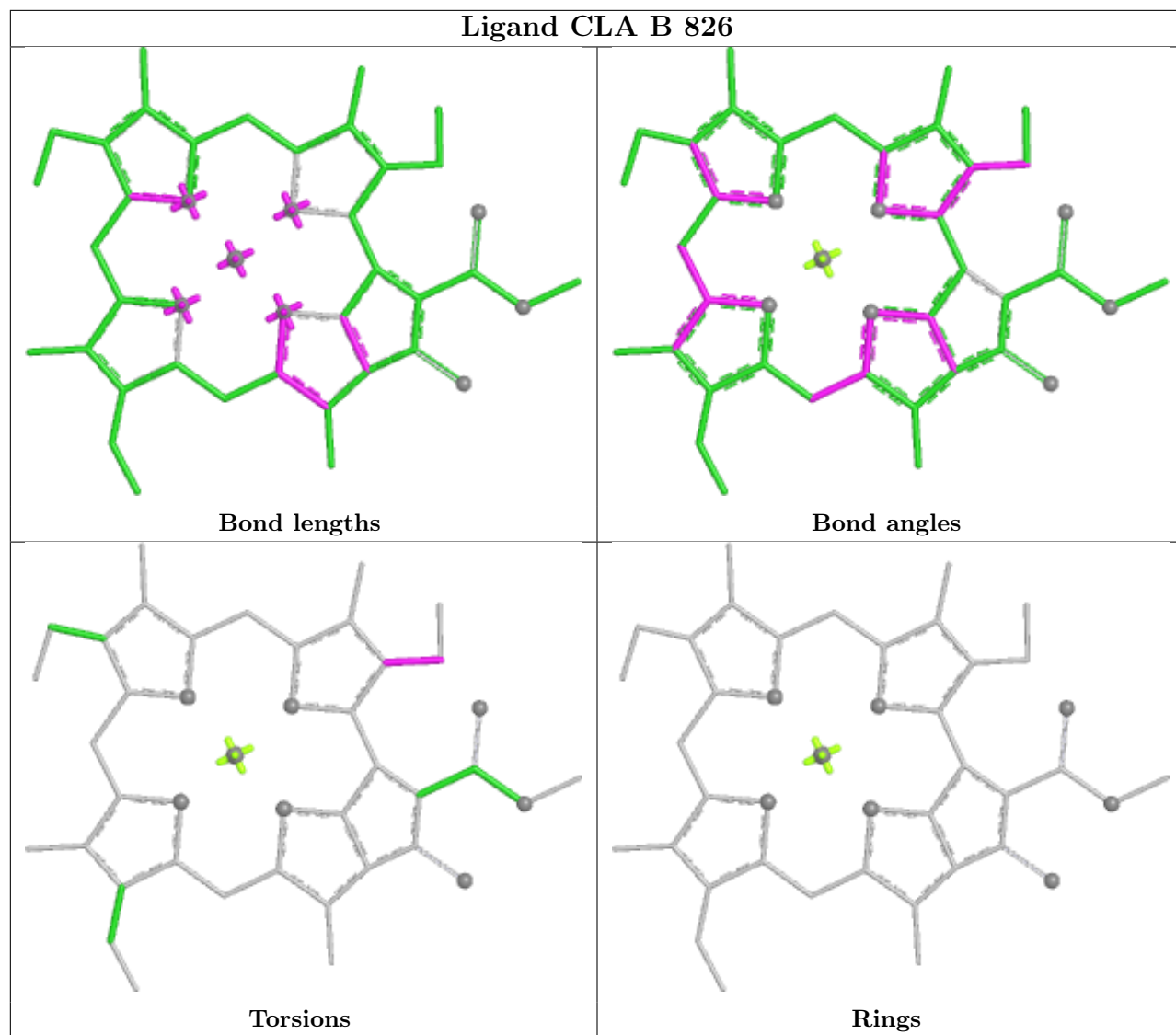


Rings

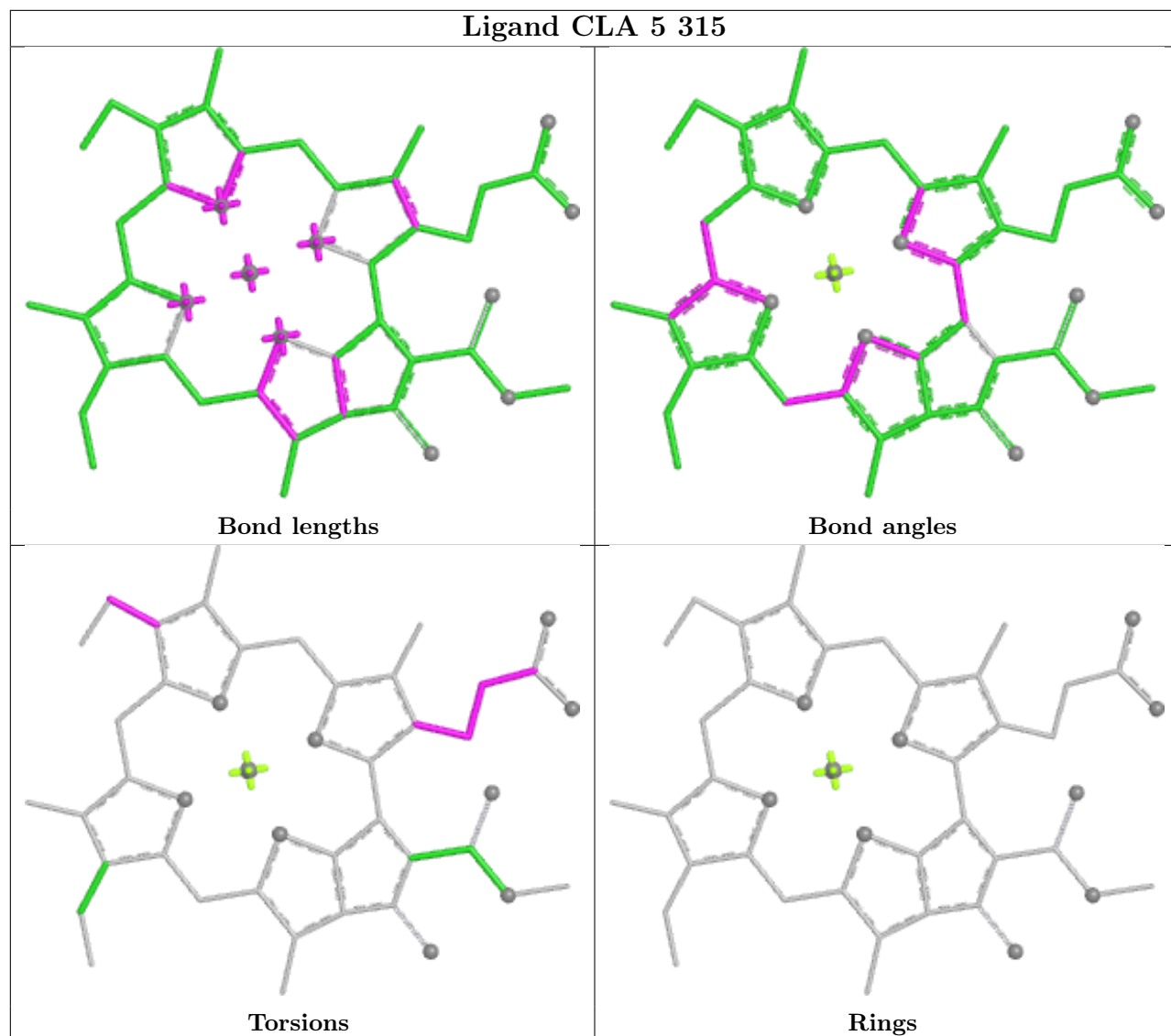
Ligand CLA A 836



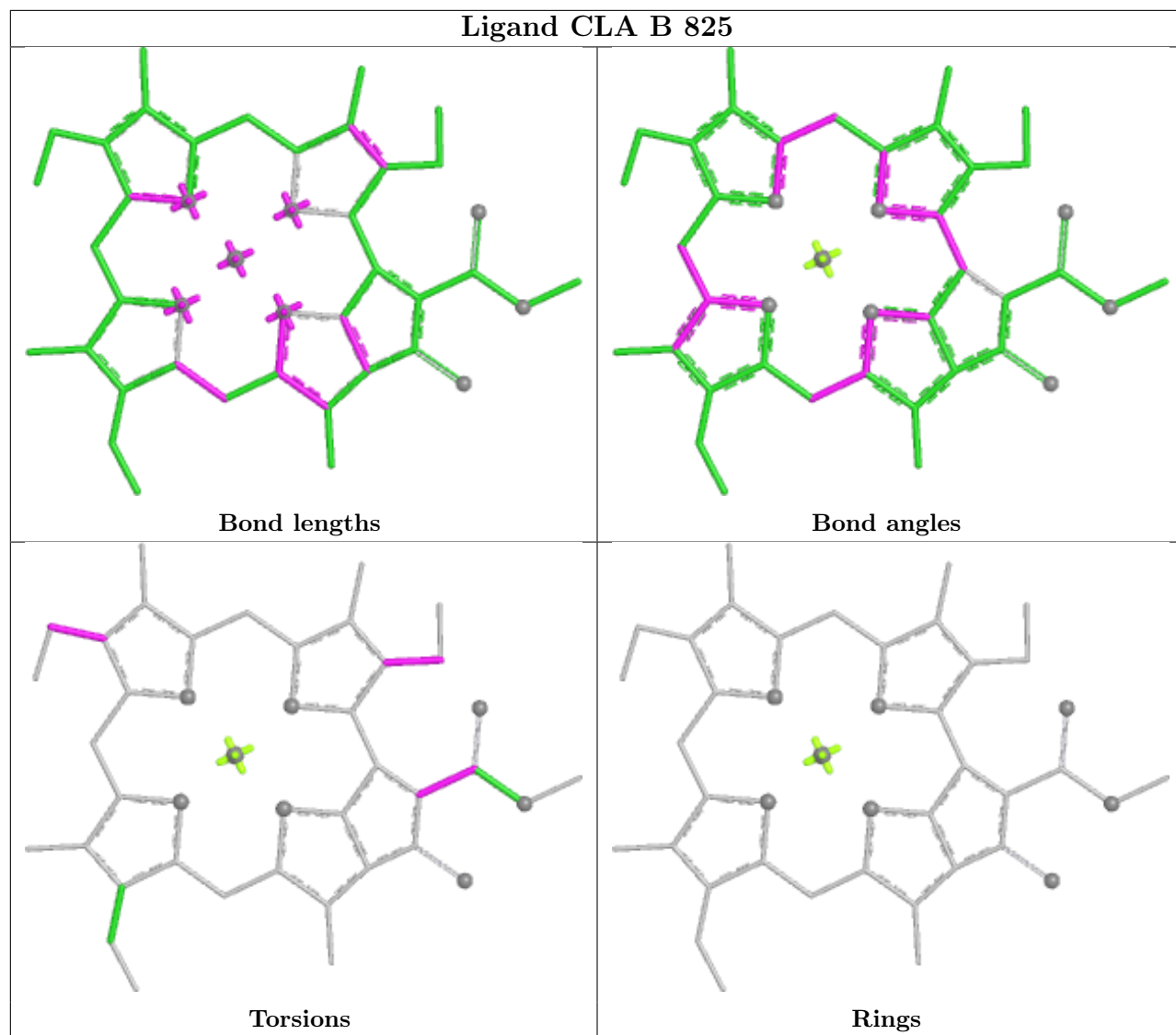
Ligand CLA B 826

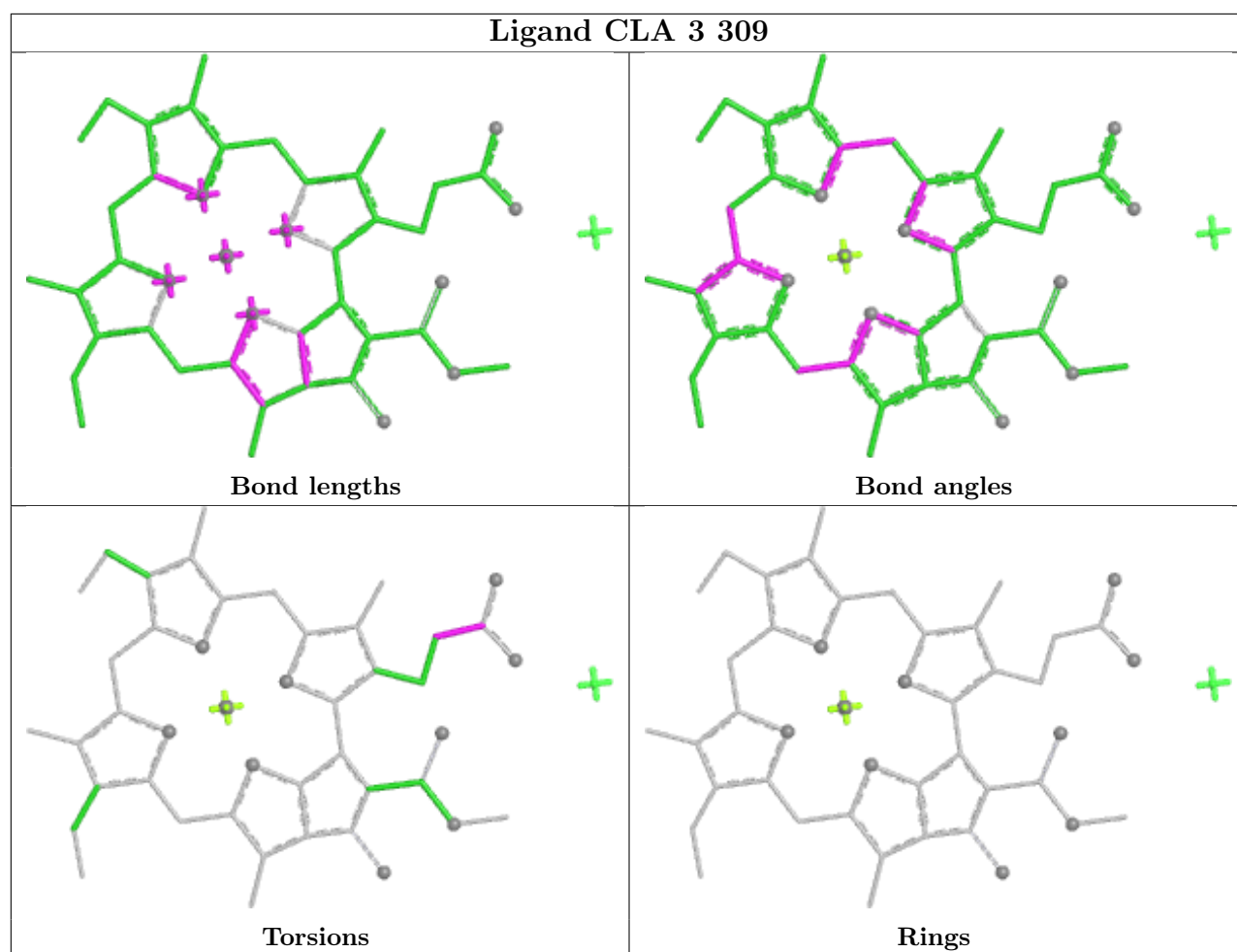


Ligand CLA 5 315

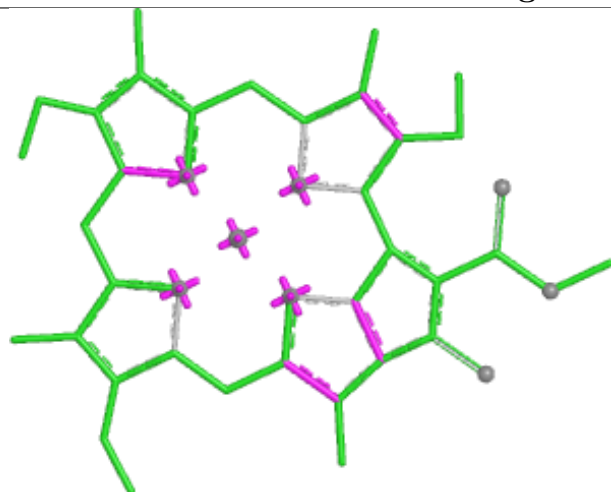


Ligand CLA B 825

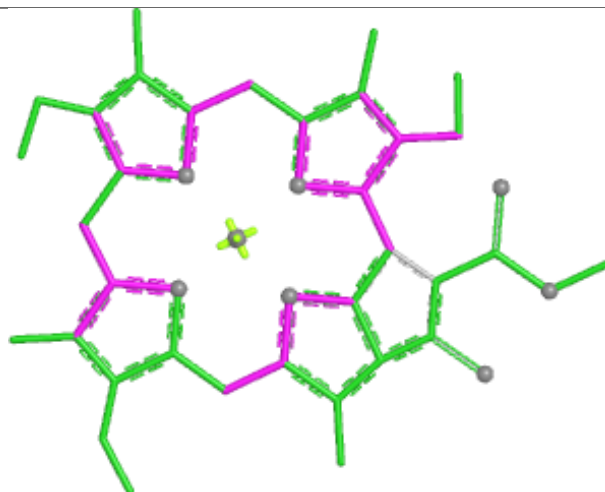




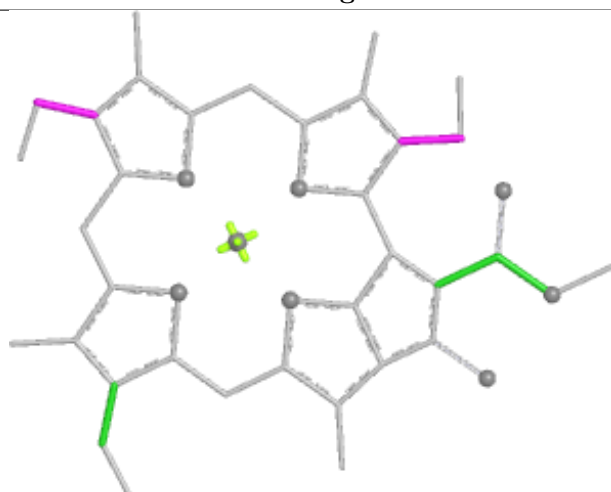
Ligand CLA 3 313



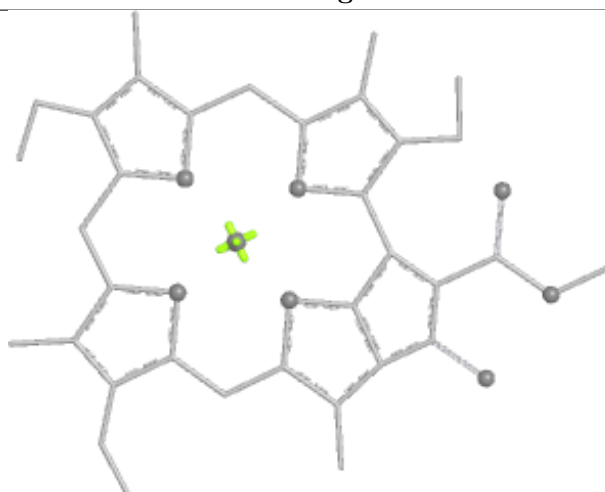
Bond lengths



Bond angles

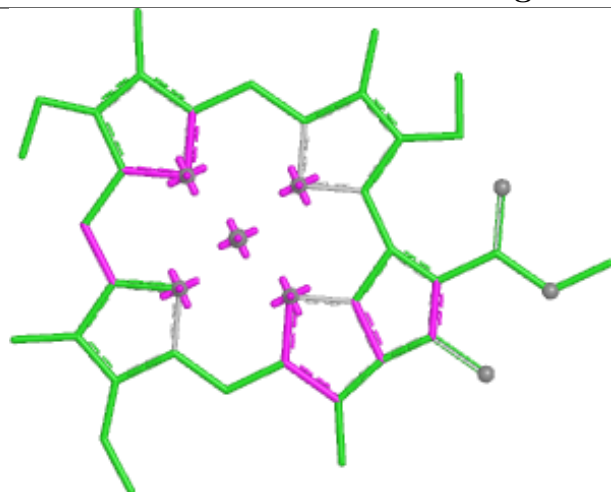


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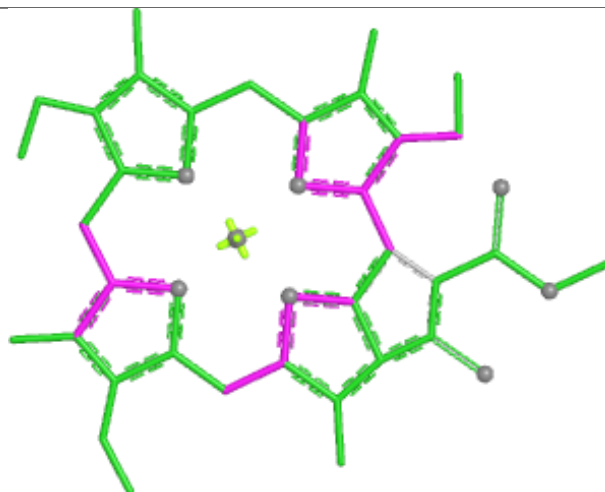


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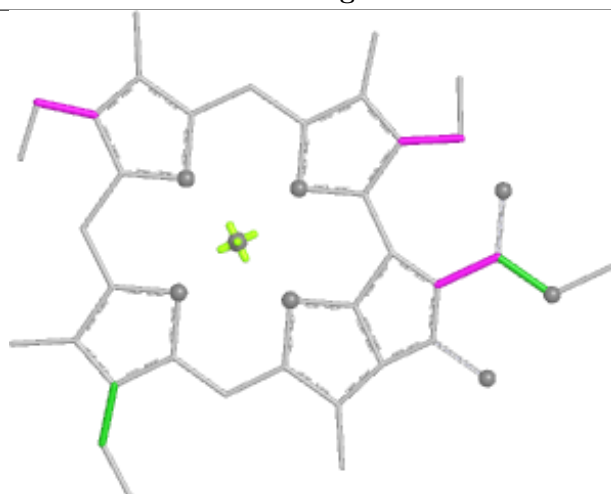
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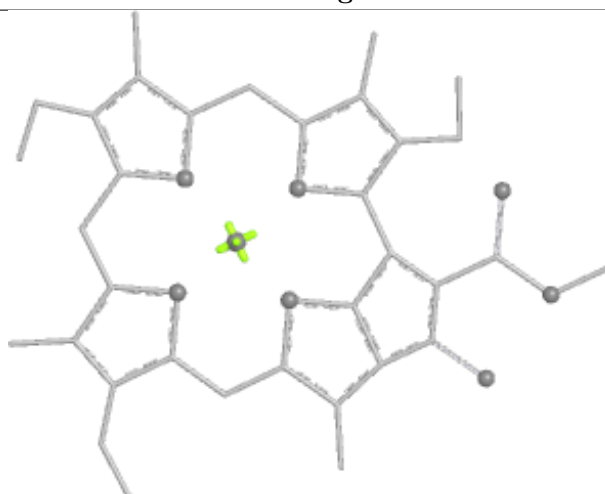
Bond lengths



Bond angles

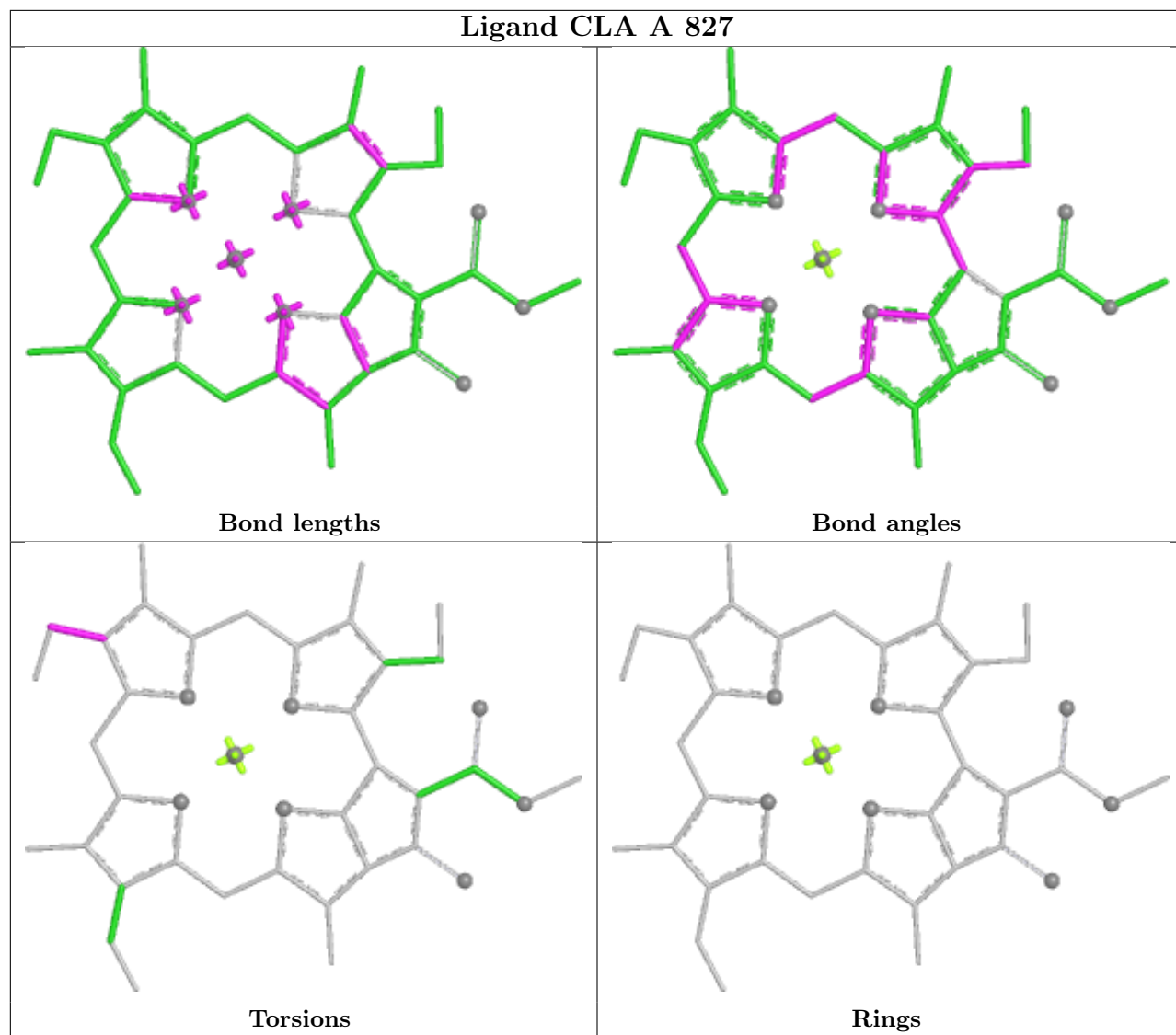


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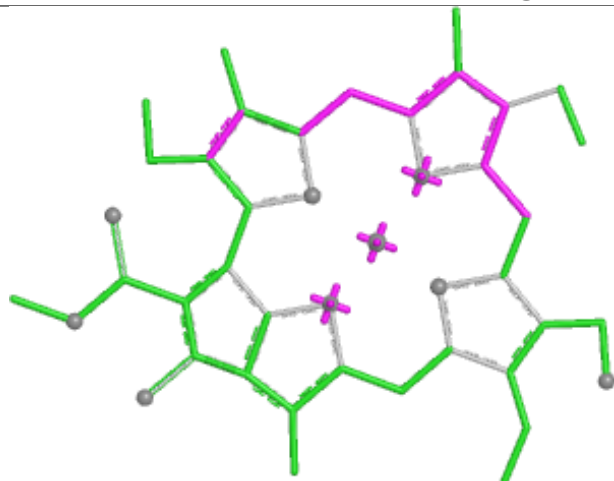


Rings

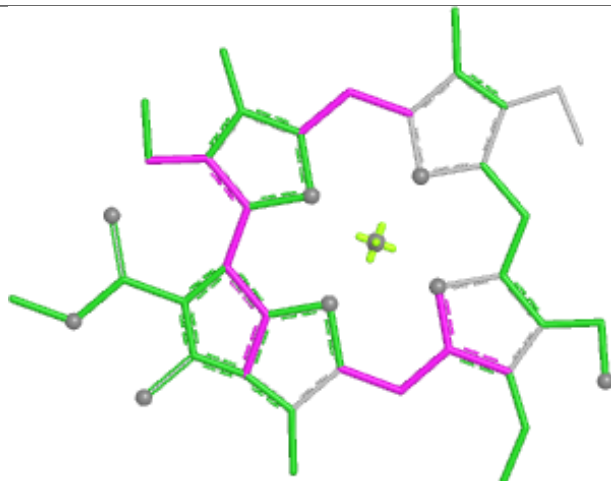
Ligand CLA A 827



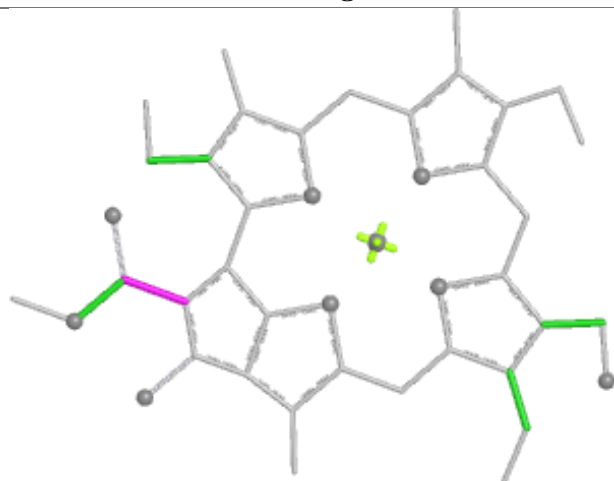
Ligand CHL 8 606



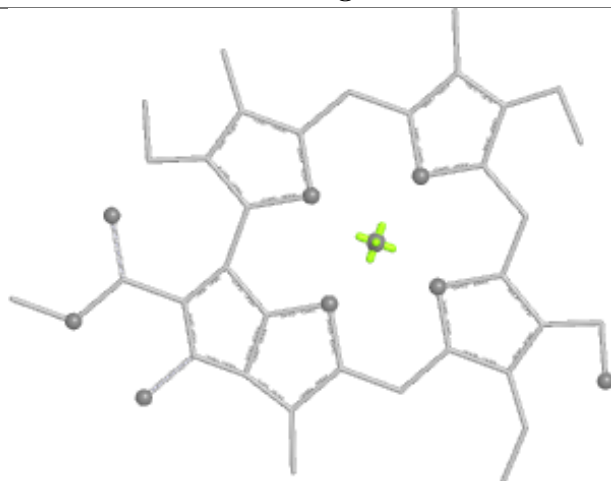
Bond lengths



Bond angles

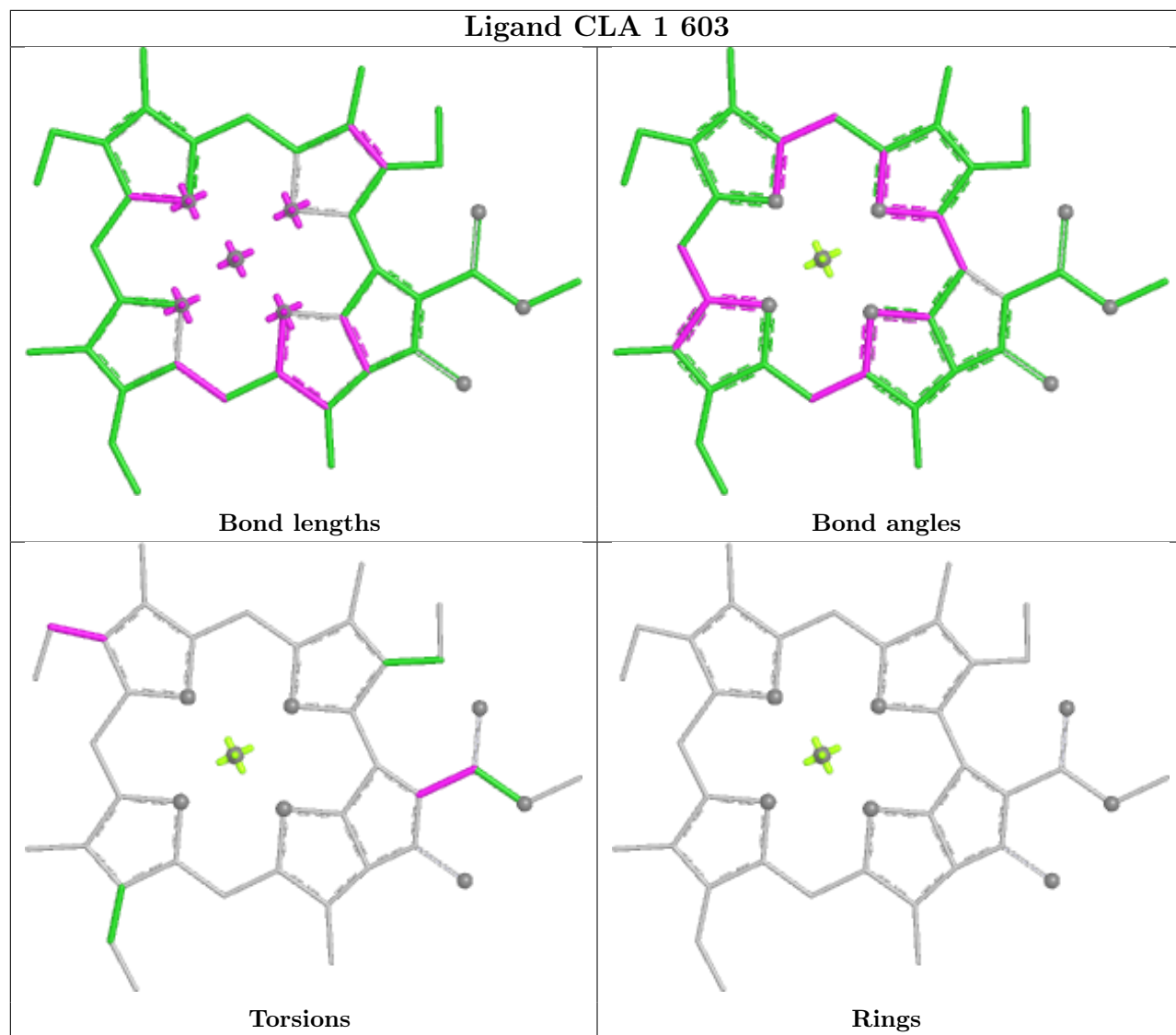


Torsions

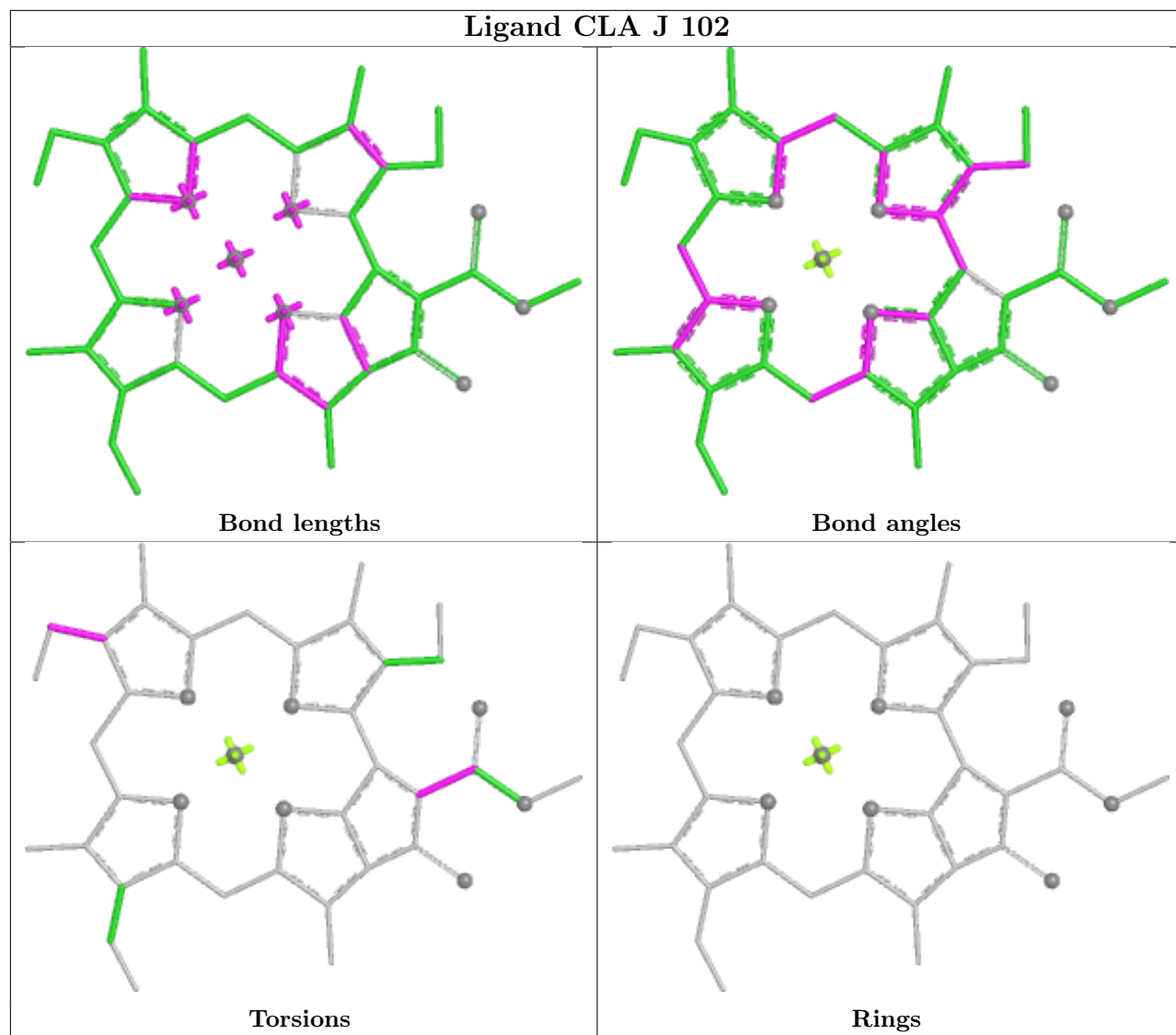


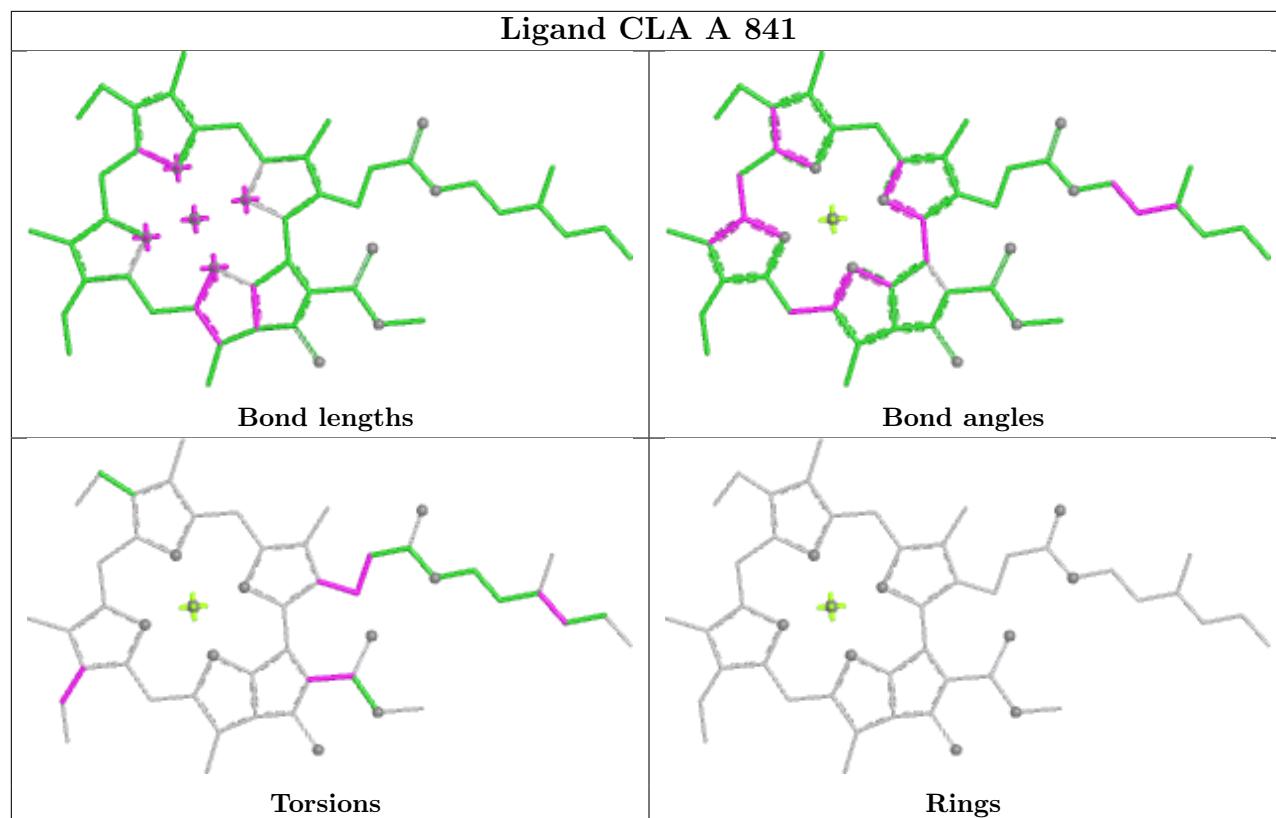
Rings

Ligand CLA 1 603

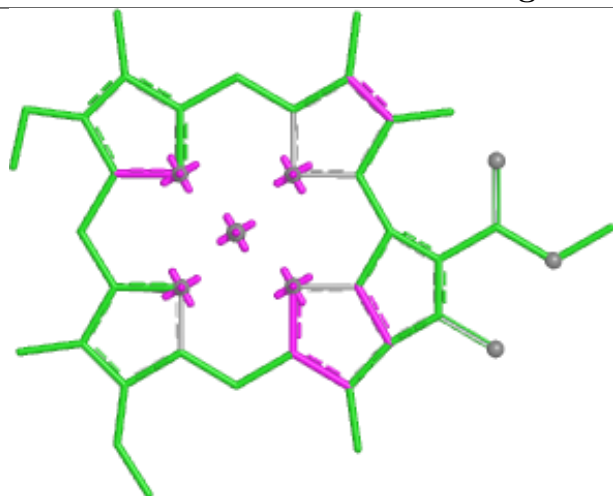


Ligand CLA J 102

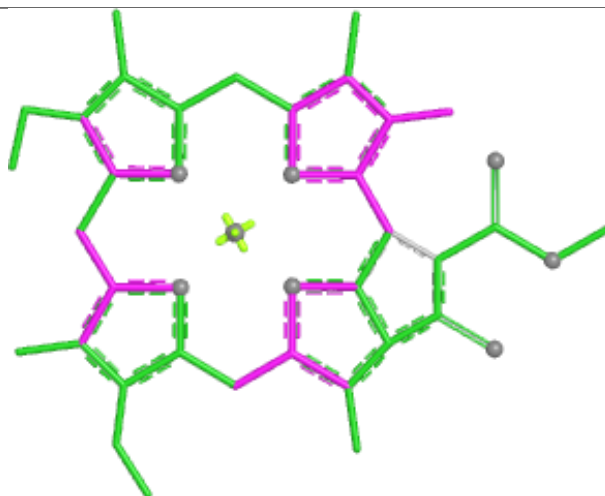




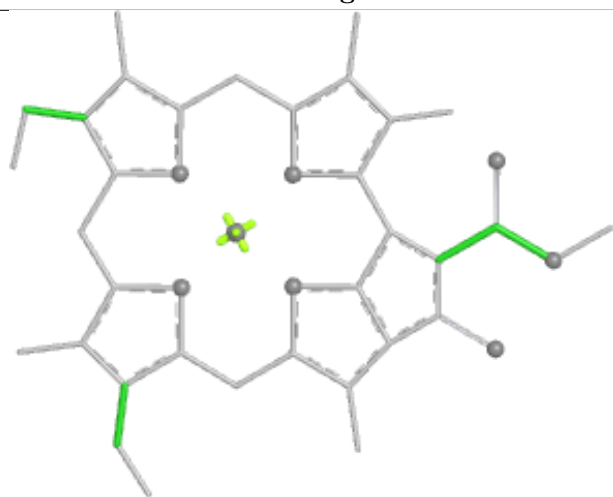
Ligand CLA 3 310



Bond lengths



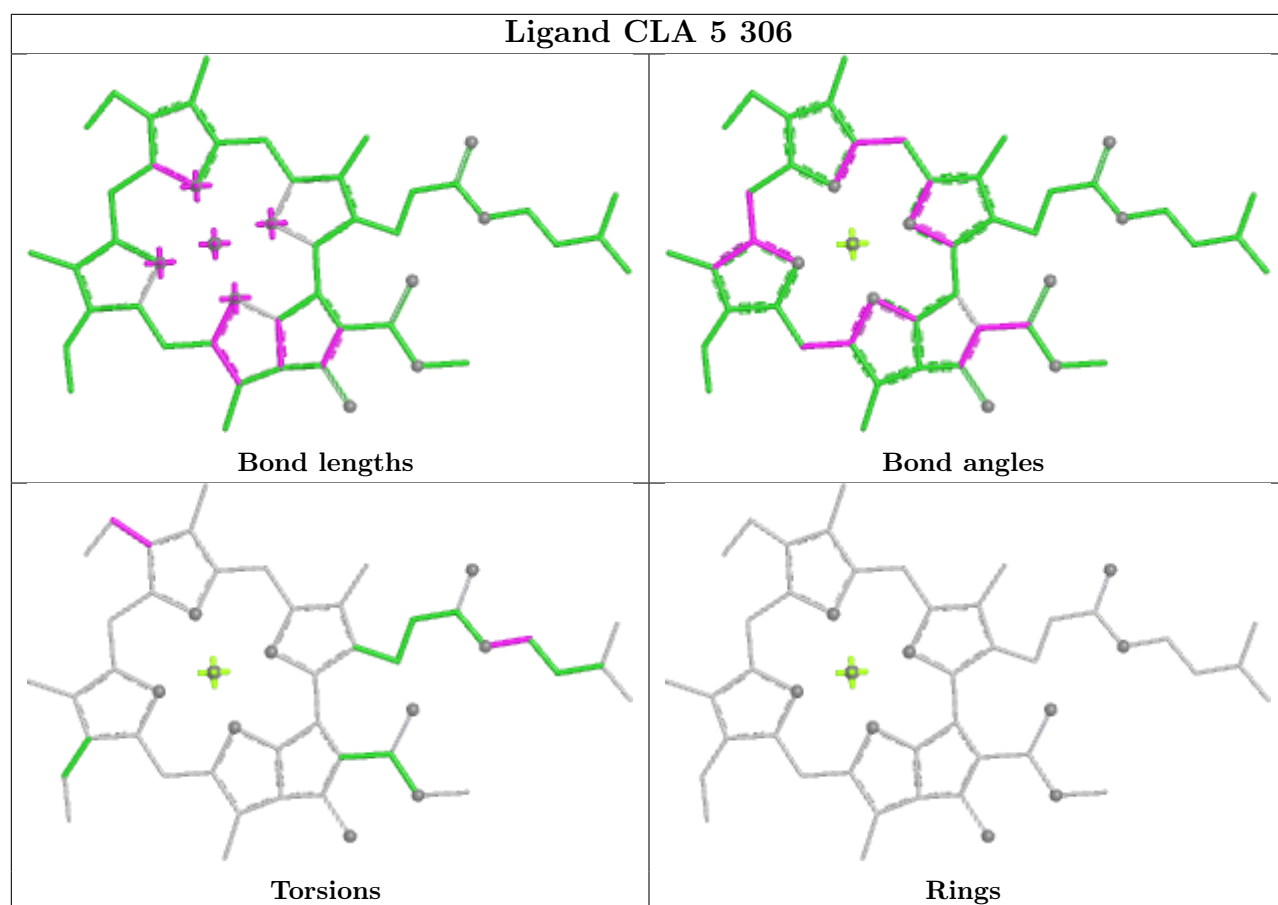
Bond angles



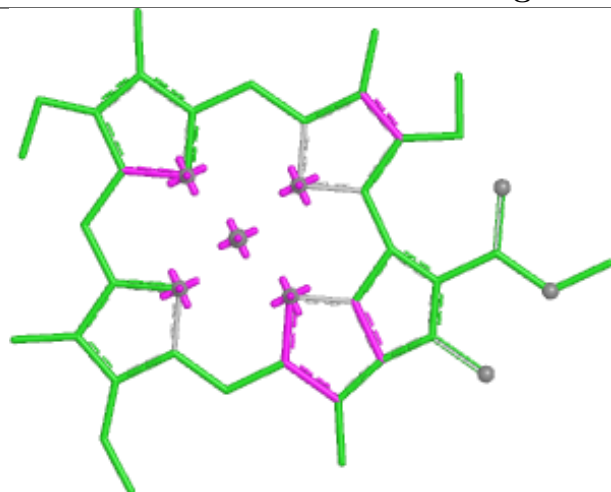
Torsions



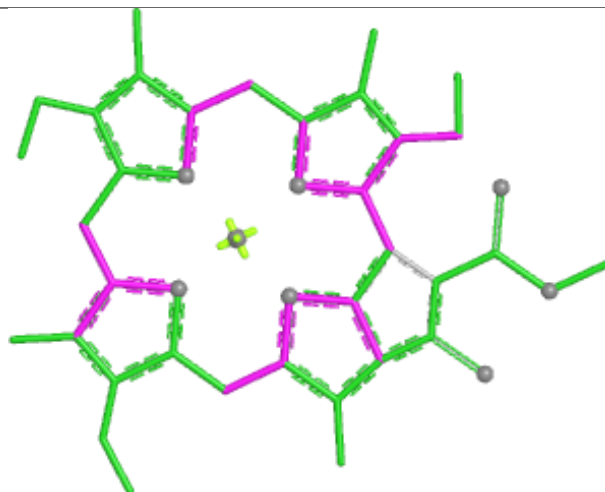
Rings



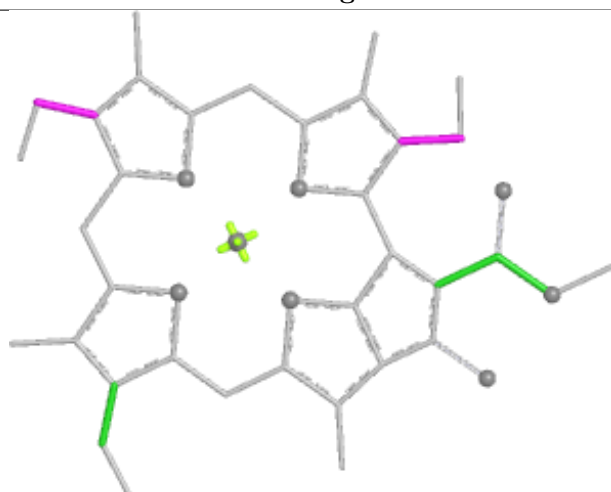
Ligand CLA A 805



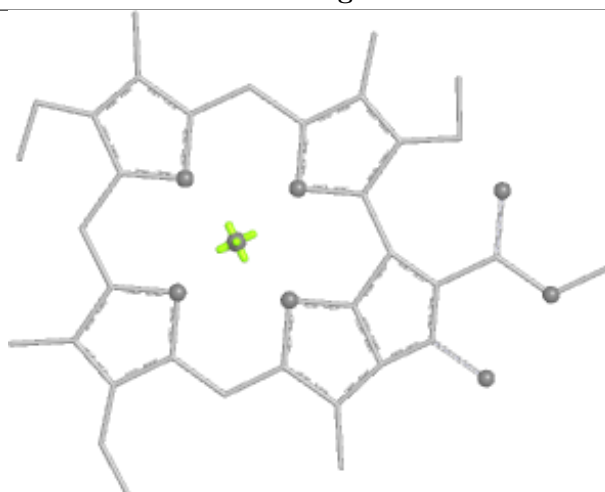
Bond lengths



Bond angles

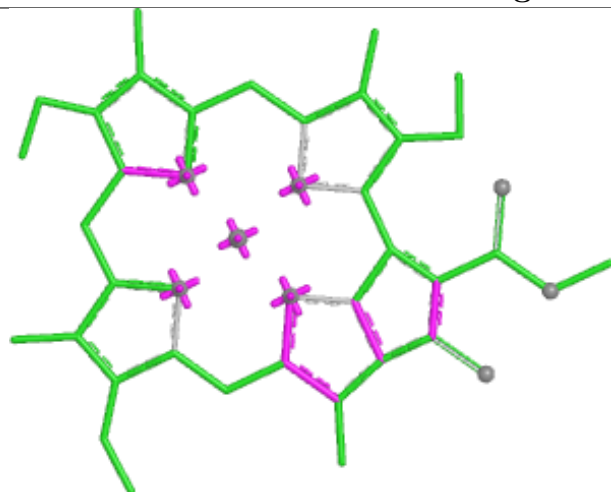


Torsions

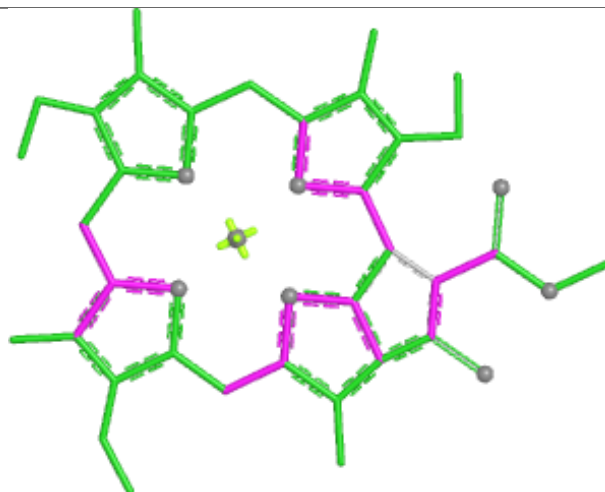


Rings

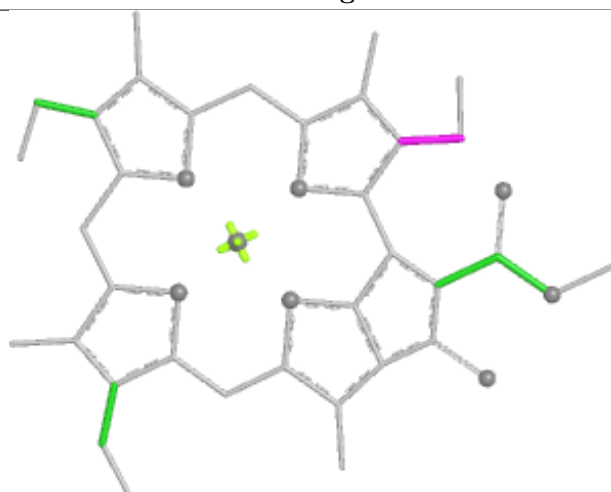
Ligand CLA A 838



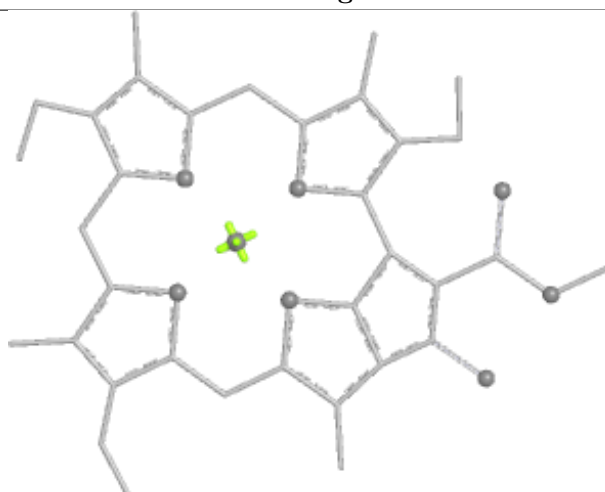
Bond lengths



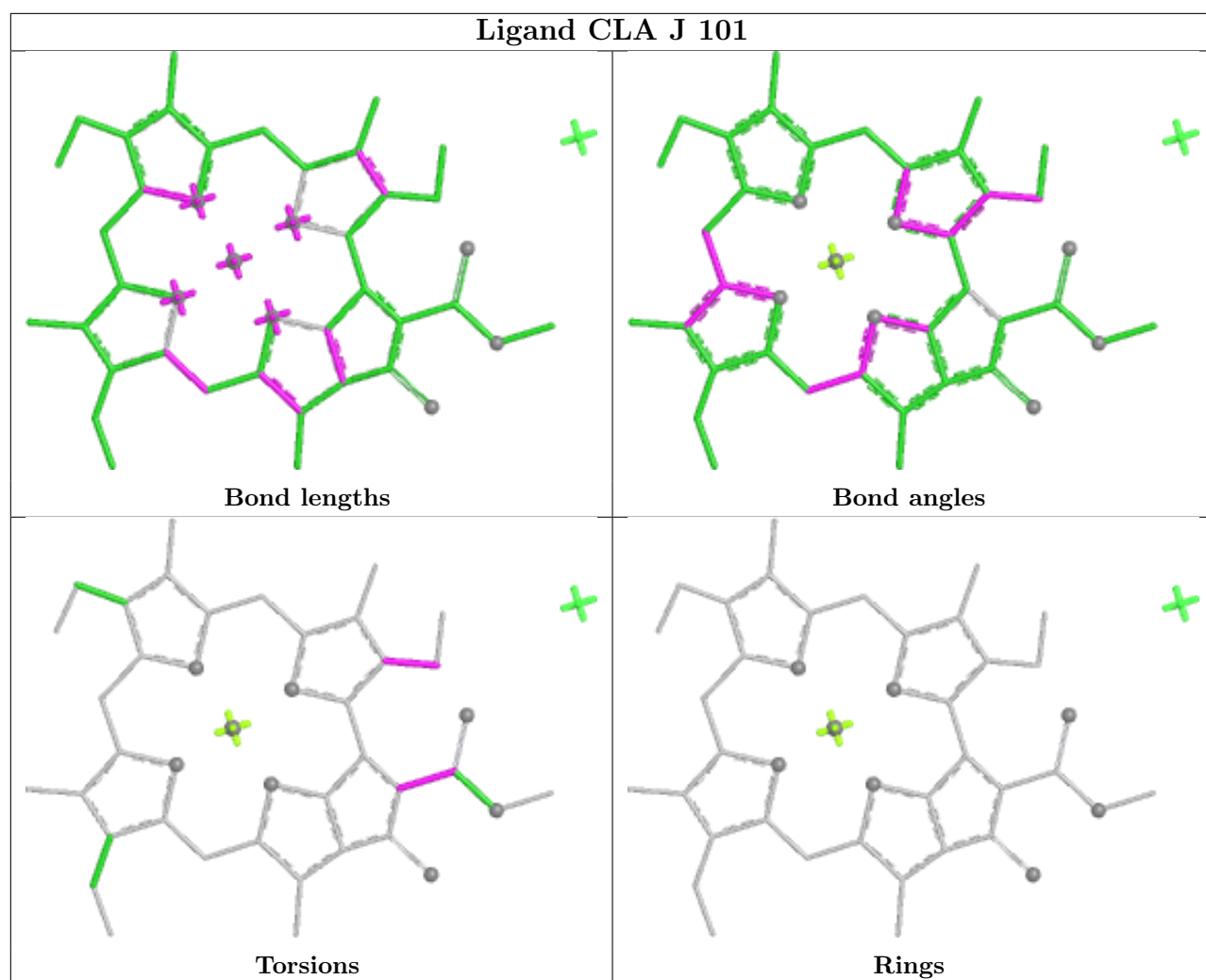
Bond angles



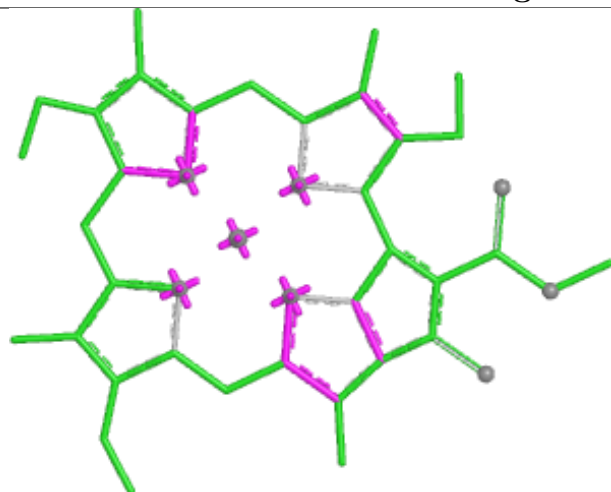
Torsions



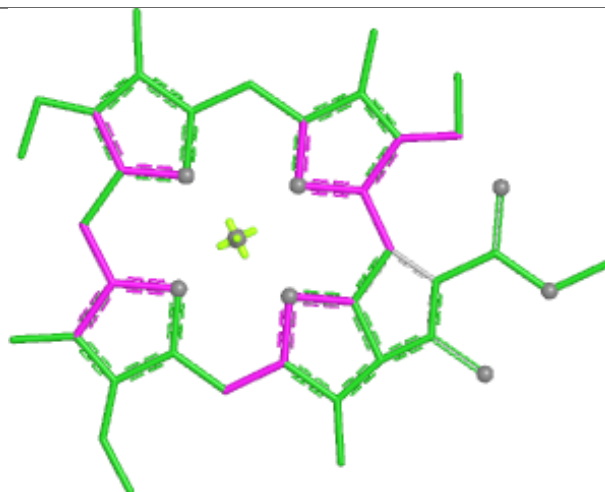
Rings



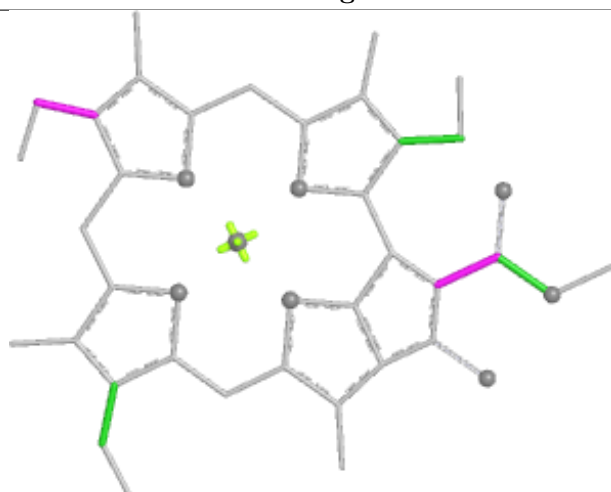
Ligand CLA A 807



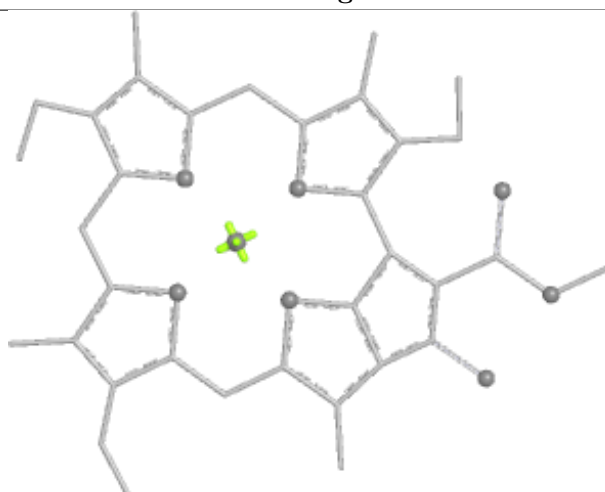
Bond lengths



Bond angles

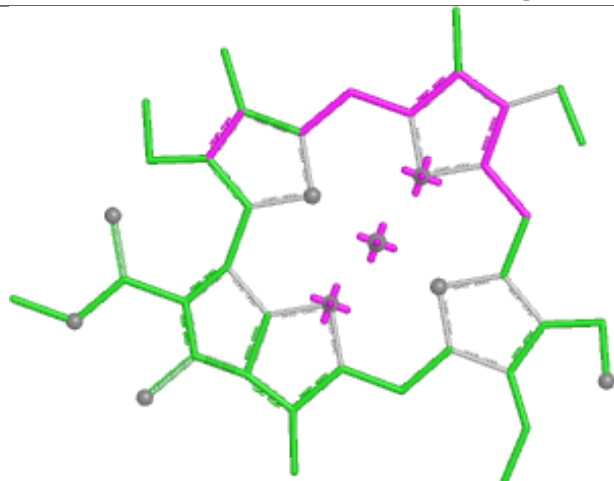


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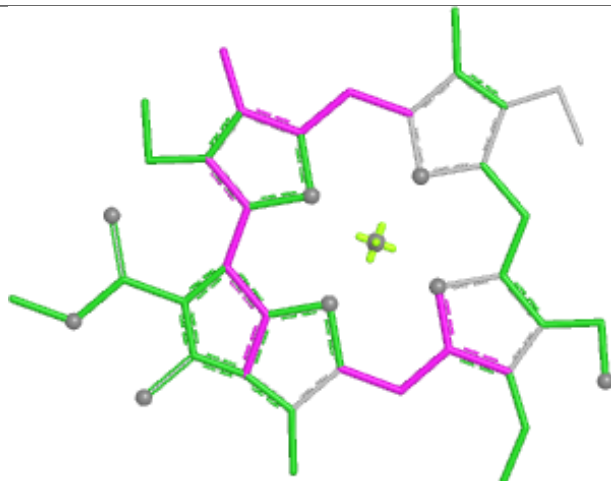


Rings

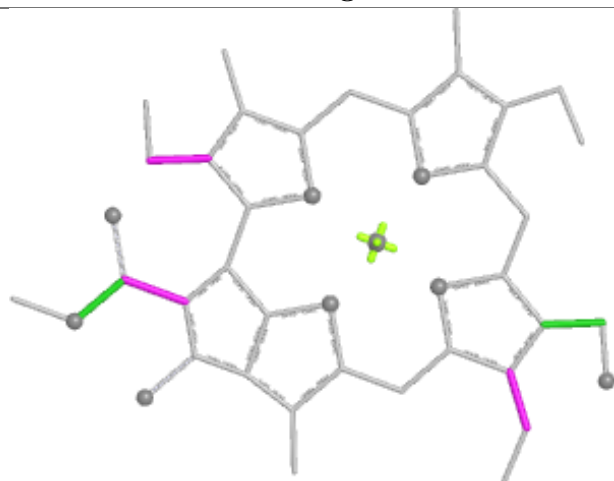
Ligand CHL 6 606



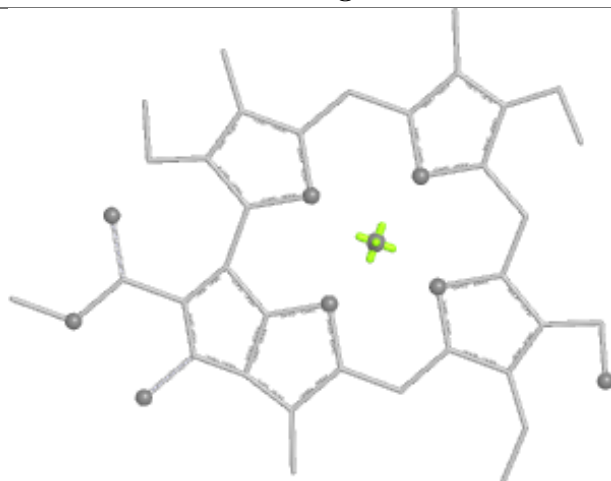
Bond lengths



Bond angles

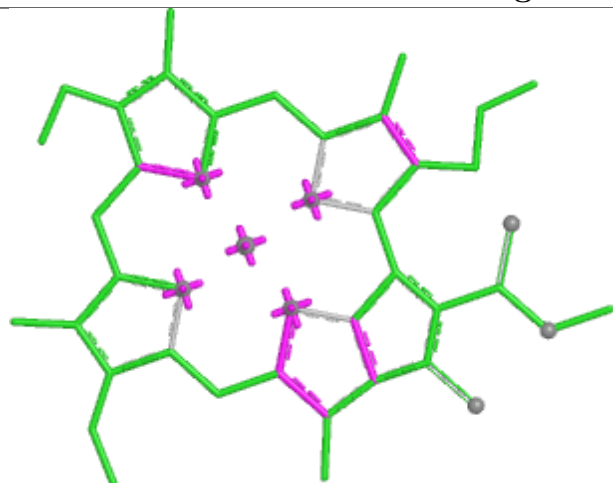


Torsions

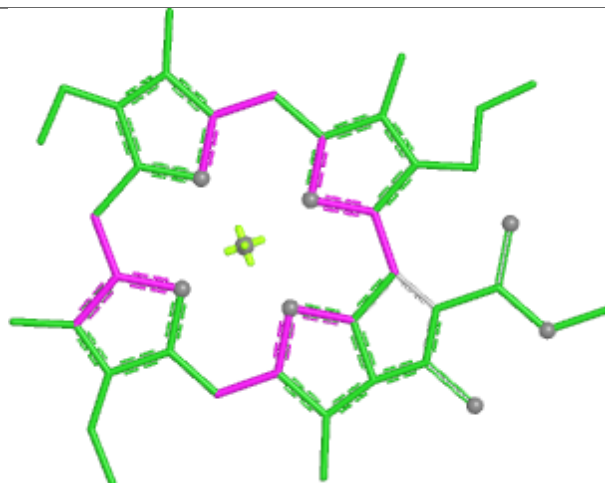


Rings

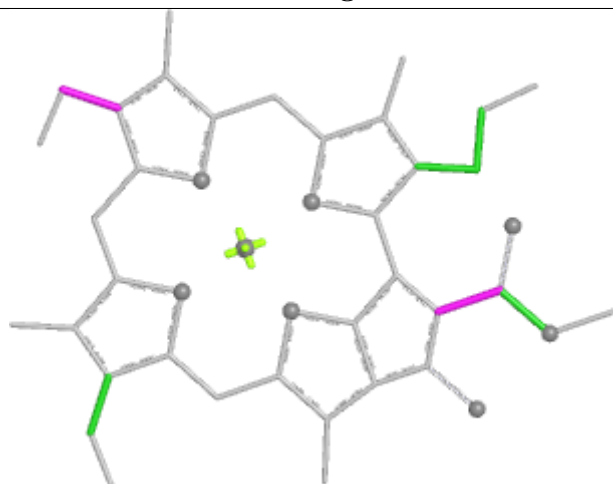
Ligand CLA B 835



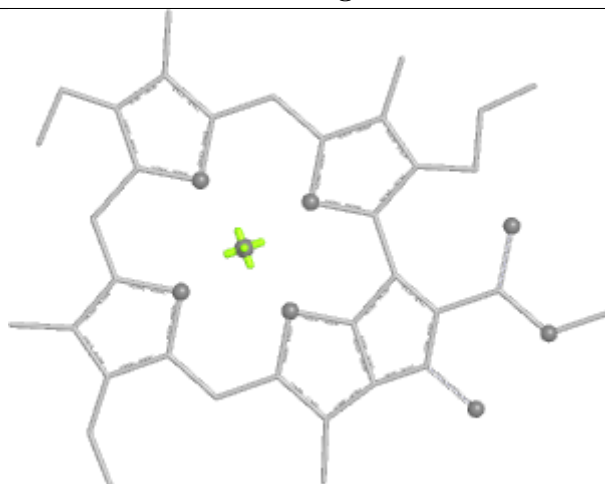
Bond lengths



Bond angles

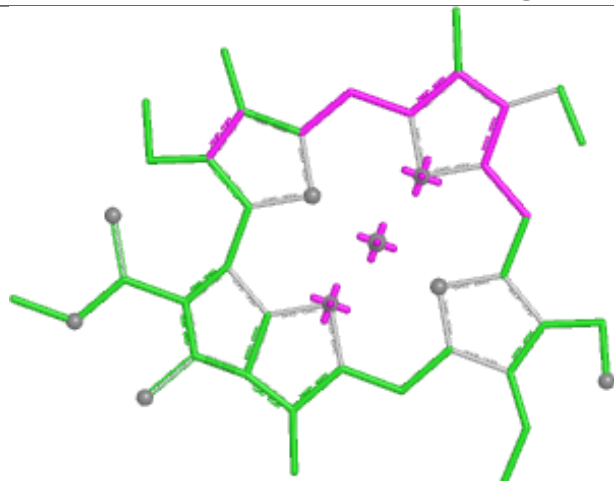


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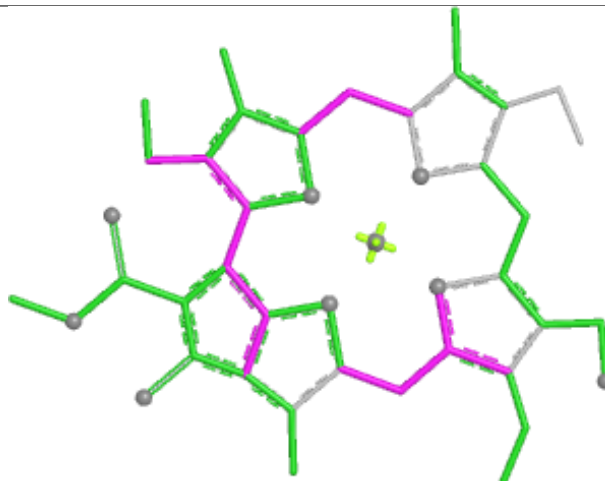


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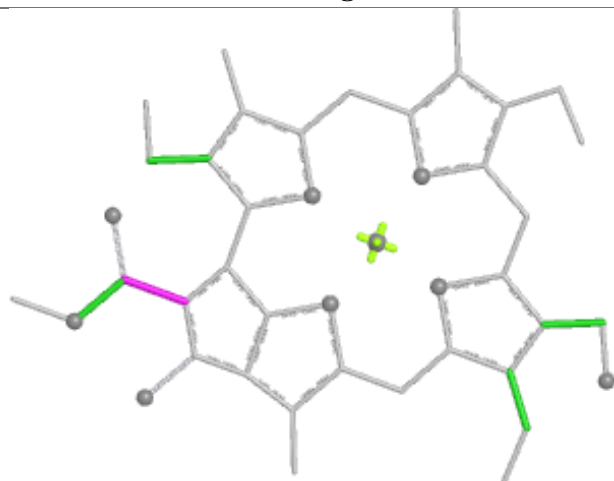
Ligand CHL 6 605



Bond lengths



Bond angles

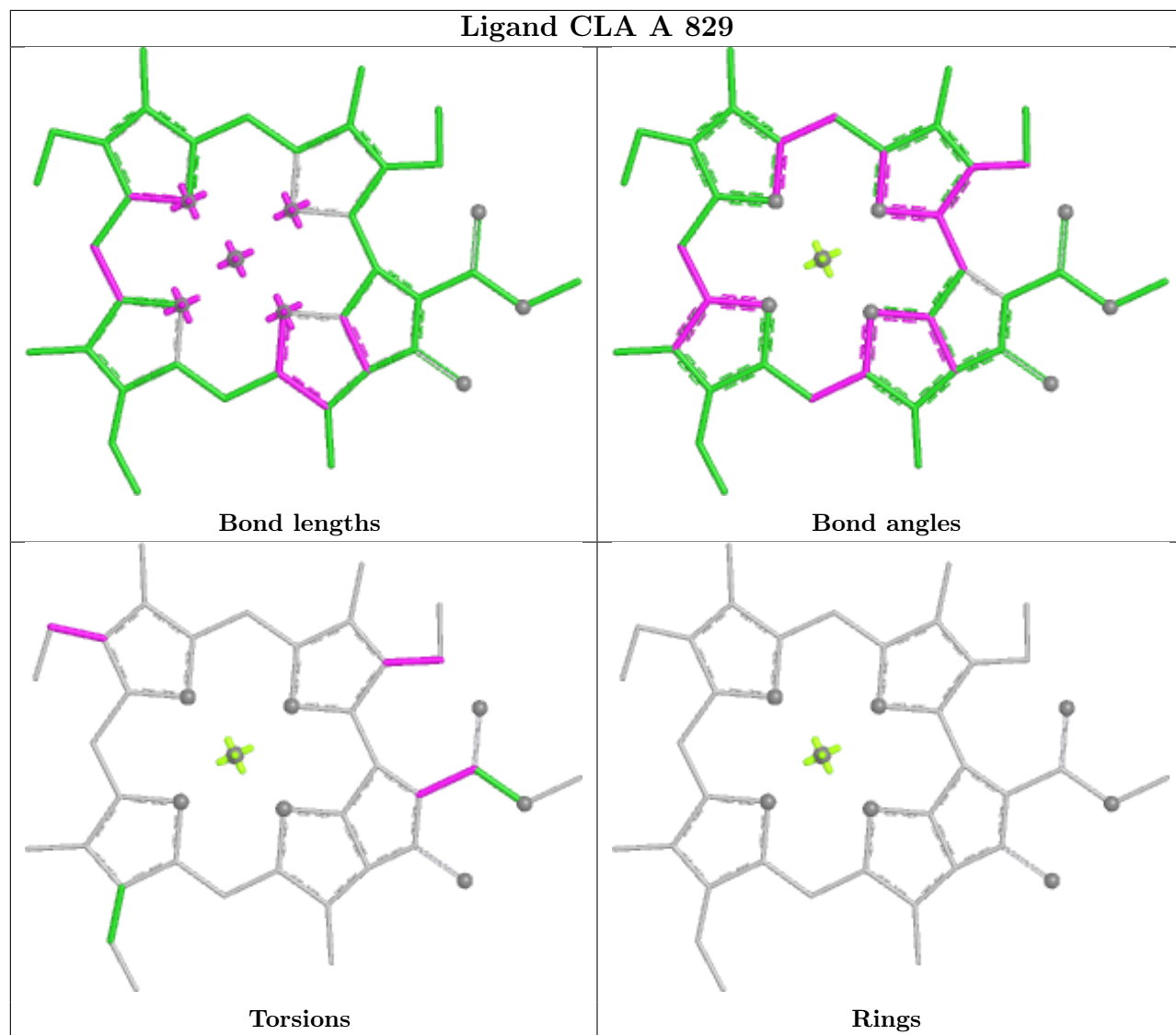


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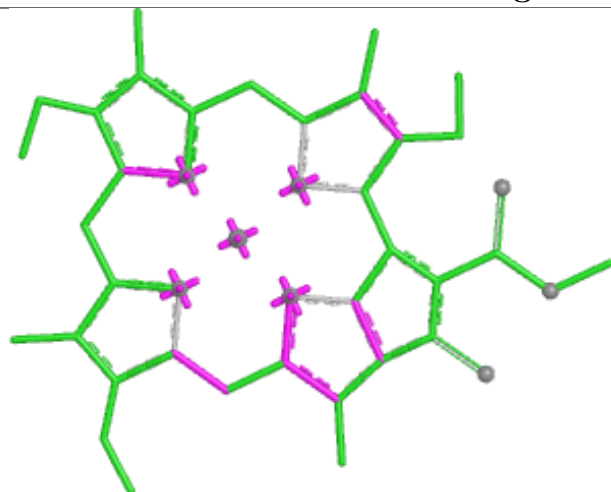


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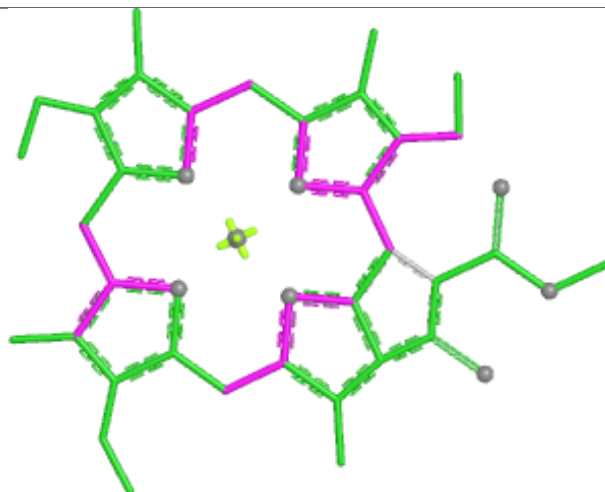
Ligand CLA A 829



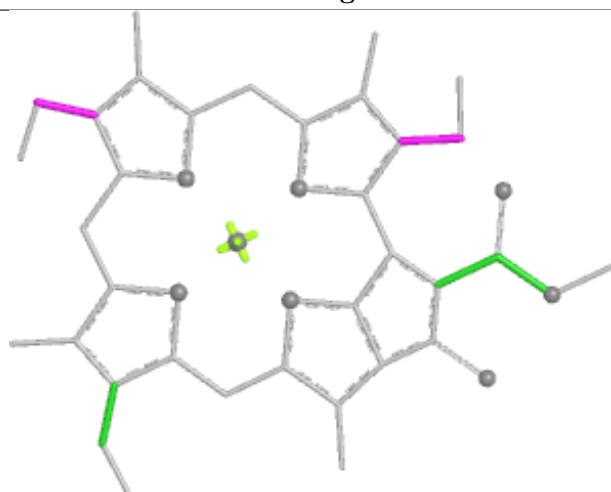
Ligand CLA A 806



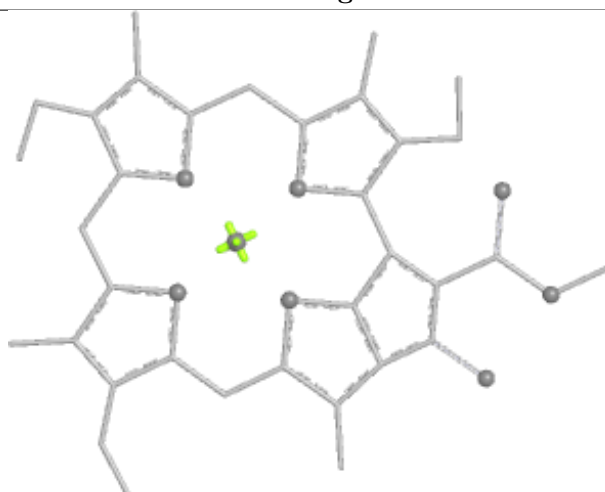
Bond lengths



Bond angles

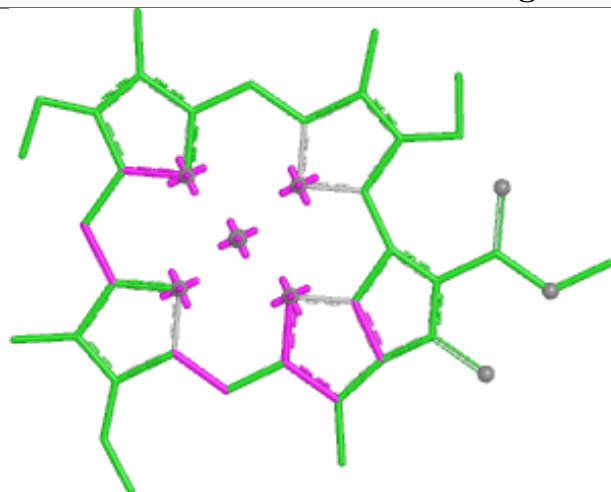


Torsions

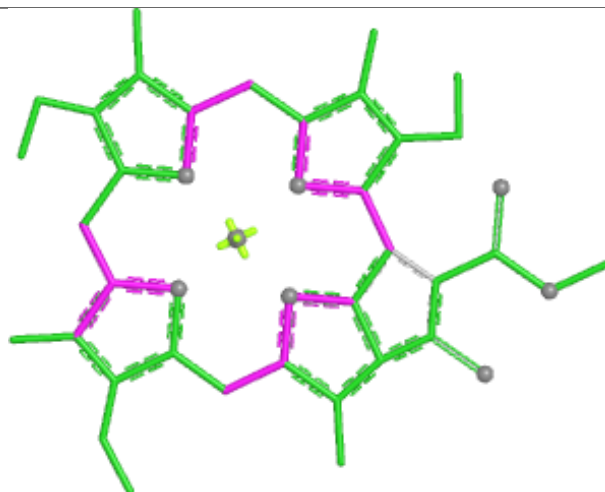


Rings

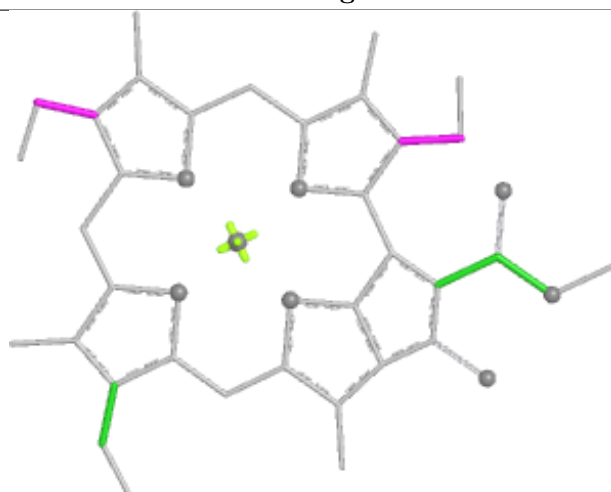
Ligand CLA 5 302



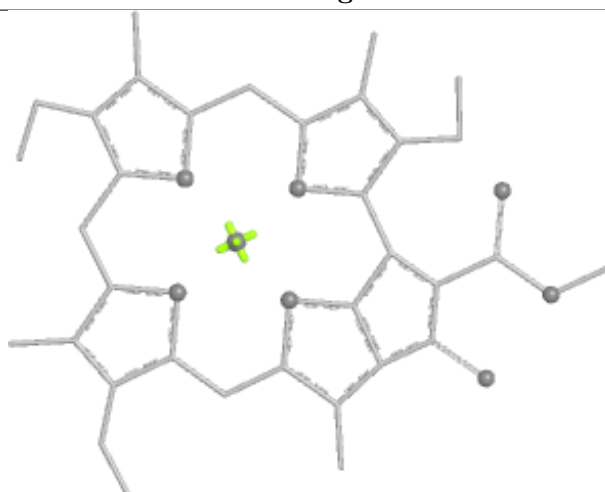
Bond lengths



Bond angles

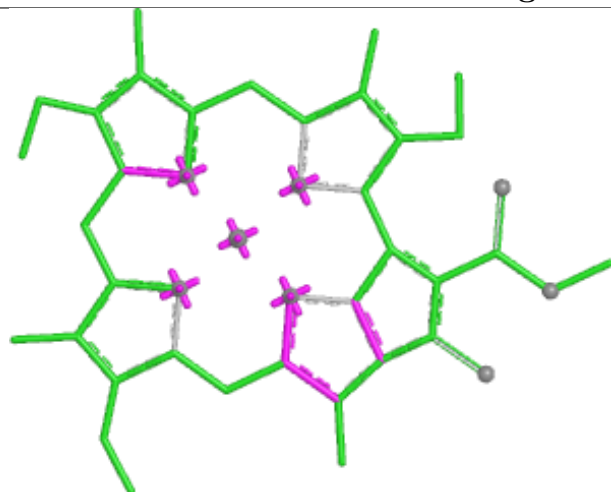


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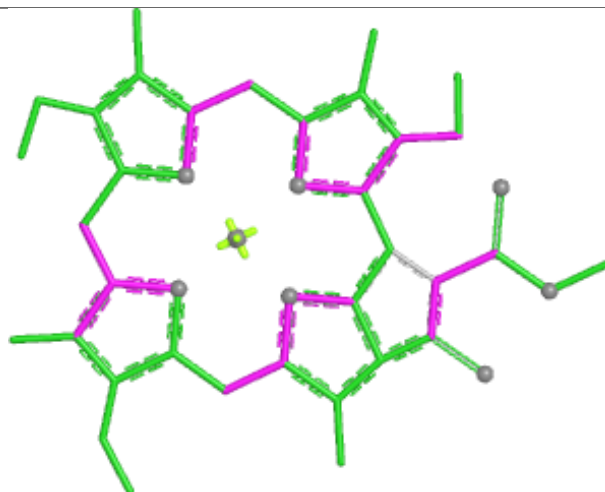


Rings

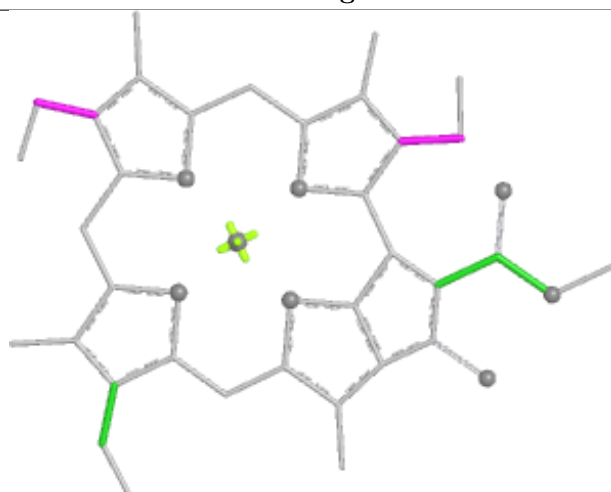
Ligand CLA 7 609



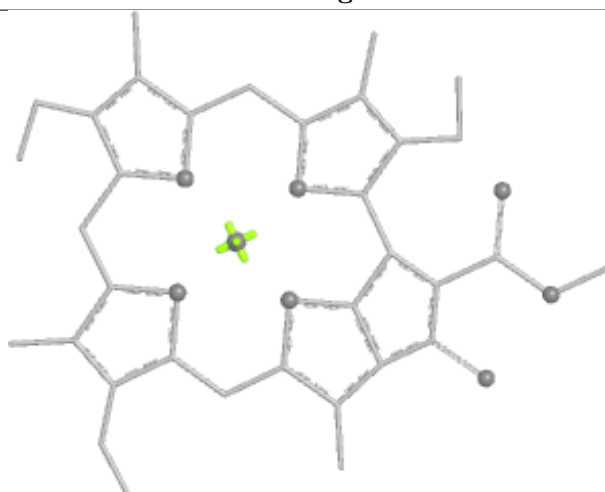
Bond lengths



Bond angles

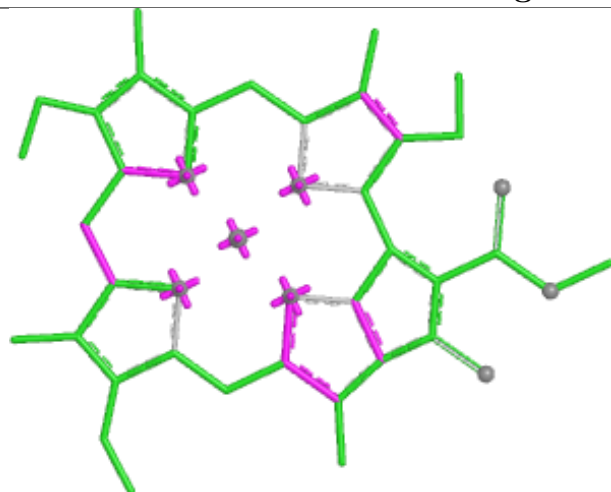


Torsions

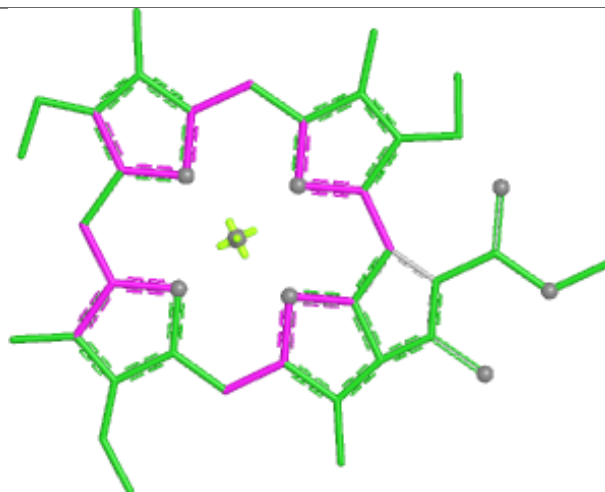


Rings

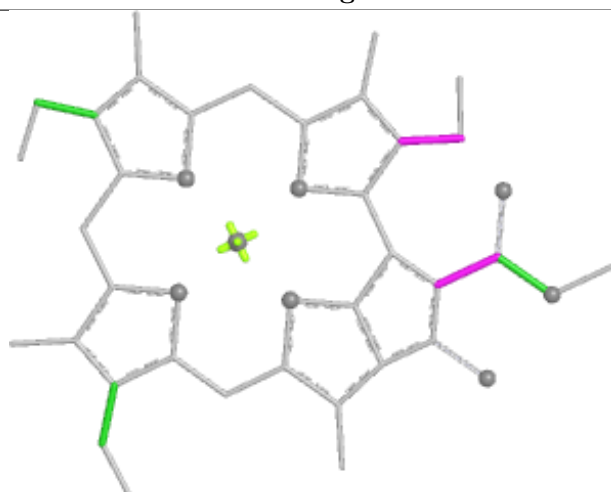
Ligand CLA B 836



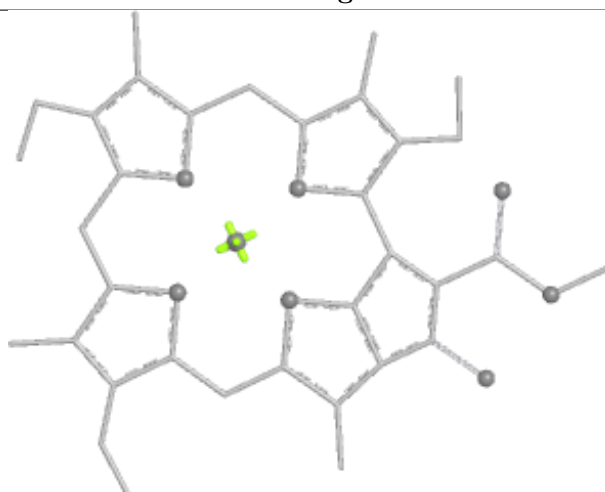
Bond lengths



Bond angles

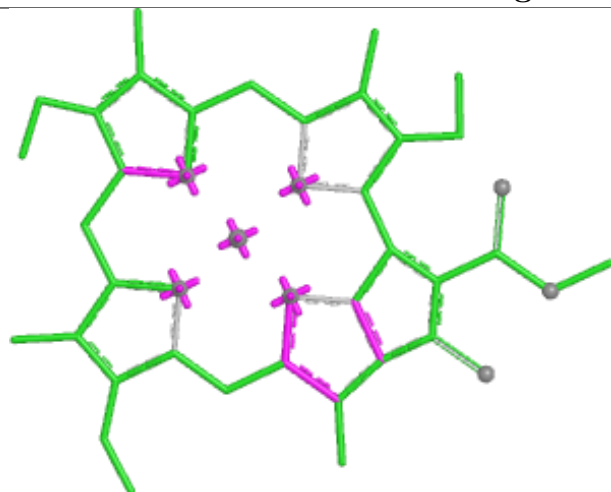


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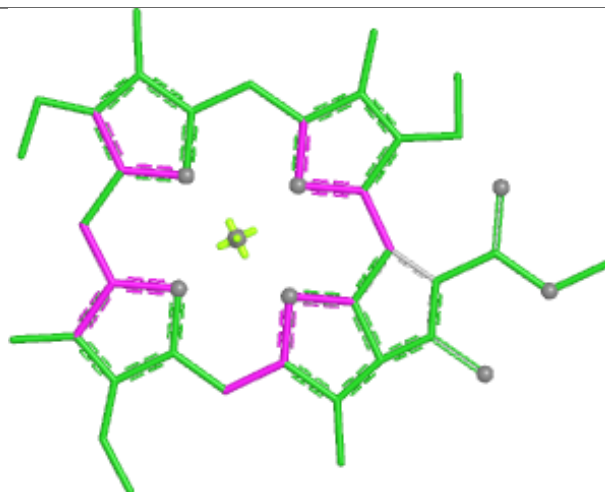


Rings

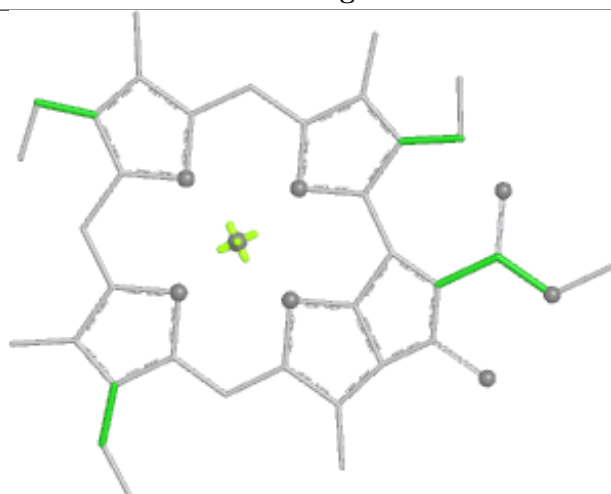
Ligand CLA B 833



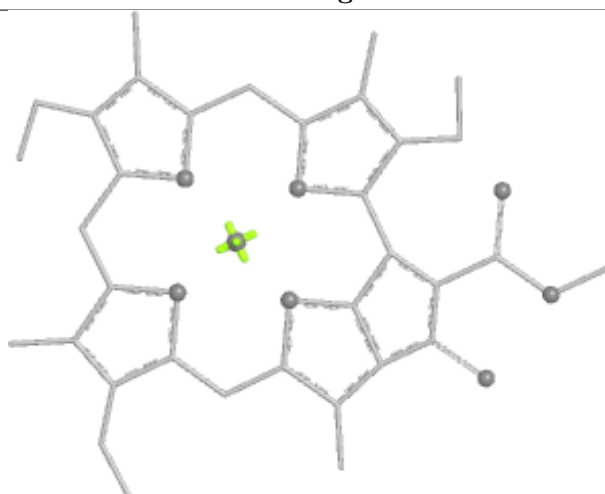
Bond lengths



Bond angles

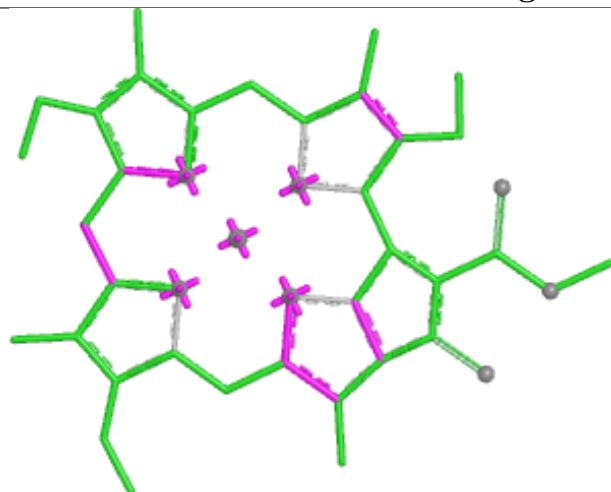


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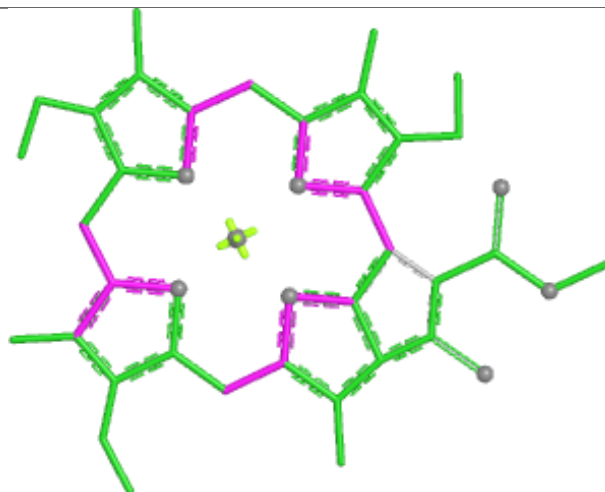


Rings

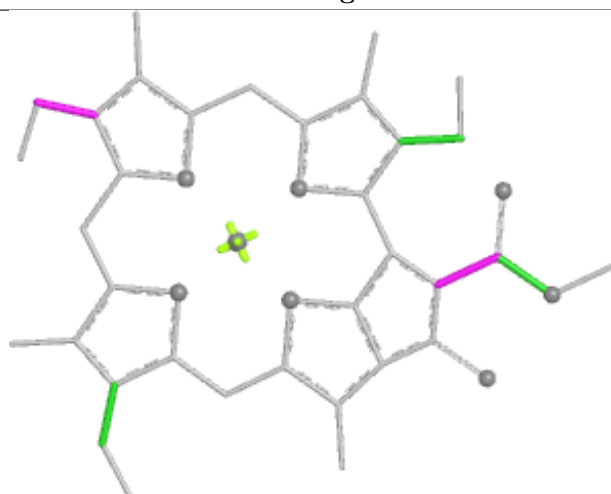
Ligand CLA 7 601



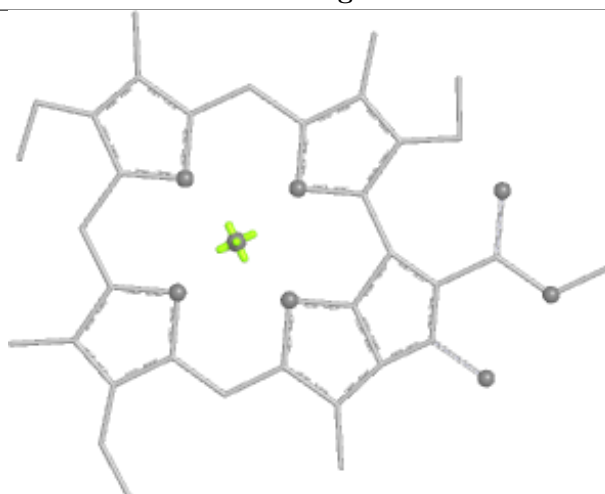
Bond lengths



Bond angles

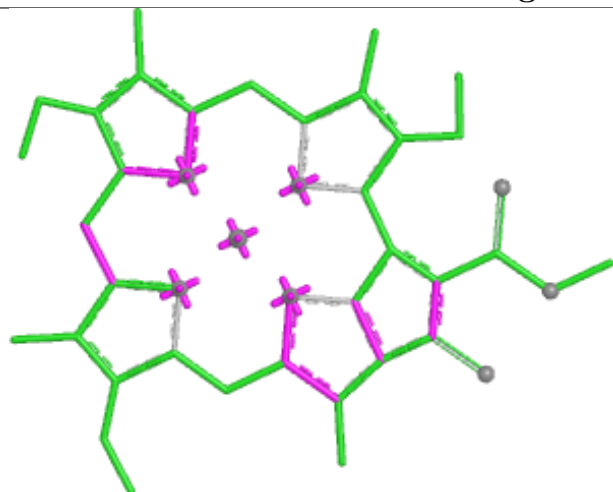


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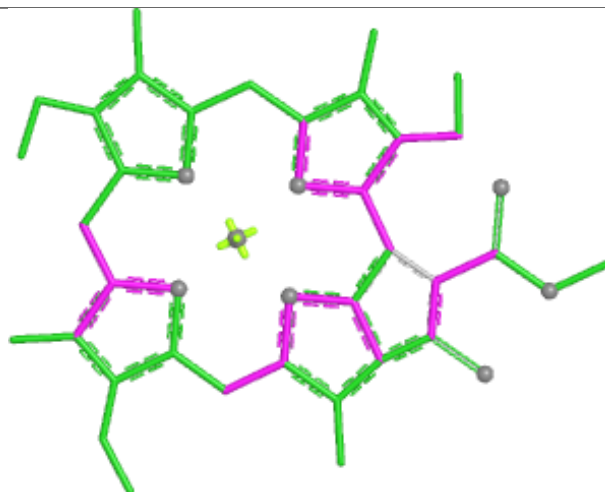


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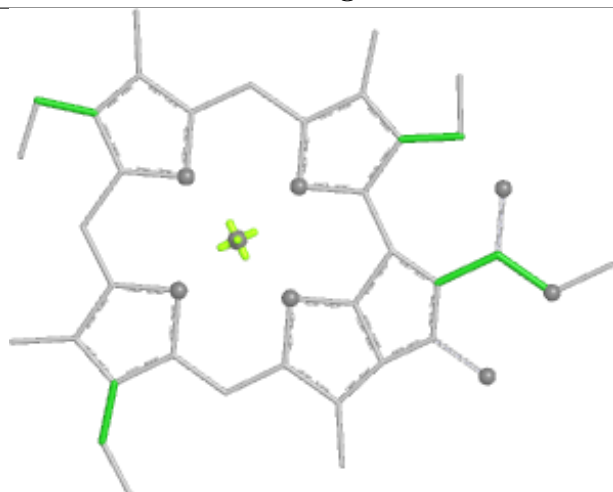
Ligand CLA 8 608



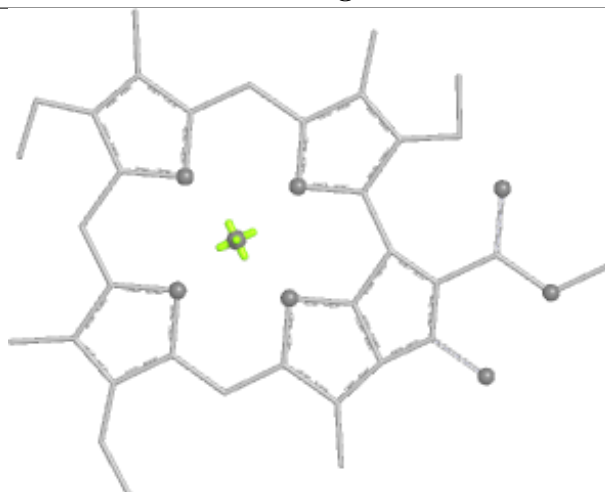
Bond lengths



Bond angles

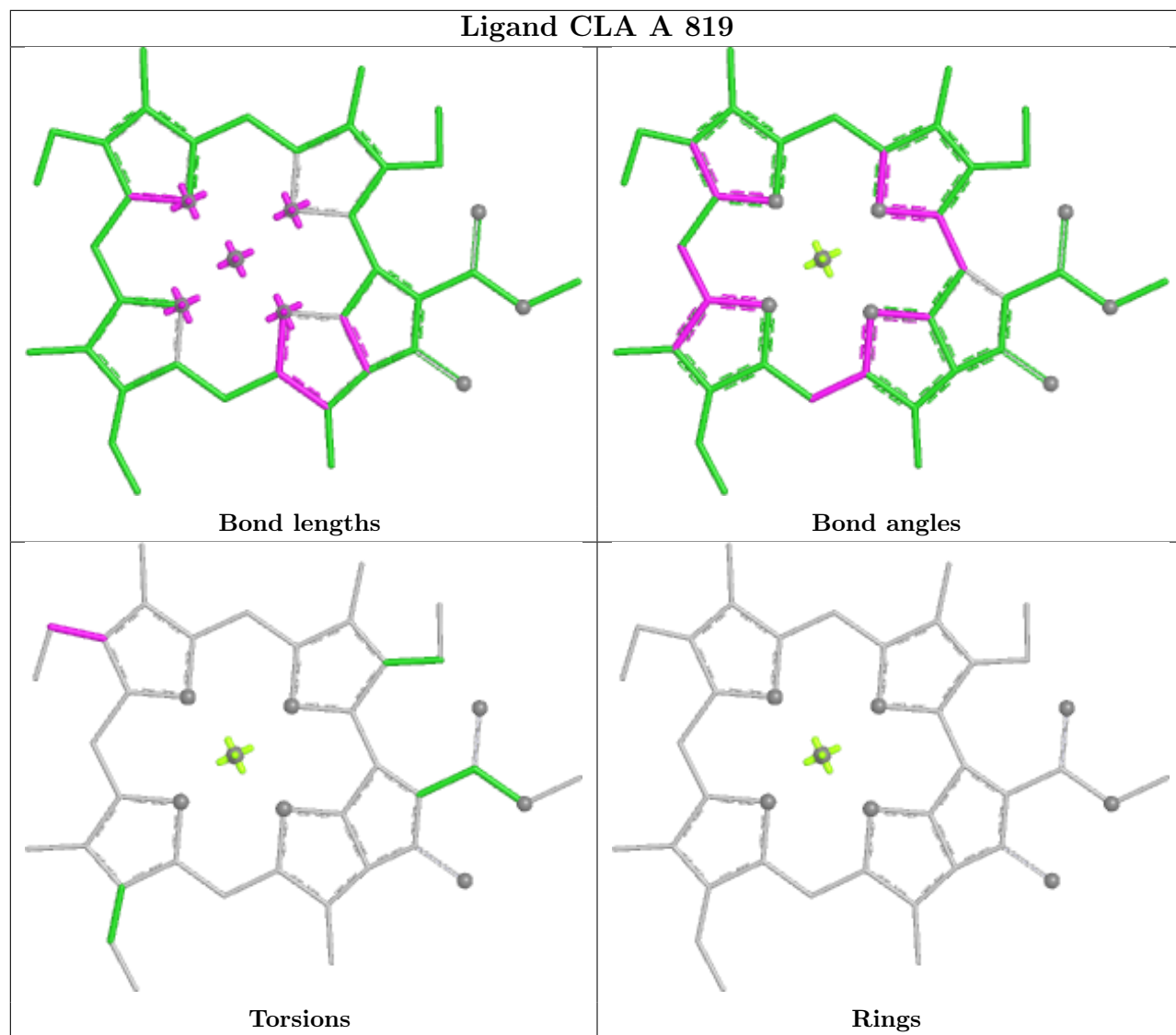


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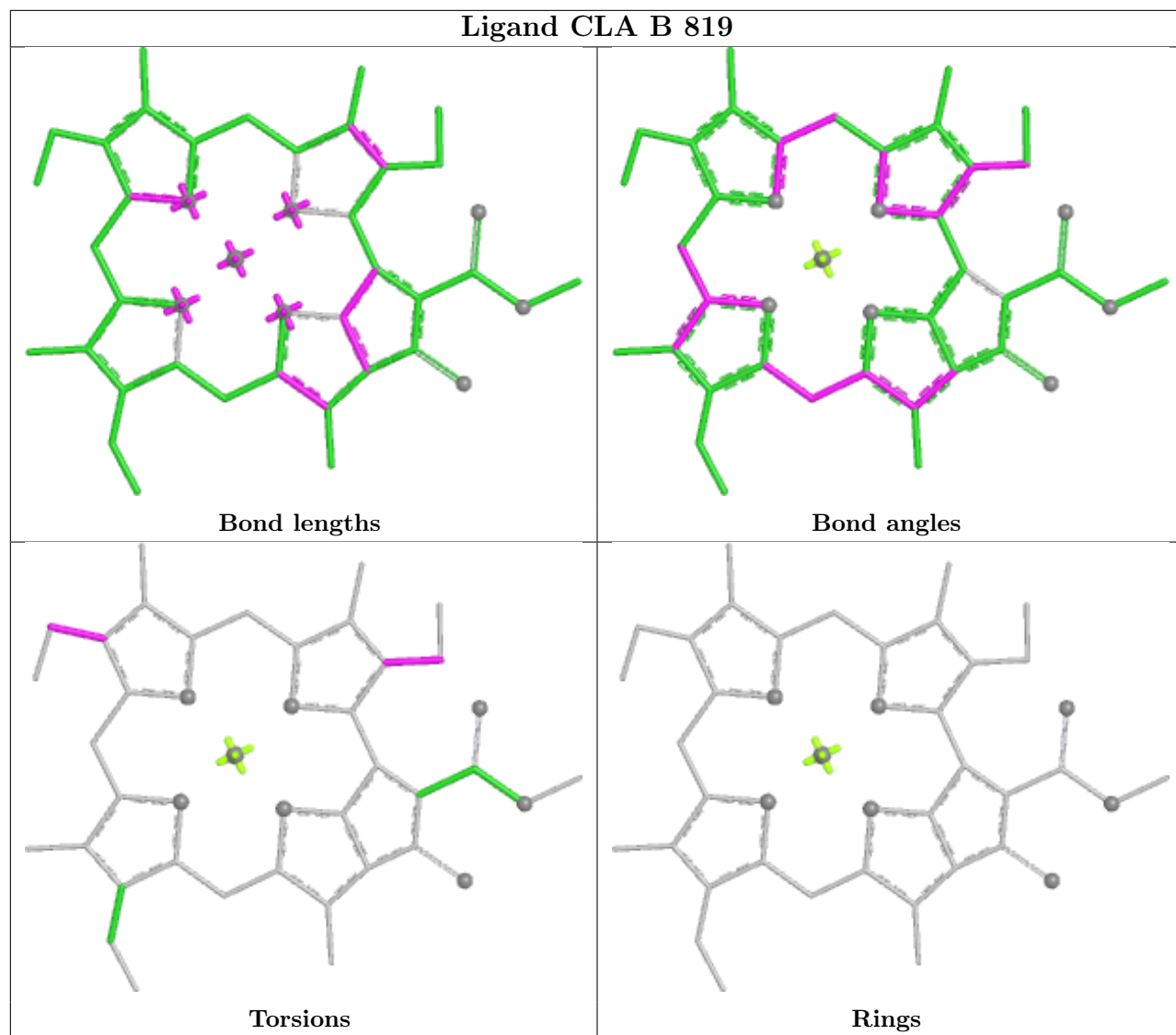


Rings

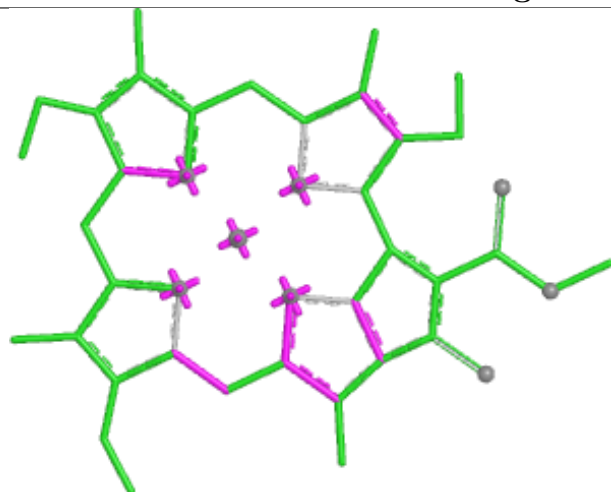
Ligand CLA A 819



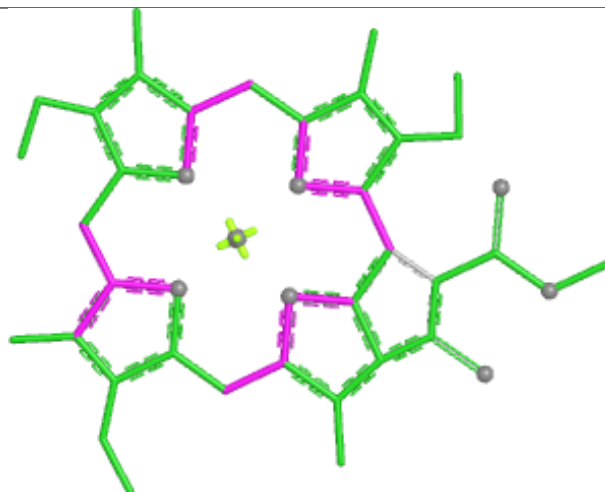
Ligand CLA B 819



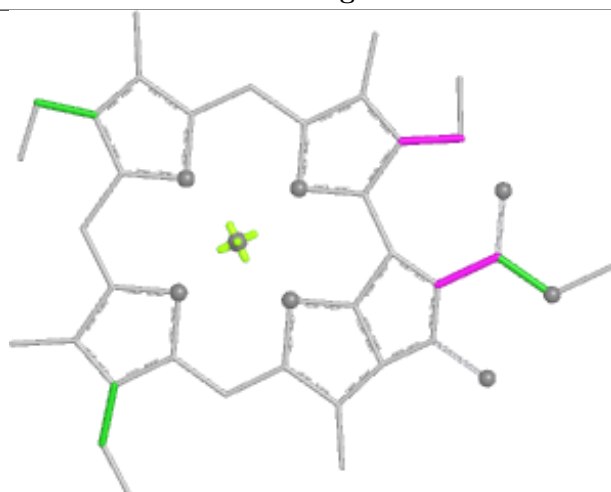
Ligand CLA A 812



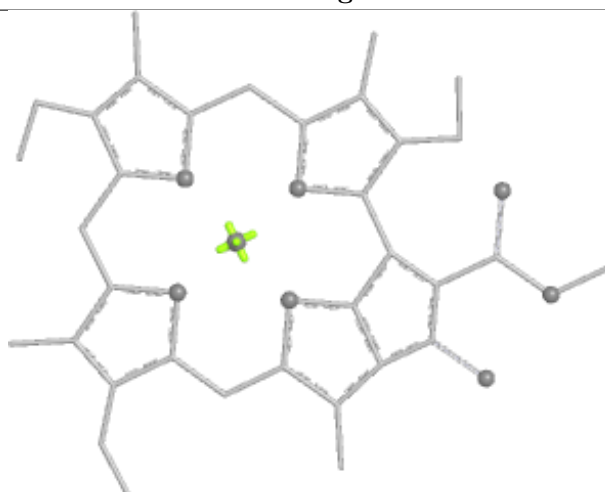
Bond lengths



Bond angles

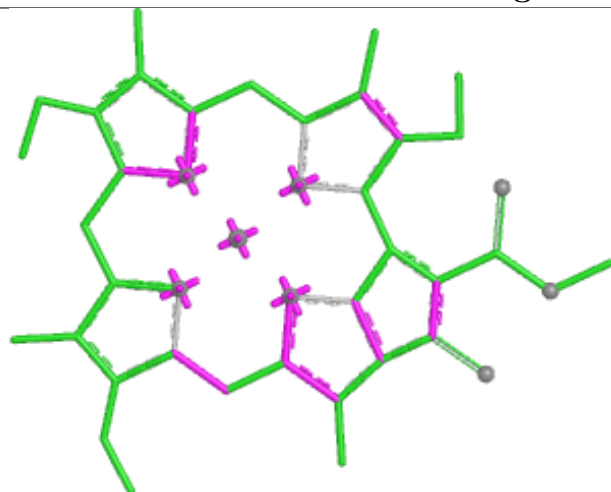


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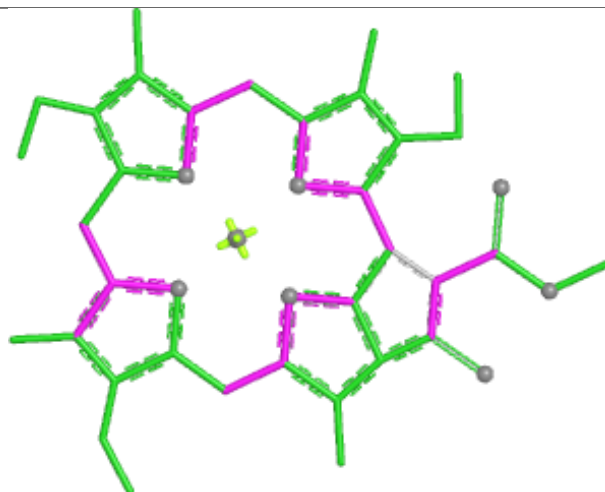


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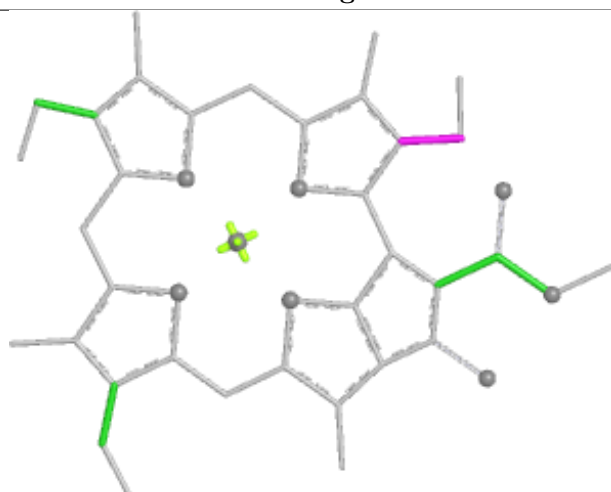
Ligand CLA A 831



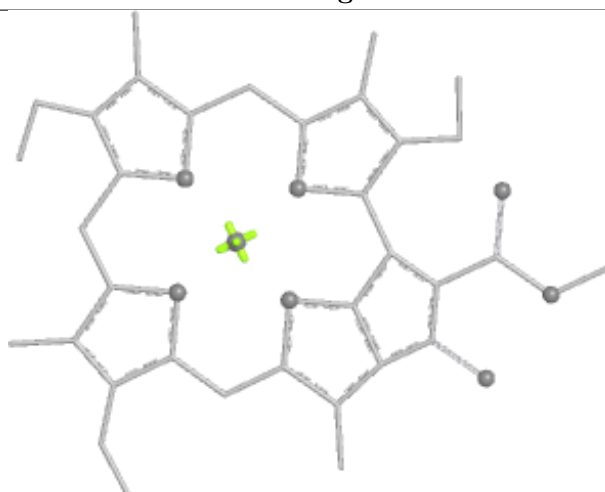
Bond lengths



Bond angles

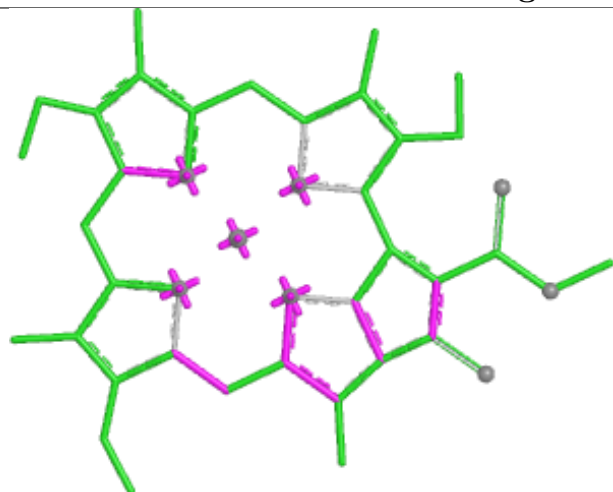


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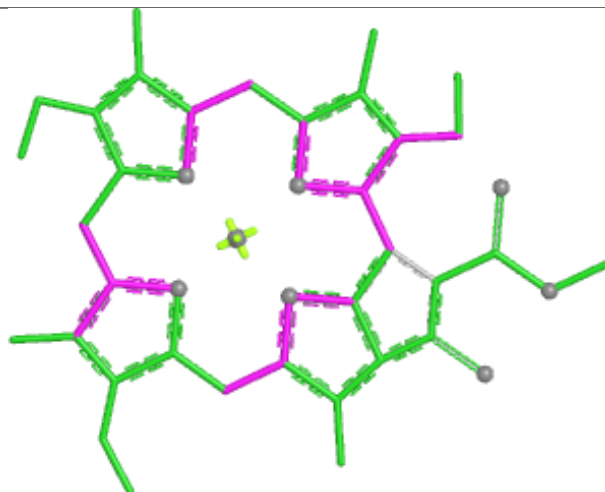


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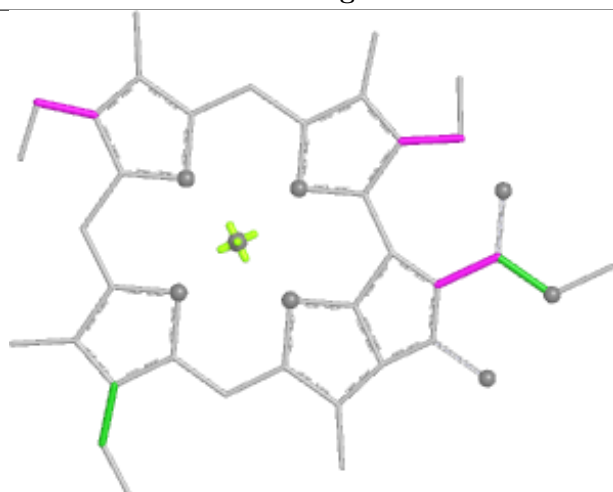
Ligand CLA 7 602



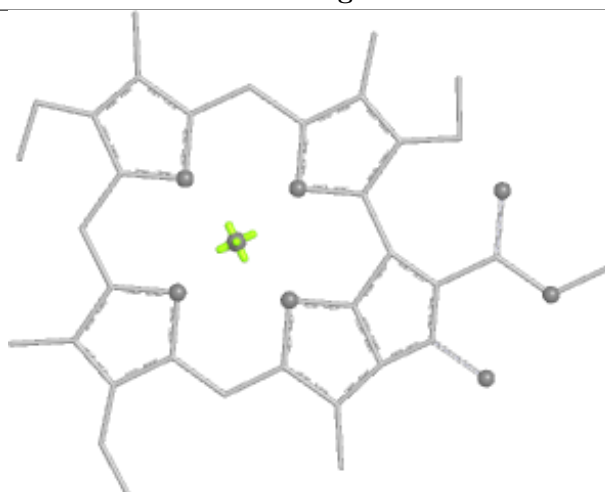
Bond lengths



Bond angles

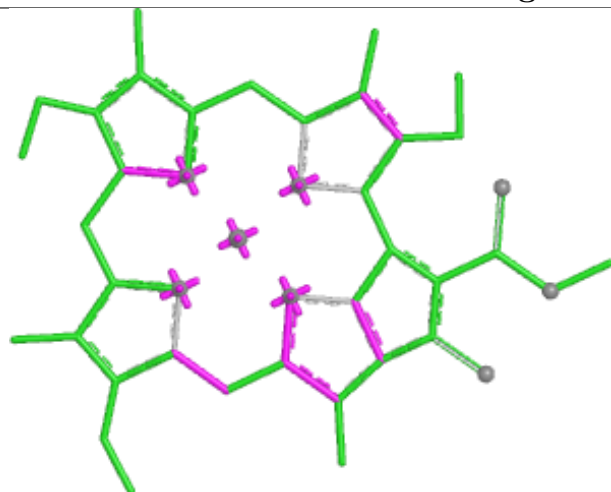


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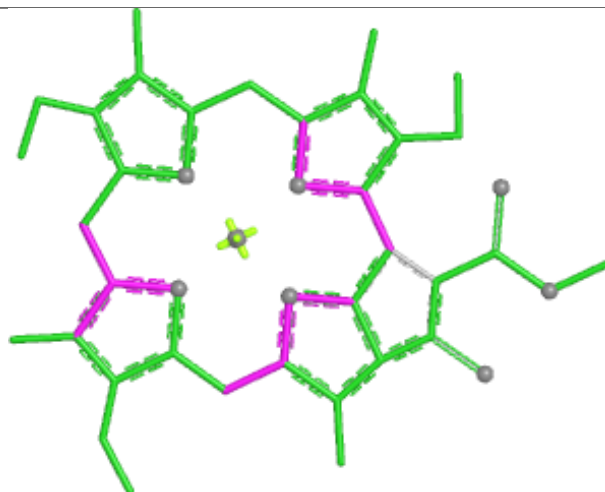


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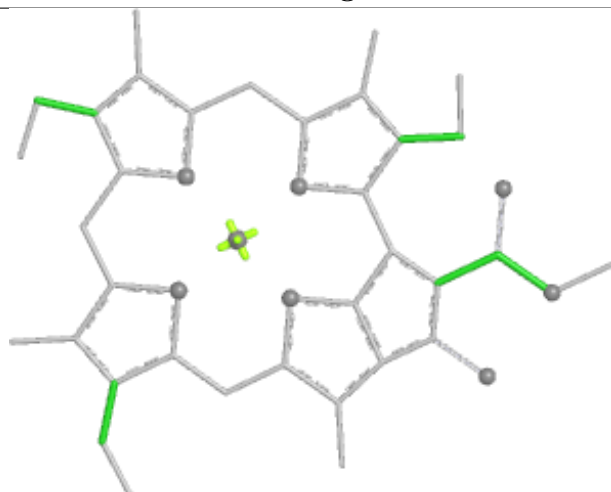
Ligand CLA 8 604



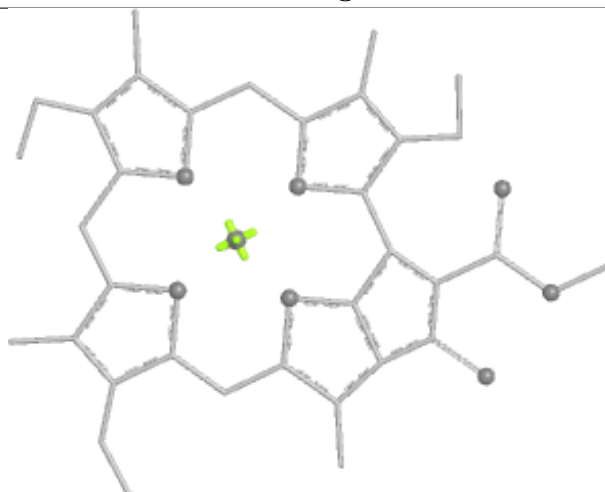
Bond lengths



Bond angles

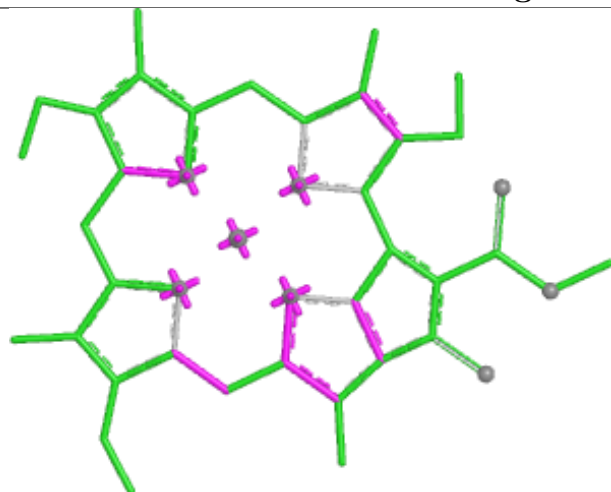


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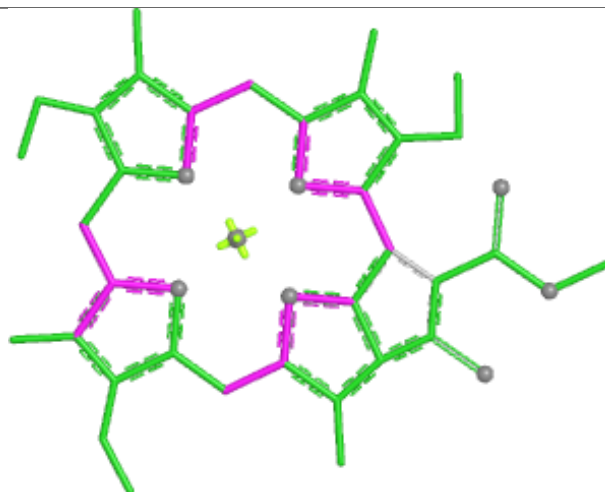


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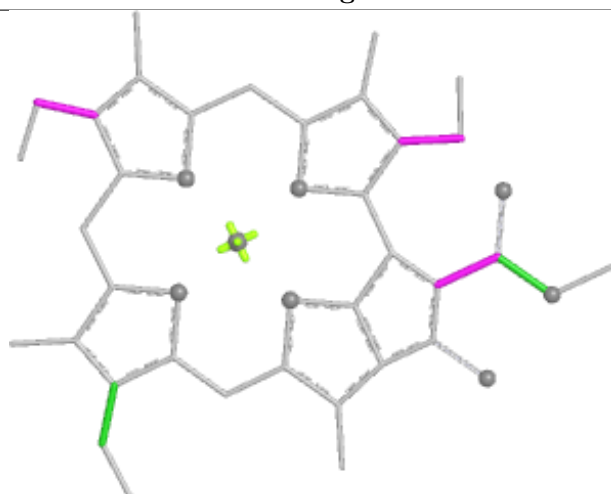
Ligand CLA B 832



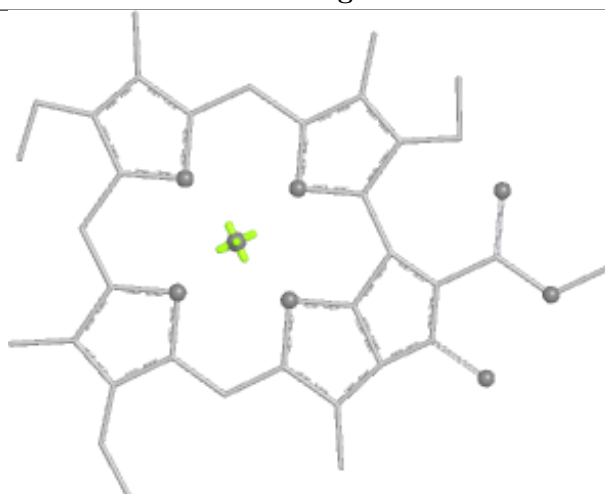
Bond lengths



Bond angles

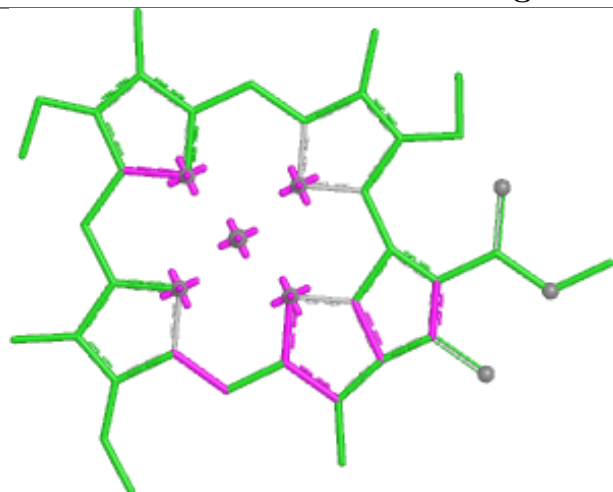


Torsions

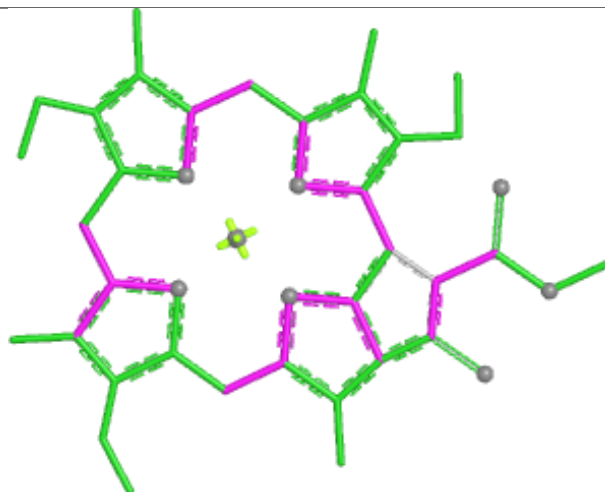


Rings

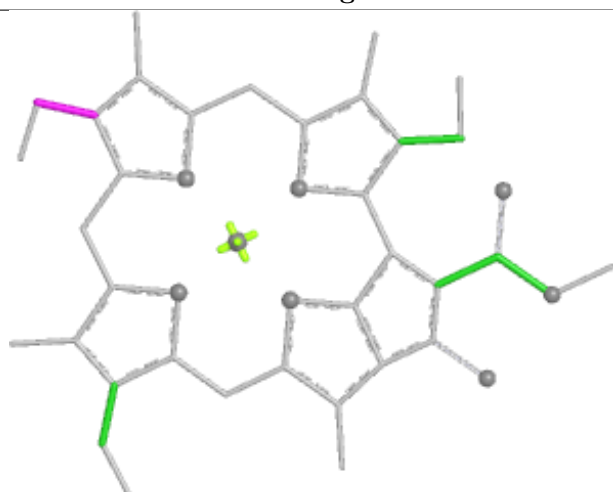
Ligand CLA A 815



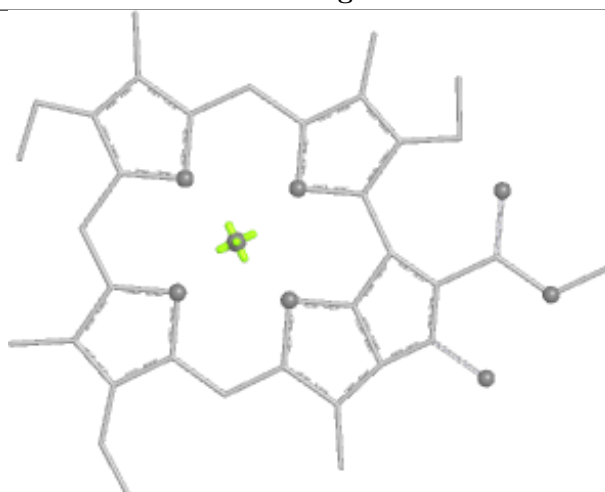
Bond lengths



Bond angles

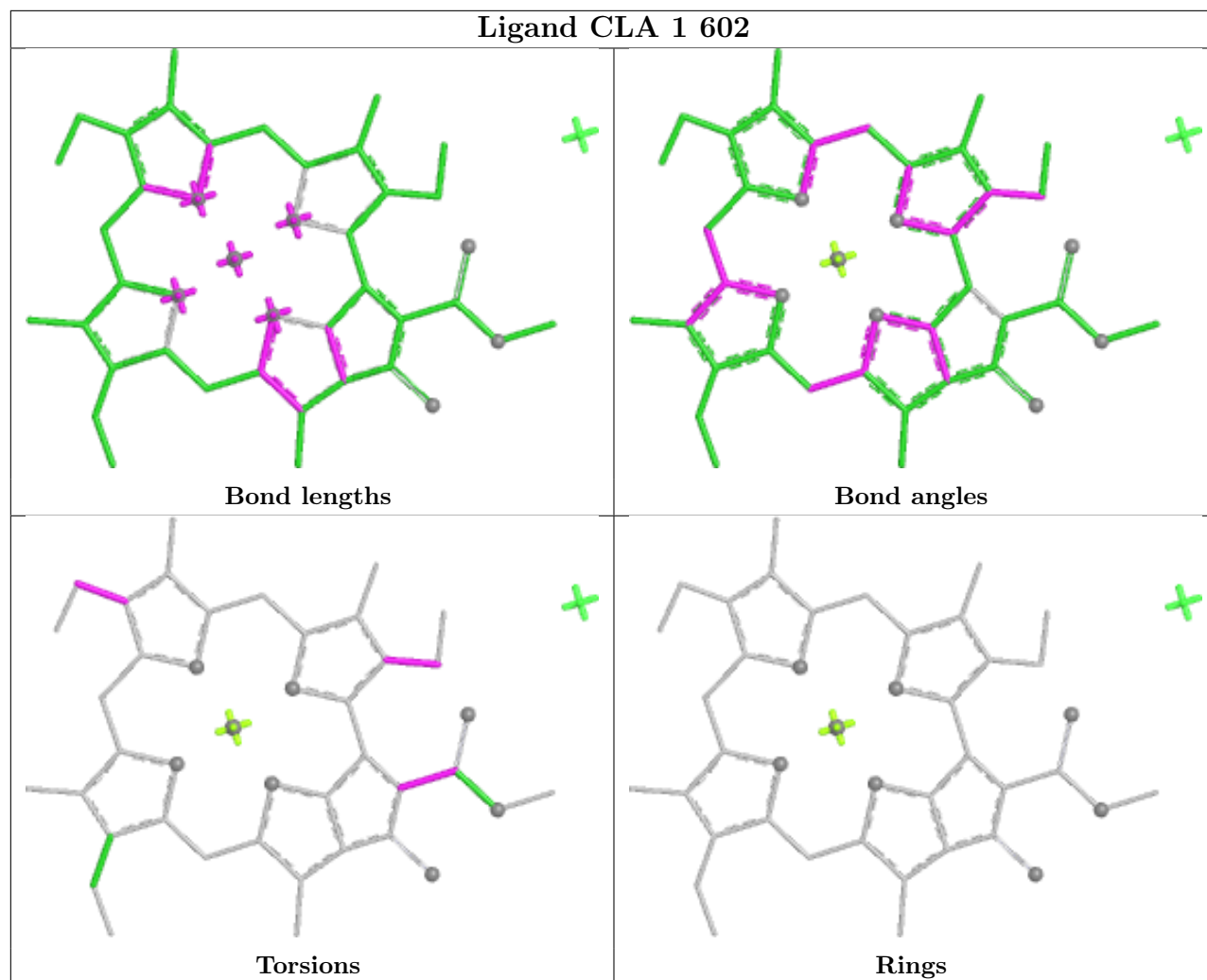


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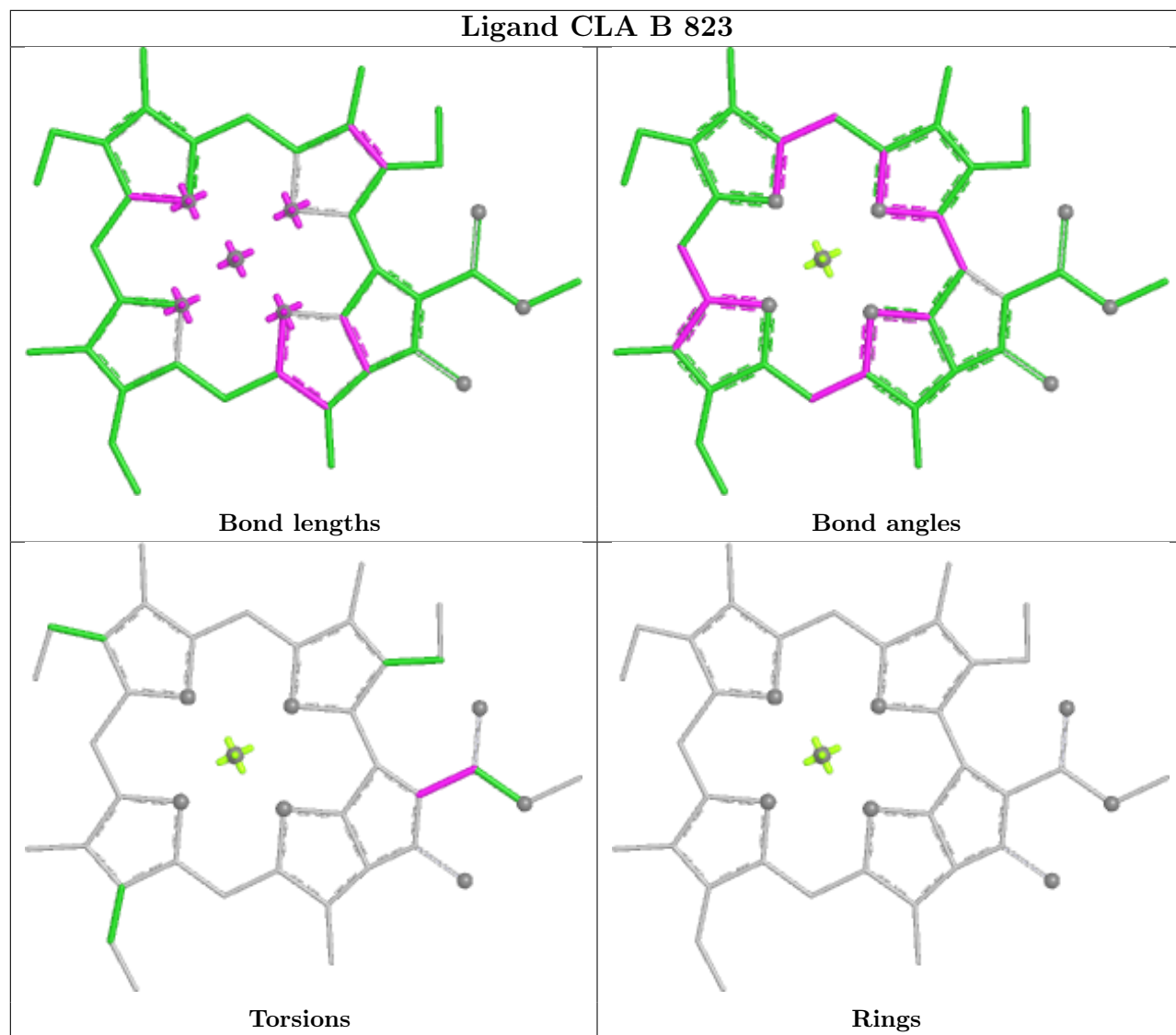


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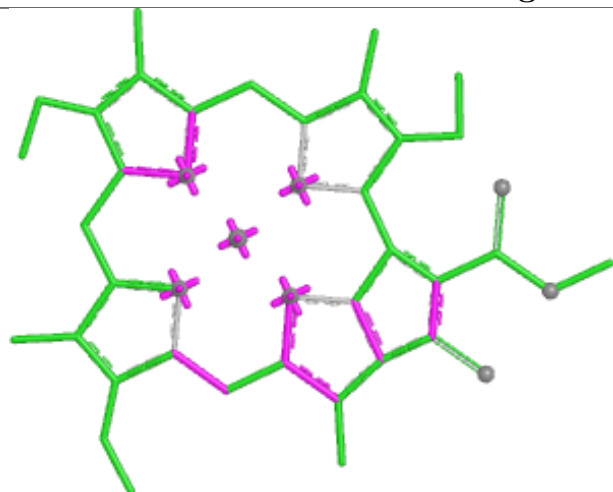
Ligand CLA 1 602



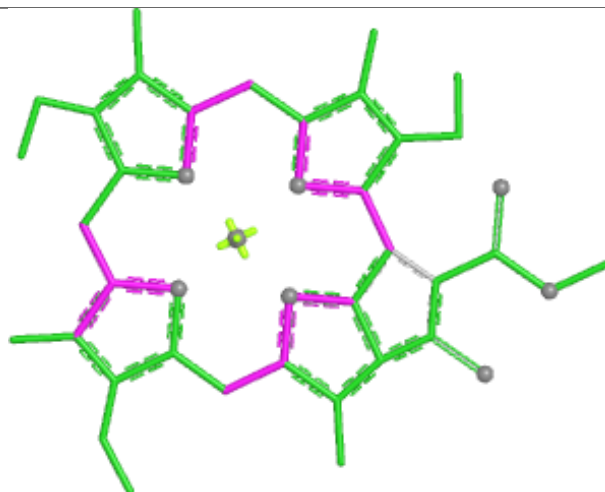
Ligand CLA B 823



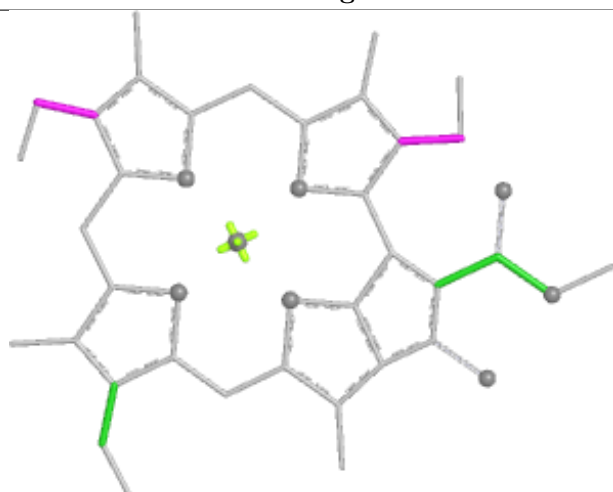
Ligand CLA 6 602



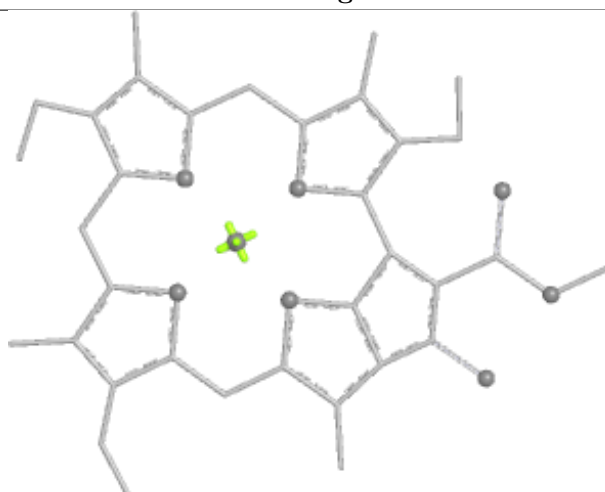
Bond lengths



Bond angles

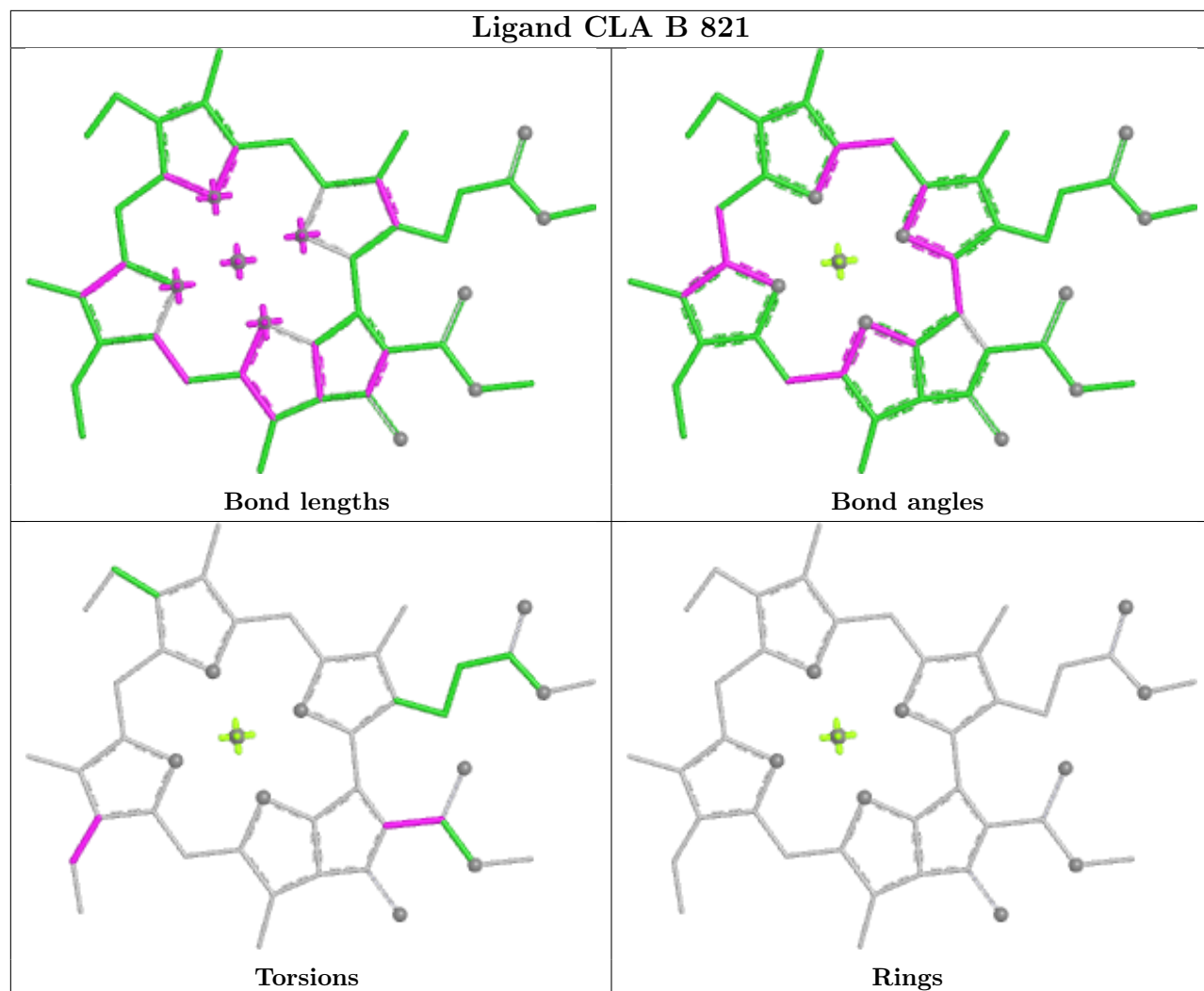


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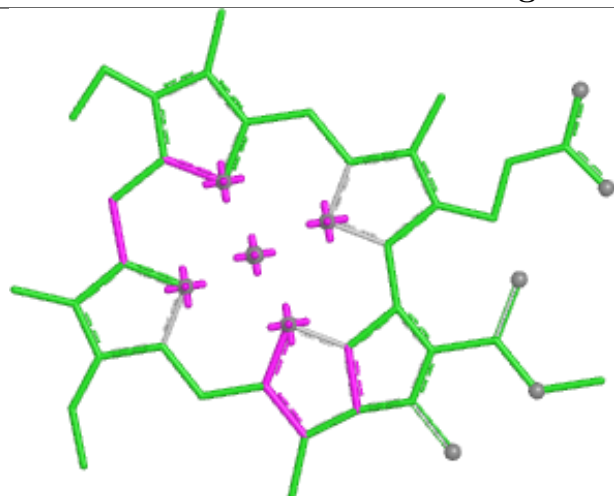


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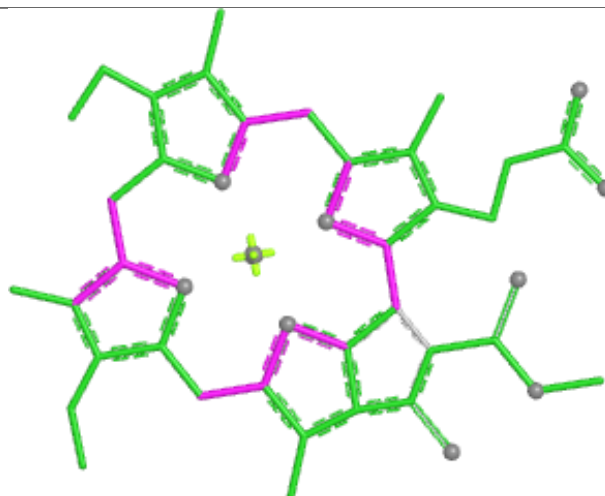
Ligand CLA B 821



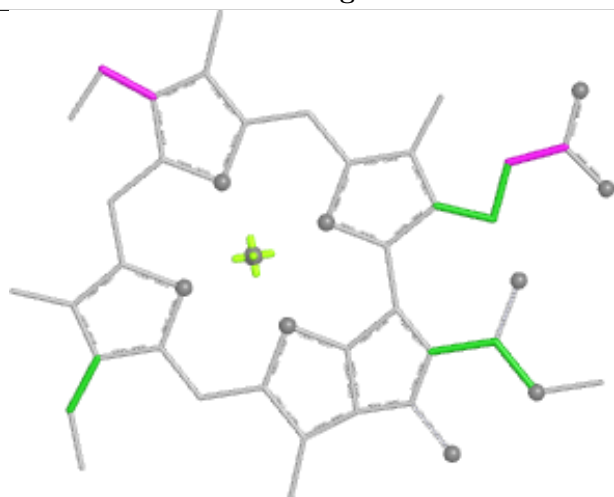
Ligand CLA 3 304



Bond lengths



Bond angles

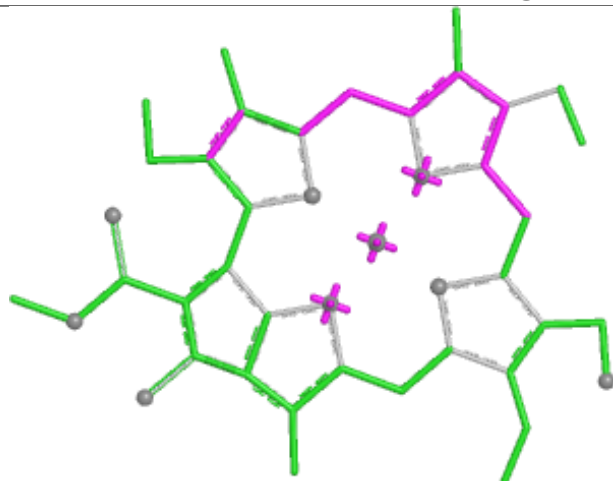


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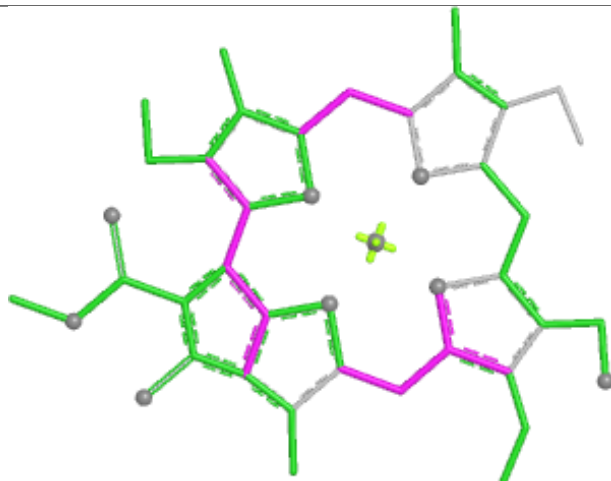


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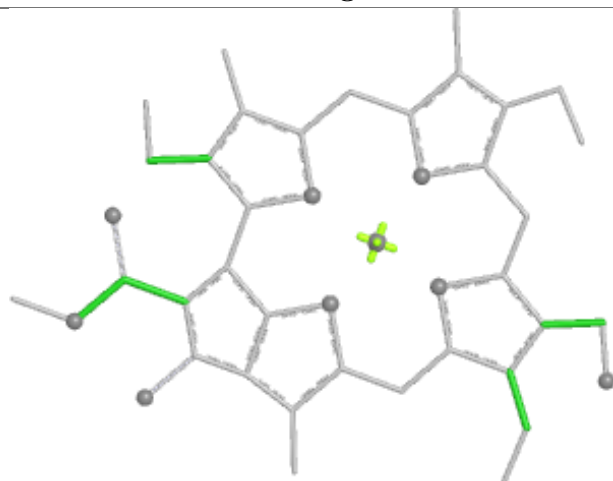
Ligand CHL 5 313



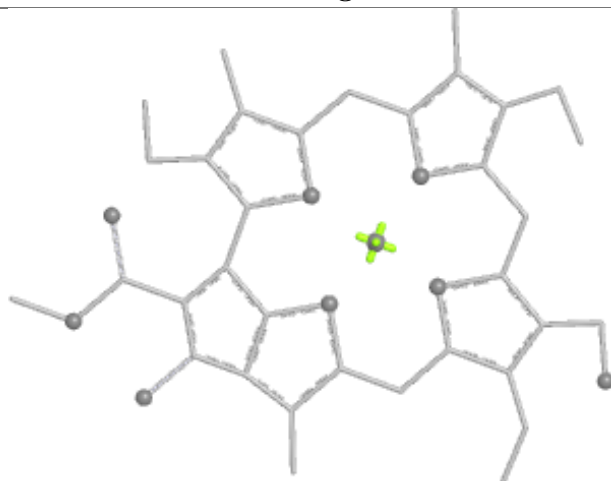
Bond lengths



Bond angles

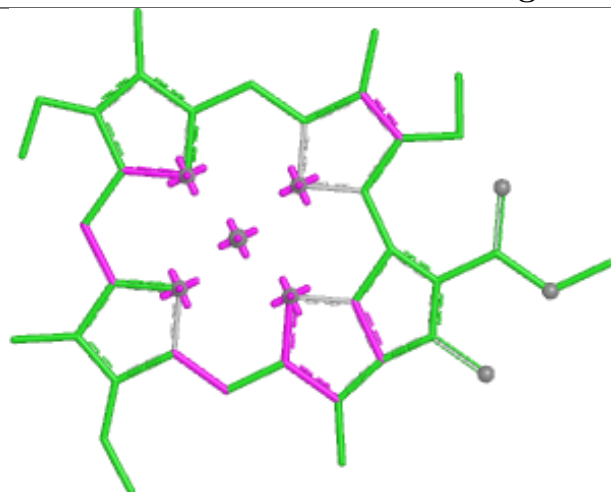


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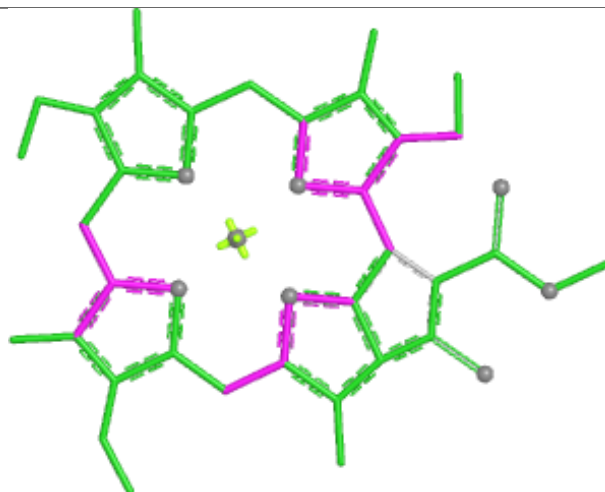


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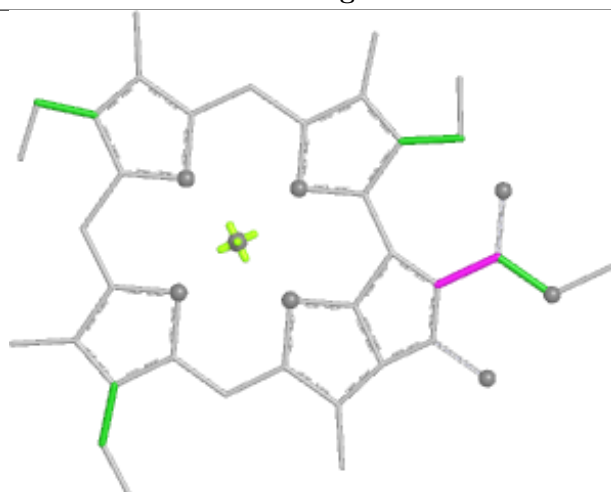
Ligand CLA 7 605



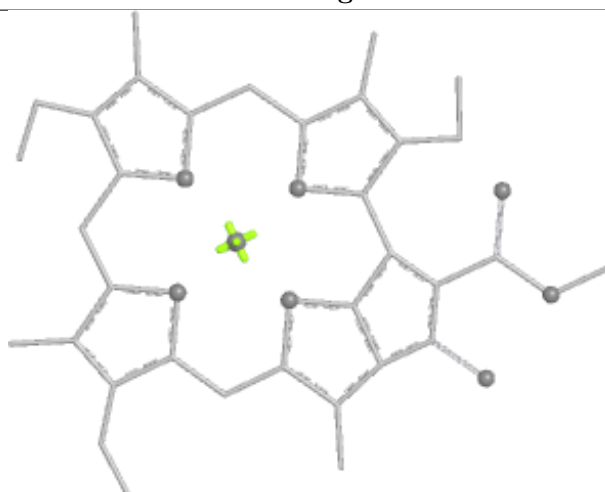
Bond lengths



Bond angles

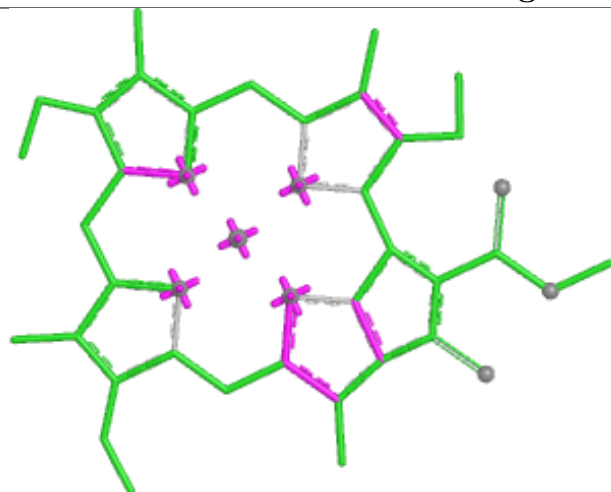


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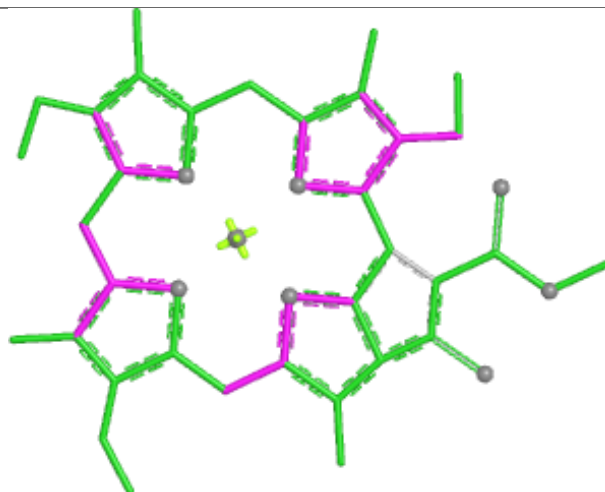


Rings

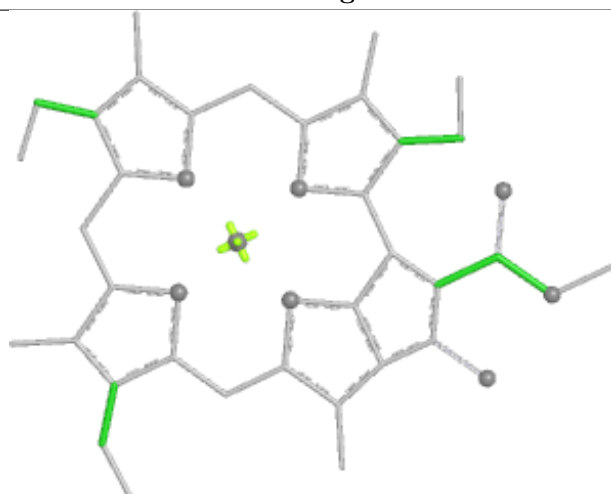
Ligand CLA 3 308



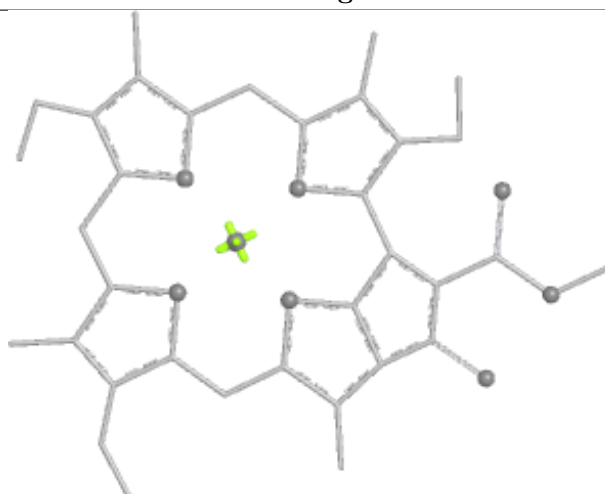
Bond lengths



Bond angles

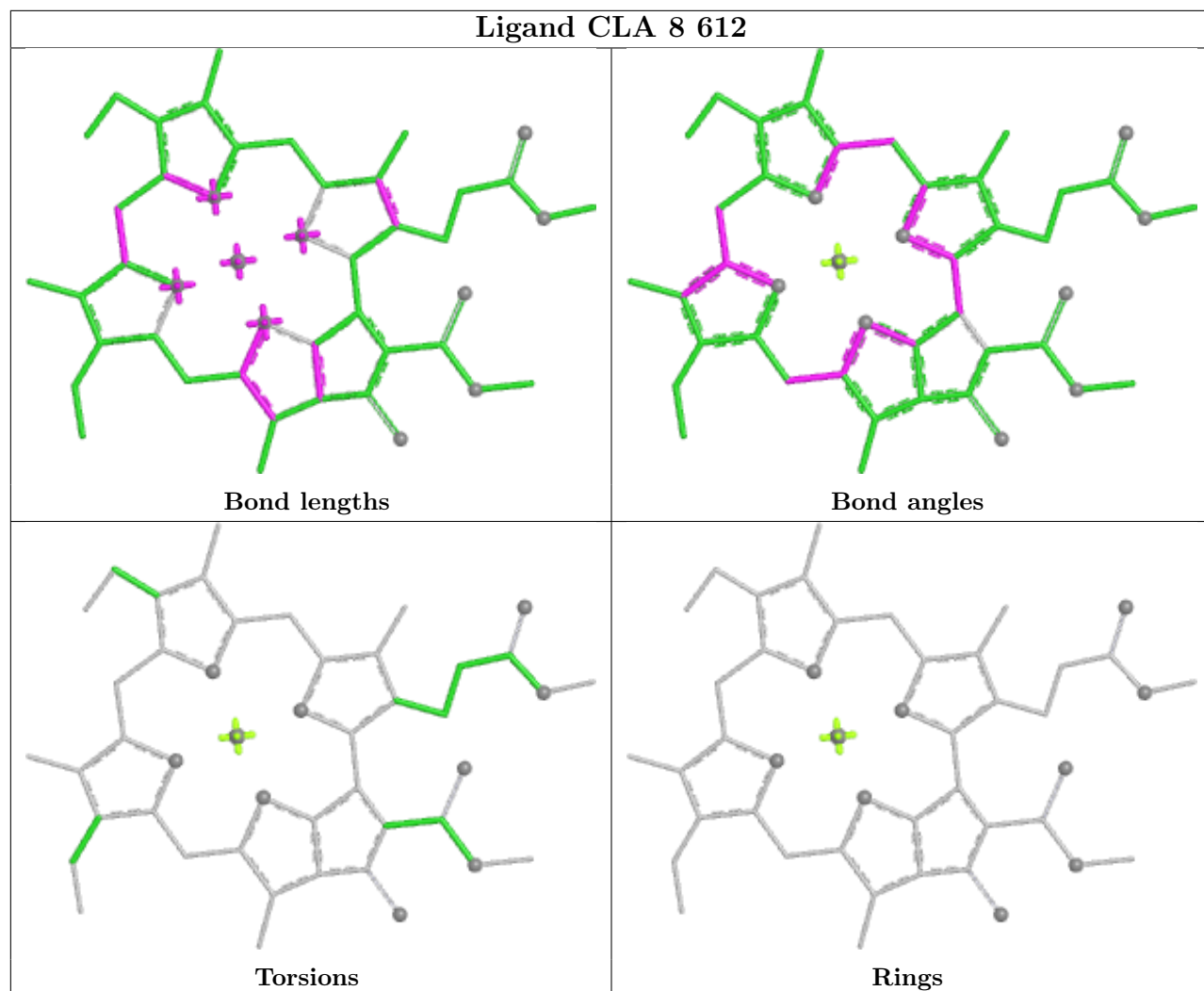


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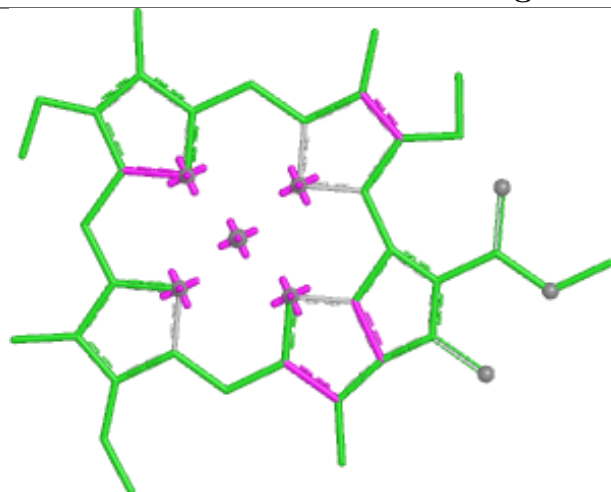


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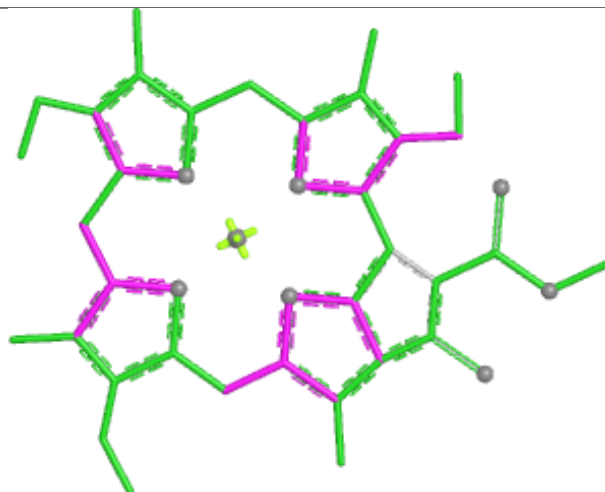
Ligand CLA 8 612



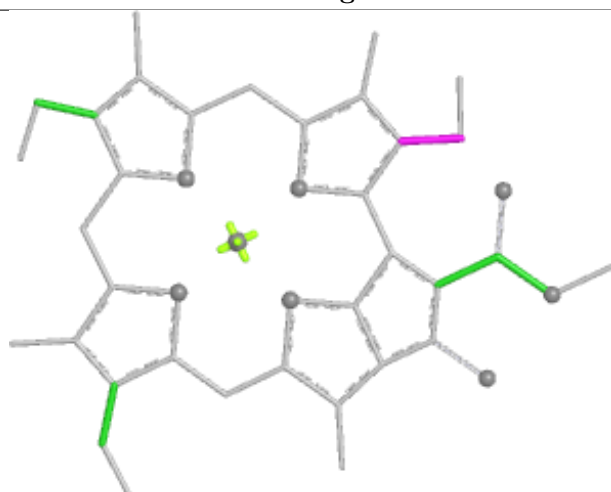
Ligand CLA B 801



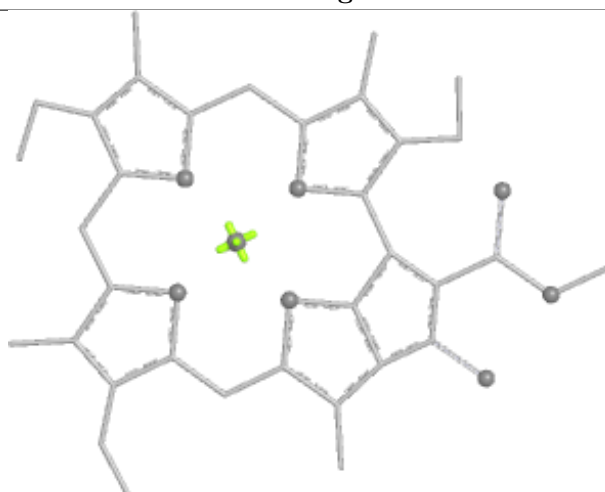
Bond lengths



Bond angles

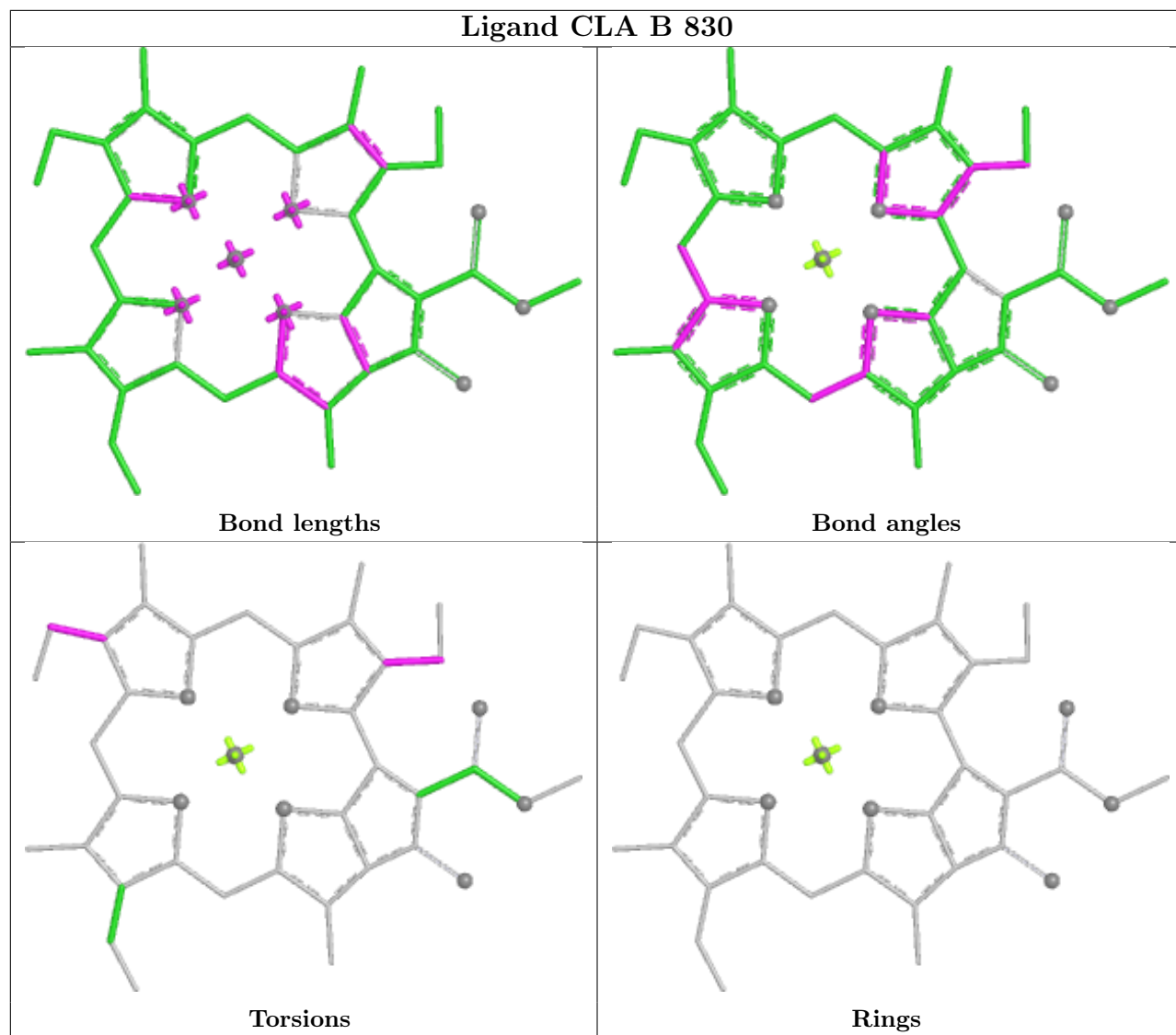


Torsions

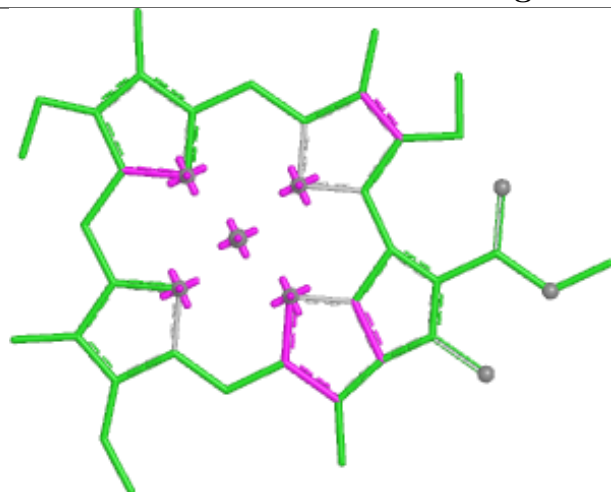


Rings

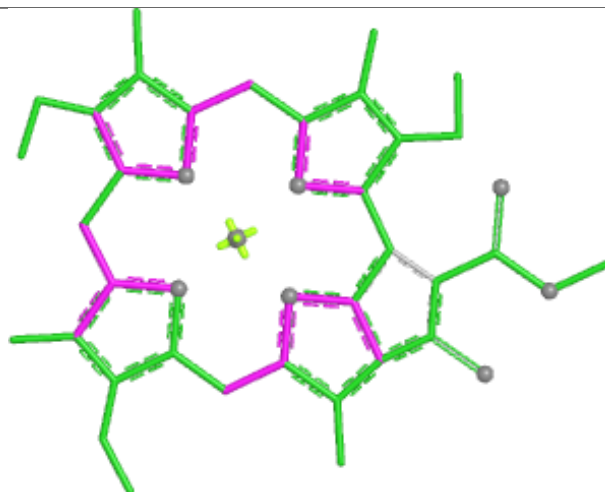
Ligand CLA B 830



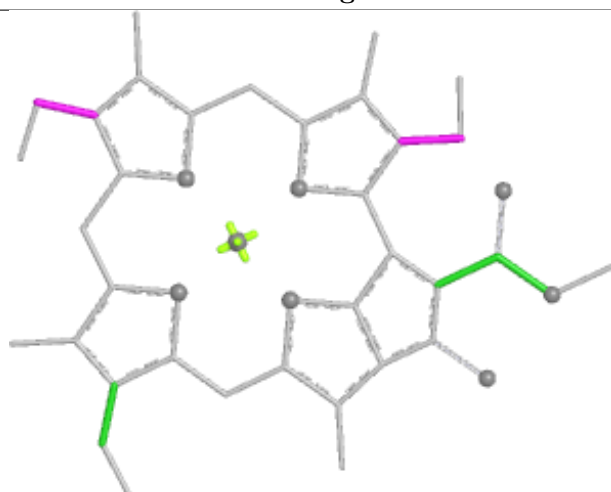
Ligand CLA B 827



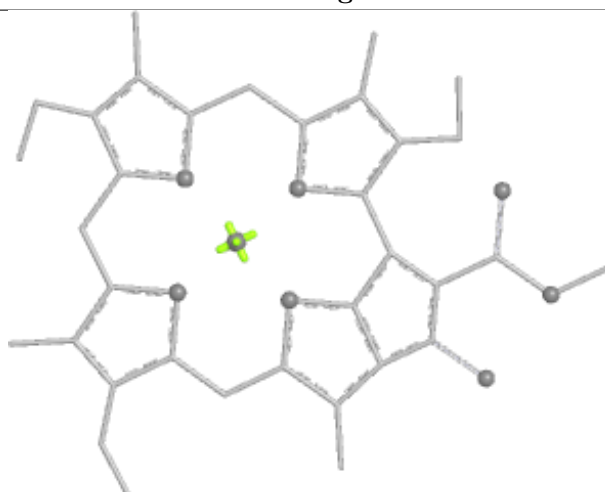
Bond lengths



Bond angles

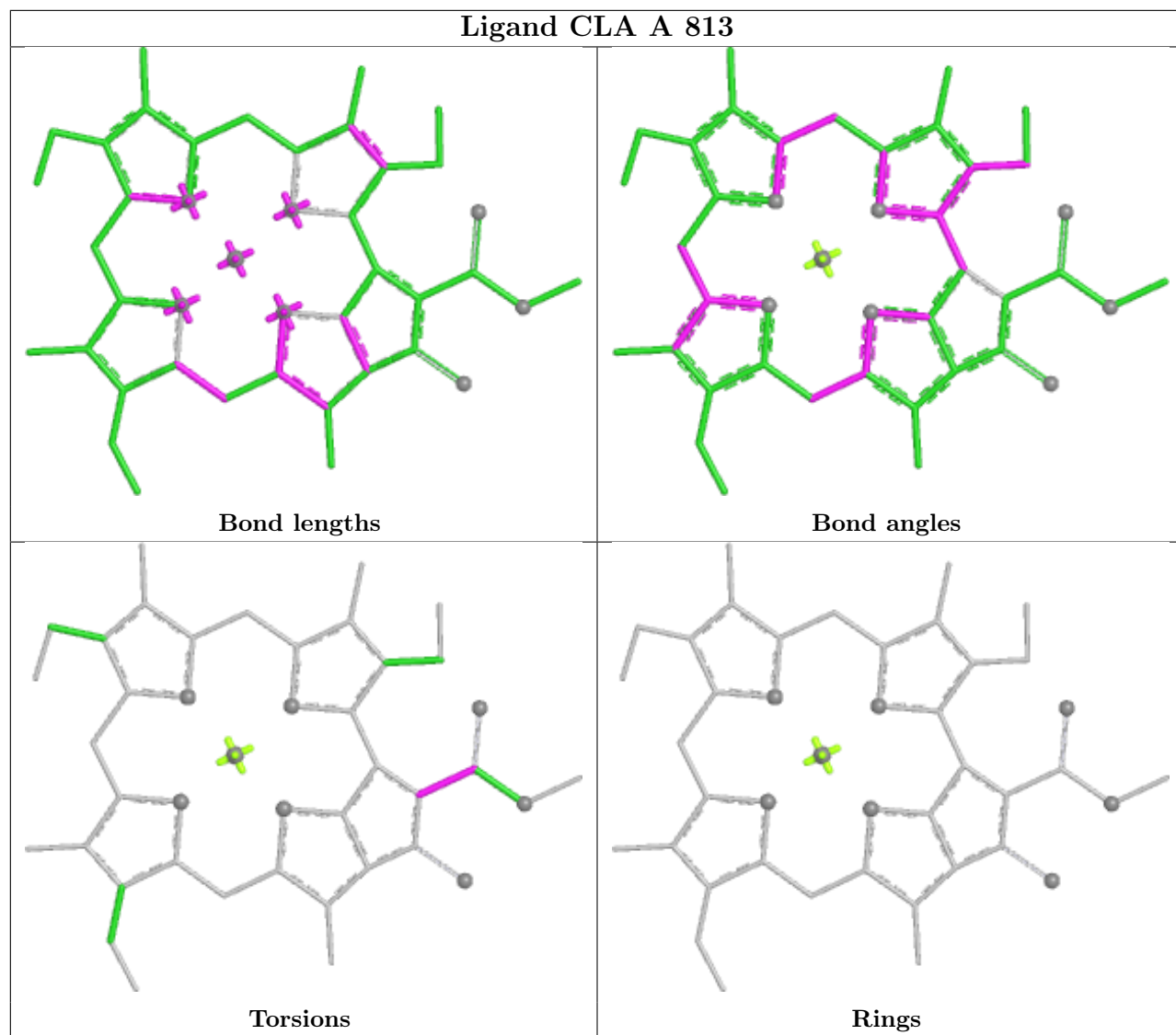


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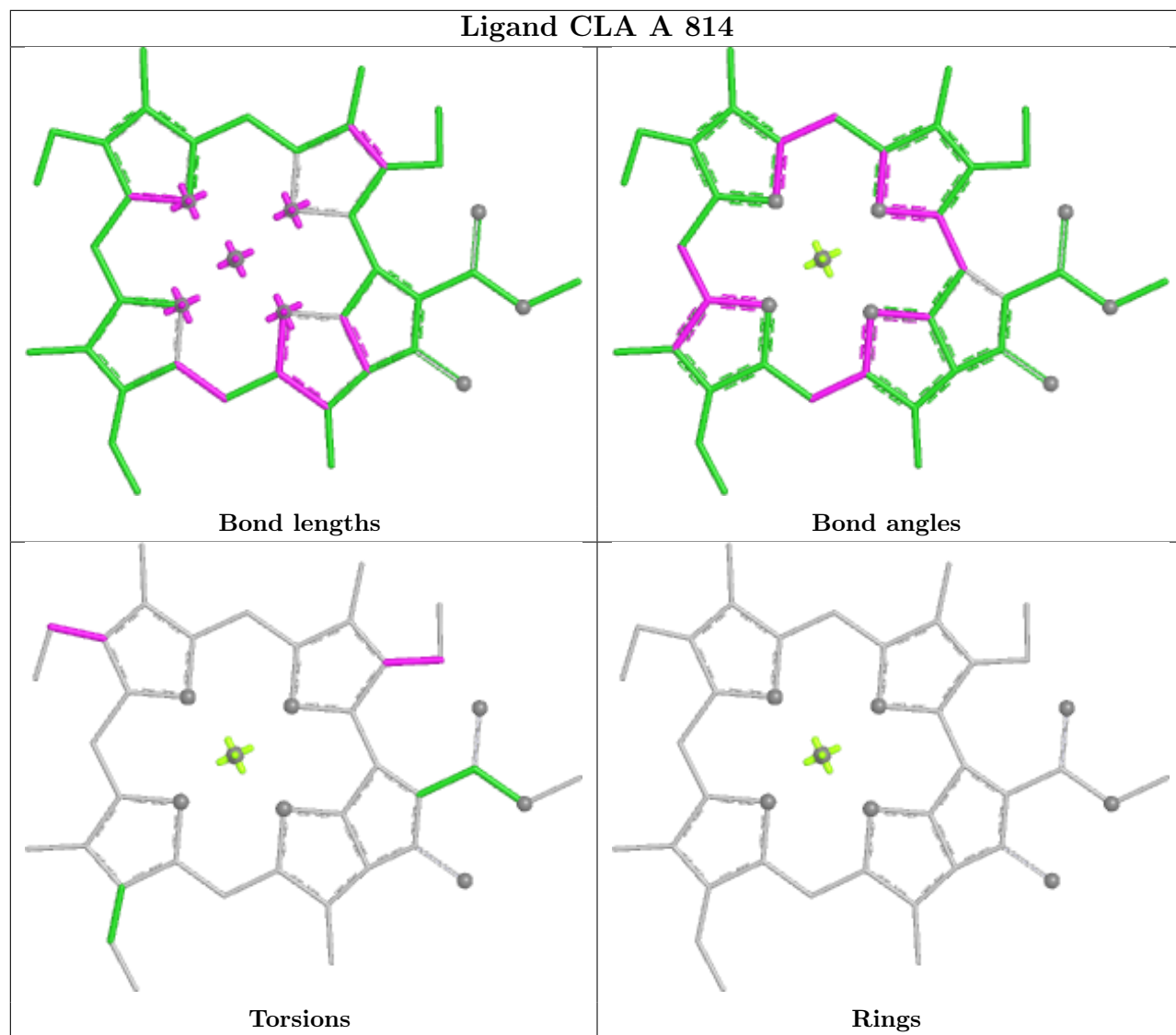


Rings

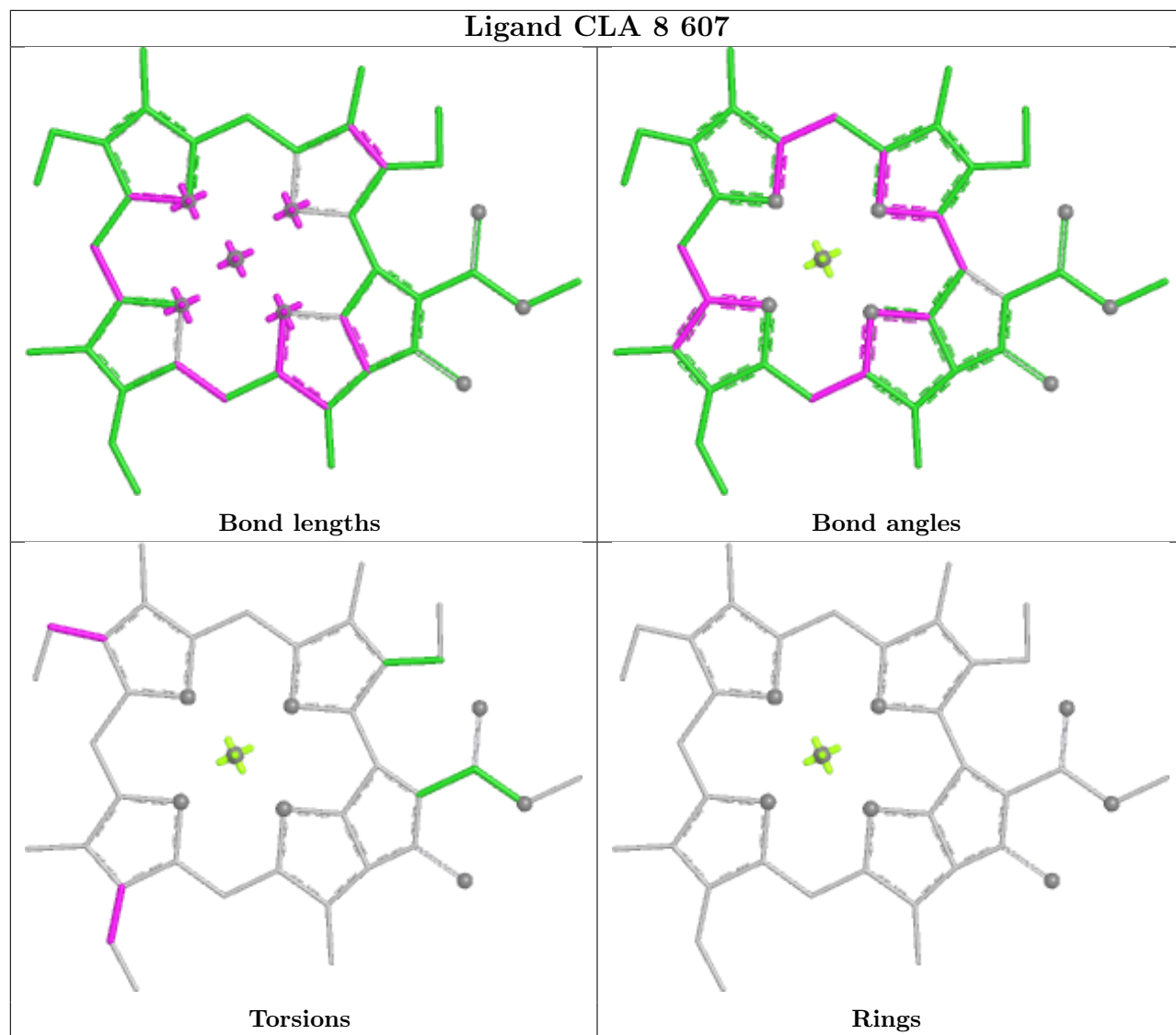
Ligand CLA A 813



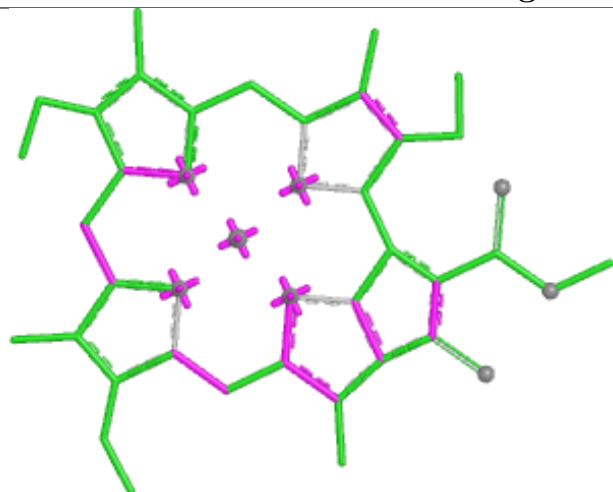
Ligand CLA A 814



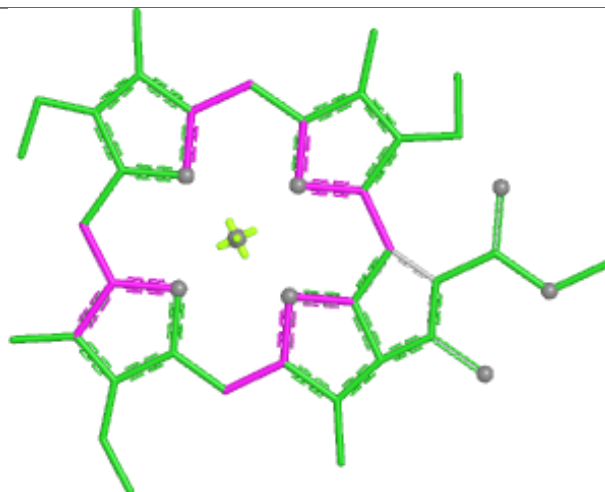
Ligand CLA 8 607



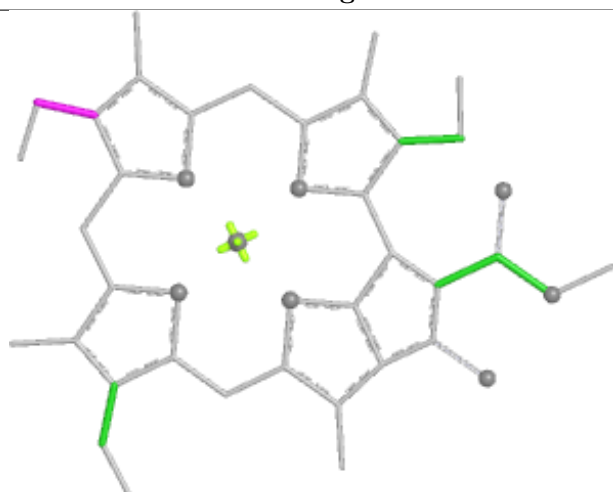
Ligand CLA 8 601



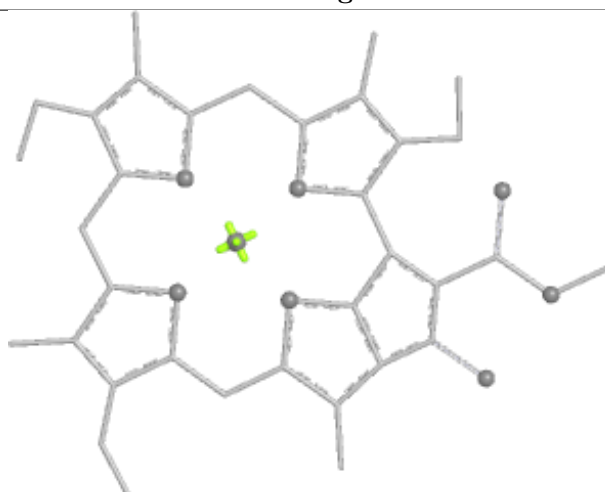
Bond lengths



Bond angles

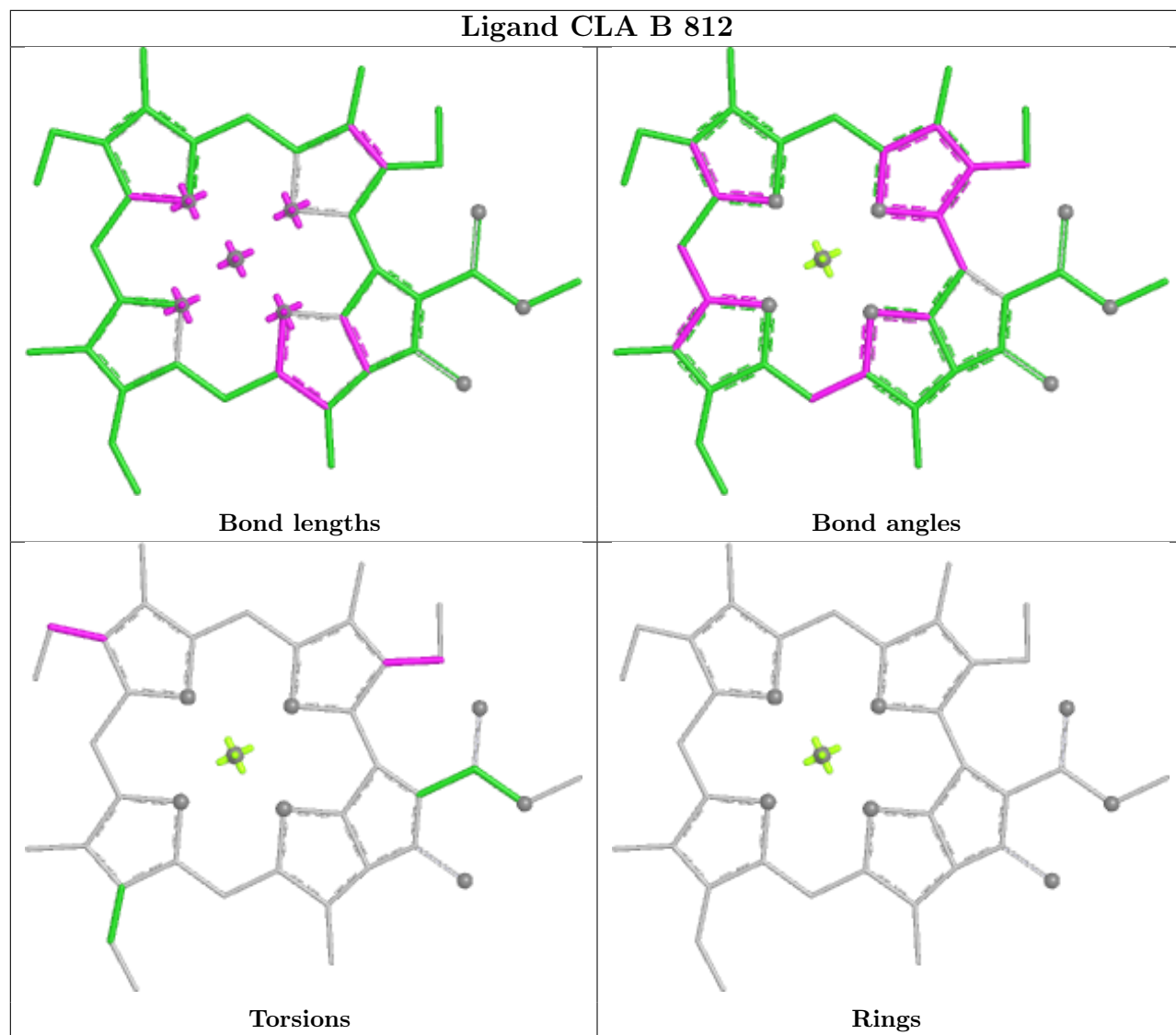


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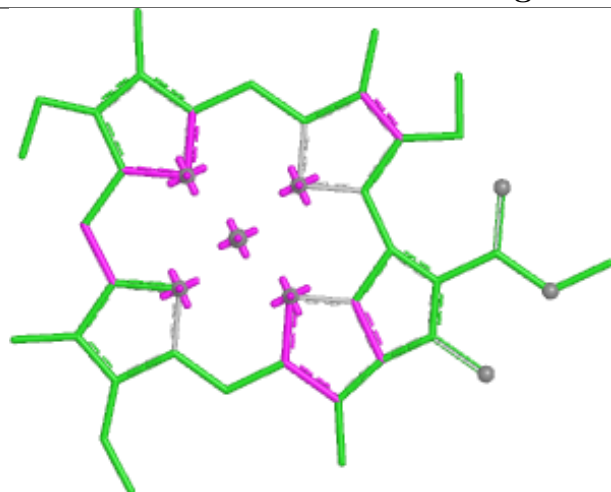


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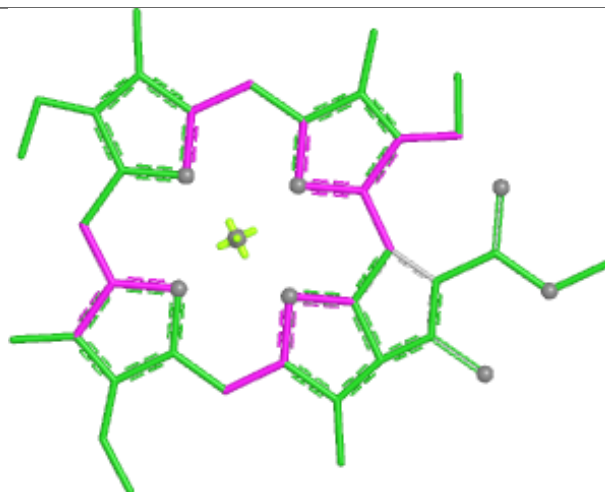
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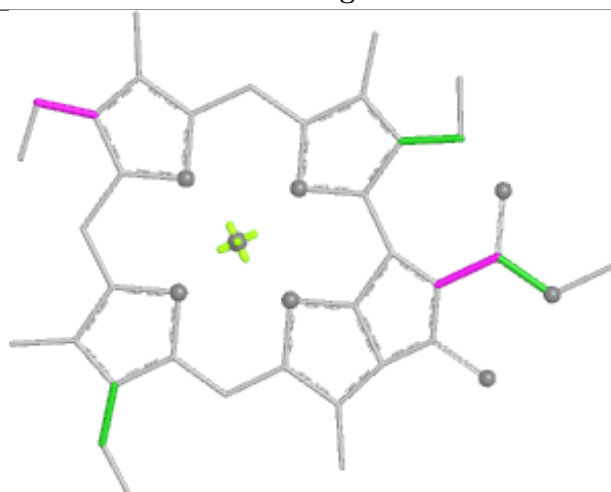
Ligand CLA B 831



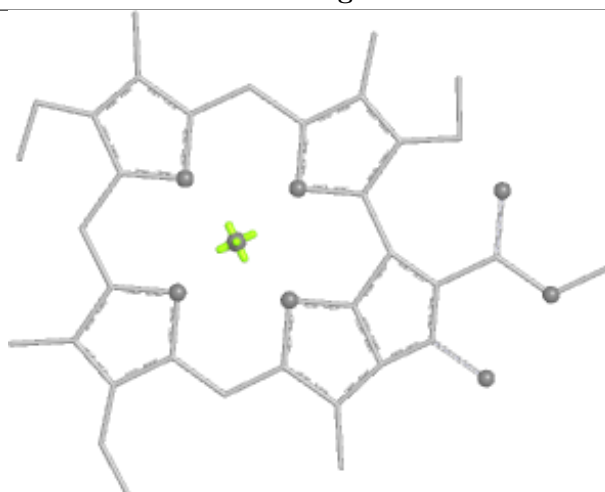
Bond lengths



Bond angles

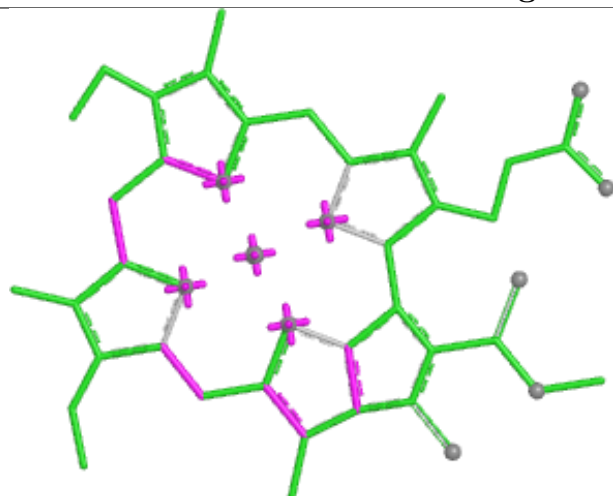


Torsions

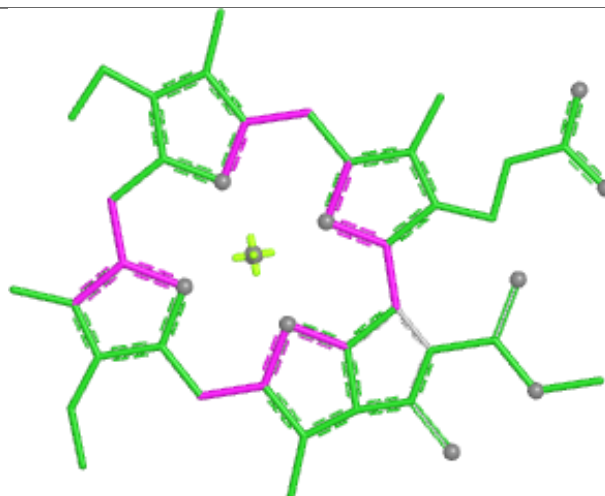


Rings

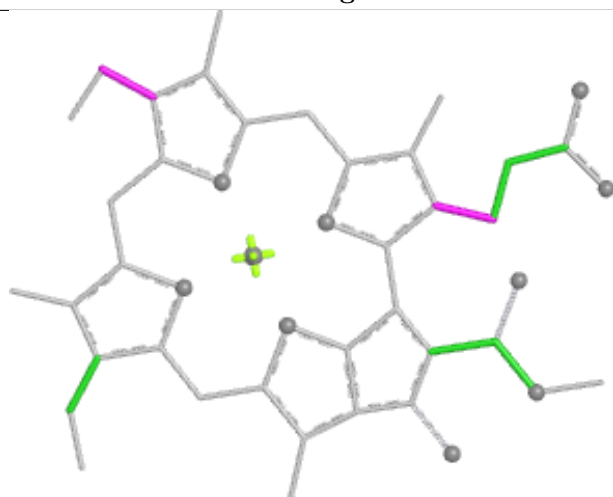
Ligand CLA 4 605



Bond lengths



Bond angles

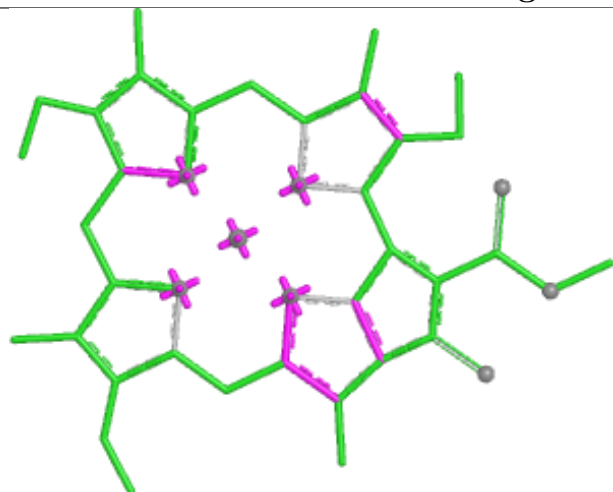


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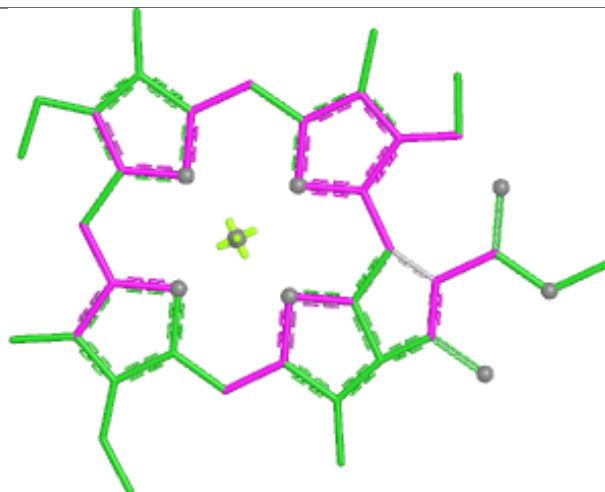


Rings

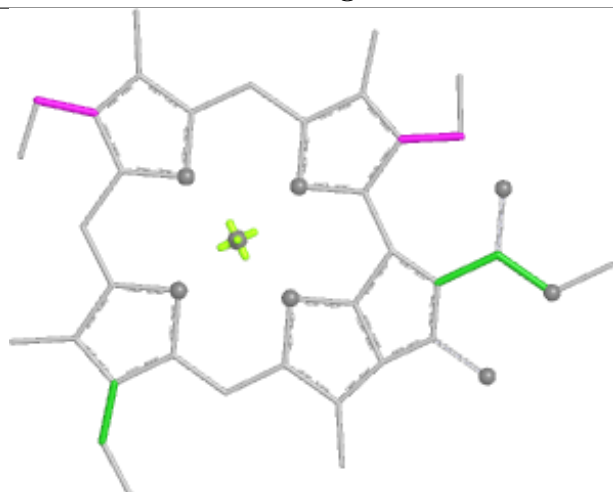
Ligand CLA 3 306



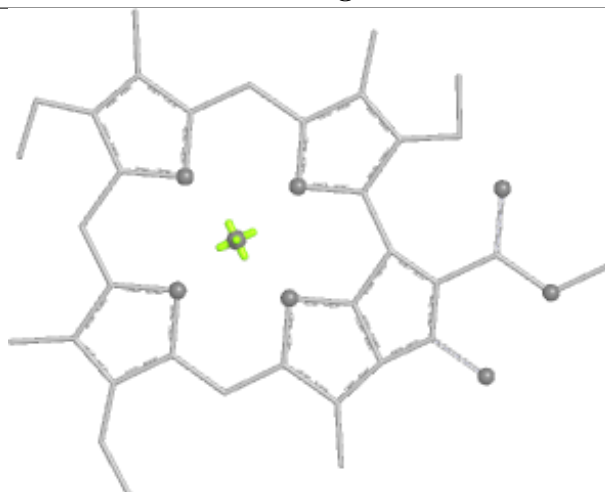
Bond lengths



Bond angles

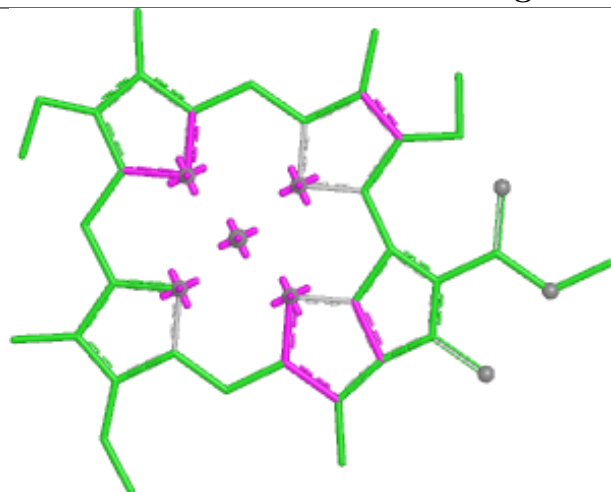


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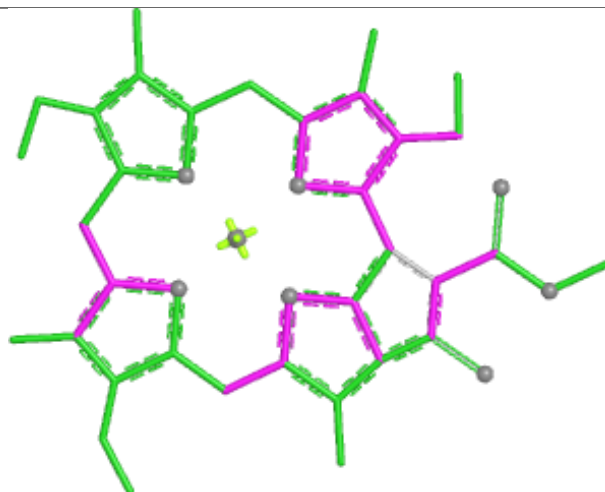


Rings

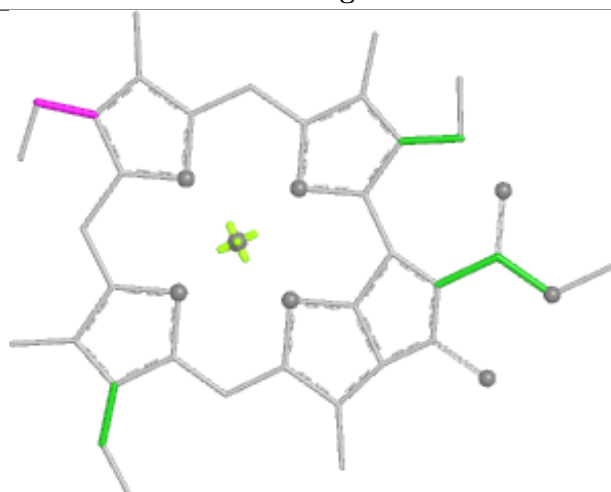
Ligand CLA B 806



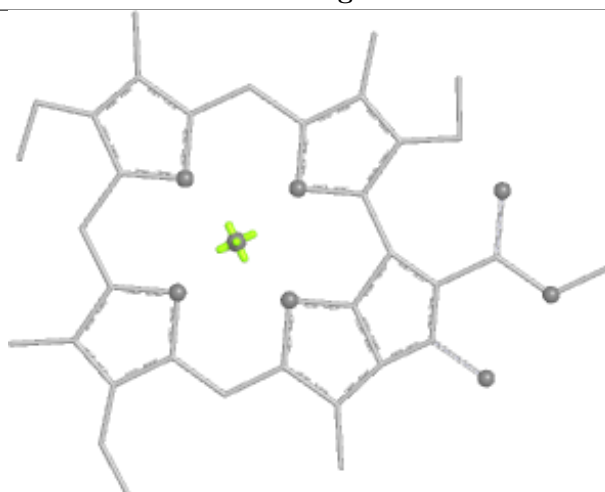
Bond lengths



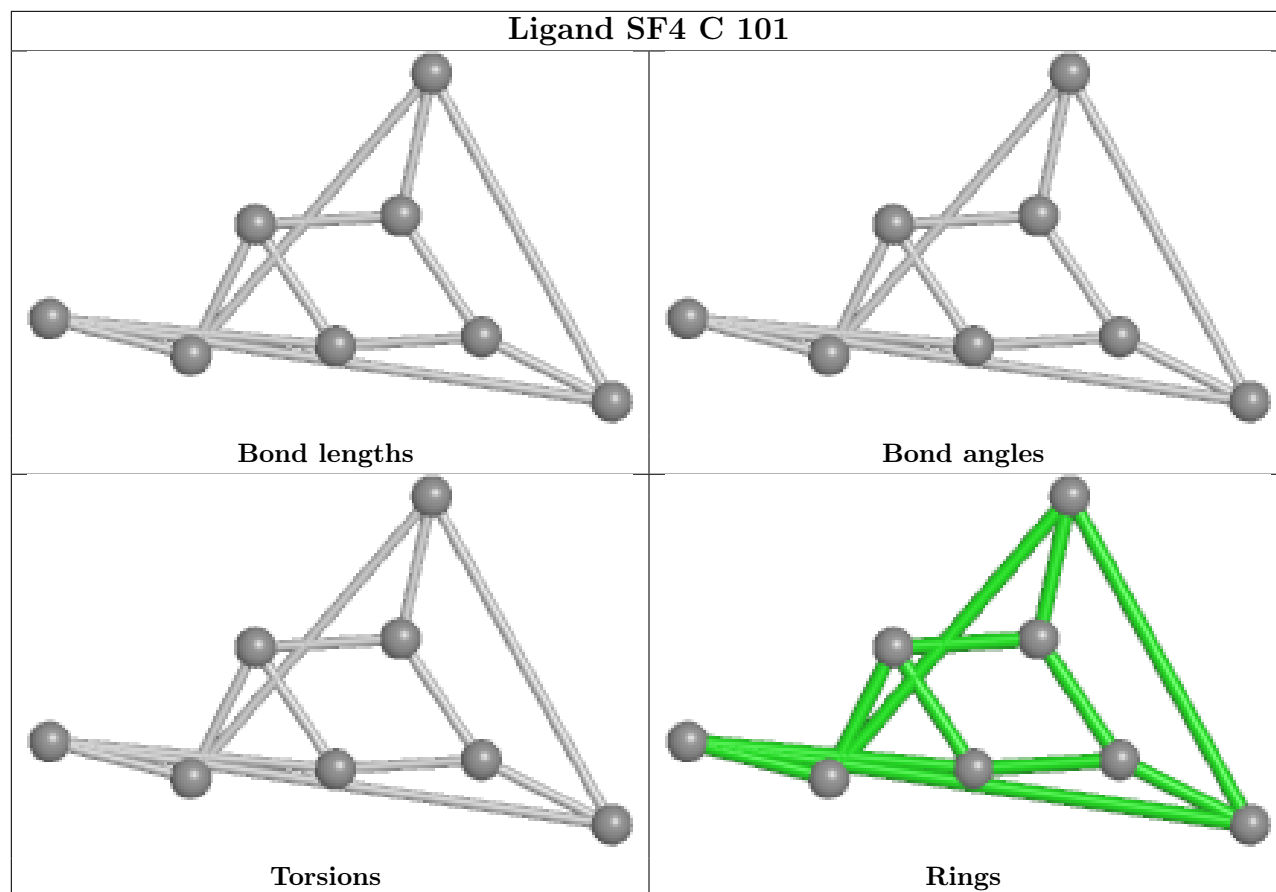
Bond angles



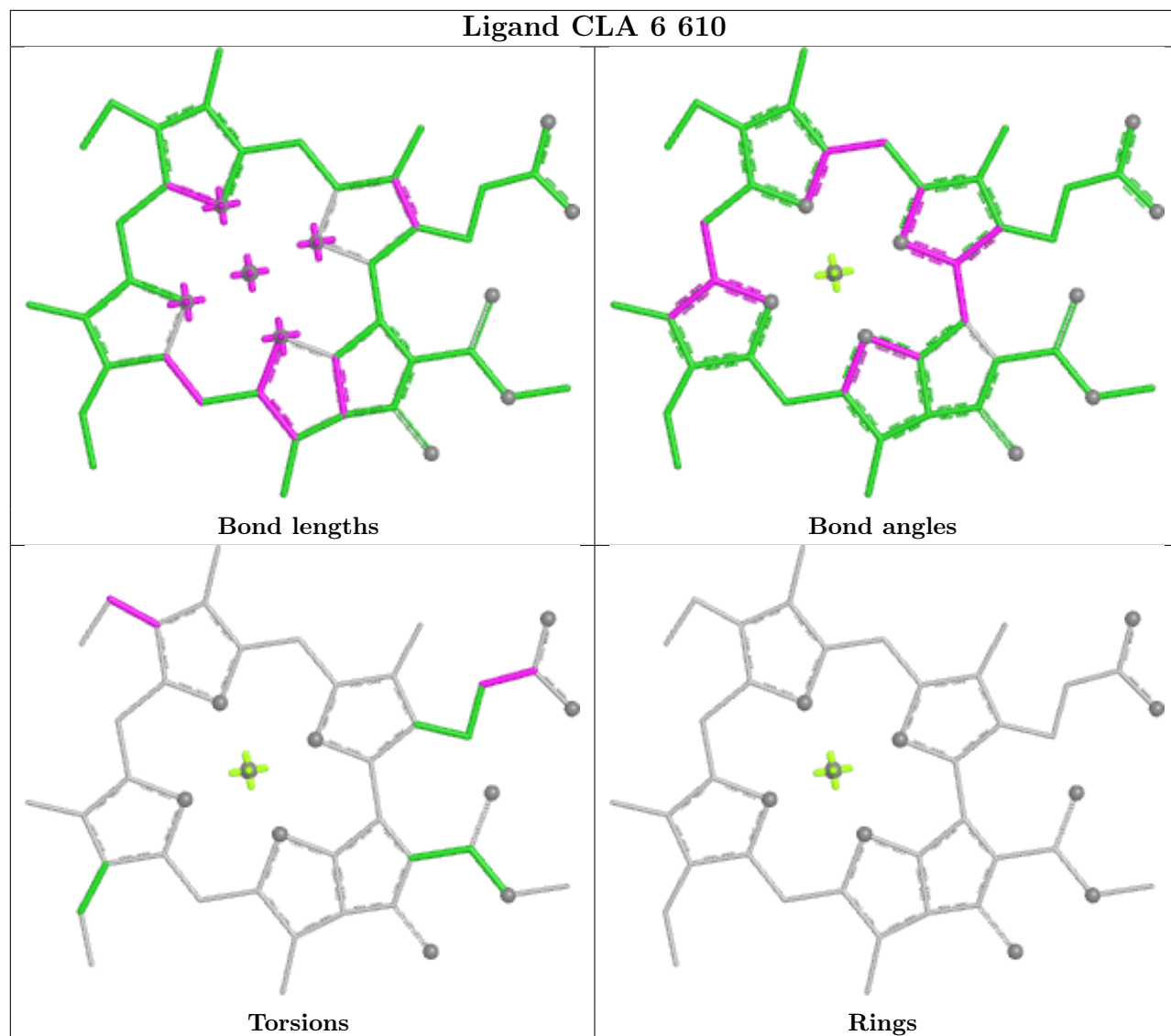
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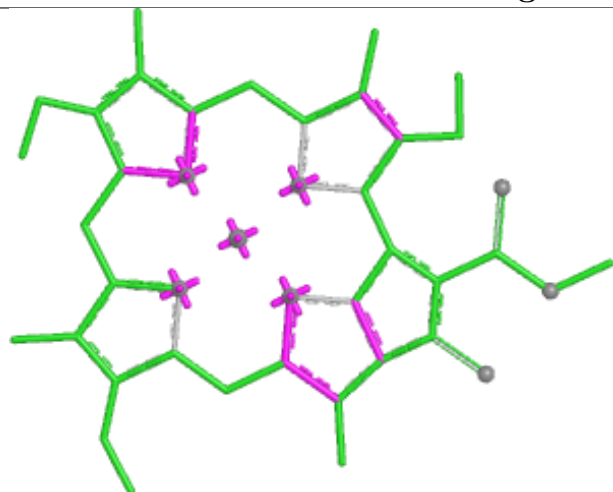
Rings



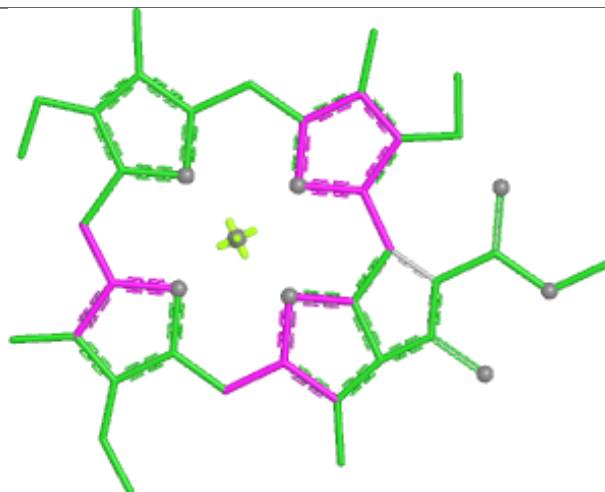
Ligand CLA 6 610



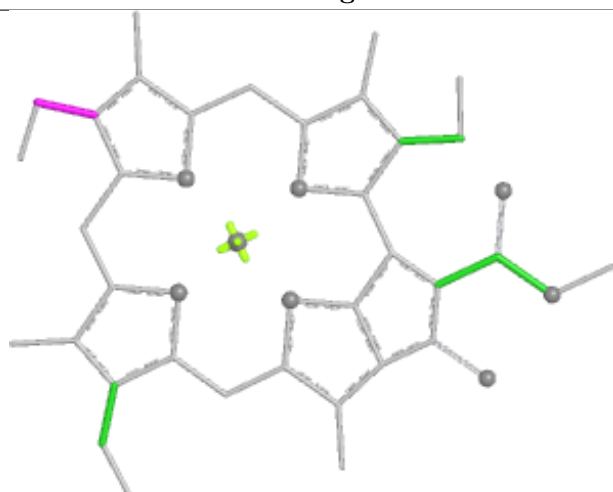
Ligand CLA 7 614



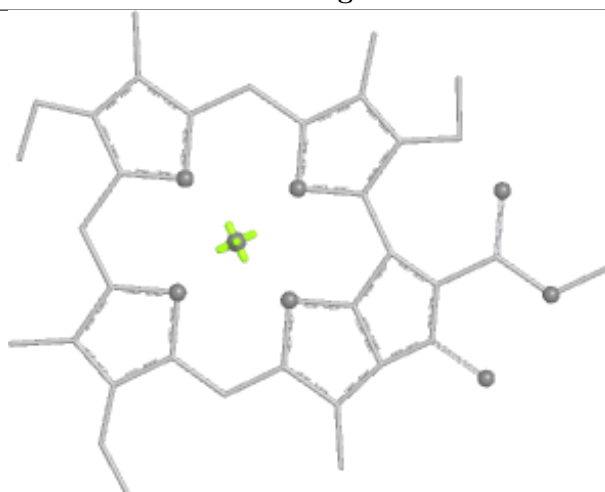
Bond lengths



Bond angles

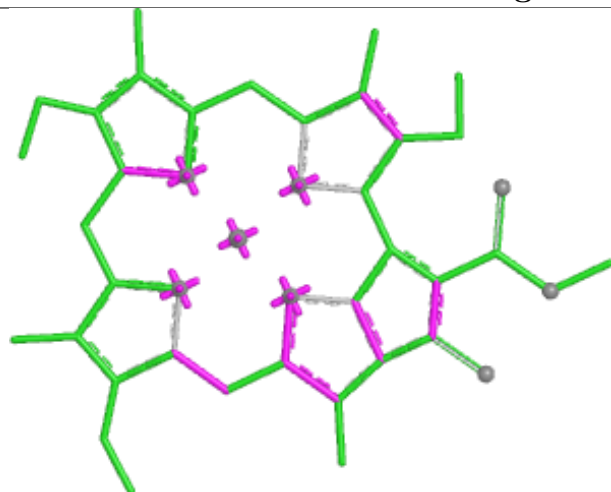


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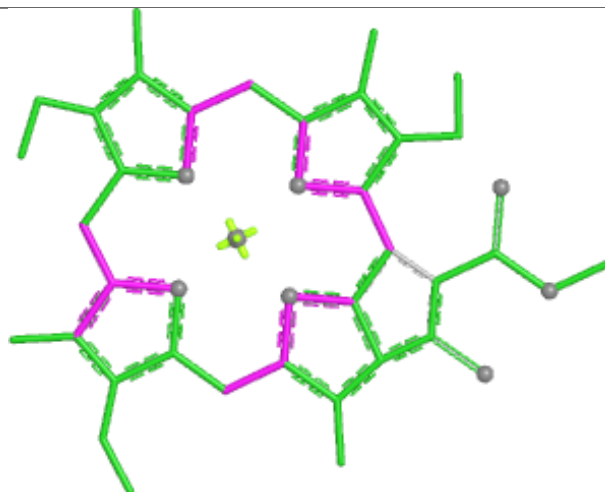


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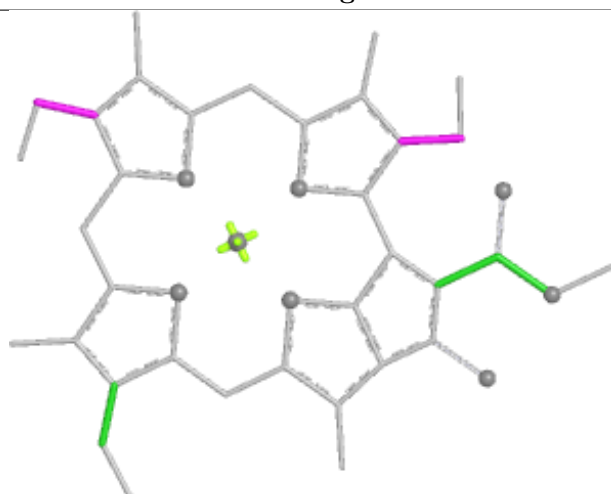
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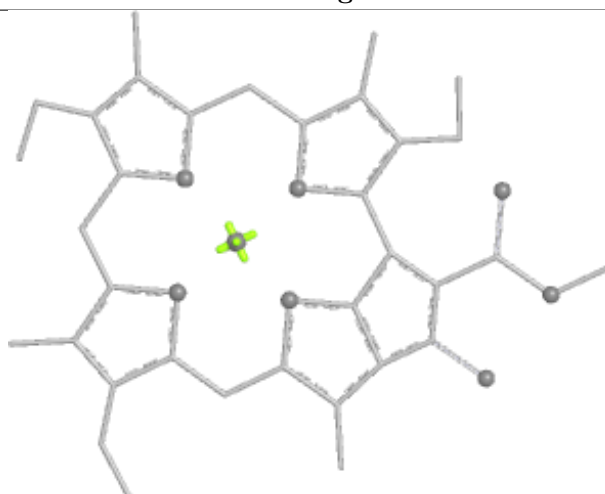
Bond lengths



Bond angles

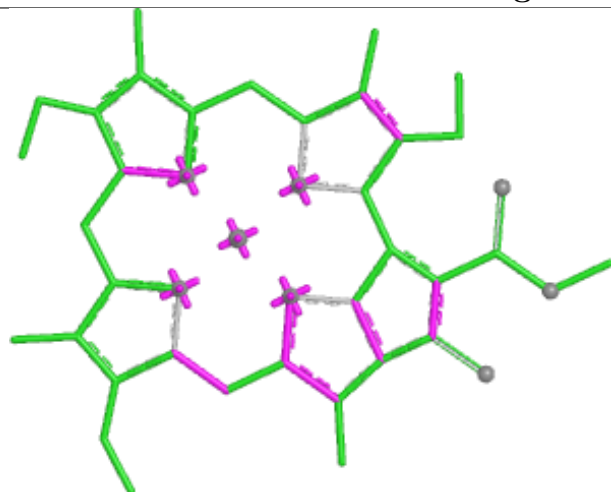


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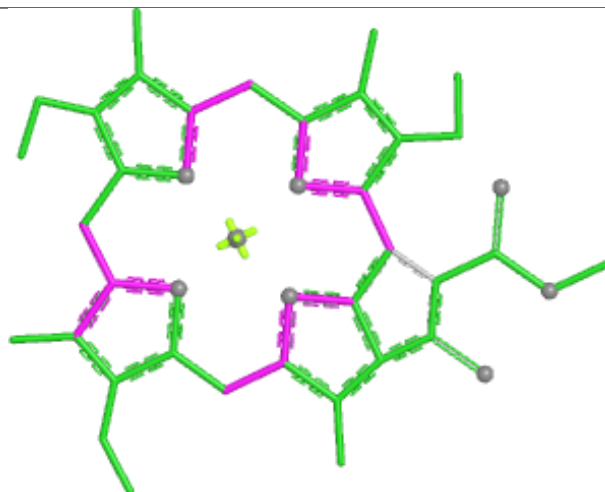


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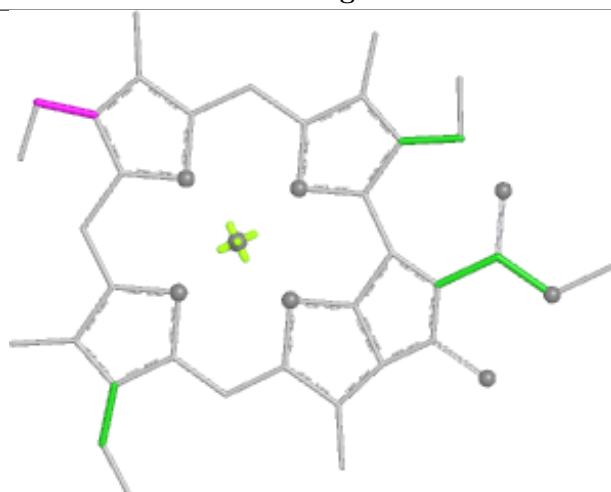
Ligand CLA A 843



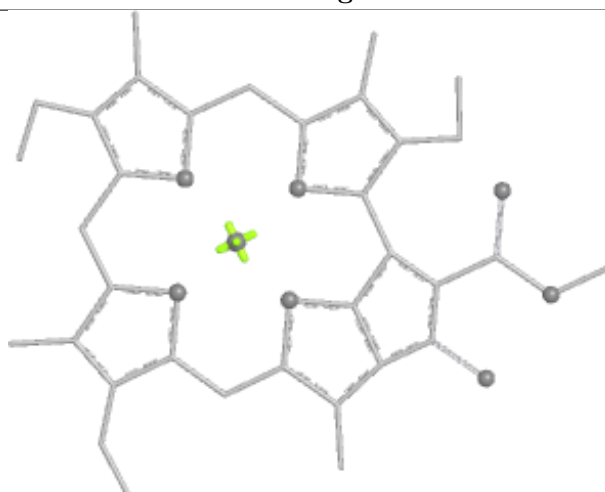
Bond lengths



Bond angles

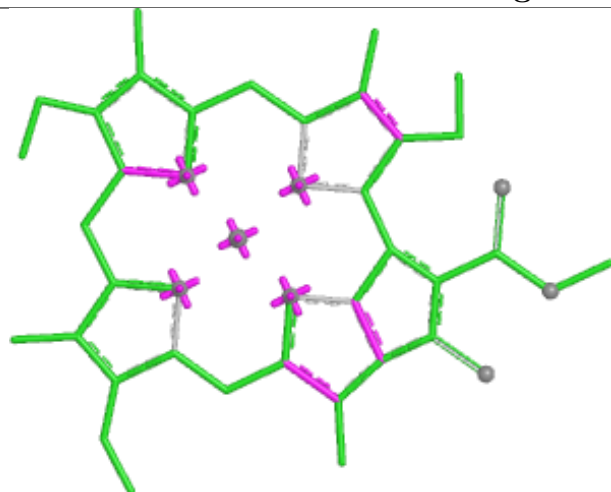


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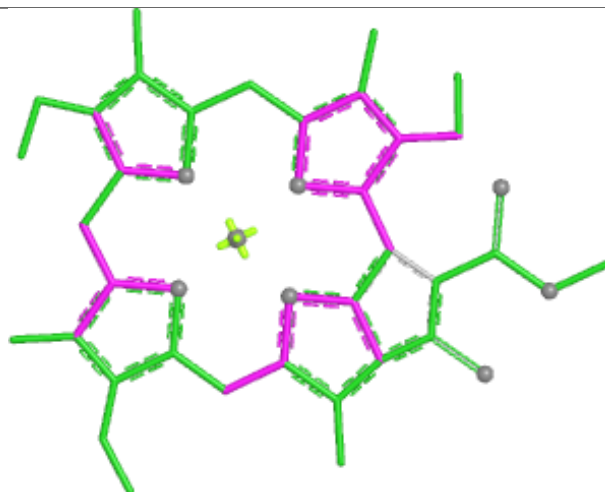


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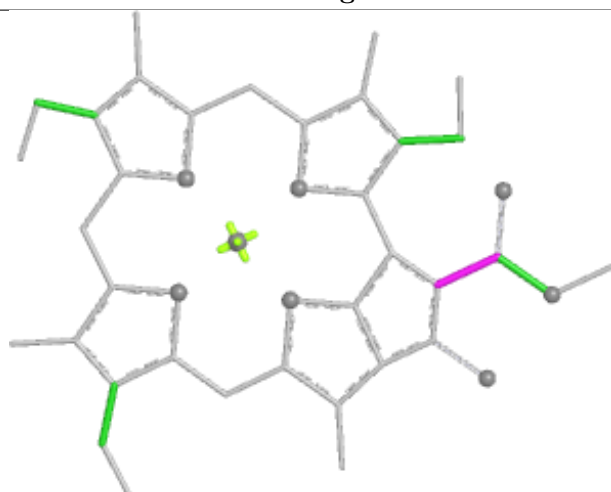
Ligand CLA A 804



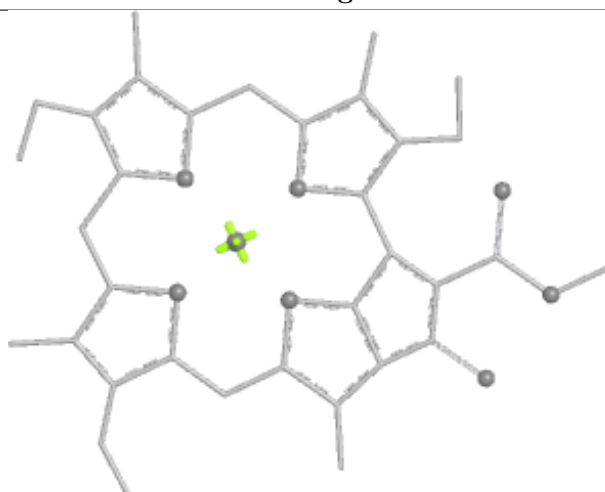
Bond lengths



Bond angles

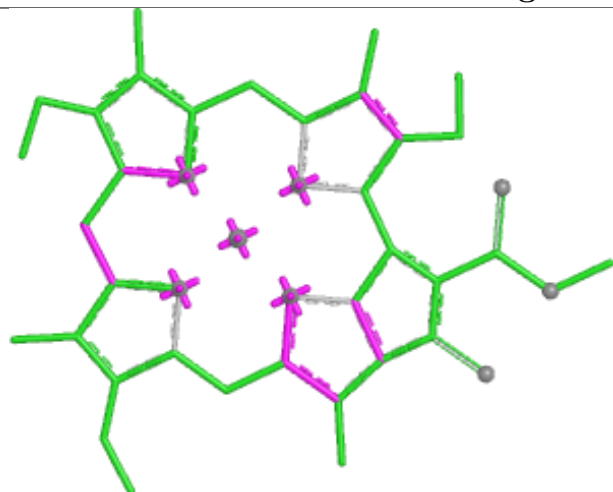


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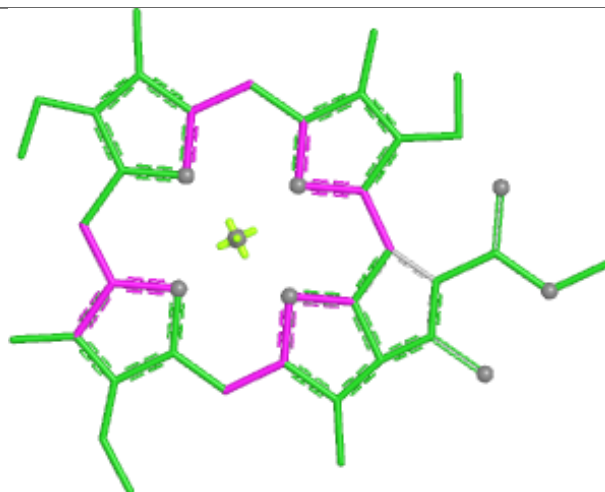


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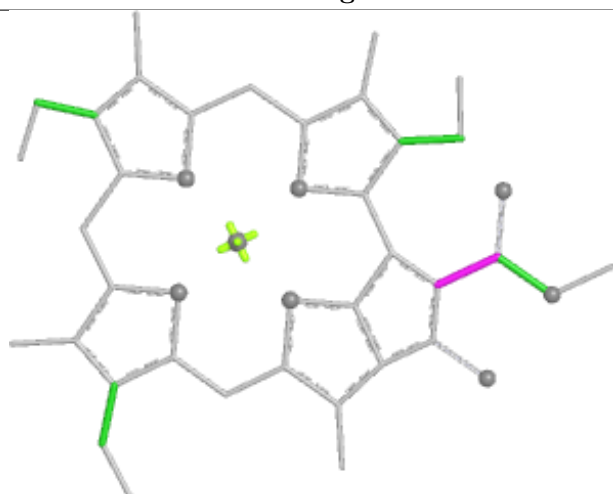
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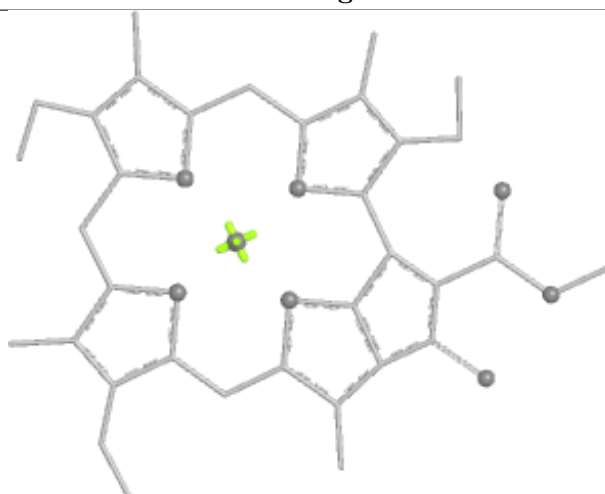
Bond lengths



Bond angles

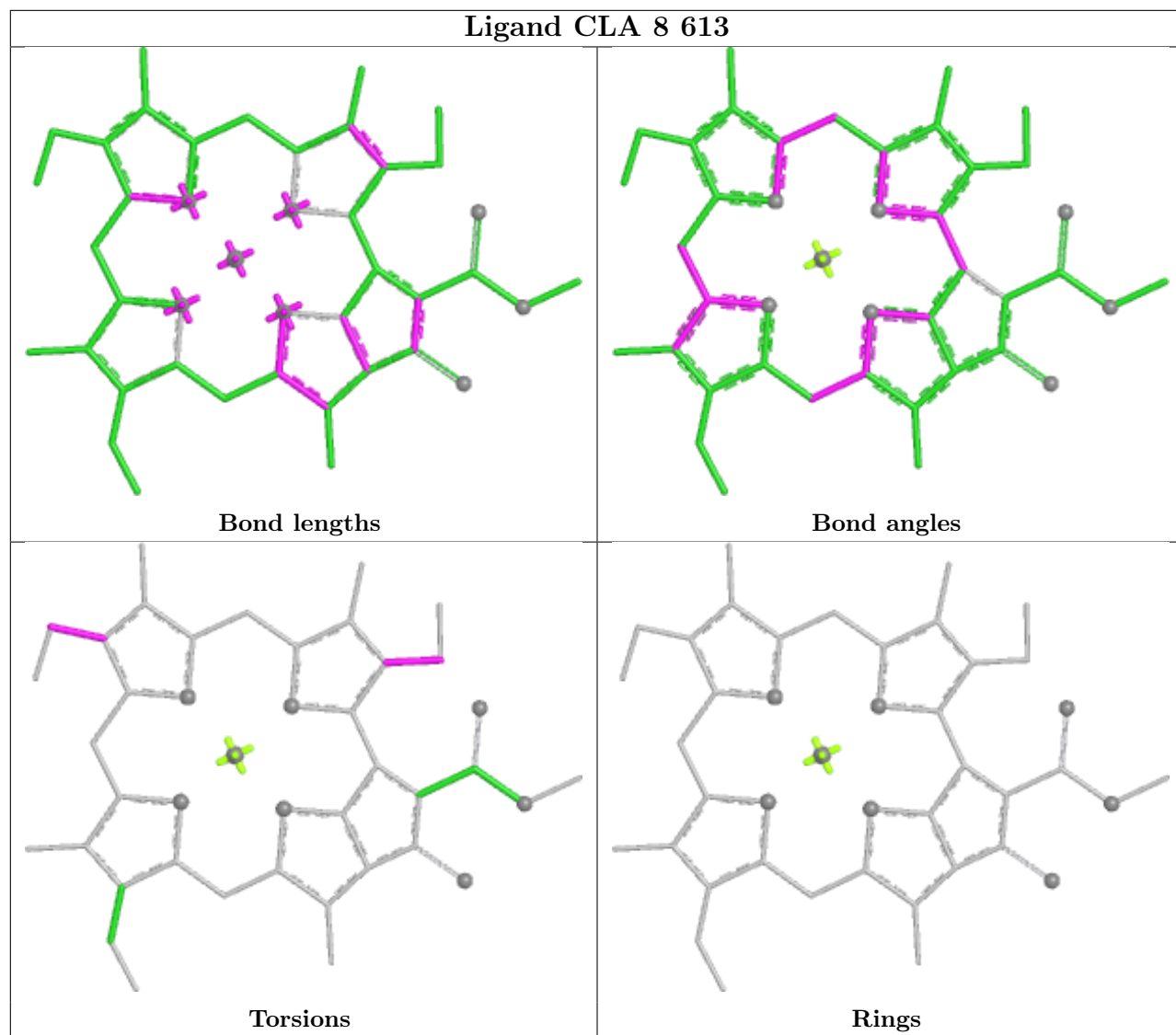


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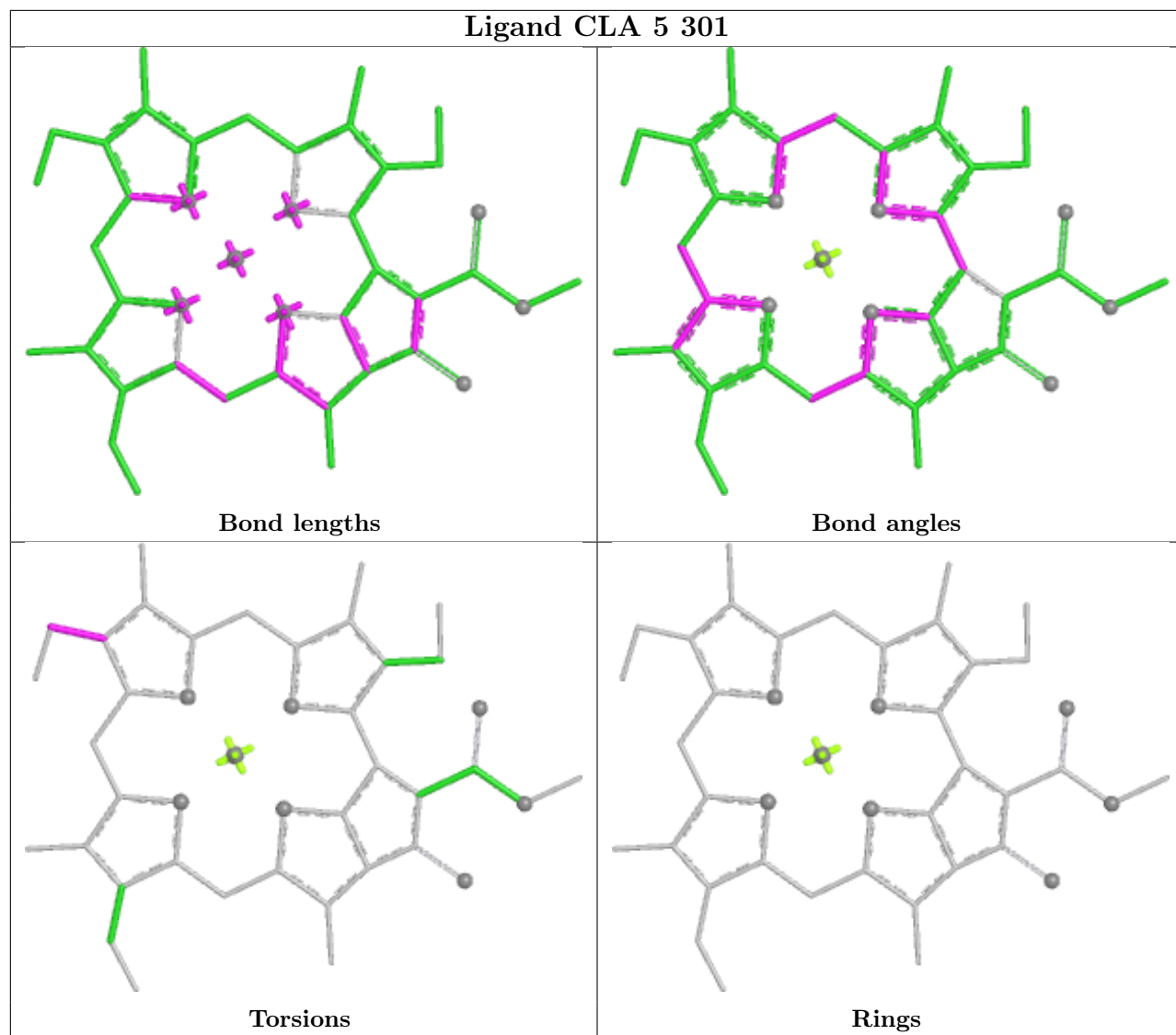


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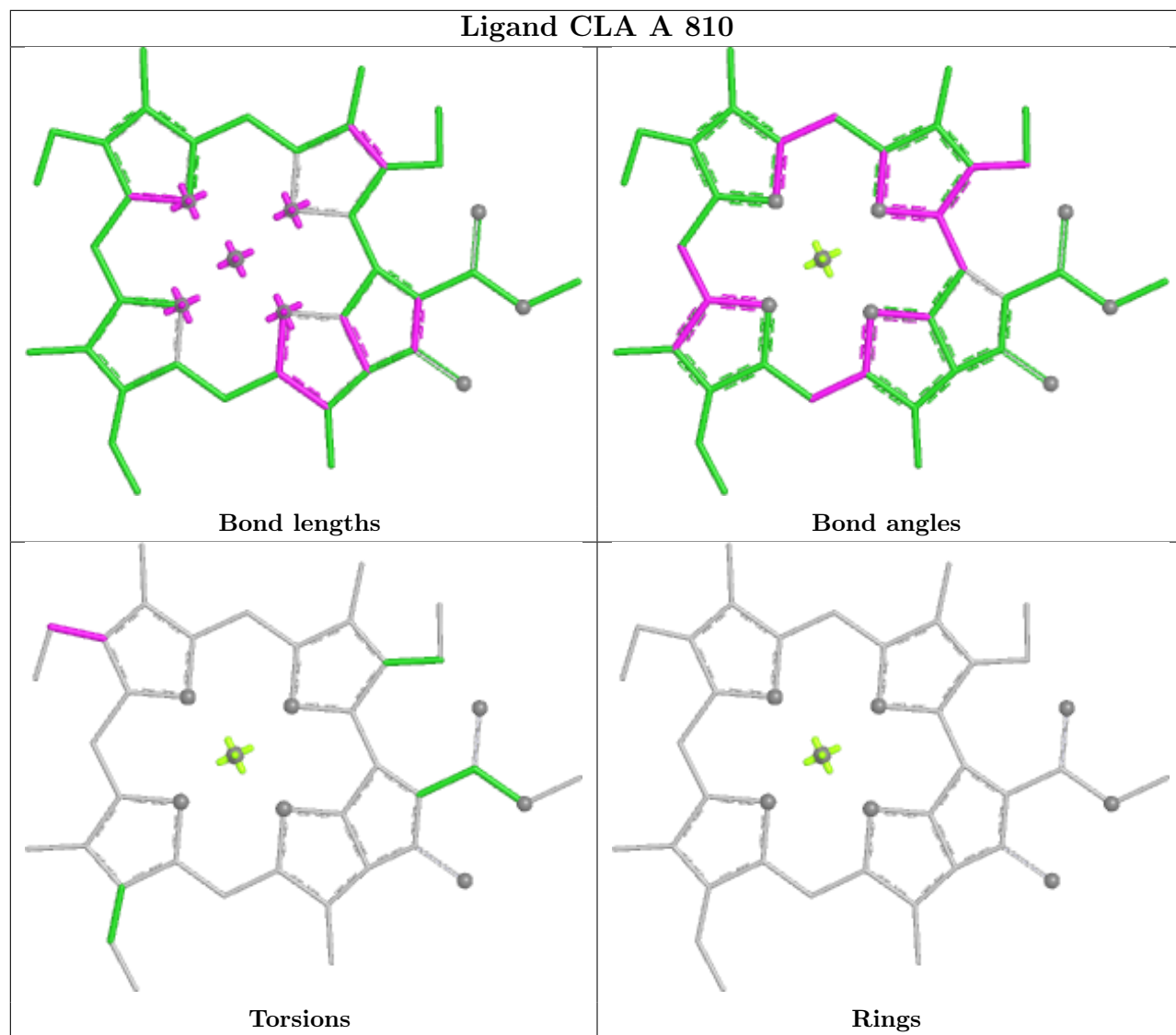
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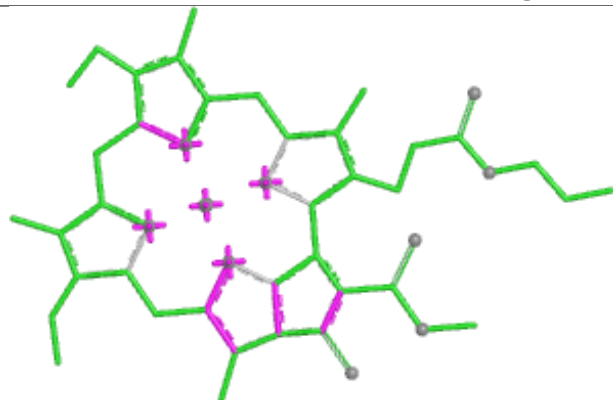
Ligand CLA 5 301



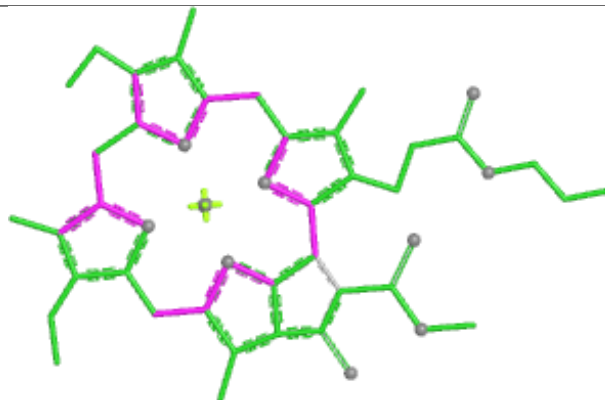
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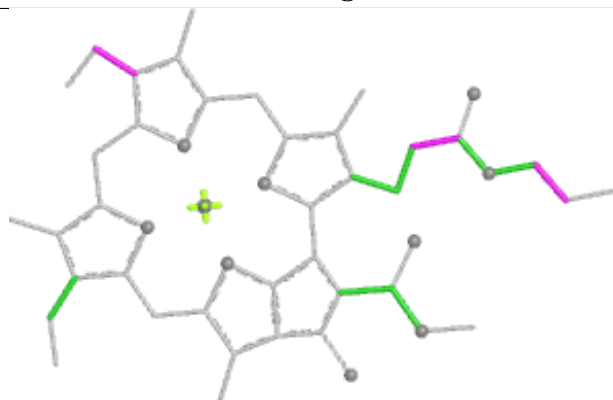
Ligand CLA 5 303



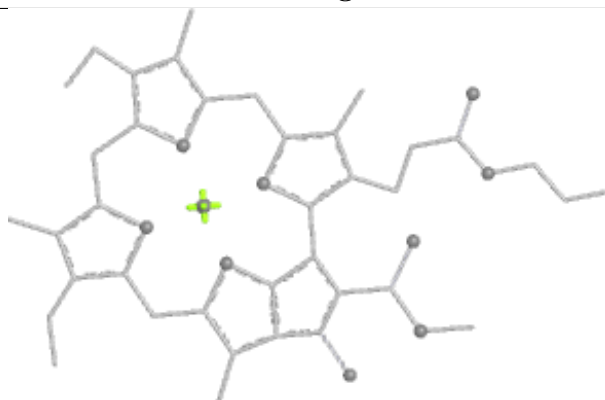
Bond lengths



Bond angles

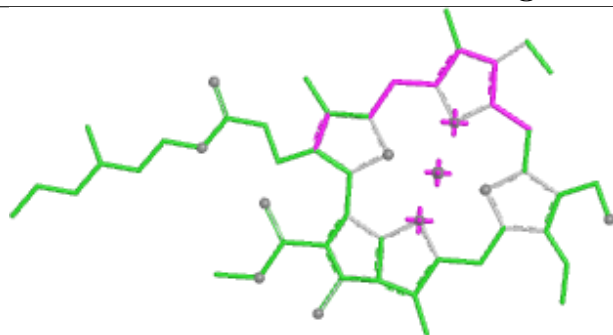


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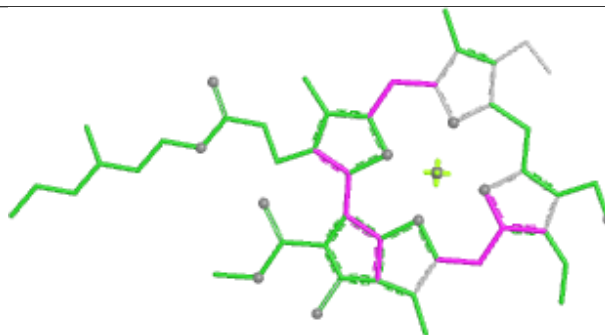


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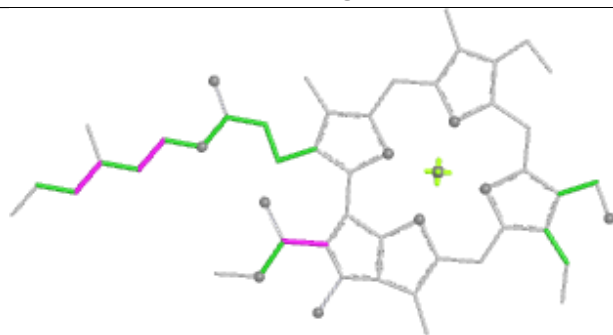
Ligand CHL 1 601



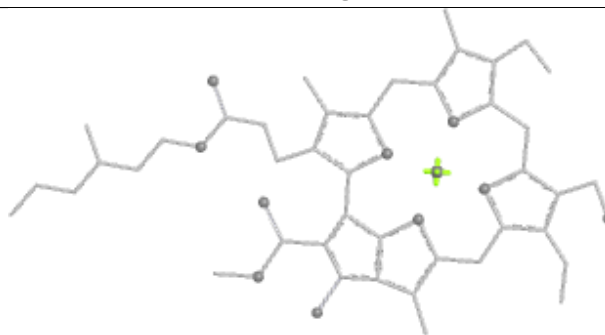
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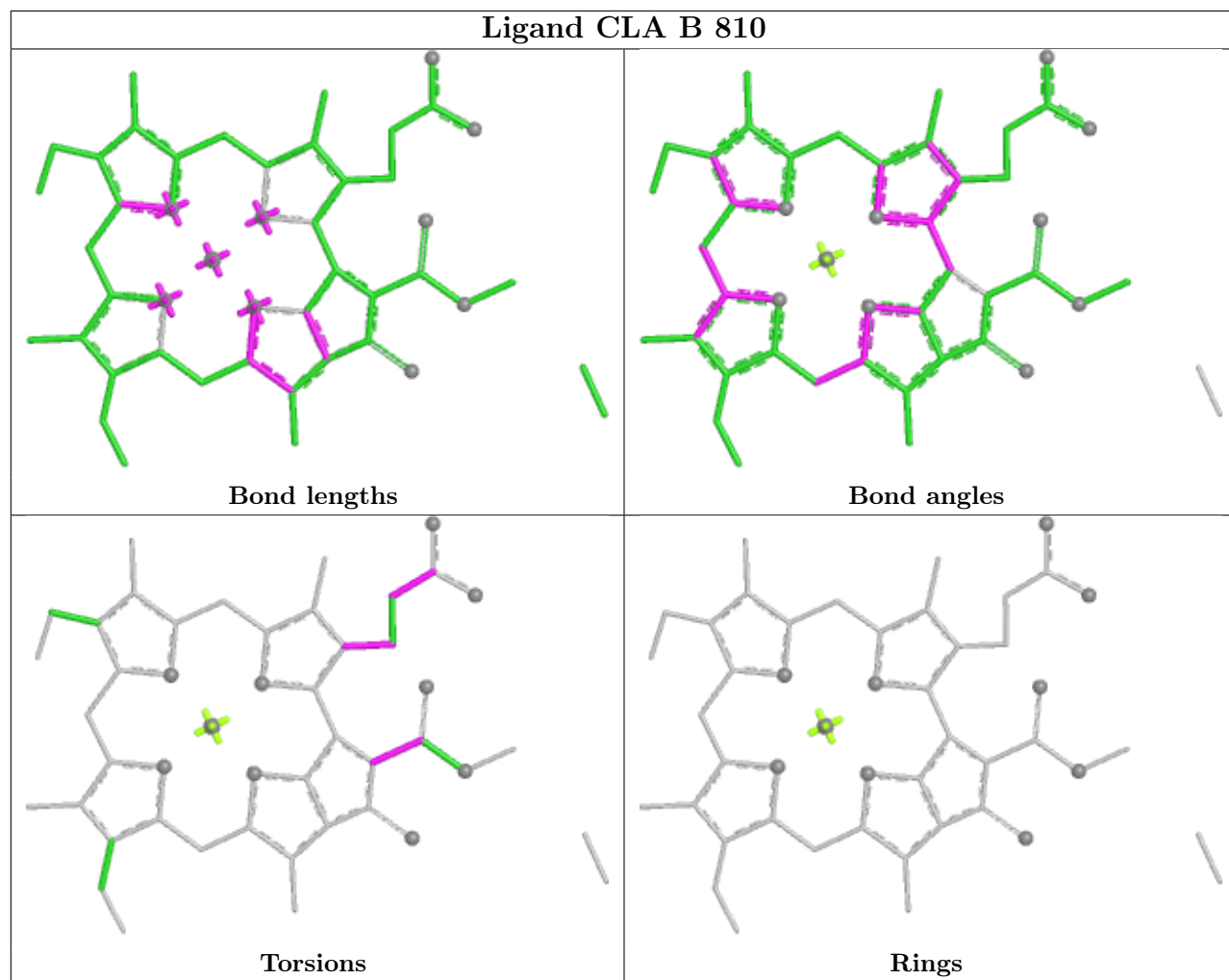
Bond angles



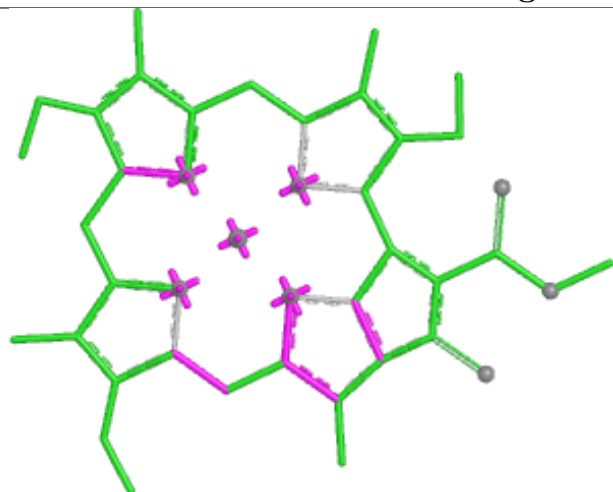
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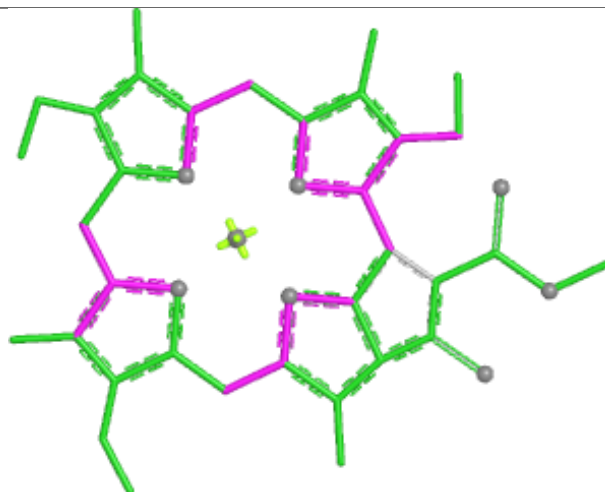
Rings



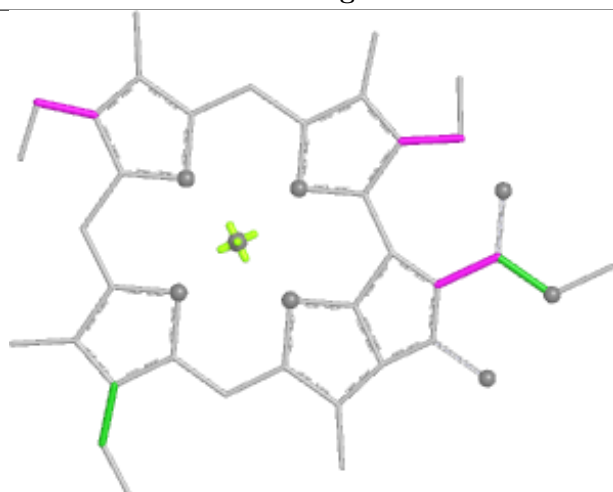
Ligand CLA 3 302



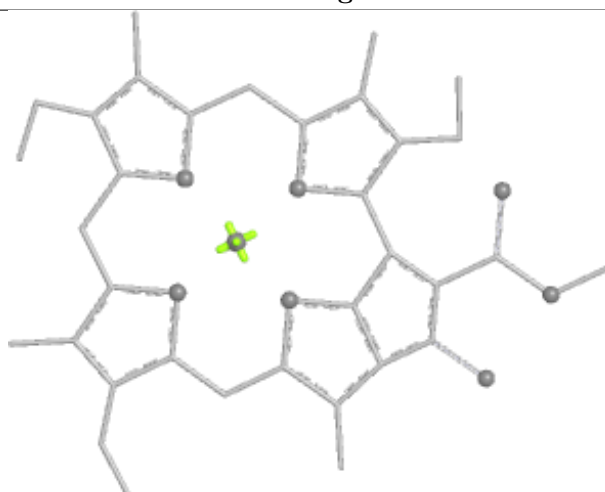
Bond lengths



Bond angles

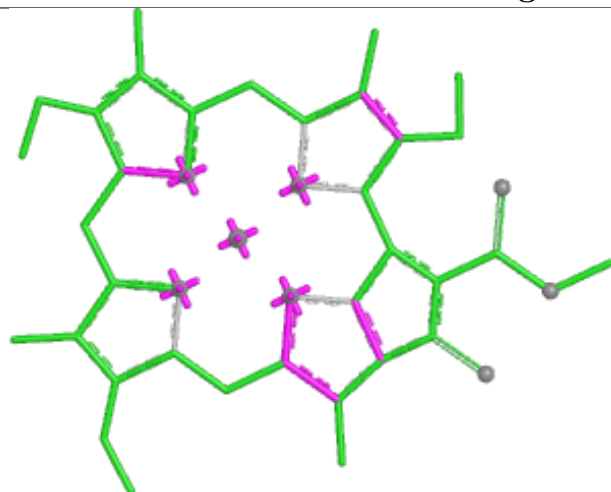


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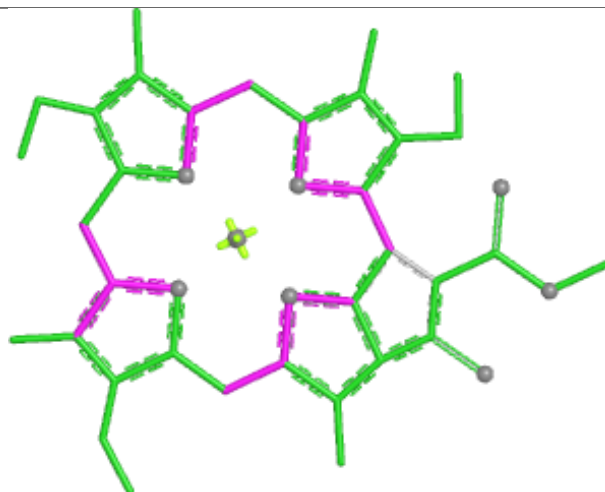


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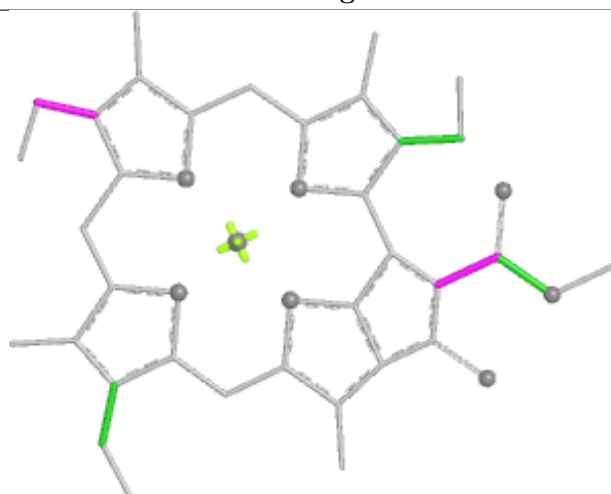
Ligand CLA 8 605



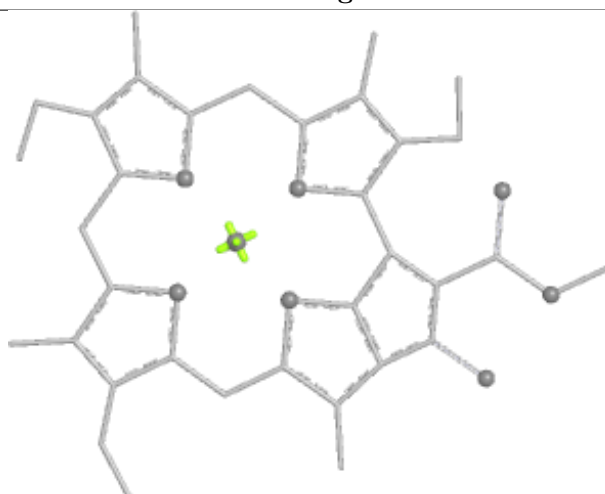
Bond lengths



Bond angles

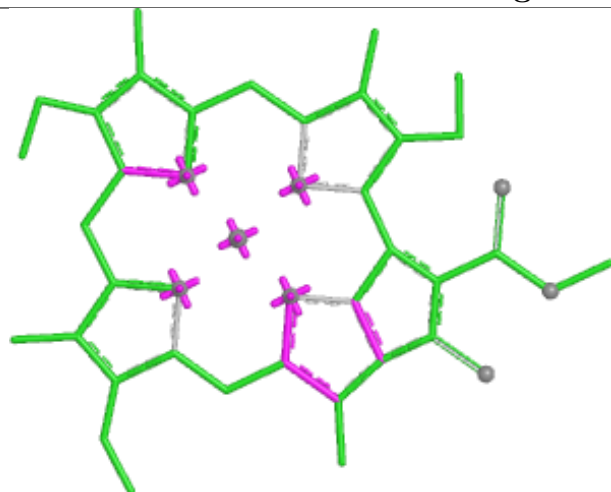


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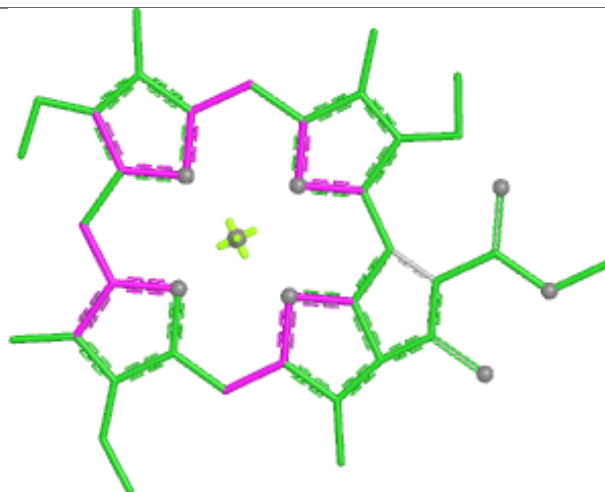


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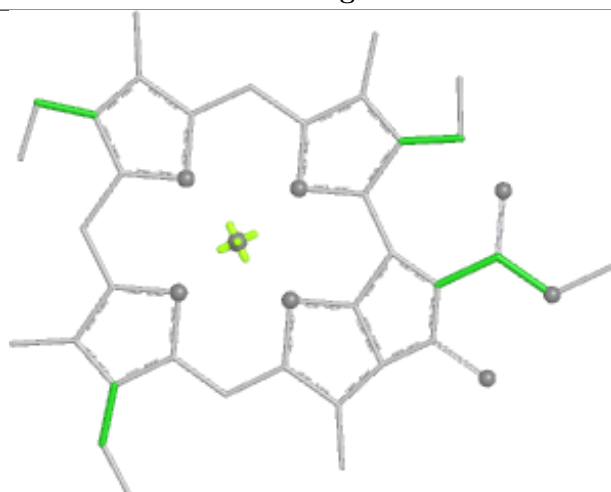
Ligand CLA A 834



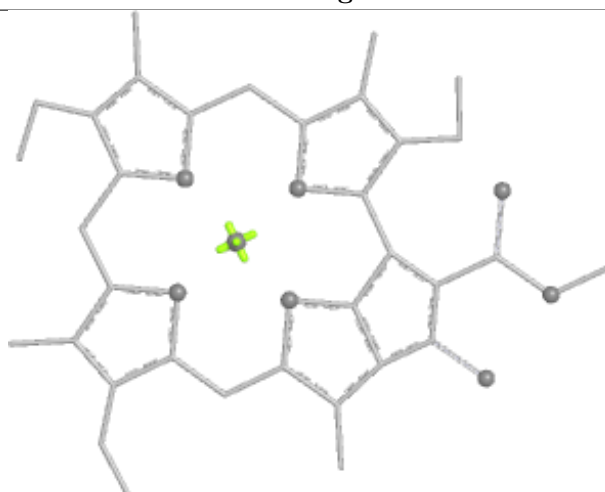
Bond lengths



Bond angles

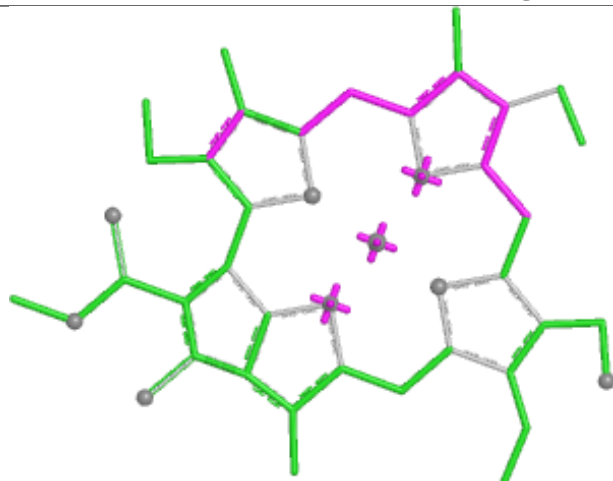


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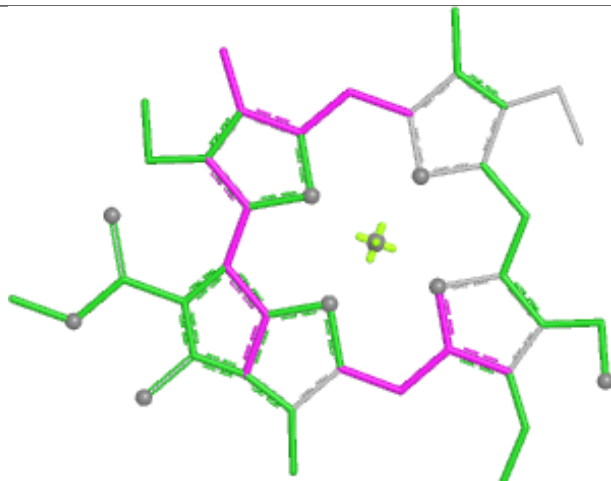


Rings

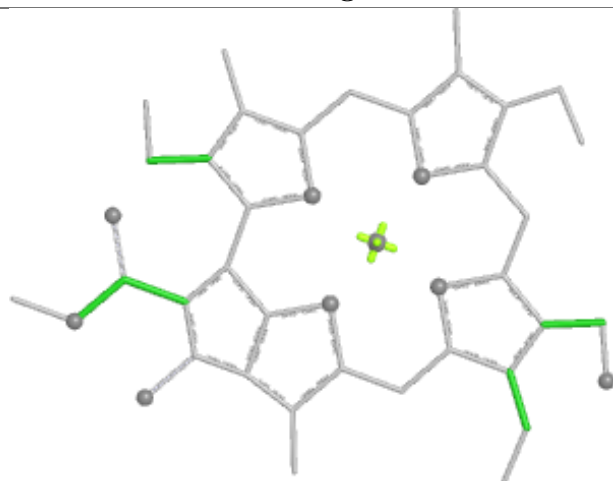
Ligand CHL 7 606



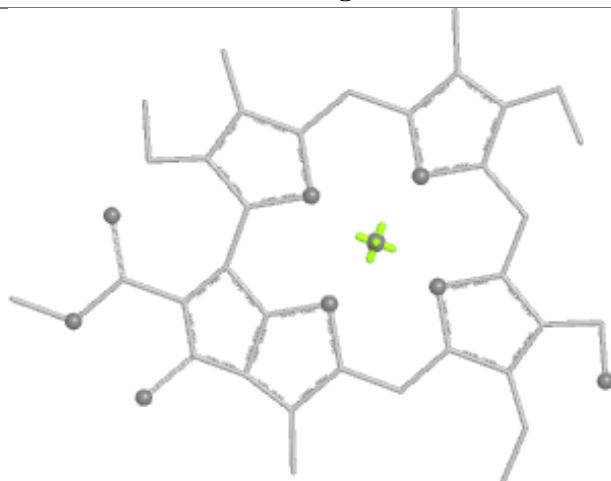
Bond lengths



Bond angles

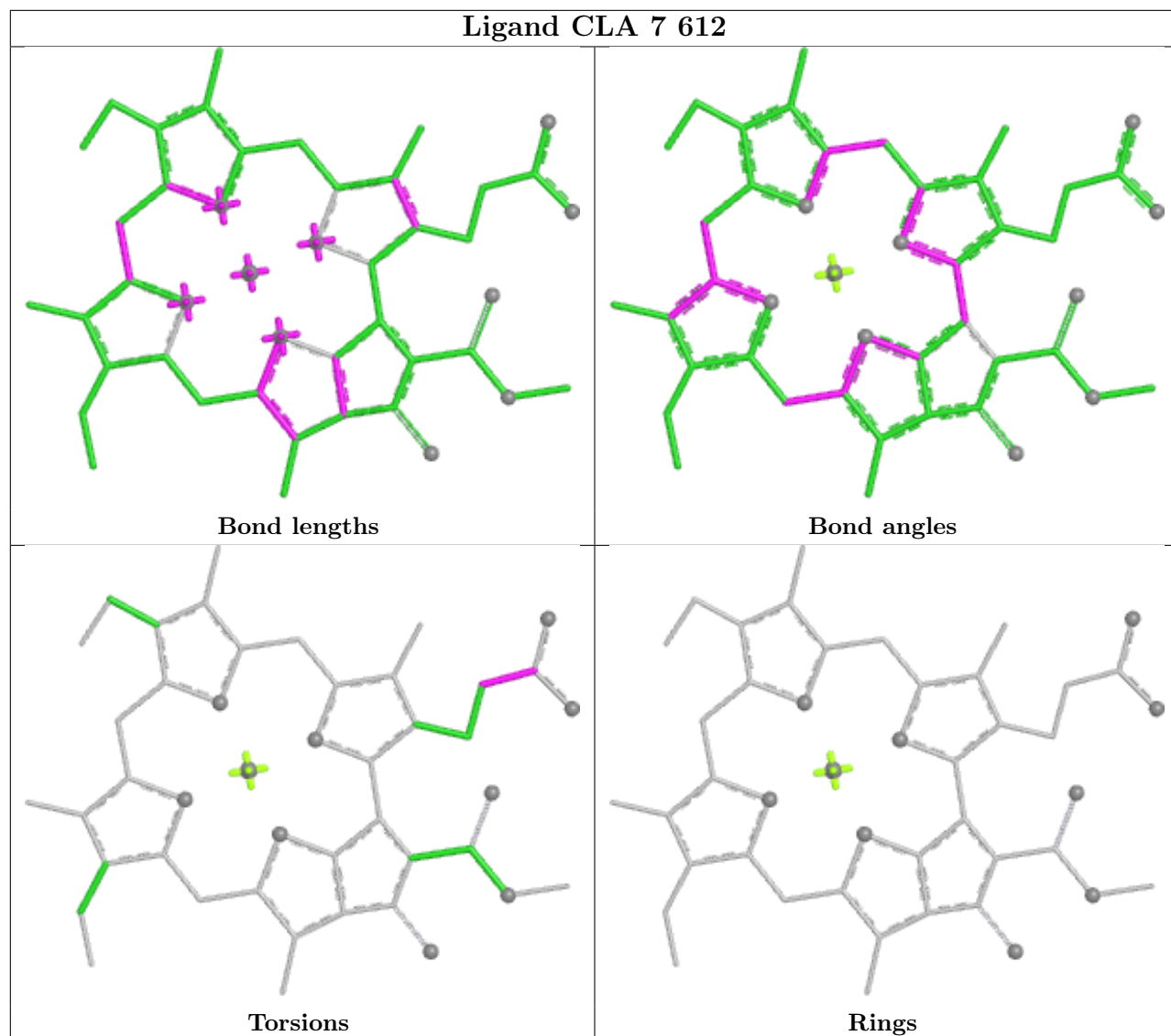


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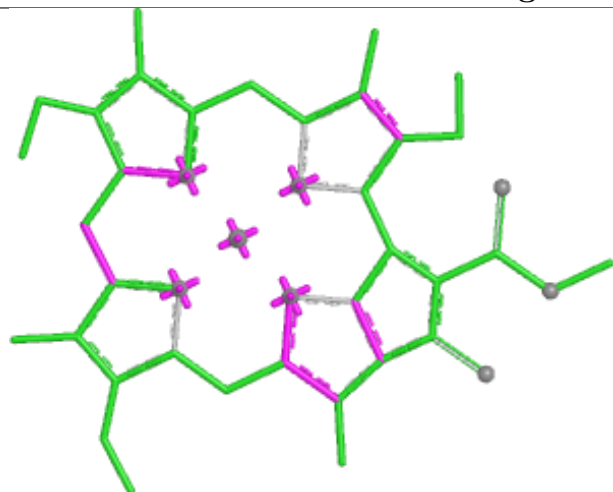


Rings

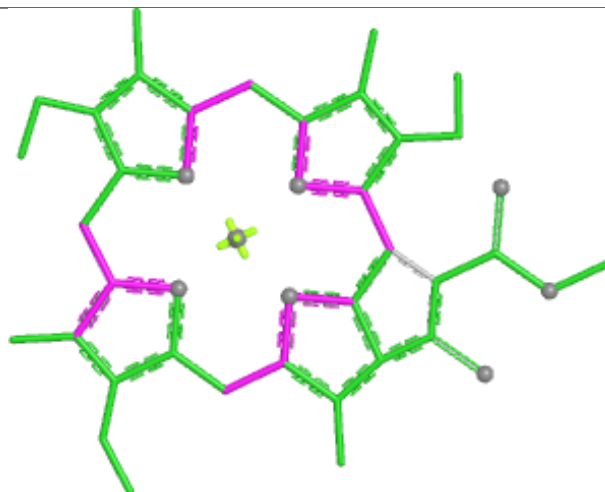
Ligand CLA 7 612



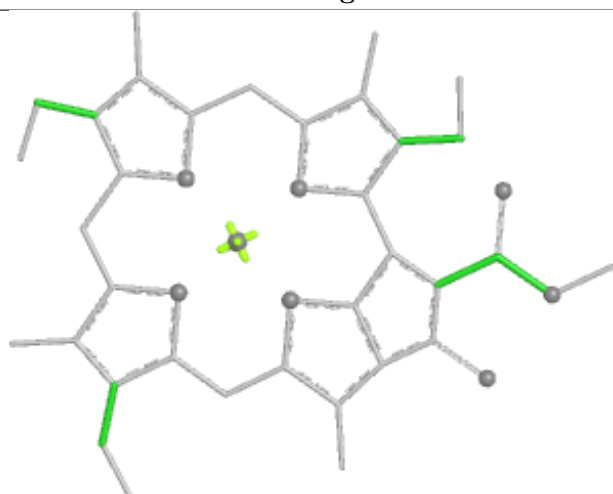
Ligand CLA 3 311



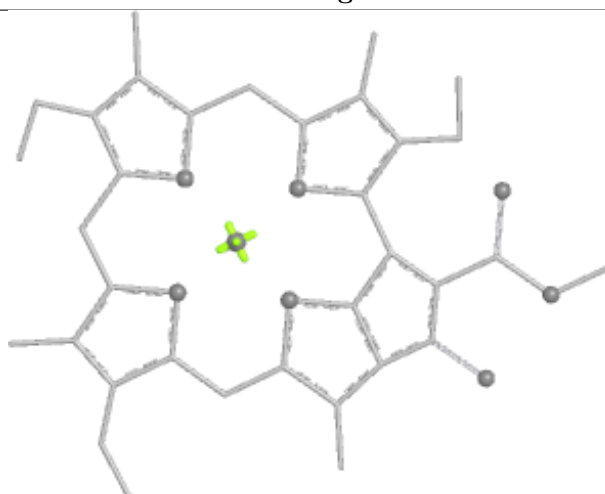
Bond lengths



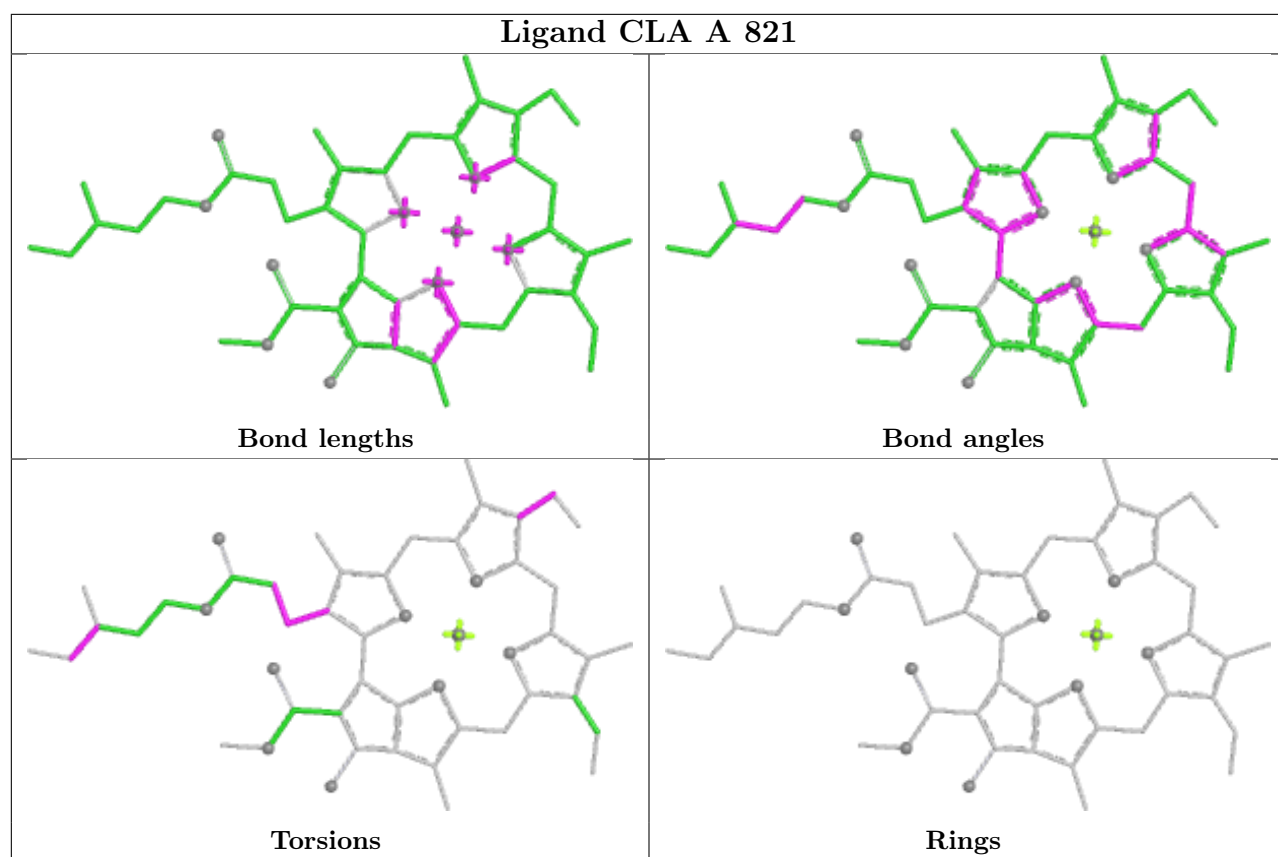
Bond angles

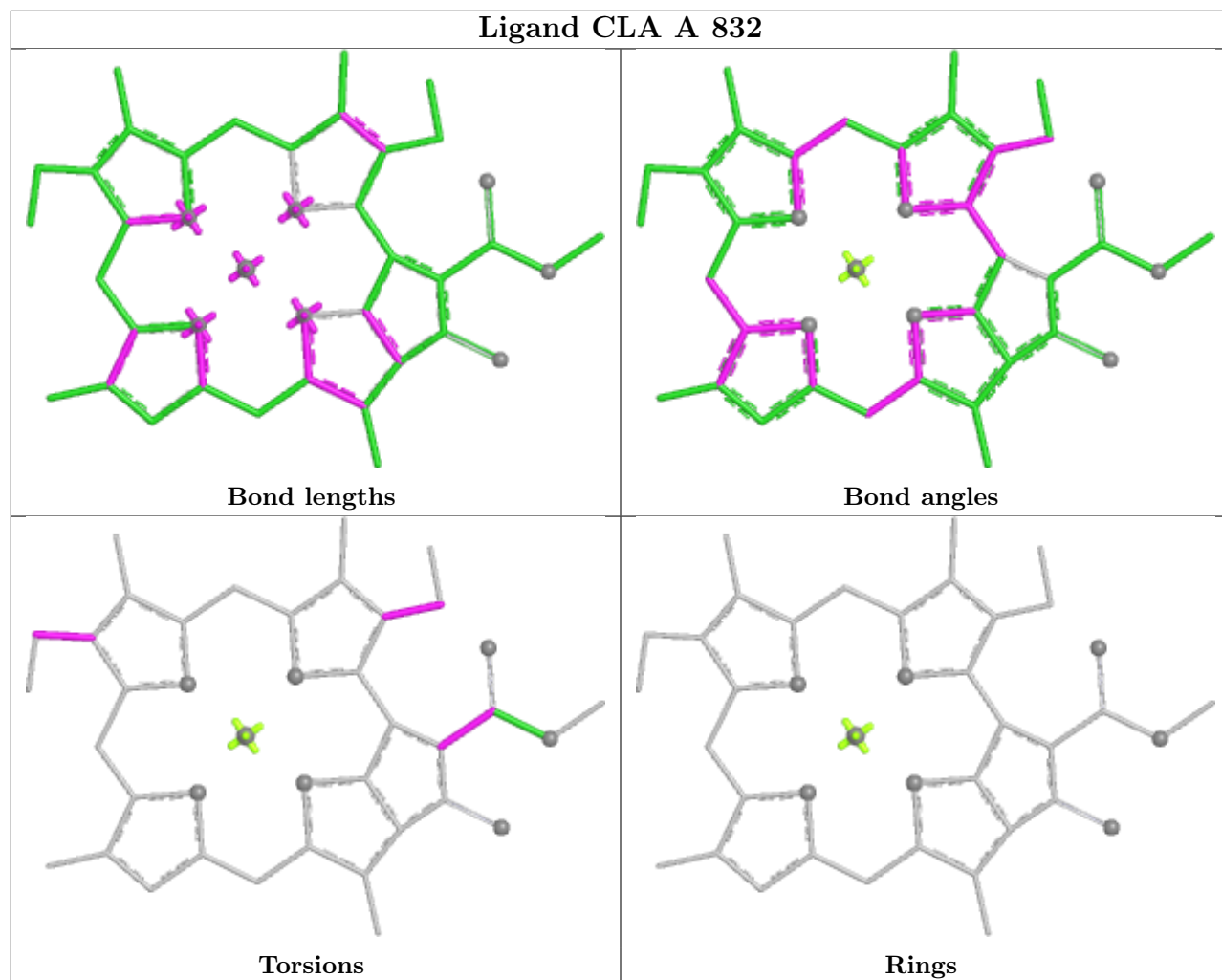


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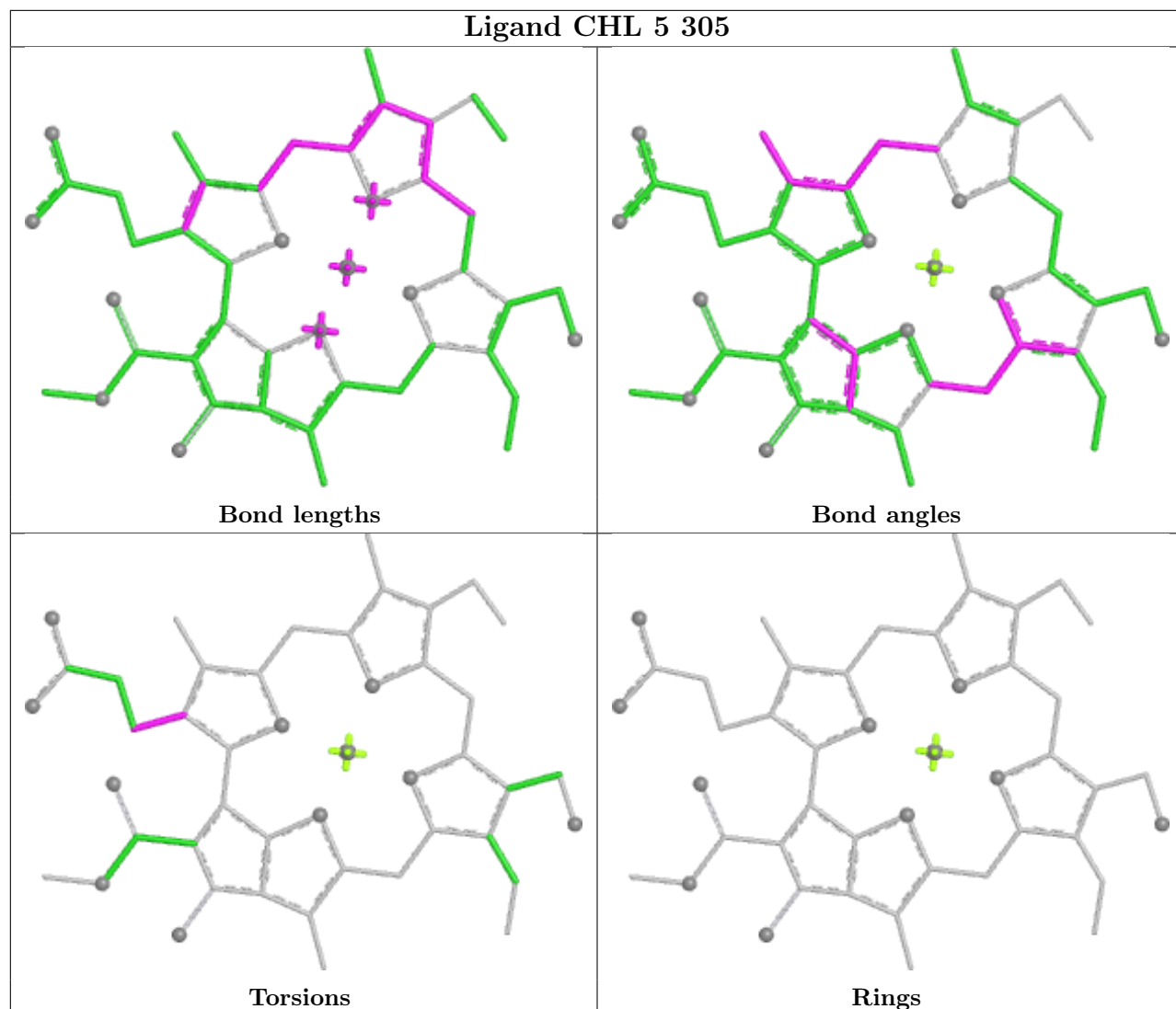


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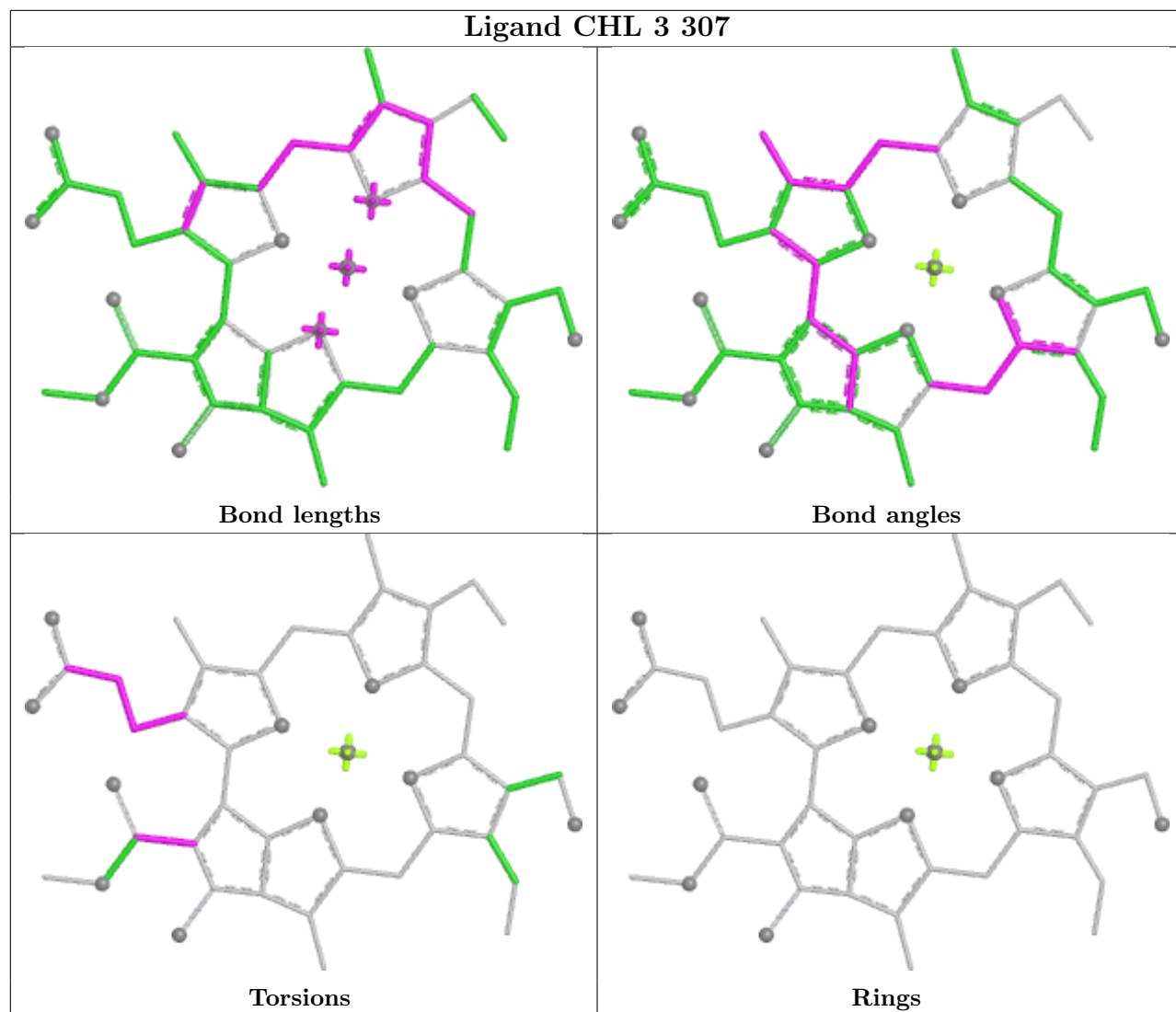




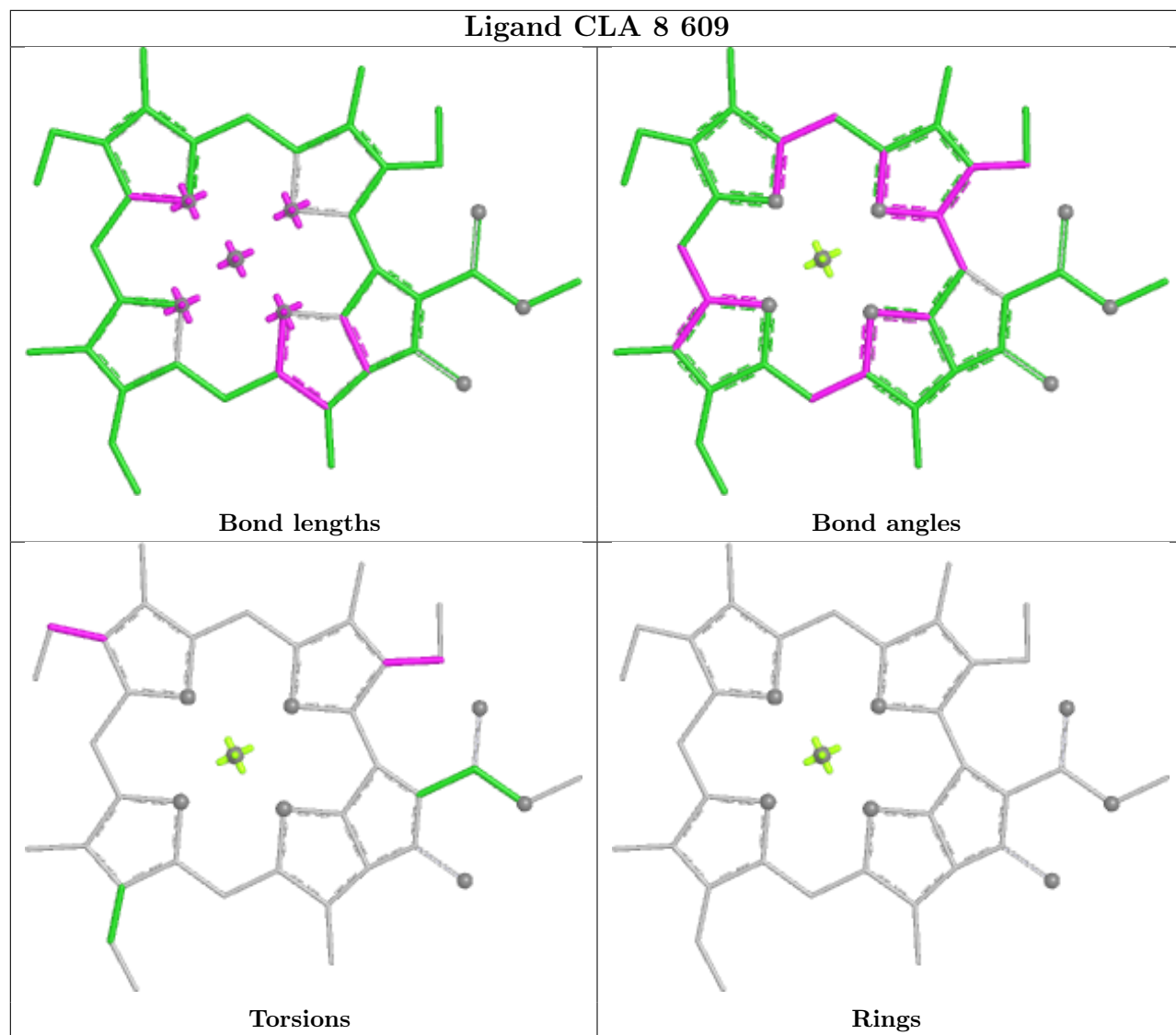
Ligand CHL 5 305



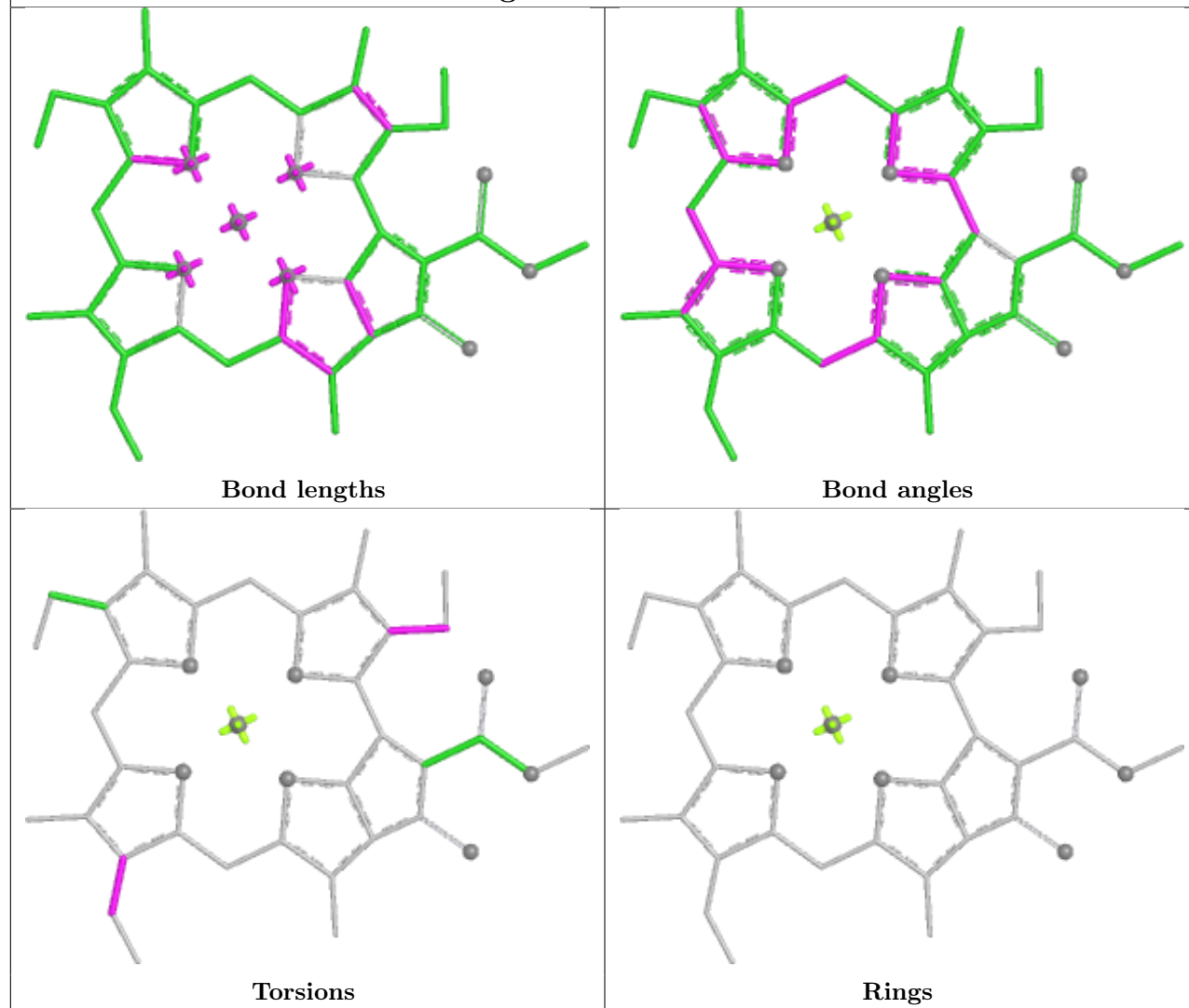
Ligand CHL 3 307



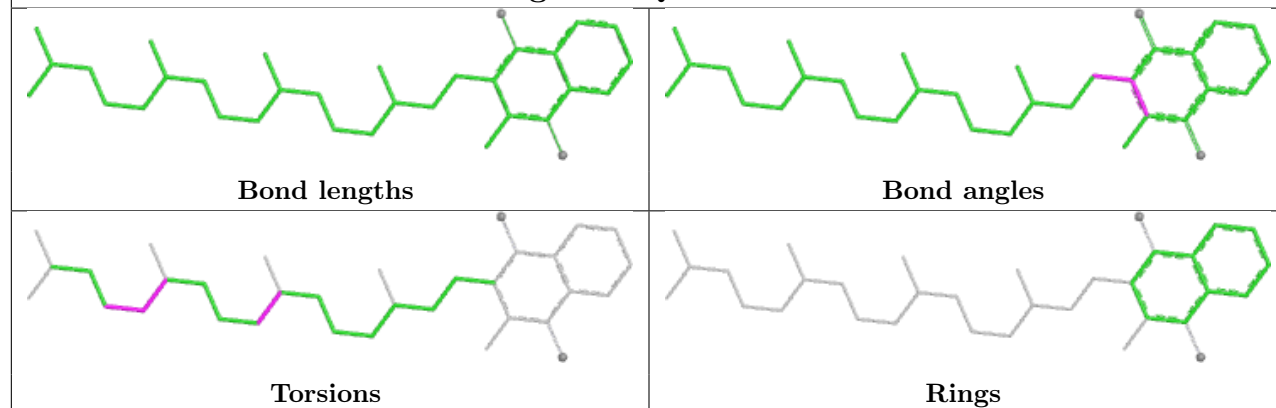
Ligand CLA 8 609



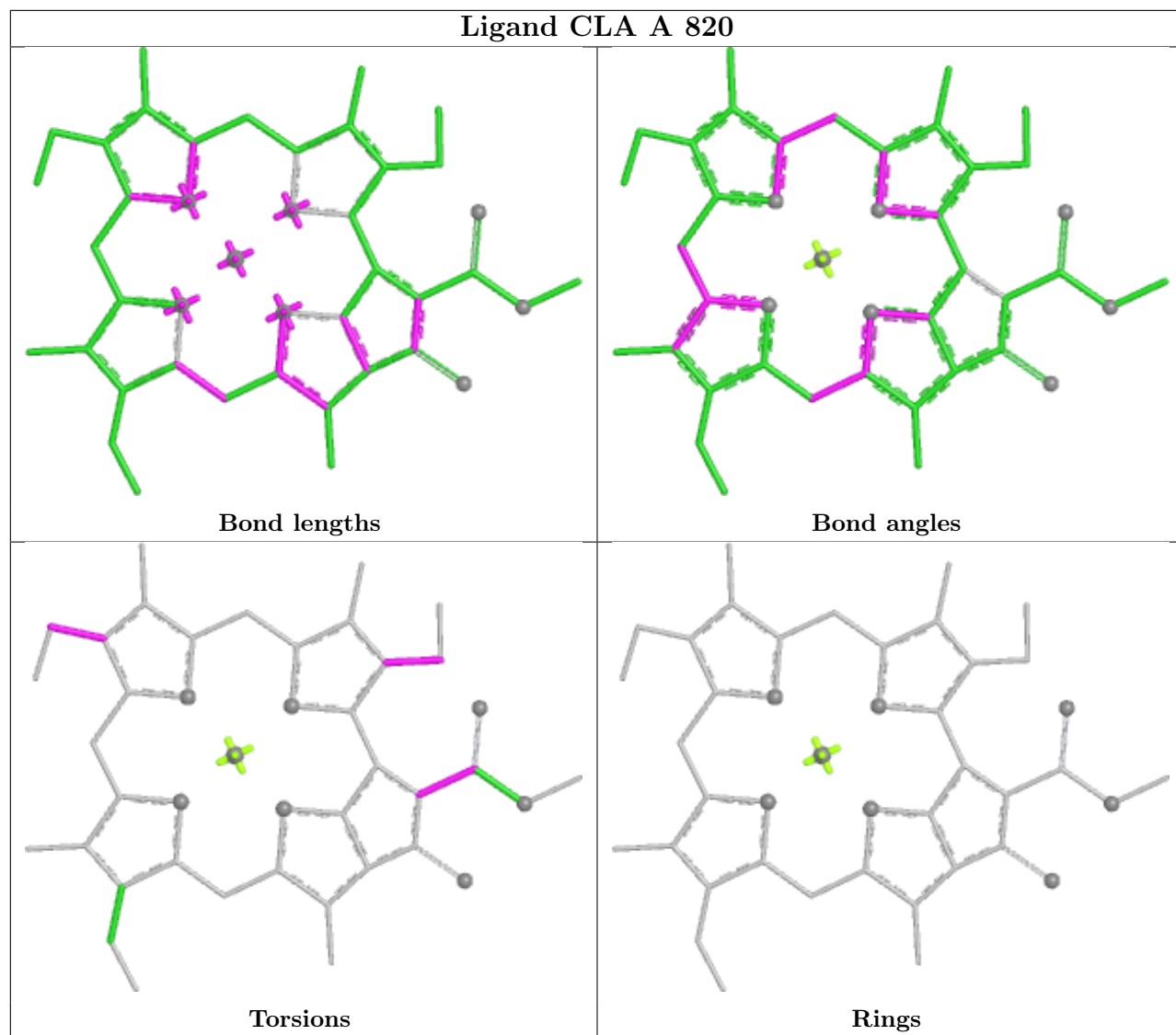
Ligand CLA 7 607



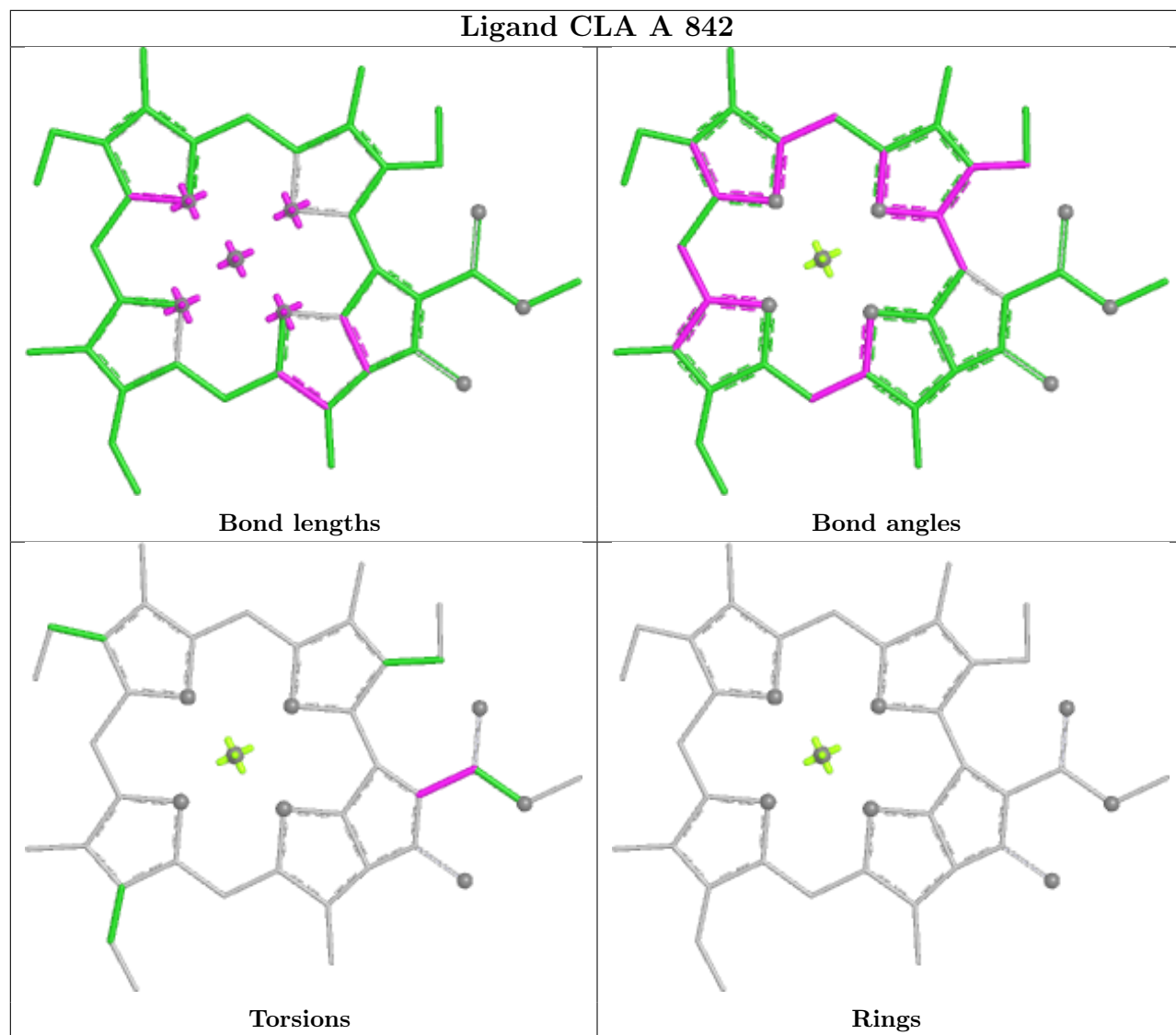
Ligand PQN A 840



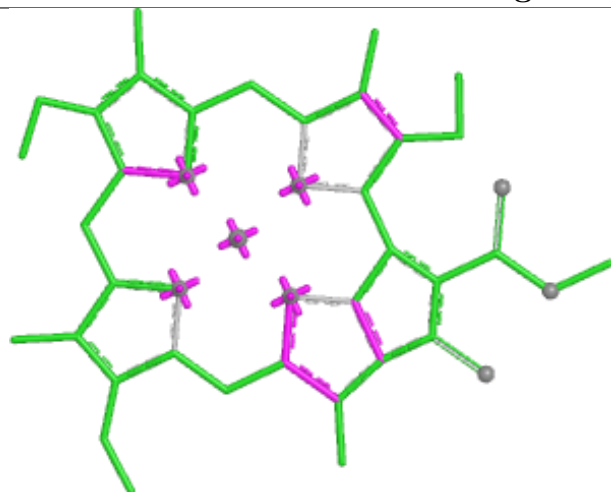
Ligand CLA A 820



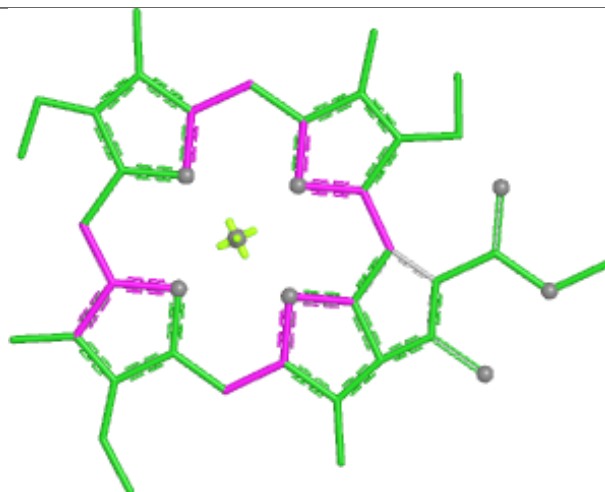
Ligand CLA A 842



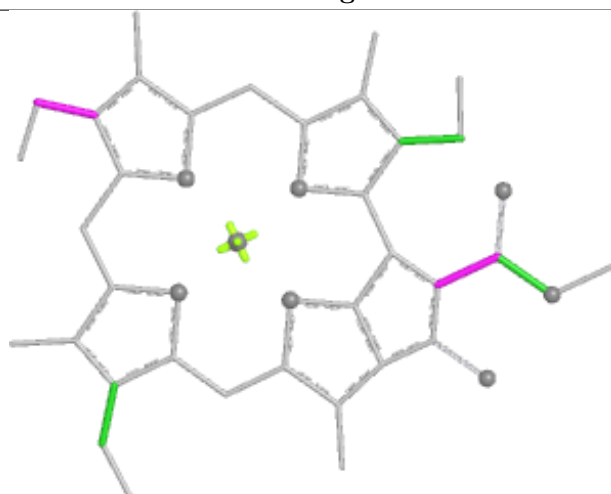
Ligand CLA B 808



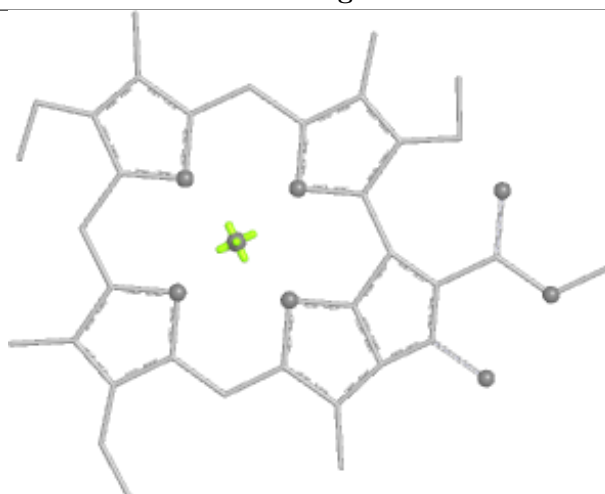
Bond lengths



Bond angles

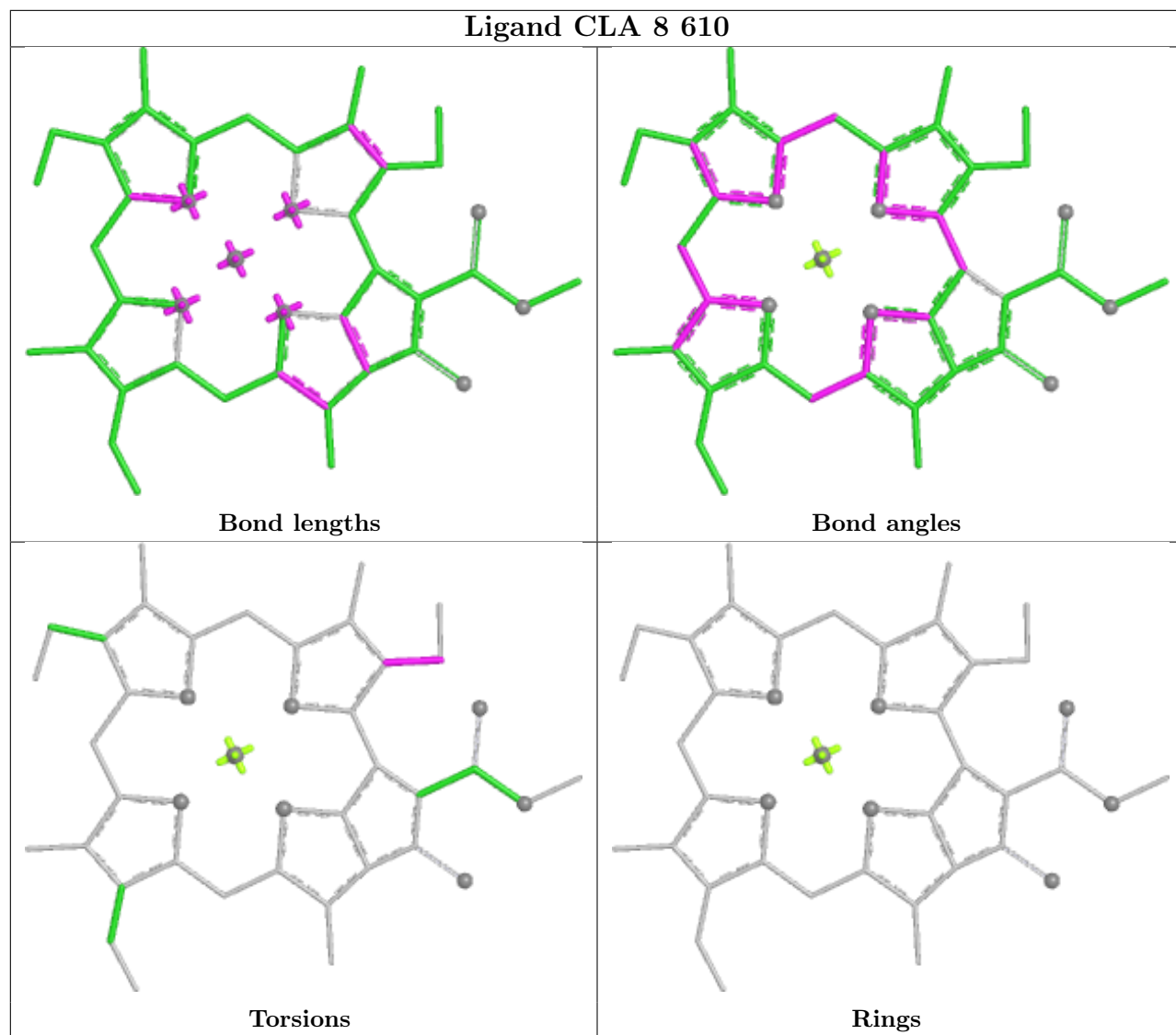


Torsions

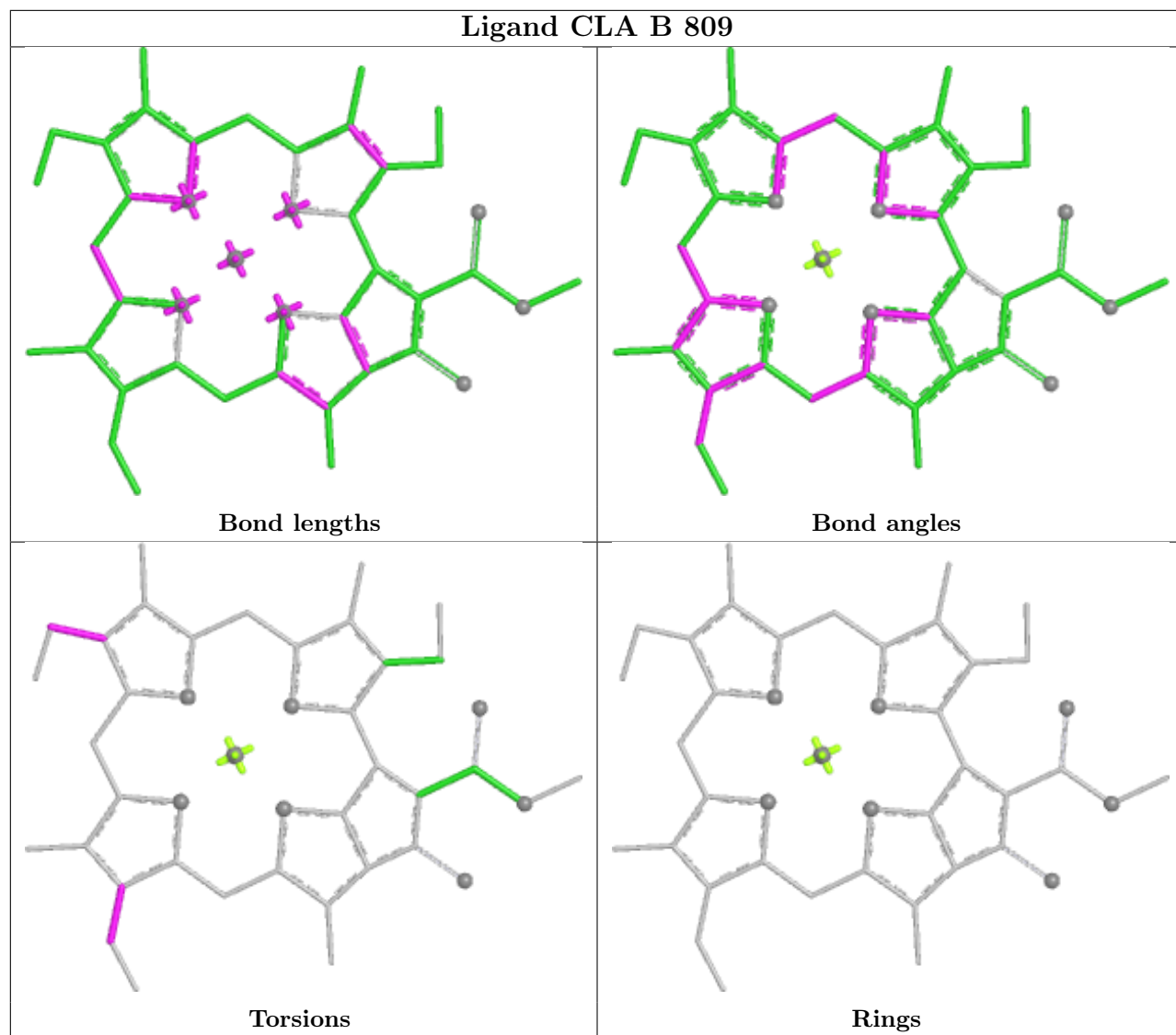


Rings

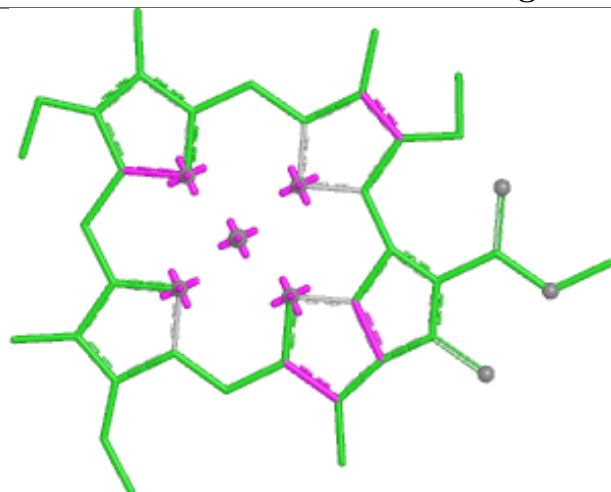
Ligand CLA 8 610



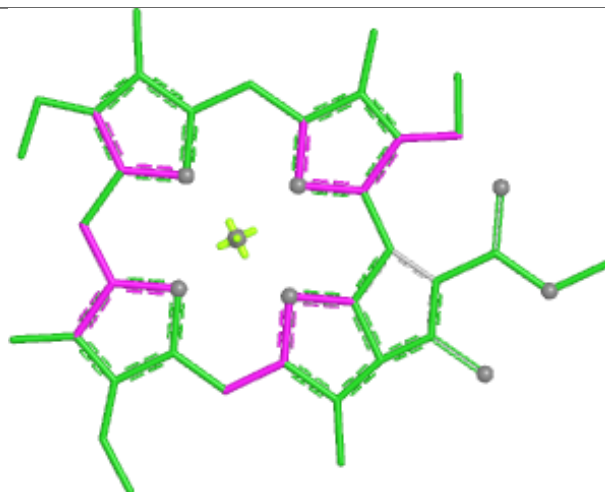
Ligand CLA B 809



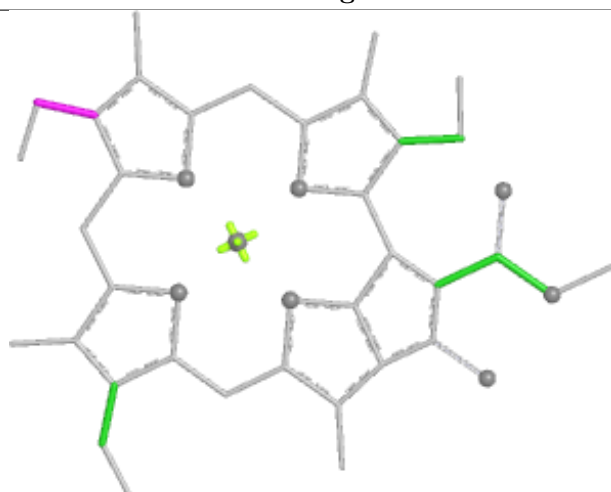
Ligand CLA 3 305



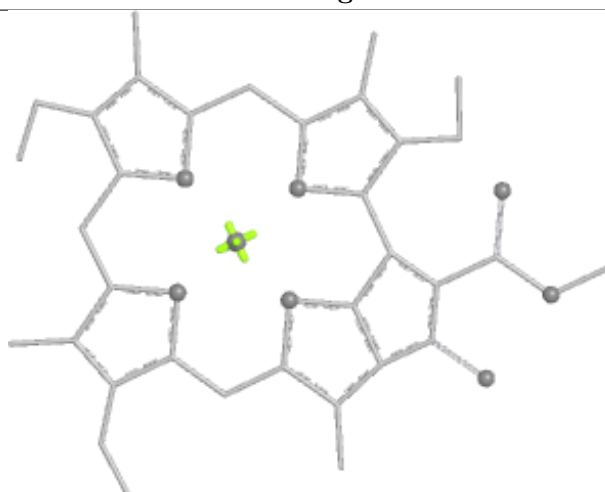
Bond lengths



Bond angles

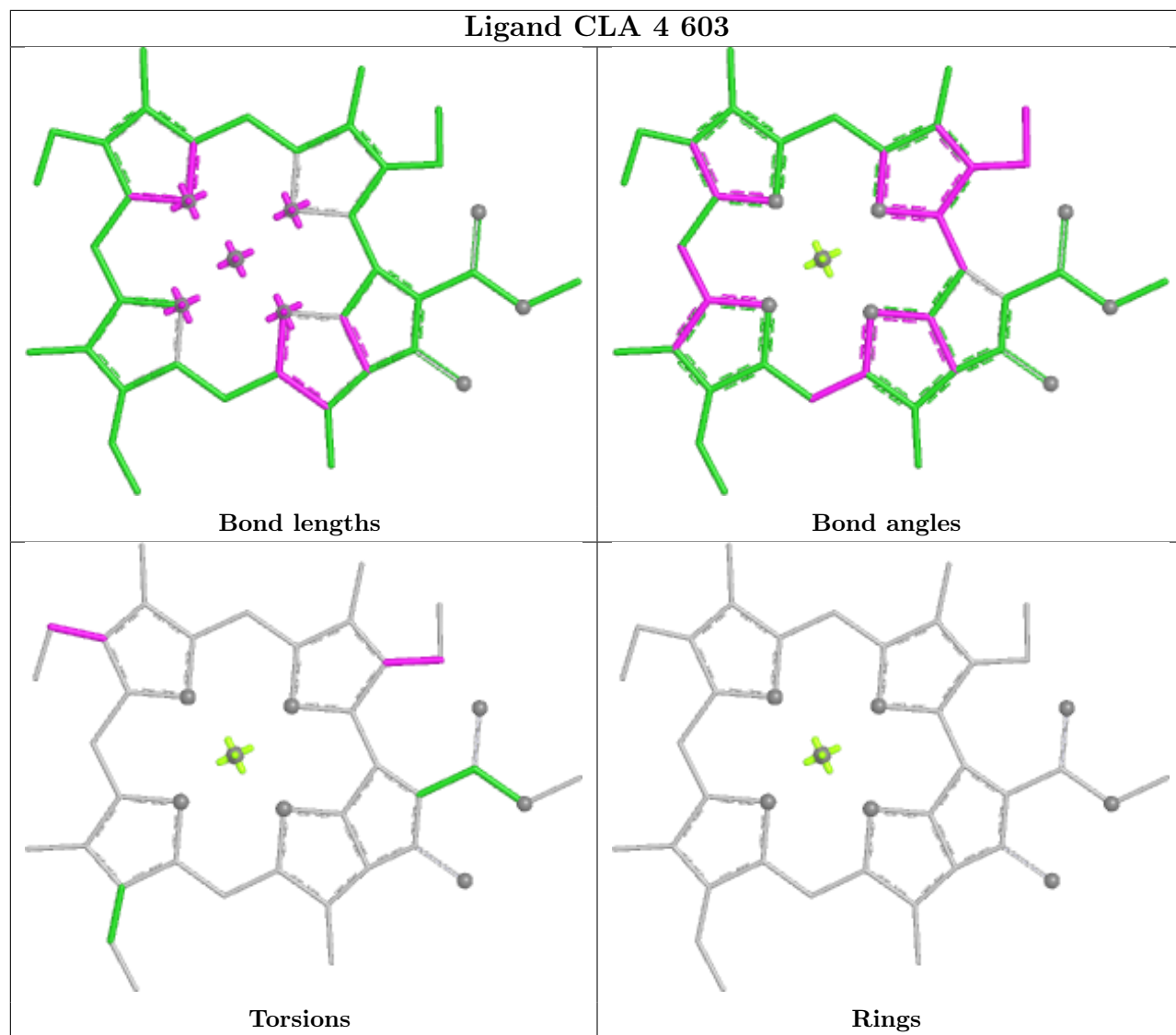


Torsions

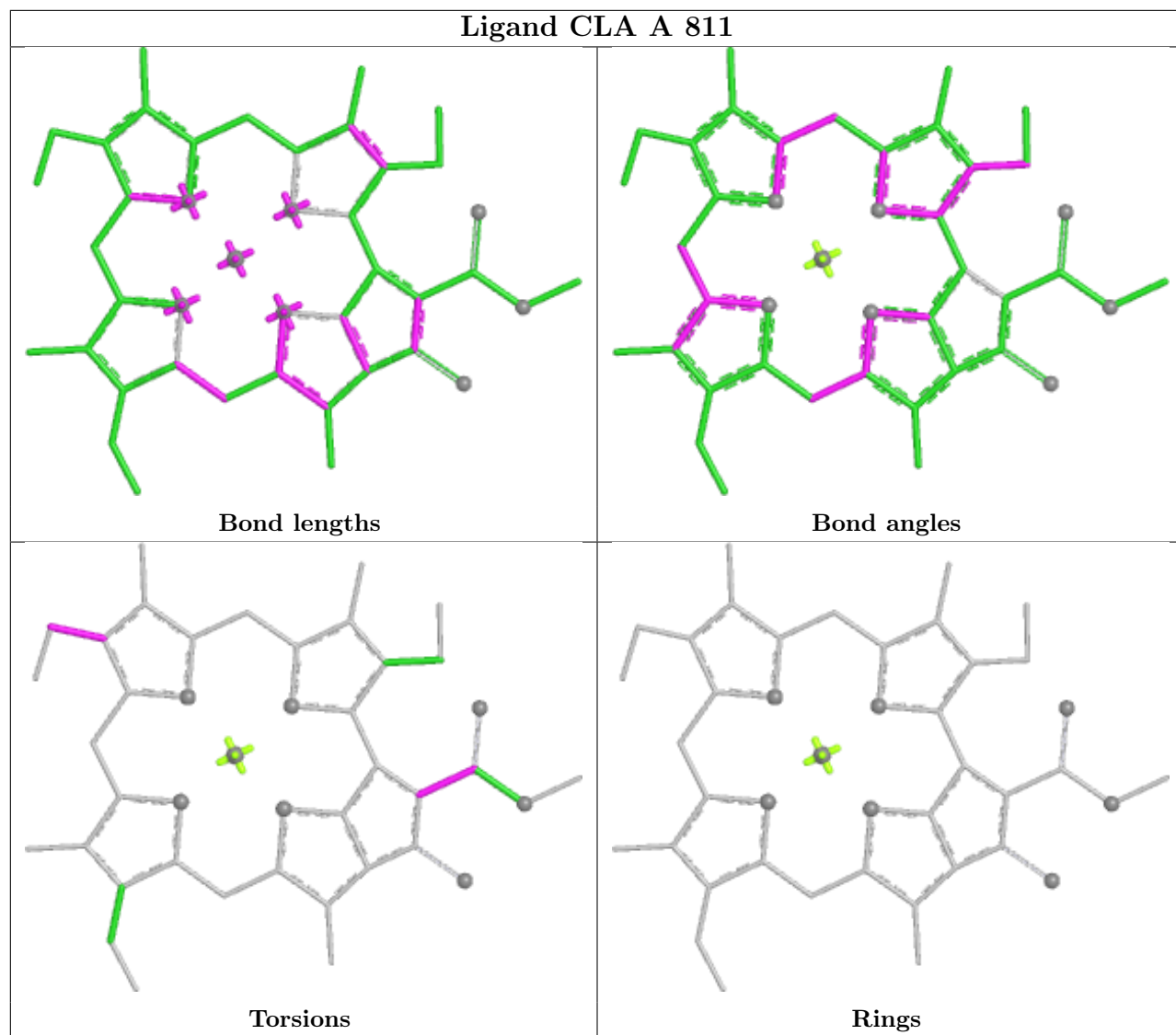


Rings

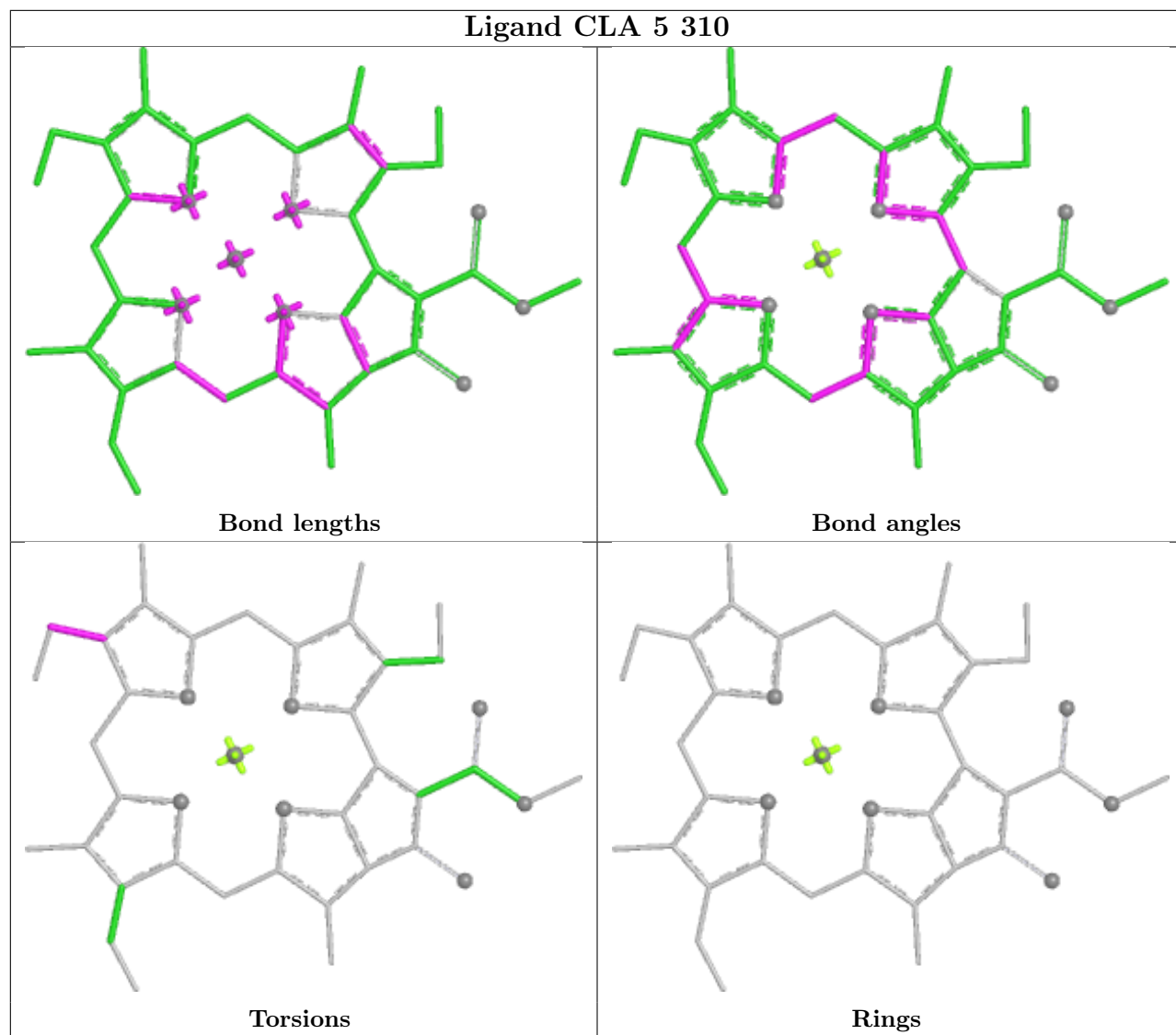
Ligand CLA 4 603



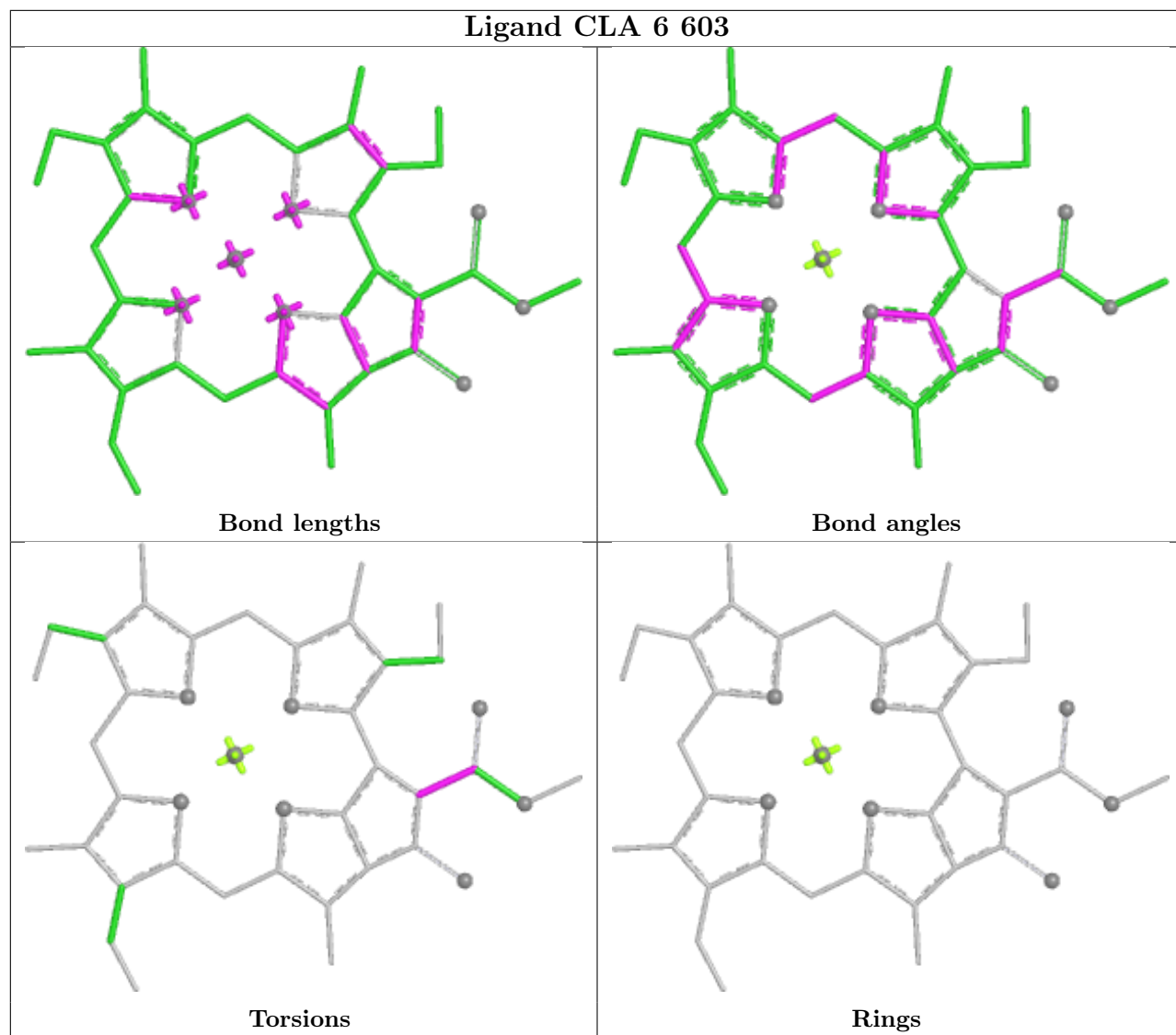
Ligand CLA A 811



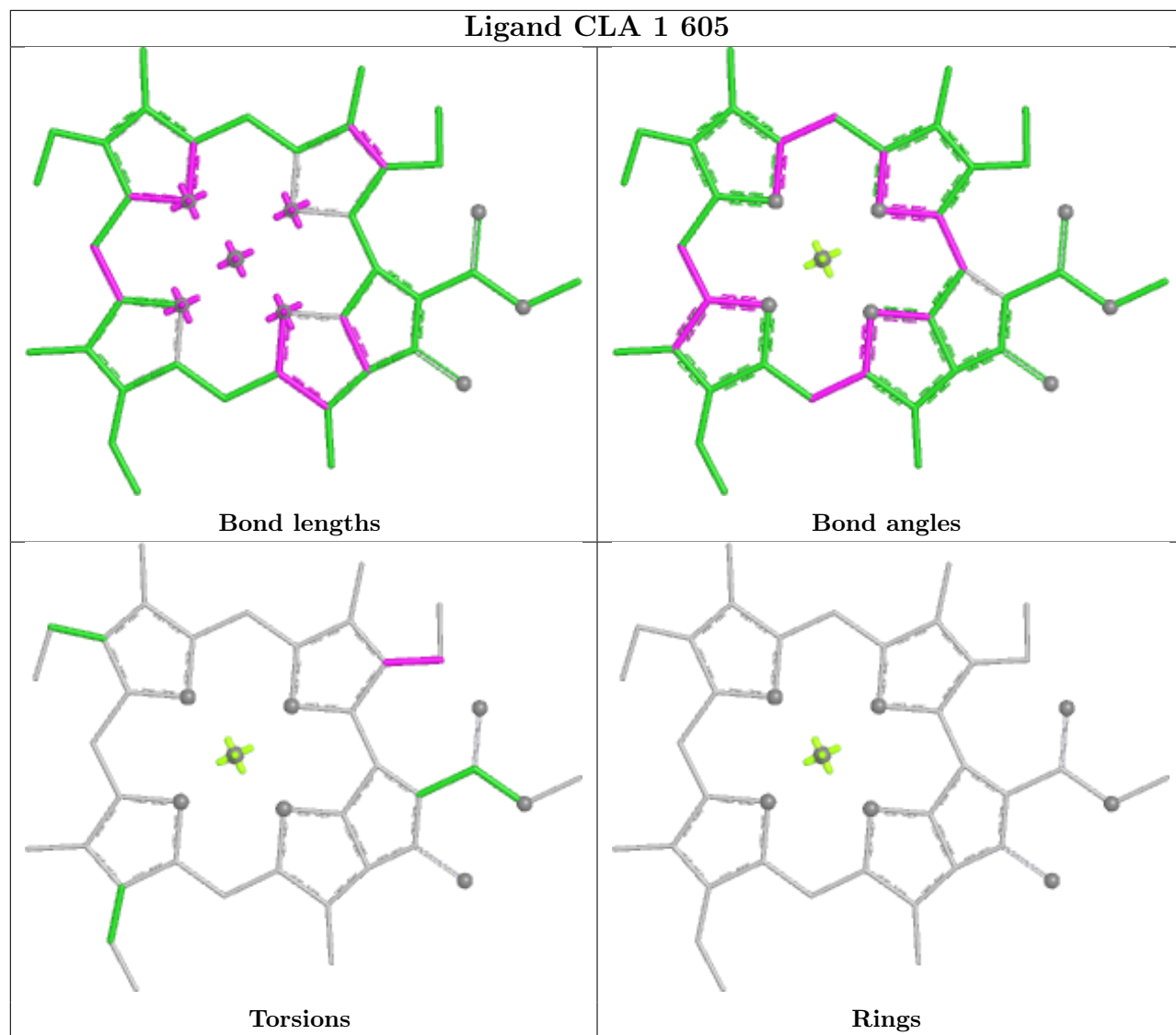
Ligand CLA 5 310



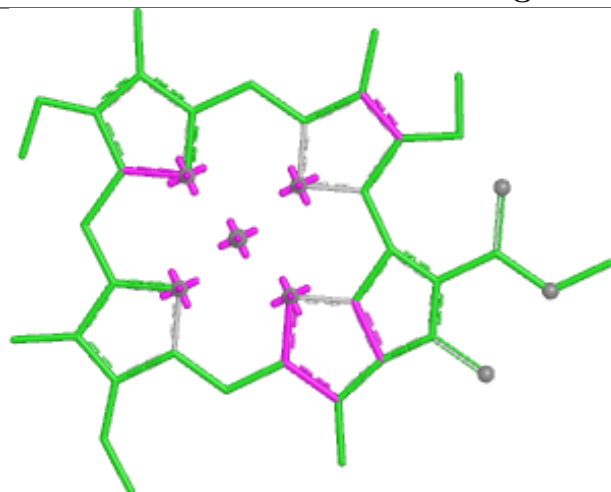
Ligand CLA 6 603



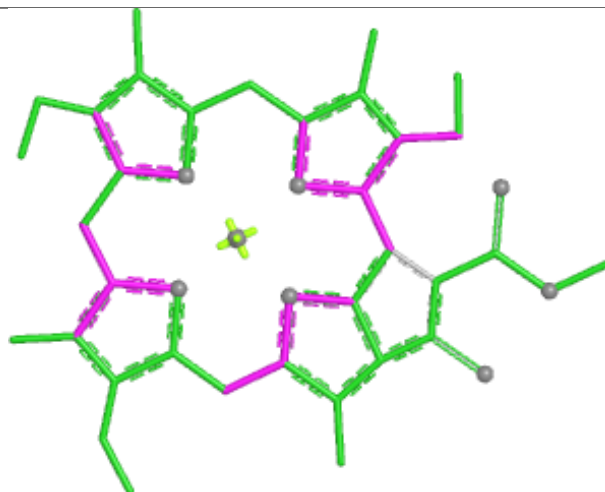
Ligand CLA 1 605



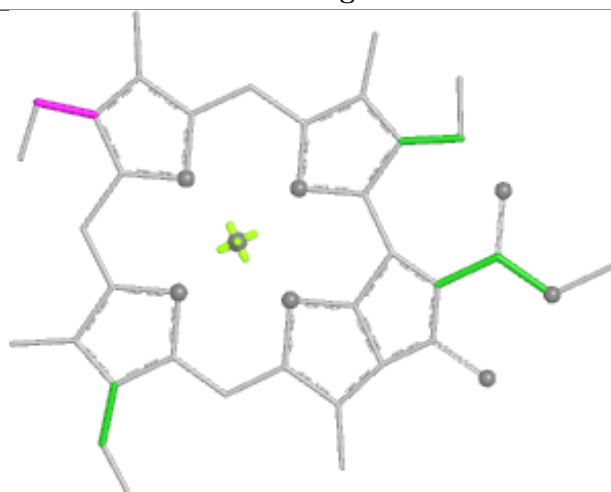
Ligand CLA A 824



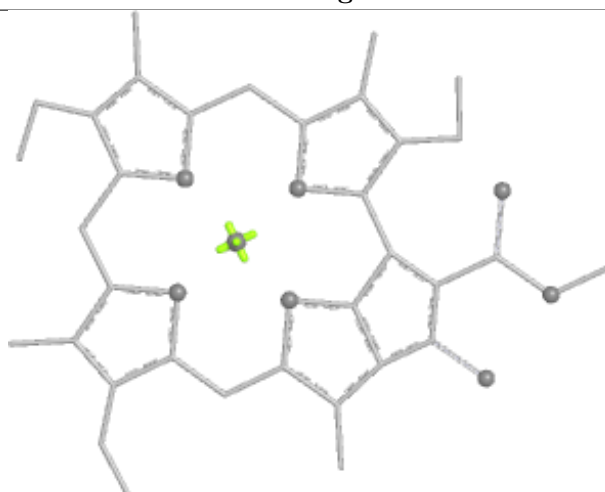
Bond lengths



Bond angles

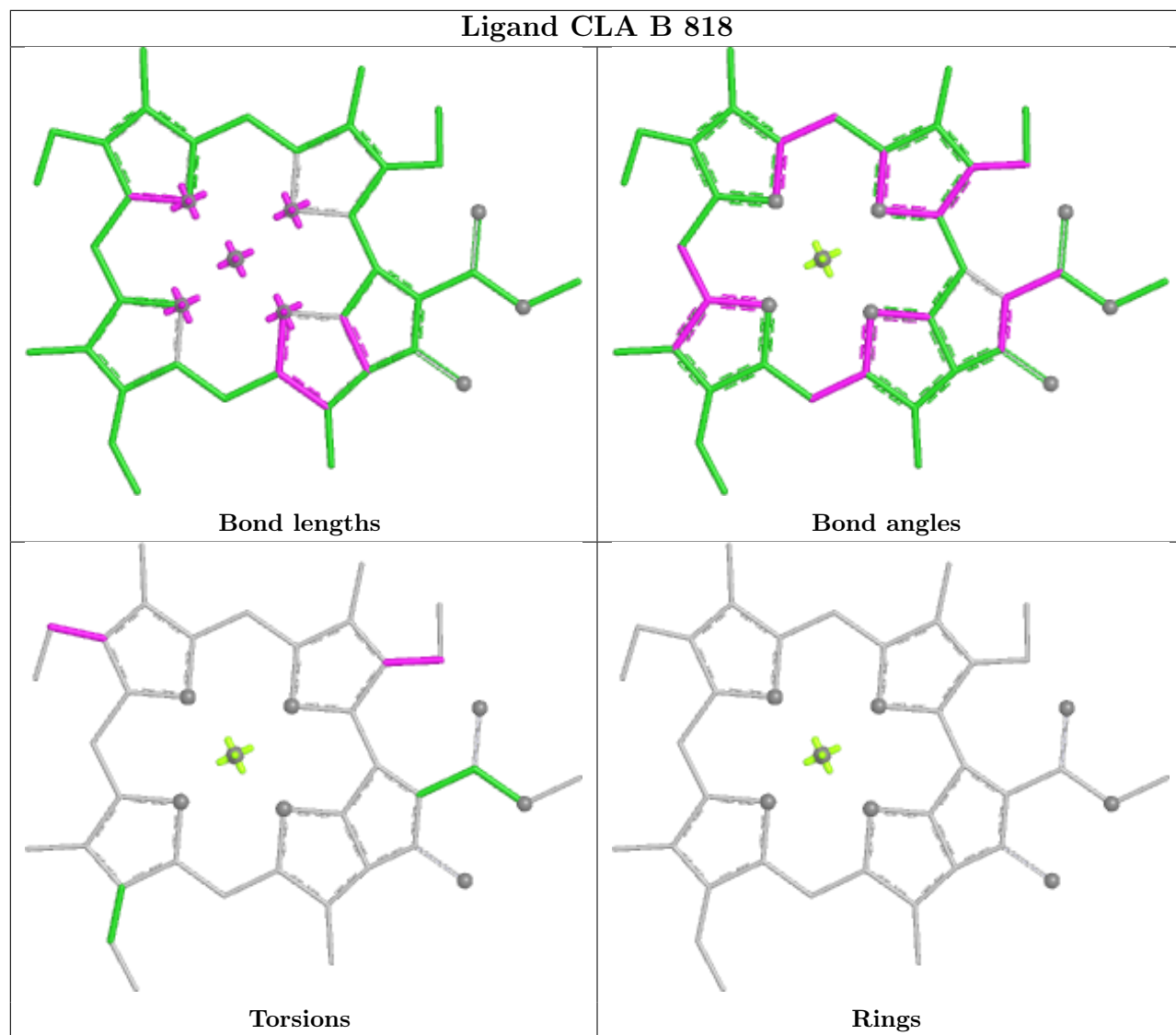


Torsions

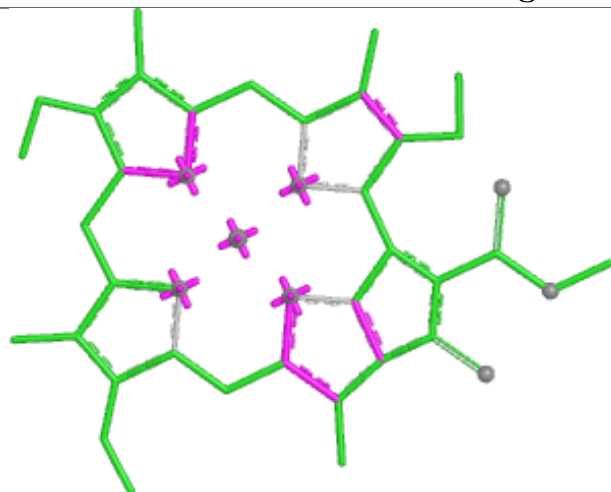


Rings

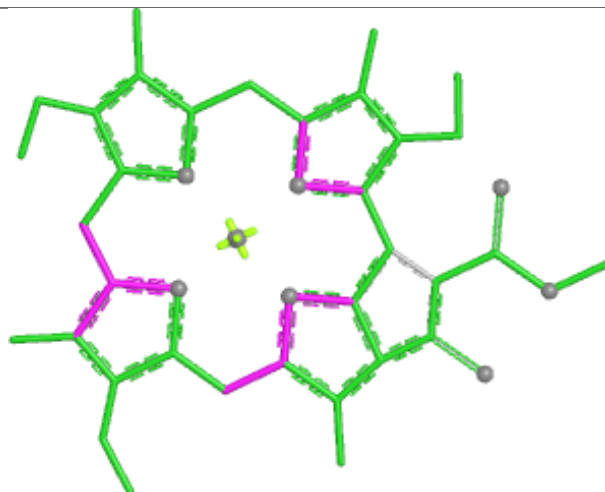
Ligand CLA B 818



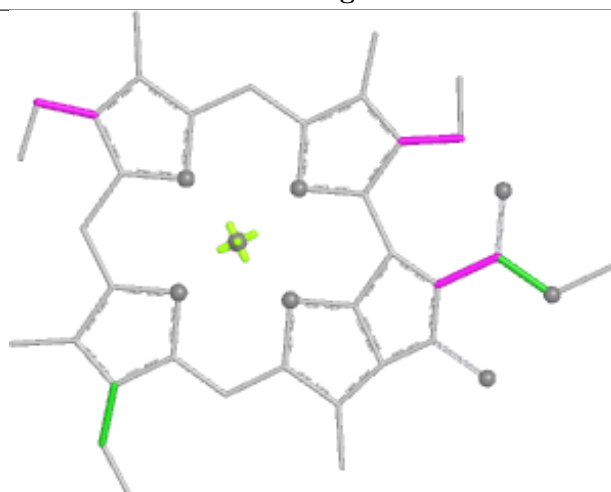
Ligand CLA 4 604



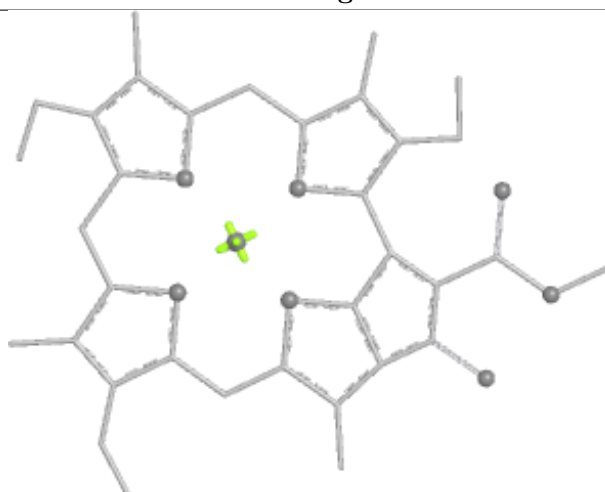
Bond lengths



Bond angles

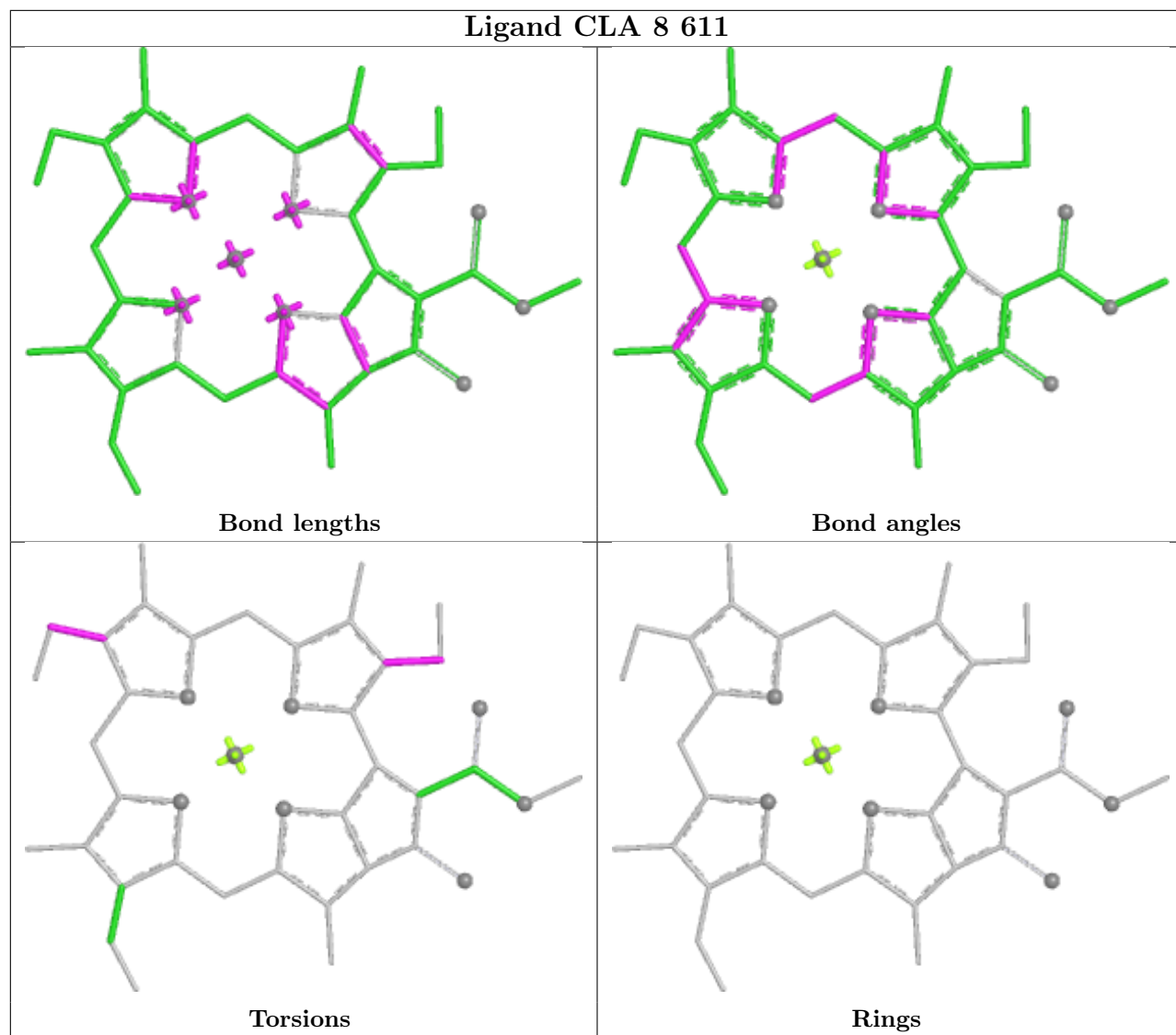


Torsions

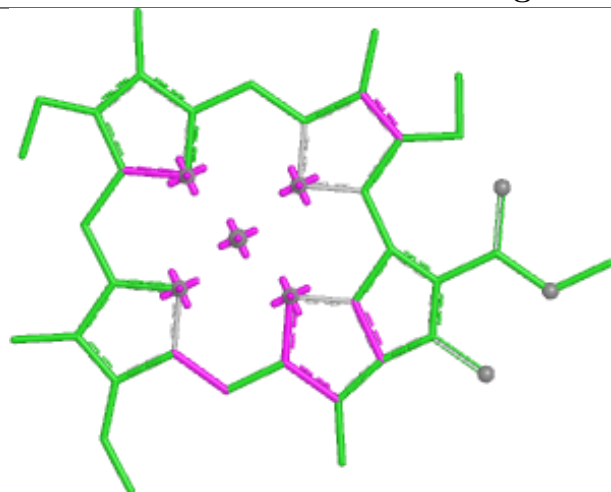


Rings

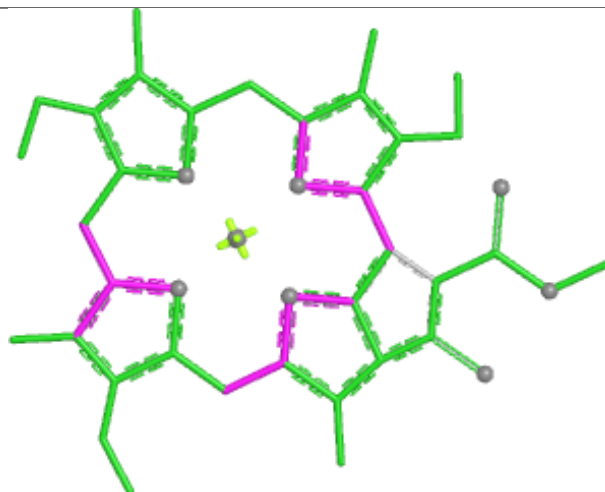
Ligand CLA 8 611



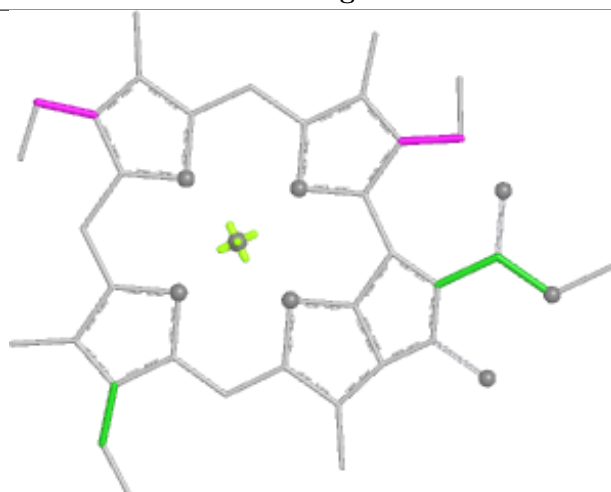
Ligand CLA A 837



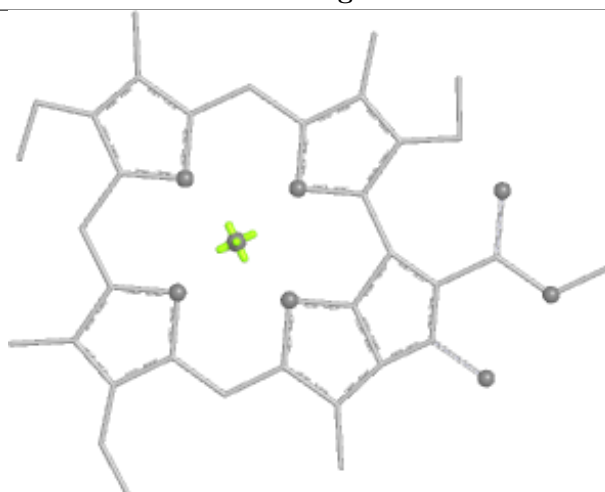
Bond lengths



Bond angles

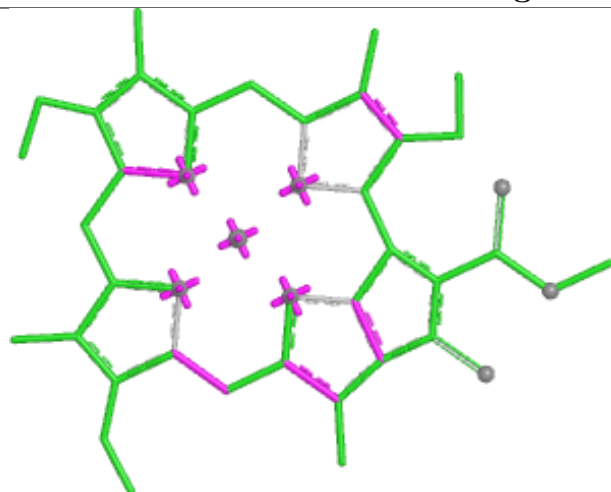


Torsions

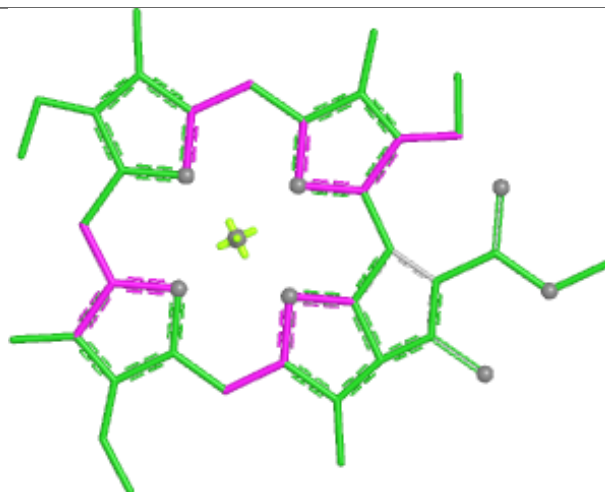


Rings

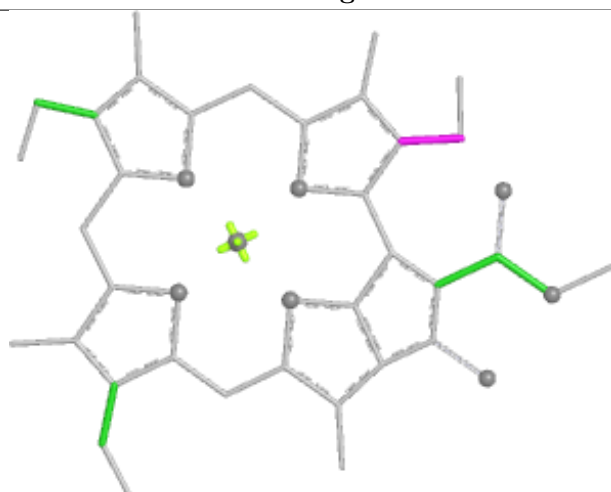
Ligand CLA A 802



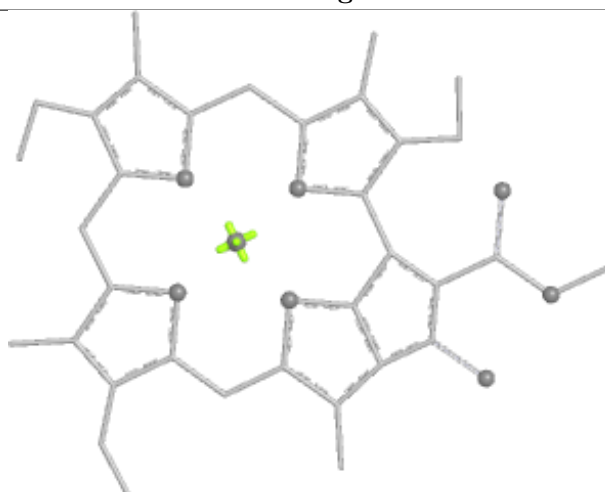
Bond lengths



Bond angles

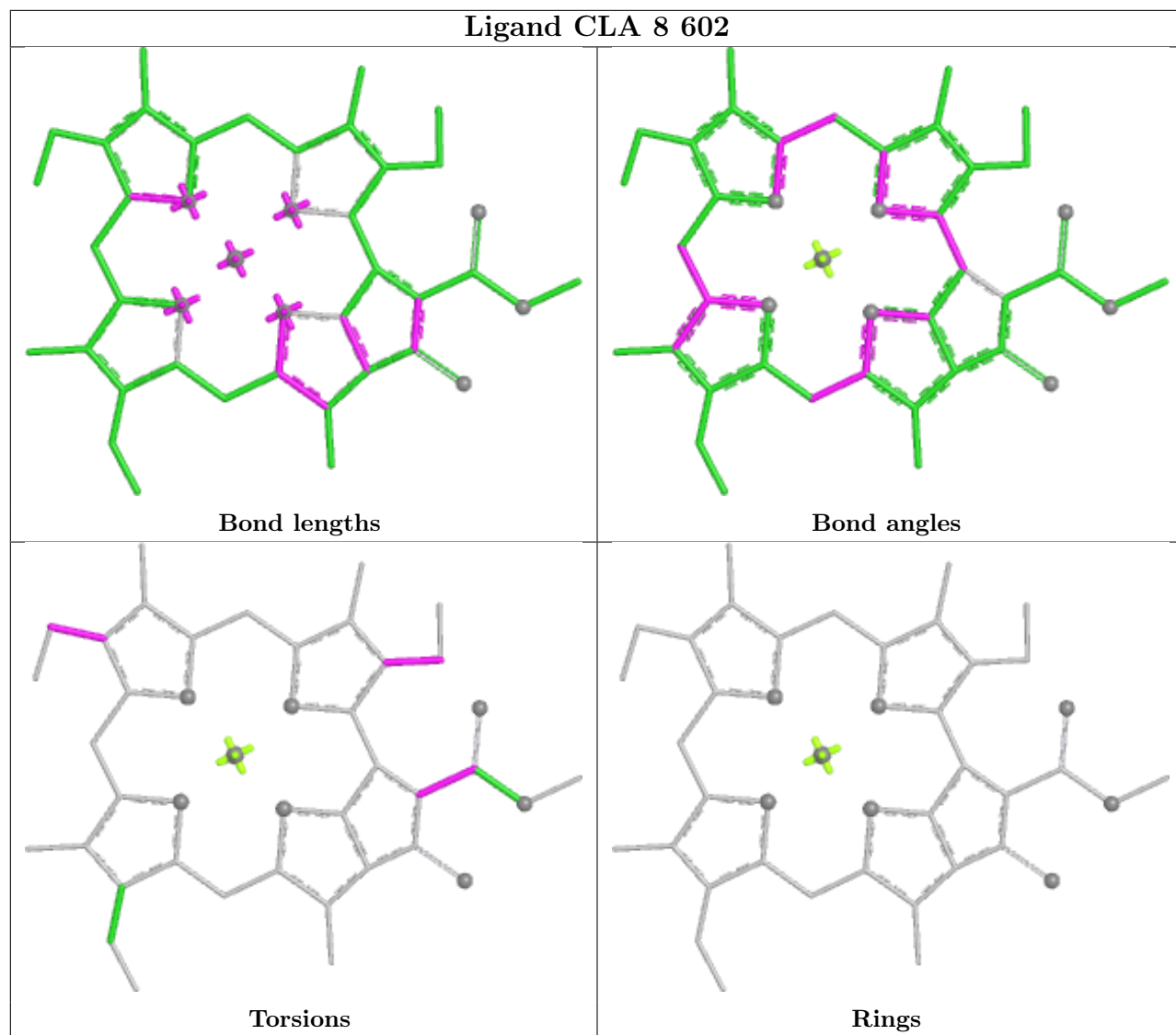


Torsions

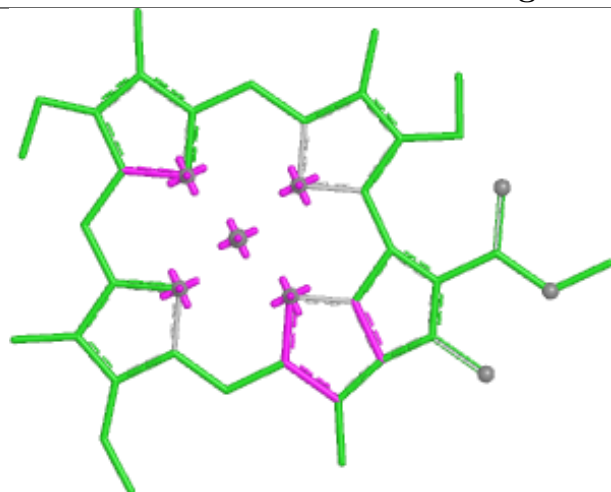


Rings

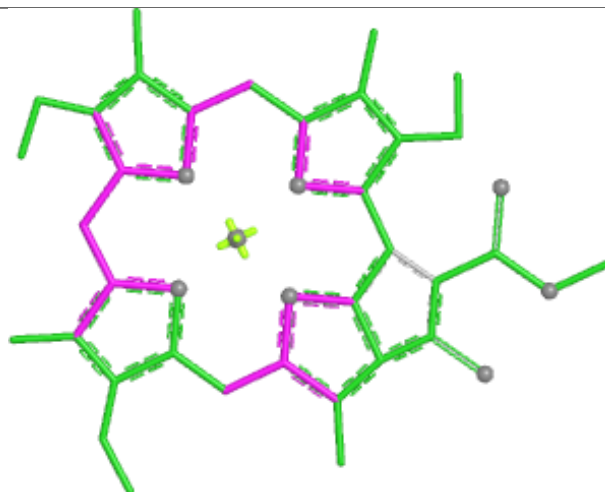
Ligand CLA 8 602



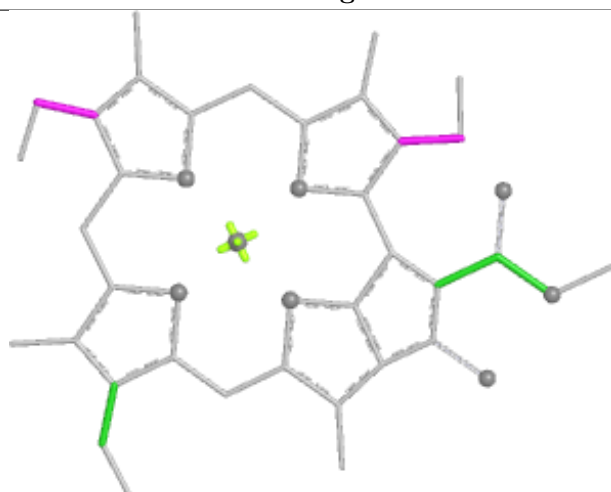
Ligand CLA 5 308



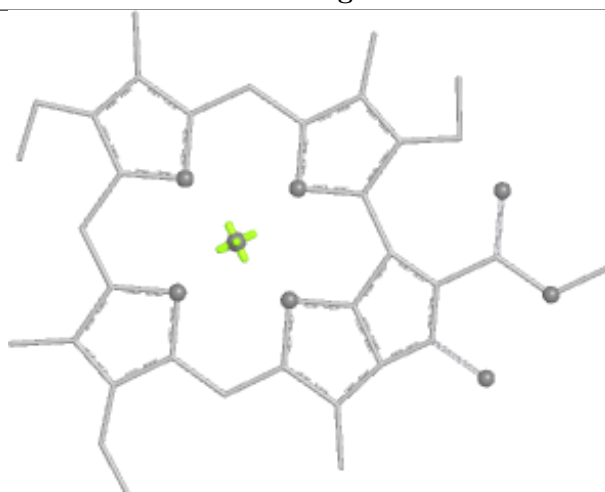
Bond lengths



Bond angles

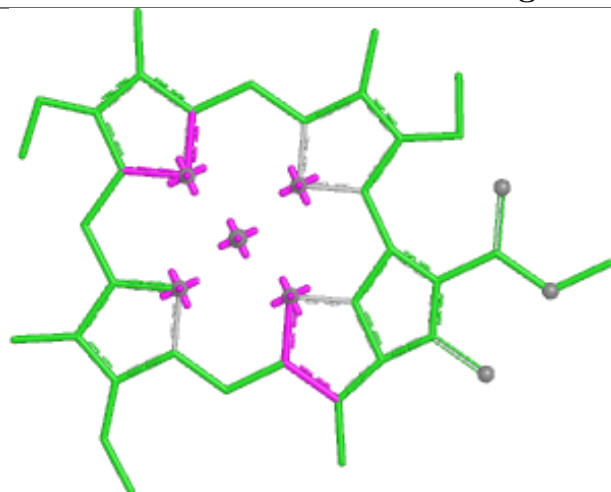


Torsions

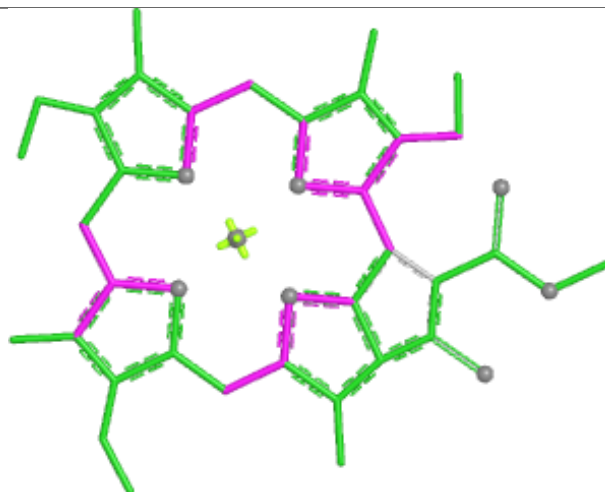


Rings

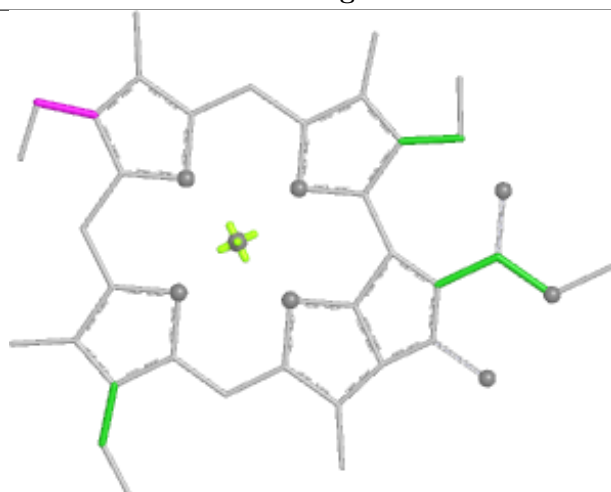
Ligand CLA 1 604



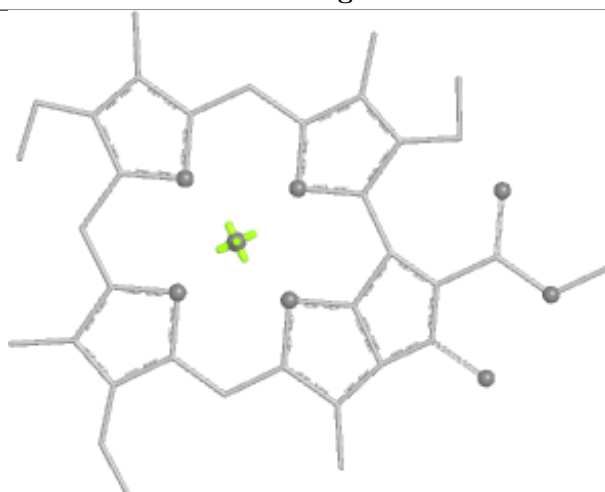
Bond lengths



Bond angles

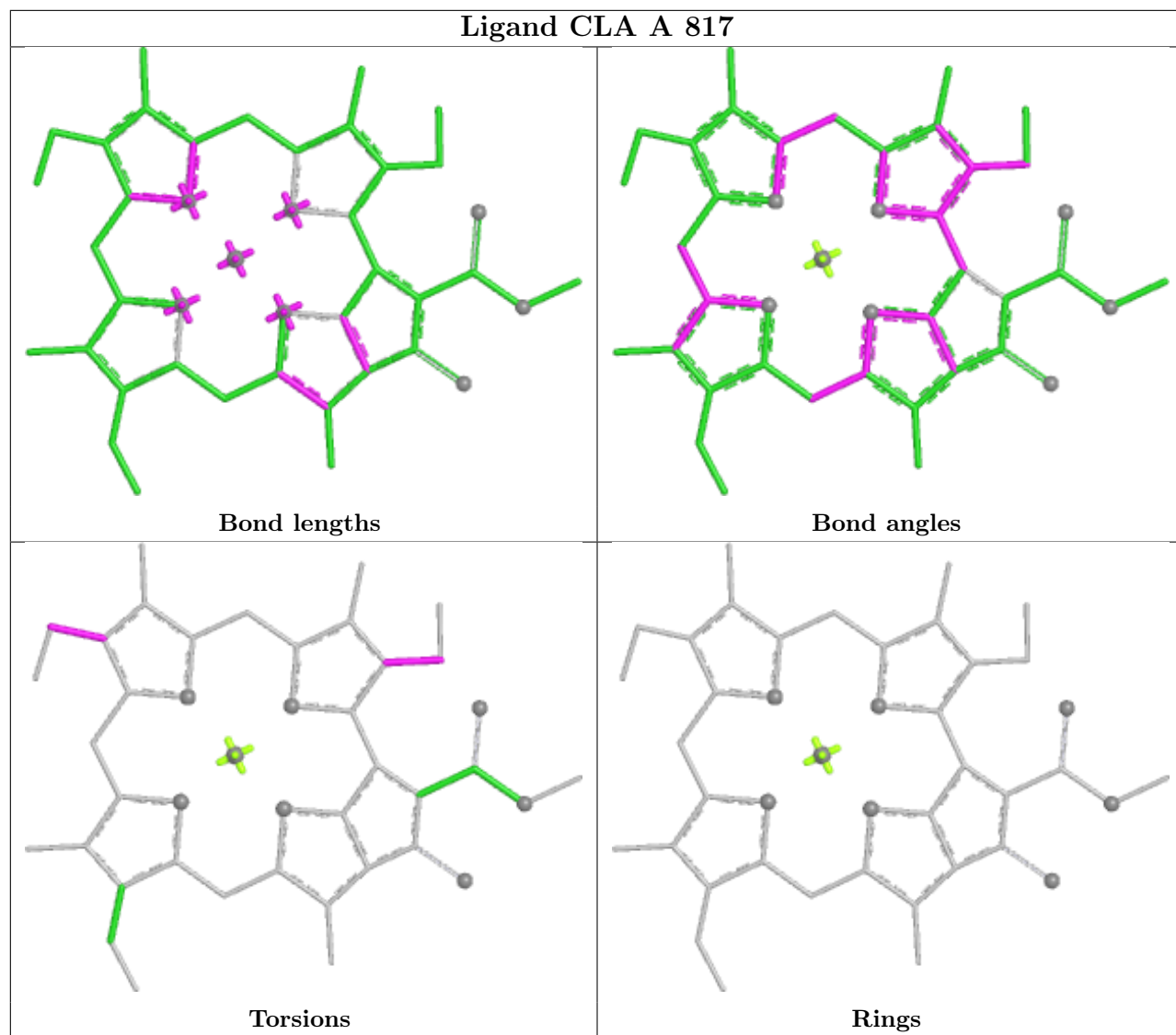


Torsions

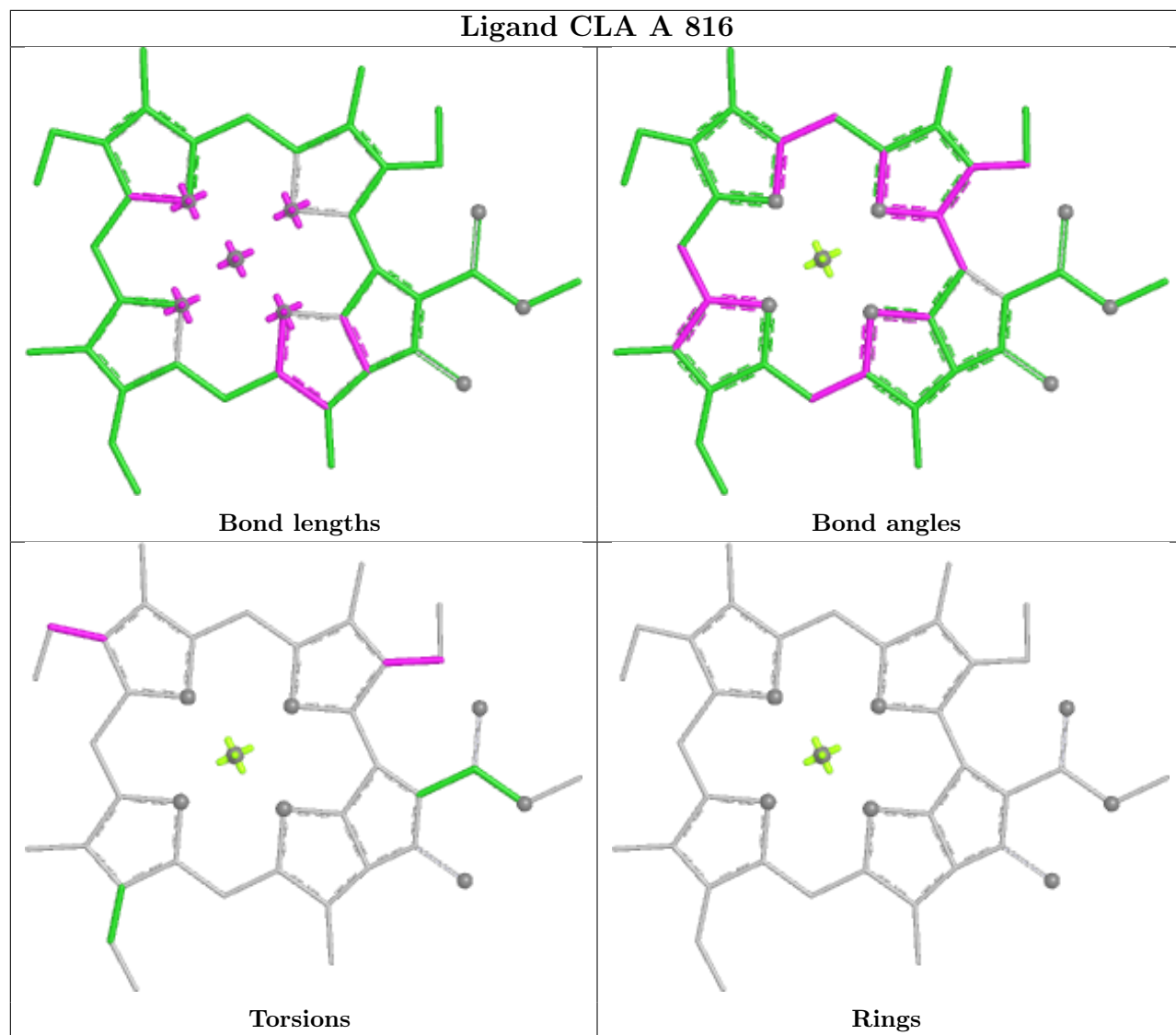


Rings

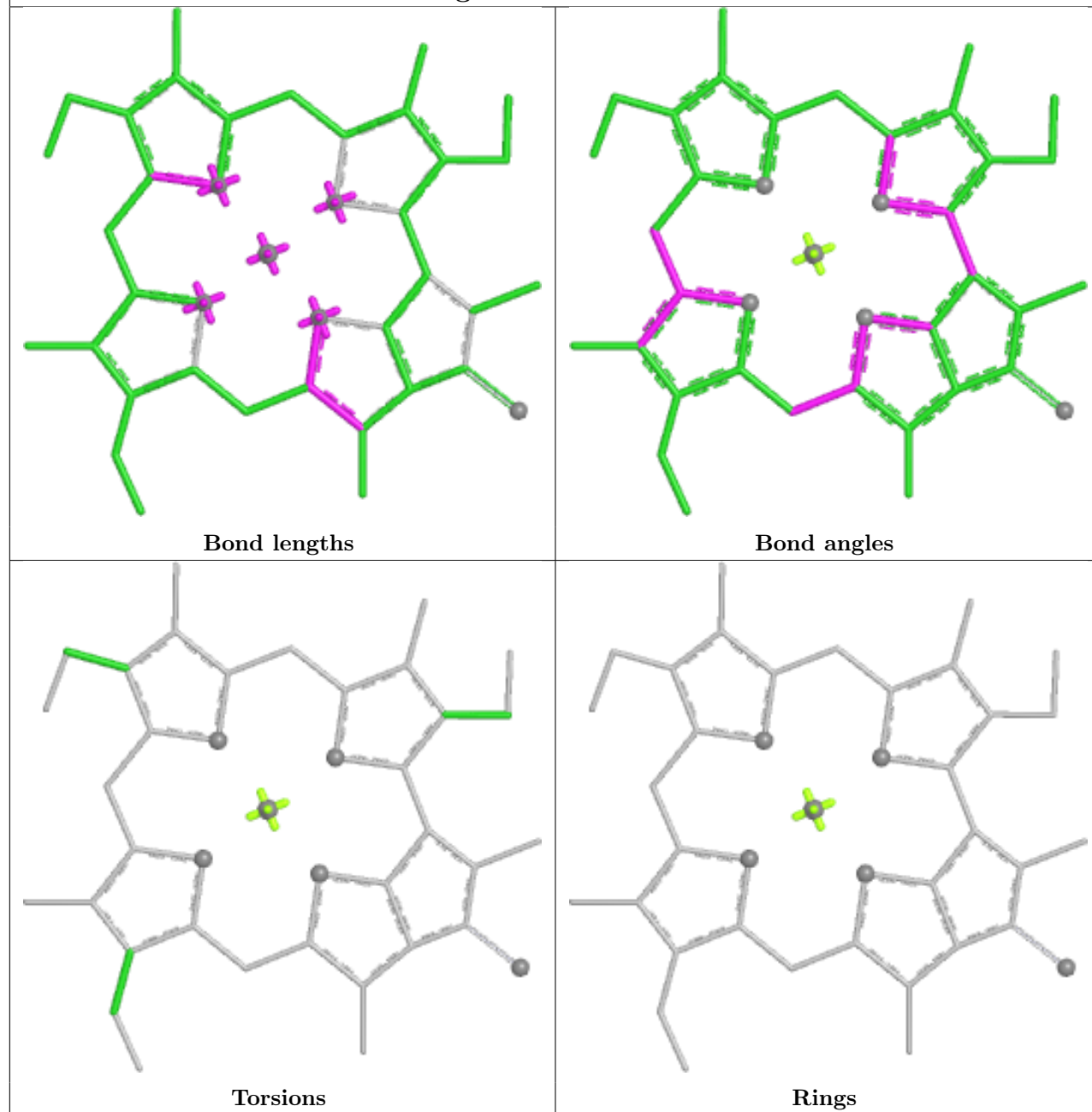
Ligand CLA A 817



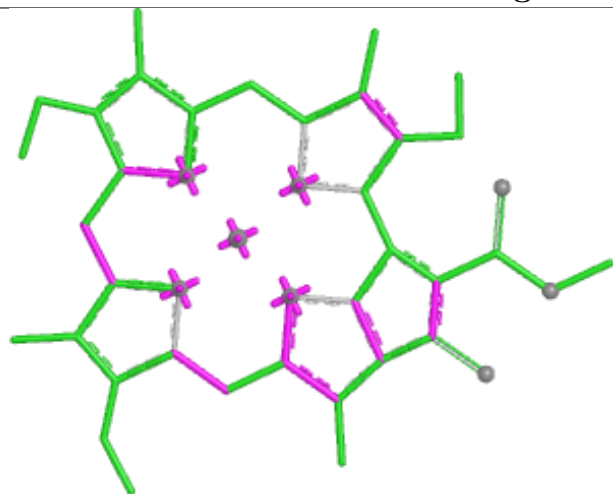
Ligand CLA A 816



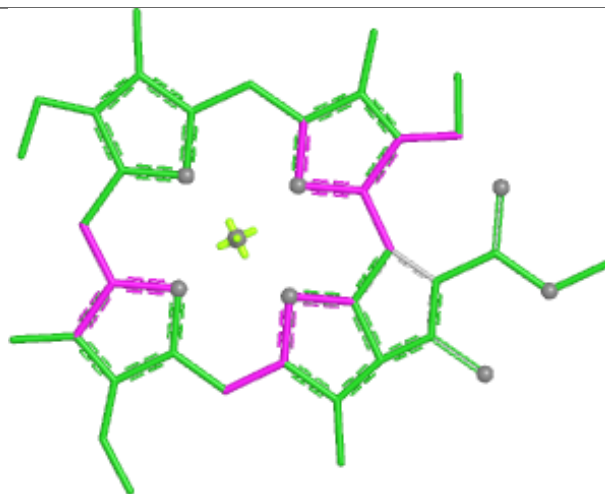
Ligand CLA B 814



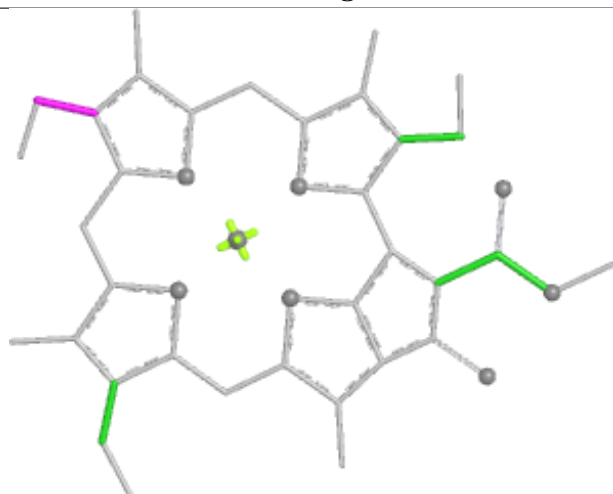
Ligand CLA A 839



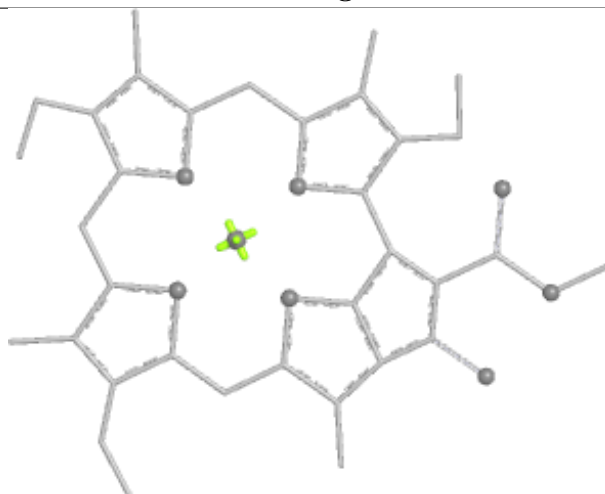
Bond lengths



Bond angles

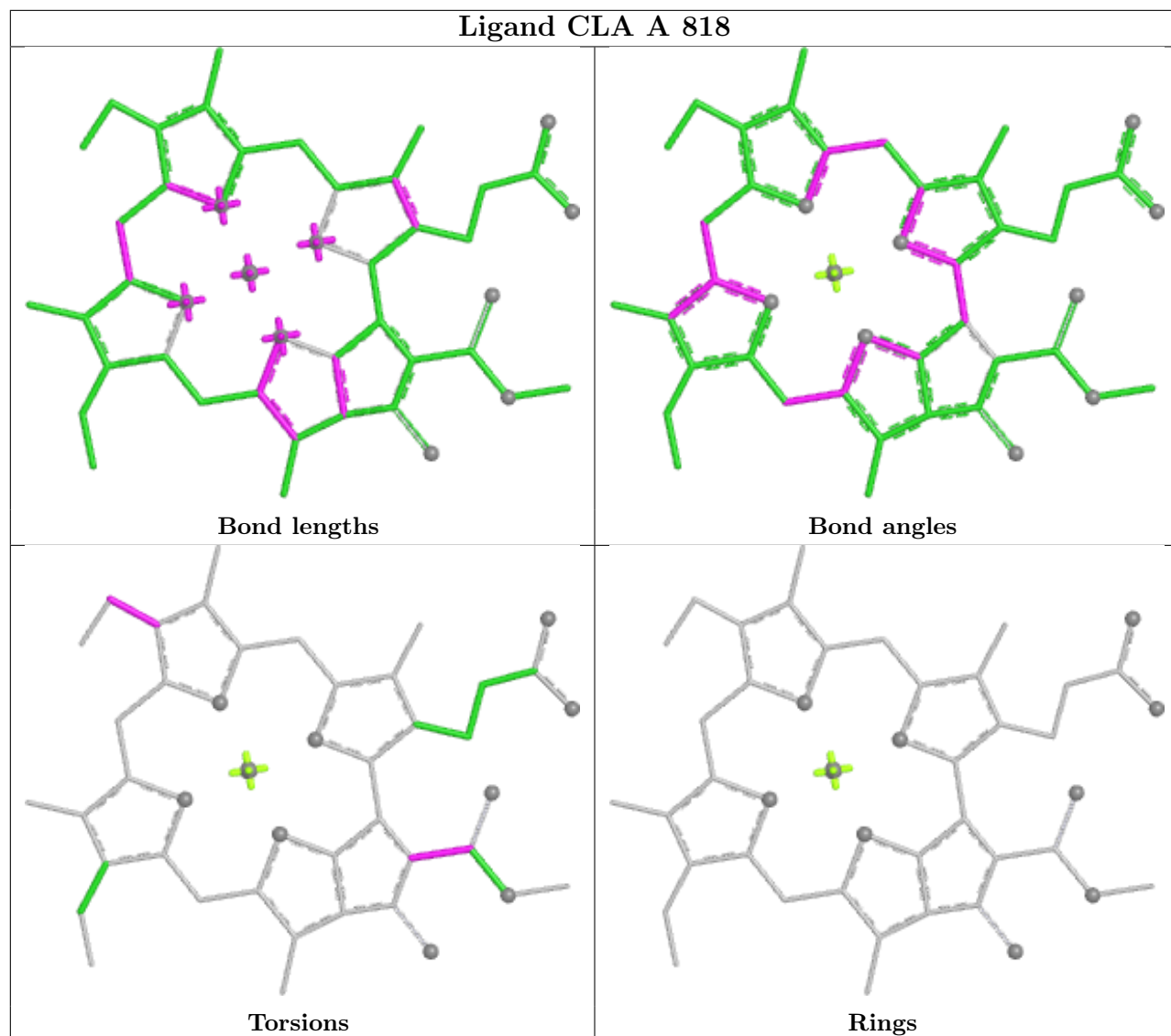


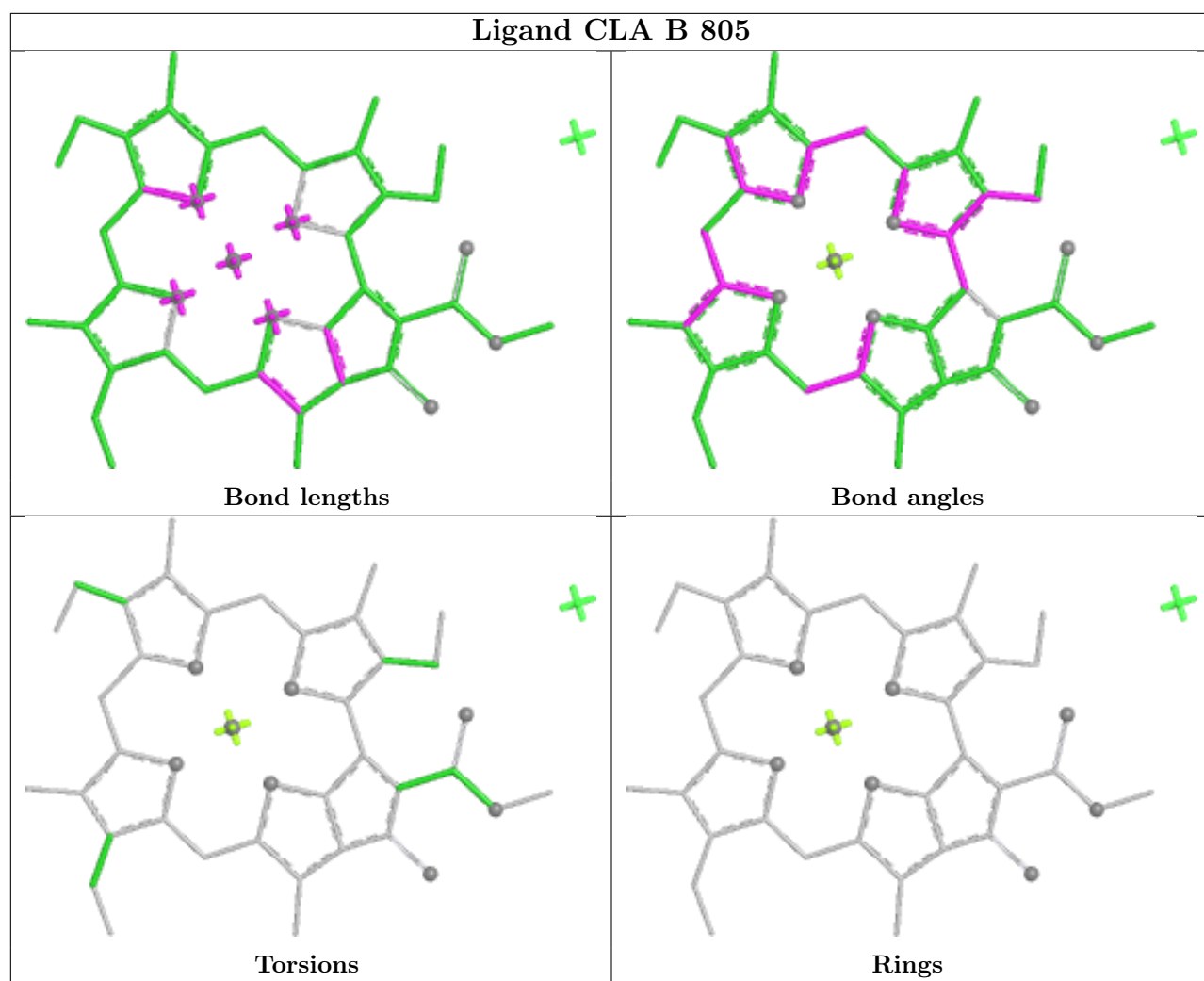
Torsions



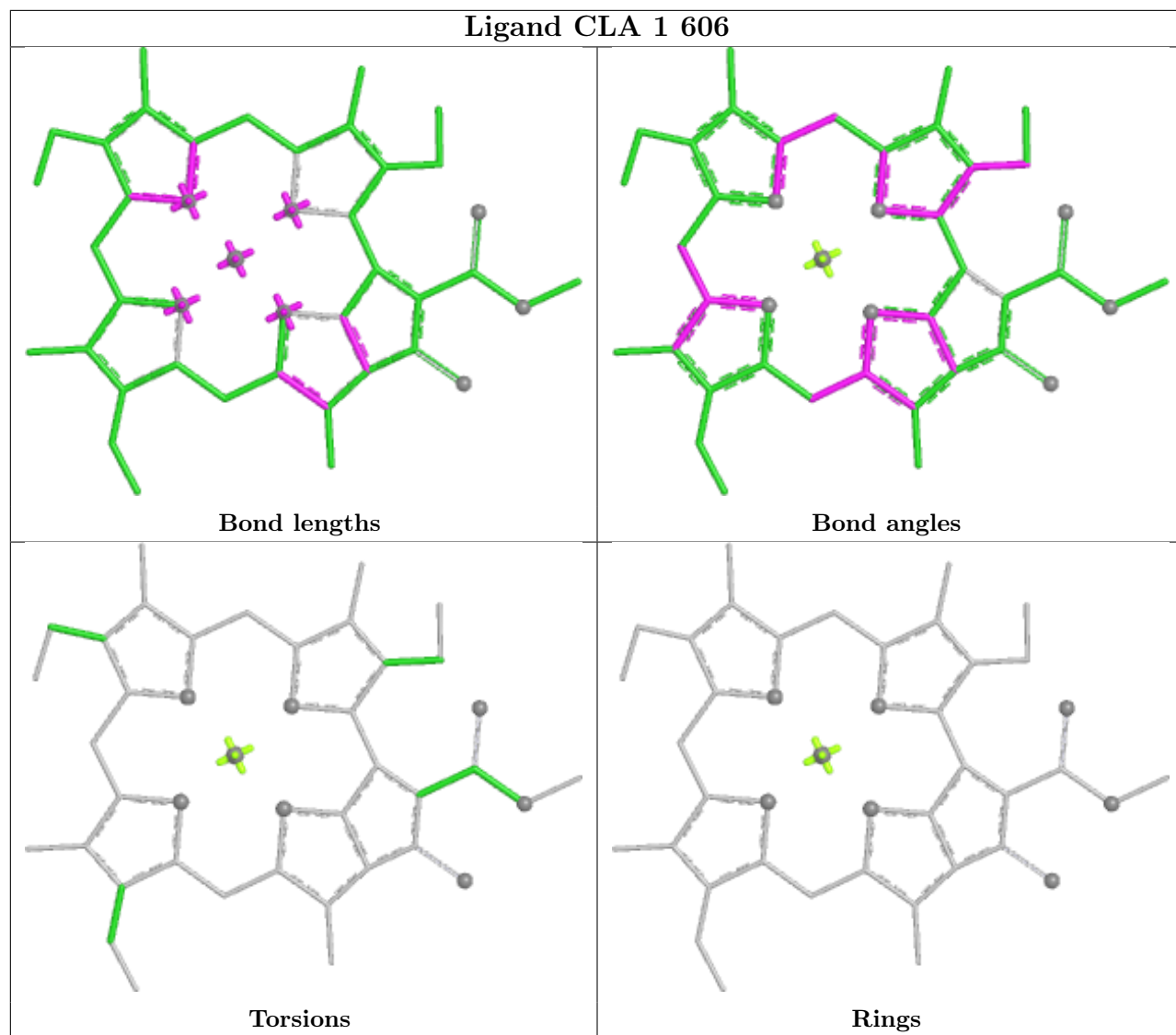
Rings

Ligand CLA A 818

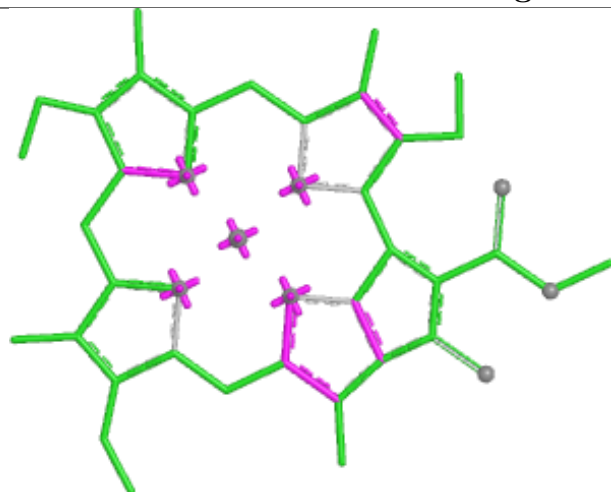




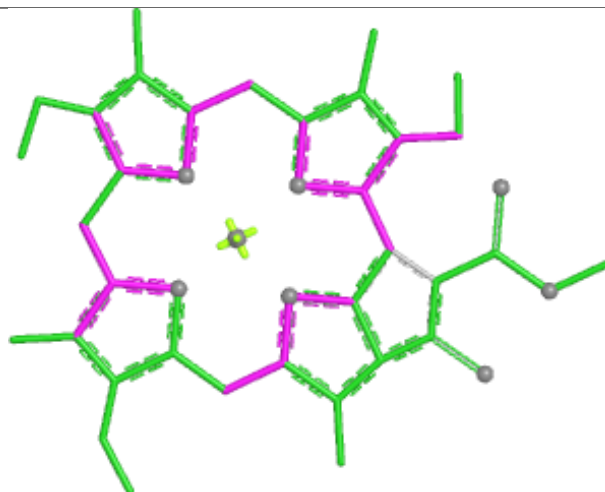
Ligand CLA 1 606



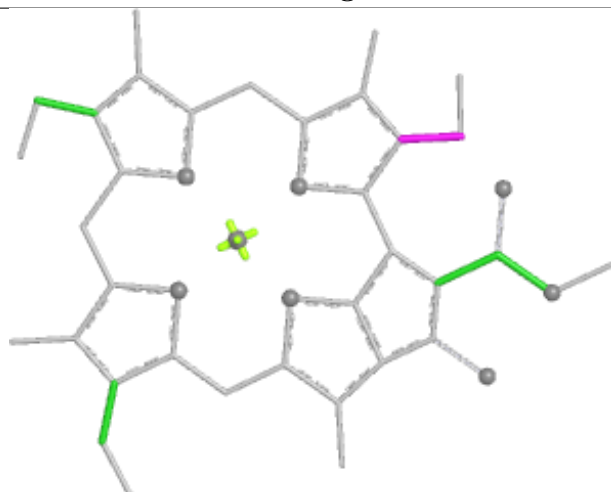
Ligand CLA B 822



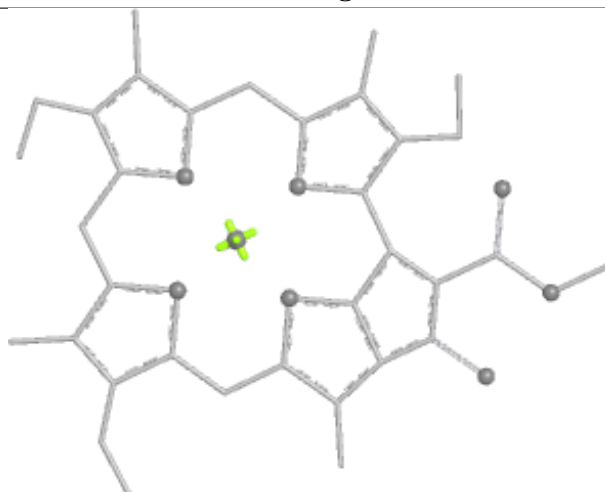
Bond lengths



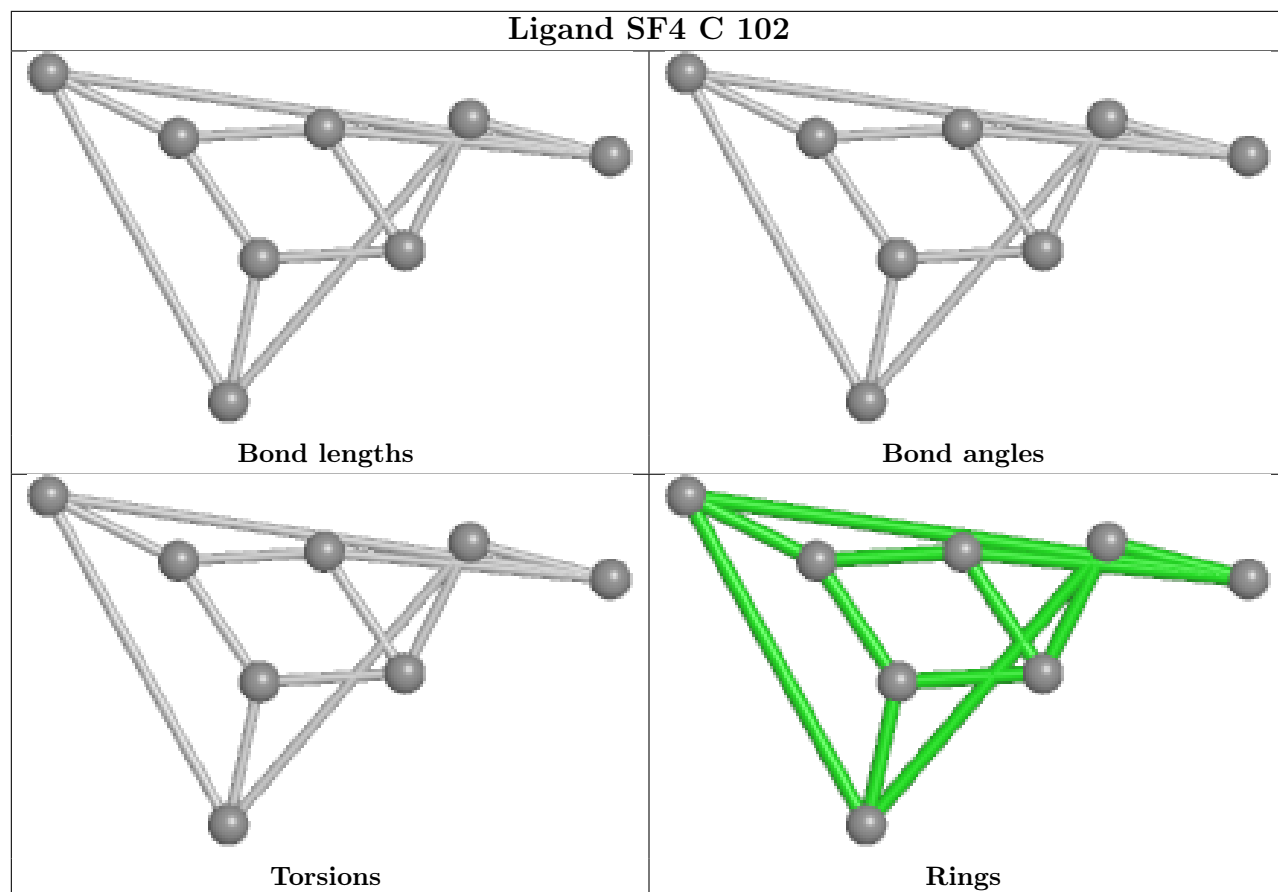
Bond angles



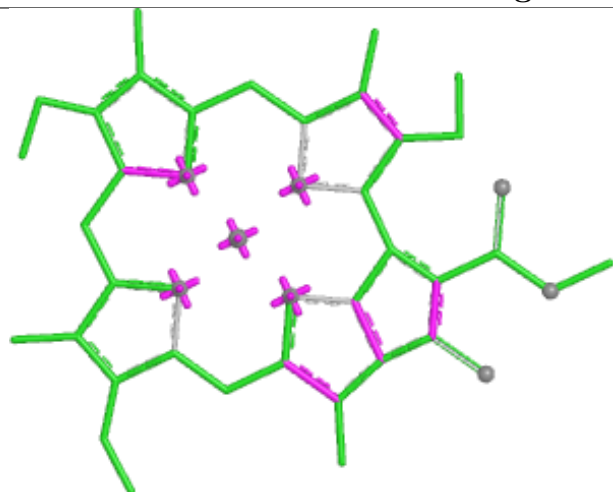
Torsions



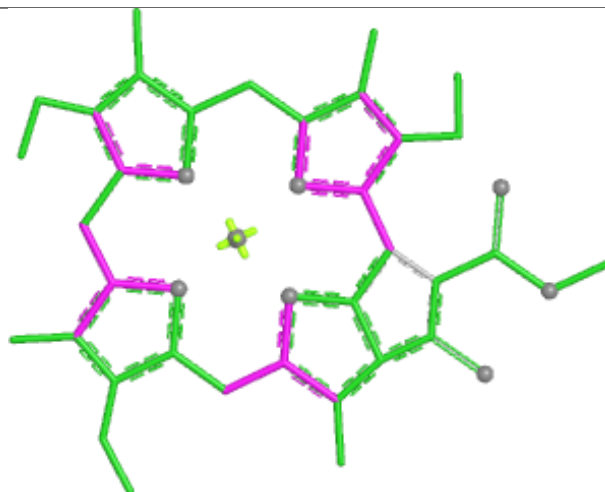
Rings



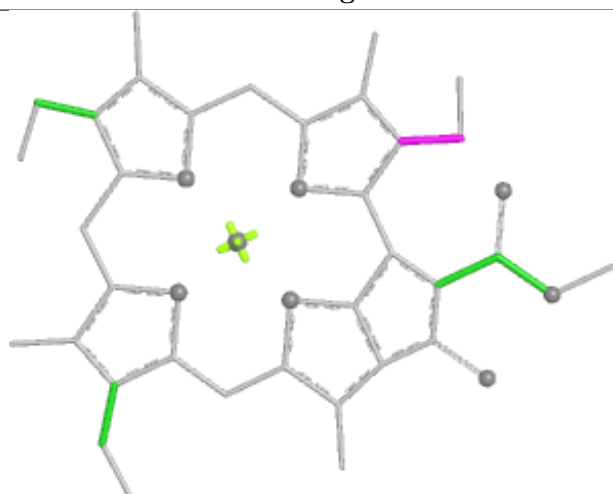
Ligand CLA B 804



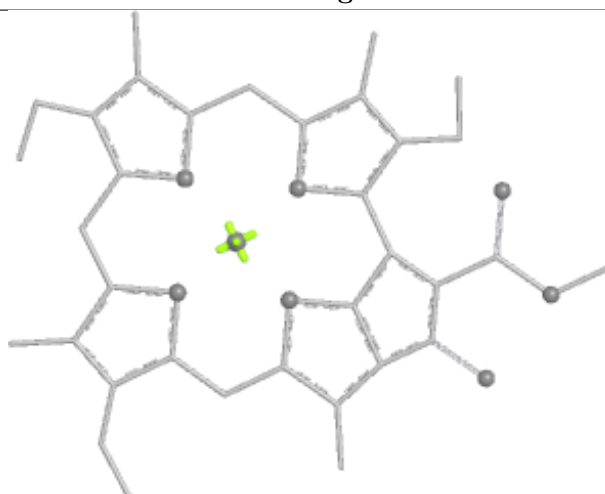
Bond lengths



Bond angles

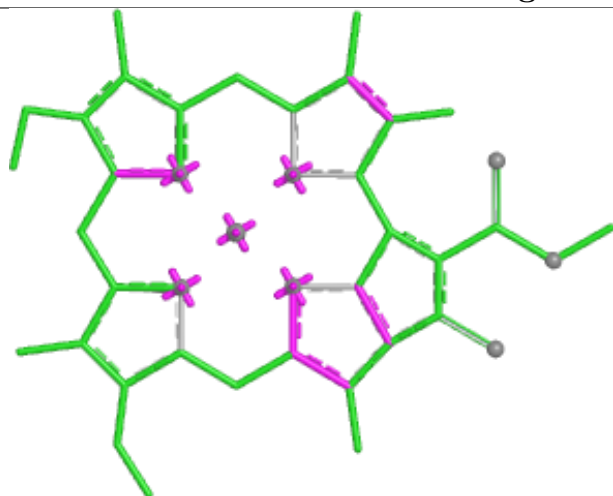


Torsions

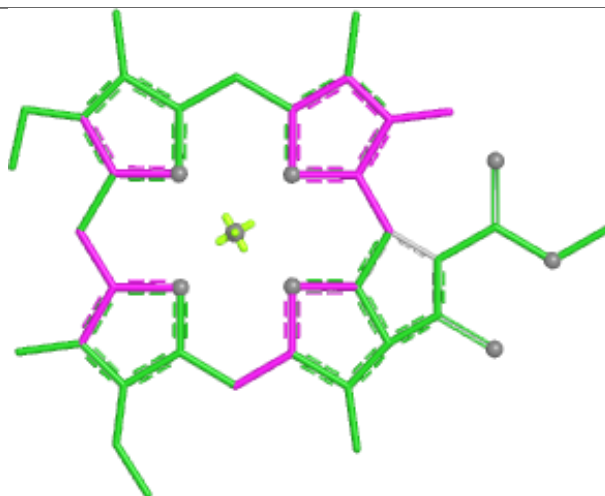


Rings

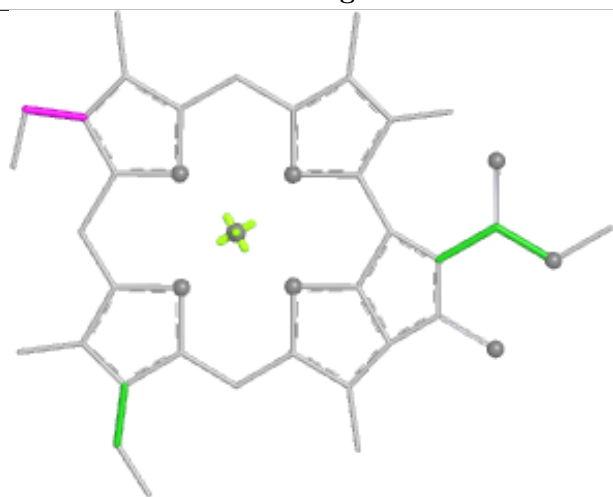
Ligand CLA 7 610



Bond lengths



Bond angles

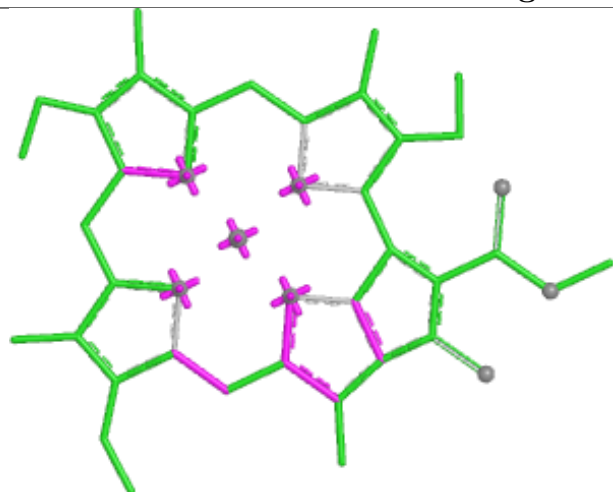


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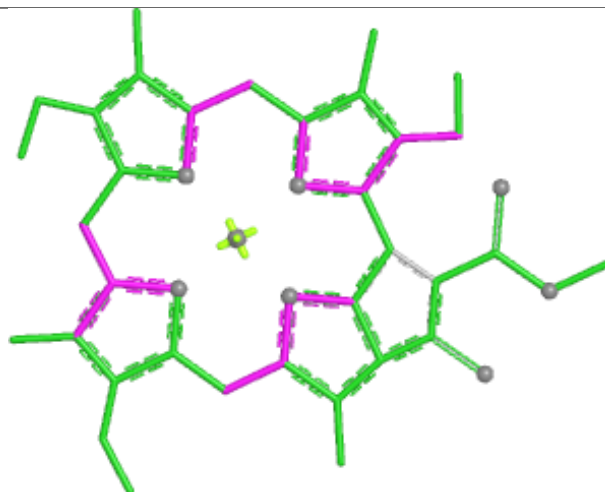


Rings

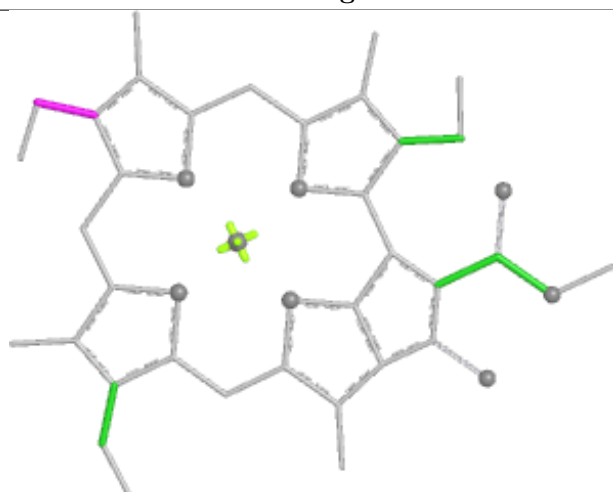
Ligand CLA 5 311



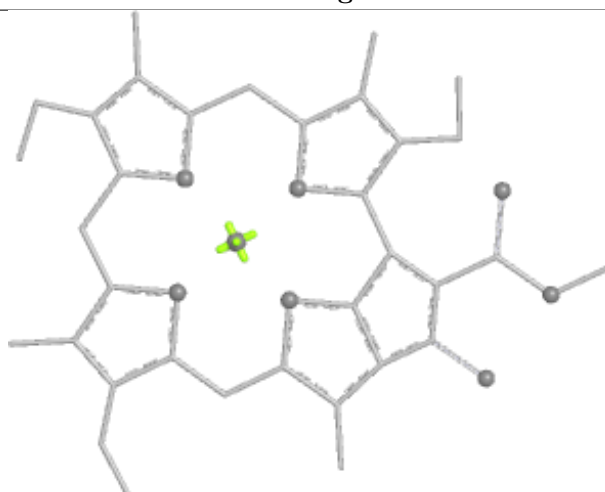
Bond lengths



Bond angles

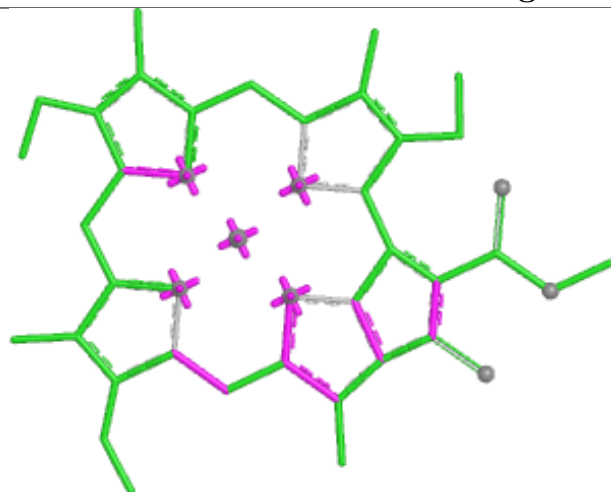


Torsions

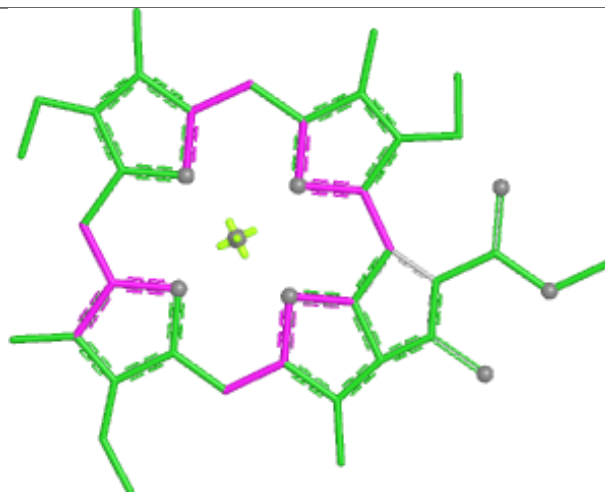


Rings

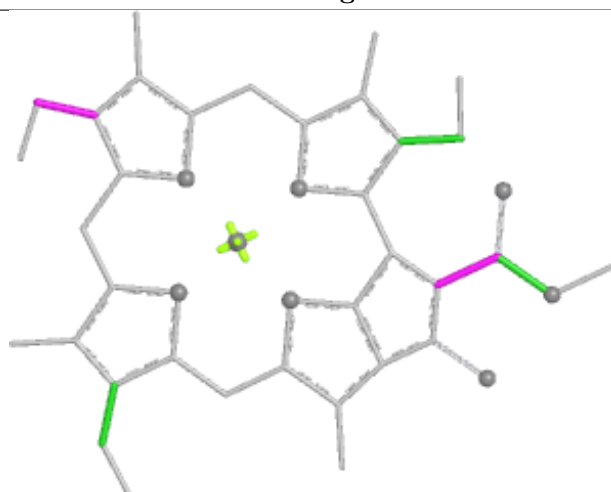
Ligand CLA 5 304



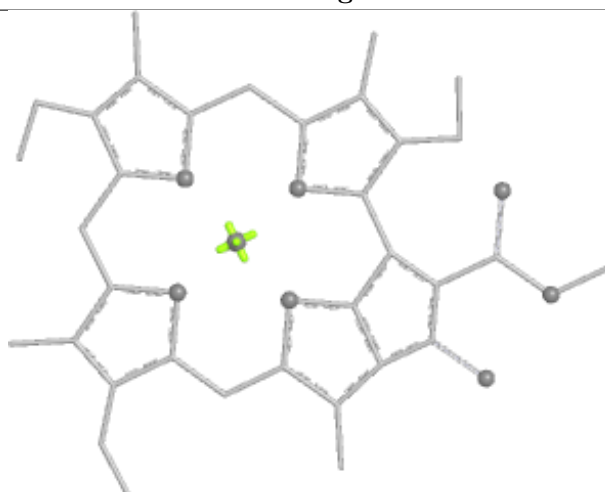
Bond lengths



Bond angles

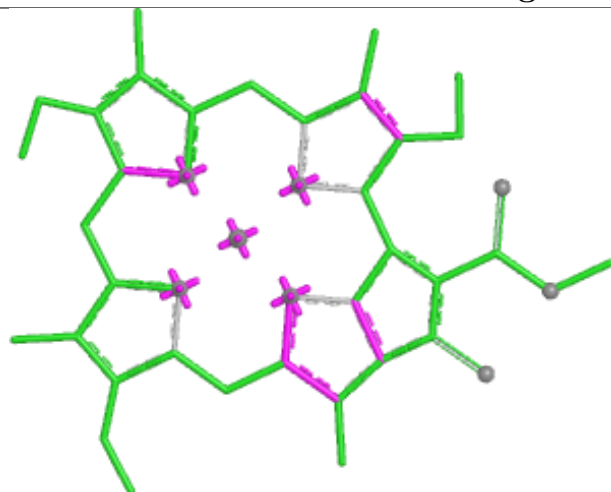


Torsions

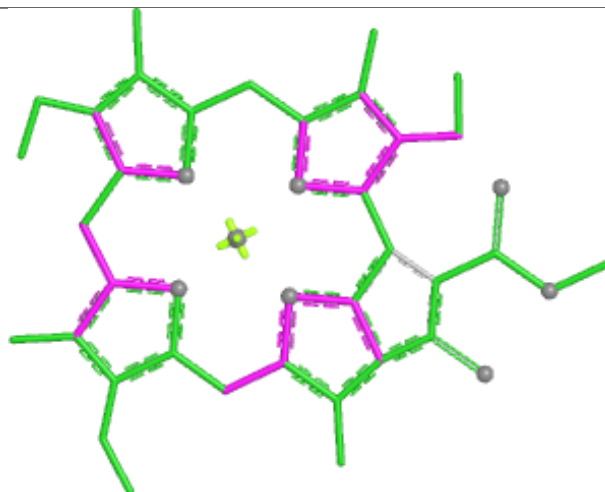


Rings

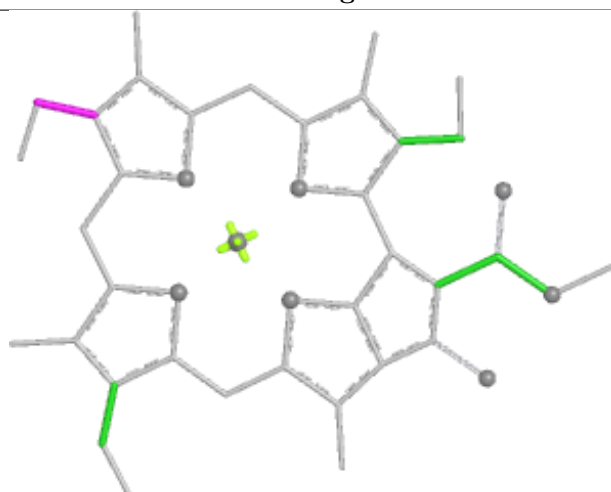
Ligand CLA 7 603



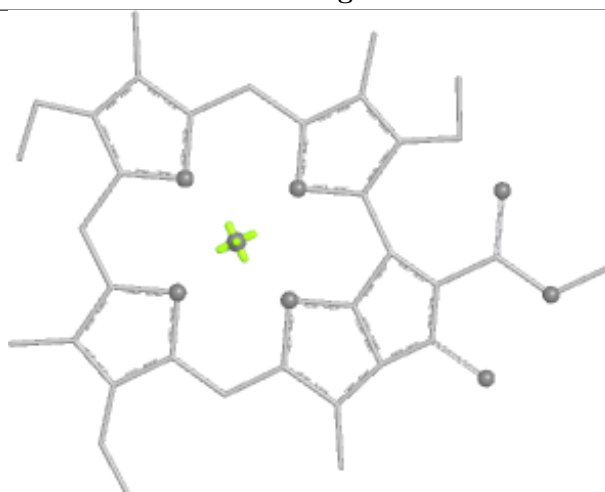
Bond lengths



Bond angles

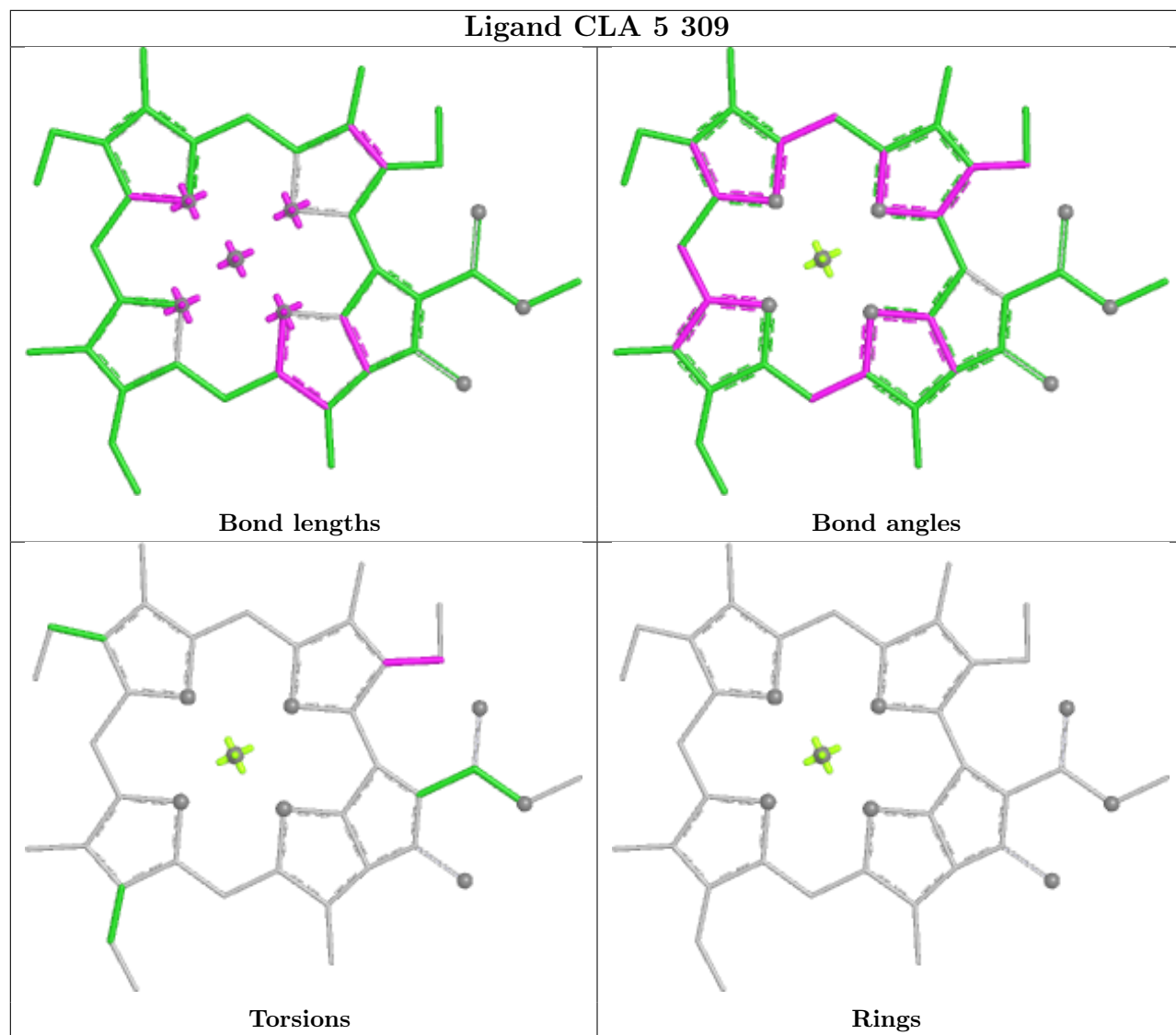


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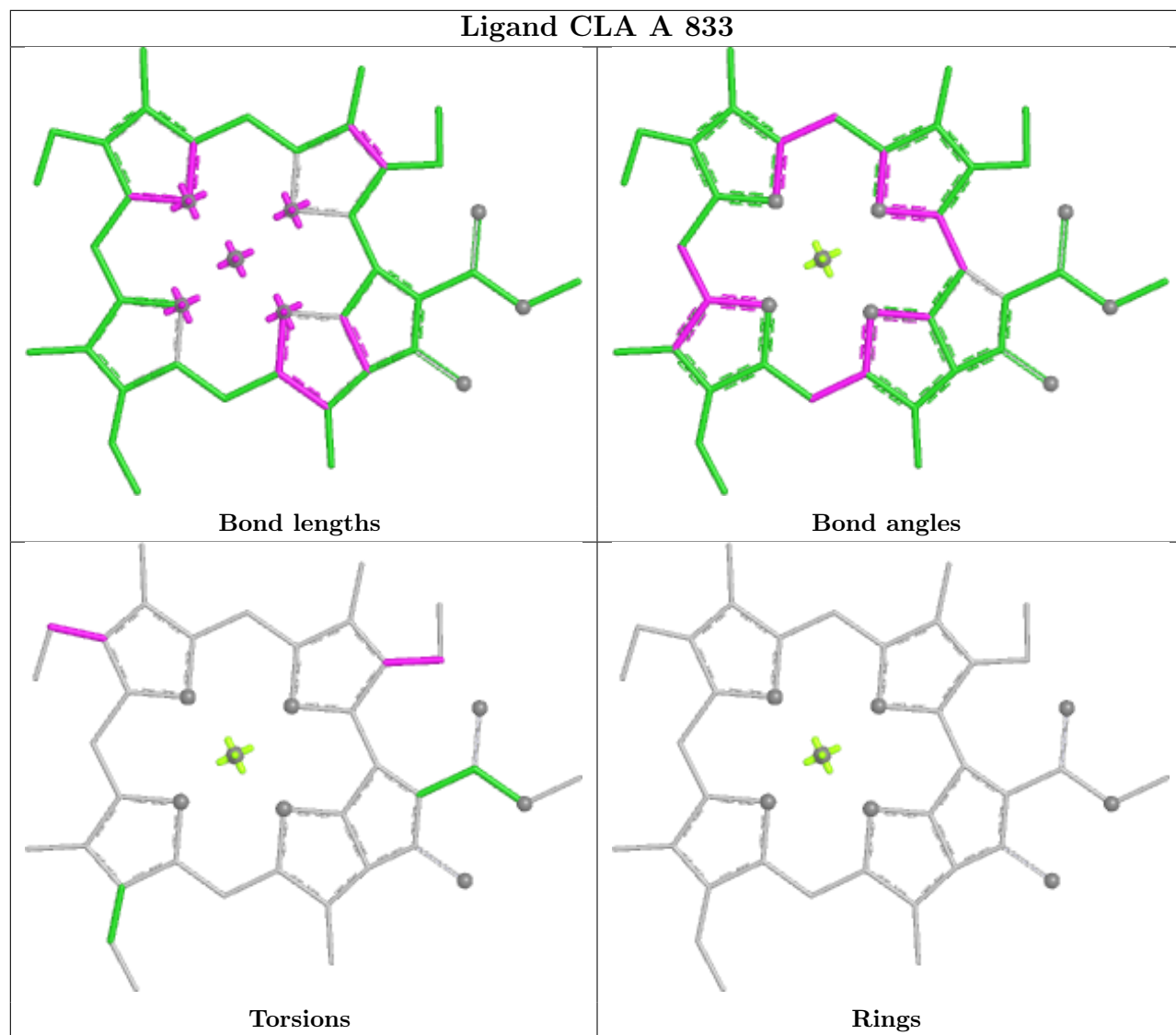


Rings

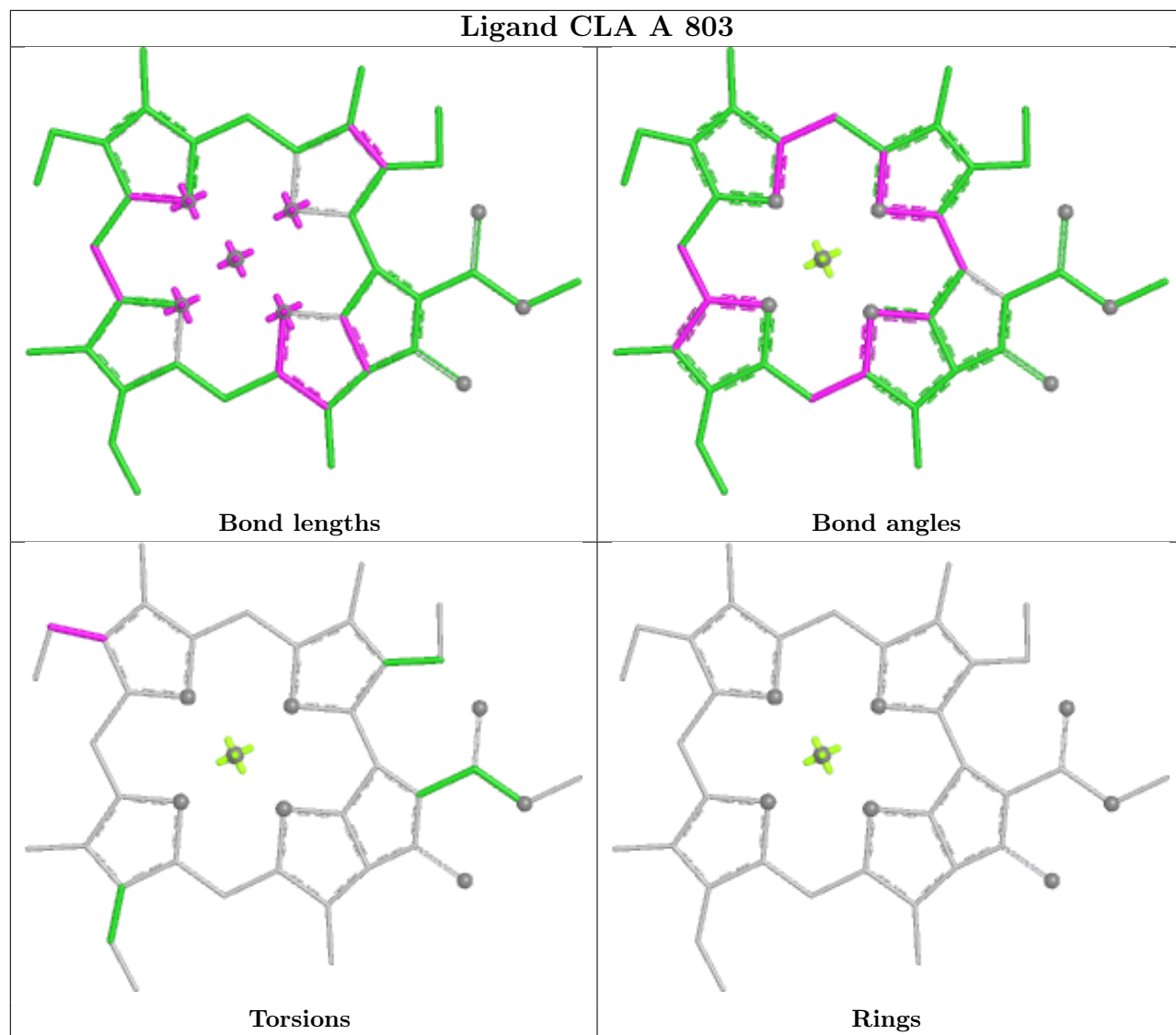
Ligand CLA 5 309



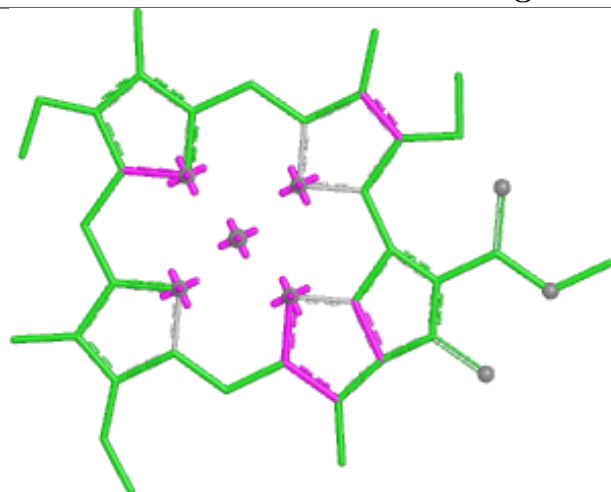
Ligand CLA A 833



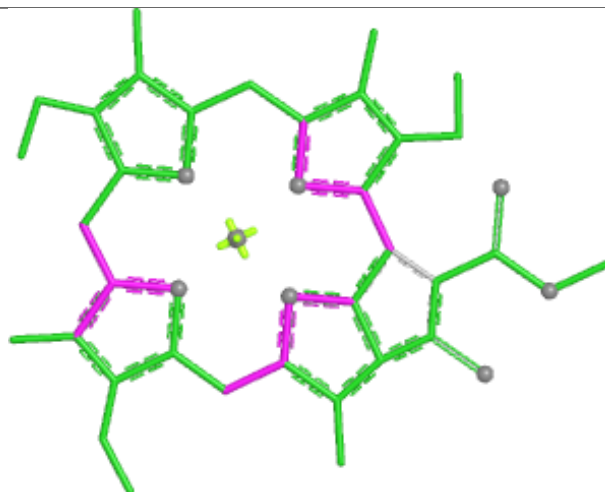
Ligand CLA A 803



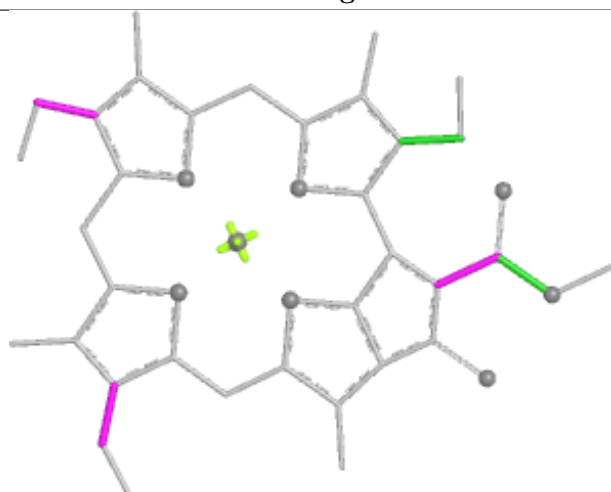
Ligand CLA B 834



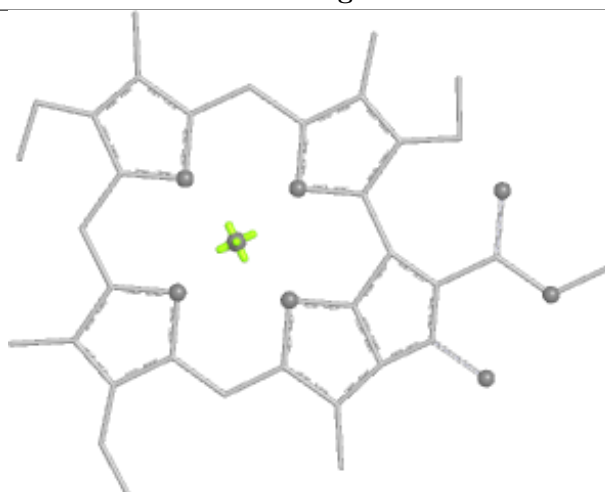
Bond lengths



Bond angles

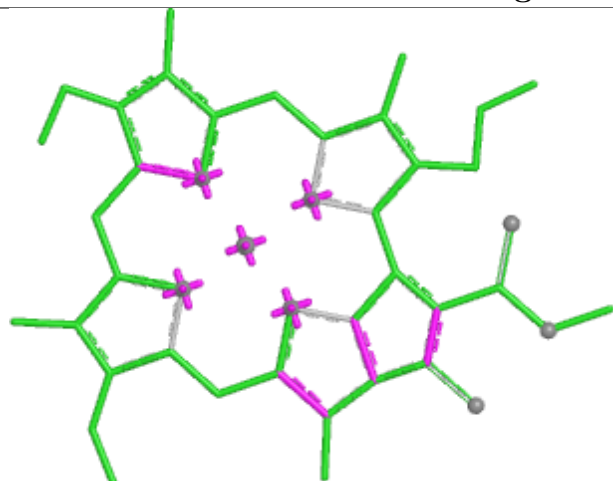


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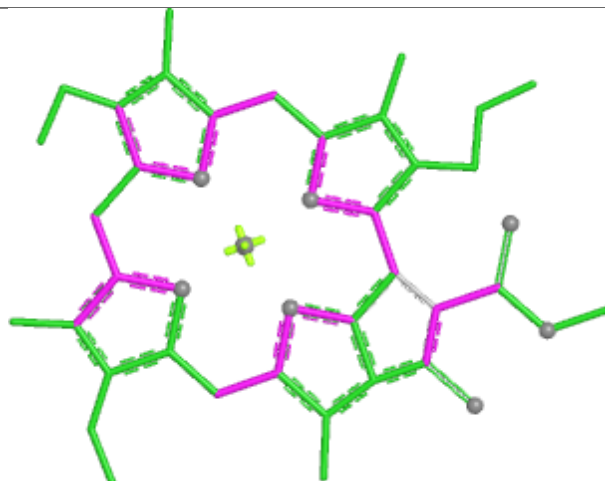


Rings

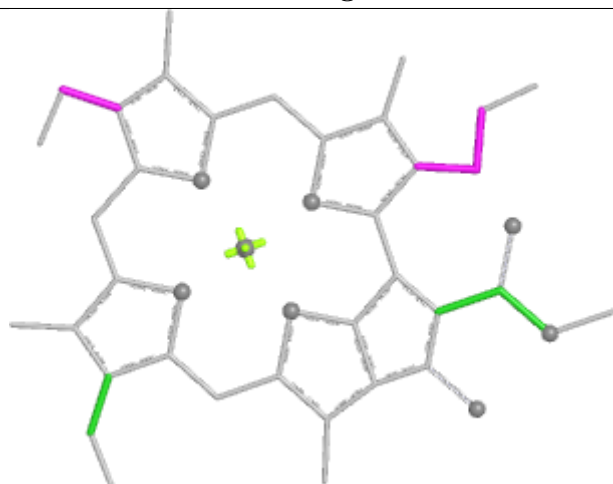
Ligand CLA B 829



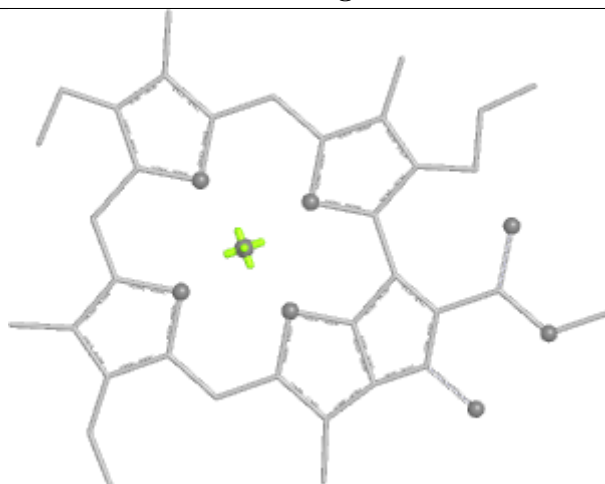
Bond lengths



Bond angles

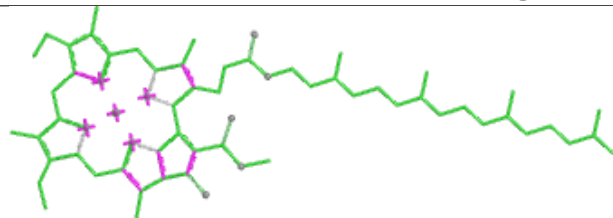


Torsions

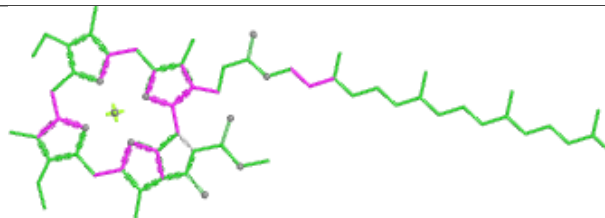


Rings

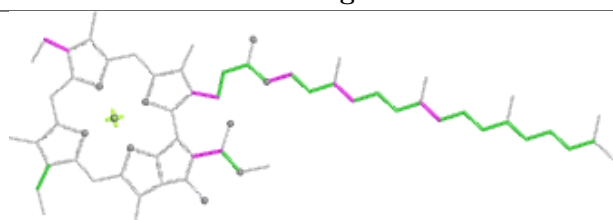
Ligand CLA B 815



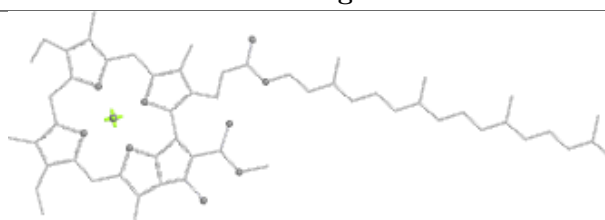
Bond lengths



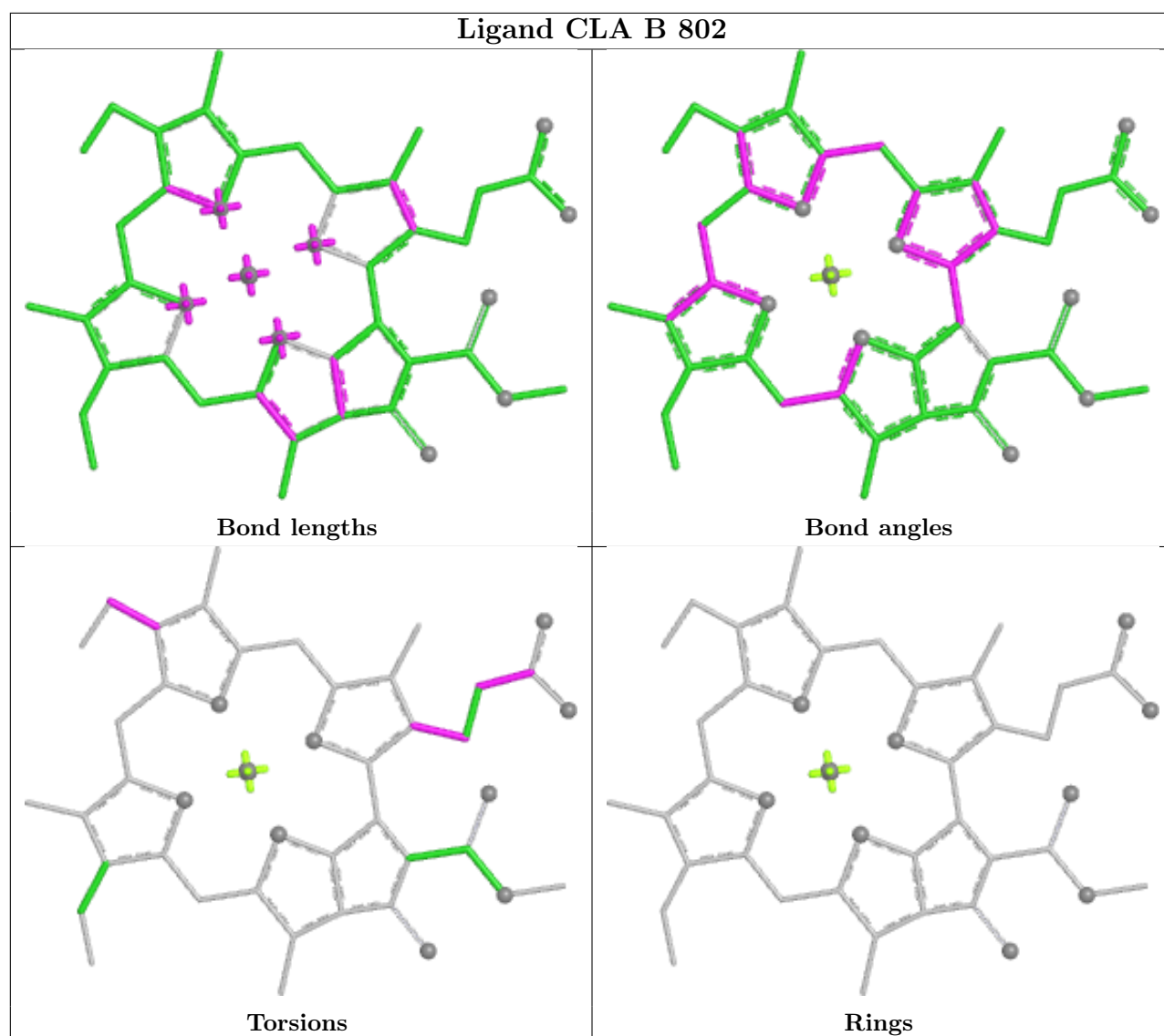
Bond angles



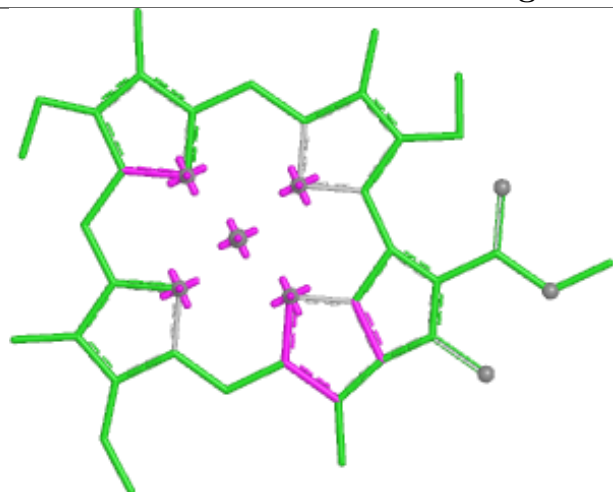
Torsions



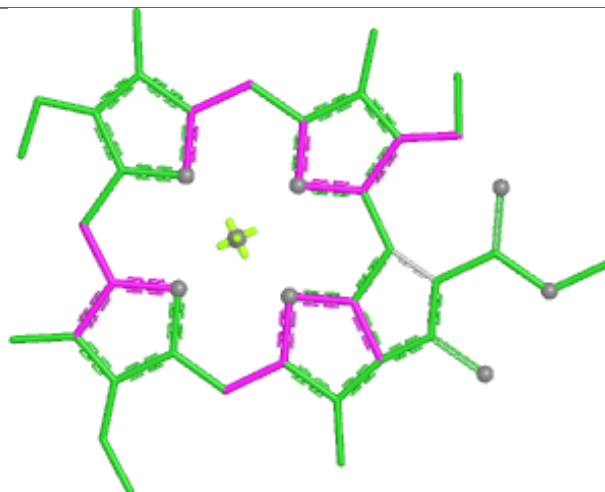
Rings



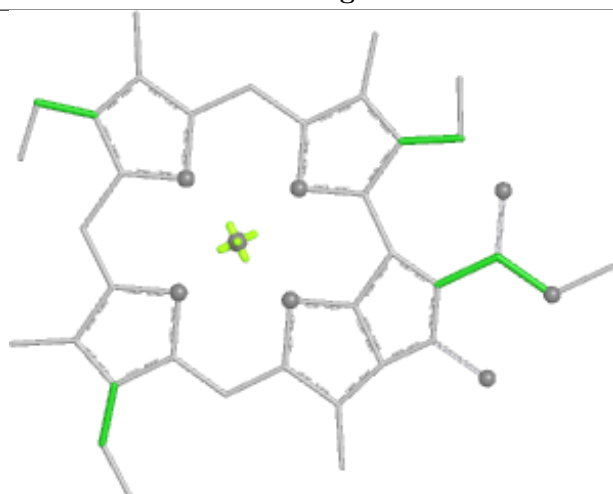
Ligand CLA 7 608



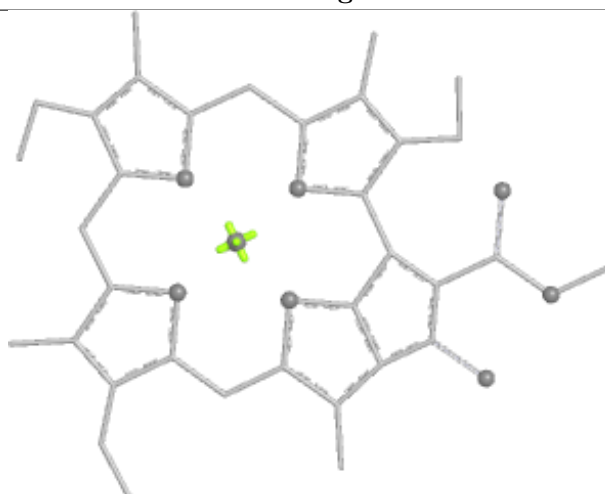
Bond lengths



Bond angles

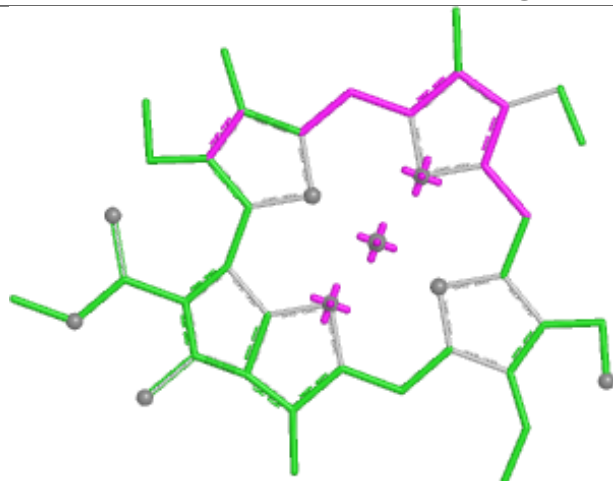


Torsions

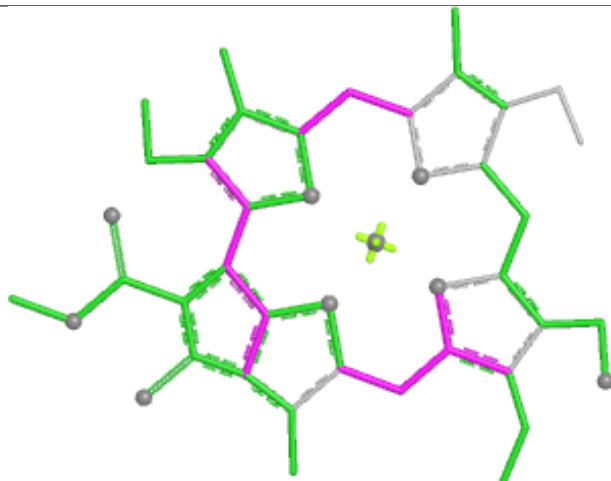


Rings

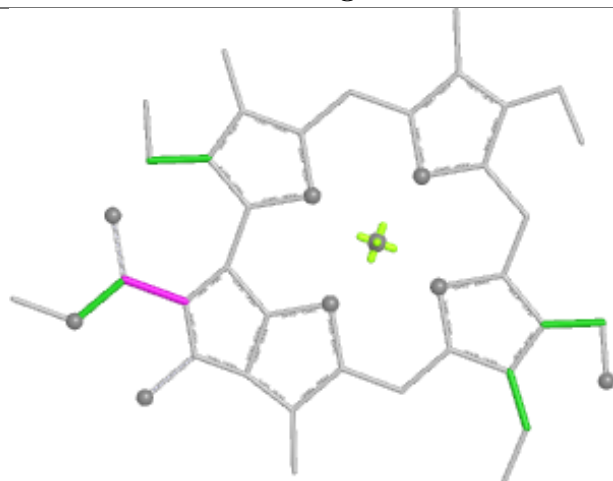
Ligand CHL Z 601



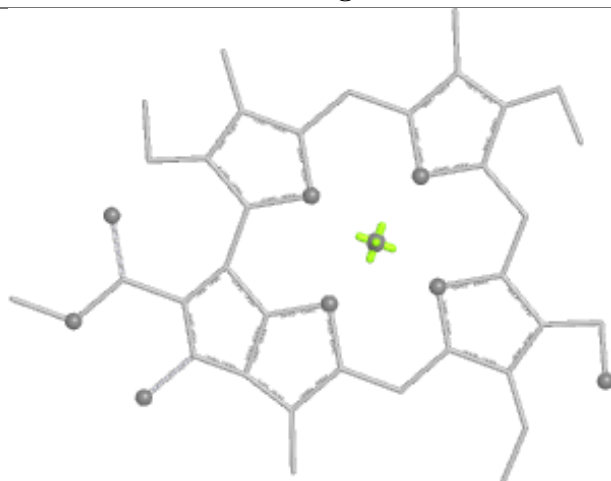
Bond lengths



Bond angles

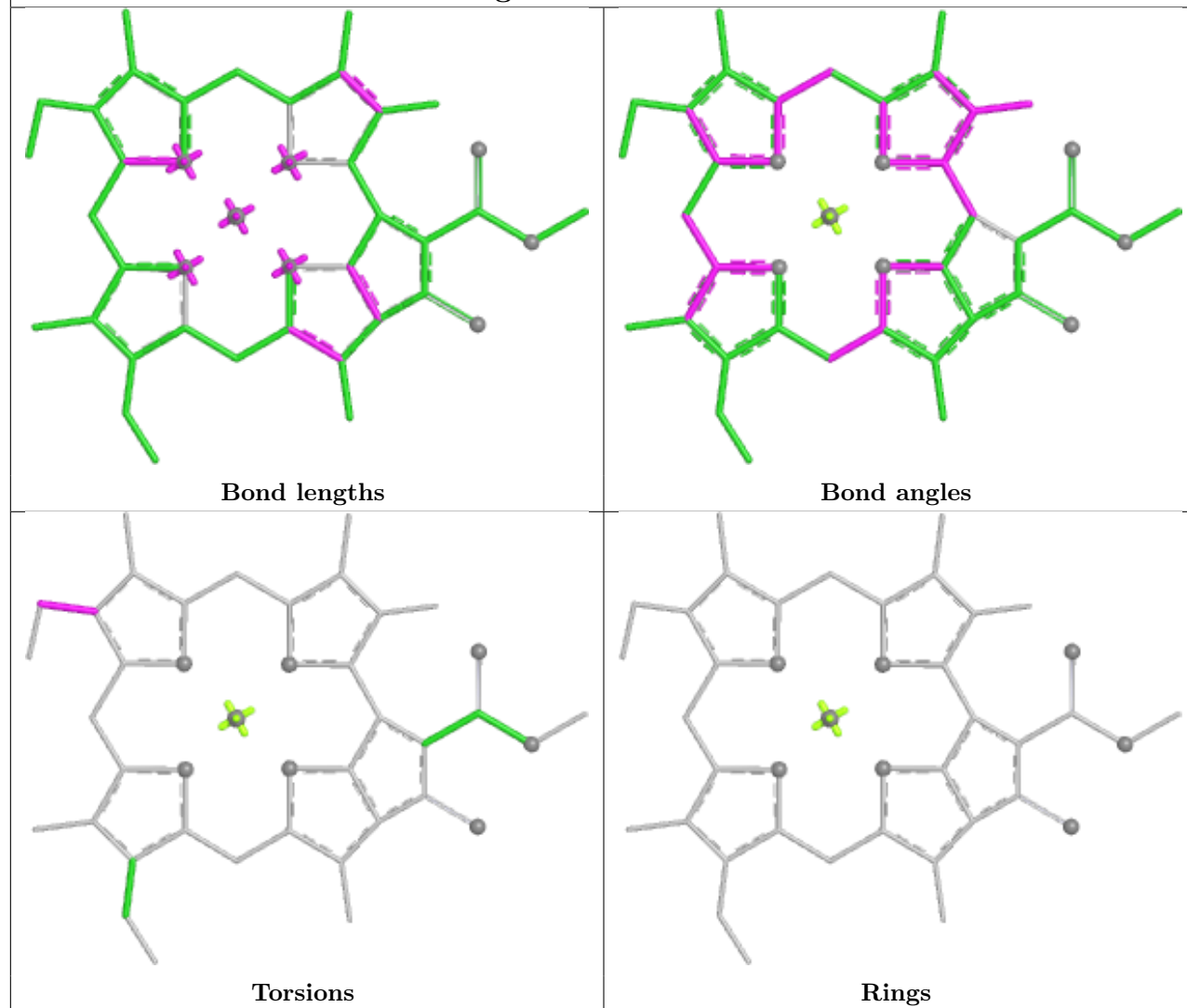


Torsions

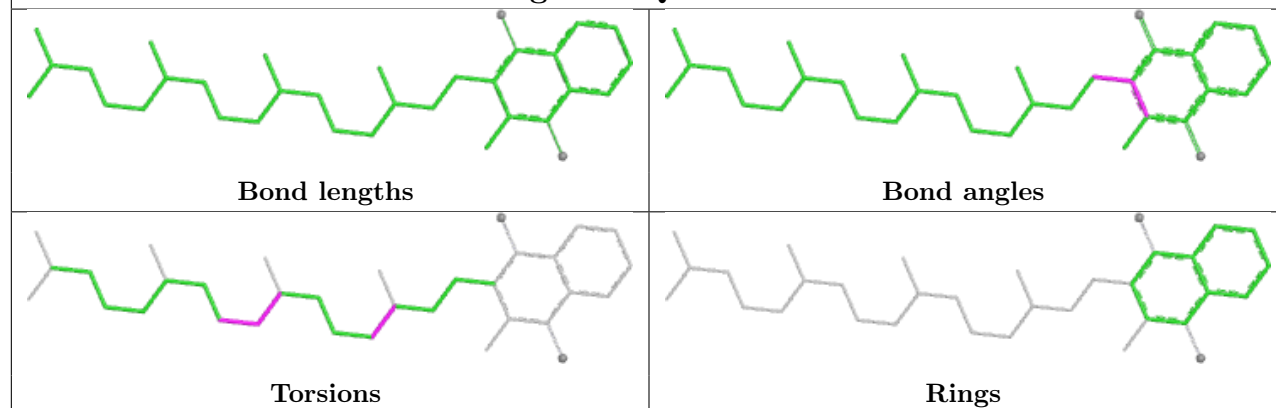


Rings

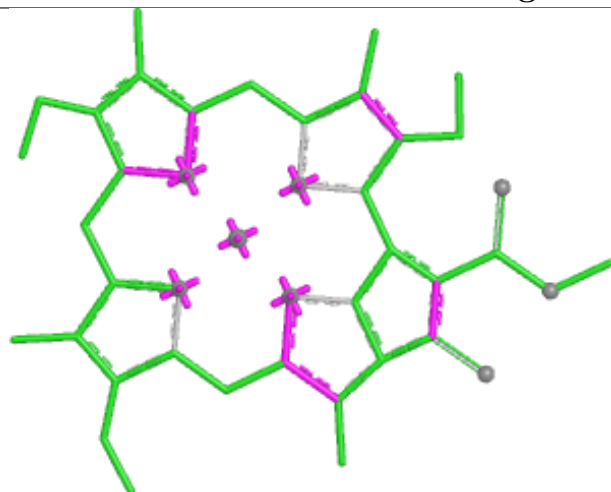
Ligand CLA B 824



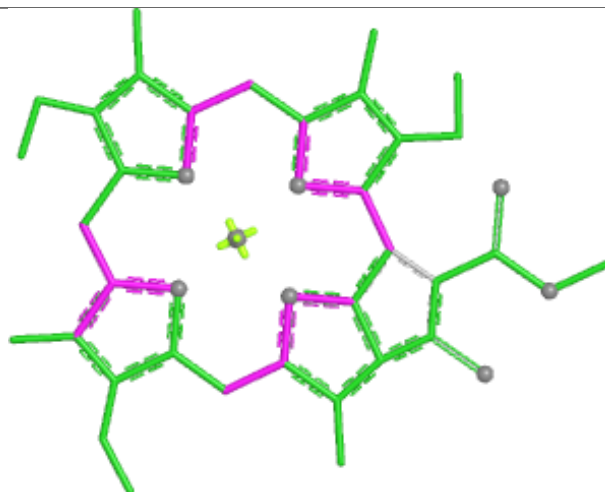
Ligand PQN B 840



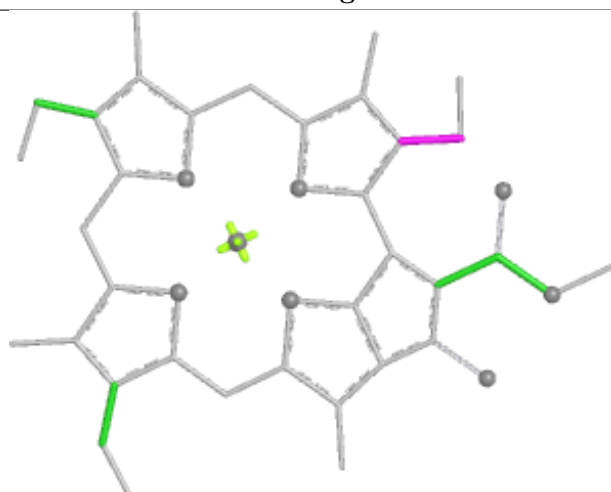
Ligand CLA 1 608



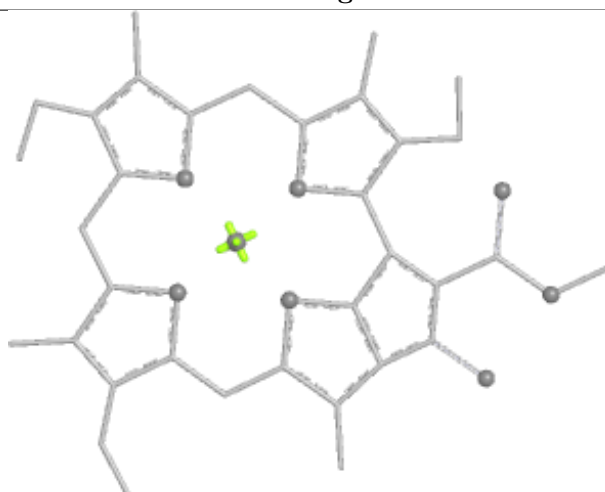
Bond lengths



Bond angles

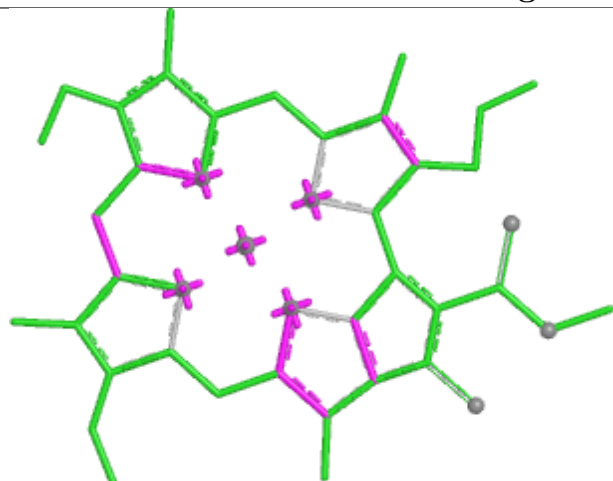


Torsions

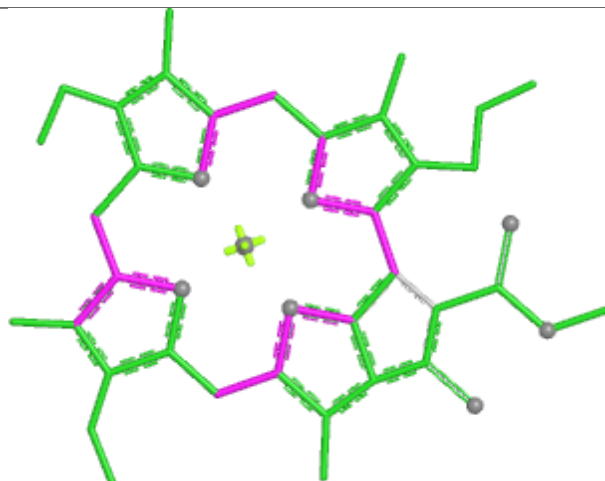


Rings

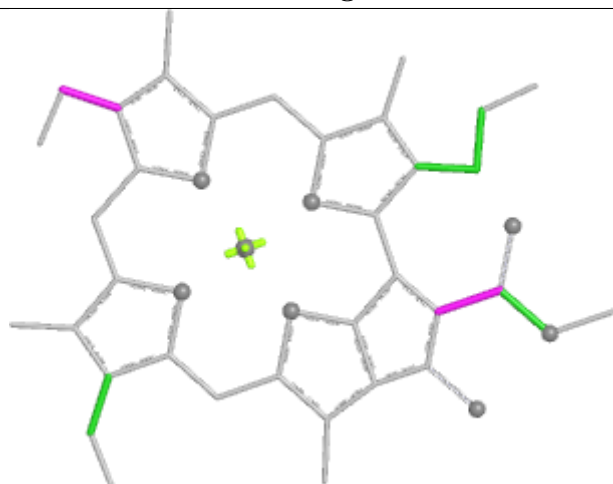
Ligand CLA 7 613



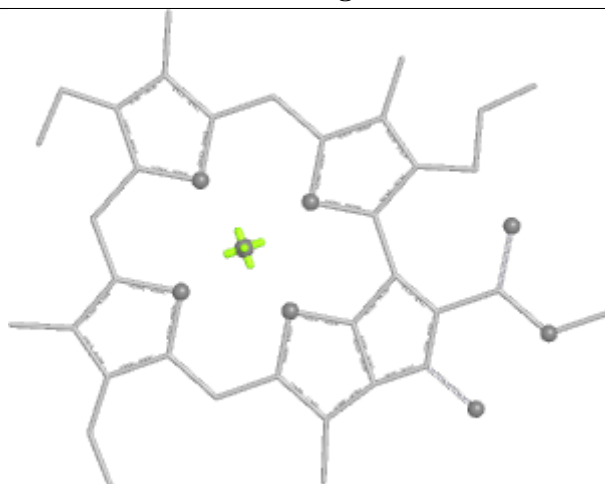
Bond lengths



Bond angles

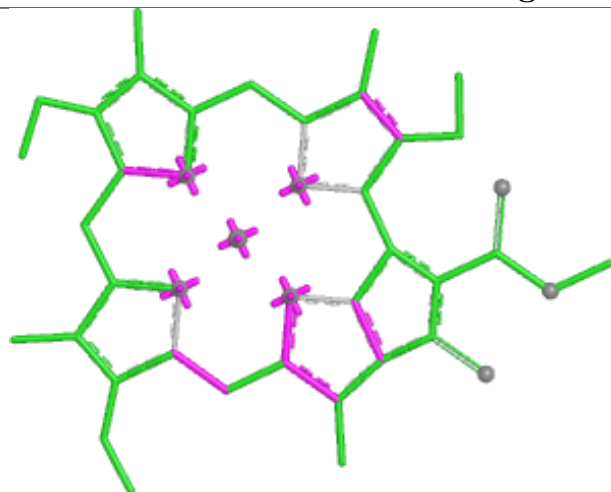


Torsions

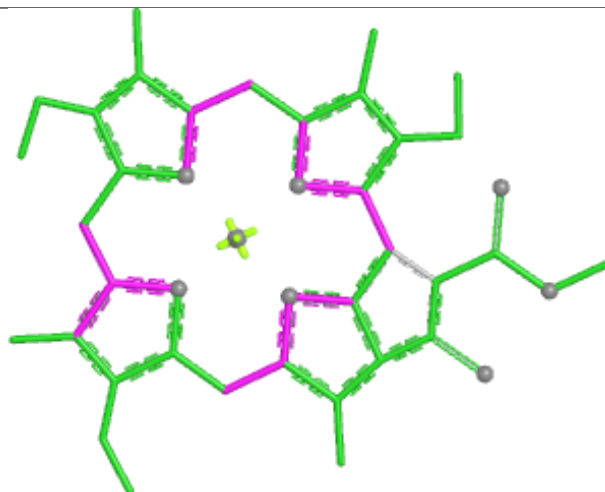


Rings

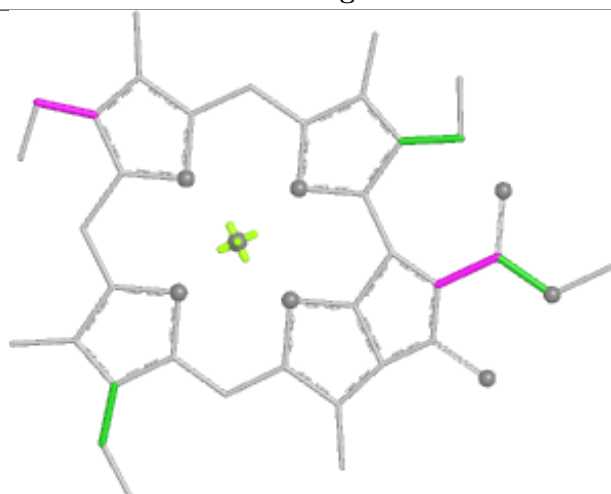
Ligand CLA 8 614



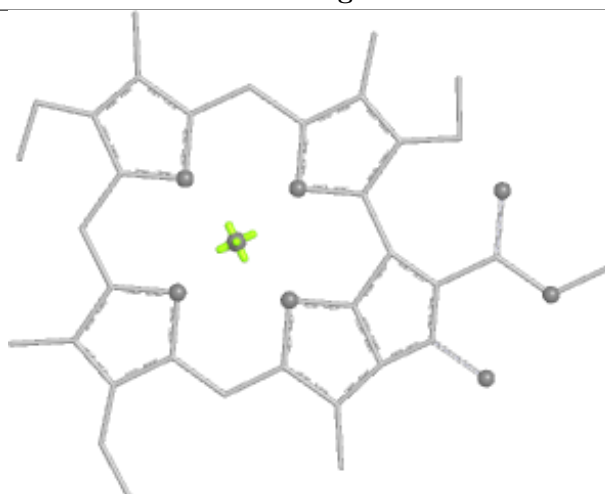
Bond lengths



Bond angles

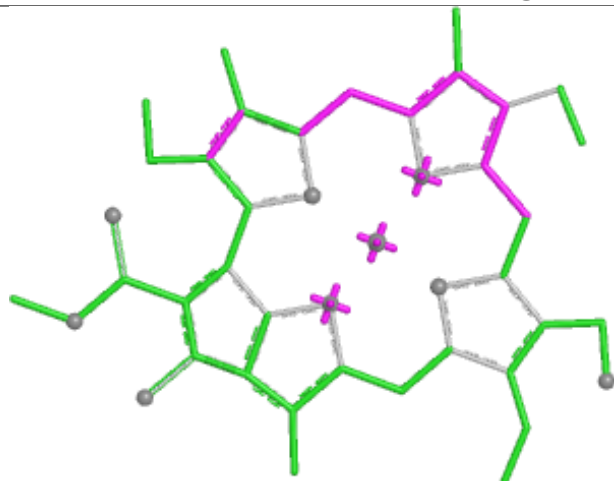


Torsions

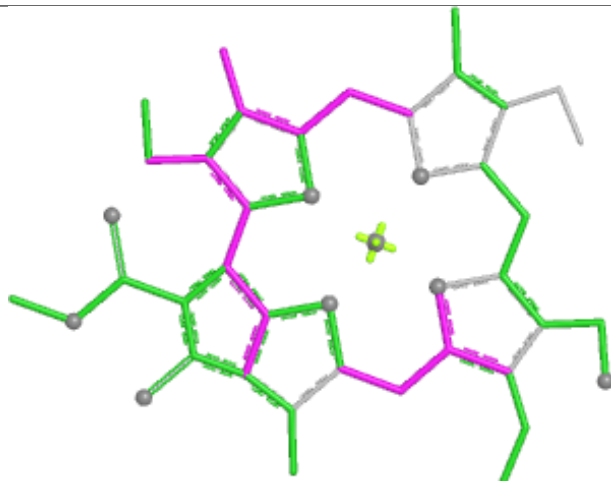


Rings

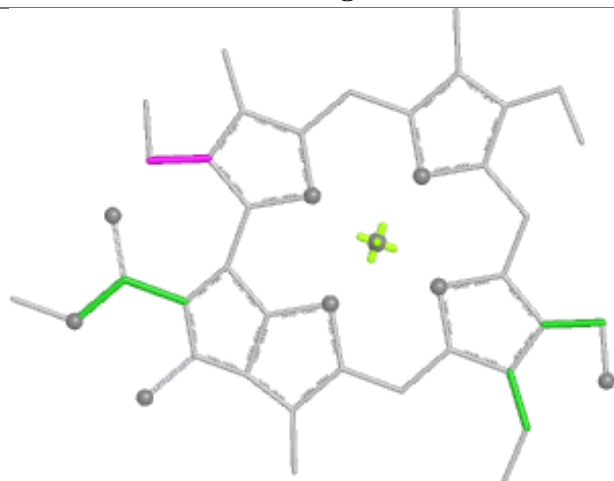
Ligand CHL 6 607



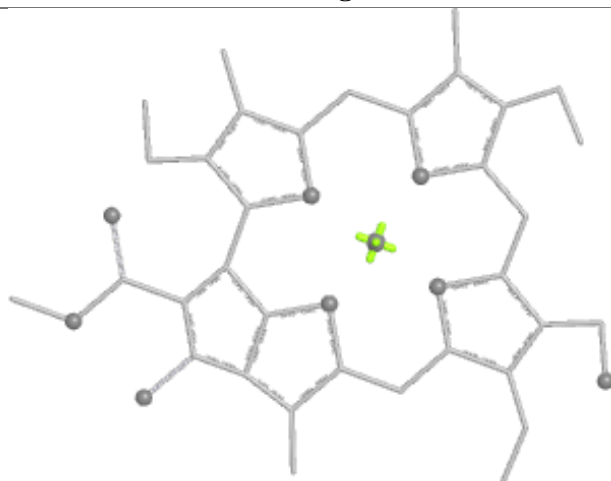
Bond lengths



Bond angles

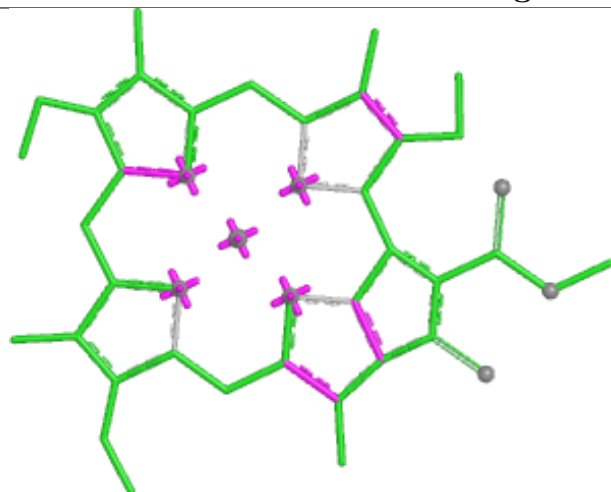


Torsions

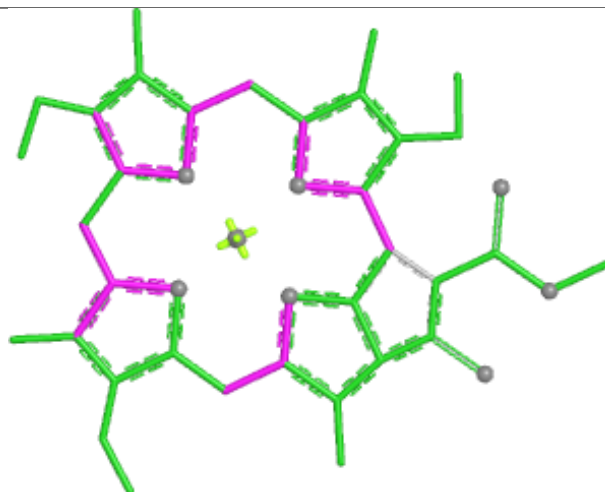


Rings

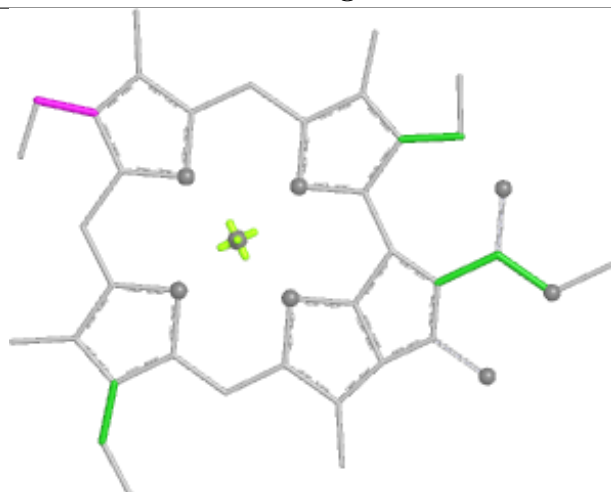
Ligand CLA A 826



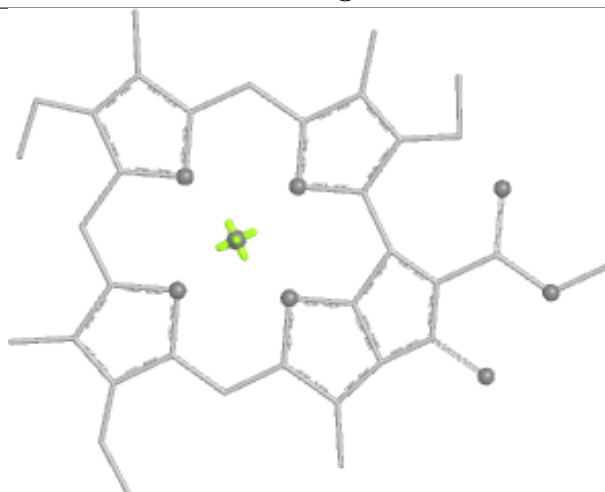
Bond lengths



Bond angles

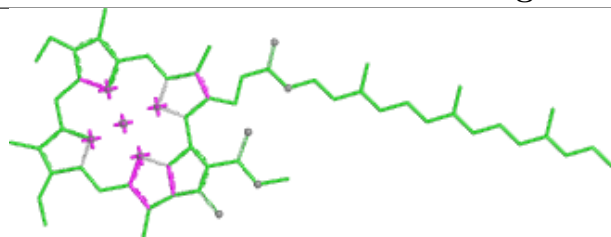


Torsions

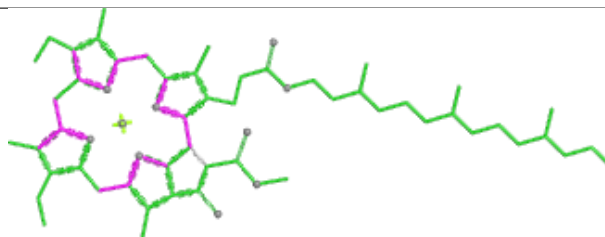


Rings

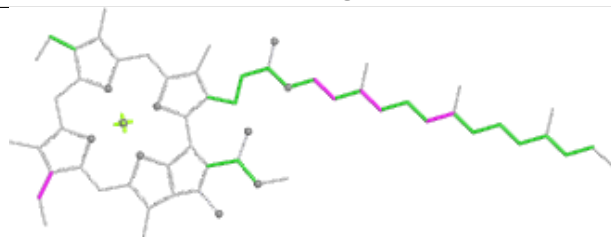
Ligand CLA F 302



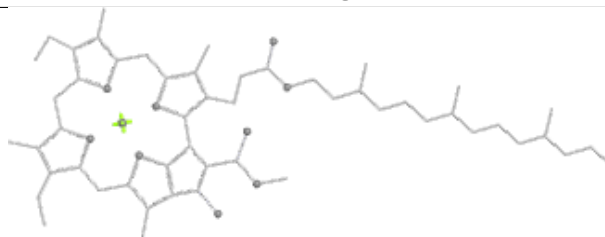
Bond lengths



Bond angles

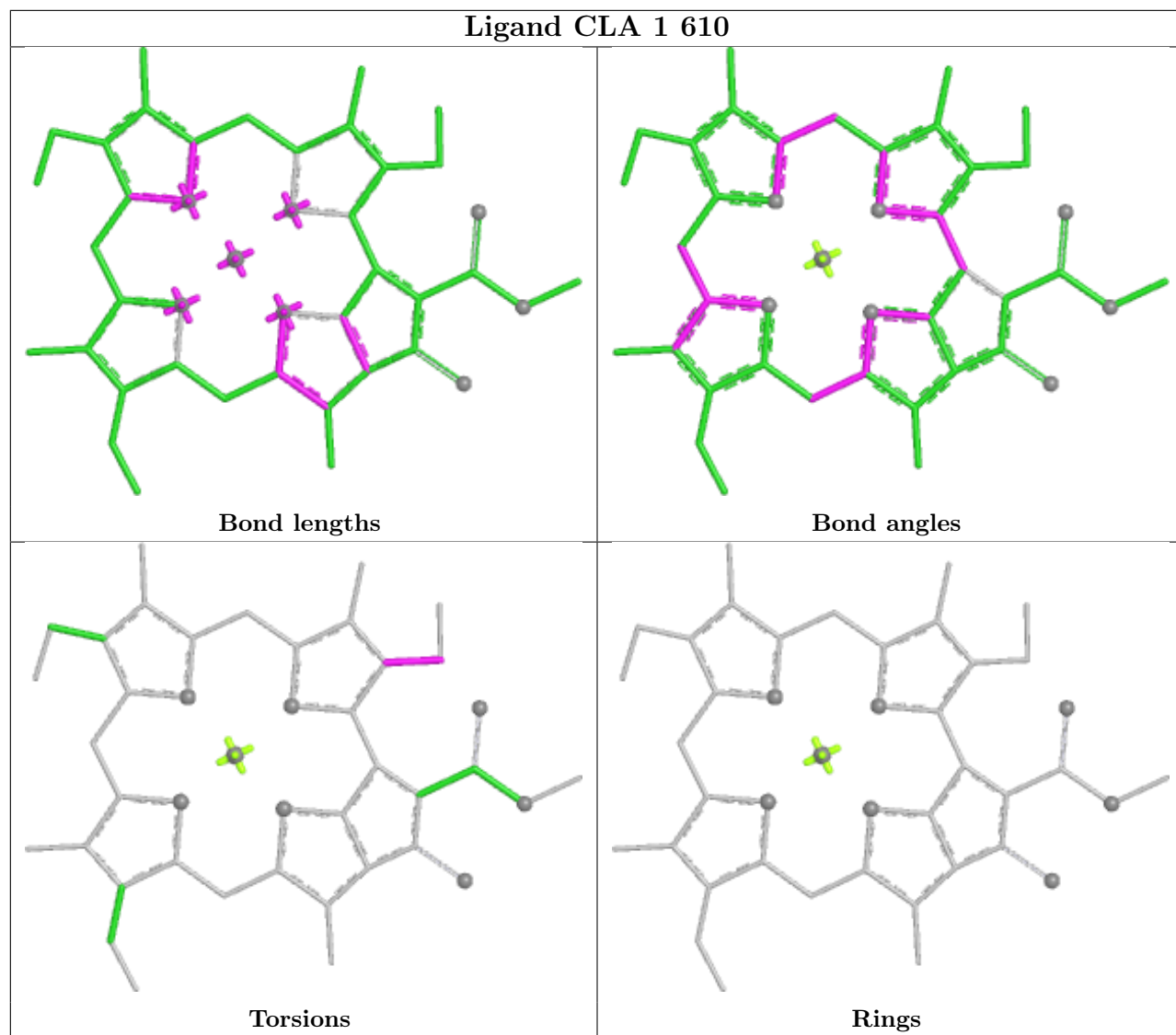


Torsions

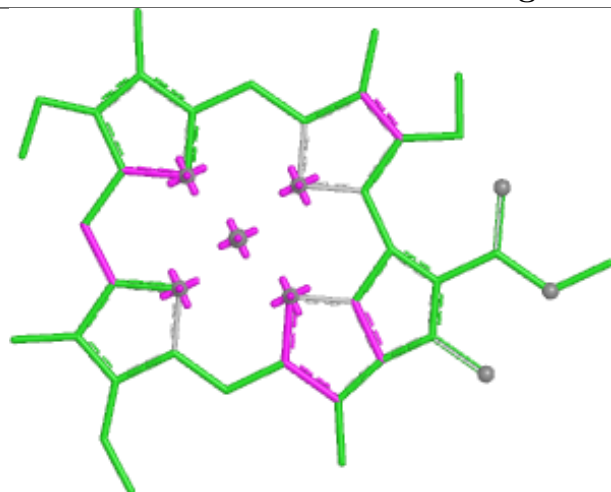


Rings

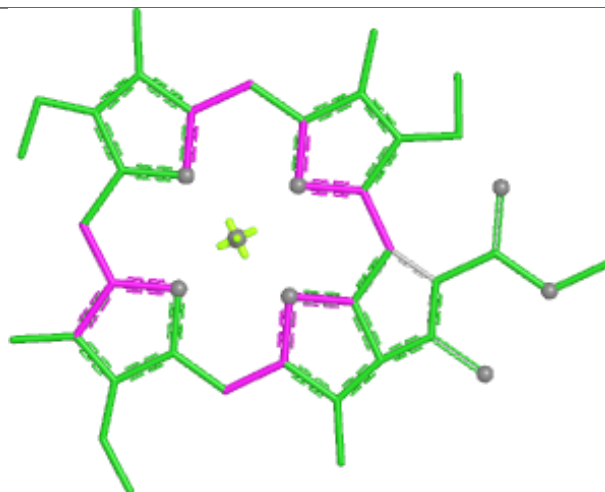
Ligand CLA 1 610



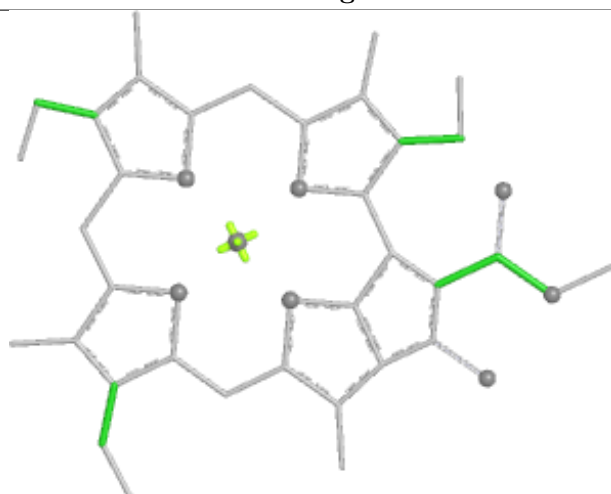
Ligand CLA 3 303



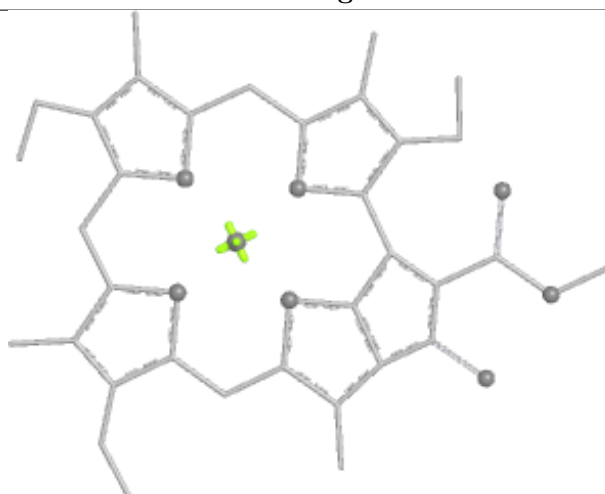
Bond lengths



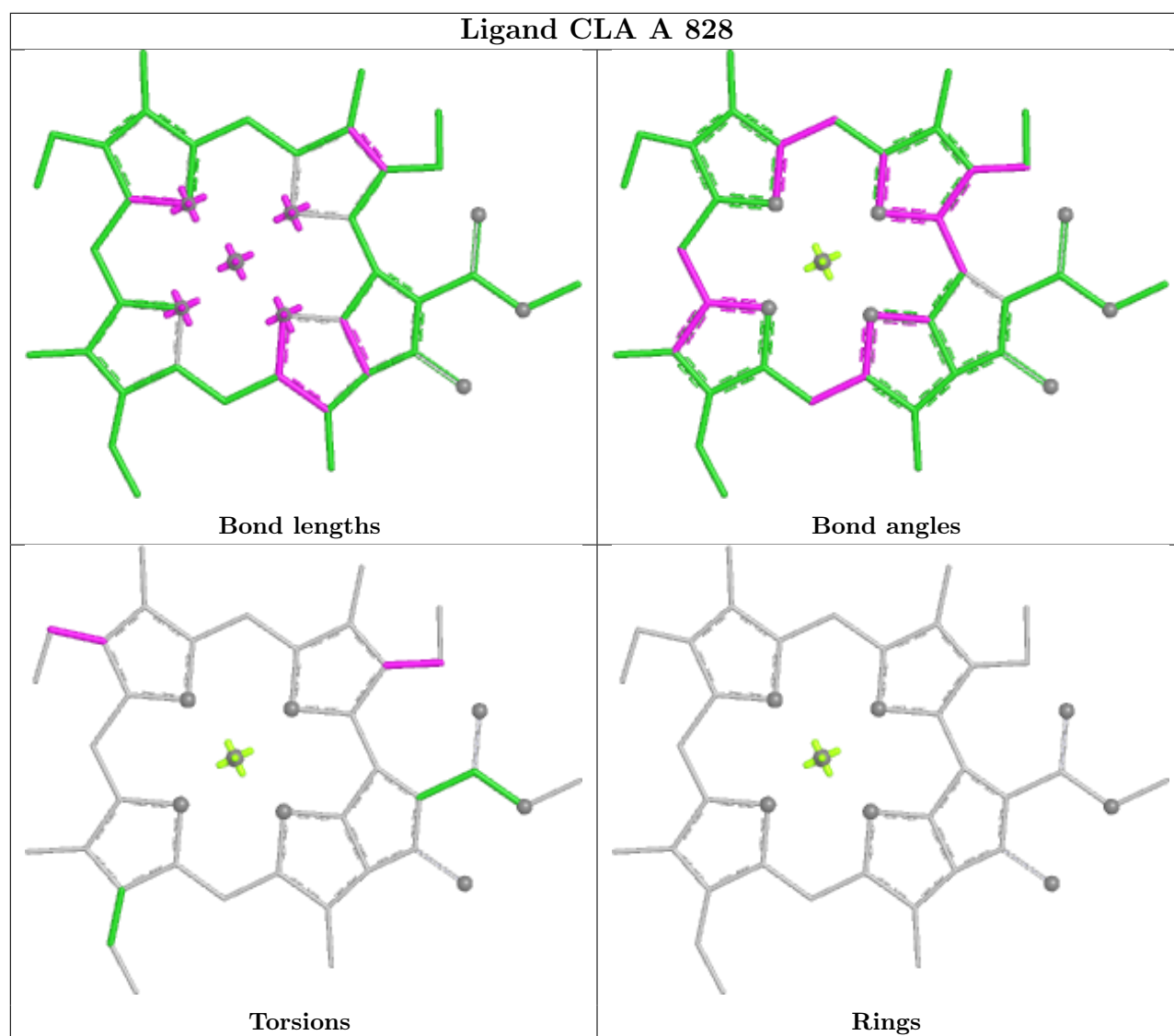
Bond angles



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.

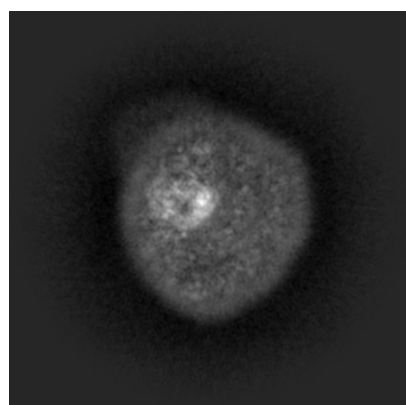
5 Map visualisation [i](#)

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.

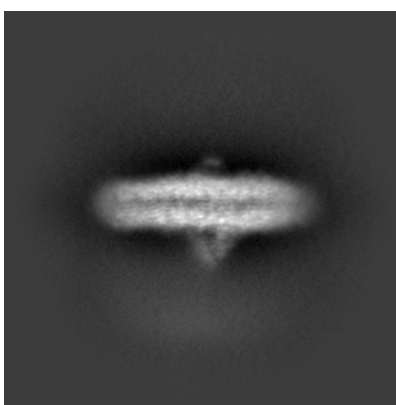
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

5.1 Orthogonal projections [i](#)

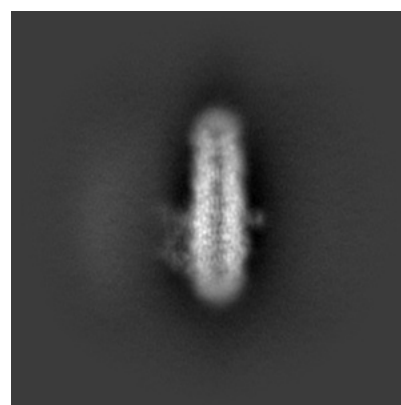
5.1.1 Primary map



X



Y

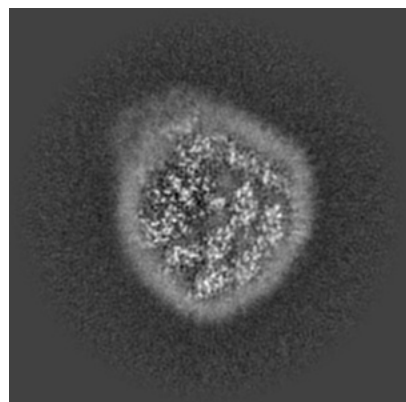


Z

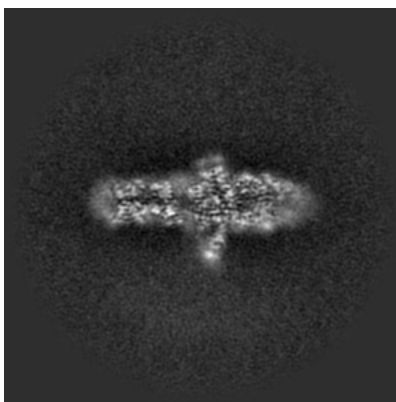
The images above show the map projected in three orthogonal directions.

5.2 Central slices [i](#)

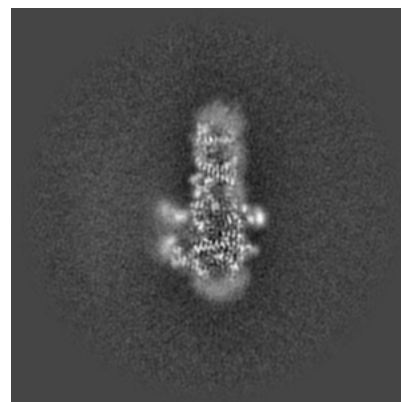
5.2.1 Primary map



X Index: 196



Y Index: 196

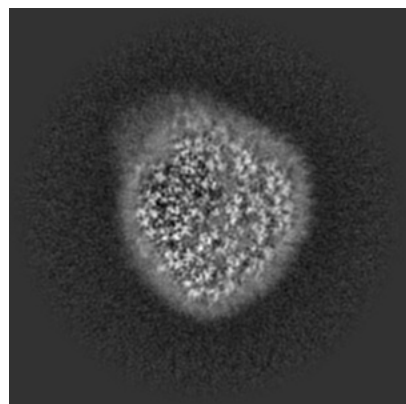


Z Index: 196

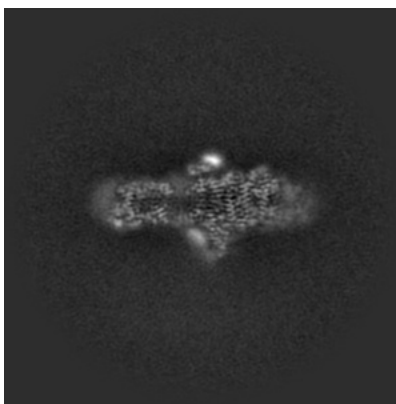
The images above show central slices of the map in three orthogonal directions.

5.3 Largest variance slices [i](#)

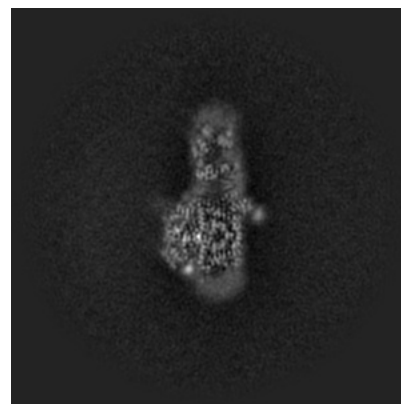
5.3.1 Primary map



X Index: 190



Y Index: 185

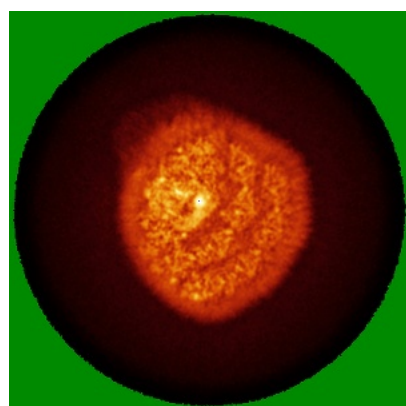


Z Index: 213

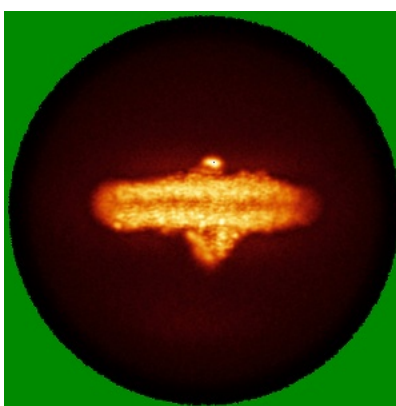
The images above show the largest variance slices of the map in three orthogonal directions.

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

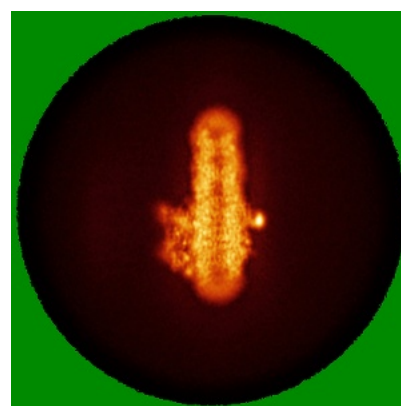
5.4.1 Primary map



X



Y

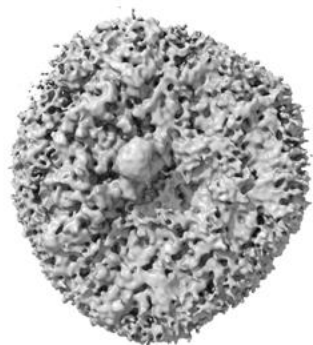


Z

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.

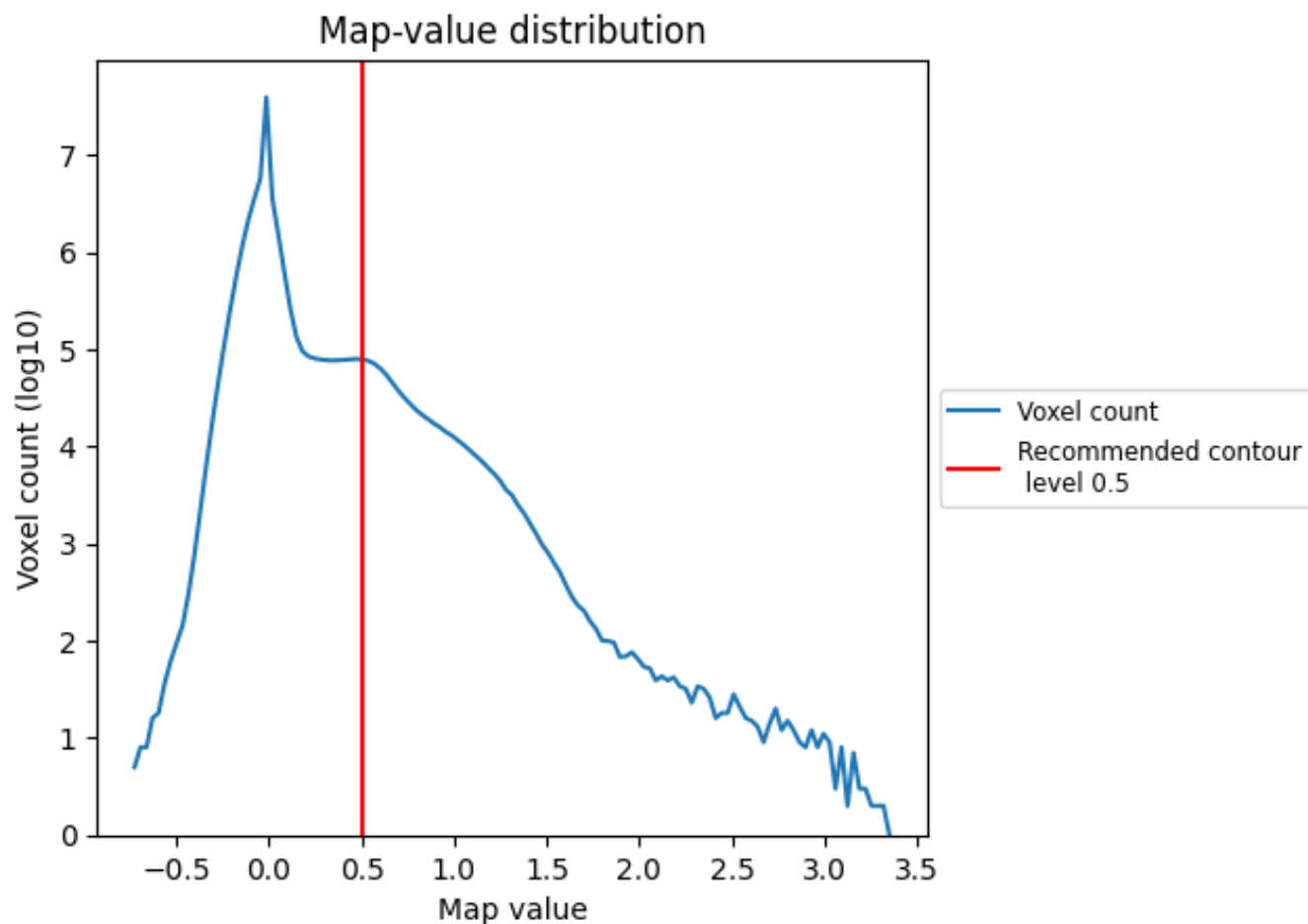
5.6 Mask visualisation [i](#)

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

6 Map analysis [i](#)

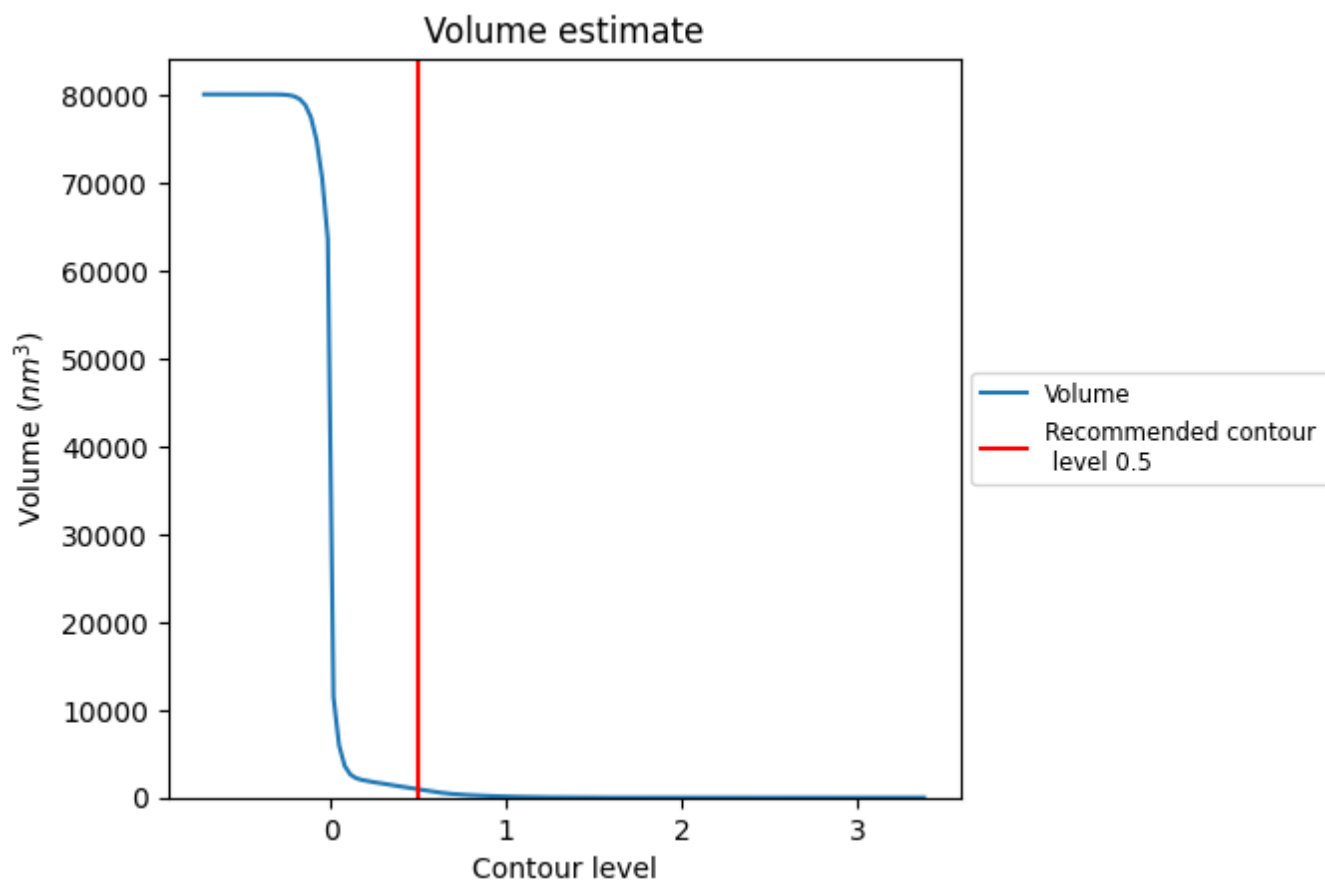
This section contains the results of statistical analysis of the map.

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.

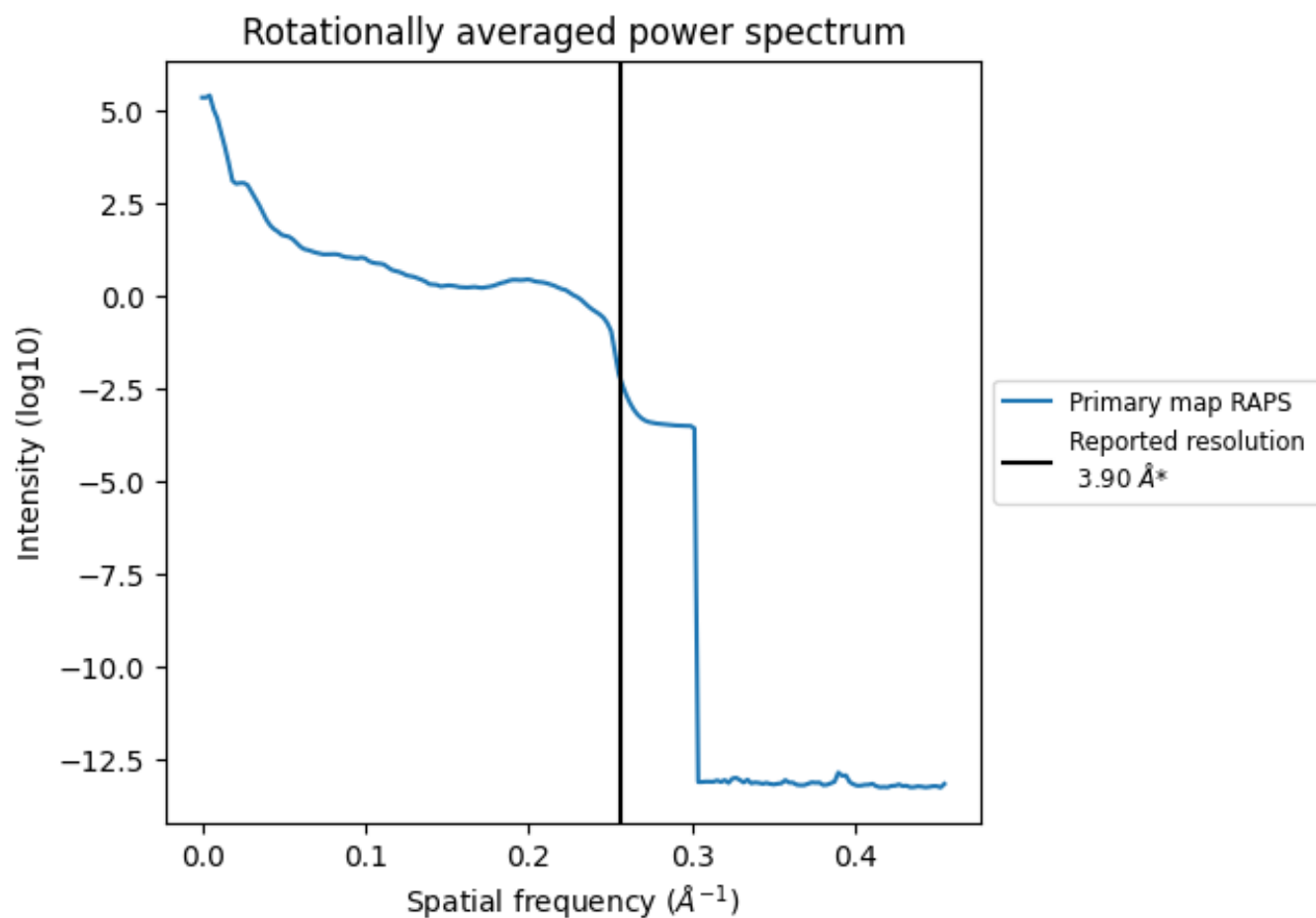
6.2 Volume estimate [i](#)



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 ⓘ

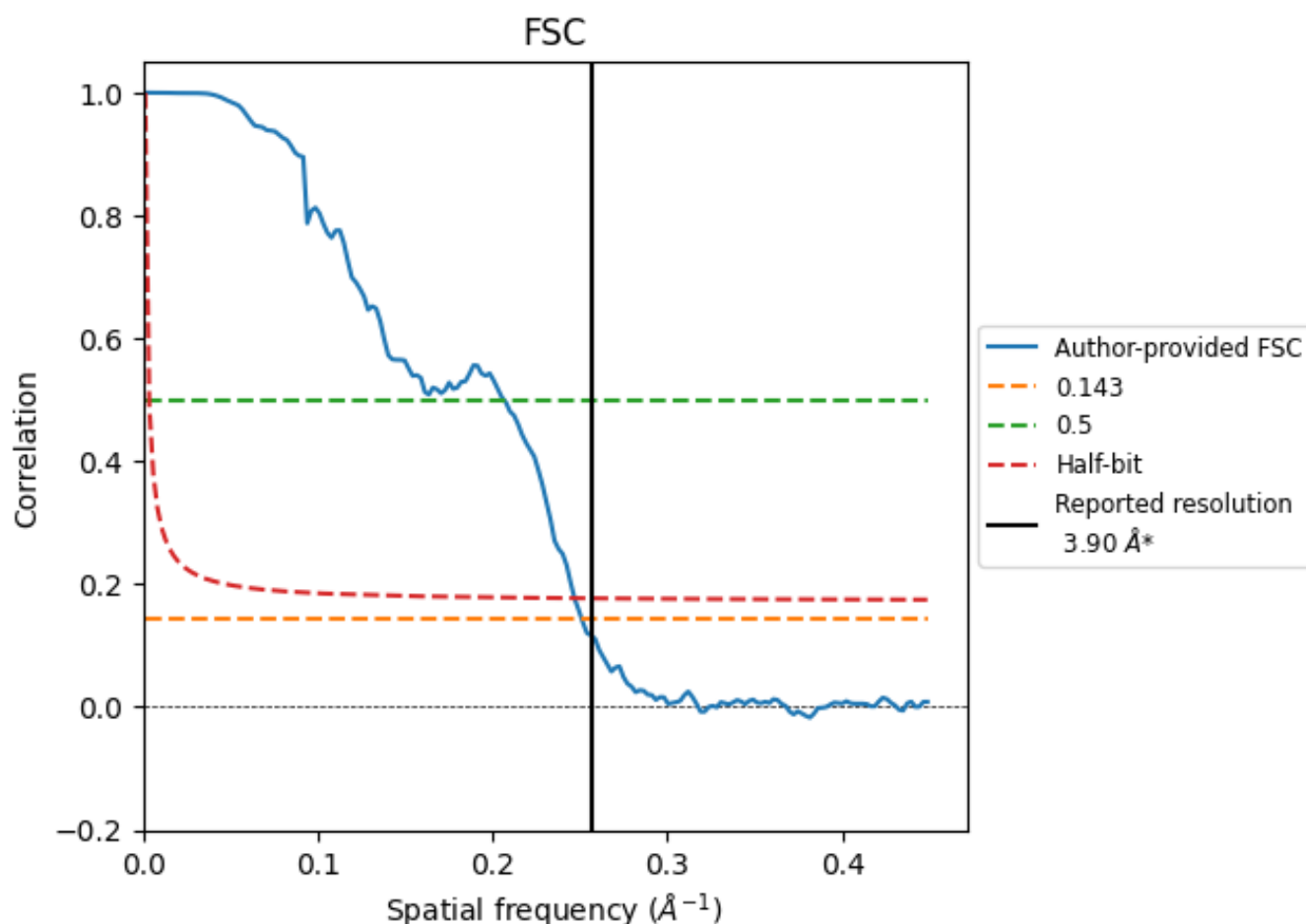


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

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 Å⁻¹

7.2 Resolution estimates [i](#)

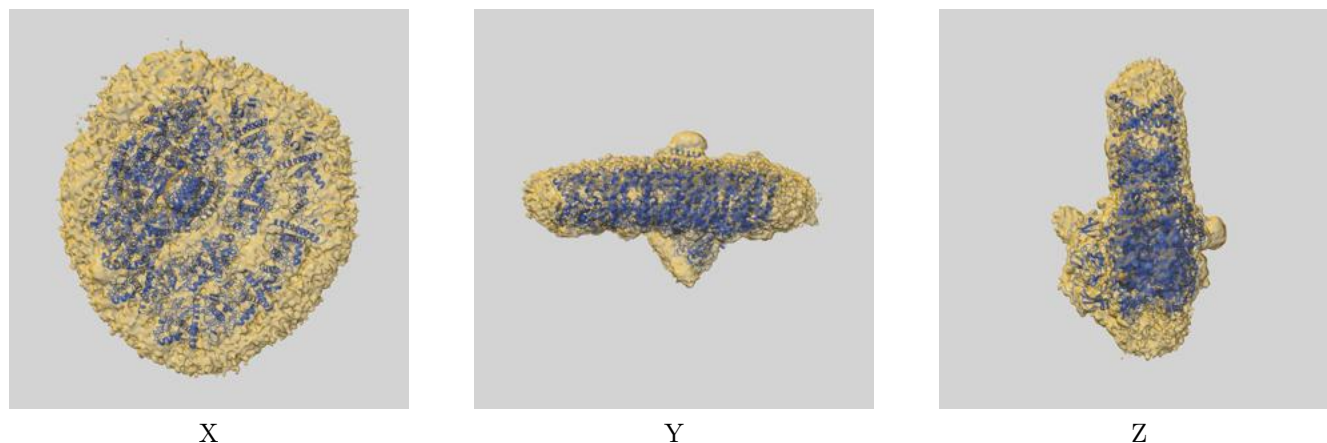
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.98	4.84	4.05
Unmasked-calculated*	-	-	-

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

8 Map-model fit [i](#)

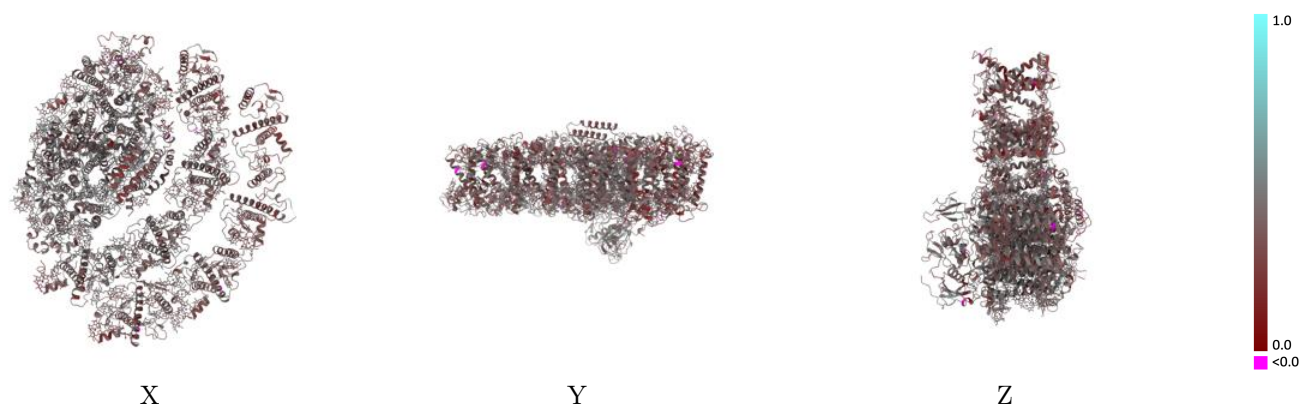
This section contains information regarding the fit between EMDB map EMD-32892 and PDB model 7WYI. Per-residue inclusion information can be found in section ?? on page ??.

8.1 Map-model overlay [i](#)



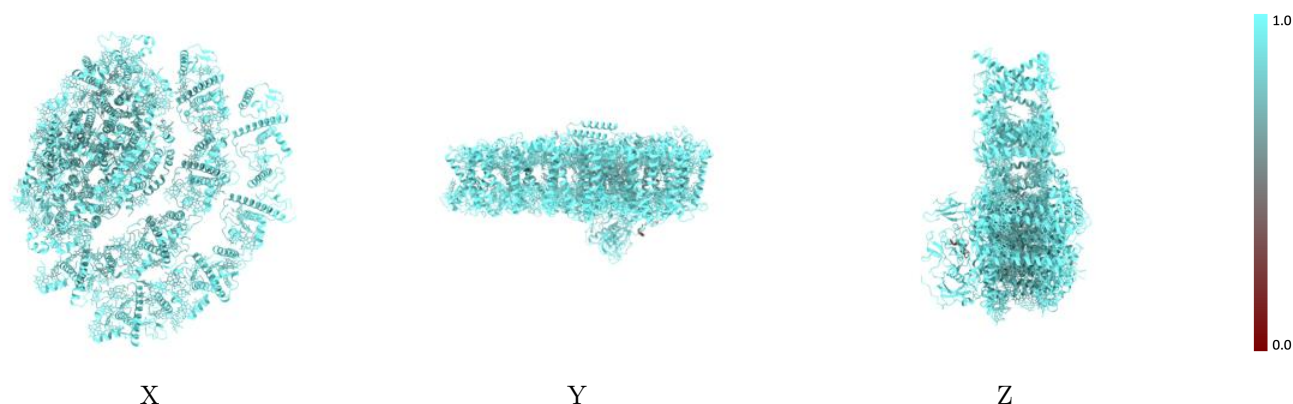
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



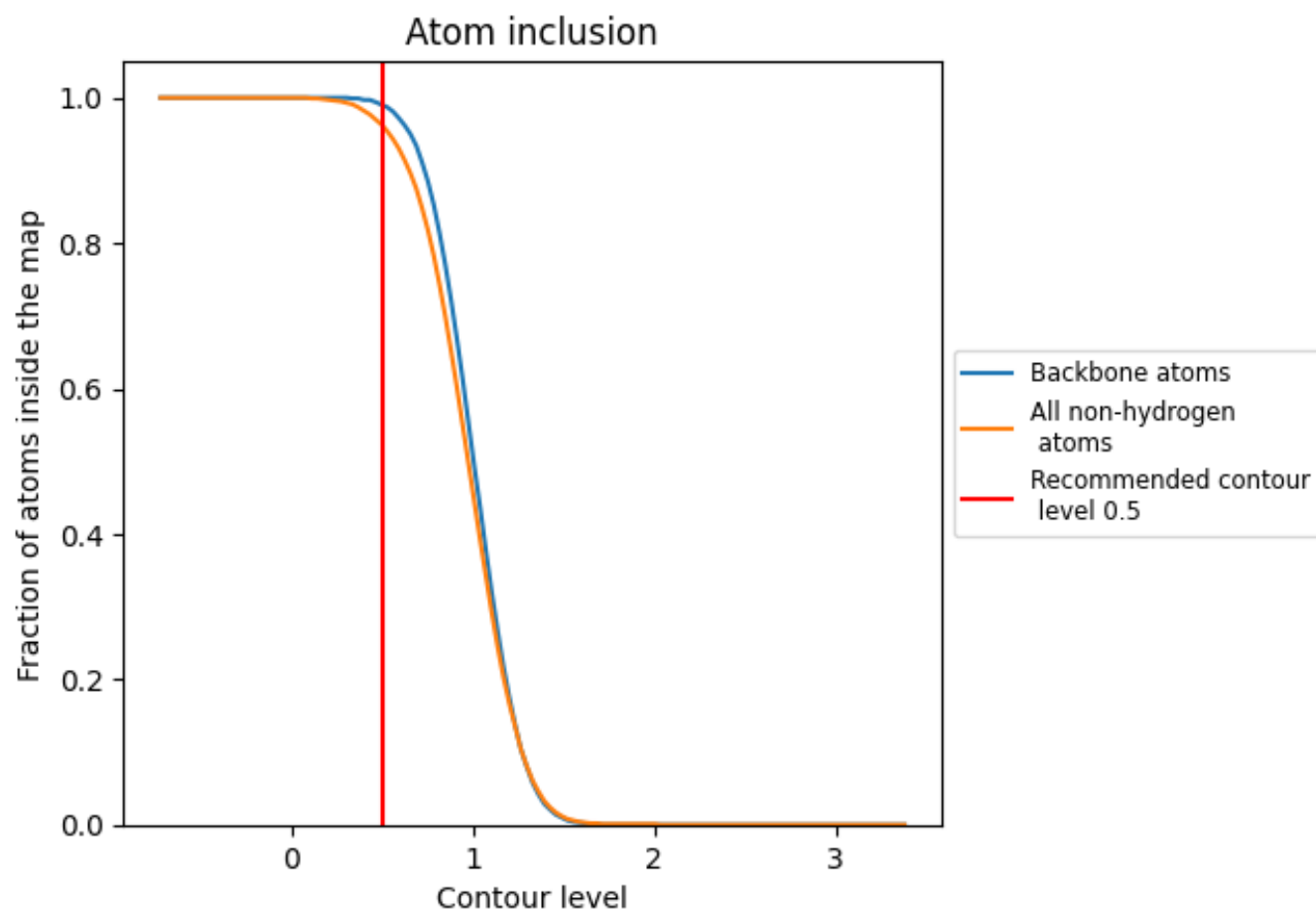
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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