



wwPDB EM Validation Summary Report ⓘ

Jun 20, 2024 – 06:20 AM JST

PDB ID : 7WYI
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.dev92
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

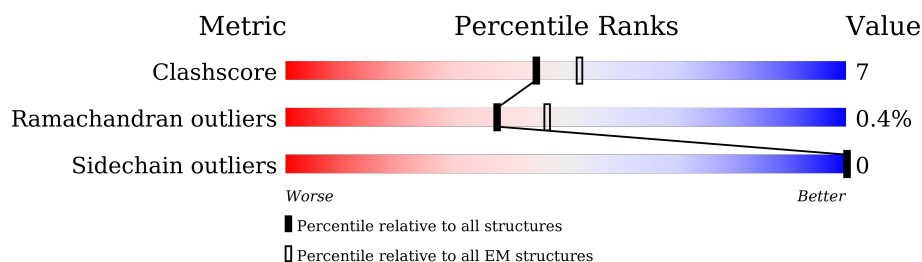
1 Overall quality at a glance

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	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	751	 94% 5% .
2	B	735	 94% 5%
3	C	81	 75% 22% ..
4	D	196	 5% 66% 7% . 27%
5	E	97	 51% 12% 37%
6	F	227	 71% . 27%
7	J	41	 93% . 5%
8	1	224	 81% 5% 13%

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Mol	Chain	Length	Quality of chain
9	3	298	
10	7	241	
11	8	243	
12	Z	228	
13	4	264	
14	5	257	
15	6	257	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CL0	A	801	X	-	-	-
17	CLA	1	602	X	-	-	-
17	CLA	1	603	X	-	-	-
17	CLA	1	604	X	-	-	-
17	CLA	1	605	X	-	-	-
17	CLA	1	606	X	-	-	-
17	CLA	1	607	X	-	-	-
17	CLA	1	608	X	-	-	-
17	CLA	1	609	X	-	-	-
17	CLA	1	610	X	-	-	-
17	CLA	3	301	X	-	-	-
17	CLA	3	302	X	-	-	-
17	CLA	3	303	X	-	-	-
17	CLA	3	304	X	-	-	-
17	CLA	3	305	X	-	-	-
17	CLA	3	306	X	-	-	-
17	CLA	3	308	X	-	-	-
17	CLA	3	309	X	-	-	-
17	CLA	3	310	X	-	-	-
17	CLA	3	311	X	-	-	-
17	CLA	3	312	X	-	-	-
17	CLA	3	313	X	-	-	-
17	CLA	4	601	X	-	-	-
17	CLA	4	602	X	-	-	-
17	CLA	4	603	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	4	604	X	-	-	-
17	CLA	4	605	X	-	-	-
17	CLA	5	301	X	-	-	-
17	CLA	5	302	X	-	-	-
17	CLA	5	303	X	-	-	-
17	CLA	5	304	X	-	-	-
17	CLA	5	306	X	-	-	-
17	CLA	5	307	X	-	-	-
17	CLA	5	308	X	-	-	-
17	CLA	5	309	X	-	-	-
17	CLA	5	310	X	-	-	-
17	CLA	5	311	X	-	-	-
17	CLA	5	312	X	-	-	-
17	CLA	5	314	X	-	-	-
17	CLA	5	315	X	-	-	-
17	CLA	6	601	X	-	-	-
17	CLA	6	602	X	-	-	-
17	CLA	6	603	X	-	-	-
17	CLA	6	604	X	-	-	-
17	CLA	6	608	X	-	-	-
17	CLA	6	609	X	-	-	-
17	CLA	6	610	X	-	-	-
17	CLA	7	601	X	-	-	-
17	CLA	7	602	X	-	-	-
17	CLA	7	603	X	-	-	-
17	CLA	7	604	X	-	-	-
17	CLA	7	605	X	-	-	-
17	CLA	7	607	X	-	-	-
17	CLA	7	608	X	-	-	-
17	CLA	7	609	X	-	-	-
17	CLA	7	610	X	-	-	-
17	CLA	7	611	X	-	-	-
17	CLA	7	612	X	-	-	-
17	CLA	7	613	X	-	-	-
17	CLA	7	614	X	-	-	-
17	CLA	8	601	X	-	-	-
17	CLA	8	602	X	-	-	-
17	CLA	8	603	X	-	-	-
17	CLA	8	604	X	-	-	-
17	CLA	8	605	X	-	-	-
17	CLA	8	607	X	-	-	-
17	CLA	8	608	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	8	609	X	-	-	-
17	CLA	8	610	X	-	-	-
17	CLA	8	611	X	-	-	-
17	CLA	8	612	X	-	-	-
17	CLA	8	613	X	-	-	-
17	CLA	8	614	X	-	-	-
17	CLA	A	802	X	-	-	-
17	CLA	A	803	X	-	-	-
17	CLA	A	804	X	-	-	-
17	CLA	A	805	X	-	-	-
17	CLA	A	806	X	-	-	-
17	CLA	A	807	X	-	-	-
17	CLA	A	808	X	-	-	-
17	CLA	A	809	X	-	-	-
17	CLA	A	810	X	-	-	-
17	CLA	A	811	X	-	-	-
17	CLA	A	812	X	-	-	-
17	CLA	A	813	X	-	-	-
17	CLA	A	814	X	-	-	-
17	CLA	A	815	X	-	-	-
17	CLA	A	816	X	-	-	-
17	CLA	A	817	X	-	-	-
17	CLA	A	818	X	-	-	-
17	CLA	A	819	X	-	-	-
17	CLA	A	820	X	-	-	-
17	CLA	A	821	X	-	-	-
17	CLA	A	822	X	-	-	-
17	CLA	A	823	X	-	-	-
17	CLA	A	824	X	-	-	-
17	CLA	A	825	X	-	-	-
17	CLA	A	826	X	-	-	-
17	CLA	A	827	X	-	-	-
17	CLA	A	828	X	-	-	-
17	CLA	A	829	X	-	-	-
17	CLA	A	830	X	-	-	-
17	CLA	A	831	X	-	-	-
17	CLA	A	832	X	-	-	-
17	CLA	A	833	X	-	-	-
17	CLA	A	834	X	-	-	-
17	CLA	A	835	X	-	-	-
17	CLA	A	836	X	-	-	-
17	CLA	A	837	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	A	838	X	-	-	-
17	CLA	A	839	X	-	-	-
17	CLA	A	841	X	-	-	-
17	CLA	A	842	X	-	-	-
17	CLA	A	843	X	-	-	-
17	CLA	B	801	X	-	-	-
17	CLA	B	802	X	-	-	-
17	CLA	B	804	X	-	-	-
17	CLA	B	805	X	-	-	-
17	CLA	B	806	X	-	-	-
17	CLA	B	807	X	-	-	-
17	CLA	B	808	X	-	-	-
17	CLA	B	809	X	-	-	-
17	CLA	B	810	X	-	-	-
17	CLA	B	811	X	-	-	-
17	CLA	B	812	X	-	-	-
17	CLA	B	813	X	-	-	-
17	CLA	B	814	X	-	-	-
17	CLA	B	815	X	-	-	-
17	CLA	B	816	X	-	-	-
17	CLA	B	817	X	-	-	-
17	CLA	B	818	X	-	-	-
17	CLA	B	819	X	-	-	-
17	CLA	B	820	X	-	-	-
17	CLA	B	821	X	-	-	-
17	CLA	B	822	X	-	-	-
17	CLA	B	823	X	-	-	-
17	CLA	B	824	X	-	-	-
17	CLA	B	825	X	-	-	-
17	CLA	B	826	X	-	-	-
17	CLA	B	827	X	-	-	-
17	CLA	B	828	X	-	-	-
17	CLA	B	829	X	-	-	-
17	CLA	B	830	X	-	-	-
17	CLA	B	831	X	-	-	-
17	CLA	B	832	X	-	-	-
17	CLA	B	833	X	-	-	-
17	CLA	B	834	X	-	-	-
17	CLA	B	835	X	-	-	-
17	CLA	B	836	X	-	-	-
17	CLA	B	837	X	-	-	-
17	CLA	B	838	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	B	839	X	-	-	-
17	CLA	F	301	X	-	-	-
17	CLA	F	302	X	-	-	-
17	CLA	J	101	X	-	-	-
17	CLA	J	102	X	-	-	-
19	SF4	C	102	-	-	X	-
20	CHL	1	601	X	-	-	-
20	CHL	3	307	X	-	-	-
20	CHL	5	305	X	-	-	-
20	CHL	5	313	X	-	-	-
20	CHL	6	605	X	-	-	-
20	CHL	6	606	X	-	-	-
20	CHL	6	607	X	-	-	-
20	CHL	7	606	X	-	-	-
20	CHL	8	606	X	-	-	-
20	CHL	Z	601	X	-	-	-

2 Entry composition

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

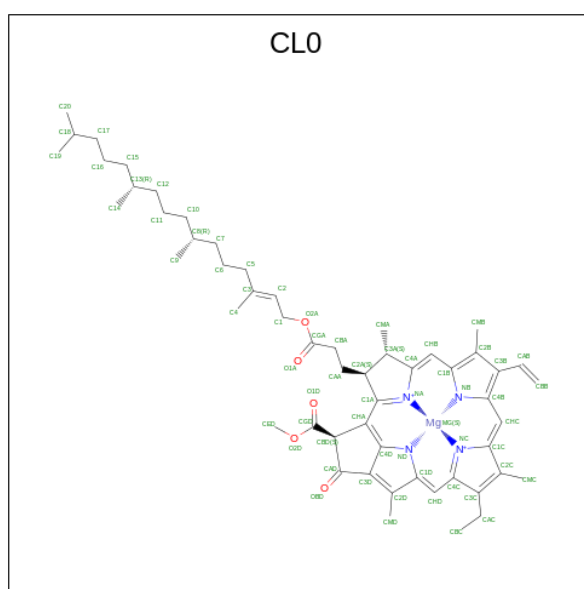
- Molecule 14 is a protein called Chlorophyll a-b binding protein, chloroplastic.

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

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

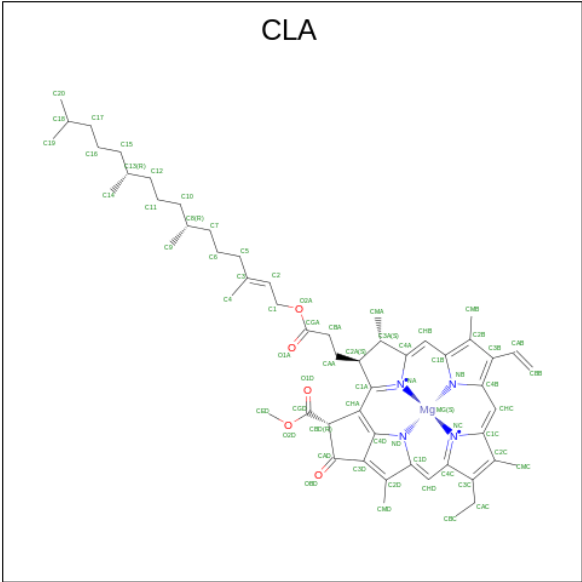
Mol	Chain	Residues	Atoms				AltConf	Trace
15	6	229	Total	C	N	O	0	0
			1122	664	229	229		

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



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

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

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

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

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

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Mol	Chain	Residues	Atoms					AltConf
17	3	1	Total 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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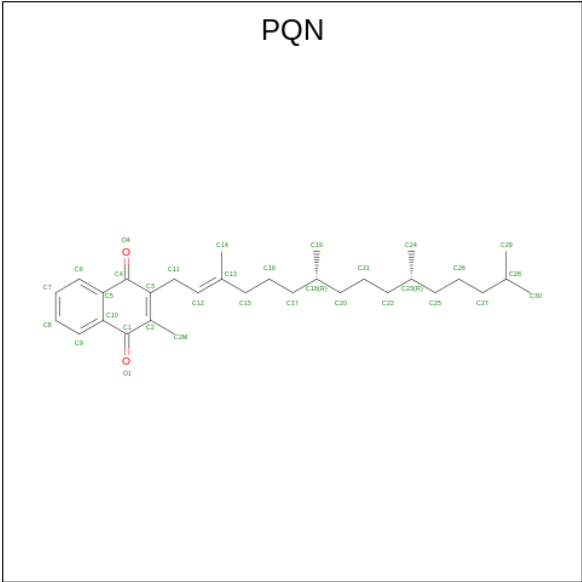
Mol	Chain	Residues	Atoms					AltConf
17	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	8	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	8	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	8	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	8	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	8	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	8	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	8	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	8	1	Total 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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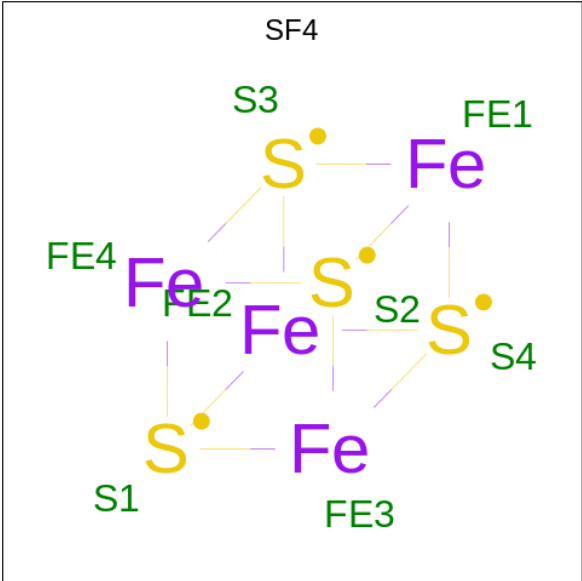
Mol	Chain	Residues	Atoms					AltConf
17	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	5	1	Total	C	Mg	N	O	0
			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 (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



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

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



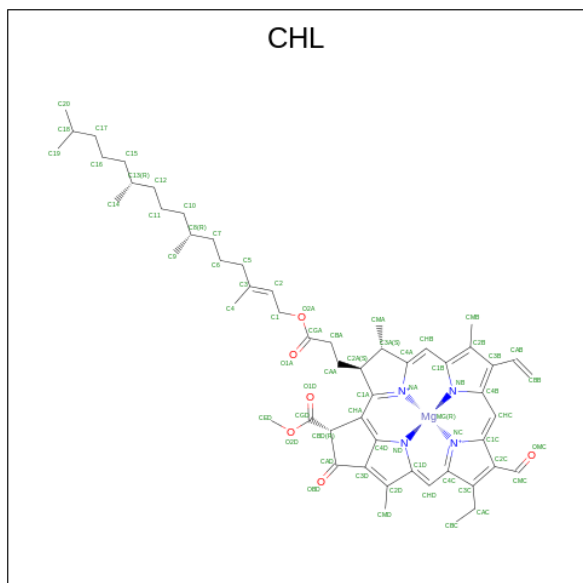
Mol	Chain	Residues	Atoms			AltConf
19	B	1	Total	Fe	S	0
			8	4	4	

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

- Molecule 20 is CHLOROPHYLL B (three-letter code: CHL) (formula: $\text{C}_{55}\text{H}_{70}\text{MgN}_4\text{O}_6$) (labeled as "Ligand of Interest" by depositor).



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

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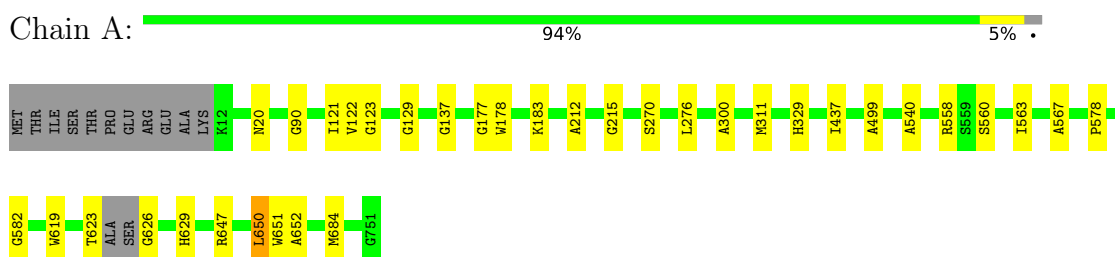
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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
20	6	1	43	34	1	4	4	0

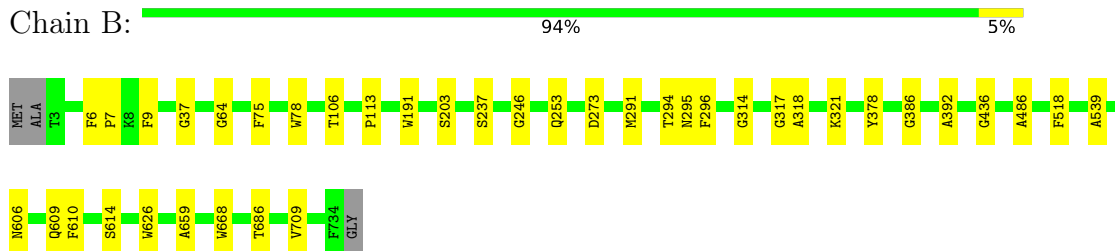
3 Residue-property plots

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

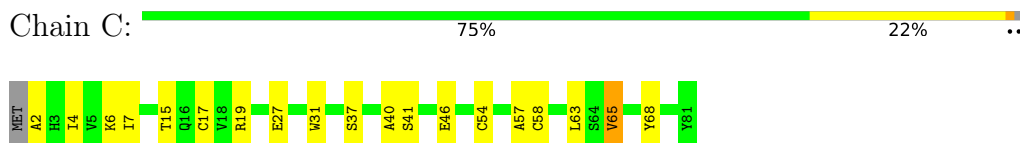
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



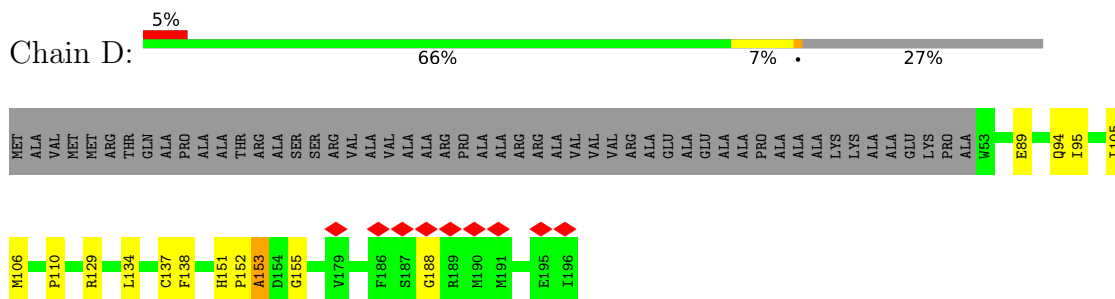
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



- Molecule 3: Photosystem I iron-sulfur center

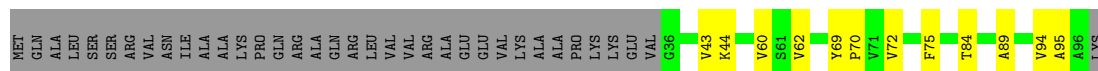


- Molecule 4: Photosystem I reaction center subunit II, chloroplastic



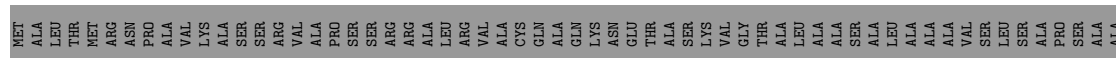
- Molecule 5: Photosystem I reaction center subunit IV, chloroplastic

Chain E:  51% 12% 37%



- Molecule 6: Photosystem I reaction center subunit III, chloroplastic

Chain F:  71% 27%




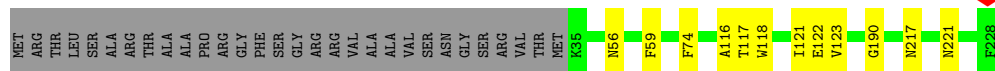
- Molecule 7: Photosystem I reaction center subunit IX

Chain J:  93% 5%



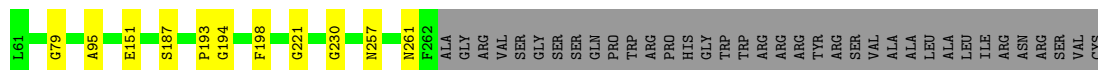
- Molecule 8: Chlorophyll a-b binding protein, chloroplastic

Chain 1:  81% 5% 13%




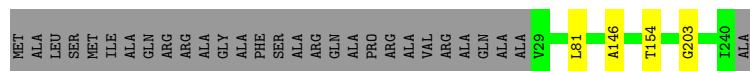
- Molecule 9: Chlorophyll a-b binding protein, chloroplastic

Chain 3:  64% 32%




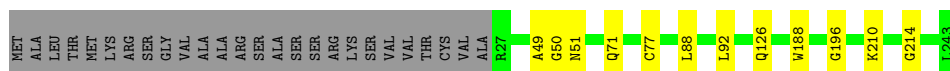
- Molecule 10: Chlorophyll a-b binding protein, chloroplastic

Chain 7:  86% 12%




- Molecule 11: Chlorophyll a-b binding protein, chloroplastic

Chain 8:  84% 5% 11%



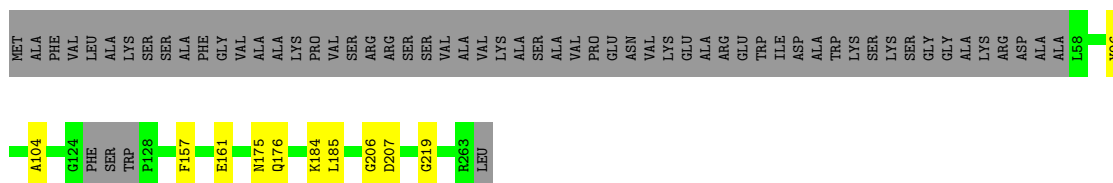
- Molecule 12: Chlorophyll a-b binding protein, chloroplastic

Chain Z:  81% 16%




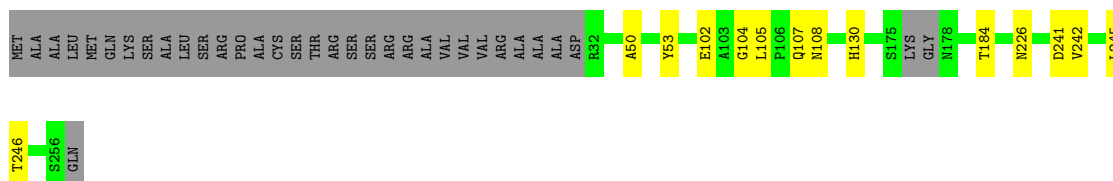
- Molecule 13: Chlorophyll a-b binding protein, chloroplastic

Chain 4:  73% 23%




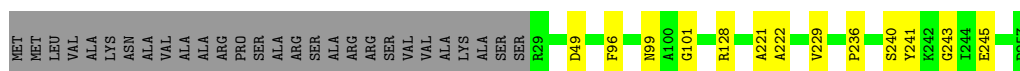
- Molecule 14: Chlorophyll a-b binding protein, chloroplastic

Chain 5:  81% 5% 13%



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

Chain 6:  84% 5% 11%



4 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 (\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 (\AA)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CLA, PQN, CHL, SF4, CL0

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.34	0/3628	0.51	0/5034
2	B	0.35	0/3602	0.50	0/5001
3	C	0.43	0/394	0.72	0/547
4	D	0.37	0/705	0.54	0/977
5	E	0.30	0/299	0.51	0/414
6	F	0.32	0/809	0.47	0/1122
7	J	0.30	0/193	0.44	0/268
8	1	0.30	0/941	0.47	0/1299
9	3	0.34	0/984	0.49	0/1361
10	7	0.34	0/1032	0.48	0/1427
11	8	0.33	0/1058	0.47	0/1464
12	Z	0.31	0/932	0.46	0/1286
13	4	0.34	0/990	0.48	0/1369
14	5	0.33	0/1089	0.51	0/1507
15	6	0.32	0/1121	0.47	0/1554
All	All	0.34	0/17777	0.50	0/24630

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
13	4	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	4	206	GLY	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3628	0	1728	30	0
2	B	3601	0	1715	29	0
3	C	395	0	178	11	0
4	D	706	0	316	11	0
5	E	300	0	135	6	0
6	F	810	0	404	2	0
7	J	194	0	87	1	0
8	1	942	0	489	9	0
9	3	985	0	480	7	0
10	7	1033	0	498	4	0
11	8	1059	0	527	8	0
12	Z	934	0	482	4	0
13	4	992	0	471	5	0
14	5	1091	0	504	13	0
15	6	1122	0	524	9	0
16	A	42	0	31	4	0
17	1	379	0	279	12	0
17	3	510	0	374	10	0
17	4	216	0	159	4	0
17	5	567	0	416	10	0
17	6	301	0	221	5	0
17	7	549	0	405	7	0
17	8	553	0	407	14	0
17	A	1743	0	1290	52	0
17	B	1630	0	1223	50	0
17	F	104	0	94	4	0
17	J	85	0	62	2	0
18	A	33	0	46	0	0
18	B	33	0	46	3	0
19	B	8	0	0	0	0
19	C	16	0	0	2	0
20	1	53	0	41	0	0
20	3	46	0	31	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	5	89	0	60	1	0
20	6	129	0	87	5	0
20	7	43	0	29	2	0
20	8	43	0	29	2	0
20	Z	43	0	29	0	0
All	All	25007	0	13897	264	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 264 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:7:81:LEU:CB	17:7:604:CLA:HBB2	1.90	1.01
4:D:138:PHE:H	4:D:151:HIS:CB	1.83	0.90
15:6:240:SER:HA	15:6:245:GLU:HA	1.56	0.86
14:5:105:LEU:CB	14:5:108:ASN:CB	2.53	0.86
14:5:226:ASN:CB	17:5:311:CLA:HED3	2.07	0.84

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	734/751 (98%)	671 (91%)	61 (8%)	2 (0%)	41	75
2	B	730/735 (99%)	660 (90%)	66 (9%)	4 (0%)	29	67
3	C	78/81 (96%)	62 (80%)	13 (17%)	3 (4%)	3	28
4	D	142/196 (72%)	122 (86%)	18 (13%)	2 (1%)	11	46
5	E	59/97 (61%)	53 (90%)	6 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	163/227 (72%)	156 (96%)	7 (4%)	0	100	100
7	J	37/41 (90%)	34 (92%)	3 (8%)	0	100	100
8	1	192/224 (86%)	175 (91%)	17 (9%)	0	100	100
9	3	200/298 (67%)	183 (92%)	17 (8%)	0	100	100
10	7	210/241 (87%)	186 (89%)	24 (11%)	0	100	100
11	8	215/243 (88%)	202 (94%)	12 (6%)	1 (0%)	29	67
12	Z	188/228 (82%)	172 (92%)	16 (8%)	0	100	100
13	4	199/264 (75%)	181 (91%)	17 (8%)	1 (0%)	29	67
14	5	219/257 (85%)	195 (89%)	24 (11%)	0	100	100
15	6	227/257 (88%)	213 (94%)	13 (6%)	1 (0%)	34	71
All	All	3593/4140 (87%)	3265 (91%)	314 (9%)	14 (0%)	38	71

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	VAL
2	B	6	PHE
4	D	152	PRO
2	B	9	PHE
1	A	650	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1/610 (0%)	1 (100%)	0	100	100
2	B	1/597 (0%)	1 (100%)	0	100	100
All	All	2/1207 (0%)	2 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are

no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	B	838	-	42,50,73	2.68	11 (26%)	48,85,113	1.53	8 (16%)
17	CLA	5	314	-	46,54,73	2.35	10 (21%)	53,90,113	1.57	8 (15%)
17	CLA	A	839	-	42,50,73	2.69	11 (26%)	48,85,113	1.54	10 (20%)
20	CHL	6	607	-	43,51,74	2.49	10 (23%)	45,86,114	1.73	9 (20%)
17	CLA	B	807	-	42,50,73	2.70	10 (23%)	48,85,113	1.89	9 (18%)
17	CLA	4	605	-	45,53,73	2.56	10 (22%)	52,89,113	1.38	8 (15%)
17	CLA	8	610	-	42,50,73	2.54	9 (21%)	48,85,113	1.55	8 (16%)
17	CLA	8	604	-	42,50,73	2.84	10 (23%)	48,85,113	1.47	8 (16%)
17	CLA	A	829	-	42,50,73	2.69	9 (21%)	48,85,113	1.59	9 (18%)
17	CLA	B	816	-	42,50,73	2.83	10 (23%)	48,85,113	1.54	7 (14%)
17	CLA	B	813	-	41,49,73	2.62	9 (21%)	51,84,113	1.50	8 (15%)
17	CLA	B	828	-	43,51,73	2.77	9 (20%)	49,86,113	1.46	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	3	308	-	42,50,73	2.67	9 (21%)	48,85,113	1.90	8 (16%)
17	CLA	A	816	-	42,50,73	2.62	9 (21%)	48,85,113	1.44	9 (18%)
19	SF4	C	102	-	0,12,12	-	-	-		
17	CLA	1	603	-	42,50,73	2.76	11 (26%)	48,85,113	1.43	7 (14%)
17	CLA	7	601	10	42,50,73	2.73	10 (23%)	48,85,113	1.55	8 (16%)
17	CLA	A	809	-	42,50,73	2.73	9 (21%)	48,85,113	1.56	9 (18%)
20	CHL	3	307	-	46,54,74	2.38	11 (23%)	49,90,114	1.76	9 (18%)
17	CLA	B	804	-	42,50,73	2.69	9 (21%)	48,85,113	1.69	7 (14%)
17	CLA	B	814	-	38,47,73	3.00	8 (21%)	45,81,113	1.49	8 (17%)
17	CLA	B	832	-	42,50,73	2.81	11 (26%)	48,85,113	1.52	8 (16%)
17	CLA	7	613	-	43,51,73	2.71	10 (23%)	49,86,113	1.45	8 (16%)
20	CHL	5	313	-	43,51,74	2.47	10 (23%)	45,86,114	1.79	8 (17%)
17	CLA	A	806	-	42,50,73	2.85	11 (26%)	48,85,113	1.48	7 (14%)
17	CLA	6	610	-	45,53,73	2.73	11 (24%)	52,89,113	1.43	8 (15%)
17	CLA	A	808	-	42,50,73	2.74	11 (26%)	48,85,113	1.47	7 (14%)
17	CLA	7	604	-	42,50,73	2.87	9 (21%)	48,85,113	1.57	11 (22%)
17	CLA	F	302	-	62,70,73	2.17	8 (12%)	72,109,113	1.22	8 (11%)
17	CLA	J	102	-	42,50,73	2.82	9 (21%)	48,85,113	1.60	9 (18%)
17	CLA	7	609	-	42,50,73	2.75	9 (21%)	48,85,113	1.52	9 (18%)
17	CLA	A	810	-	42,50,73	2.84	10 (23%)	48,85,113	1.52	9 (18%)
17	CLA	A	823	-	42,50,73	2.83	10 (23%)	48,85,113	1.58	9 (18%)
17	CLA	7	605	-	42,50,73	2.79	11 (26%)	48,85,113	1.47	10 (20%)
18	PQN	B	840	-	34,34,34	0.23	0	42,45,45	0.23	0
17	CLA	B	810	-	46,54,73	2.52	9 (19%)	52,89,113	1.54	8 (15%)
17	CLA	3	310	-	41,49,73	2.73	9 (21%)	47,84,113	2.12	13 (27%)
17	CLA	B	830	-	42,50,73	2.67	9 (21%)	48,85,113	1.57	8 (16%)
17	CLA	8	602	-	42,50,73	2.72	9 (21%)	48,85,113	1.49	7 (14%)
17	CLA	B	802	-	45,53,73	2.47	7 (15%)	52,89,113	1.69	7 (13%)
17	CLA	8	605	-	42,50,73	2.75	10 (23%)	48,85,113	1.44	8 (16%)
17	CLA	A	815	-	42,50,73	2.91	10 (23%)	48,85,113	1.52	7 (14%)
20	CHL	8	606	-	43,51,74	2.49	10 (23%)	45,86,114	1.82	7 (15%)
17	CLA	B	827	-	42,50,73	2.67	10 (23%)	48,85,113	1.45	7 (14%)
17	CLA	1	604	-	42,50,73	2.77	7 (16%)	48,85,113	1.42	9 (18%)
17	CLA	3	305	-	42,50,73	2.58	8 (19%)	48,85,113	1.62	8 (16%)
19	SF4	C	101	-	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	A	802	-	42,50,73	2.77	10 (23%)	48,85,113	1.74	9 (18%)
17	CLA	A	807	-	42,50,73	2.80	9 (21%)	48,85,113	1.77	10 (20%)
16	CL0	A	801	-	42,50,73	2.68	10 (23%)	48,85,113	1.61	8 (16%)
17	CLA	3	301	-	42,50,73	2.76	10 (23%)	48,85,113	1.60	9 (18%)
17	CLA	B	817	-	42,50,73	2.79	9 (21%)	48,85,113	1.56	9 (18%)
17	CLA	A	831	-	42,50,73	2.83	10 (23%)	48,85,113	1.47	9 (18%)
17	CLA	6	604	-	42,50,73	2.75	10 (23%)	48,85,113	1.44	9 (18%)
17	CLA	5	301	-	42,50,73	2.72	10 (23%)	48,85,113	1.46	7 (14%)
17	CLA	B	811	-	42,50,73	2.73	10 (23%)	48,85,113	1.50	10 (20%)
17	CLA	1	602	-	42,50,73	2.67	9 (21%)	48,85,113	1.54	8 (16%)
17	CLA	A	830	-	42,50,73	2.72	10 (23%)	48,85,113	1.59	9 (18%)
17	CLA	4	604	-	42,50,73	2.84	9 (21%)	48,85,113	1.46	8 (16%)
17	CLA	8	609	-	42,50,73	2.67	9 (21%)	48,85,113	1.46	8 (16%)
17	CLA	8	608	-	42,50,73	2.80	9 (21%)	48,85,113	1.65	11 (22%)
17	CLA	B	837	-	42,50,73	2.74	9 (21%)	48,85,113	1.61	8 (16%)
17	CLA	A	832	-	41,48,73	2.93	11 (26%)	46,82,113	2.12	11 (23%)
17	CLA	A	819	-	42,50,73	2.72	9 (21%)	48,85,113	1.46	9 (18%)
17	CLA	7	607	-	42,50,73	2.74	10 (23%)	48,85,113	1.45	8 (16%)
17	CLA	7	612	-	45,53,73	2.71	10 (22%)	52,89,113	1.36	7 (13%)
17	CLA	A	804	-	42,50,73	2.59	9 (21%)	48,85,113	2.01	10 (20%)
17	CLA	A	811	-	42,50,73	2.77	11 (26%)	48,85,113	1.49	7 (14%)
17	CLA	B	834	-	42,50,73	2.69	10 (23%)	48,85,113	1.62	8 (16%)
17	CLA	6	602	-	42,50,73	2.74	9 (21%)	48,85,113	1.50	8 (16%)
17	CLA	6	603	-	42,50,73	2.71	10 (23%)	48,85,113	1.59	7 (14%)
17	CLA	1	606	-	42,50,73	2.78	7 (16%)	48,85,113	1.76	9 (18%)
20	CHL	7	606	-	43,51,74	2.48	10 (23%)	45,86,114	1.86	8 (17%)
17	CLA	1	608	-	42,50,73	2.96	9 (21%)	48,85,113	1.49	9 (18%)
17	CLA	A	834	1	42,50,73	2.71	9 (21%)	48,85,113	1.54	7 (14%)
17	CLA	7	611	-	42,50,73	2.85	10 (23%)	48,85,113	1.53	8 (16%)
17	CLA	8	603	-	45,53,73	2.79	11 (24%)	52,89,113	1.47	8 (15%)
17	CLA	B	824	-	41,49,73	2.82	9 (21%)	47,84,113	1.74	10 (21%)
17	CLA	5	304	-	42,50,73	2.80	10 (23%)	48,85,113	1.38	7 (14%)
17	CLA	3	303	-	42,50,73	2.82	10 (23%)	48,85,113	1.48	8 (16%)
17	CLA	B	821	-	46,54,73	2.76	10 (21%)	53,90,113	1.37	7 (13%)
17	CLA	A	826	-	42,50,73	2.59	9 (21%)	48,85,113	1.44	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	A	841	-	52,60,73	2.49	9 (17%)	60,97,113	1.48	10 (16%)
17	CLA	8	601	11	42,50,73	2.75	11 (26%)	48,85,113	1.51	7 (14%)
17	CLA	B	822	-	42,50,73	2.68	10 (23%)	48,85,113	1.47	8 (16%)
17	CLA	6	608	-	42,50,73	2.54	8 (19%)	48,85,113	1.53	9 (18%)
17	CLA	B	819	-	42,50,73	2.79	9 (21%)	48,85,113	1.71	10 (20%)
17	CLA	A	821	-	51,59,73	2.46	9 (17%)	59,96,113	1.58	10 (16%)
17	CLA	B	835	-	43,51,73	2.64	9 (20%)	49,86,113	1.47	8 (16%)
17	CLA	B	808	-	42,50,73	2.69	10 (23%)	48,85,113	1.53	8 (16%)
17	CLA	A	813	-	42,50,73	2.80	11 (26%)	48,85,113	1.54	10 (20%)
17	CLA	B	809	-	42,50,73	2.82	10 (23%)	48,85,113	1.57	7 (14%)
19	SF4	B	803	-	0,12,12	-	-	-	-	-
17	CLA	A	822	-	42,50,73	2.71	10 (23%)	48,85,113	1.64	9 (18%)
17	CLA	B	825	-	42,50,73	2.79	10 (23%)	48,85,113	1.43	8 (16%)
17	CLA	B	815	-	65,73,73	2.29	8 (12%)	76,113,113	1.62	14 (18%)
17	CLA	A	837	-	42,50,73	2.73	11 (26%)	48,85,113	1.49	7 (14%)
17	CLA	A	825	-	42,50,73	2.60	10 (23%)	48,85,113	1.67	9 (18%)
17	CLA	1	610	-	42,50,73	2.80	9 (21%)	48,85,113	1.46	8 (16%)
17	CLA	B	831	-	42,50,73	2.84	10 (23%)	48,85,113	1.78	9 (18%)
17	CLA	5	307	-	42,50,73	2.75	9 (21%)	48,85,113	1.48	8 (16%)
17	CLA	3	311	-	42,50,73	2.83	9 (21%)	48,85,113	1.45	8 (16%)
20	CHL	6	605	-	43,51,74	2.53	10 (23%)	45,86,114	1.78	9 (20%)
17	CLA	A	836	-	42,50,73	2.75	10 (23%)	48,85,113	1.53	8 (16%)
17	CLA	B	812	-	42,50,73	2.72	10 (23%)	48,85,113	2.04	10 (20%)
20	CHL	Z	601	12	43,51,74	2.50	10 (23%)	45,86,114	1.74	7 (15%)
17	CLA	A	833	-	42,50,73	2.74	10 (23%)	48,85,113	1.61	8 (16%)
17	CLA	A	828	-	42,50,73	2.74	10 (23%)	48,85,113	1.41	8 (16%)
17	CLA	5	312	-	42,50,73	2.71	10 (23%)	48,85,113	1.45	8 (16%)
17	CLA	A	803	-	42,50,73	2.75	10 (23%)	48,85,113	1.61	7 (14%)
17	CLA	7	614	10	42,50,73	2.72	9 (21%)	48,85,113	1.90	11 (22%)
17	CLA	B	839	-	42,50,73	2.67	9 (21%)	48,85,113	1.50	8 (16%)
17	CLA	B	829	-	43,51,73	2.55	9 (20%)	49,86,113	1.59	9 (18%)
20	CHL	5	305	-	46,54,74	2.33	11 (23%)	49,90,114	1.85	9 (18%)
20	CHL	6	606	-	43,51,74	2.45	11 (25%)	45,86,114	1.86	8 (17%)
20	CHL	1	601	8	53,61,74	2.25	10 (18%)	57,98,114	1.54	7 (12%)
17	CLA	3	306	-	42,50,73	2.69	9 (21%)	48,85,113	1.95	13 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	B	826	-	42,50,73	2.62	9 (21%)	48,85,113	1.79	7 (14%)
17	CLA	5	311	-	42,50,73	2.74	9 (21%)	48,85,113	1.50	8 (16%)
17	CLA	A	843	-	42,50,73	2.73	11 (26%)	48,85,113	1.39	7 (14%)
17	CLA	4	601	-	42,50,73	2.73	10 (23%)	48,85,113	1.53	8 (16%)
17	CLA	5	308	-	42,50,73	2.49	8 (19%)	48,85,113	1.46	7 (14%)
17	CLA	3	309	-	45,53,73	2.54	8 (17%)	52,89,113	1.47	7 (13%)
17	CLA	3	302	-	42,50,73	2.78	10 (23%)	48,85,113	1.45	8 (16%)
17	CLA	5	309	-	42,50,73	2.69	10 (23%)	48,85,113	1.64	8 (16%)
17	CLA	8	607	-	42,50,73	2.71	11 (26%)	48,85,113	1.54	8 (16%)
17	CLA	B	806	-	42,50,73	2.81	10 (23%)	48,85,113	2.02	12 (25%)
18	PQN	A	840	-	34,34,34	0.21	0	42,45,45	0.26	0
17	CLA	7	603	-	42,50,73	2.77	9 (21%)	48,85,113	1.74	10 (20%)
17	CLA	A	814	-	42,50,73	2.70	11 (26%)	48,85,113	1.46	7 (14%)
17	CLA	A	817	-	42,50,73	2.75	9 (21%)	48,85,113	1.73	10 (20%)
17	CLA	F	301	-	42,50,73	2.67	9 (21%)	48,85,113	1.61	9 (18%)
17	CLA	B	833	-	42,50,73	2.67	9 (21%)	48,85,113	1.53	8 (16%)
17	CLA	1	607	-	42,50,73	2.83	8 (19%)	48,85,113	1.94	9 (18%)
17	CLA	1	609	-	42,50,73	2.90	8 (19%)	48,85,113	1.39	7 (14%)
17	CLA	5	310	-	42,50,73	2.82	11 (26%)	48,85,113	1.42	8 (16%)
17	CLA	8	611	-	42,50,73	2.79	10 (23%)	48,85,113	1.59	7 (14%)
17	CLA	8	613	-	42,50,73	2.67	10 (23%)	48,85,113	1.51	8 (16%)
17	CLA	B	823	-	42,50,73	2.78	10 (23%)	48,85,113	1.58	10 (20%)
17	CLA	B	801	-	42,50,73	2.49	8 (19%)	48,85,113	1.72	9 (18%)
17	CLA	J	101	-	42,50,73	2.83	11 (26%)	48,85,113	1.62	9 (18%)
17	CLA	B	805	-	42,50,73	2.66	7 (16%)	48,85,113	1.55	8 (16%)
17	CLA	5	302	14	42,50,73	2.76	10 (23%)	48,85,113	1.48	8 (16%)
17	CLA	5	306	-	50,58,73	2.55	9 (18%)	58,95,113	1.36	7 (12%)
17	CLA	5	315	-	45,53,73	2.63	10 (22%)	52,89,113	1.53	8 (15%)
17	CLA	3	313	-	42,50,73	2.73	10 (23%)	48,85,113	1.77	10 (20%)
17	CLA	A	824	-	42,50,73	2.62	10 (23%)	48,85,113	1.73	9 (18%)
17	CLA	A	842	-	42,50,73	2.64	7 (16%)	48,85,113	1.34	9 (18%)
17	CLA	A	838	-	42,50,73	2.76	9 (21%)	48,85,113	1.67	10 (20%)
17	CLA	B	820	-	42,50,73	2.65	8 (19%)	48,85,113	1.62	9 (18%)
17	CLA	B	818	-	42,50,73	2.72	9 (21%)	48,85,113	1.66	10 (20%)
17	CLA	B	836	-	42,50,73	2.74	10 (23%)	48,85,113	1.61	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	A	818	-	45,53,73	2.65	10 (22%)	52,89,113	1.48	9 (17%)
17	CLA	8	612	-	46,54,73	2.68	10 (21%)	53,90,113	1.39	7 (13%)
17	CLA	A	835	-	42,50,73	2.69	11 (26%)	48,85,113	1.46	9 (18%)
17	CLA	7	610	-	41,49,73	2.88	10 (24%)	47,84,113	2.00	11 (23%)
17	CLA	7	602	-	42,50,73	2.71	10 (23%)	48,85,113	1.51	8 (16%)
17	CLA	A	812	-	42,50,73	2.76	11 (26%)	48,85,113	1.49	8 (16%)
17	CLA	3	312	-	42,50,73	2.67	9 (21%)	48,85,113	1.63	8 (16%)
17	CLA	7	608	-	42,50,73	2.76	8 (19%)	48,85,113	1.59	8 (16%)
17	CLA	8	614	11	42,50,73	2.79	10 (23%)	48,85,113	1.65	8 (16%)
17	CLA	6	609	15	46,54,73	2.73	10 (21%)	53,90,113	1.42	8 (15%)
17	CLA	4	602	-	45,53,73	2.69	7 (15%)	52,89,113	1.45	8 (15%)
17	CLA	6	601	15	42,50,73	2.80	10 (23%)	48,85,113	1.47	8 (16%)
17	CLA	5	303	-	48,56,73	2.49	9 (18%)	55,92,113	1.33	8 (14%)
17	CLA	A	805	-	42,50,73	2.80	10 (23%)	48,85,113	1.69	9 (18%)
17	CLA	A	827	-	42,50,73	2.66	11 (26%)	48,85,113	1.49	9 (18%)
17	CLA	3	304	-	45,53,73	2.60	9 (20%)	52,89,113	1.39	8 (15%)
17	CLA	4	603	-	42,50,73	2.82	8 (19%)	48,85,113	1.94	10 (20%)
17	CLA	A	820	-	42,50,73	2.90	10 (23%)	48,85,113	1.50	6 (12%)
17	CLA	1	605	-	42,50,73	2.85	9 (21%)	48,85,113	1.52	9 (18%)

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	B	838	-	1/1/10/20	2/10/88/115	-
17	CLA	5	314	-	1/1/11/20	7/15/93/115	-
17	CLA	A	839	-	1/1/10/20	1/10/88/115	-
20	CHL	6	607	-	3/3/15/26	2/12/110/137	-
17	CLA	B	807	-	1/1/10/20	4/10/88/115	-
17	CLA	4	605	-	1/1/11/20	1/13/91/115	-
17	CLA	8	610	-	1/1/10/20	3/10/88/115	-
17	CLA	8	604	-	1/1/10/20	0/10/88/115	-
17	CLA	A	829	-	1/1/10/20	3/10/88/115	-
17	CLA	B	816	-	1/1/10/20	3/10/88/115	-
17	CLA	B	813	-	1/1/10/20	1/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	B	828	-	1/1/10/20	1/11/89/115	-
17	CLA	3	308	-	1/1/10/20	1/10/88/115	-
17	CLA	A	816	-	1/1/10/20	3/10/88/115	-
19	SF4	C	102	-	-	-	0/6/5/5
17	CLA	1	603	-	1/1/10/20	2/10/88/115	-
17	CLA	7	601	10	1/1/10/20	3/10/88/115	-
17	CLA	A	809	-	1/1/10/20	2/10/88/115	-
20	CHL	3	307	-	3/3/16/26	5/15/113/137	-
17	CLA	B	804	-	1/1/10/20	1/10/88/115	-
17	CLA	B	814	-	1/1/9/20	0/4/82/115	-
17	CLA	B	832	-	1/1/10/20	2/10/88/115	-
17	CLA	7	613	-	1/1/10/20	1/11/89/115	-
20	CHL	5	313	-	3/3/15/26	2/12/110/137	-
17	CLA	A	806	-	1/1/10/20	1/10/88/115	-
17	CLA	6	610	-	1/1/11/20	3/13/91/115	-
17	CLA	A	808	-	1/1/10/20	0/10/88/115	-
17	CLA	7	604	-	1/1/10/20	0/10/88/115	-
17	CLA	F	302	-	1/1/14/20	8/34/112/115	-
17	CLA	J	102	-	1/1/10/20	2/10/88/115	-
17	CLA	7	609	-	1/1/10/20	1/10/88/115	-
17	CLA	A	810	-	1/1/10/20	1/10/88/115	-
17	CLA	A	823	-	1/1/10/20	3/10/88/115	-
17	CLA	7	605	-	1/1/10/20	3/10/88/115	-
18	PQN	B	840	-	-	4/23/43/43	0/2/2/2
17	CLA	B	810	-	1/1/11/20	5/13/91/115	-
17	CLA	3	310	-	1/1/10/20	2/8/86/115	-
17	CLA	B	830	-	1/1/10/20	2/10/88/115	-
17	CLA	8	602	-	1/1/10/20	3/10/88/115	-
17	CLA	B	802	-	1/1/11/20	5/13/91/115	-
17	CLA	8	605	-	1/1/10/20	2/10/88/115	-
17	CLA	A	815	-	1/1/10/20	0/10/88/115	-
20	CHL	8	606	-	3/3/15/26	0/12/110/137	-
17	CLA	B	827	-	1/1/10/20	4/10/88/115	-
17	CLA	1	604	-	1/1/10/20	1/10/88/115	-
17	CLA	3	305	-	1/1/10/20	1/10/88/115	-
19	SF4	C	101	-	-	-	0/6/5/5
17	CLA	A	802	-	1/1/10/20	4/10/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	A	807	-	1/1/10/20	2/10/88/115	-
16	CL0	A	801	-	3/3/15/25	3/10/108/135	-
17	CLA	3	301	-	1/1/10/20	3/10/88/115	-
17	CLA	B	817	-	1/1/10/20	3/10/88/115	-
17	CLA	A	831	-	1/1/10/20	3/10/88/115	-
17	CLA	6	604	-	1/1/10/20	0/10/88/115	-
17	CLA	5	301	-	1/1/10/20	2/10/88/115	-
17	CLA	B	811	-	1/1/10/20	0/10/88/115	-
17	CLA	1	602	-	1/1/10/20	3/10/88/115	-
17	CLA	A	830	-	1/1/10/20	1/10/88/115	-
17	CLA	4	604	-	1/1/10/20	1/10/88/115	-
17	CLA	8	609	-	1/1/10/20	1/10/88/115	-
17	CLA	8	608	-	1/1/10/20	0/10/88/115	-
17	CLA	B	837	-	1/1/10/20	1/10/88/115	-
17	CLA	A	832	-	1/1/10/20	4/8/86/115	-
17	CLA	A	819	-	1/1/10/20	2/10/88/115	-
17	CLA	7	607	-	1/1/10/20	3/10/88/115	-
17	CLA	7	612	-	1/1/11/20	4/13/91/115	-
17	CLA	A	804	-	1/1/10/20	3/10/88/115	-
17	CLA	A	811	-	1/1/10/20	2/10/88/115	-
17	CLA	B	834	-	1/1/10/20	5/10/88/115	-
17	CLA	6	602	-	1/1/10/20	3/10/88/115	-
17	CLA	6	603	-	1/1/10/20	3/10/88/115	-
17	CLA	1	606	-	1/1/10/20	0/10/88/115	-
20	CHL	7	606	-	3/3/15/26	0/12/110/137	-
17	CLA	1	608	-	1/1/10/20	3/10/88/115	-
17	CLA	A	834	1	1/1/10/20	0/10/88/115	-
17	CLA	7	611	-	1/1/10/20	3/10/88/115	-
17	CLA	8	603	-	1/1/11/20	2/13/91/115	-
17	CLA	B	824	-	1/1/10/20	1/8/86/115	-
17	CLA	5	304	-	1/1/10/20	2/10/88/115	-
17	CLA	3	303	-	1/1/10/20	0/10/88/115	-
17	CLA	B	821	-	1/1/11/20	3/15/93/115	-
17	CLA	A	826	-	1/1/10/20	0/10/88/115	-
17	CLA	A	841	-	1/1/12/20	9/22/100/115	-
17	CLA	8	601	11	1/1/10/20	1/10/88/115	-
17	CLA	B	822	-	1/1/10/20	3/10/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	6	608	-	1/1/10/20	2/10/88/115	-
17	CLA	B	819	-	1/1/10/20	3/10/88/115	-
17	CLA	A	821	-	1/1/12/20	5/21/99/115	-
17	CLA	B	835	-	1/1/10/20	3/11/89/115	-
17	CLA	B	808	-	1/1/10/20	1/10/88/115	-
17	CLA	A	813	-	1/1/10/20	3/10/88/115	-
17	CLA	B	809	-	1/1/10/20	4/10/88/115	-
19	SF4	B	803	-	-	-	0/6/5/5
17	CLA	A	822	-	1/1/10/20	2/10/88/115	-
17	CLA	B	825	-	1/1/10/20	4/10/88/115	-
17	CLA	B	815	-	1/1/15/20	10/37/115/115	-
17	CLA	A	837	-	1/1/10/20	3/10/88/115	-
17	CLA	A	825	-	1/1/10/20	2/10/88/115	-
17	CLA	1	610	-	1/1/10/20	3/10/88/115	-
17	CLA	B	831	-	1/1/10/20	0/10/88/115	-
17	CLA	5	307	-	1/1/10/20	3/10/88/115	-
17	CLA	3	311	-	1/1/10/20	3/10/88/115	-
20	CHL	6	605	-	3/3/15/26	1/12/110/137	-
17	CLA	A	836	-	1/1/10/20	2/10/88/115	-
17	CLA	B	812	-	1/1/10/20	4/10/88/115	-
20	CHL	Z	601	12	3/3/15/26	3/12/110/137	-
17	CLA	A	833	-	1/1/10/20	1/10/88/115	-
17	CLA	A	828	-	1/1/10/20	1/10/88/115	-
17	CLA	5	312	-	1/1/10/20	1/10/88/115	-
17	CLA	A	803	-	1/1/10/20	2/10/88/115	-
17	CLA	7	614	10	1/1/10/20	2/10/88/115	-
17	CLA	B	839	-	1/1/10/20	1/10/88/115	-
17	CLA	B	829	-	1/1/10/20	5/11/89/115	-
20	CHL	5	305	-	3/3/16/26	3/15/113/137	-
20	CHL	6	606	-	3/3/15/26	3/12/110/137	-
20	CHL	1	601	8	3/3/17/26	6/24/122/137	-
17	CLA	3	306	-	1/1/10/20	2/10/88/115	-
17	CLA	B	826	-	1/1/10/20	2/10/88/115	-
17	CLA	5	311	-	1/1/10/20	3/10/88/115	-
17	CLA	A	843	-	1/1/10/20	2/10/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	4	601	-	1/1/10/20	2/10/88/115	-
17	CLA	5	308	-	1/1/10/20	3/10/88/115	-
17	CLA	3	309	-	1/1/11/20	0/13/91/115	-
17	CLA	3	302	-	1/1/10/20	2/10/88/115	-
17	CLA	5	309	-	1/1/10/20	3/10/88/115	-
17	CLA	8	607	-	1/1/10/20	2/10/88/115	-
17	CLA	B	806	-	1/1/10/20	2/10/88/115	-
18	PQN	A	840	-	-	5/23/43/43	0/2/2/2
17	CLA	7	603	-	1/1/10/20	2/10/88/115	-
17	CLA	A	814	-	1/1/10/20	1/10/88/115	-
17	CLA	A	817	-	1/1/10/20	2/10/88/115	-
17	CLA	F	301	-	1/1/10/20	2/10/88/115	-
17	CLA	B	833	-	1/1/10/20	1/10/88/115	-
17	CLA	1	607	-	1/1/10/20	3/10/88/115	-
17	CLA	1	609	-	1/1/10/20	2/10/88/115	-
17	CLA	5	310	-	1/1/10/20	0/10/88/115	-
17	CLA	8	611	-	1/1/10/20	3/10/88/115	-
17	CLA	8	613	-	1/1/10/20	3/10/88/115	-
17	CLA	B	823	-	1/1/10/20	4/10/88/115	-
17	CLA	B	801	-	1/1/10/20	3/10/88/115	-
17	CLA	J	101	-	1/1/10/20	4/10/88/115	-
17	CLA	B	805	-	1/1/10/20	0/10/88/115	-
17	CLA	5	302	14	1/1/10/20	2/10/88/115	-
17	CLA	5	306	-	1/1/12/20	3/19/97/115	-
17	CLA	5	315	-	1/1/11/20	4/13/91/115	-
17	CLA	3	313	-	1/1/10/20	1/10/88/115	-
17	CLA	A	824	-	1/1/10/20	0/10/88/115	-
17	CLA	A	842	-	1/1/10/20	3/10/88/115	-
17	CLA	A	838	-	1/1/10/20	2/10/88/115	-
17	CLA	B	820	-	1/1/10/20	3/10/88/115	-
17	CLA	B	818	-	1/1/10/20	3/10/88/115	-
17	CLA	B	836	-	1/1/10/20	2/10/88/115	-
17	CLA	A	818	-	1/1/11/20	3/13/91/115	-
17	CLA	8	612	-	1/1/11/20	0/15/93/115	-
17	CLA	A	835	-	1/1/10/20	4/10/88/115	-
17	CLA	7	610	-	1/1/10/20	3/8/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	7	602	-	1/1/10/20	3/10/88/115	-
17	CLA	A	812	-	1/1/10/20	2/10/88/115	-
17	CLA	3	312	-	1/1/10/20	1/10/88/115	-
17	CLA	7	608	-	1/1/10/20	1/10/88/115	-
17	CLA	8	614	11	1/1/10/20	1/10/88/115	-
17	CLA	6	609	15	1/1/11/20	1/15/93/115	-
17	CLA	4	602	-	1/1/11/20	4/13/91/115	-
17	CLA	6	601	15	1/1/10/20	3/10/88/115	-
17	CLA	5	303	-	1/1/11/20	5/17/95/115	-
17	CLA	A	805	-	1/1/10/20	2/10/88/115	-
17	CLA	A	827	-	1/1/10/20	0/10/88/115	-
17	CLA	3	304	-	1/1/11/20	2/13/91/115	-
17	CLA	4	603	-	1/1/10/20	4/10/88/115	-
17	CLA	A	820	-	1/1/10/20	4/10/88/115	-
17	CLA	1	605	-	1/1/10/20	2/10/88/115	-

The worst 5 of 1588 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	608	CLA	C4B-NB	14.91	1.48	1.35
17	7	604	CLA	C4B-NB	14.47	1.48	1.35
17	B	821	CLA	C4B-NB	14.31	1.48	1.35
17	B	814	CLA	C4B-NB	14.30	1.48	1.35
17	1	609	CLA	C4B-NB	14.16	1.47	1.35

The worst 5 of 1401 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	804	CLA	C4A-NA-C1A	-9.73	102.33	106.71
17	3	310	CLA	C4A-NA-C1A	-9.32	102.52	106.71
17	A	832	CLA	C1C-NC-C4C	-9.00	102.66	106.71
17	B	815	CLA	C4A-NA-C1A	-8.93	102.69	106.71
17	B	812	CLA	C4A-NA-C1A	-8.85	102.72	106.71

5 of 188 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
16	A	801	CL0	NA
16	A	801	CL0	ND

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

5 of 396 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	A	802	CLA	C1A-C2A-CAA-CBA
17	A	802	CLA	CHA-CBD-CGD-O1D
17	A	802	CLA	CHA-CBD-CGD-O2D
17	A	803	CLA	CHA-CBD-CGD-O1D
17	A	803	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

118 monomers are involved in 179 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	B	838	CLA	1	0
17	A	839	CLA	1	0
20	6	607	CHL	1	0
17	B	807	CLA	2	0
17	4	605	CLA	2	0
17	8	610	CLA	1	0
17	8	604	CLA	2	0
17	A	829	CLA	1	0
17	B	816	CLA	1	0
17	B	828	CLA	4	0
19	C	102	SF4	2	0
17	1	603	CLA	2	0
17	A	809	CLA	3	0
20	3	307	CHL	1	0
17	B	804	CLA	3	0
17	B	814	CLA	2	0
17	B	832	CLA	1	0
17	7	613	CLA	1	0
20	5	313	CHL	1	0
17	A	806	CLA	5	0
17	6	610	CLA	1	0
17	A	808	CLA	4	0
17	7	604	CLA	2	0
17	F	302	CLA	4	0
17	J	102	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	823	CLA	2	0
17	7	605	CLA	2	0
18	B	840	PQN	3	0
17	B	810	CLA	6	0
17	8	602	CLA	1	0
17	B	802	CLA	1	0
17	8	605	CLA	4	0
17	A	815	CLA	6	0
20	8	606	CHL	2	0
17	B	827	CLA	5	0
17	3	305	CLA	2	0
17	A	802	CLA	2	0
17	A	807	CLA	5	0
16	A	801	CL0	4	0
17	3	301	CLA	2	0
17	A	831	CLA	2	0
17	5	301	CLA	2	0
17	B	811	CLA	3	0
17	1	602	CLA	3	0
17	A	830	CLA	1	0
17	4	604	CLA	3	0
17	8	609	CLA	1	0
17	8	608	CLA	2	0
17	B	837	CLA	2	0
17	A	832	CLA	1	0
17	A	819	CLA	1	0
17	7	612	CLA	2	0
17	A	811	CLA	1	0
17	B	834	CLA	1	0
17	6	602	CLA	1	0
17	1	606	CLA	2	0
20	7	606	CHL	2	0
17	1	608	CLA	1	0
17	A	834	CLA	5	0
17	7	611	CLA	1	0
17	8	603	CLA	1	0
17	B	824	CLA	1	0
17	5	304	CLA	2	0
17	3	303	CLA	1	0
17	B	821	CLA	1	0
17	A	841	CLA	7	0
17	8	601	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	B	822	CLA	3	0
17	A	821	CLA	3	0
17	B	835	CLA	2	0
17	B	808	CLA	1	0
17	A	813	CLA	2	0
17	B	809	CLA	4	0
17	A	822	CLA	1	0
17	B	825	CLA	1	0
17	B	815	CLA	5	0
17	A	837	CLA	3	0
17	A	825	CLA	2	0
17	1	610	CLA	2	0
17	B	831	CLA	1	0
17	3	311	CLA	3	0
20	6	605	CHL	3	0
17	A	836	CLA	3	0
17	B	812	CLA	1	0
17	A	833	CLA	2	0
17	A	803	CLA	1	0
17	B	839	CLA	2	0
20	5	305	CHL	1	0
20	6	606	CHL	3	0
17	3	306	CLA	1	0
17	B	826	CLA	3	0
17	5	311	CLA	2	0
17	A	843	CLA	1	0
17	3	309	CLA	1	0
17	5	309	CLA	1	0
17	A	814	CLA	2	0
17	B	833	CLA	3	0
17	1	609	CLA	4	0
17	5	310	CLA	2	0
17	8	613	CLA	1	0
17	B	823	CLA	2	0
17	B	801	CLA	2	0
17	J	101	CLA	1	0
17	B	805	CLA	2	0
17	5	306	CLA	2	0
17	A	824	CLA	2	0
17	A	838	CLA	1	0
17	B	818	CLA	1	0
17	B	836	CLA	1	0

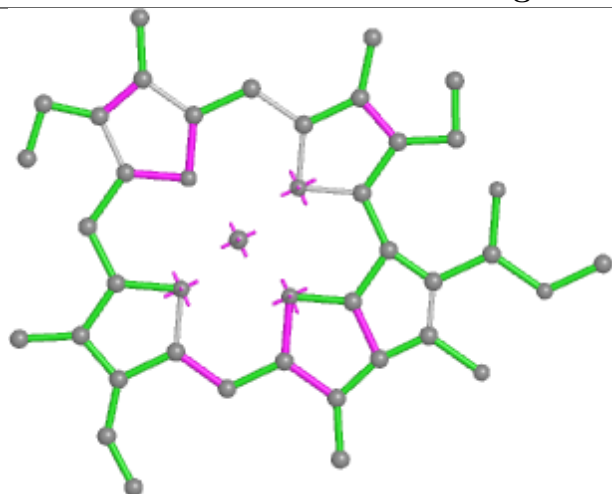
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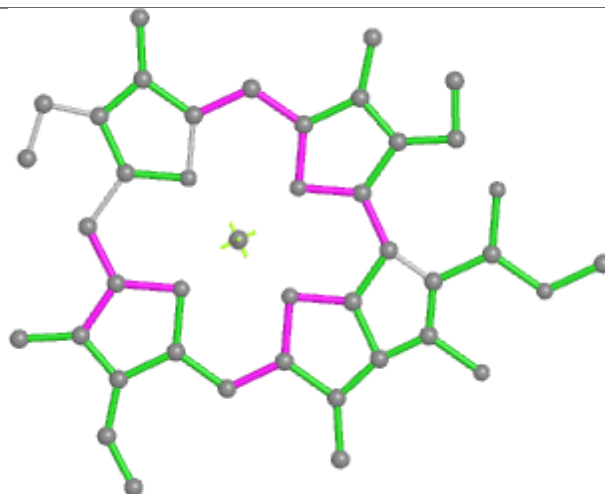
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	8	612	CLA	2	0
17	A	812	CLA	2	0
17	3	312	CLA	2	0
17	6	609	CLA	3	0
17	4	602	CLA	1	0
17	5	303	CLA	1	0
17	3	304	CLA	1	0
17	A	820	CLA	2	0
17	1	605	CLA	2	0

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

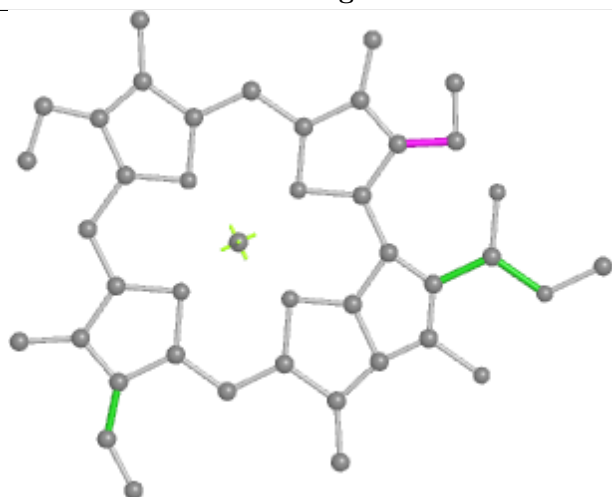
Ligand CLA B 838



Bond lengths



Bond angles

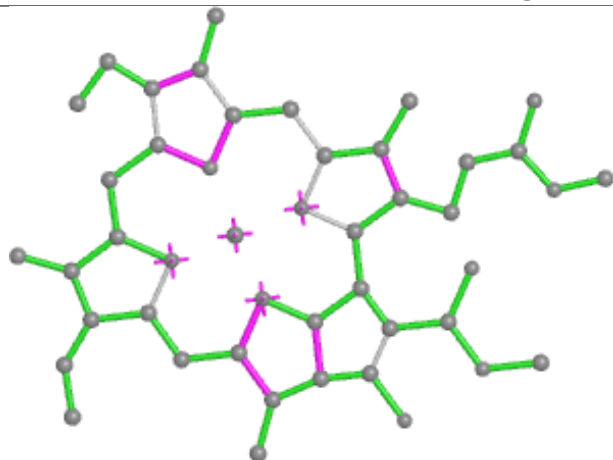


Torsions

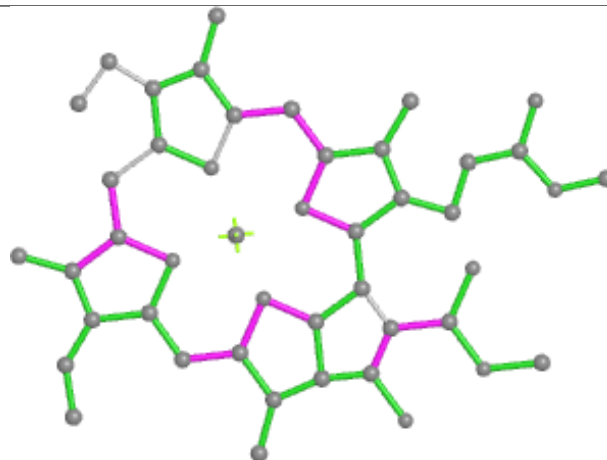


Rings

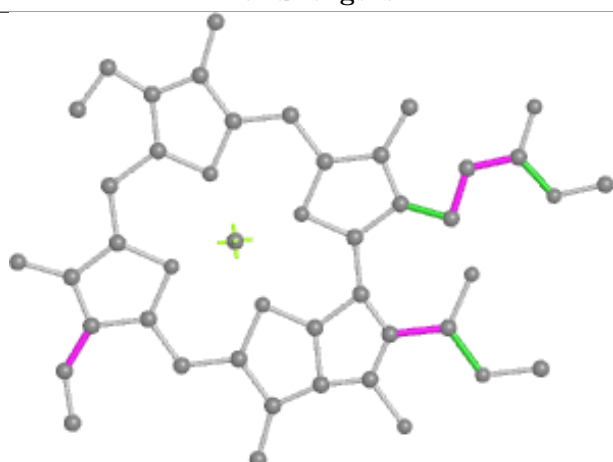
Ligand CLA 5 314



Bond lengths



Bond angles

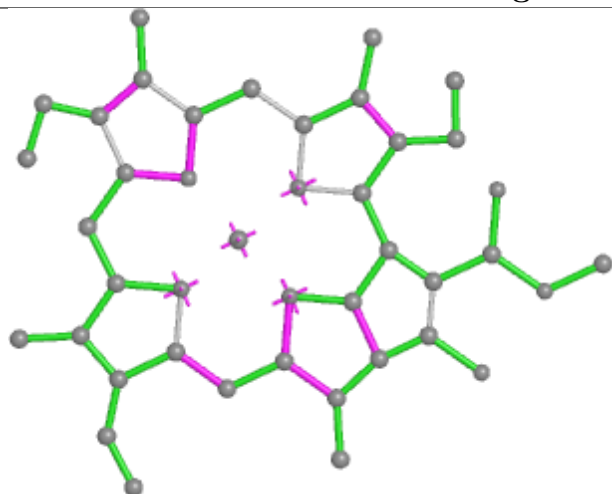


Torsions

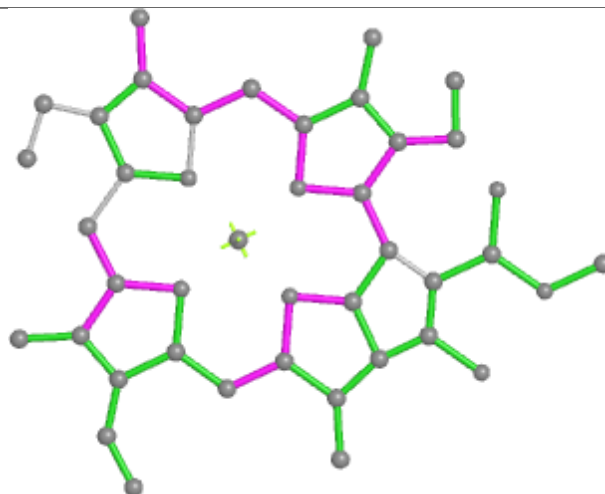


Rings

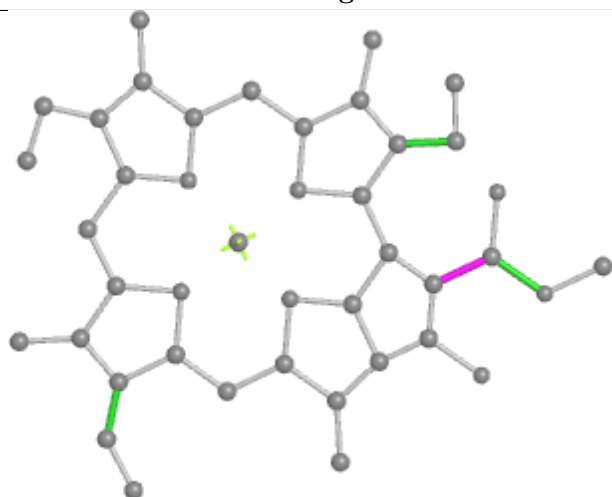
Ligand CLA A 839



Bond lengths



Bond angles

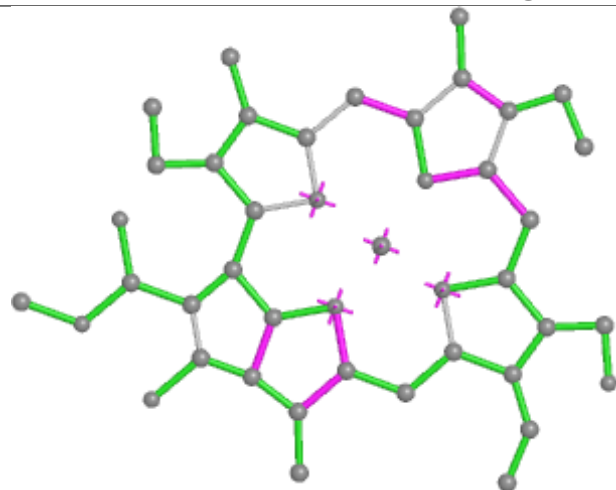


Torsions

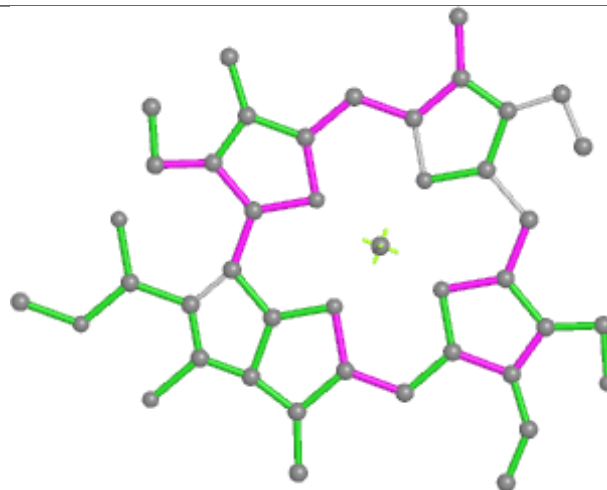


Rings

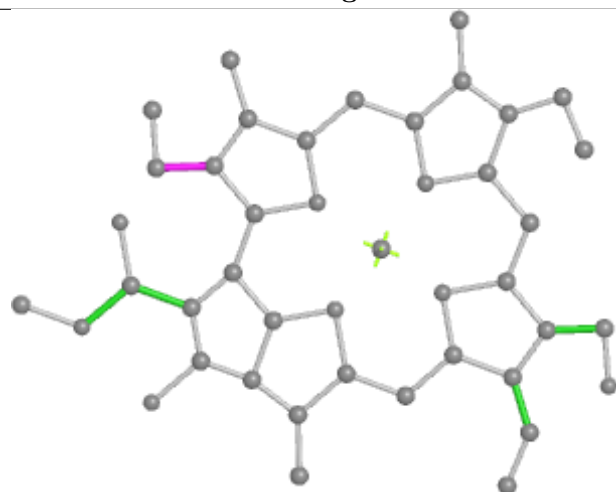
Ligand CHL 6 607



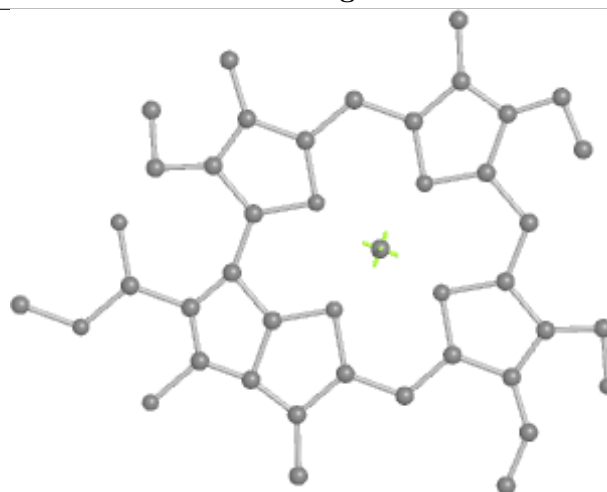
Bond lengths



Bond angles

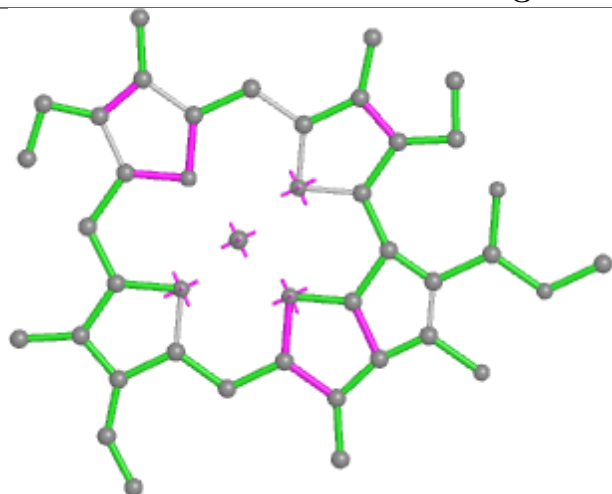


Torsions

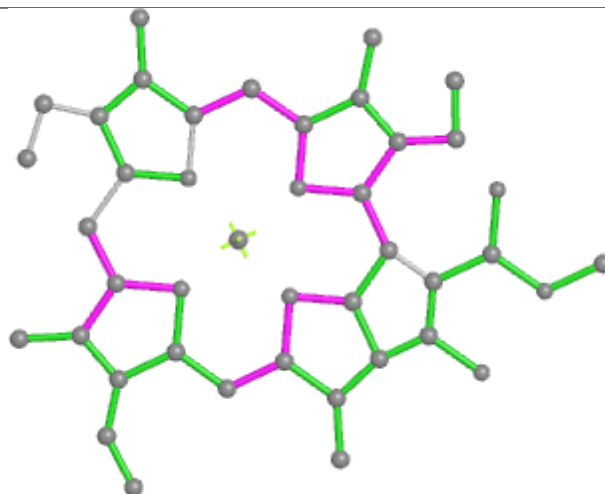


Rings

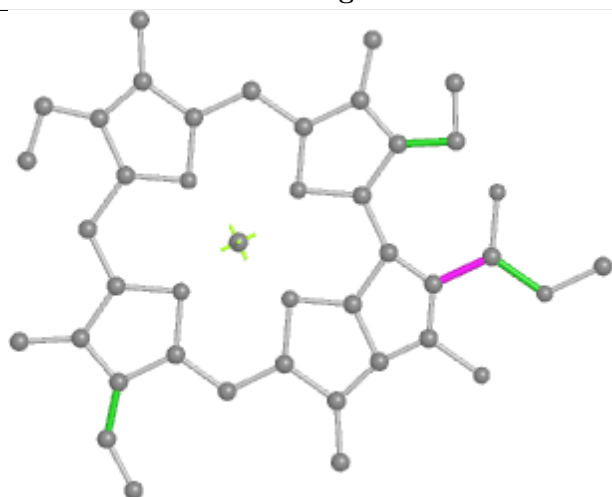
Ligand CLA B 807



Bond lengths



Bond angles

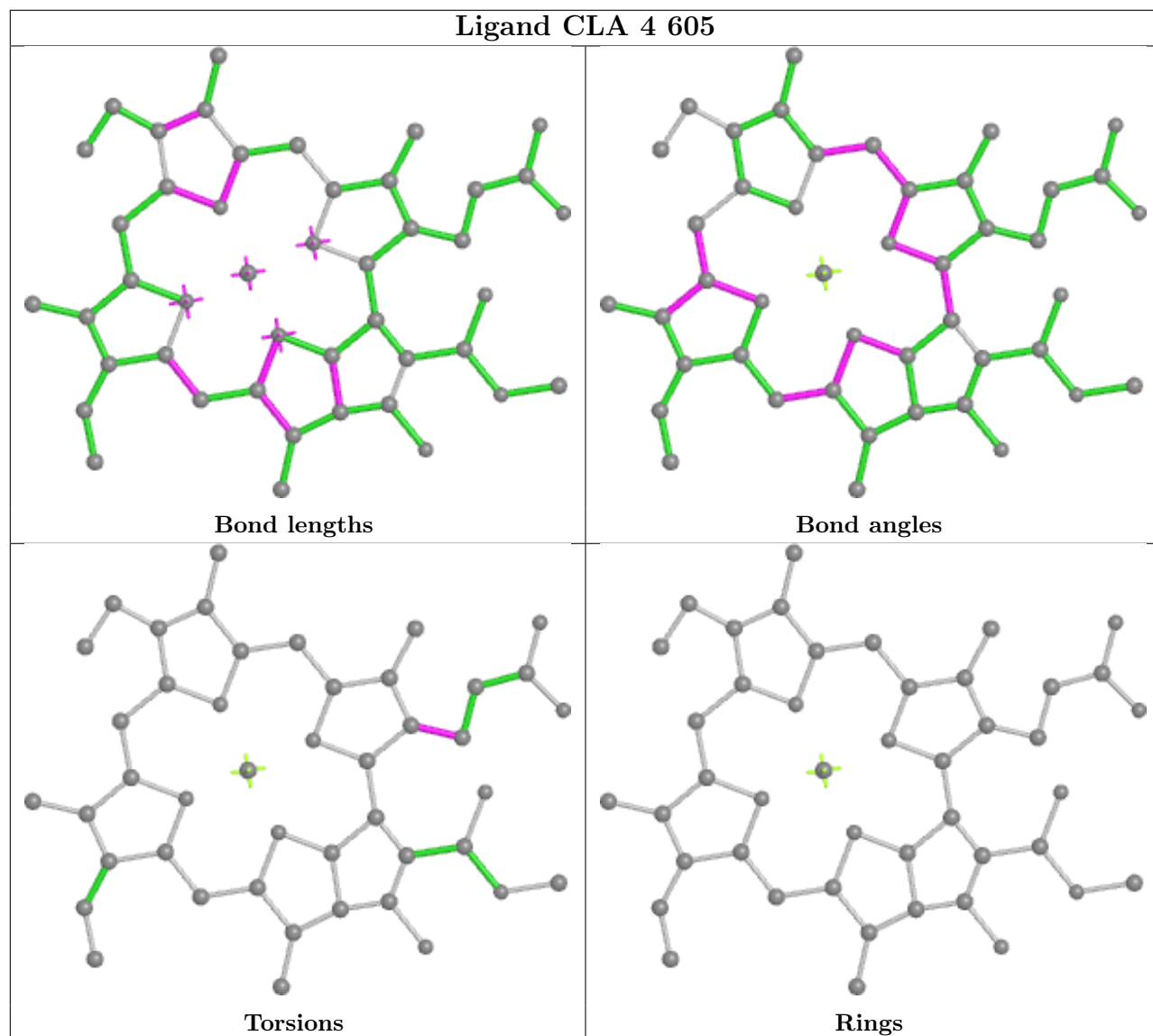


Torsions

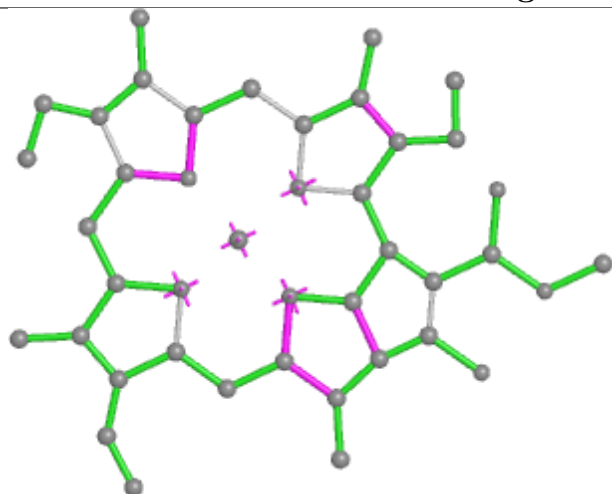


Rings

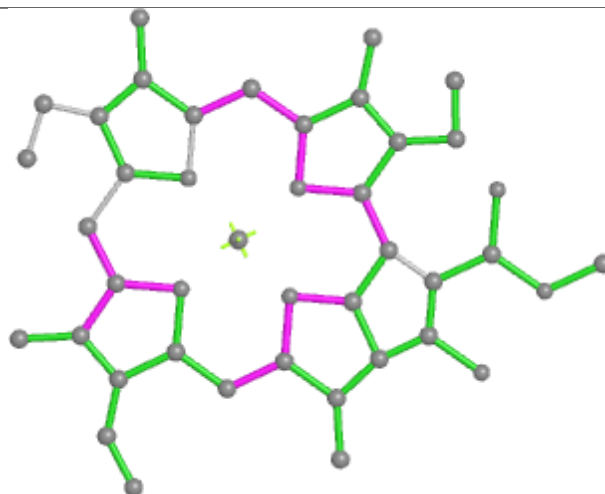
Ligand CLA 4 605



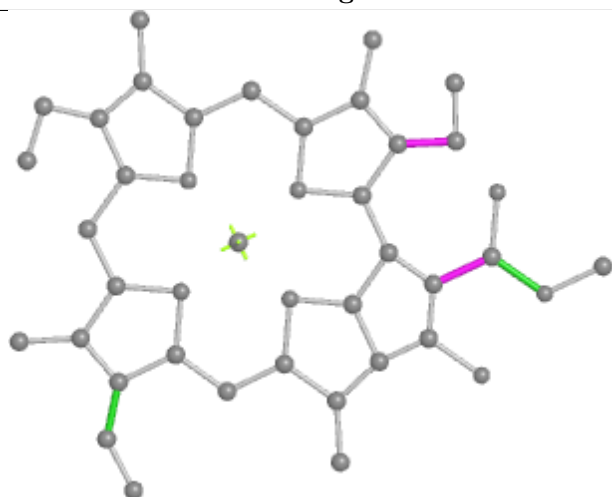
Ligand CLA 8 610



Bond lengths



Bond angles

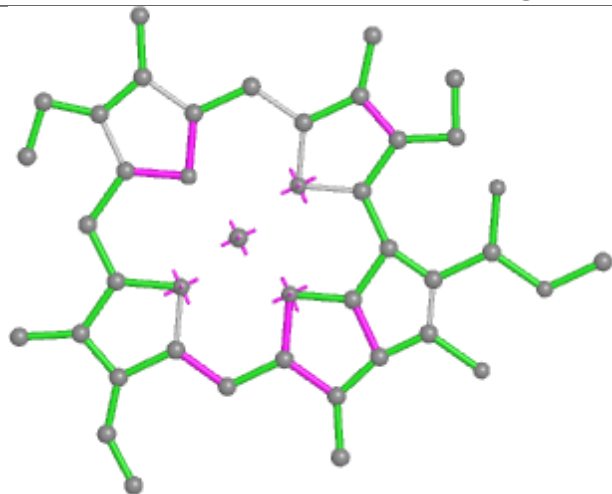


Torsions

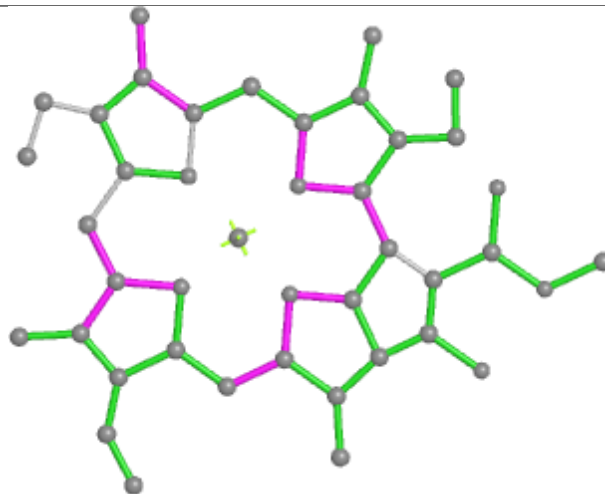


Rings

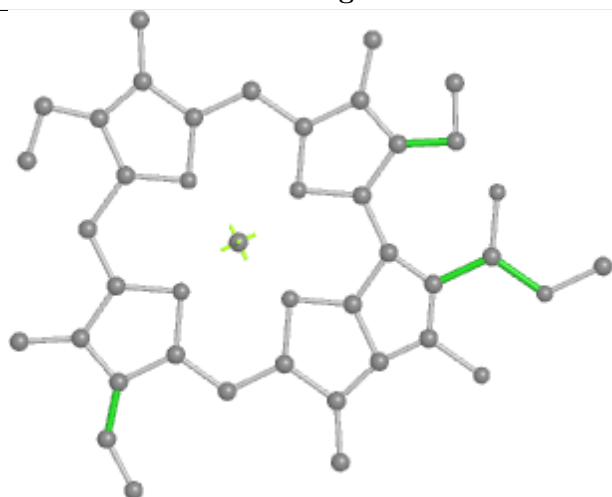
Ligand CLA 8 604



Bond lengths



Bond angles

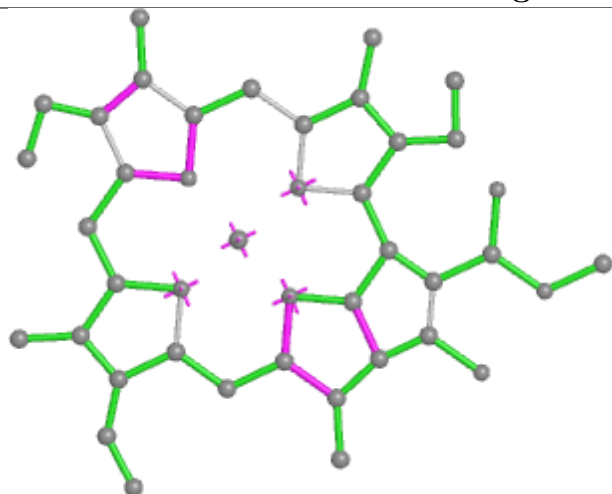


Torsions

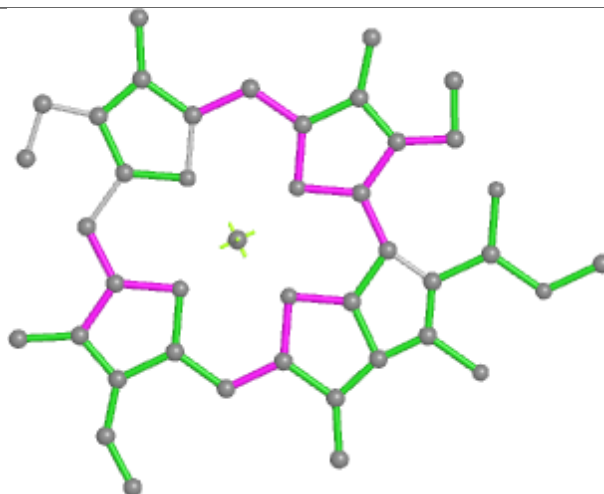


Rings

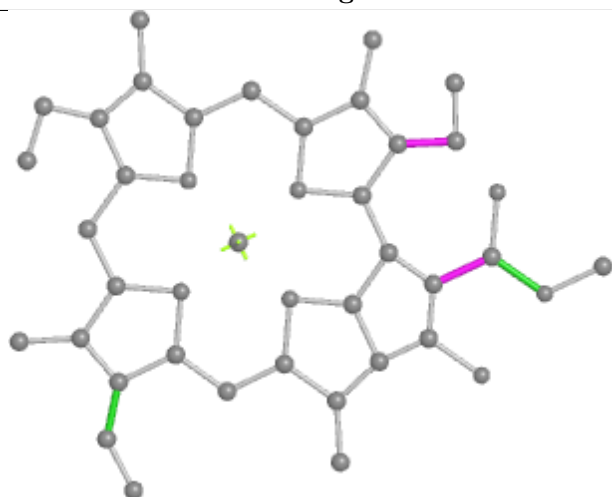
Ligand CLA A 829



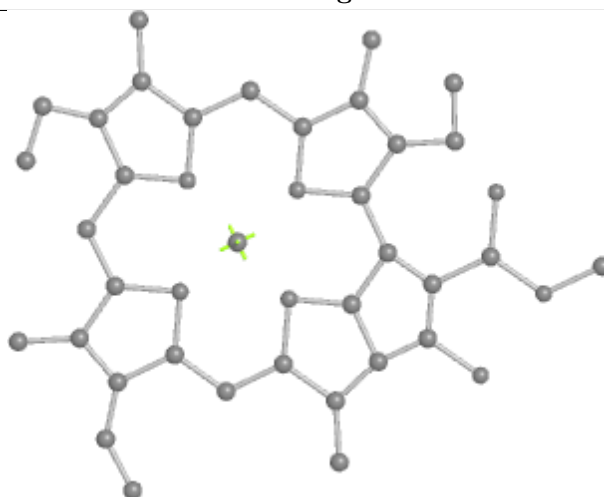
Bond lengths



Bond angles

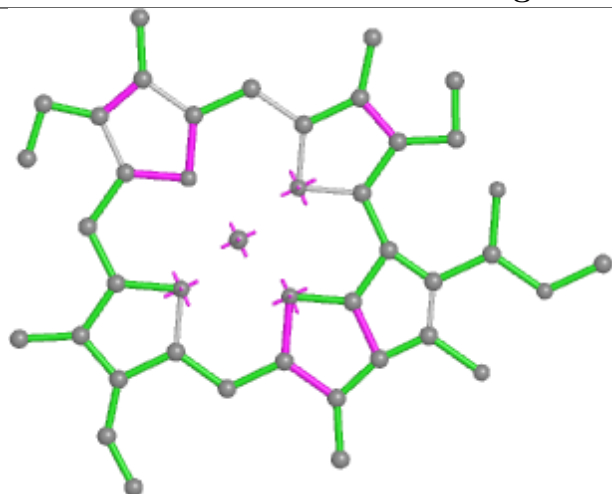


Torsions

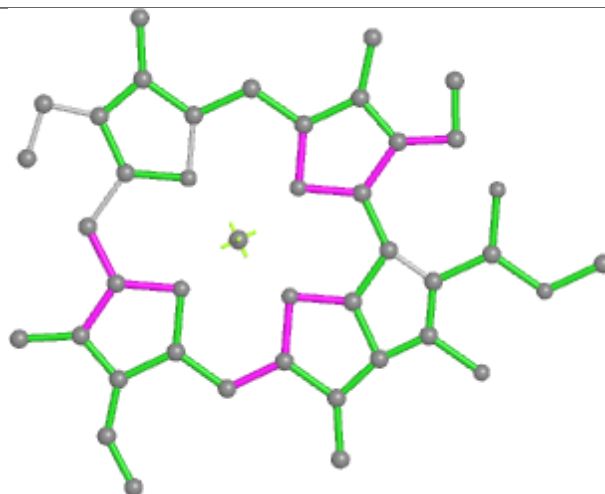


Rings

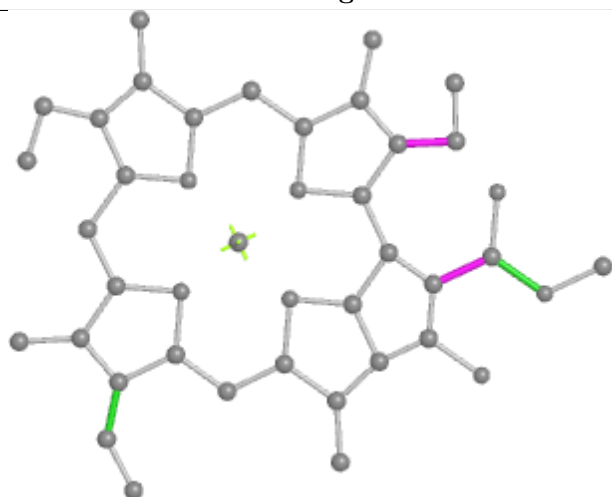
Ligand CLA B 816



Bond lengths



Bond angles

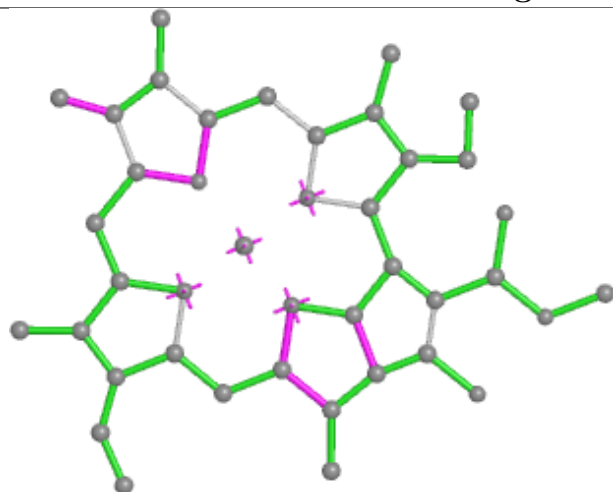


Torsions

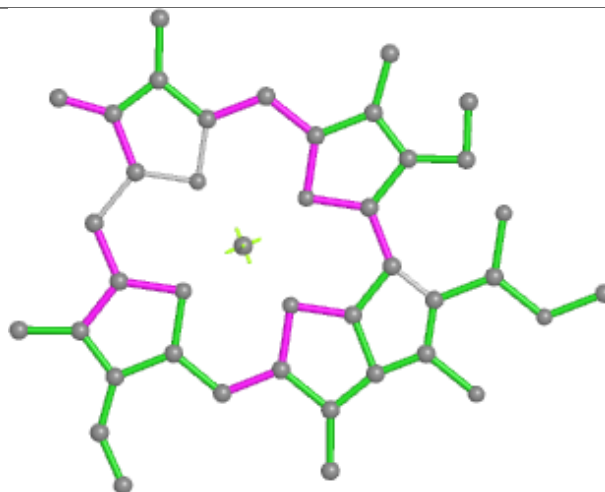


Rings

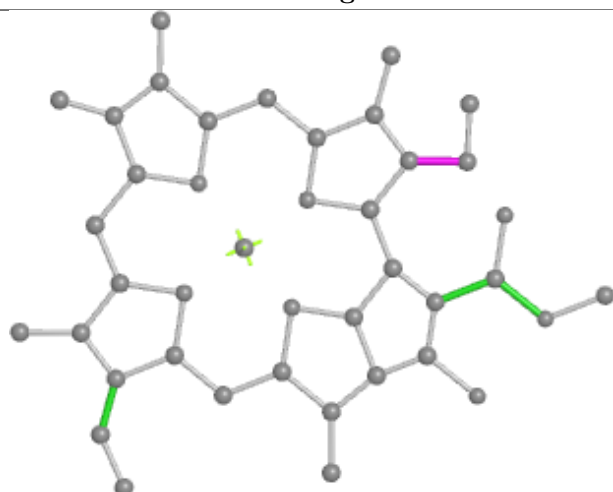
Ligand CLA B 813



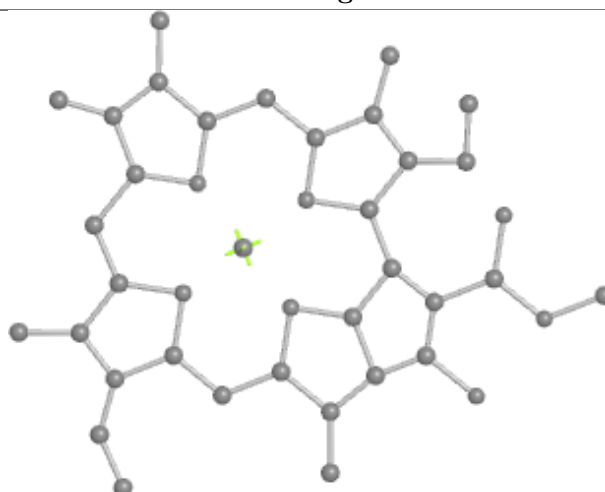
Bond lengths



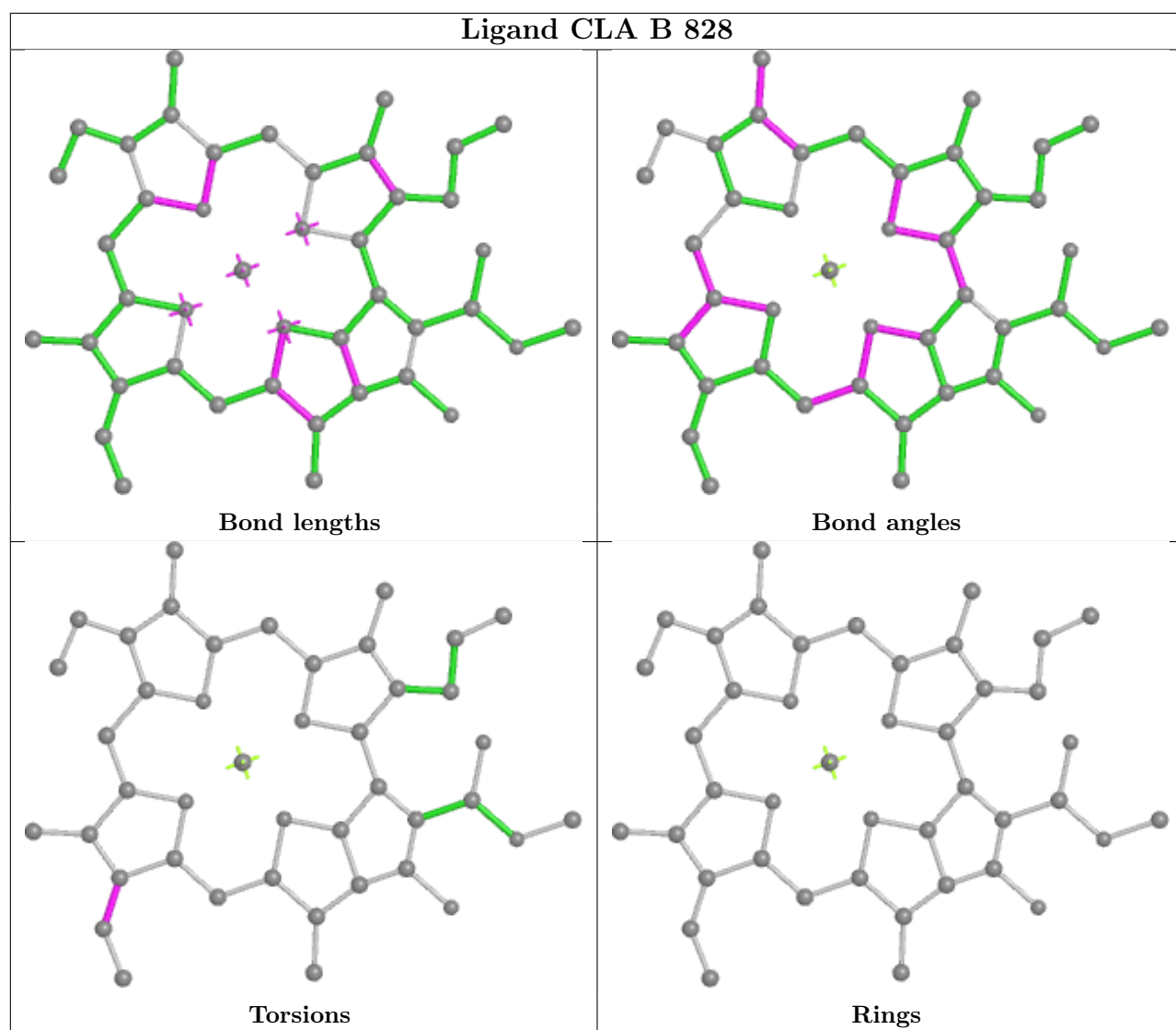
Bond angles



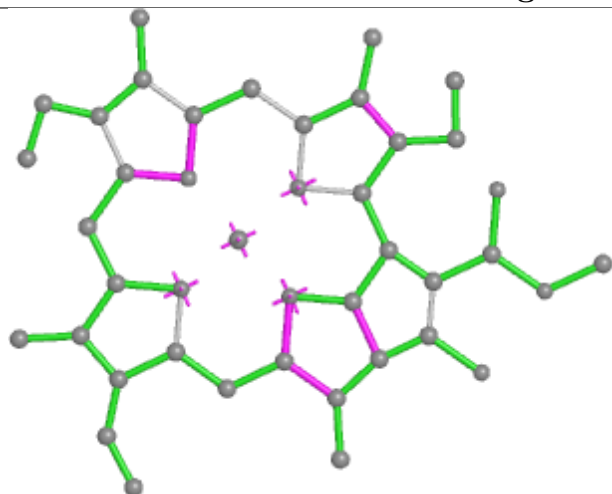
Torsions



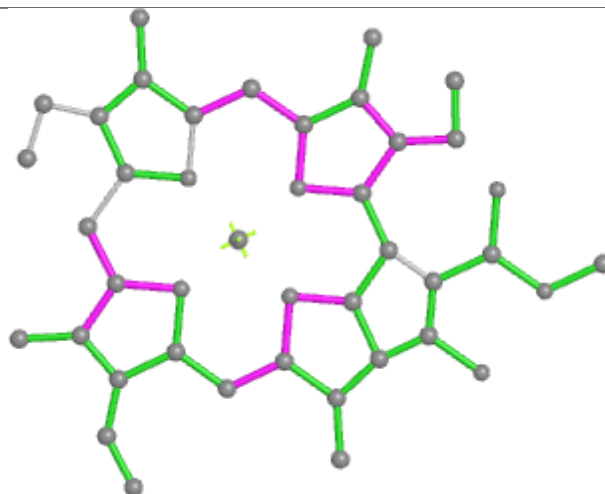
Rings



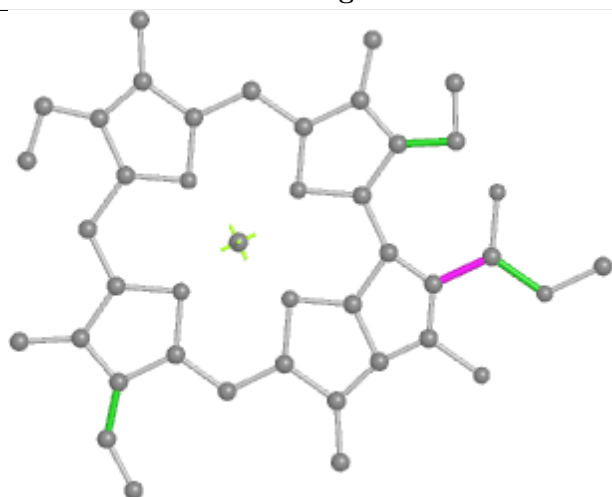
Ligand CLA 3 308



Bond lengths



Bond angles

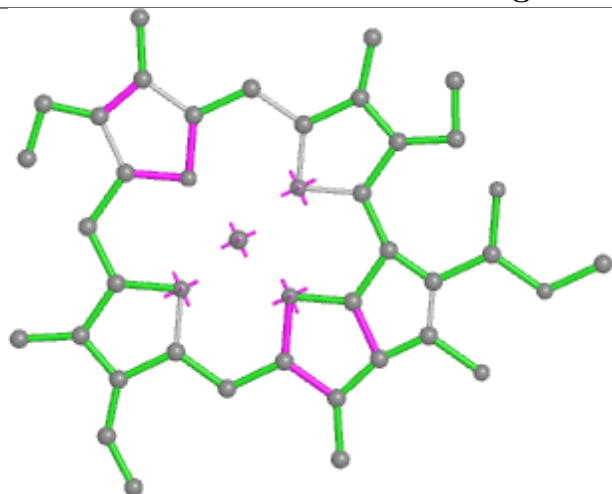


Torsions

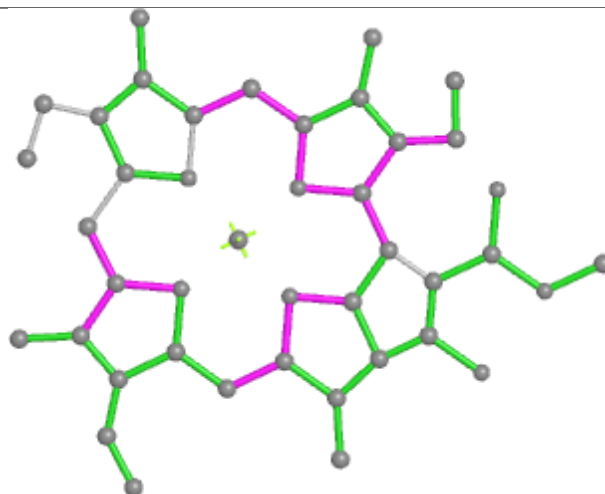


Rings

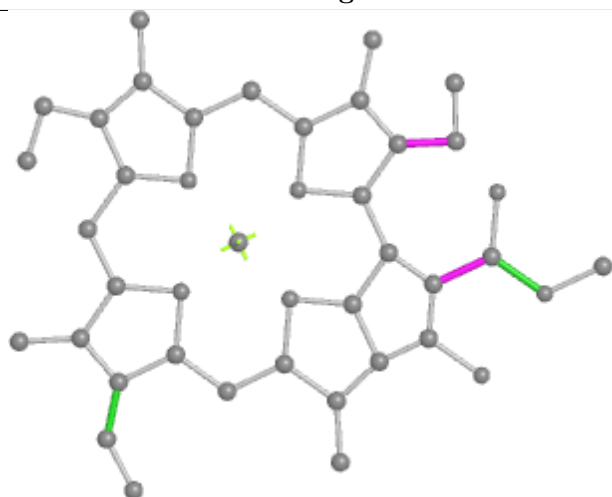
Ligand CLA A 816



Bond lengths



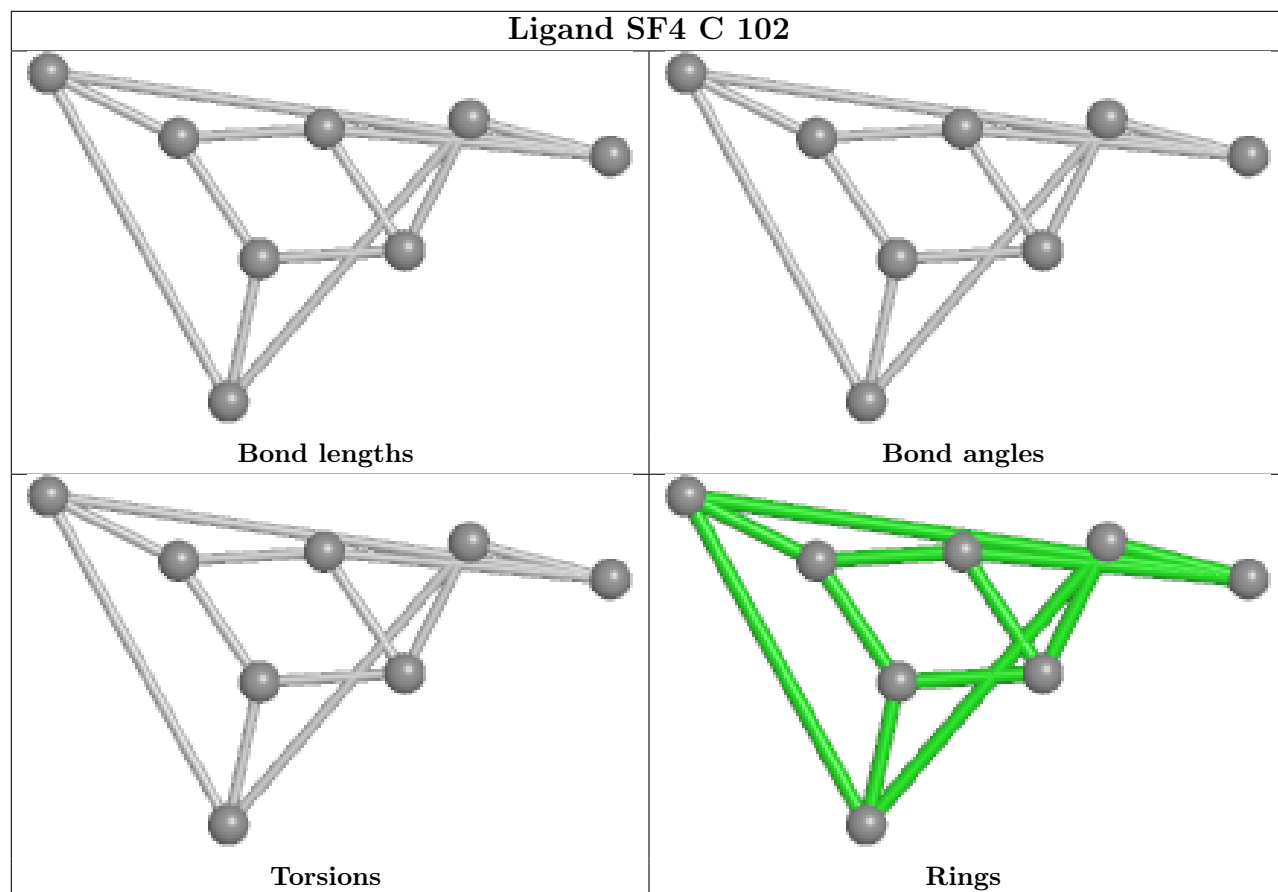
Bond angles



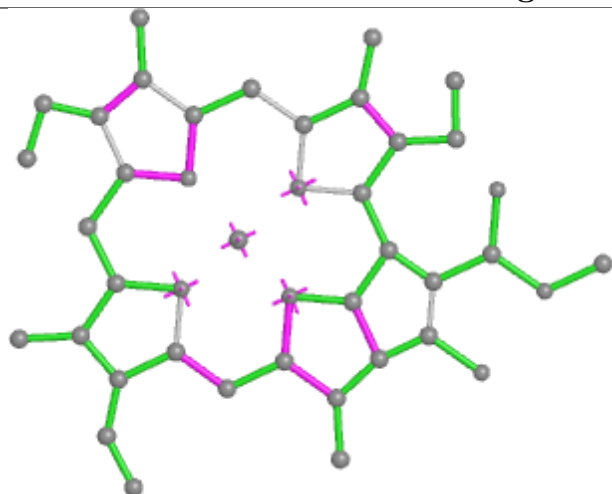
Torsions



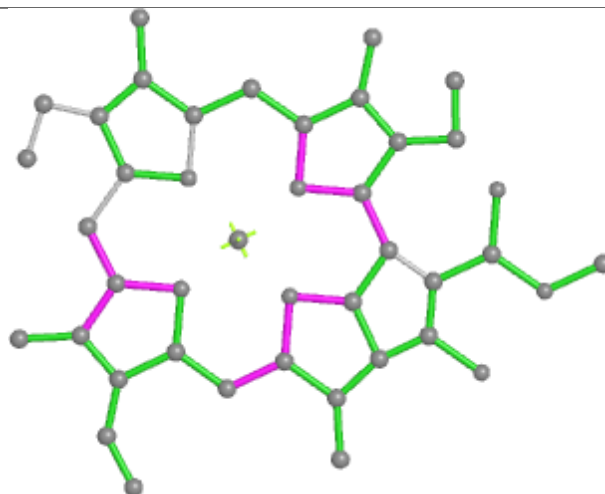
Rings



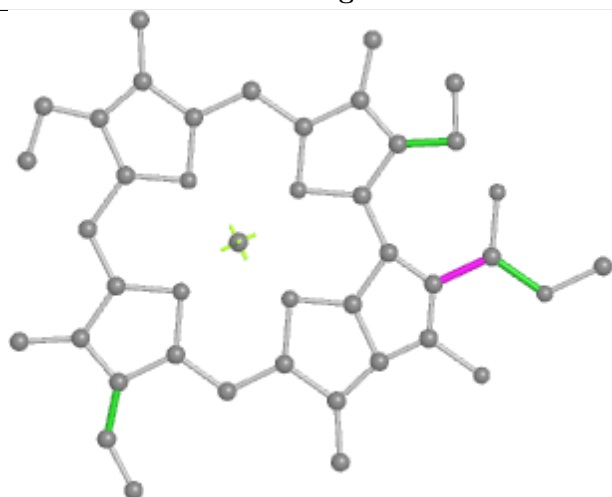
Ligand CLA 1 603



Bond lengths



Bond angles

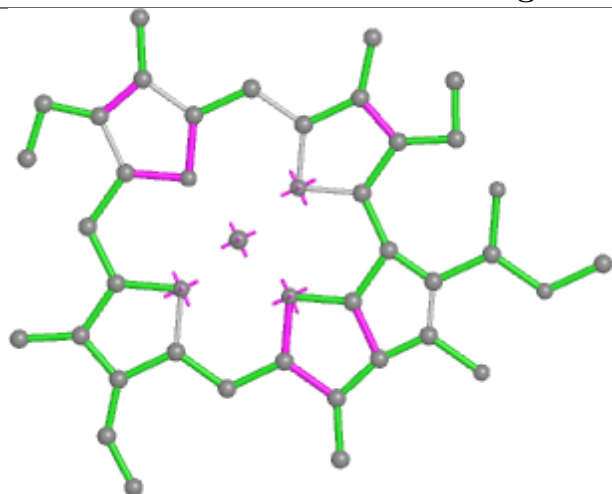


Torsions

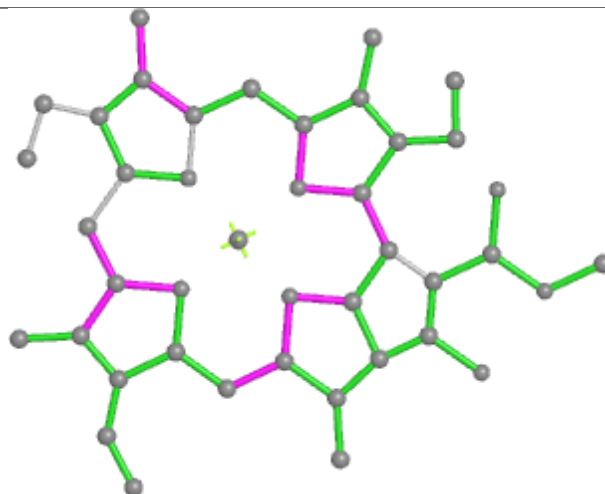


Rings

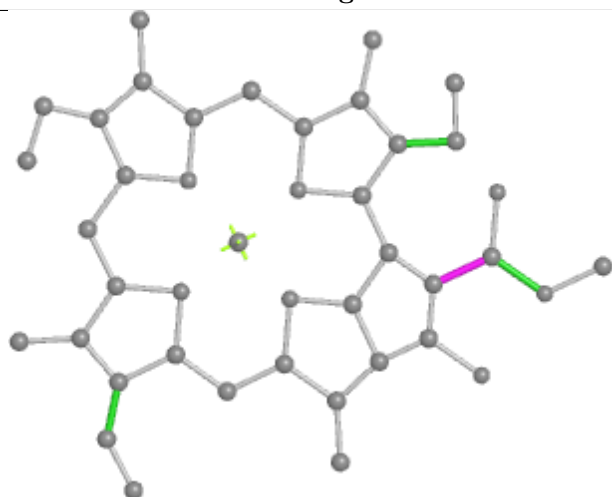
Ligand CLA 7 601



Bond lengths



Bond angles

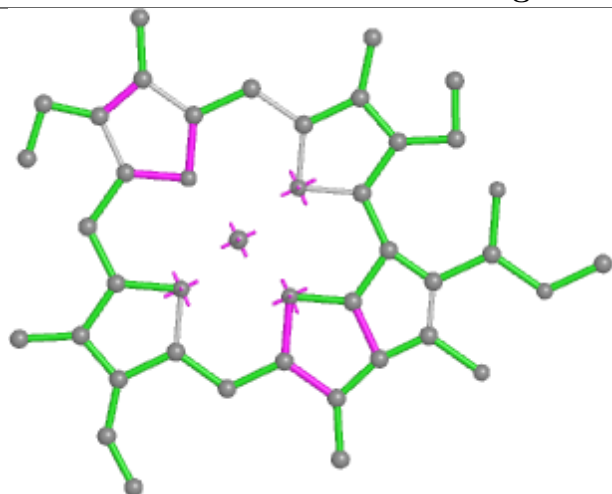


Torsions

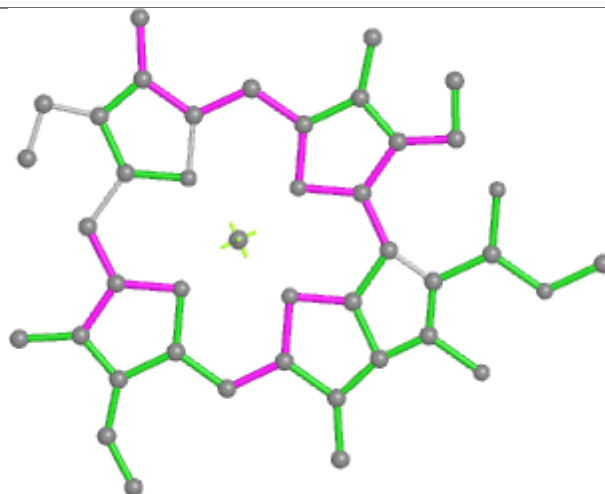


Rings

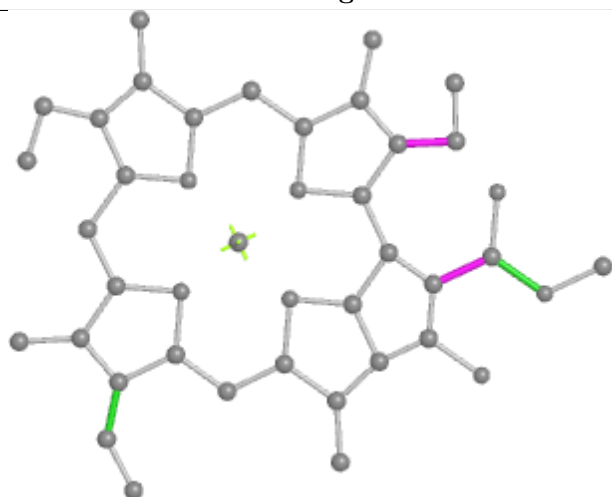
Ligand CLA A 809



Bond lengths



Bond angles

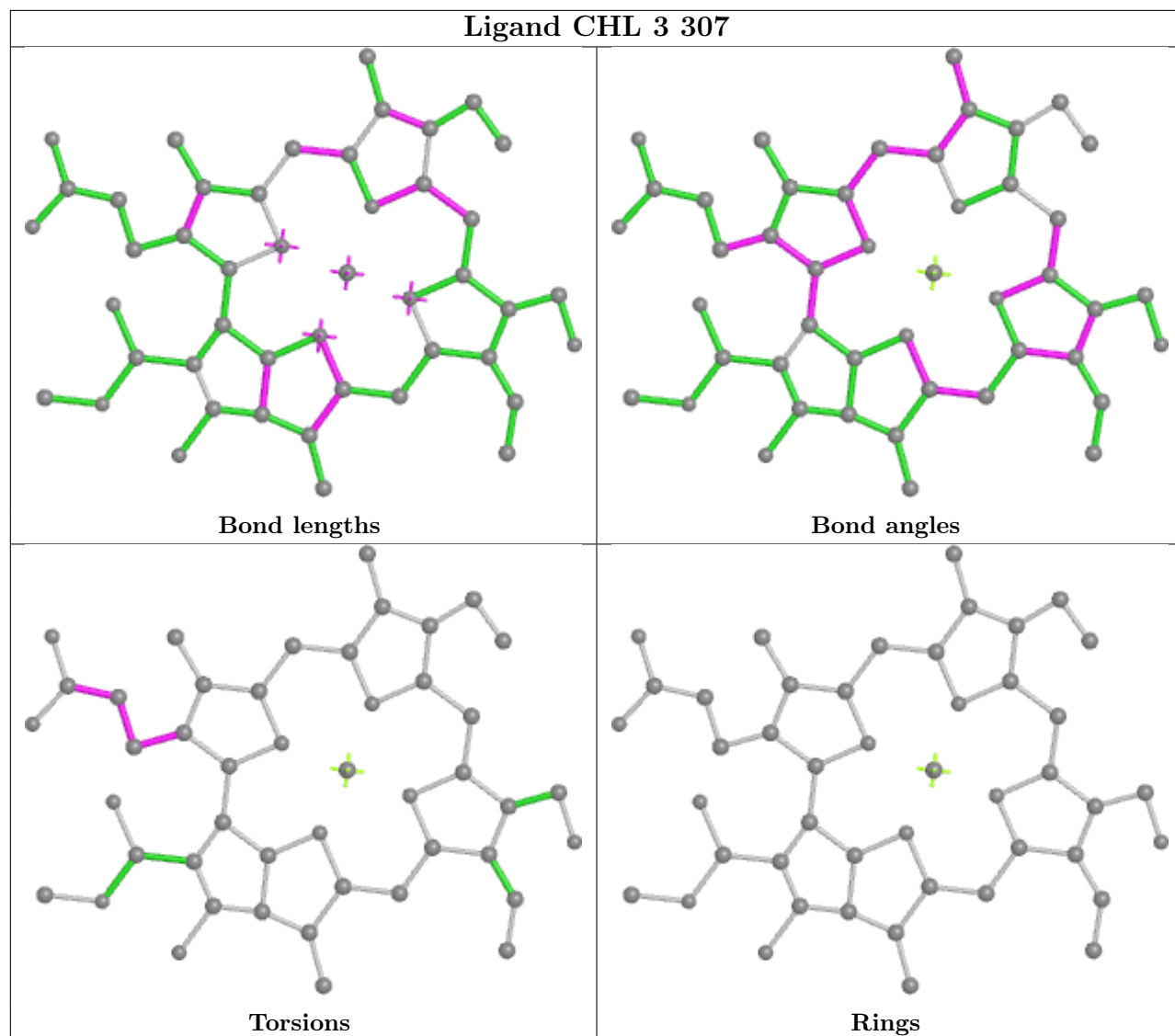


Torsions

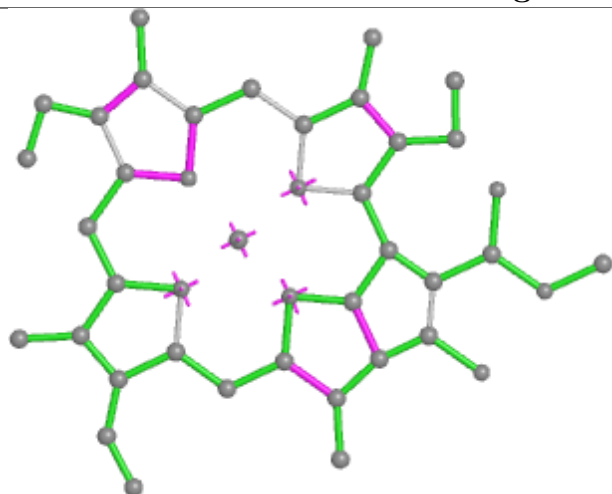


Rings

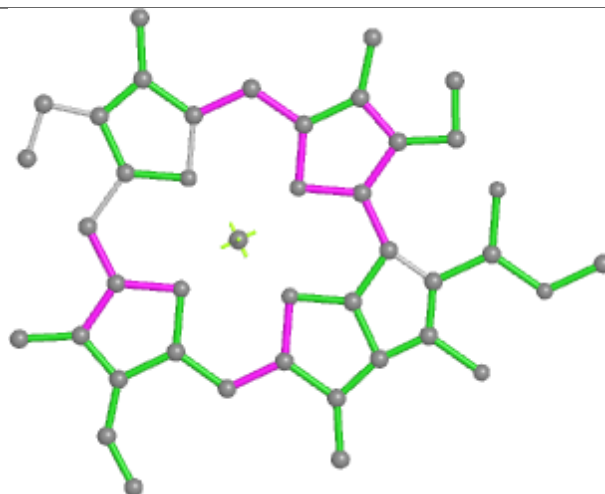
Ligand CHL 3 307



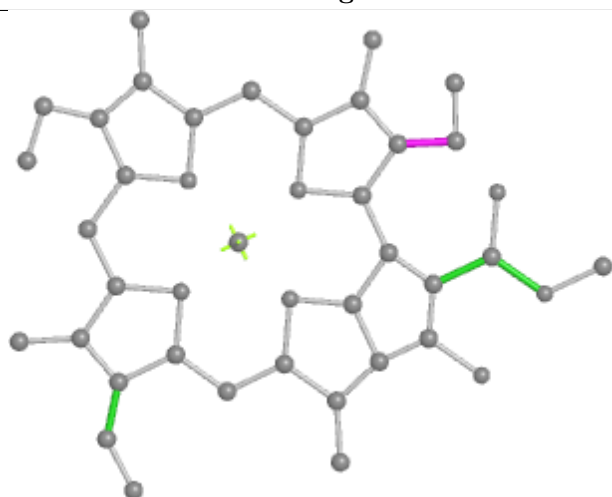
Ligand CLA B 804



Bond lengths



Bond angles

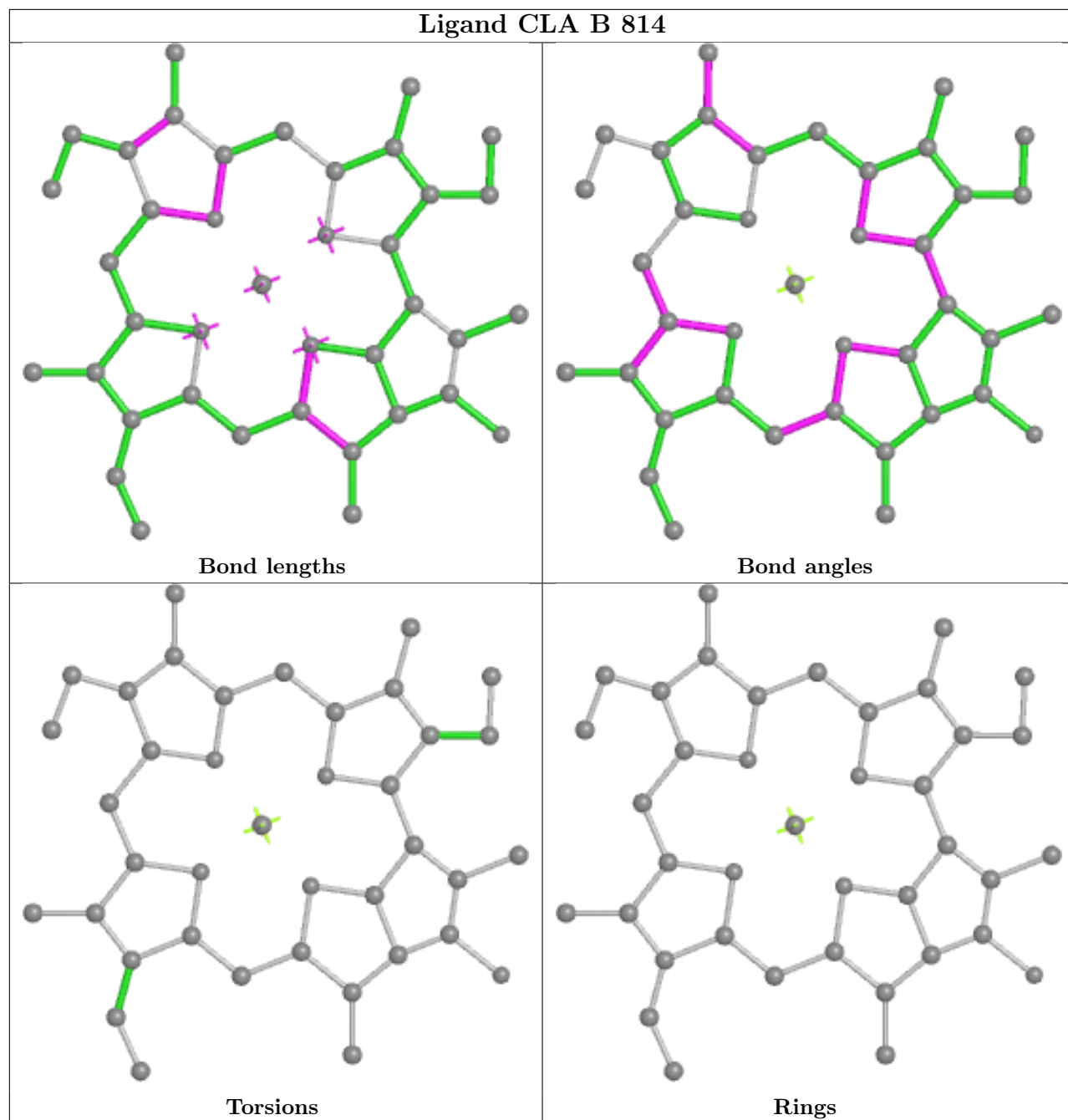


Torsions

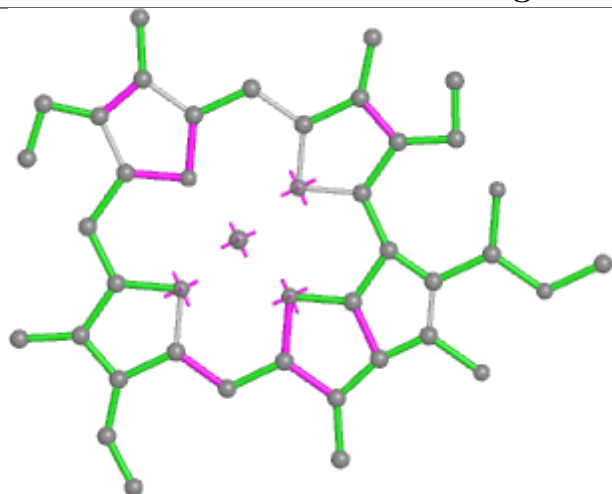


Rings

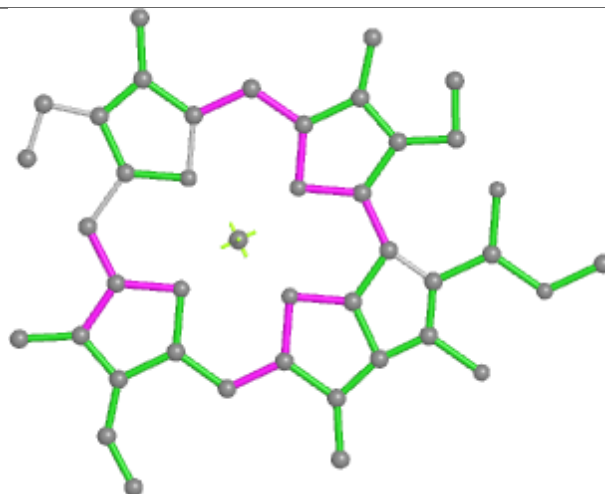
Ligand CLA B 814



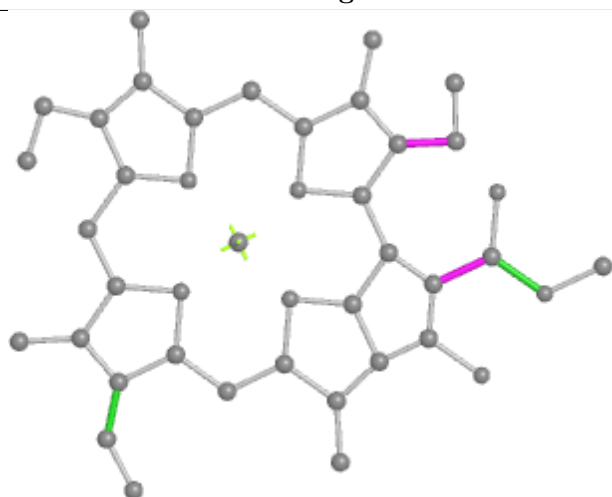
Ligand CLA B 832



Bond lengths



Bond angles

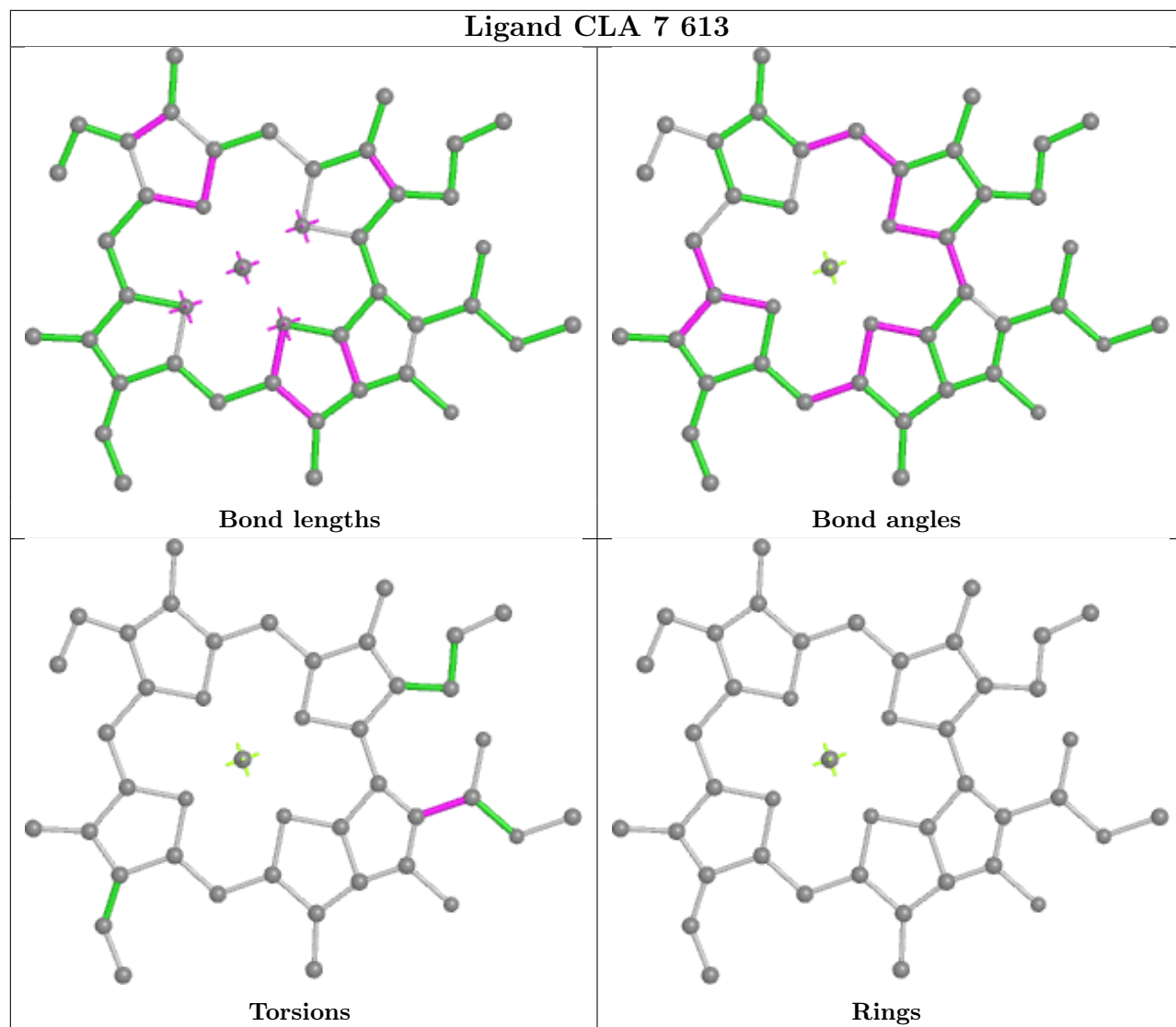


Torsions

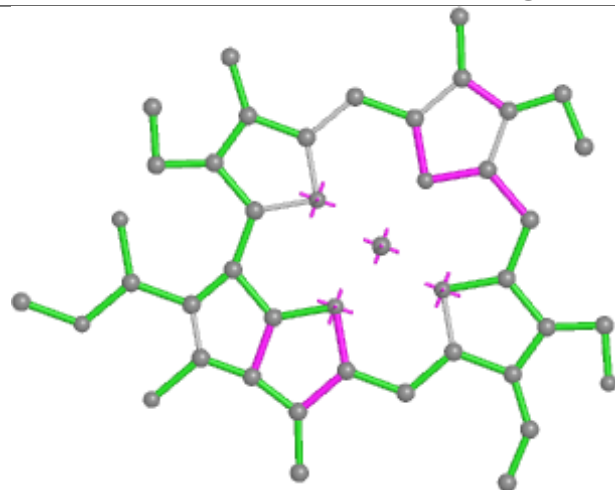


Rings

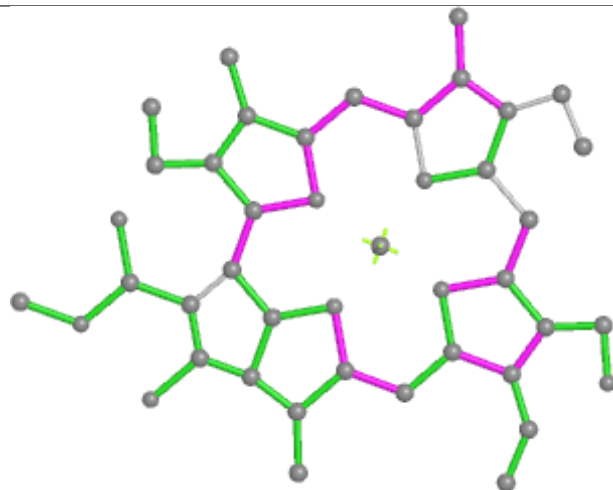
Ligand CLA 7 613



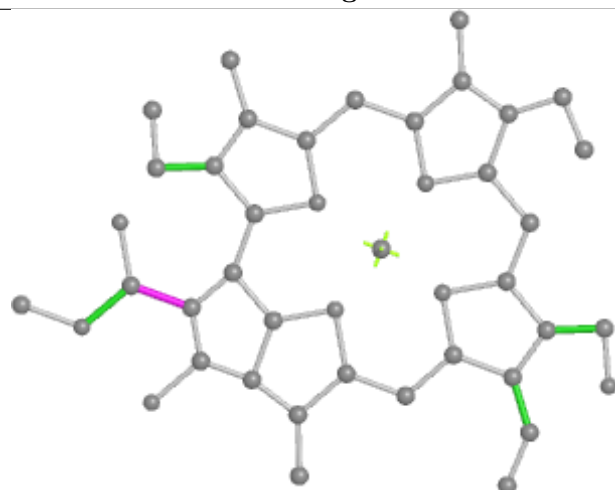
Ligand CHL 5 313



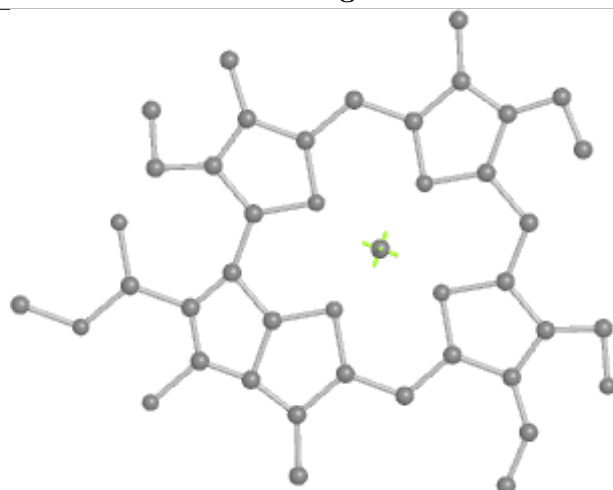
Bond lengths



Bond angles

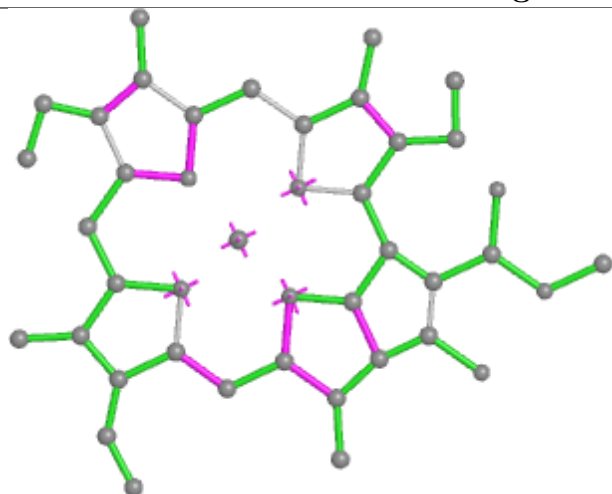


Torsions

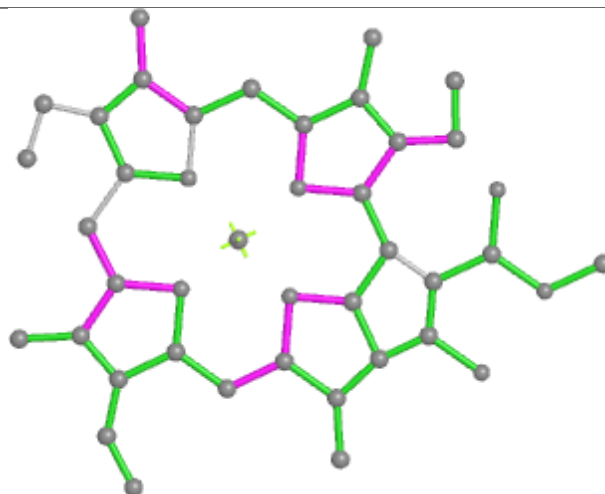


Rings

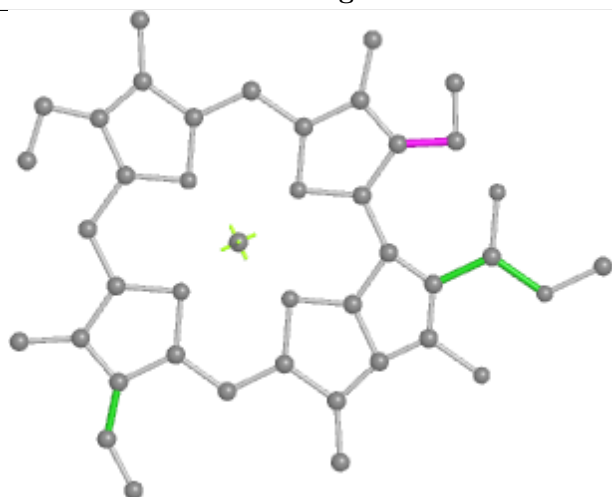
Ligand CLA A 806



Bond lengths



Bond angles

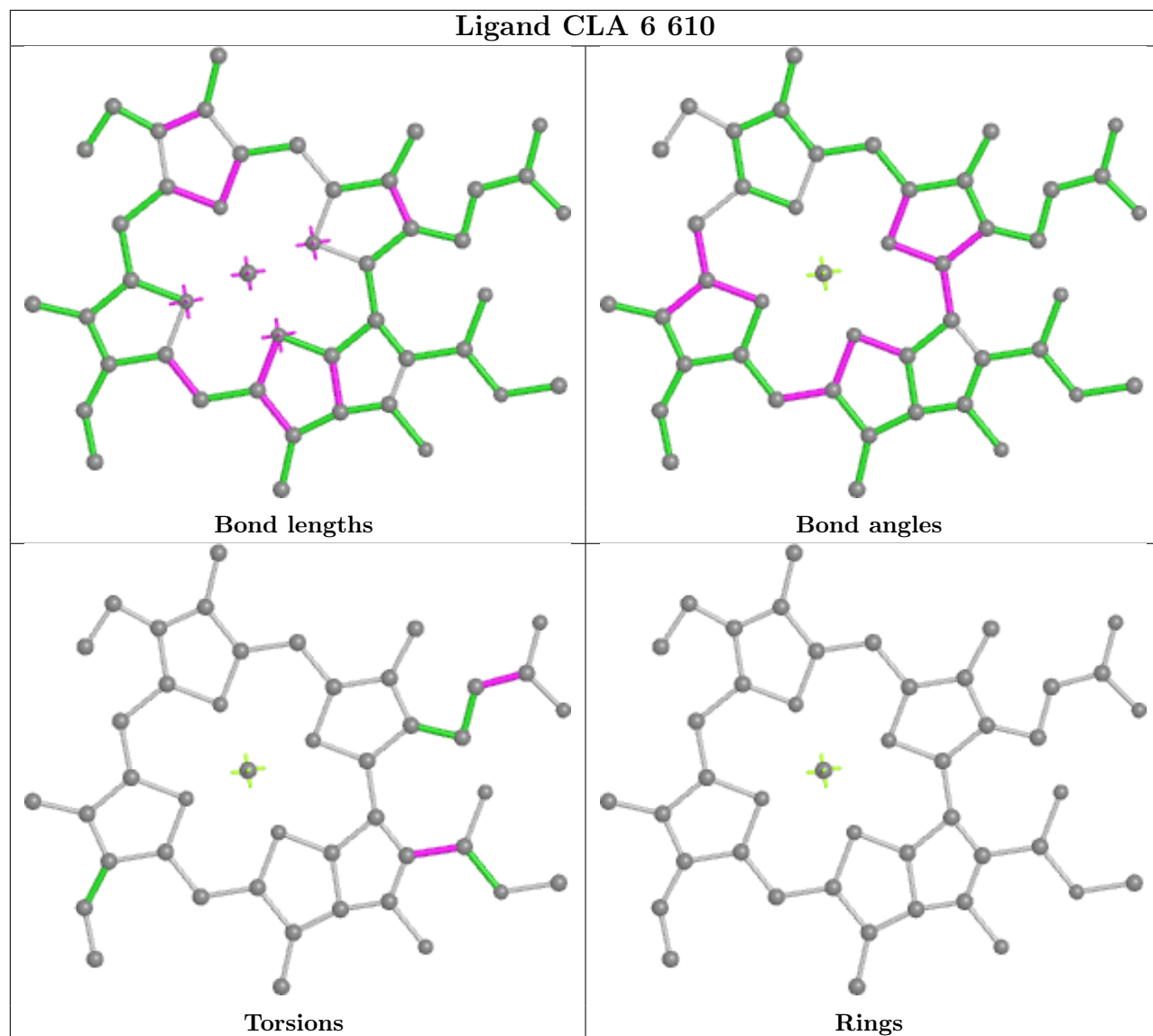


Torsions

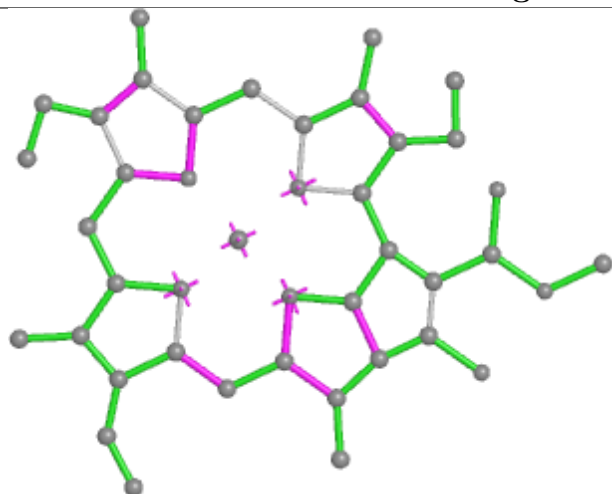


Rings

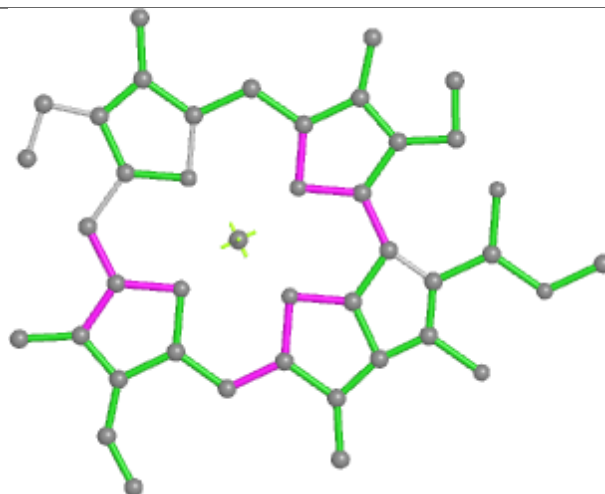
Ligand CLA 6 610



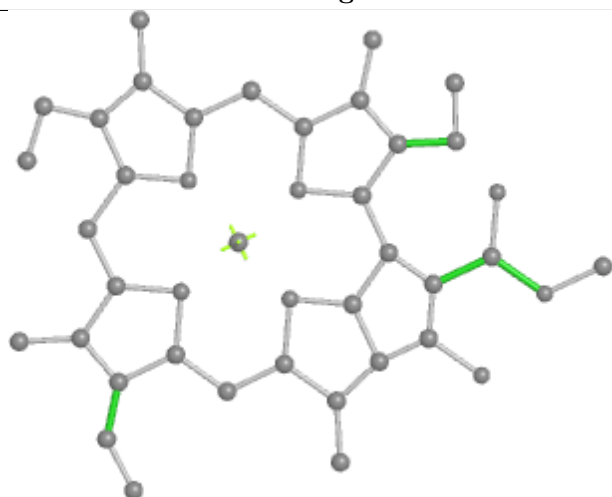
Ligand CLA A 808



Bond lengths



Bond angles

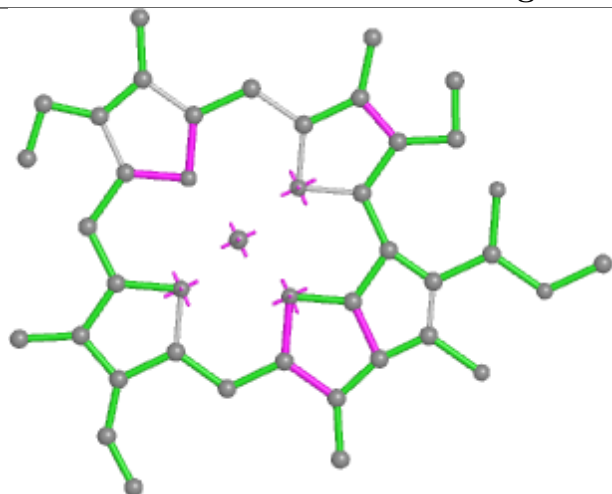


Torsions

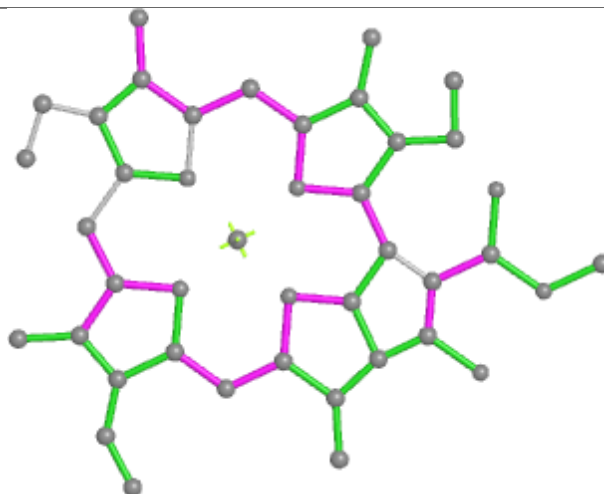


Rings

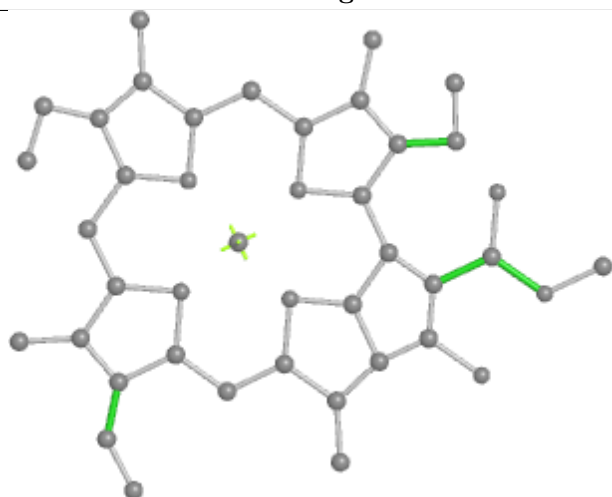
Ligand CLA 7 604



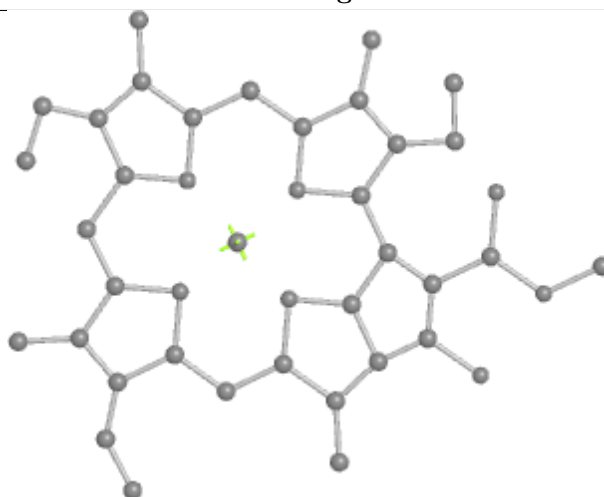
Bond lengths



Bond angles

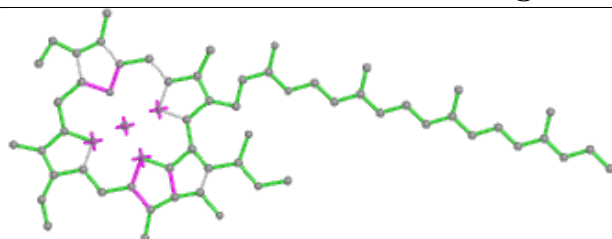


Torsions

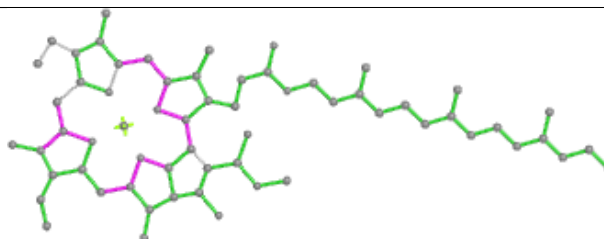


Rings

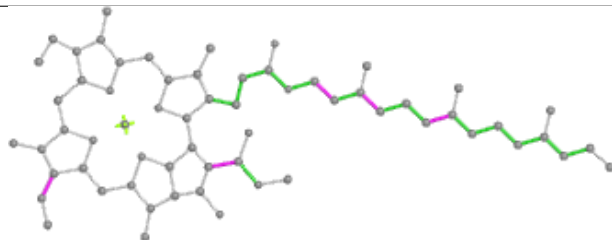
Ligand CLA F 302



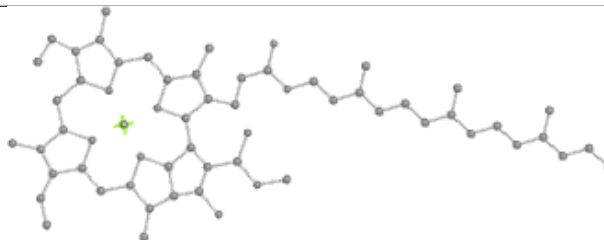
Bond lengths



Bond angles

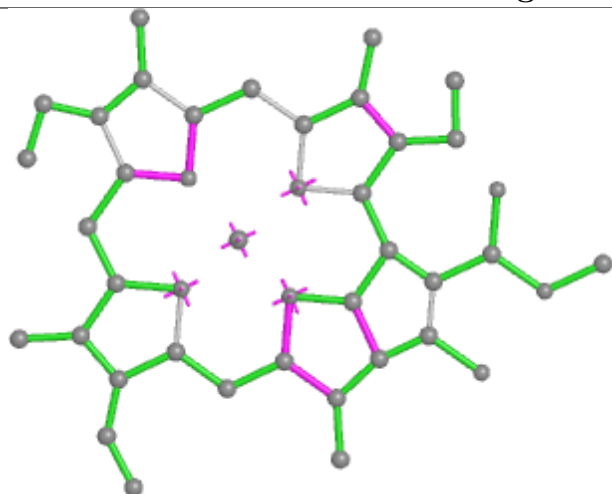


Torsions

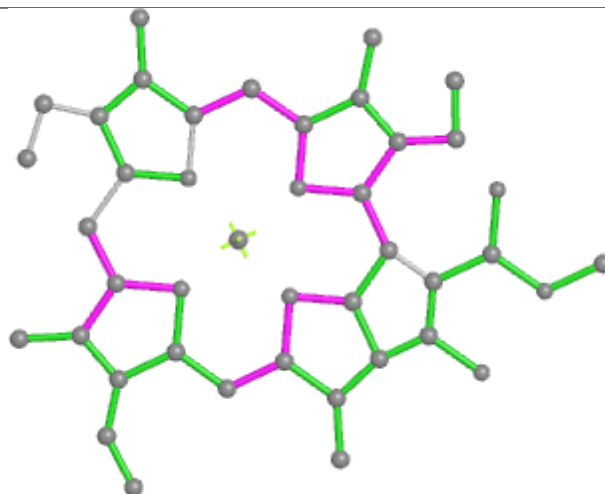


Rings

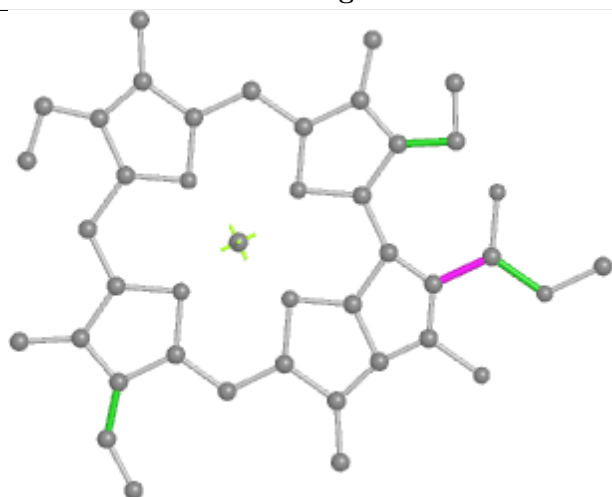
Ligand CLA J 102



Bond lengths



Bond angles

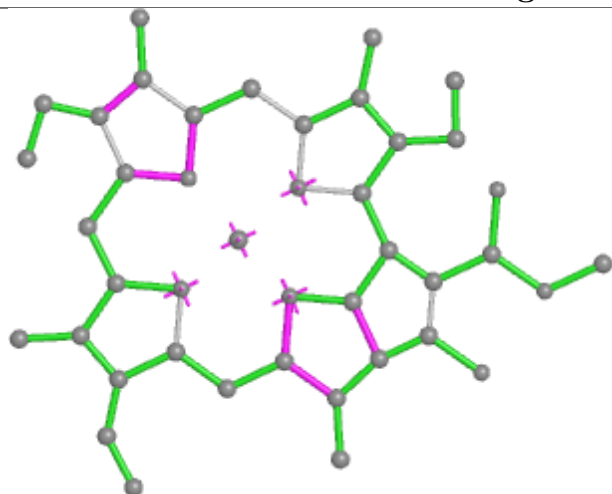


Torsions

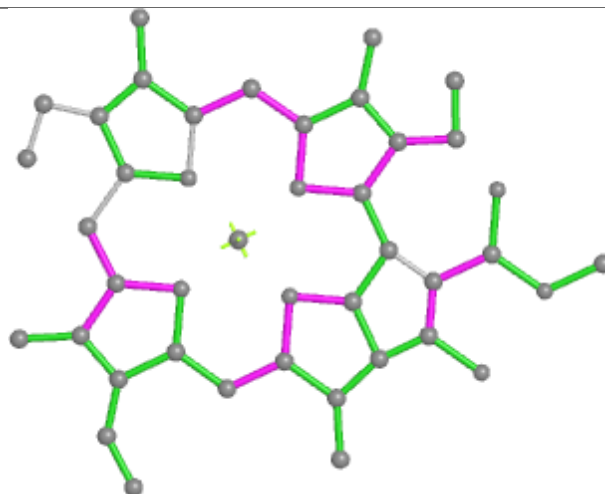


Rings

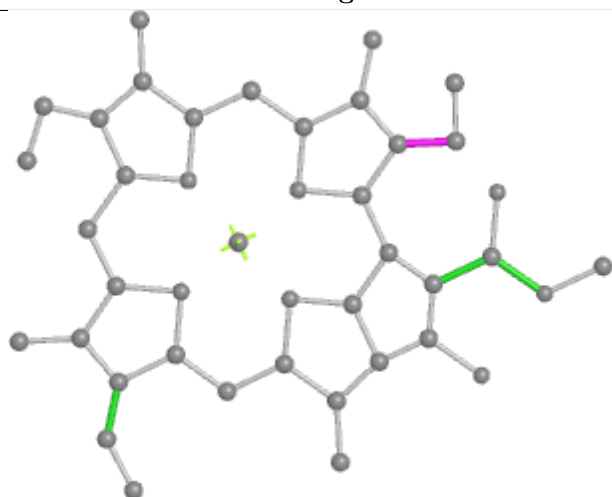
Ligand CLA 7 609



Bond lengths



Bond angles

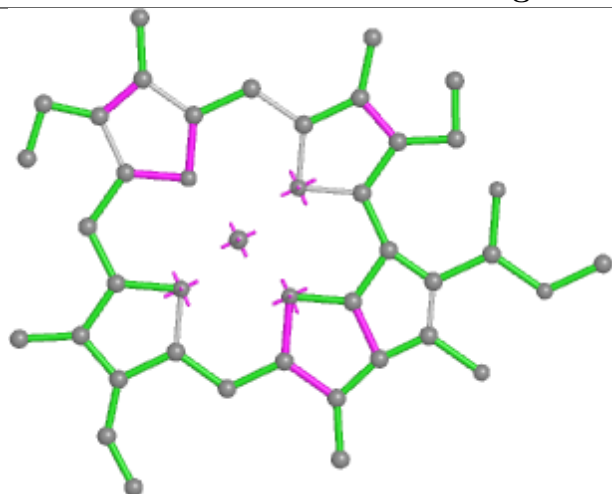


Torsions

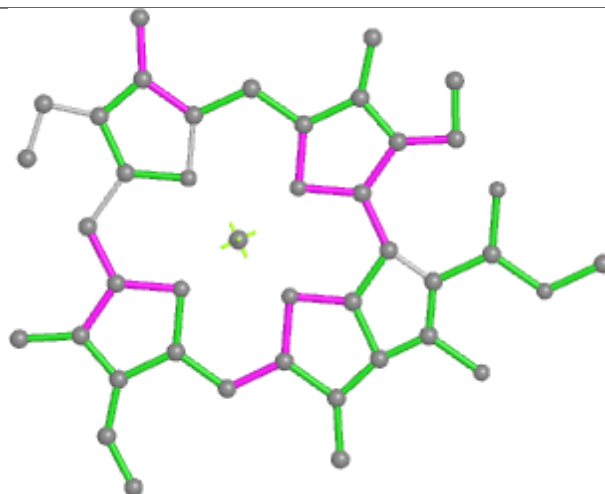


Rings

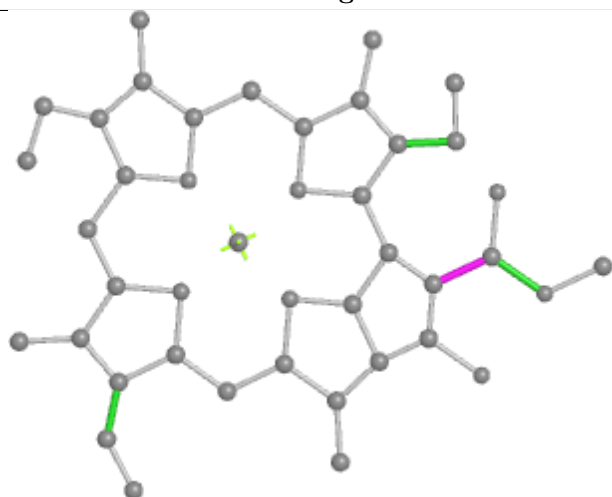
Ligand CLA A 810



Bond lengths



Bond angles

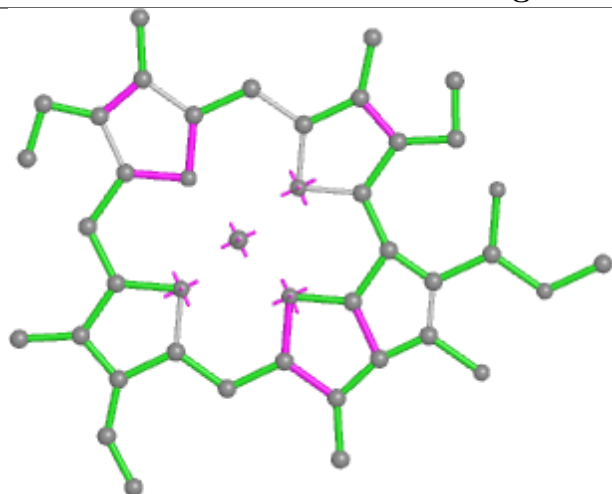


Torsions

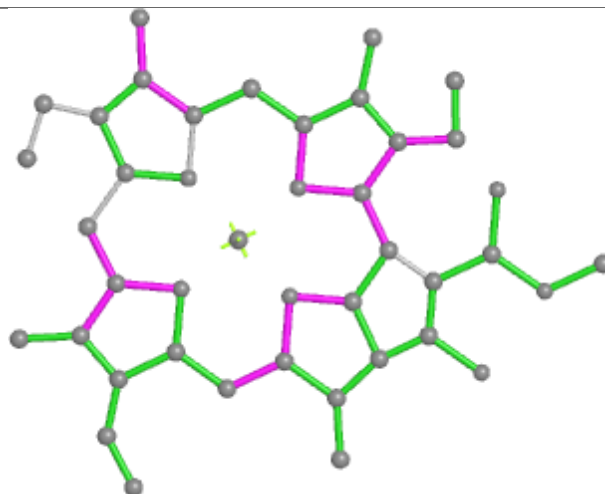


Rings

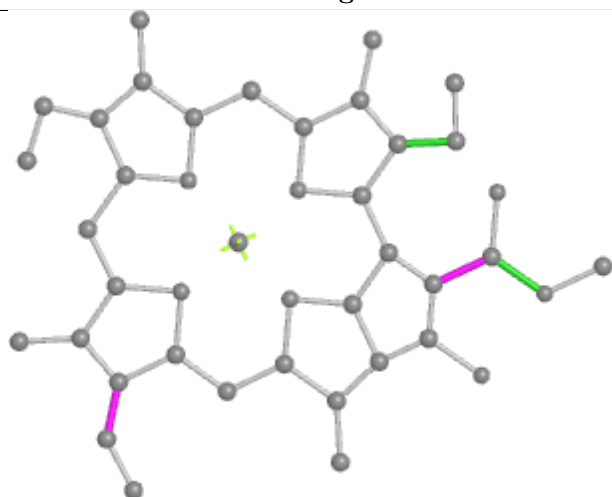
Ligand CLA A 823



Bond lengths



Bond angles

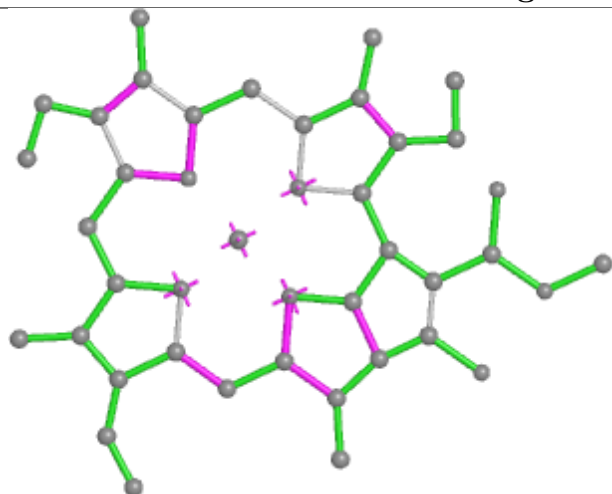


Torsions

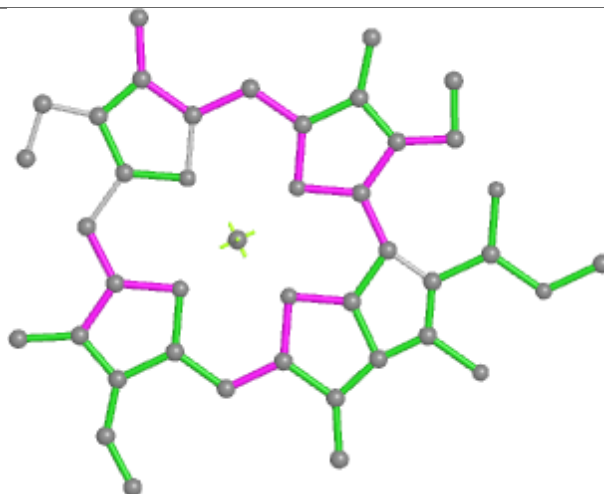


Rings

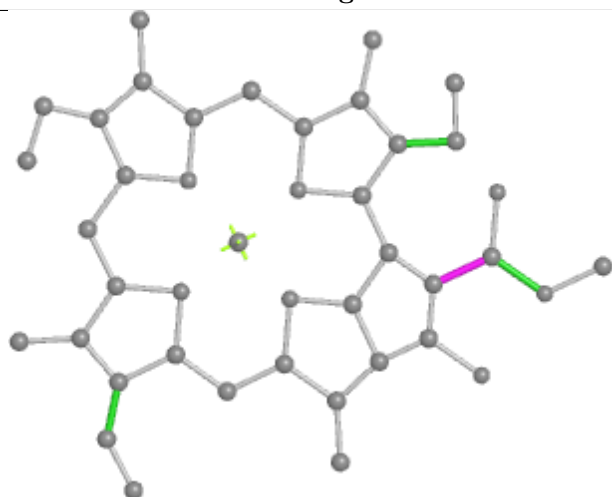
Ligand CLA 7 605



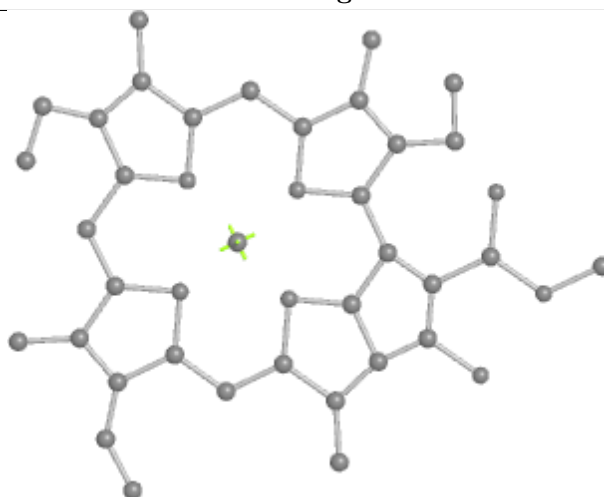
Bond lengths



Bond angles

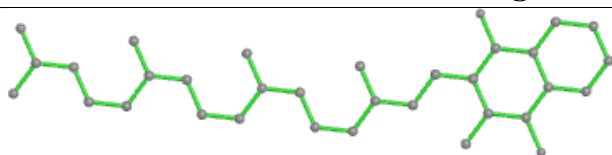


Torsions

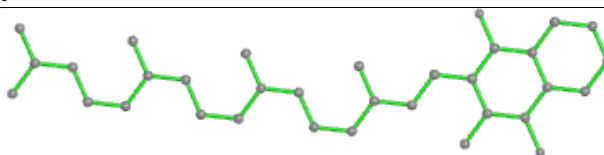


Rings

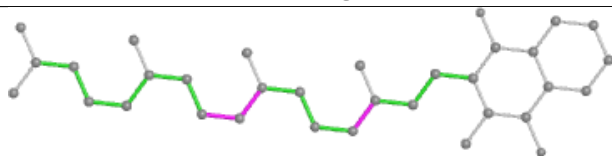
Ligand PQN B 840



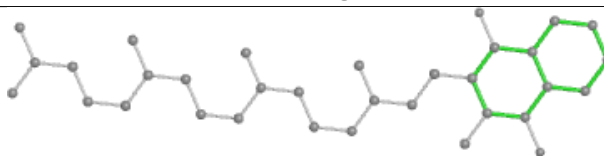
Bond lengths



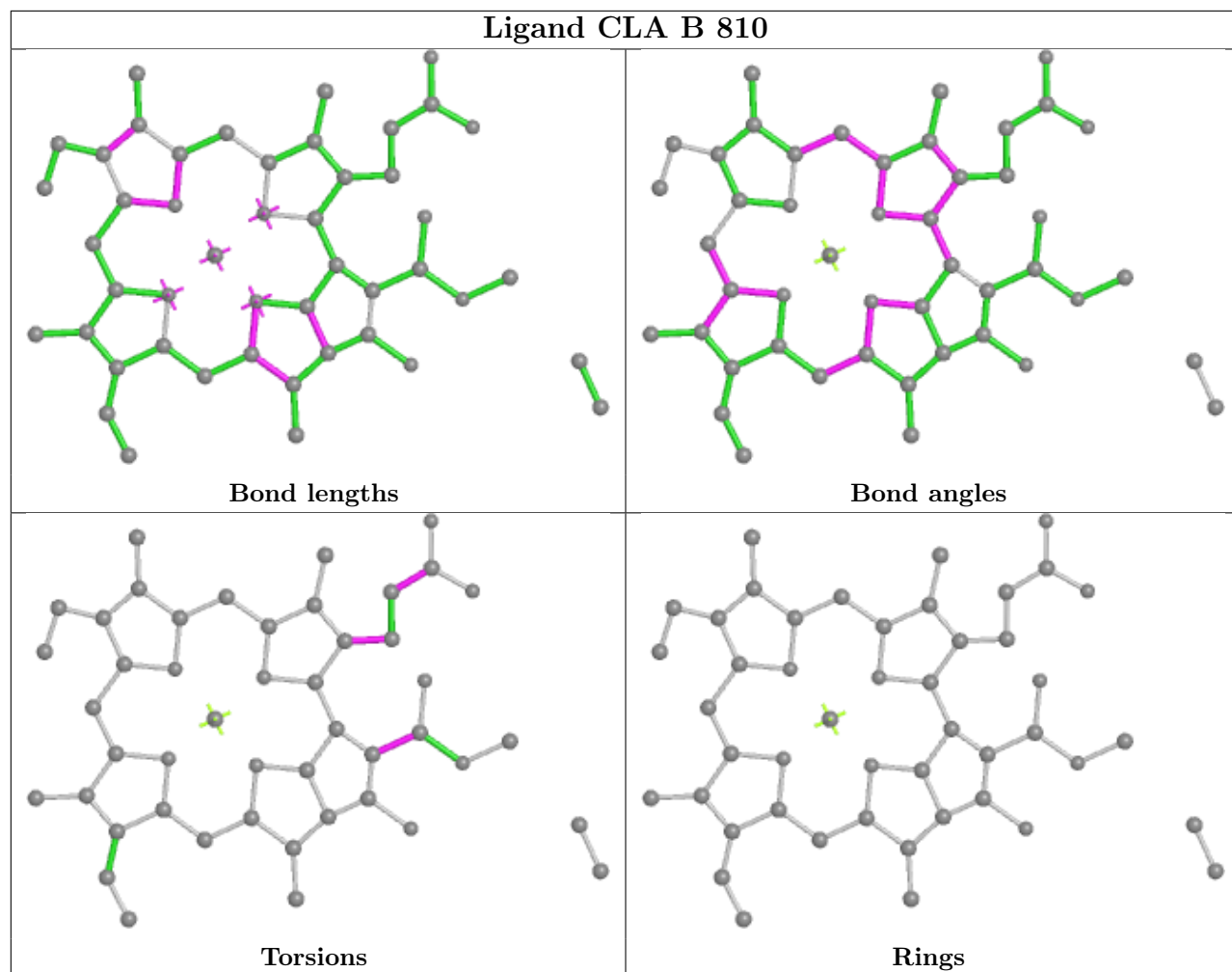
Bond angles



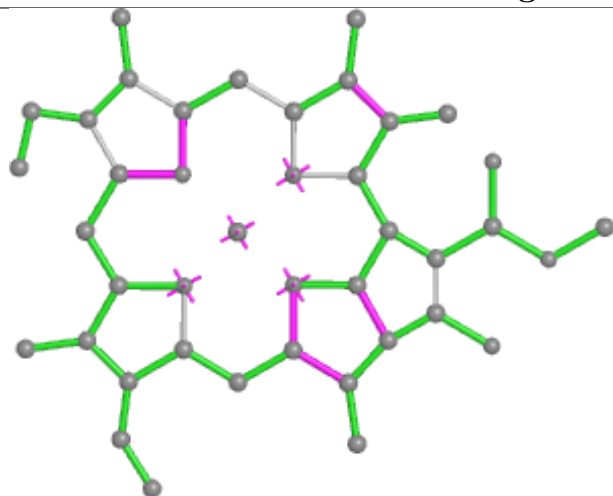
Torsions



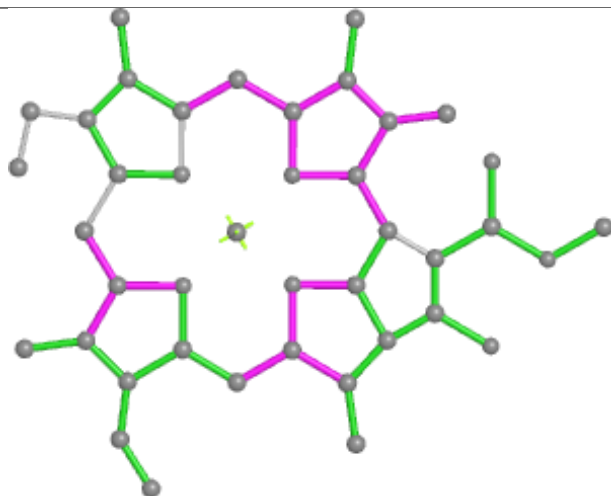
Rings



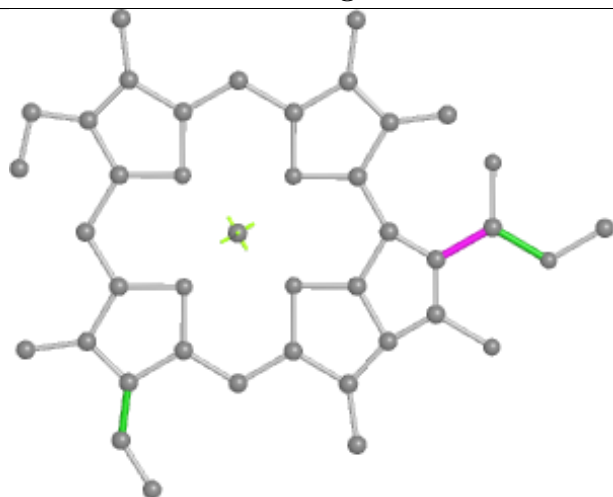
Ligand CLA 3 310



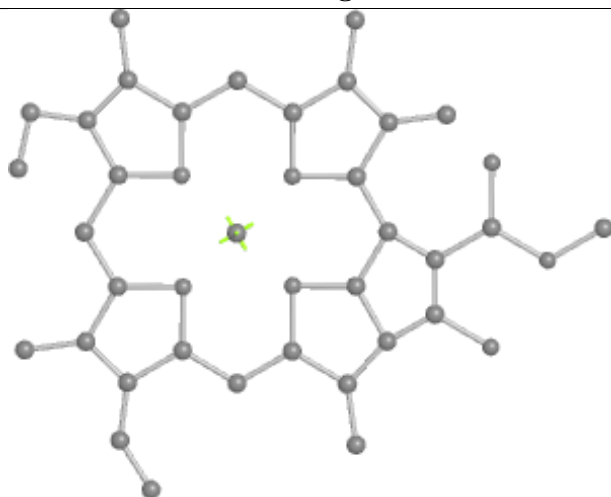
Bond lengths



Bond angles

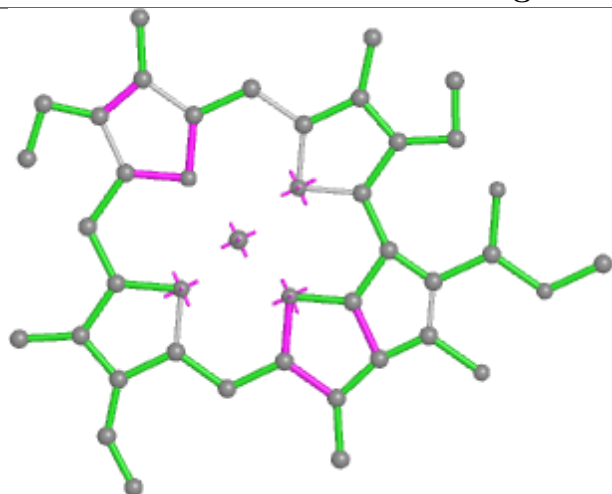


Torsions

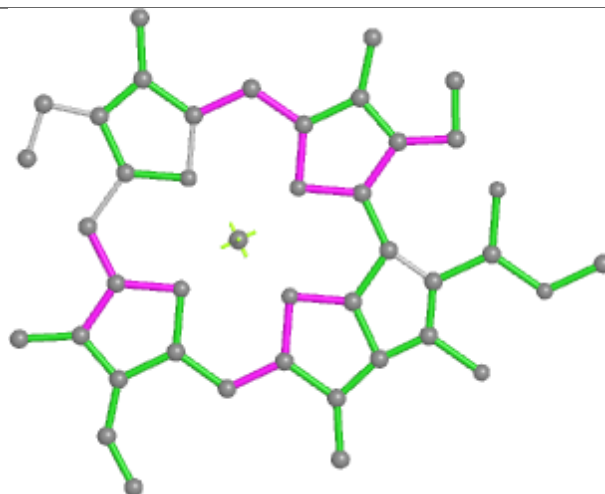


Rings

Ligand CLA B 830



Bond lengths



Bond angles

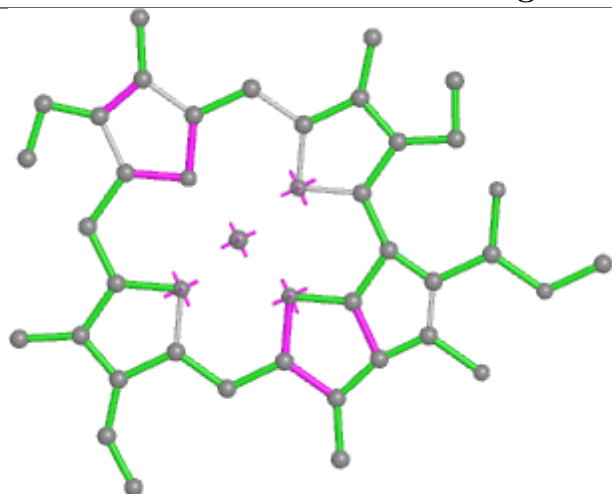


Torsions

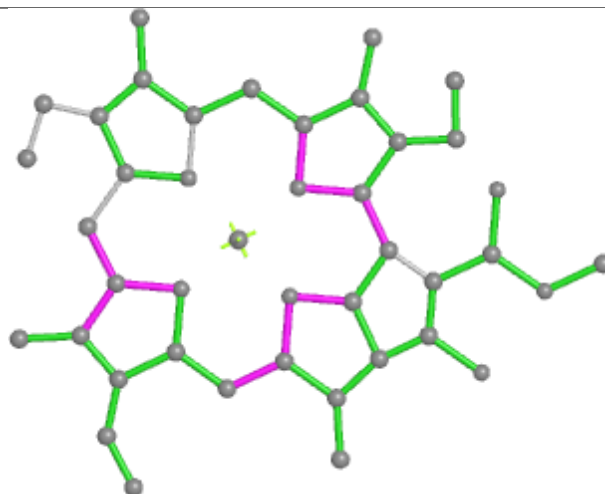


Rings

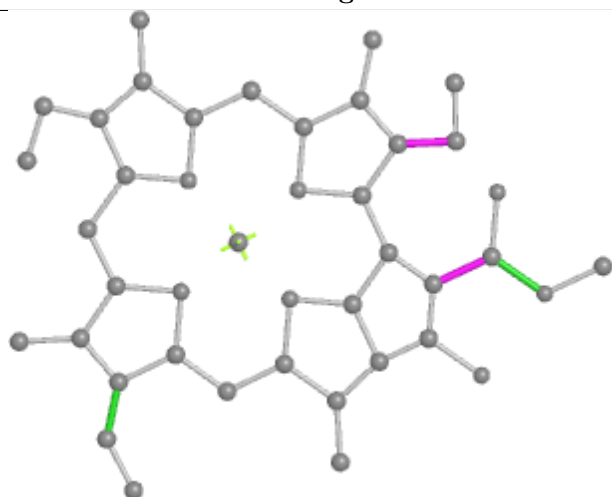
Ligand CLA 8 602



Bond lengths



Bond angles

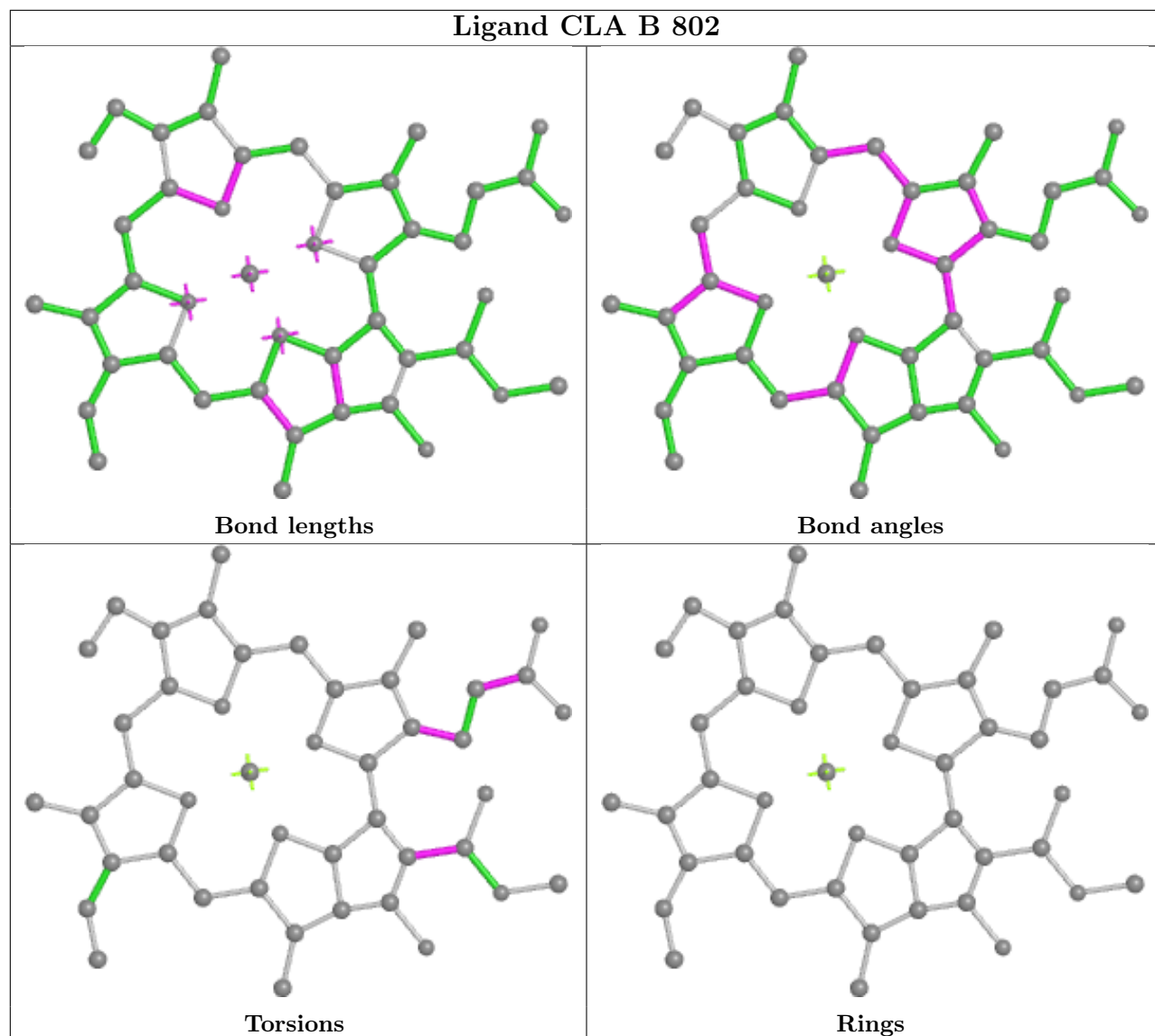


Torsions

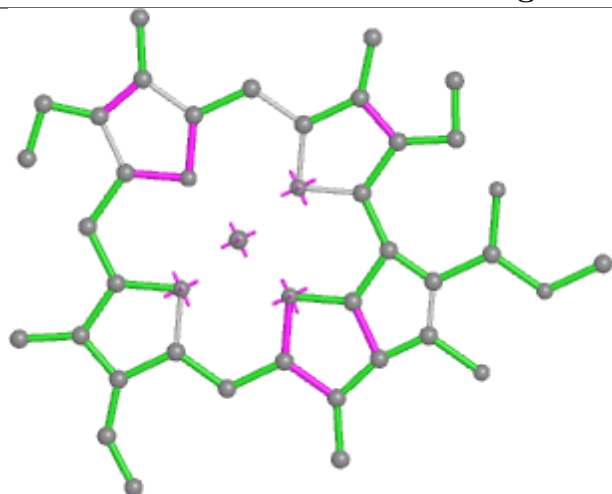


Rings

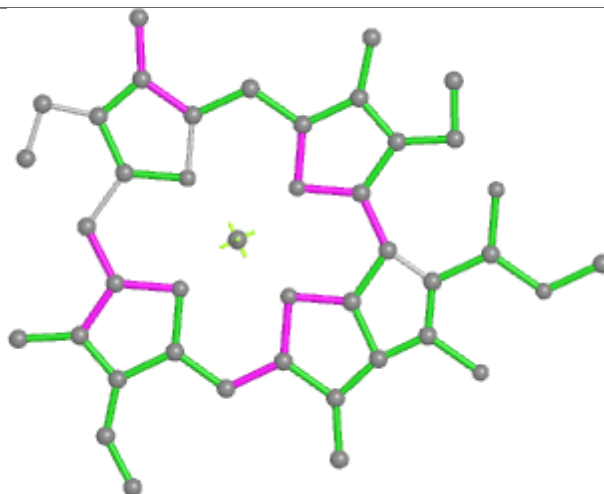
Ligand CLA B 802



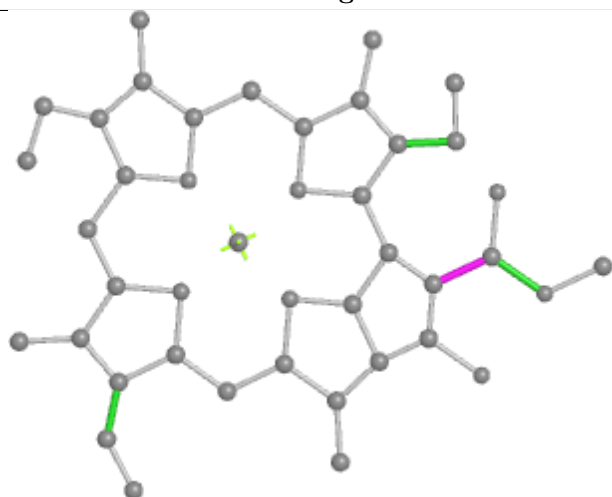
Ligand CLA 8 605



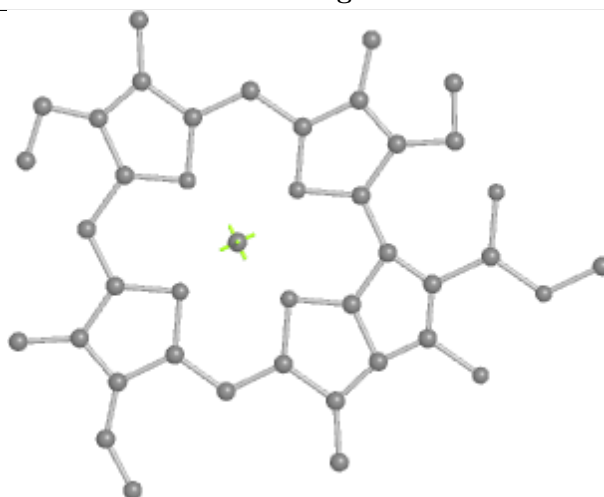
Bond lengths



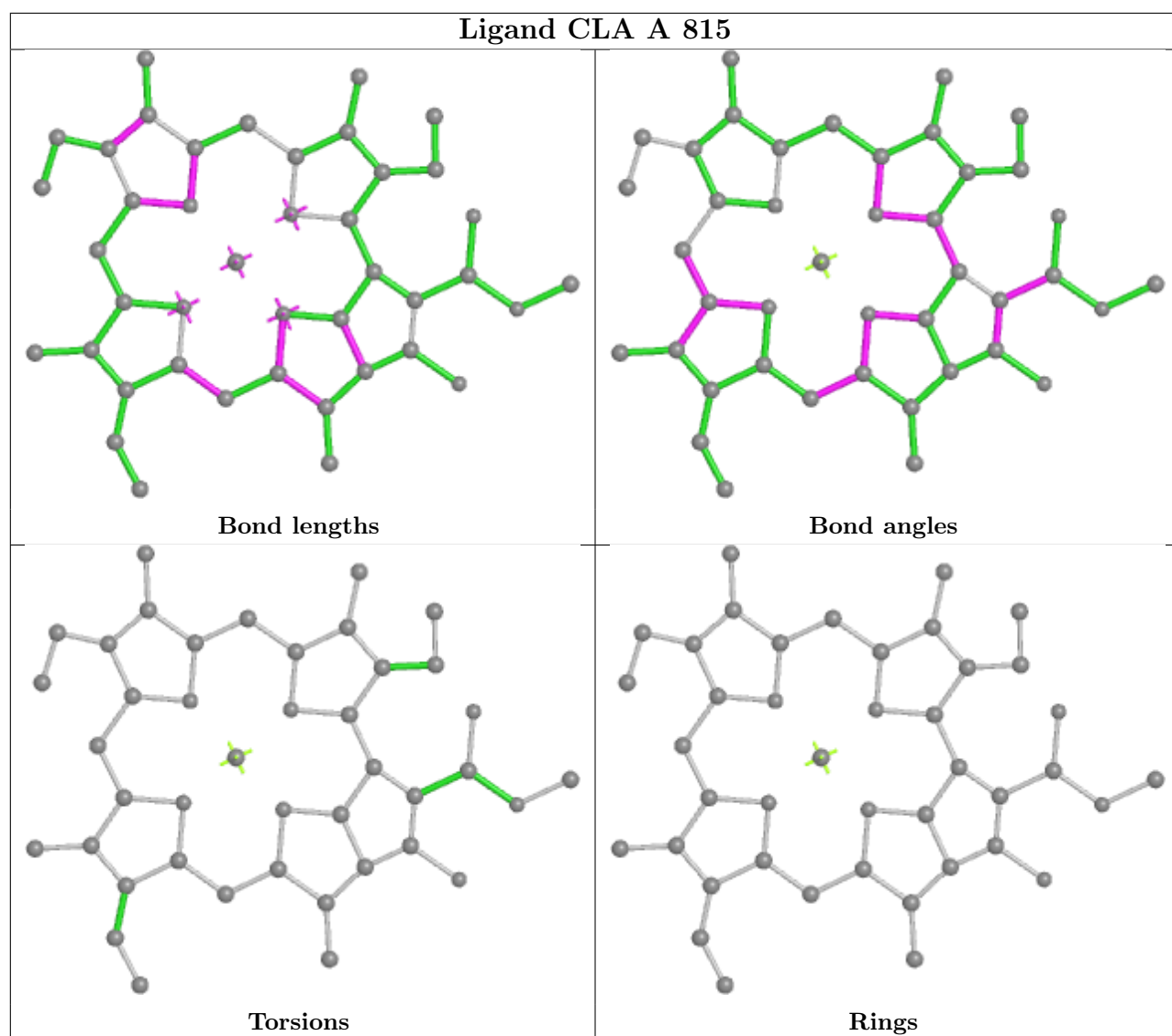
Bond angles



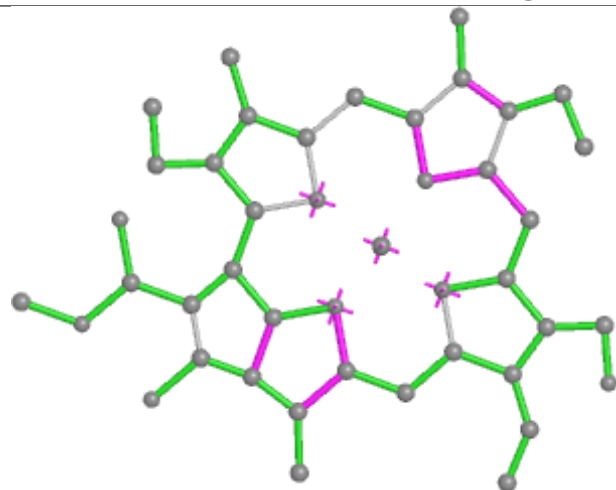
Torsions



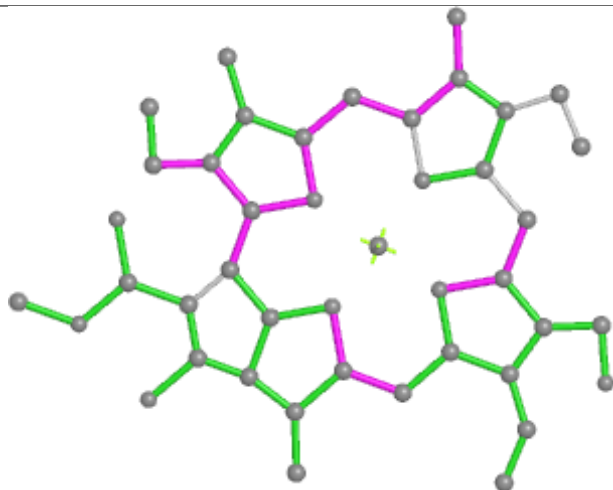
Rings



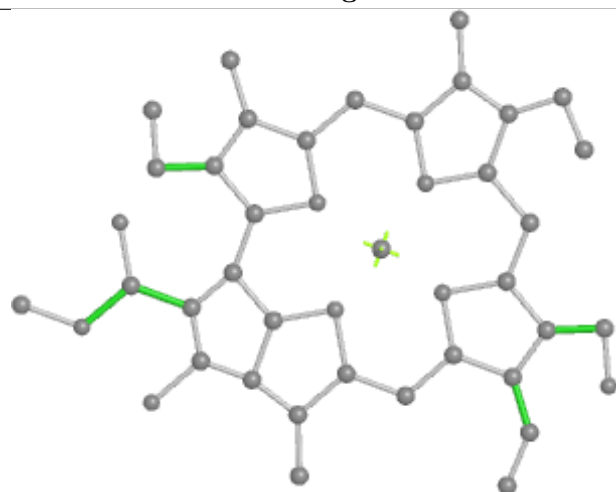
Ligand CHL 8 606



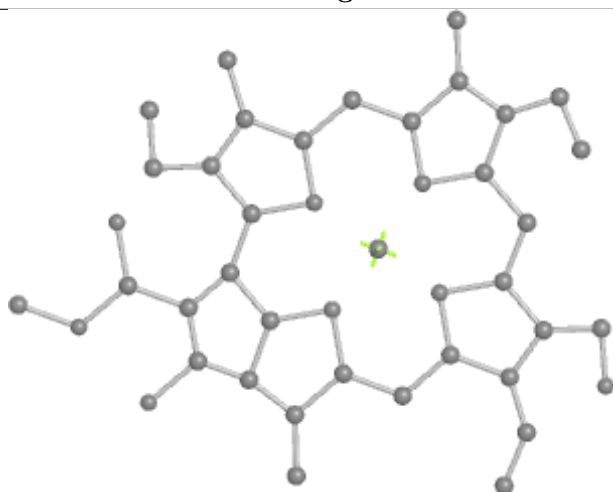
Bond lengths



Bond angles

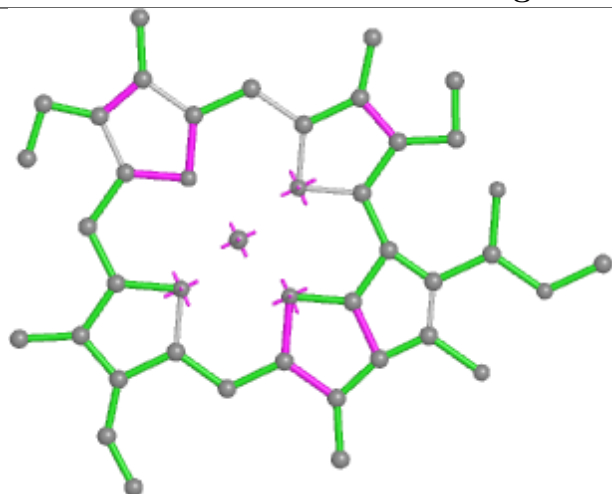


Torsions

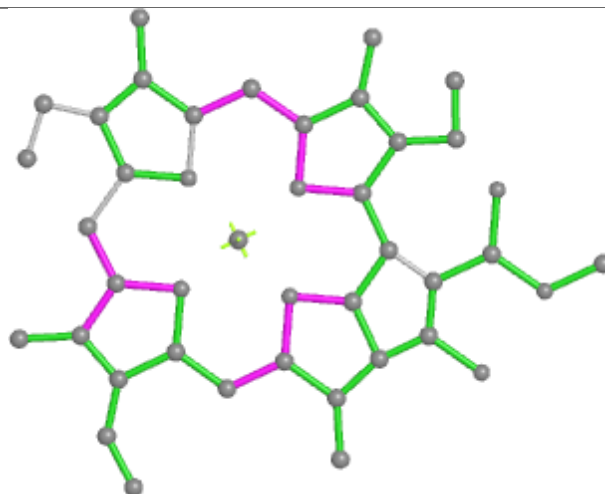


Rings

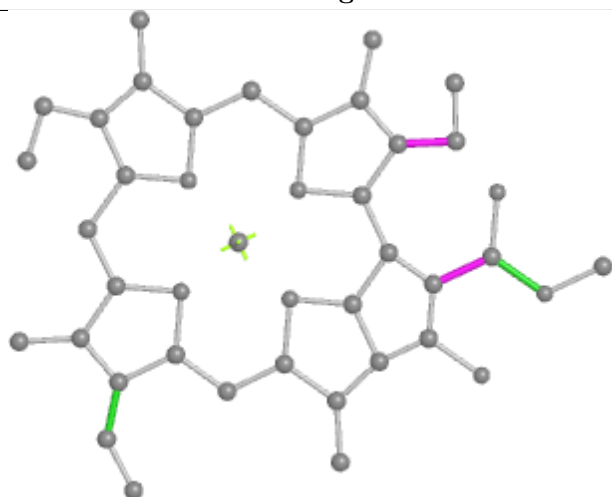
Ligand CLA B 827



Bond lengths



Bond angles

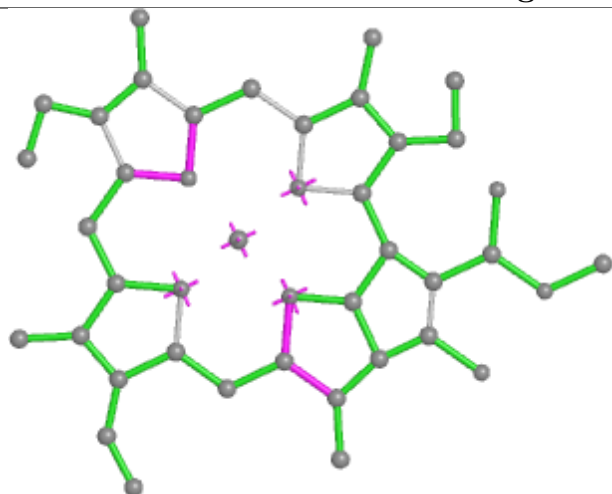


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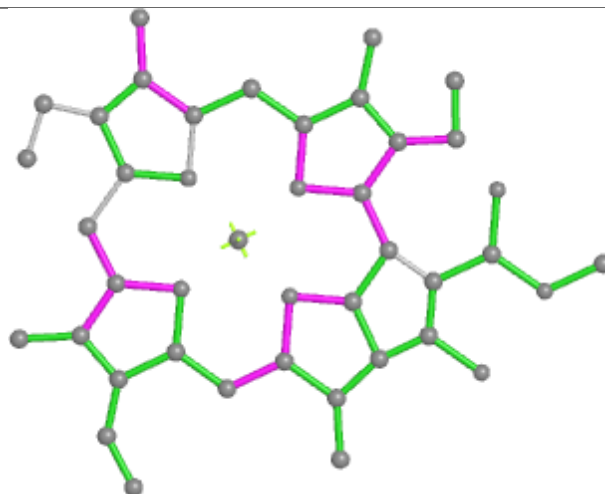


Rings

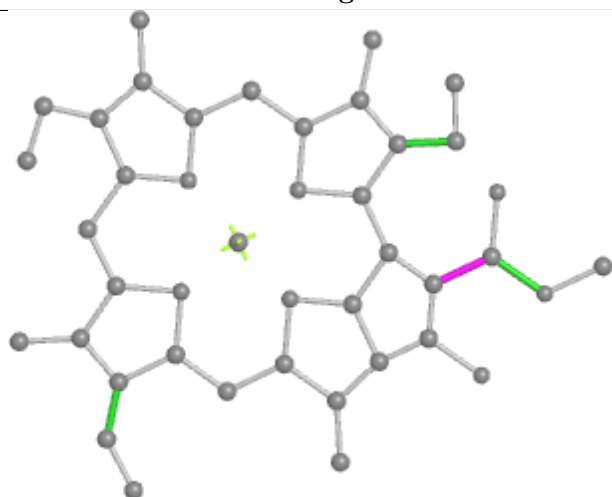
Ligand CLA 1 604



Bond lengths



Bond angles

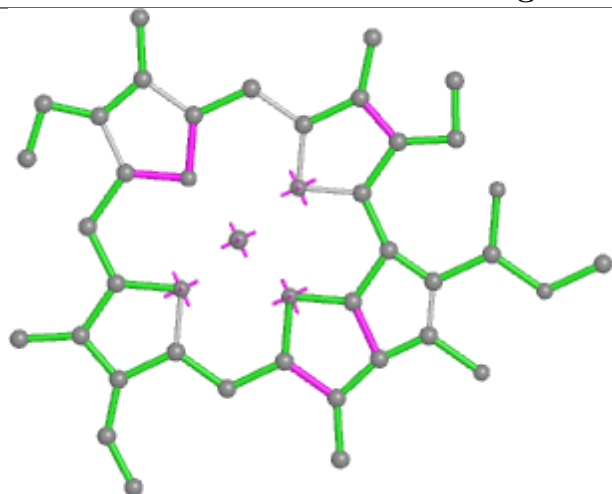


Torsions

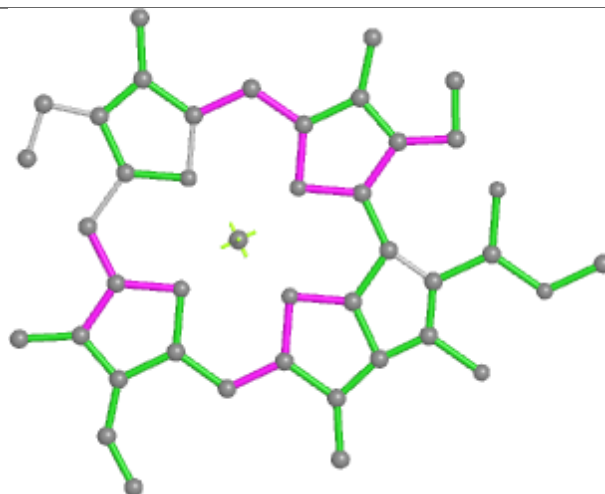


Rings

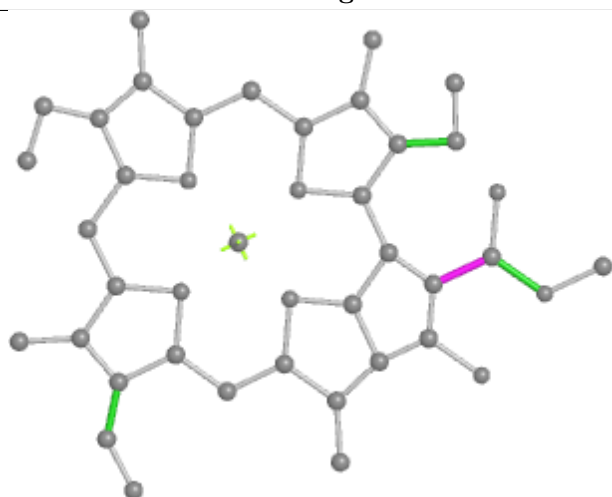
Ligand CLA 3 305



Bond lengths



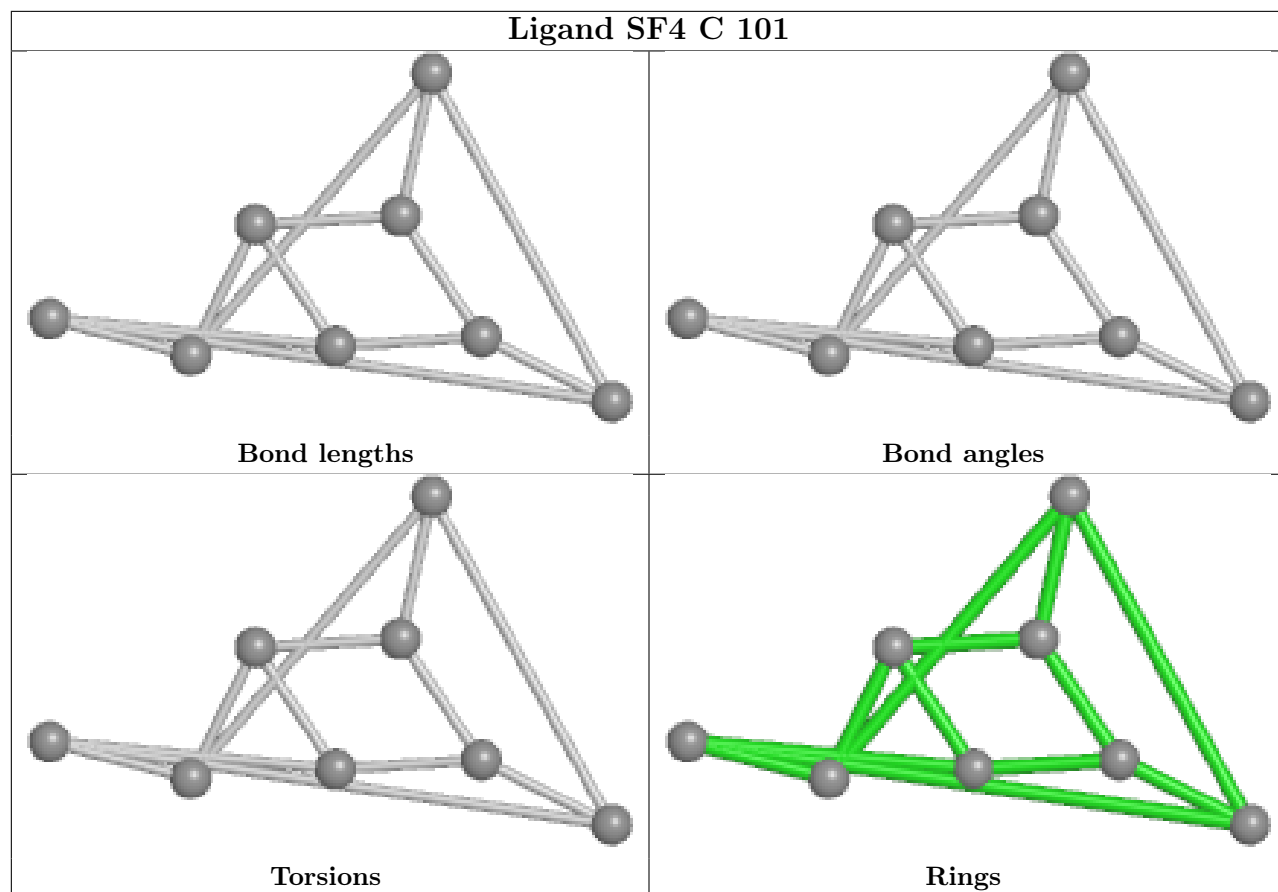
Bond angles



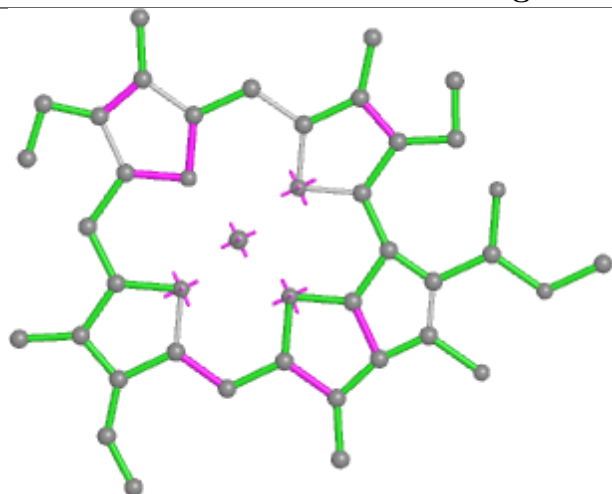
Torsions



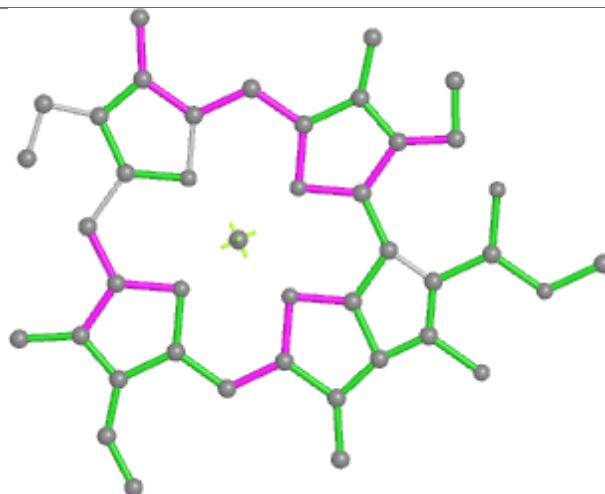
Rings



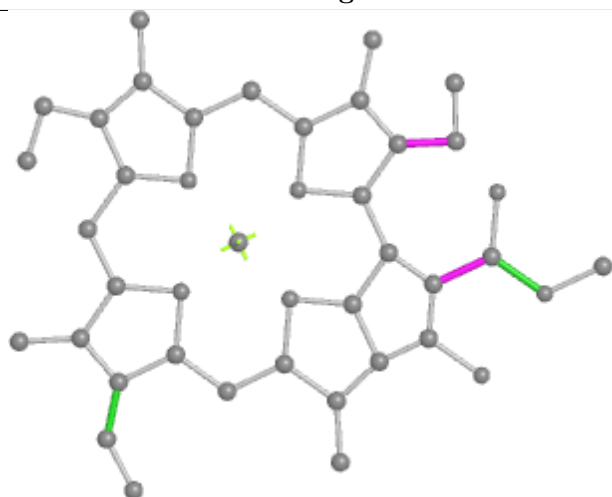
Ligand CLA A 802



Bond lengths



Bond angles

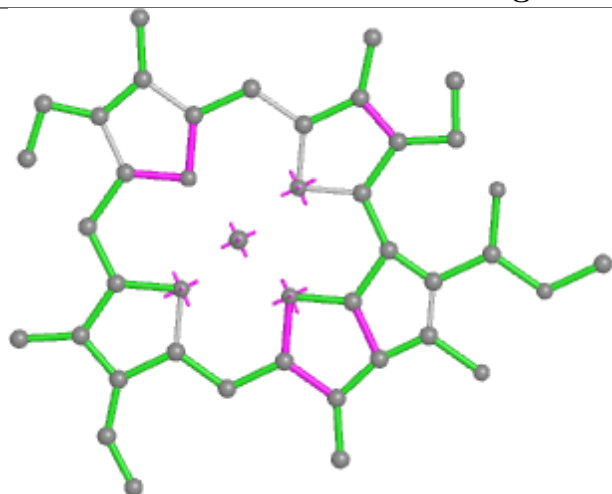


Torsions

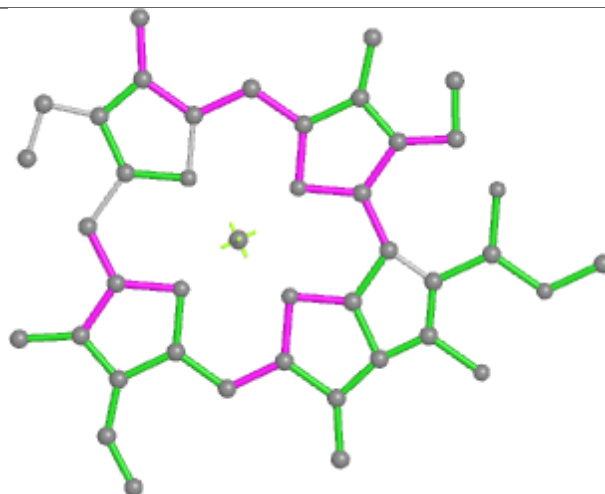


Rings

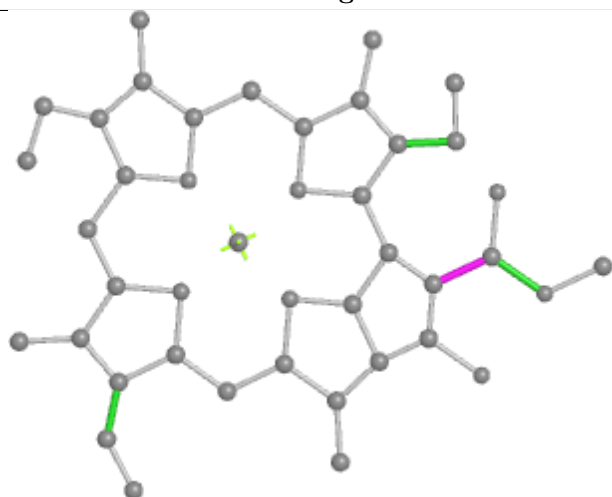
Ligand CLA A 807



Bond lengths



Bond angles

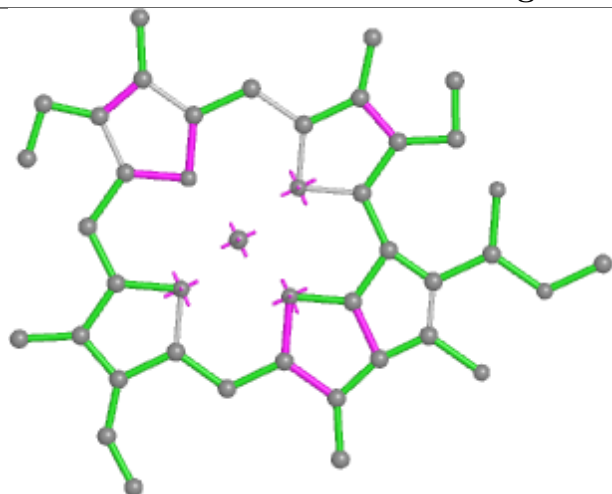


Torsions

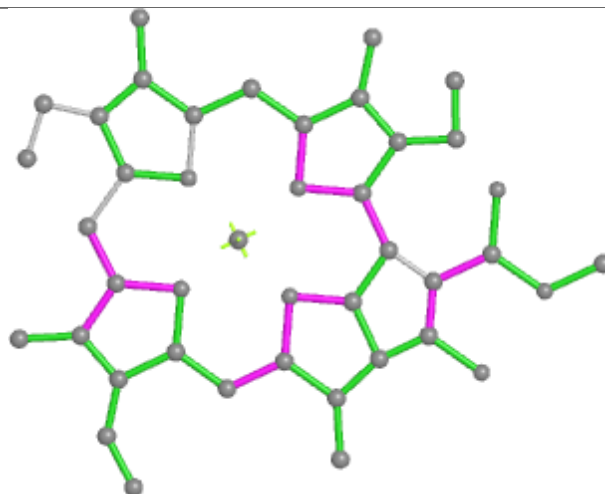


Rings

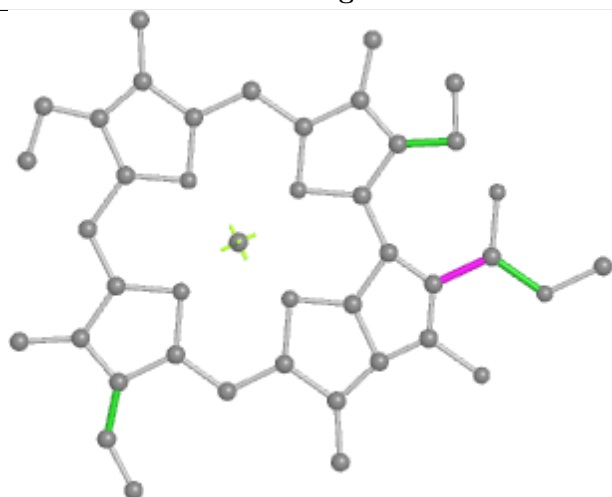
Ligand CL0 A 801



Bond lengths



Bond angles

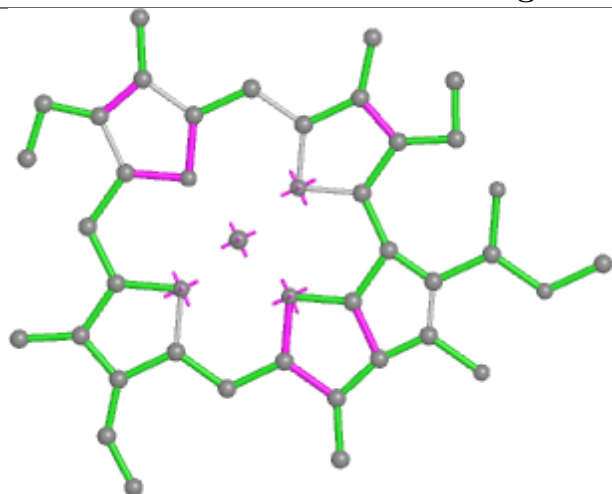


Torsions

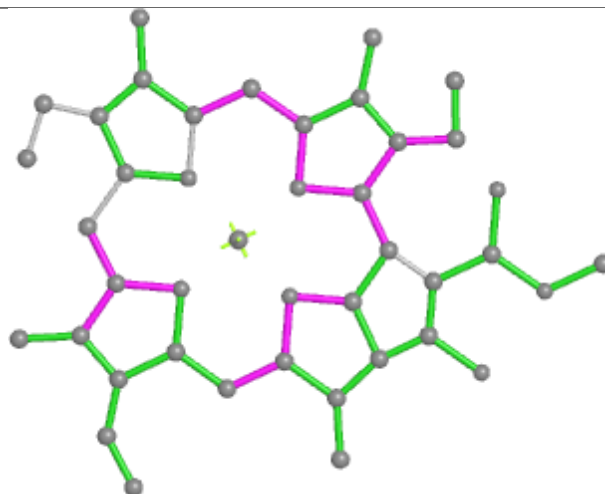


Rings

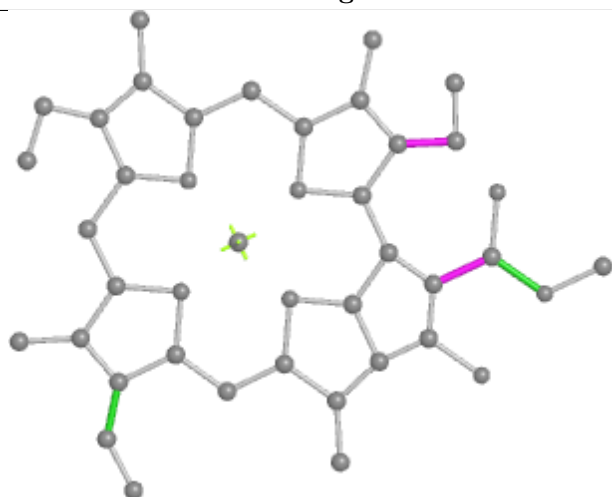
Ligand CLA 3 301



Bond lengths



Bond angles

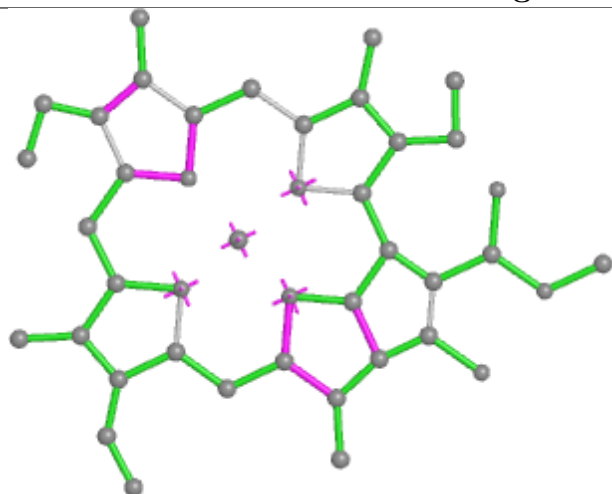


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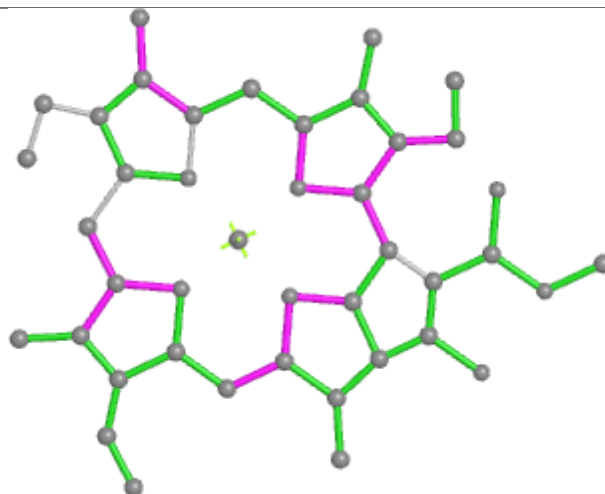


Rings

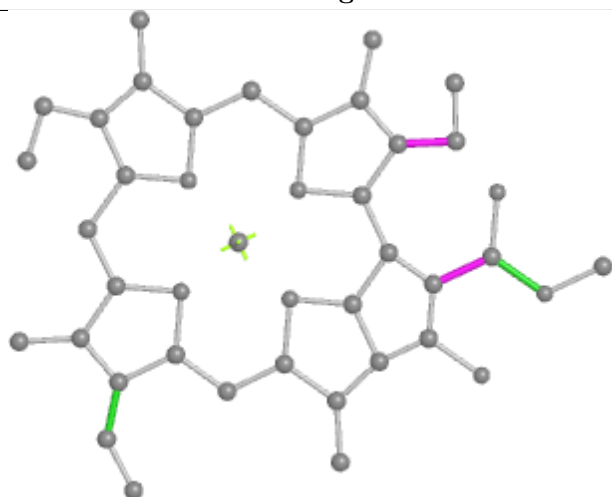
Ligand CLA B 817



Bond lengths



Bond angles

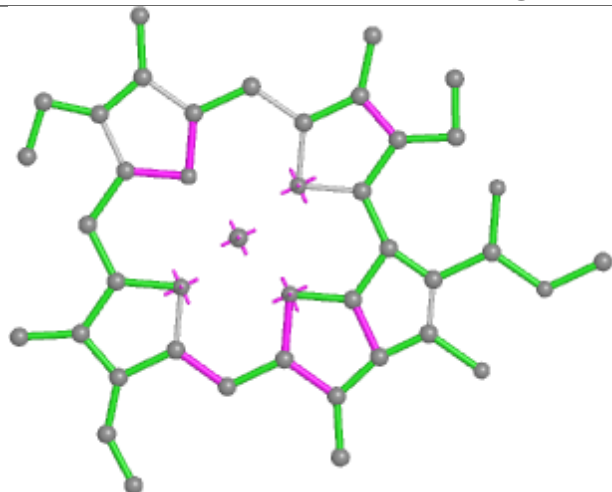


Torsions

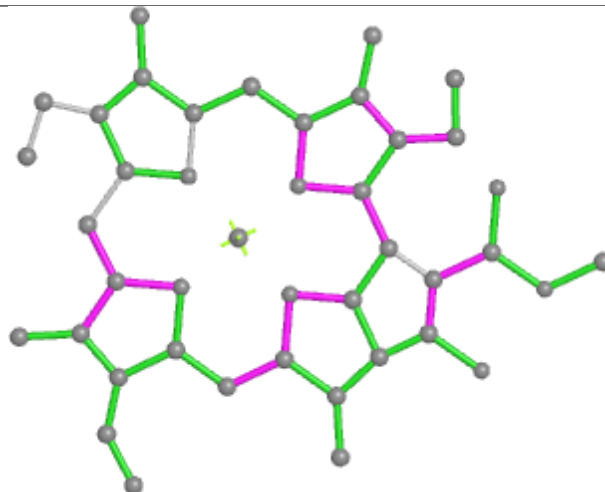


Rings

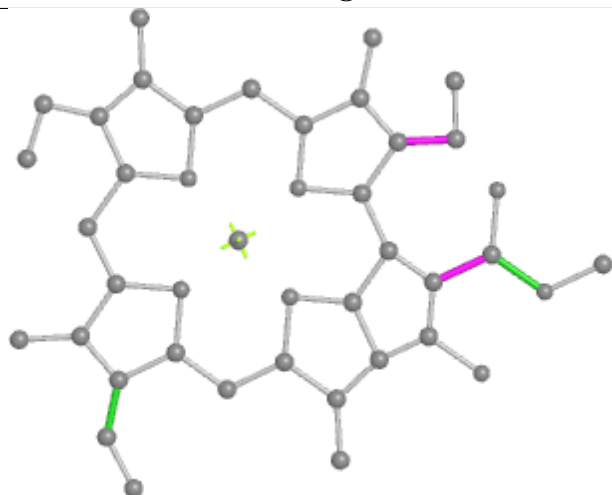
Ligand CLA A 831



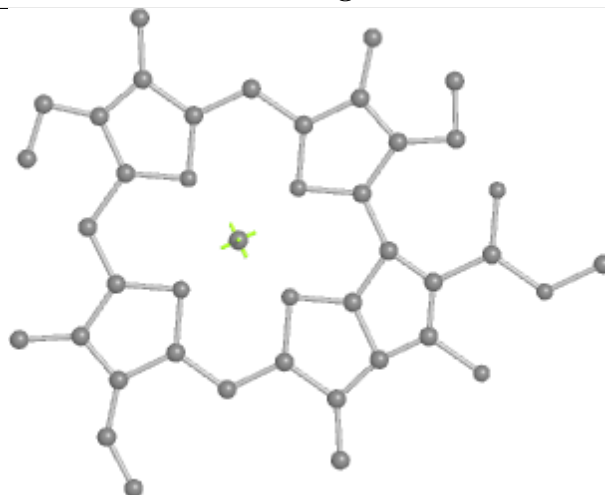
Bond lengths



Bond angles

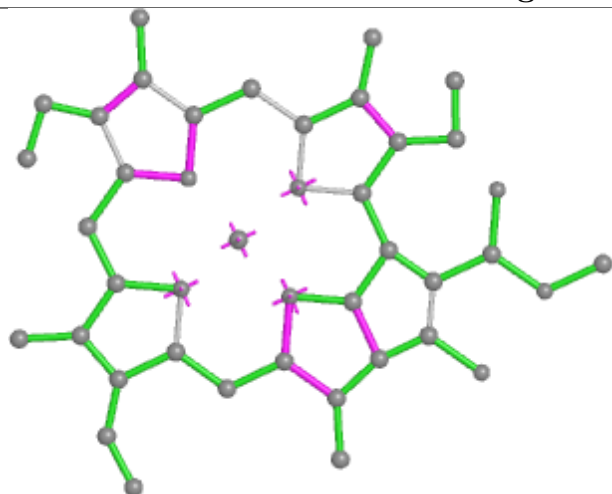


Torsions

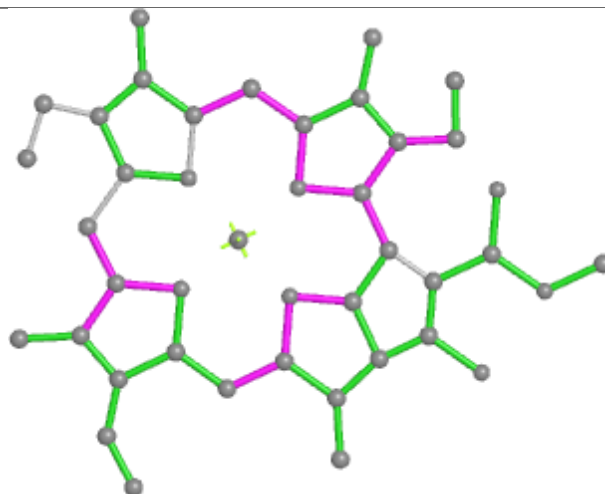


Rings

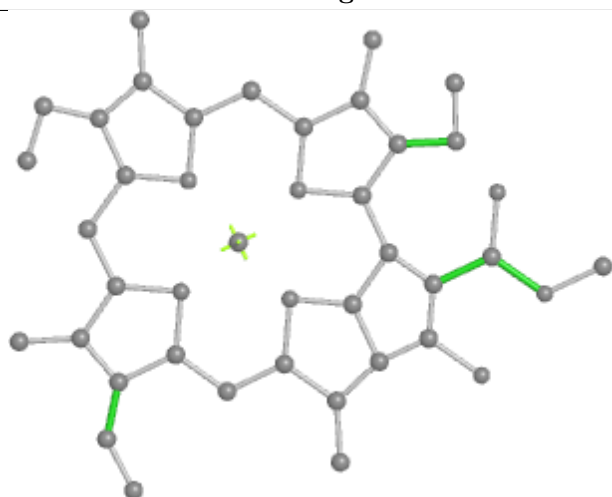
Ligand CLA 6 604



Bond lengths



Bond angles

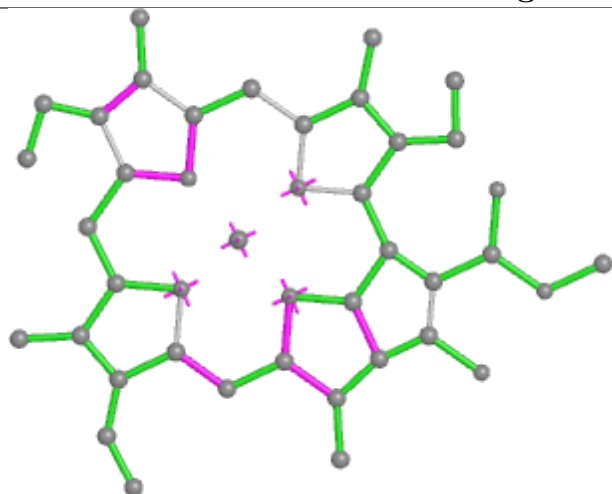


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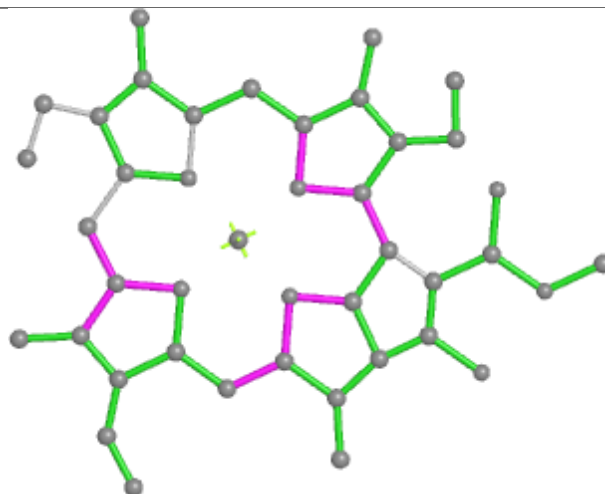


Rings

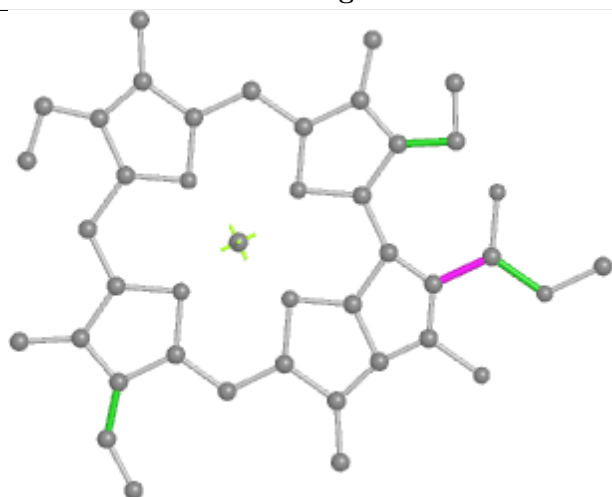
Ligand CLA 5 301



Bond lengths



Bond angles

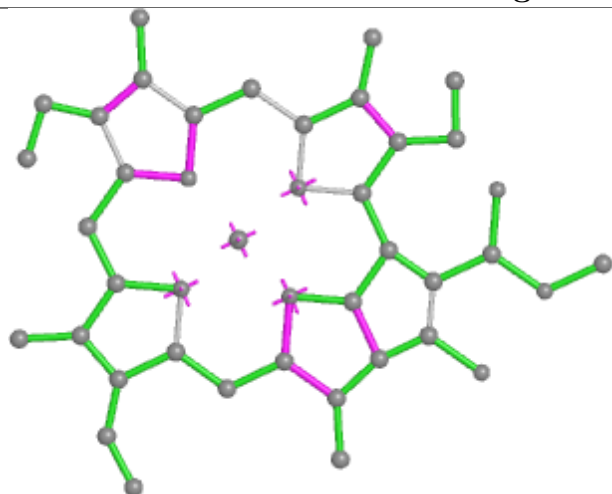


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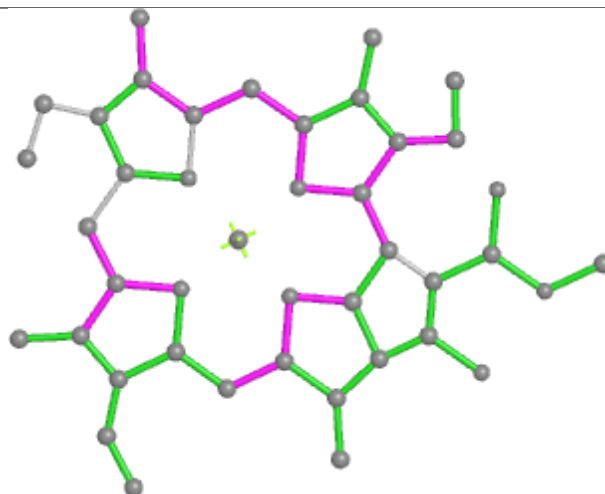


Rings

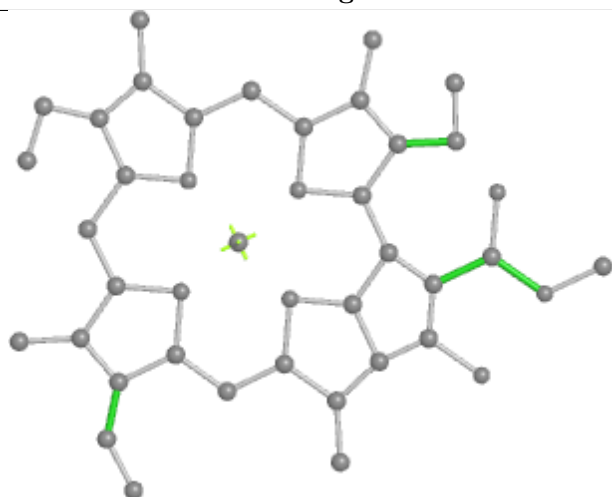
Ligand CLA B 811



Bond lengths



Bond angles

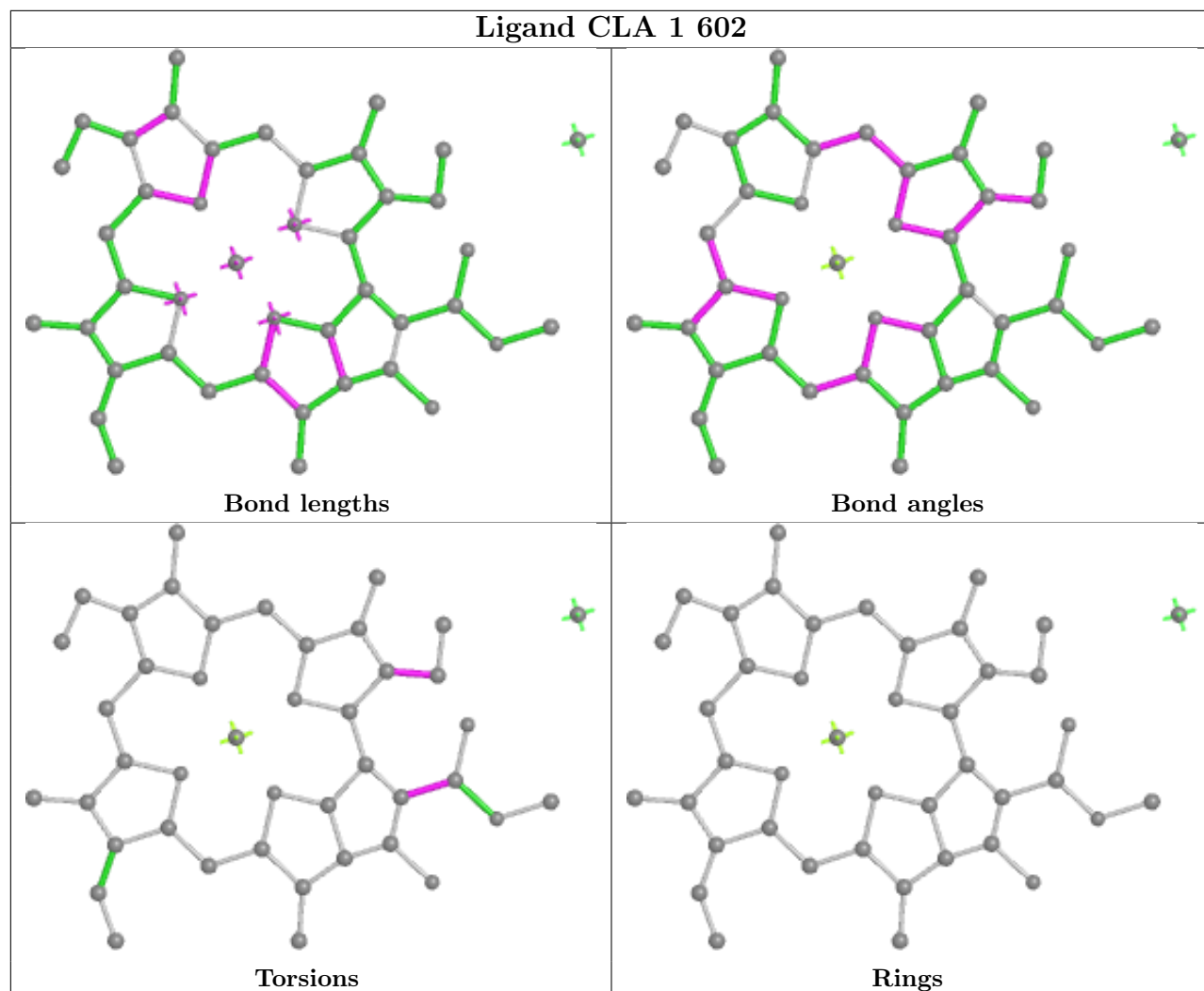


Torsions

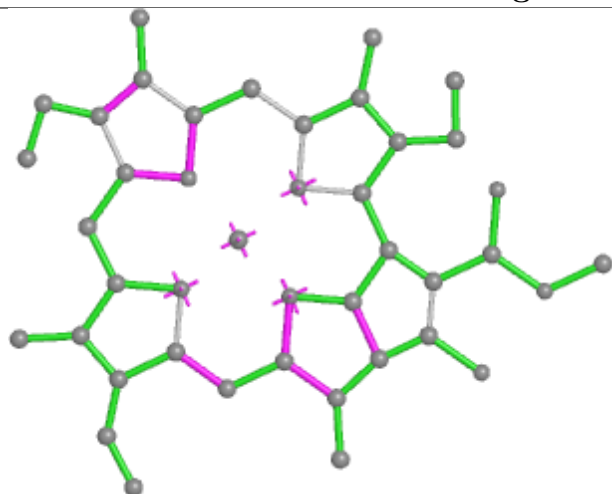


Rings

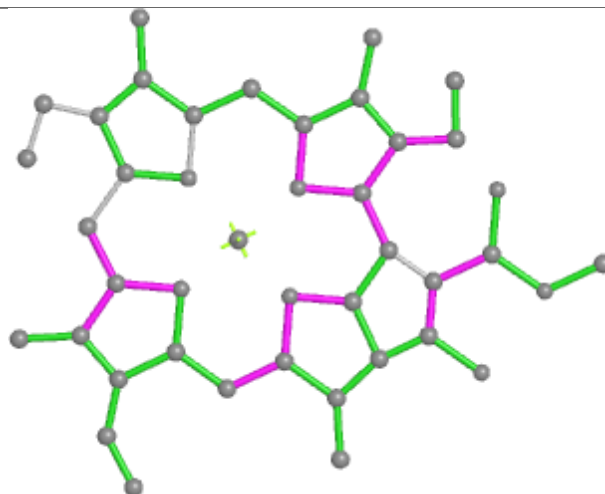
Ligand CLA 1 602



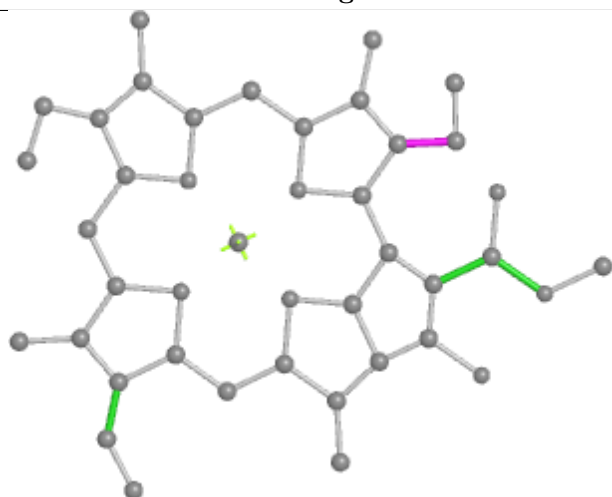
Ligand CLA A 830



Bond lengths



Bond angles

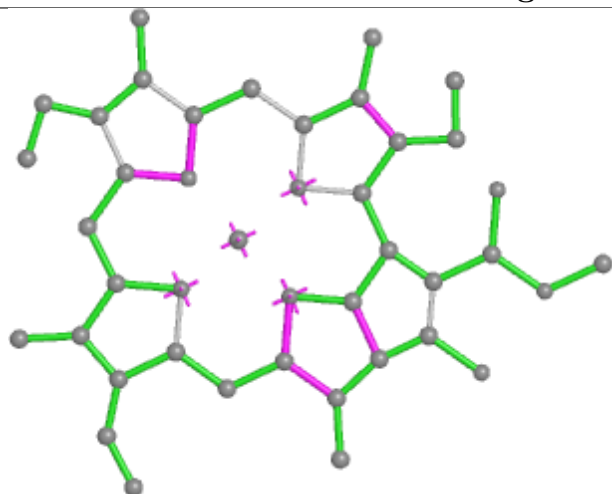


Torsions

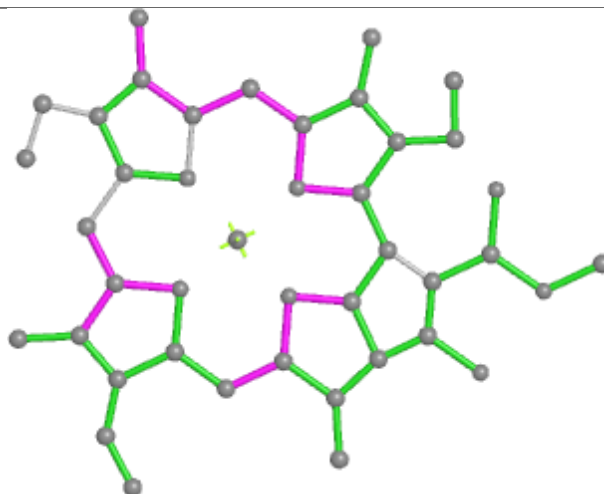


Rings

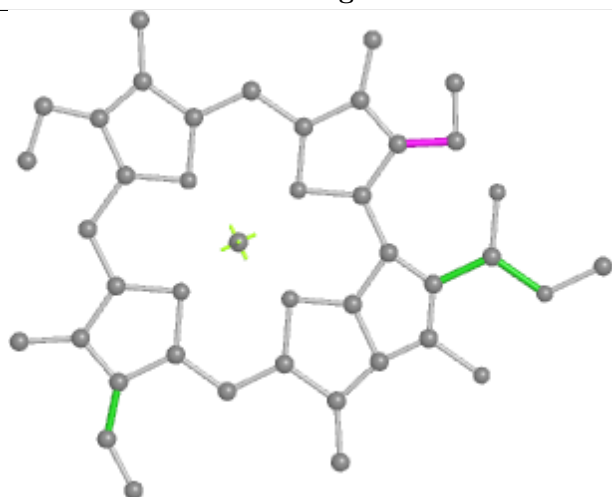
Ligand CLA 4 604



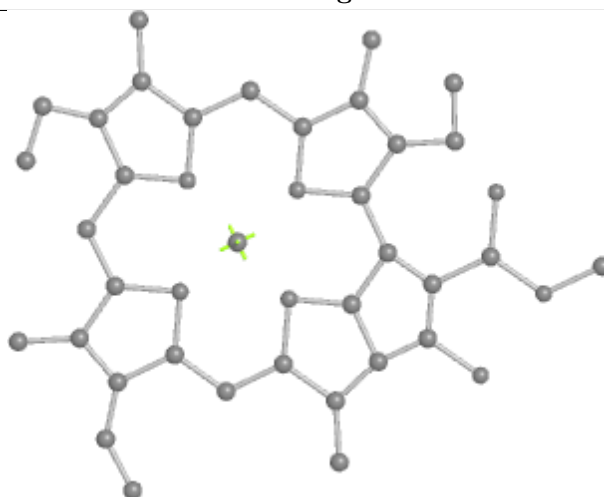
Bond lengths



Bond angles

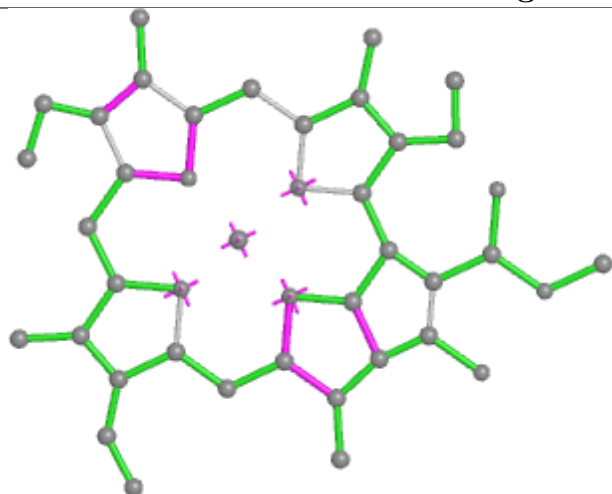


Torsions

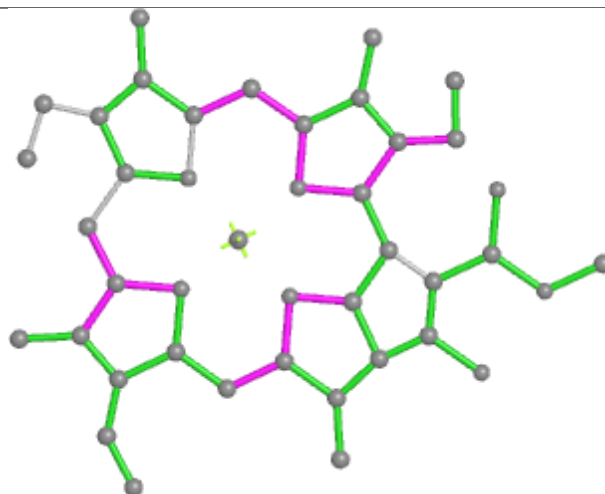


Rings

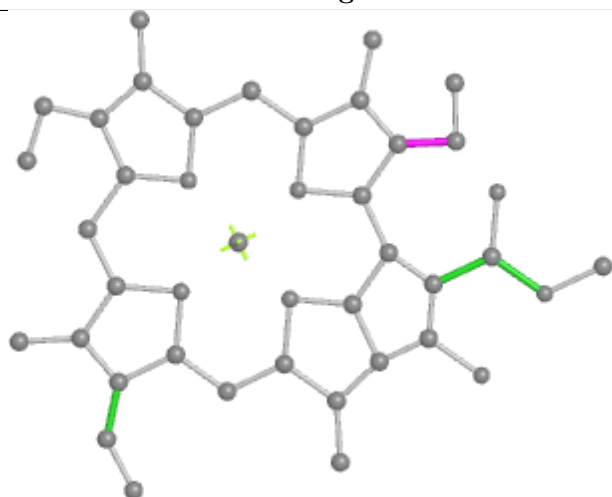
Ligand CLA 8 609



Bond lengths



Bond angles

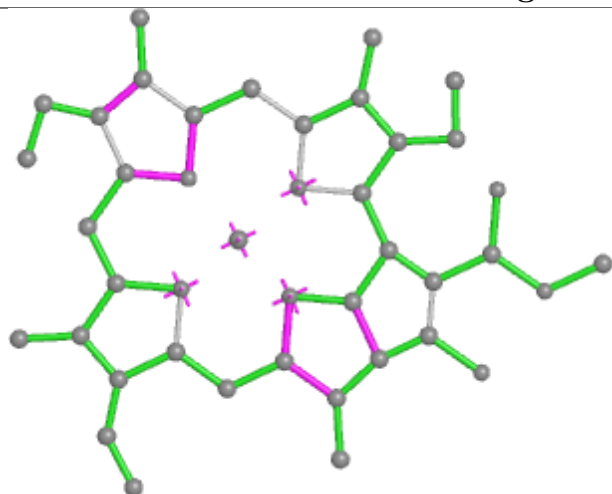


Torsions

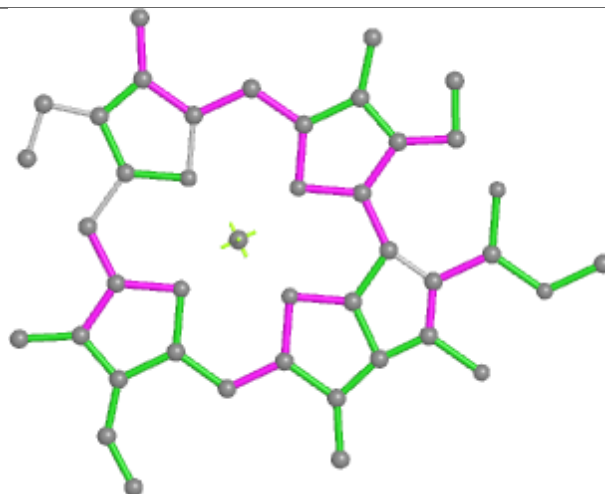


Rings

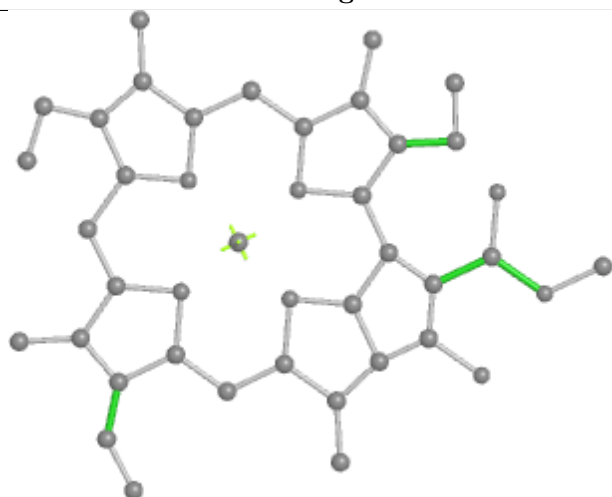
Ligand CLA 8 608



Bond lengths



Bond angles

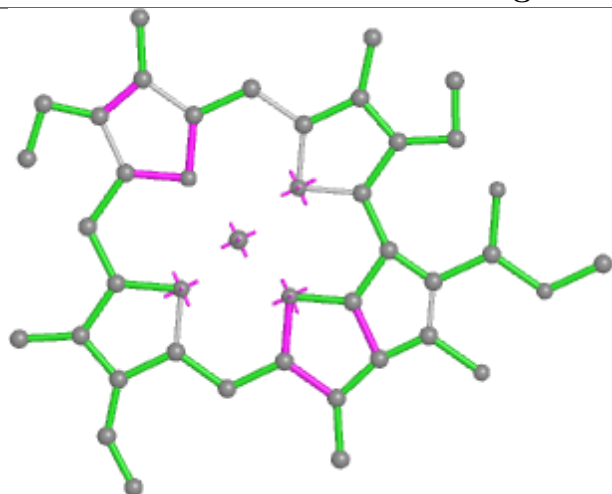


Torsions

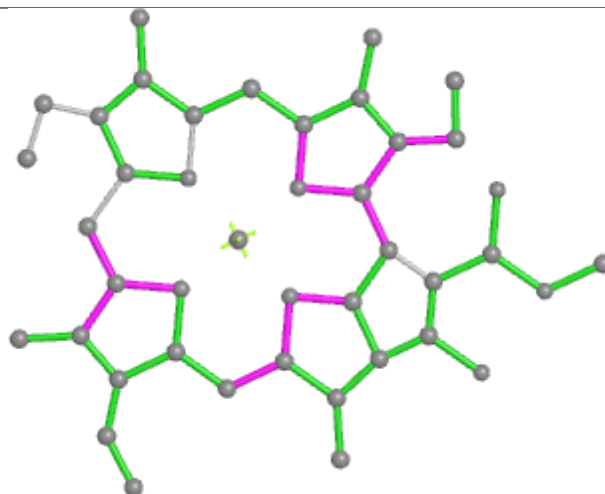


Rings

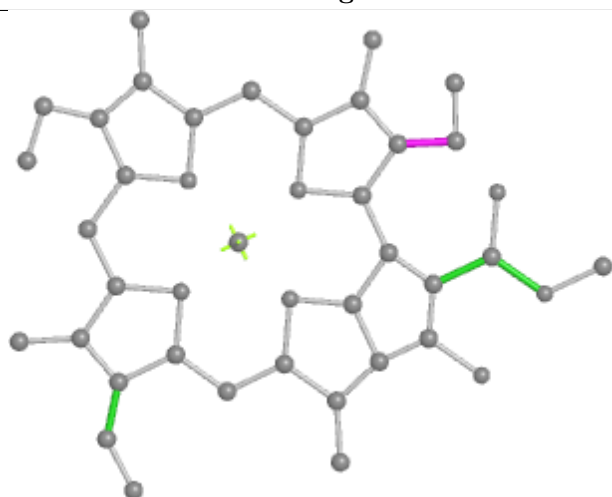
Ligand CLA B 837



Bond lengths



Bond angles

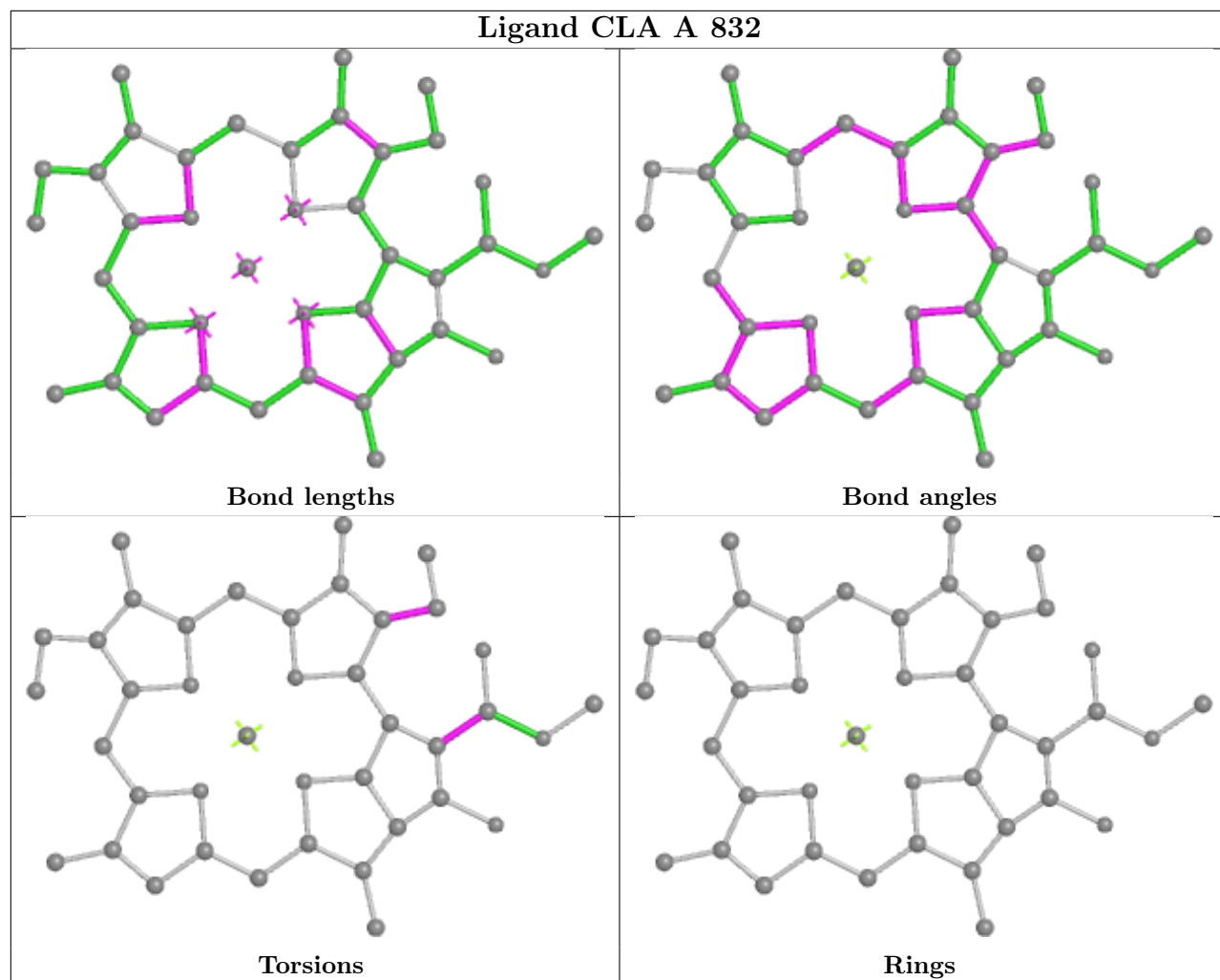


Torsions

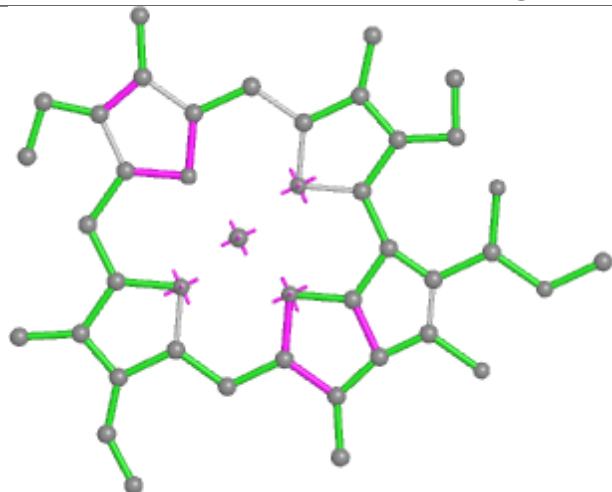


Rings

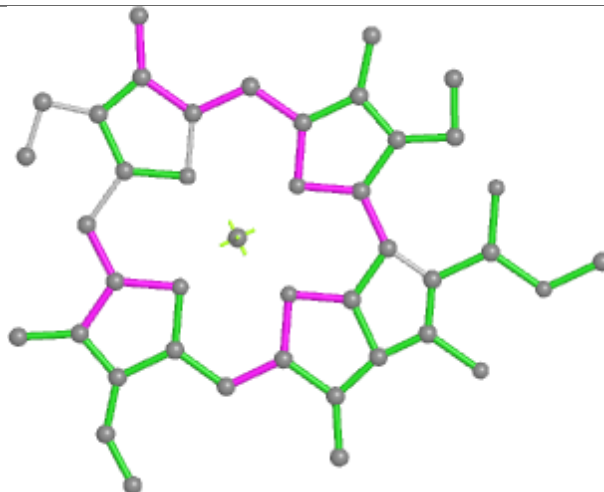
Ligand CLA A 832



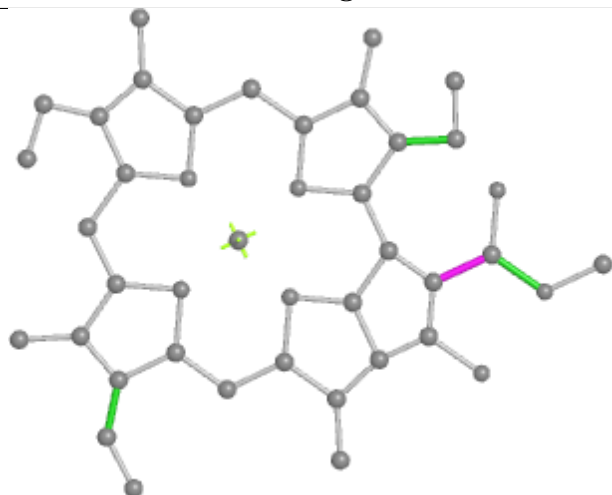
Ligand CLA A 819



Bond lengths



Bond angles

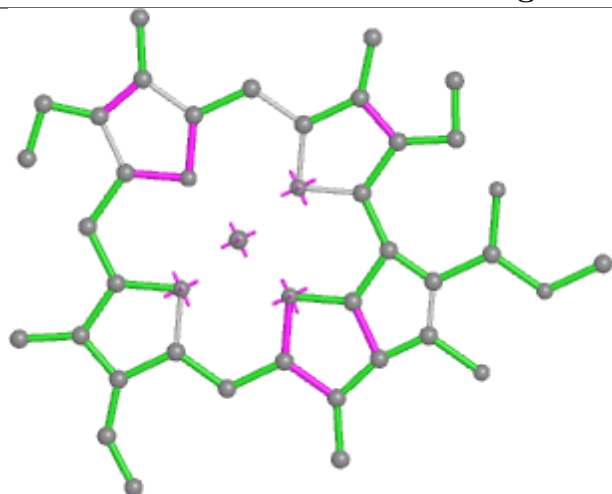


Torsions

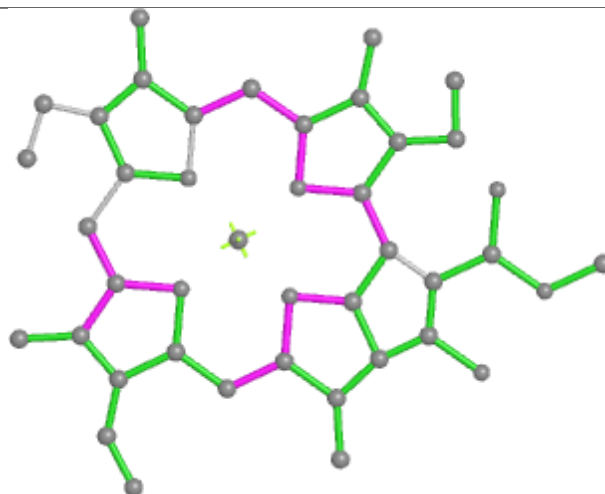


Rings

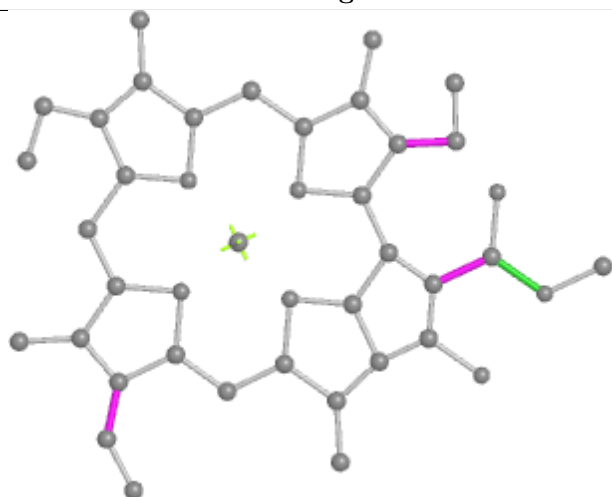
Ligand CLA 7 607



Bond lengths



Bond angles

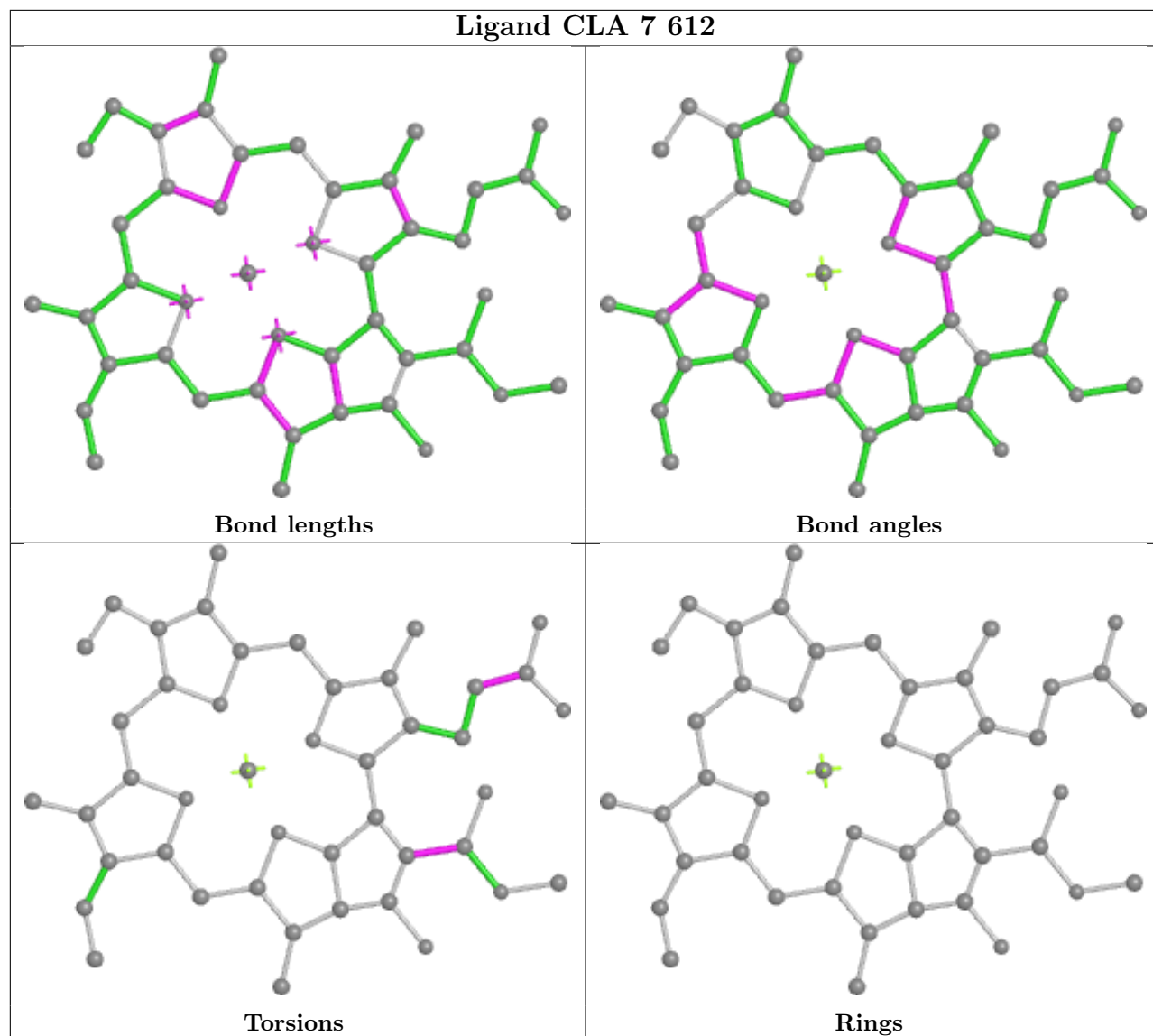


Torsions

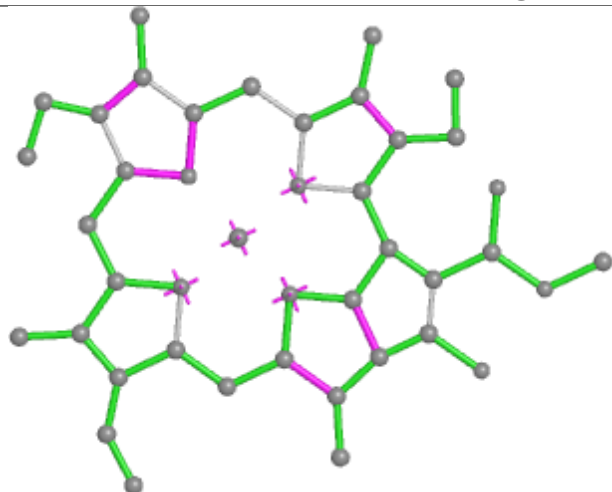


Rings

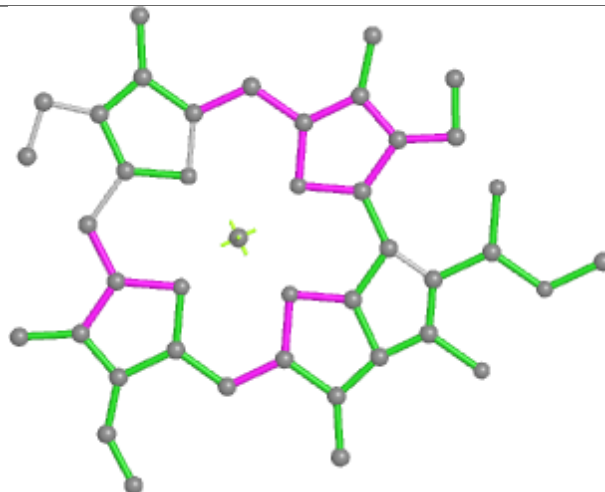
Ligand CLA 7 612



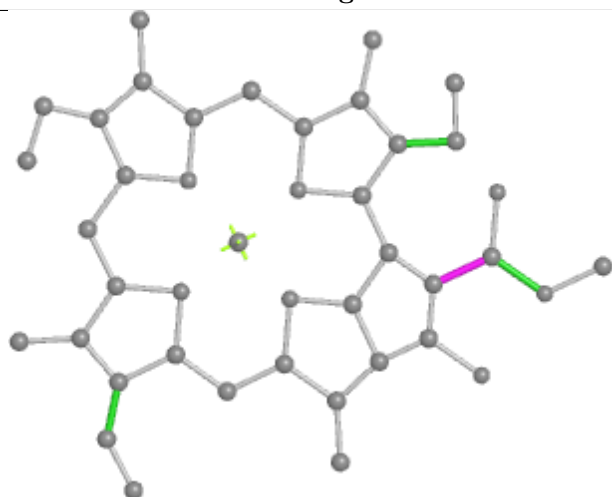
Ligand CLA A 804



Bond lengths



Bond angles

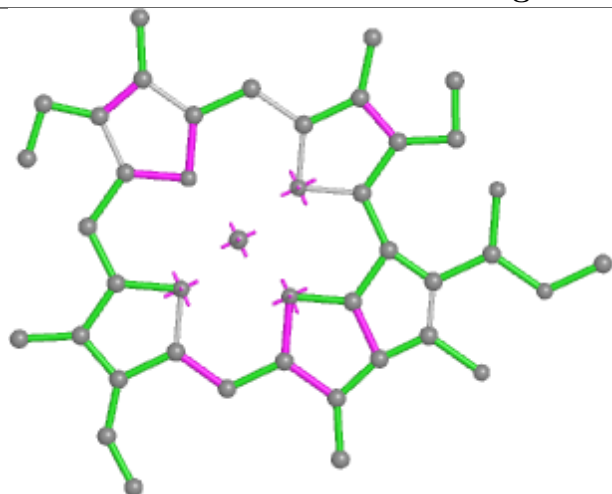


Torsions

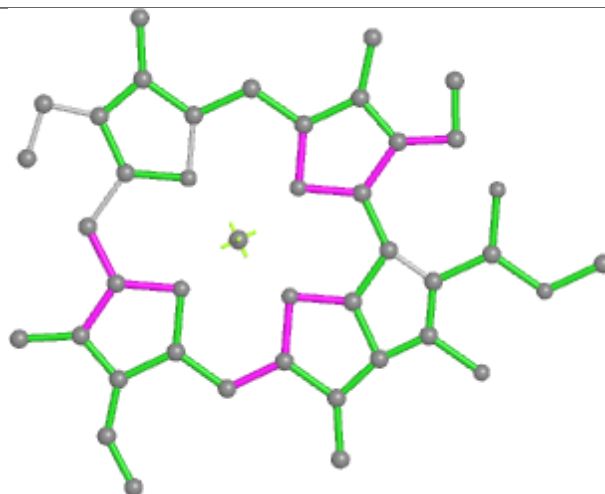


Rings

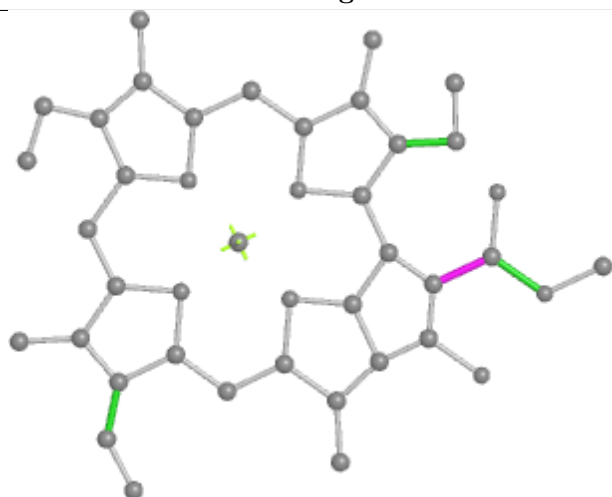
Ligand CLA A 811



Bond lengths



Bond angles

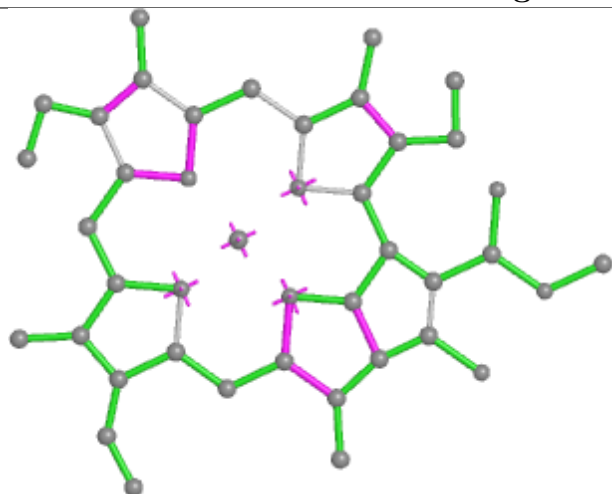


Torsions

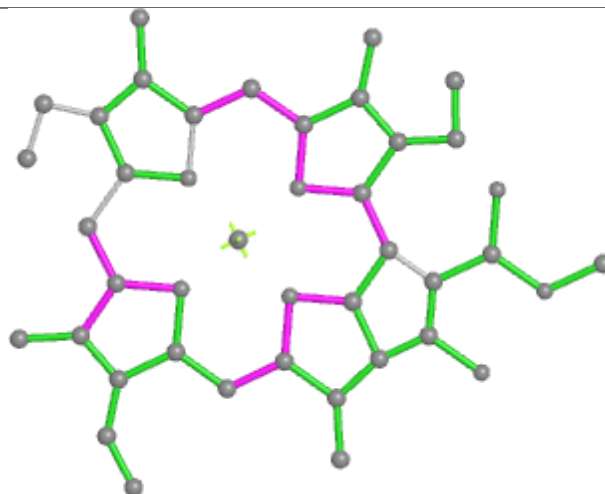


Rings

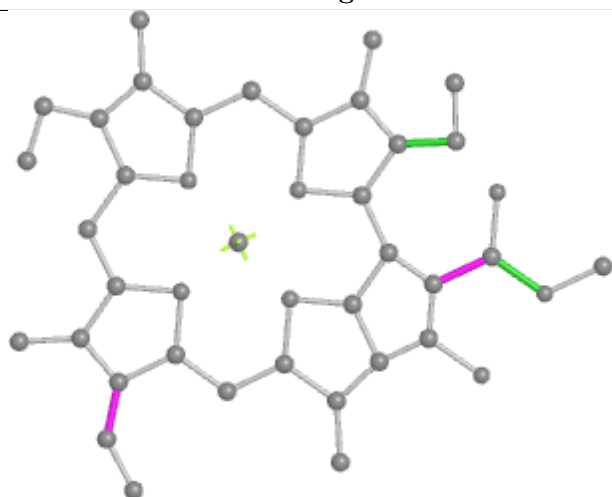
Ligand CLA B 834



Bond lengths



Bond angles

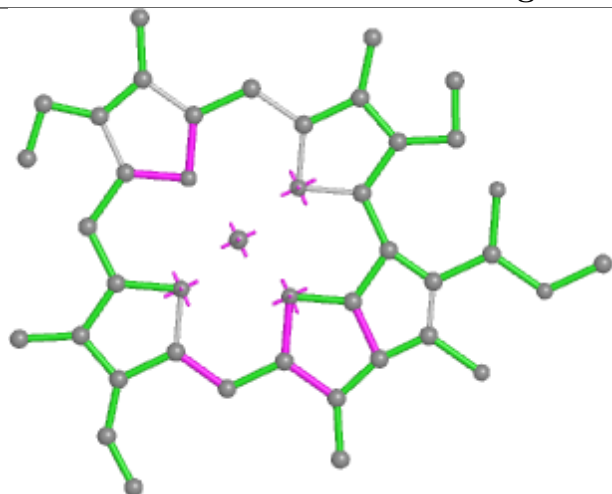


Torsions

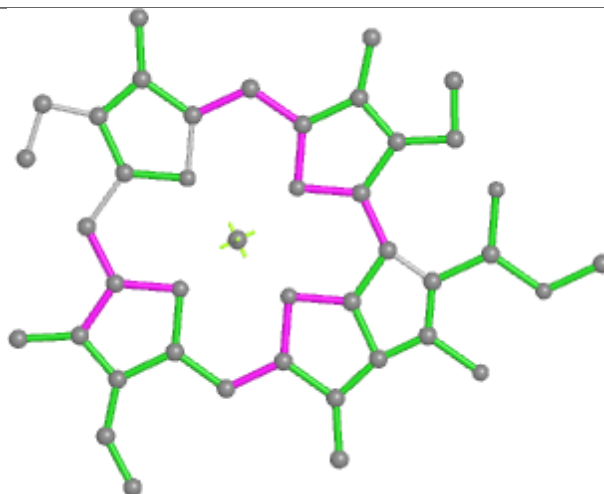


Rings

Ligand CLA 6 602



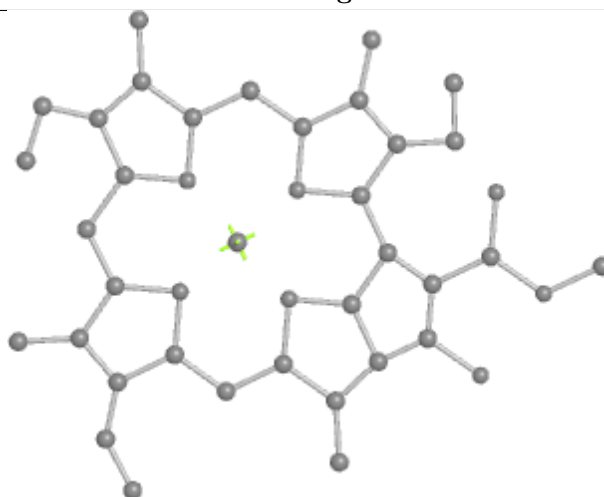
Bond lengths



Bond angles

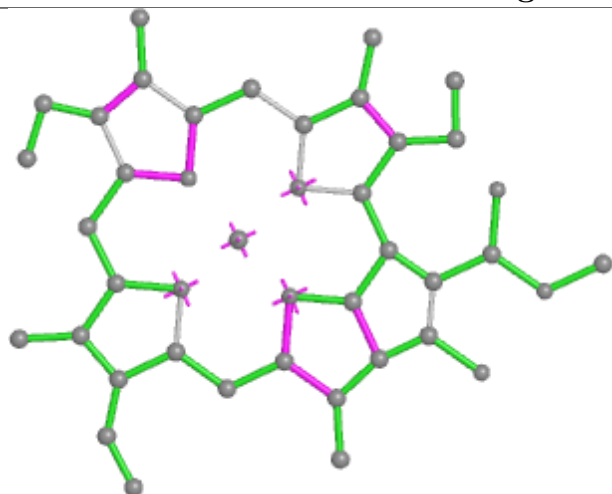


Torsions

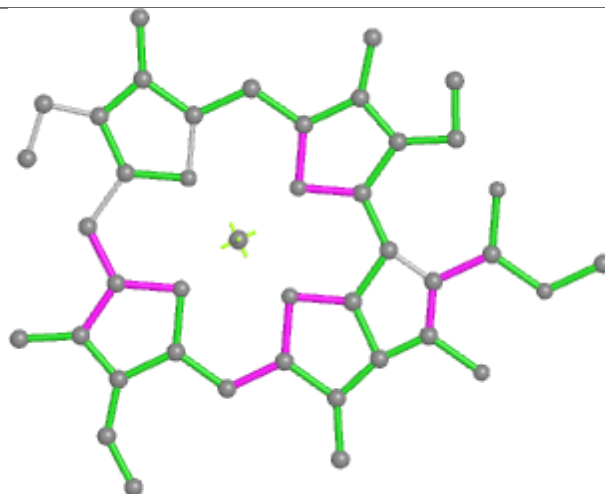


Rings

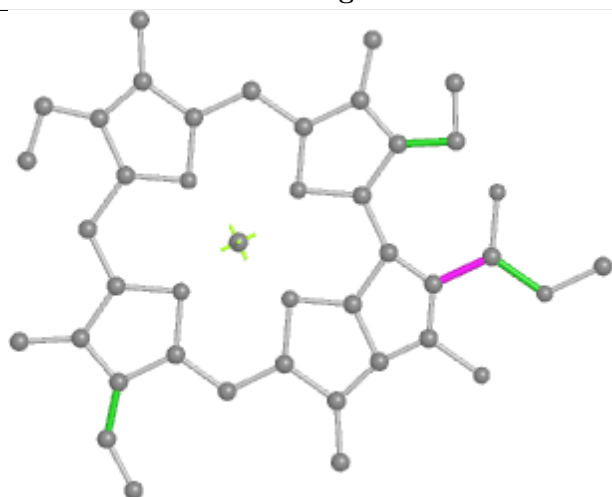
Ligand CLA 6 603



Bond lengths



Bond angles

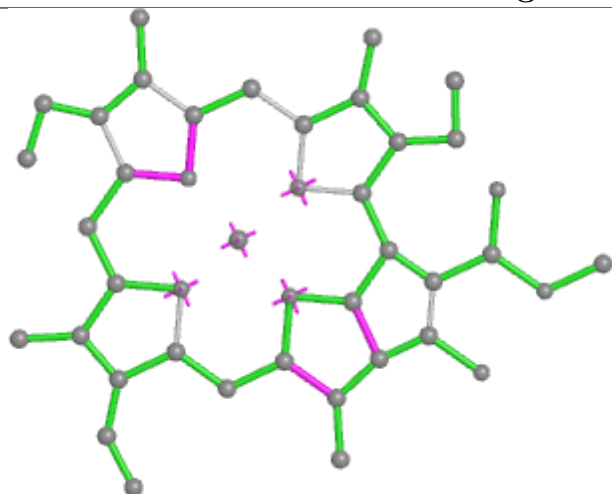


Torsions

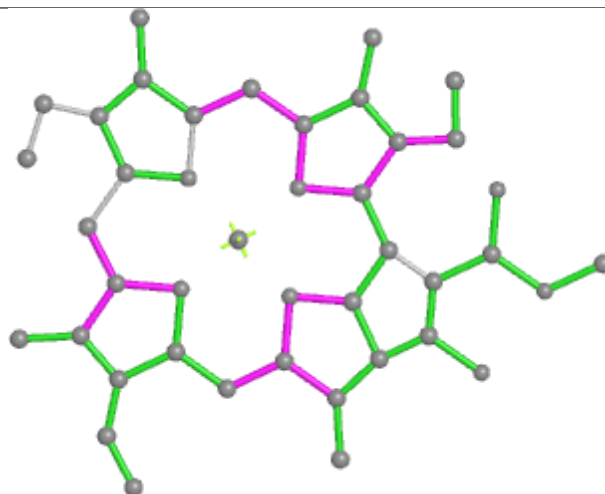


Rings

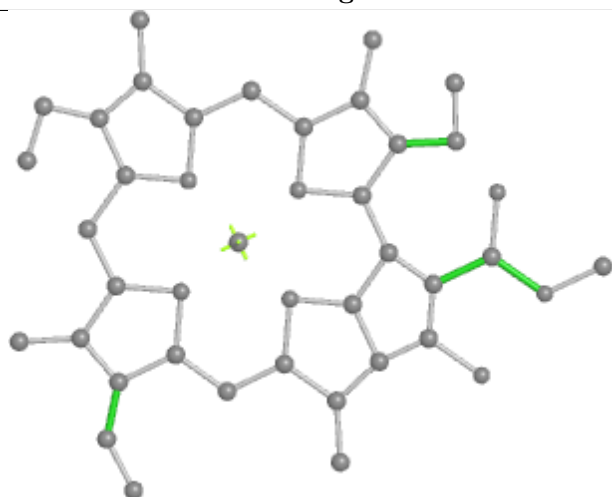
Ligand CLA 1 606



Bond lengths



Bond angles

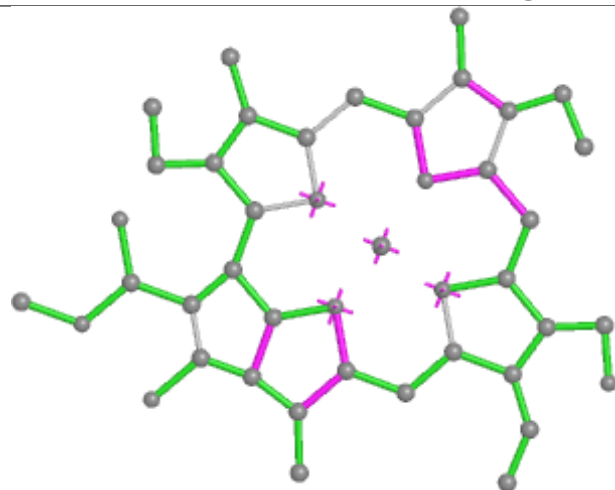


Torsions

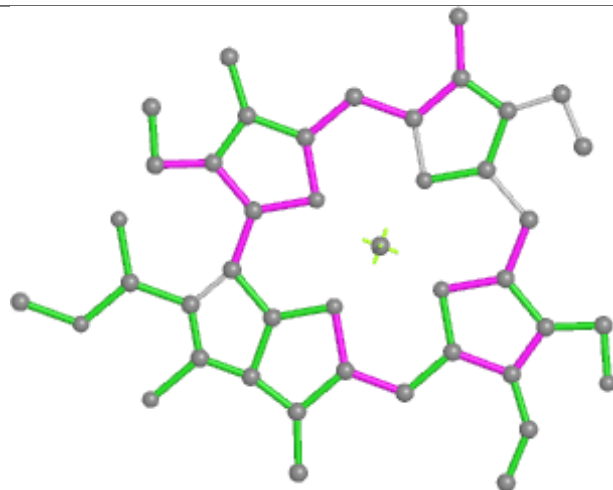


Rings

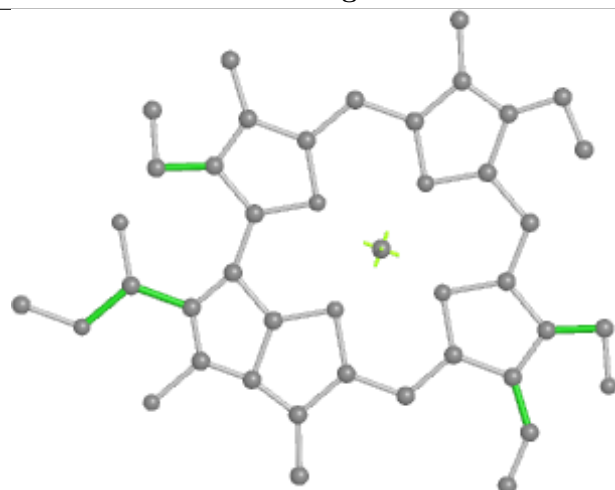
Ligand CHL 7 606



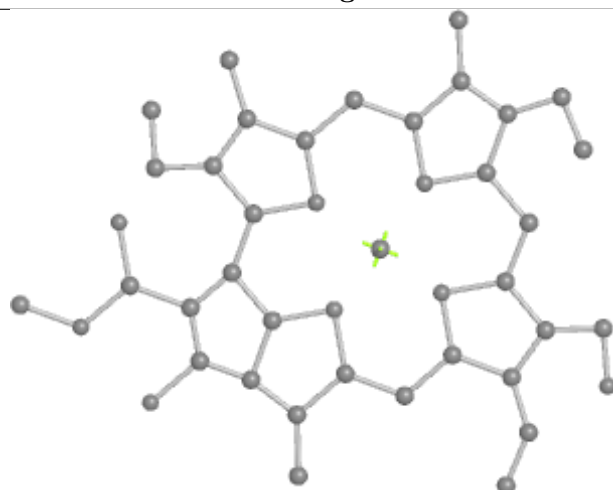
Bond lengths



Bond angles

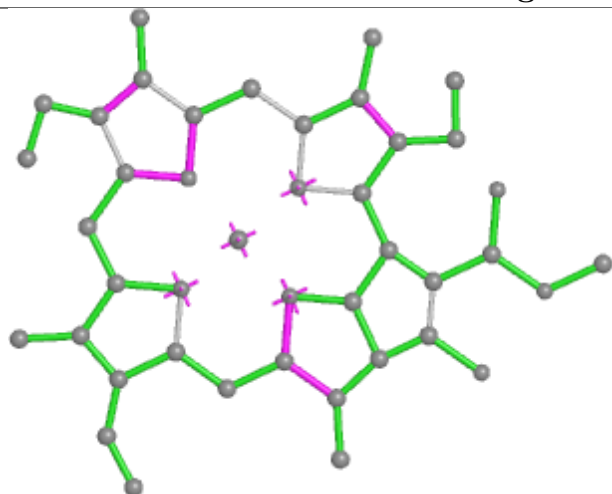


Torsions

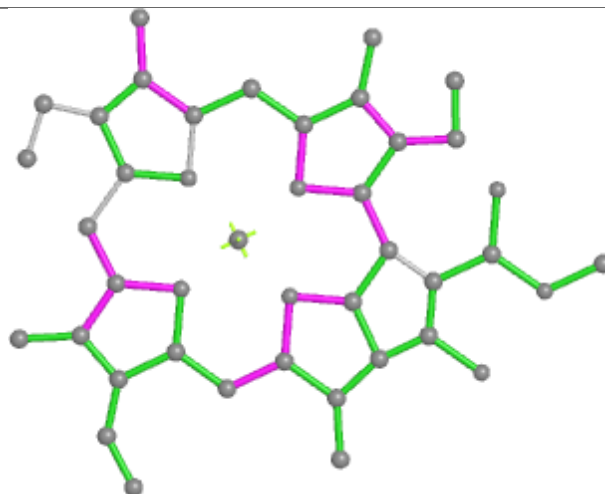


Rings

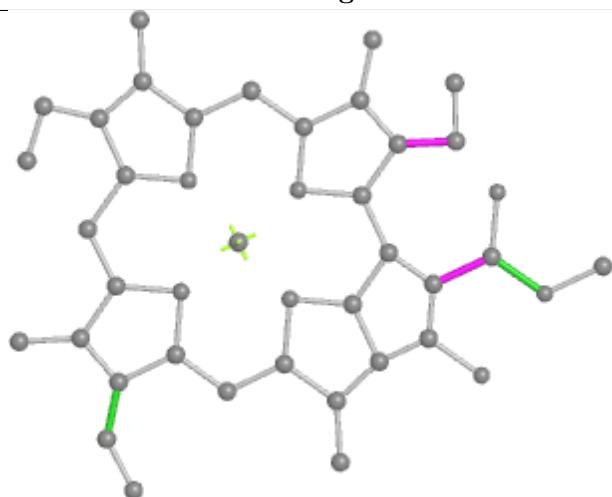
Ligand CLA 1 608



Bond lengths



Bond angles

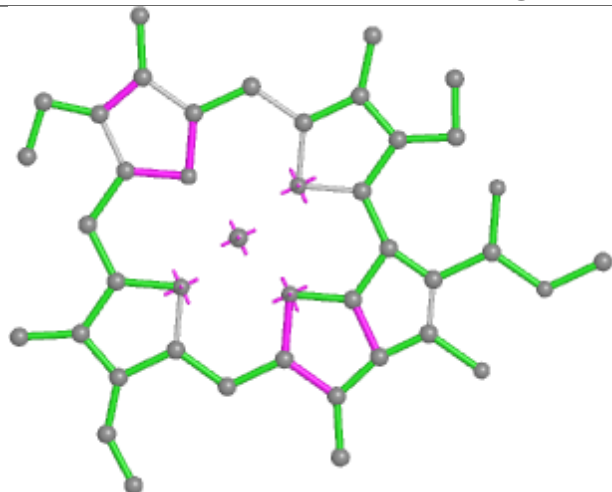


Torsions

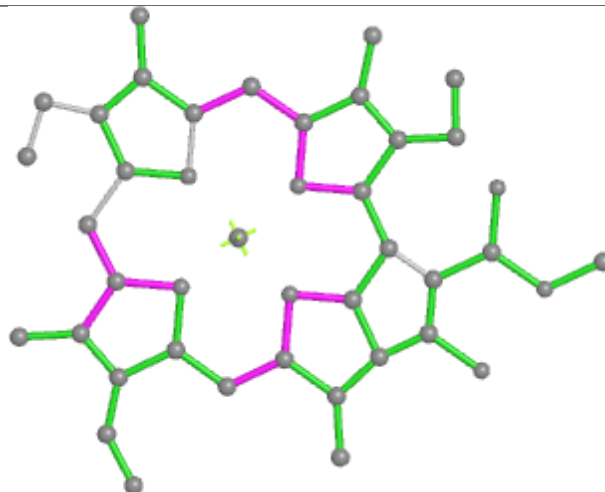


Rings

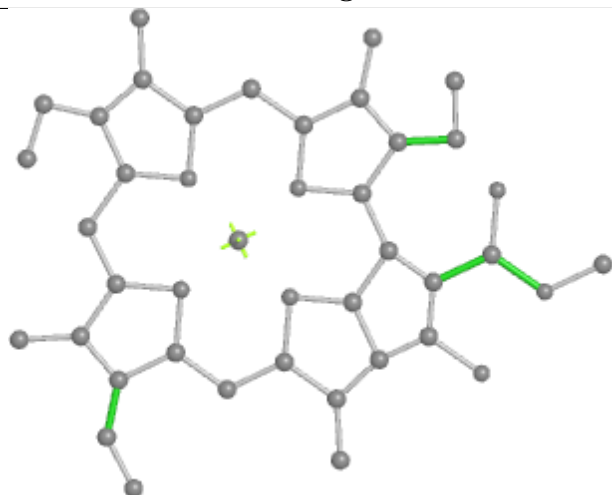
Ligand CLA A 834



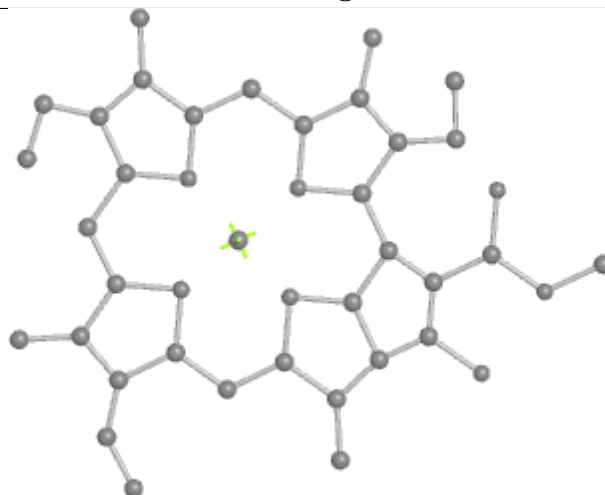
Bond lengths



Bond angles

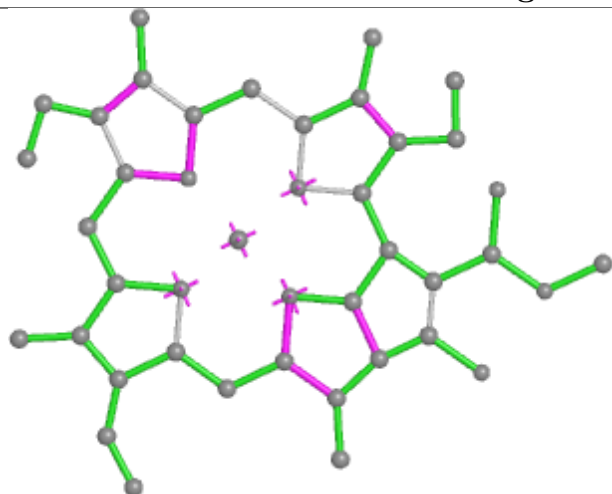


Torsions

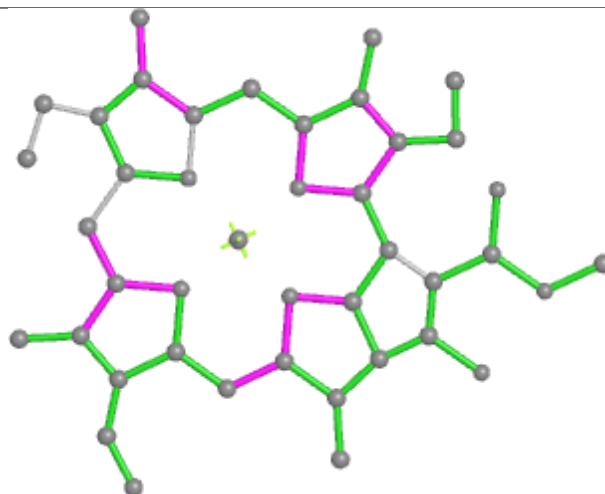


Rings

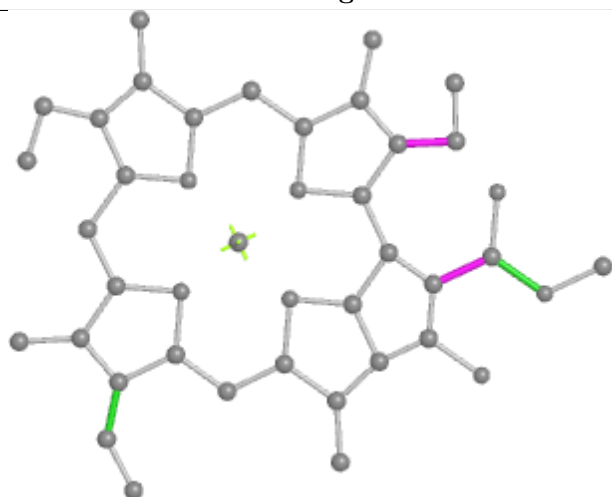
Ligand CLA 7 611



Bond lengths



Bond angles

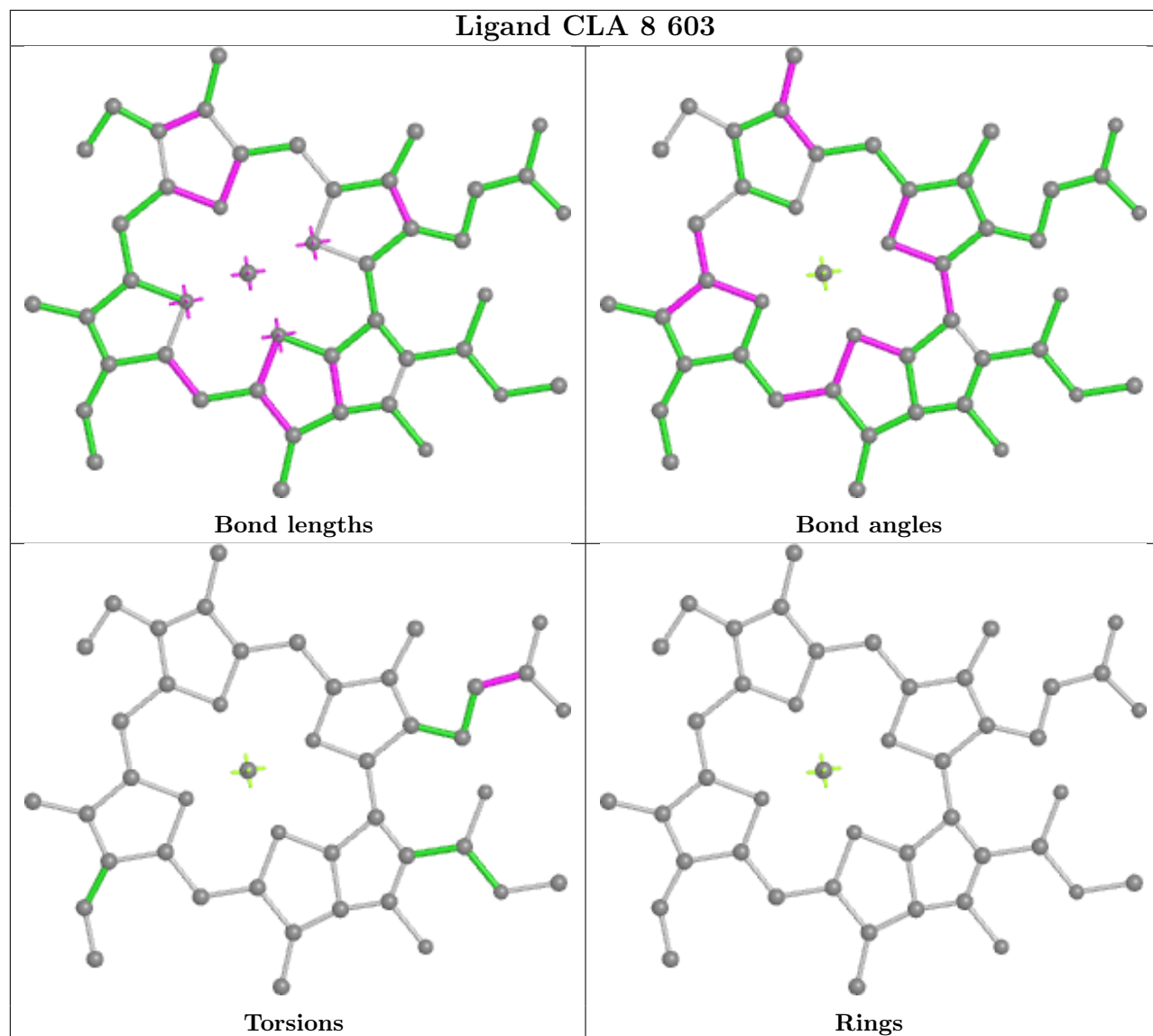


Torsions

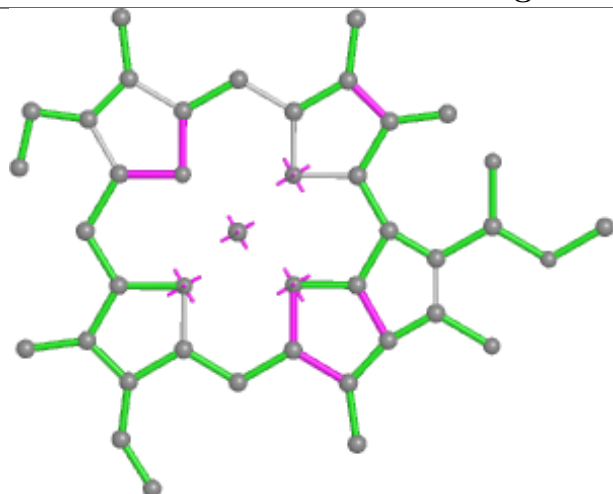


Rings

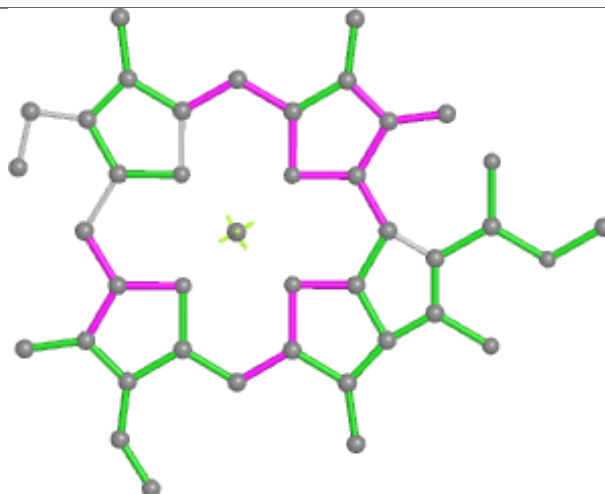
Ligand CLA 8 603



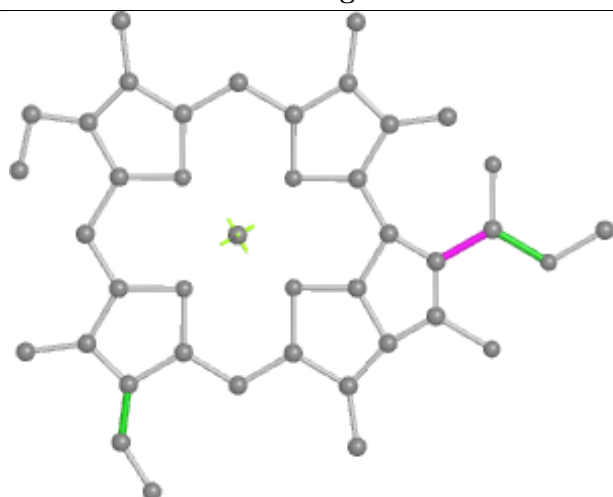
Ligand CLA B 824



Bond lengths



Bond angles

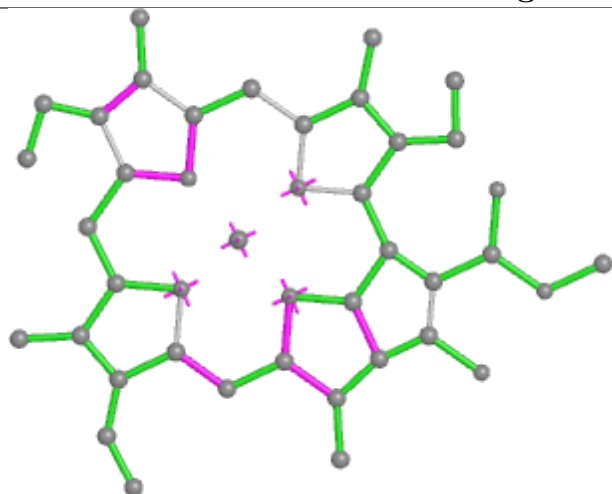


Torsions

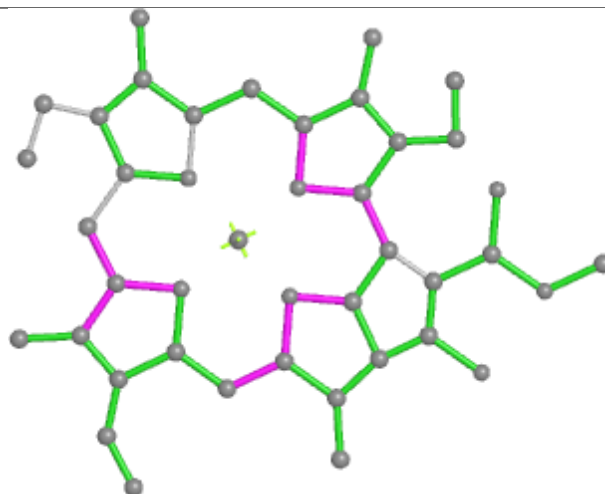


Rings

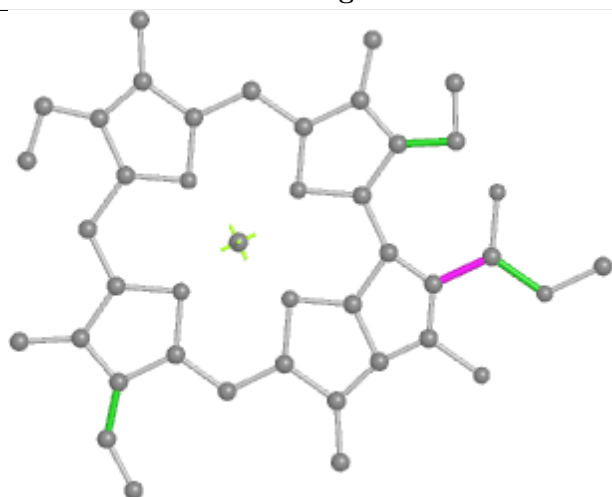
Ligand CLA 5 304



Bond lengths



Bond angles

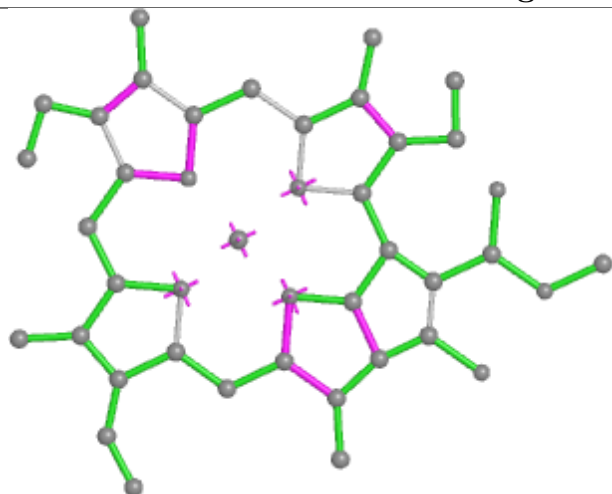


Torsions

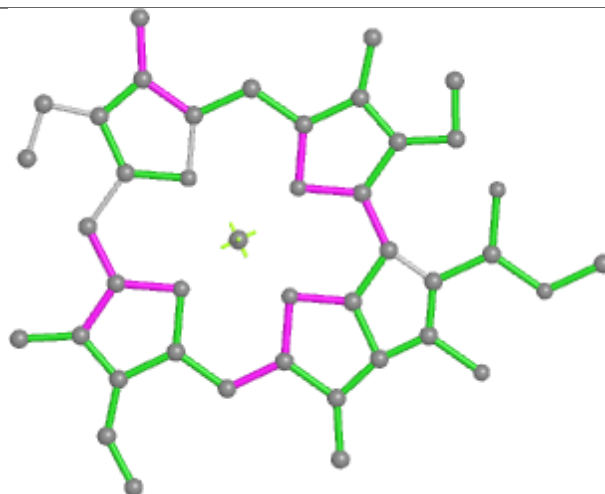


Rings

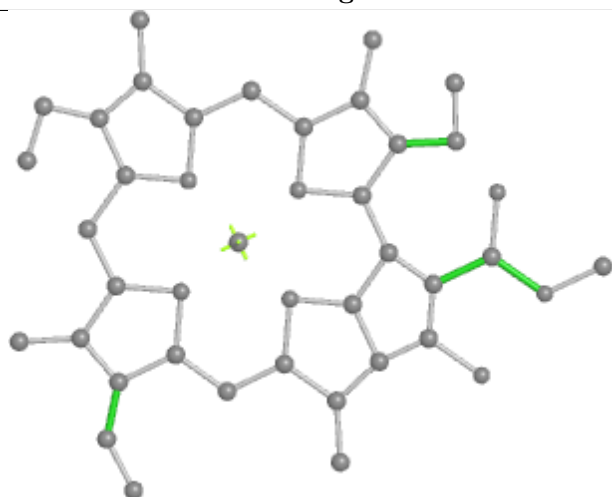
Ligand CLA 3 303



Bond lengths



Bond angles

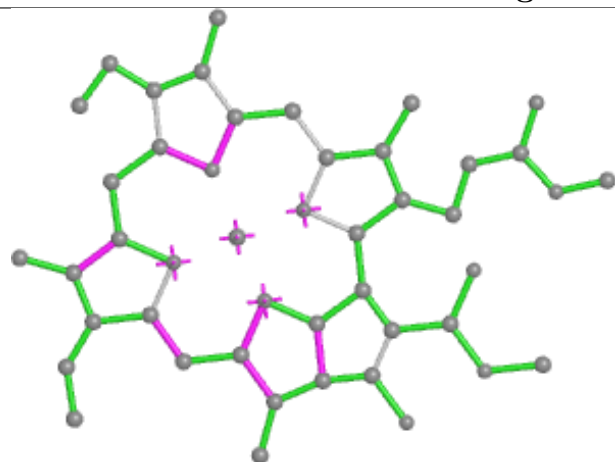


Torsions

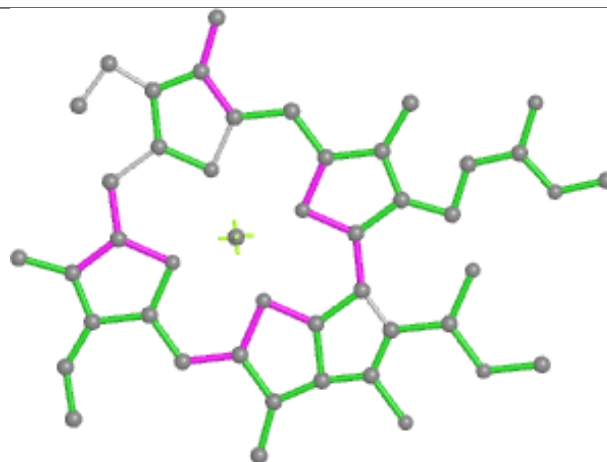


Rings

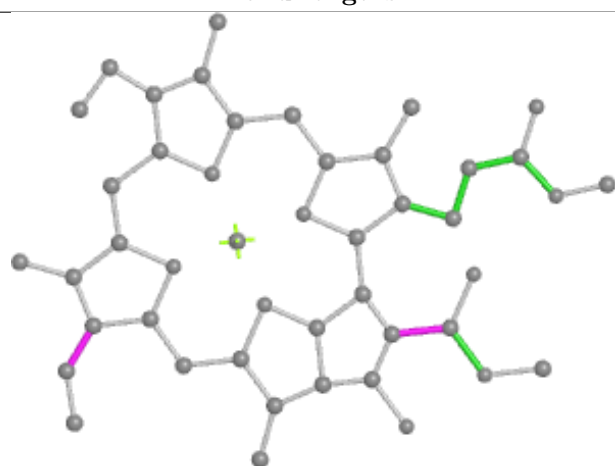
Ligand CLA B 821



Bond lengths



Bond angles

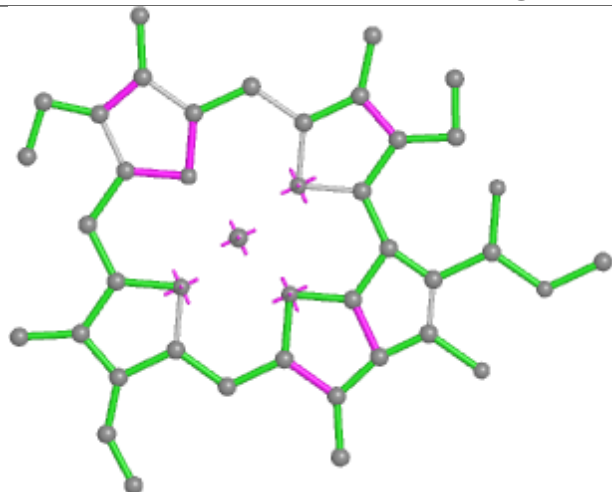


Torsions

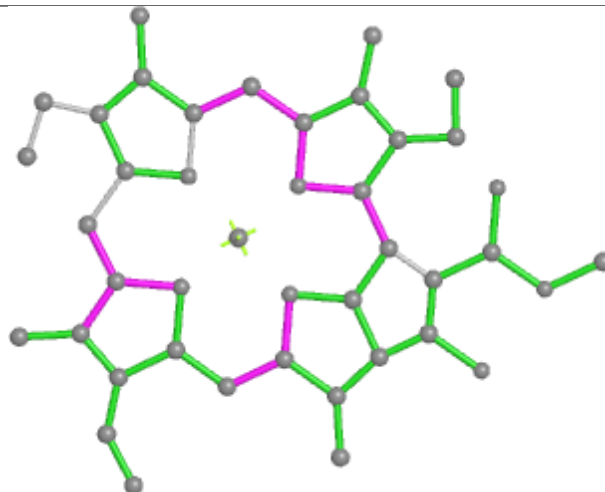


Rings

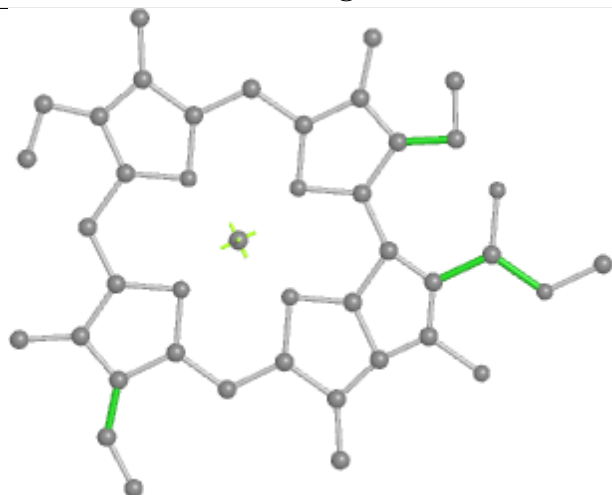
Ligand CLA A 826



Bond lengths



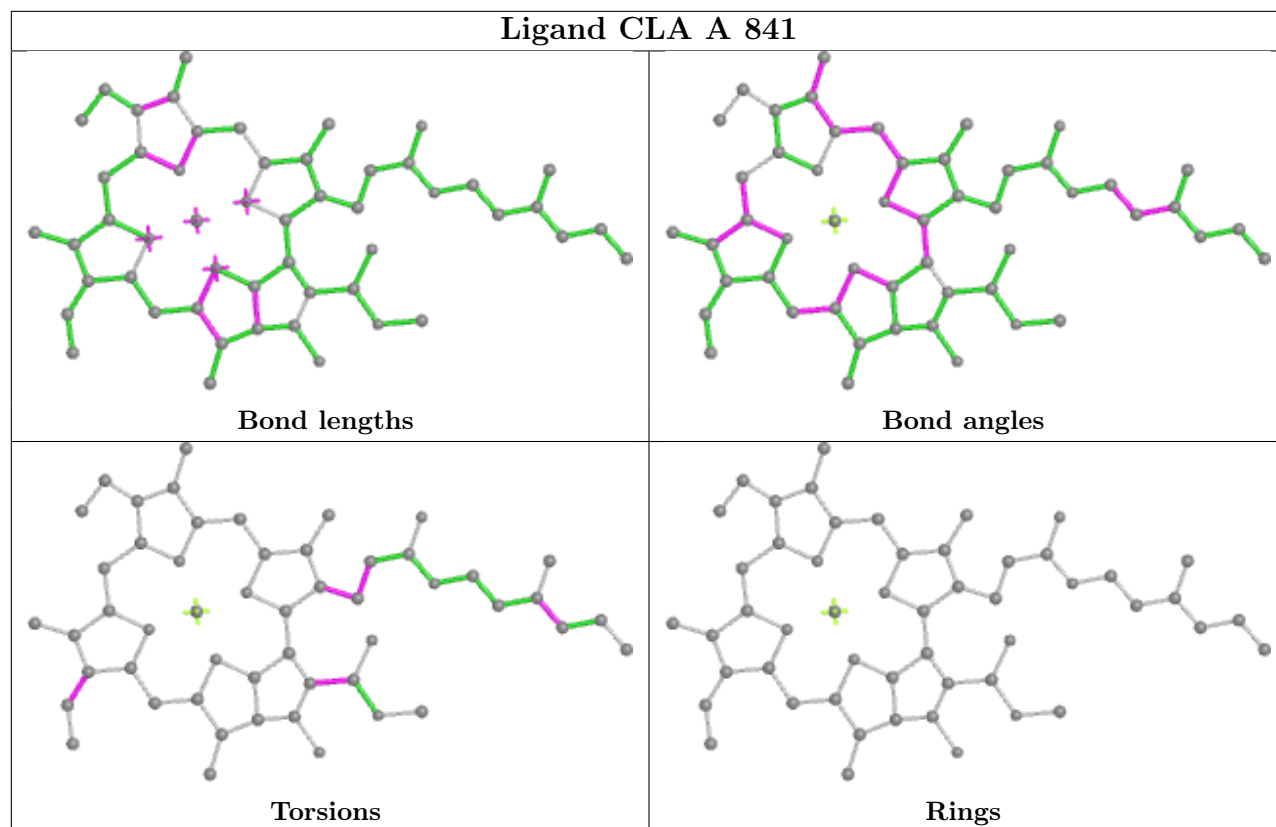
Bond angles



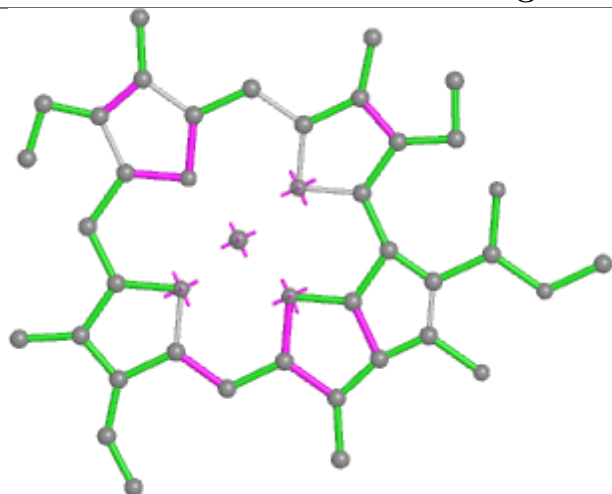
Torsions



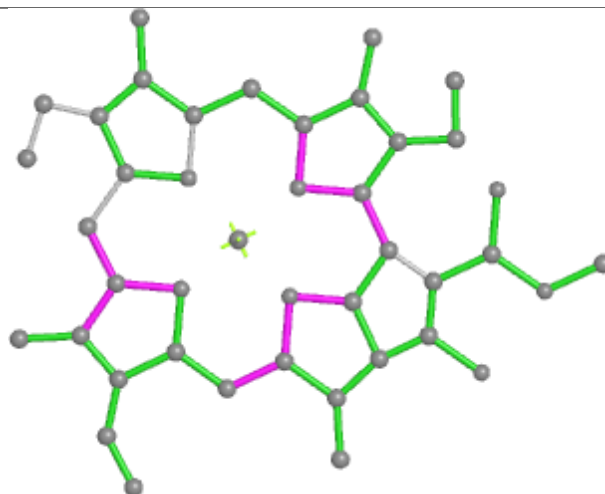
Rings



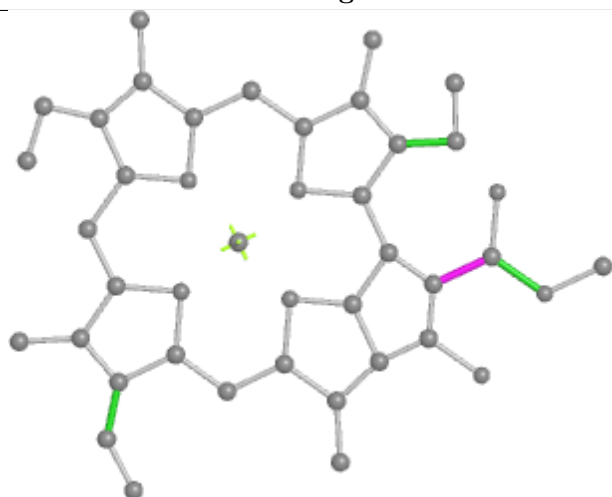
Ligand CLA 8 601



Bond lengths



Bond angles

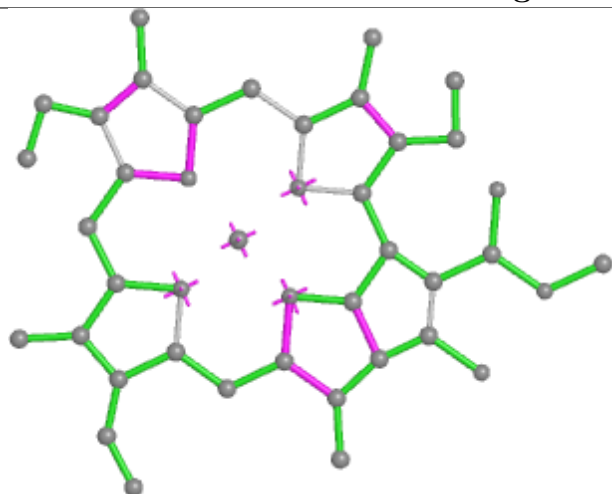


Torsions

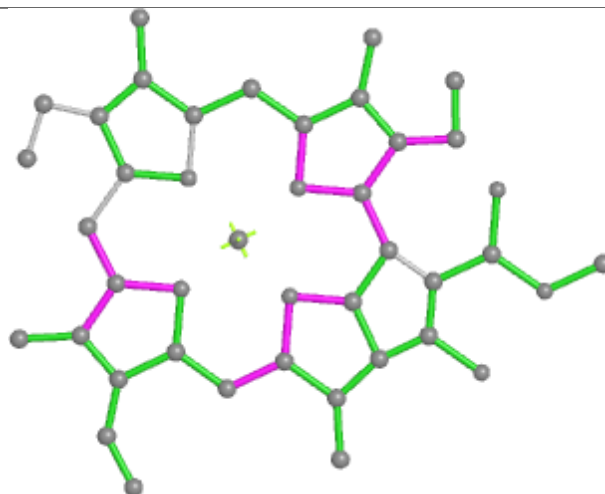


Rings

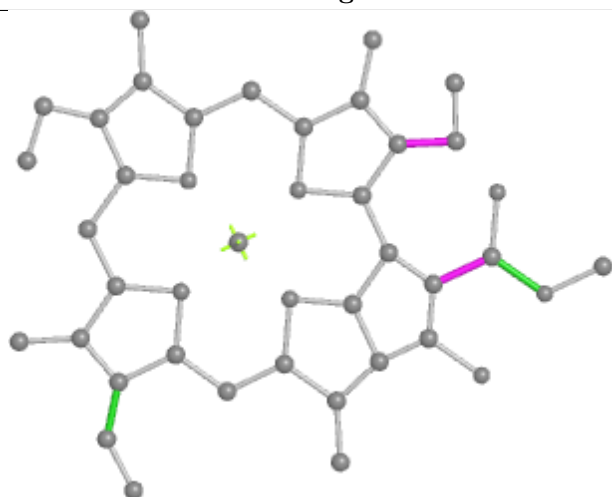
Ligand CLA B 822



Bond lengths



Bond angles

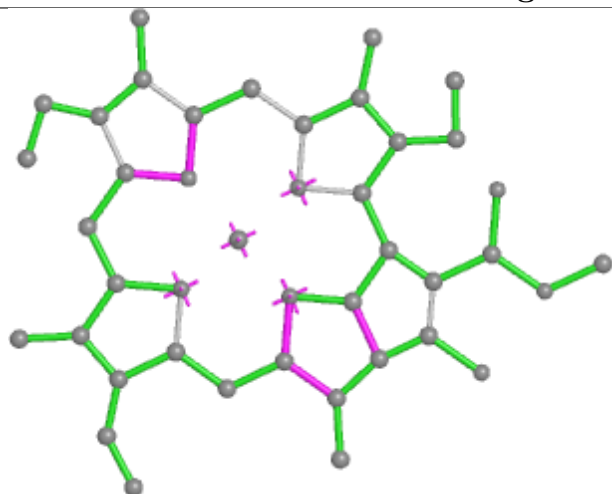


Torsions

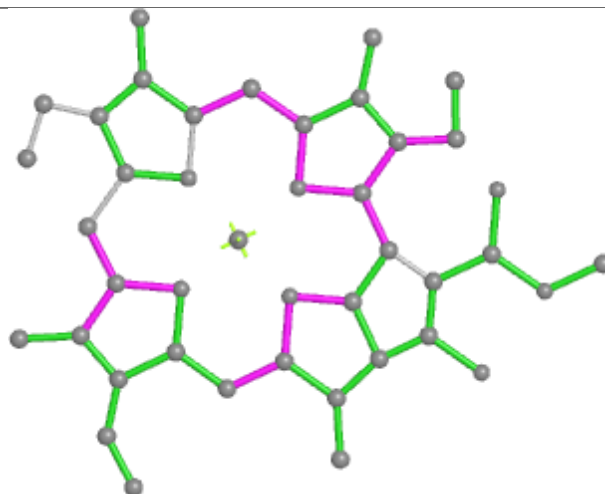


Rings

Ligand CLA 6 608



Bond lengths



Bond angles

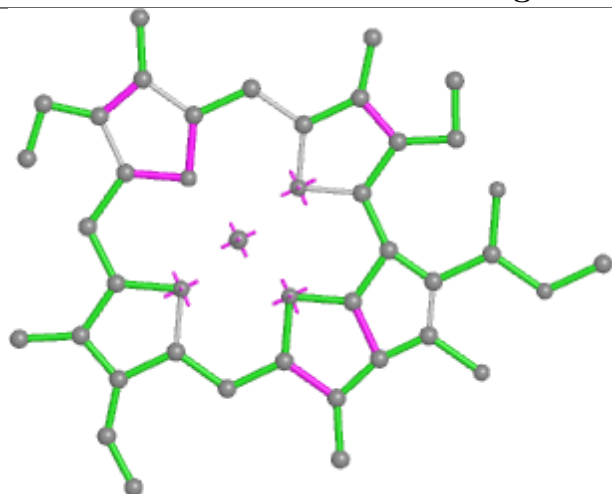


Torsions

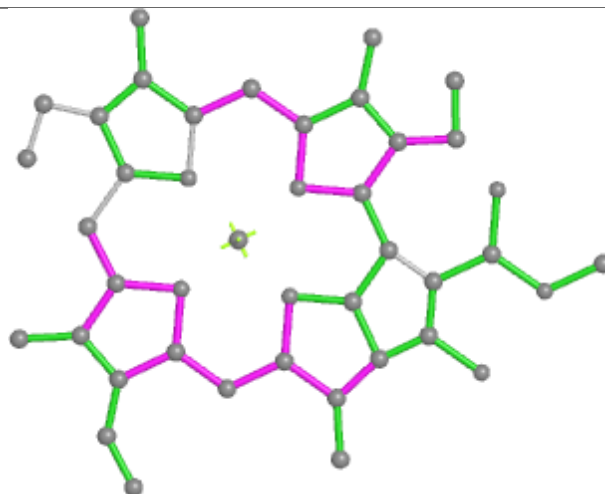


Rings

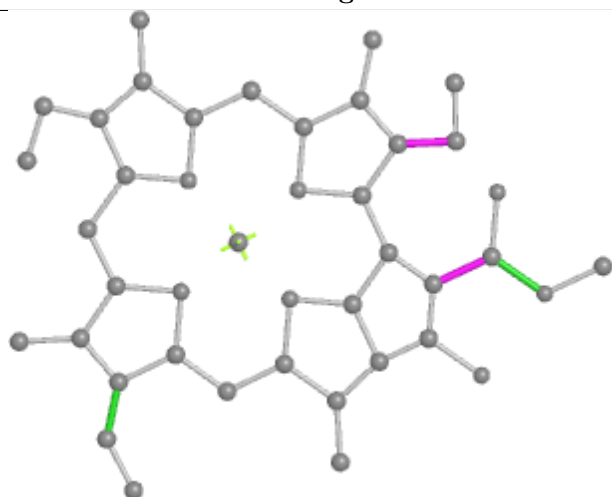
Ligand CLA B 819



Bond lengths



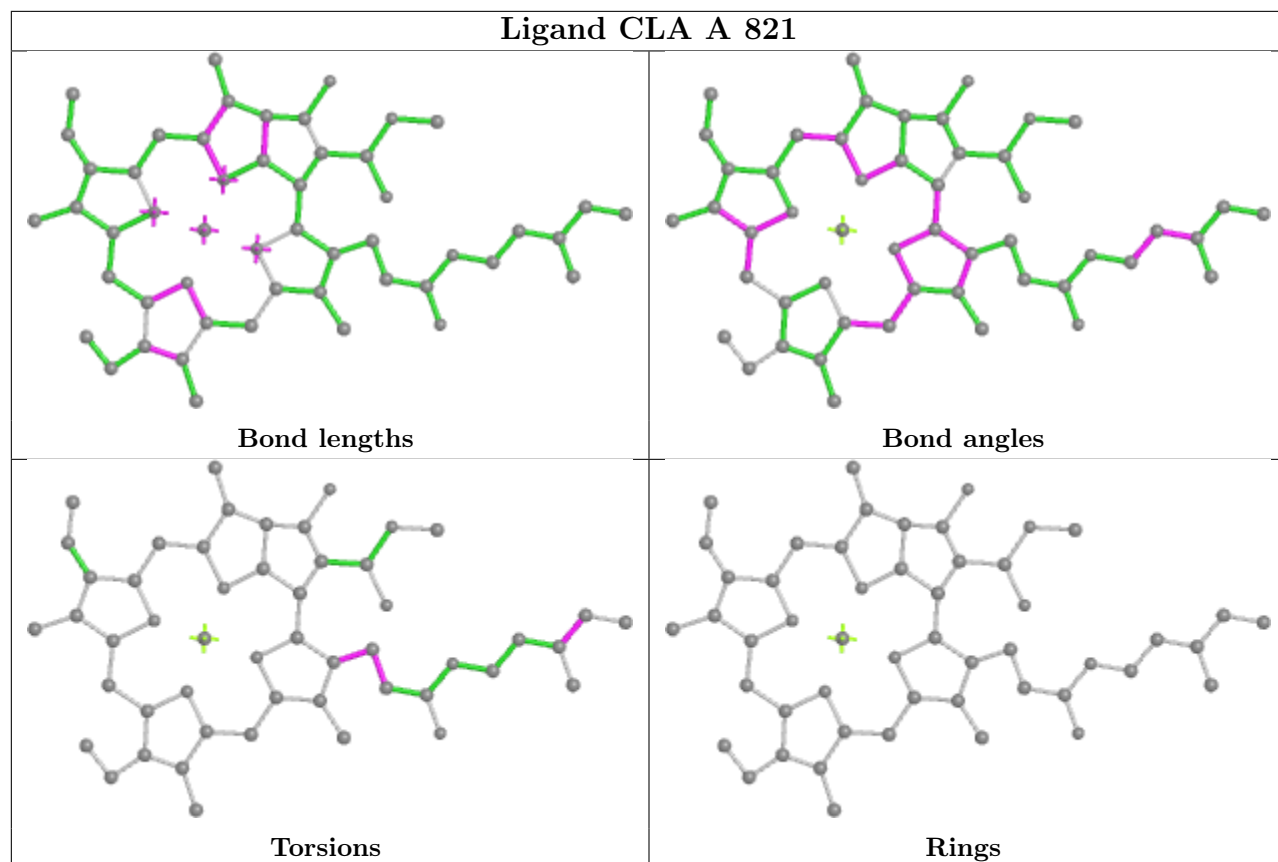
Bond angles



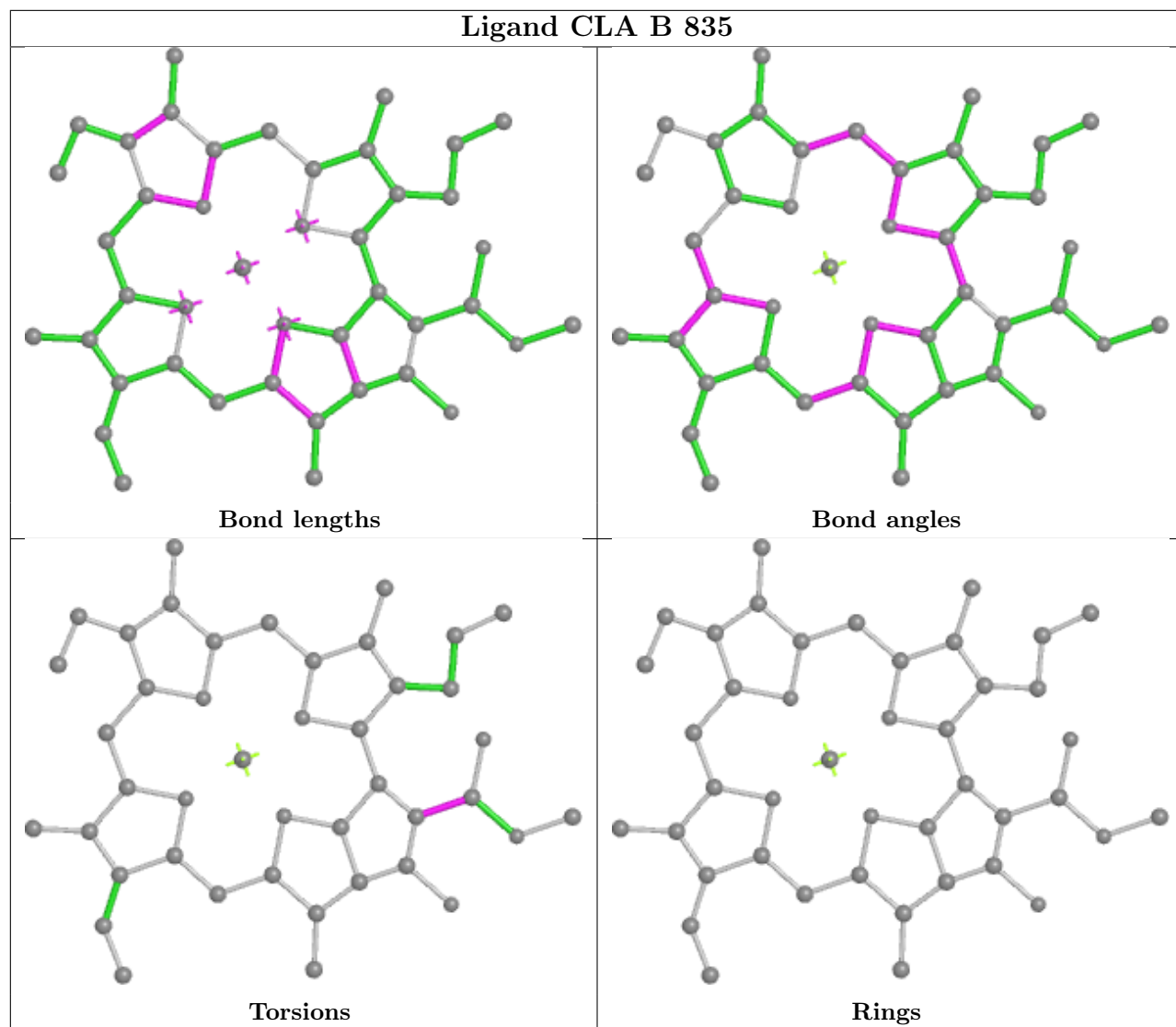
Torsions



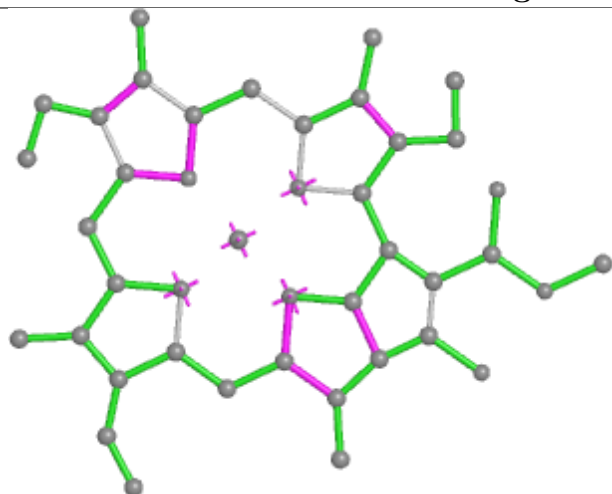
Rings



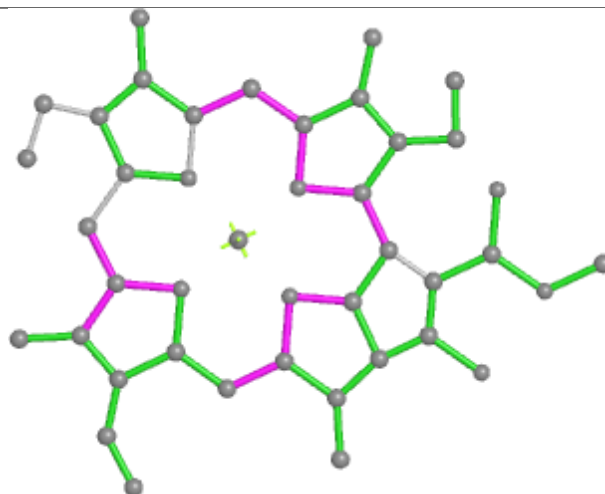
Ligand CLA B 835



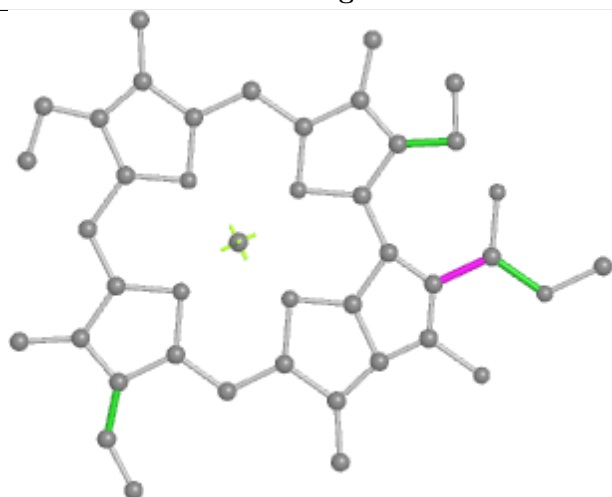
Ligand CLA B 808



Bond lengths



Bond angles

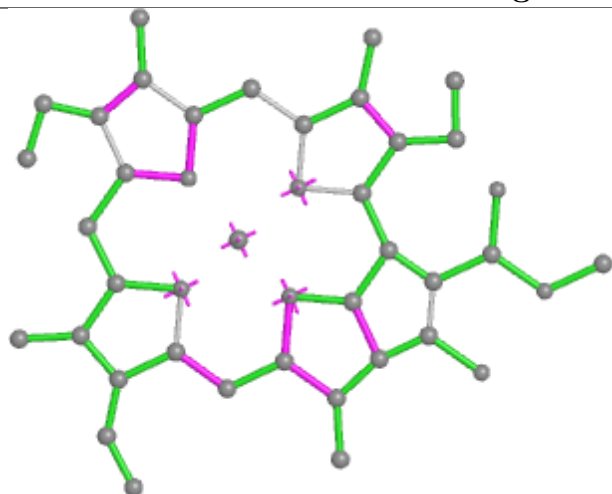


Torsions

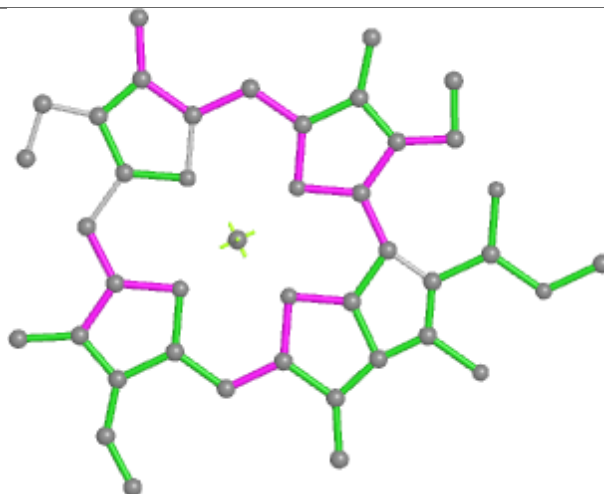


Rings

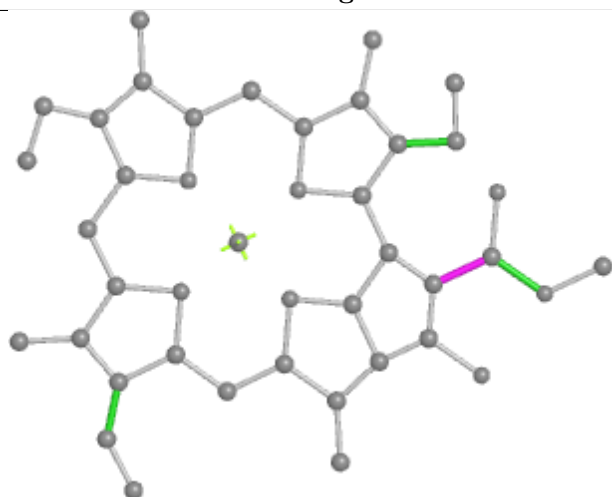
Ligand CLA A 813



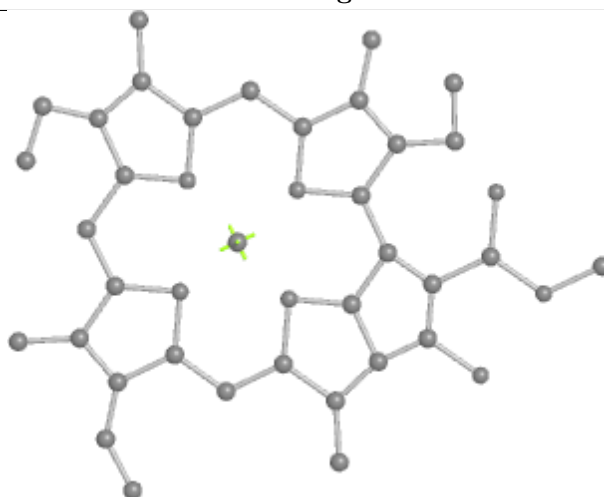
Bond lengths



Bond angles

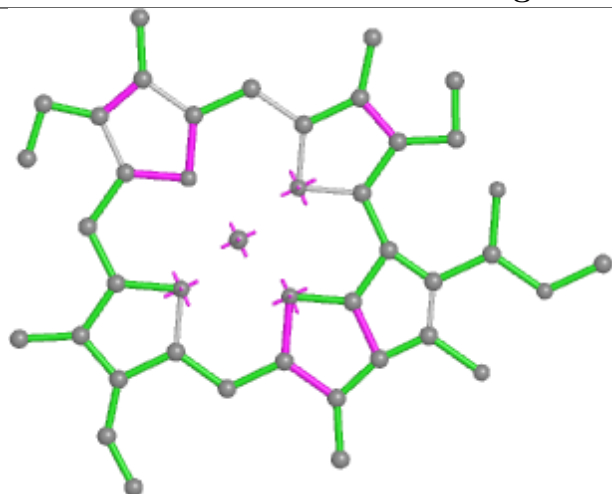


Torsions

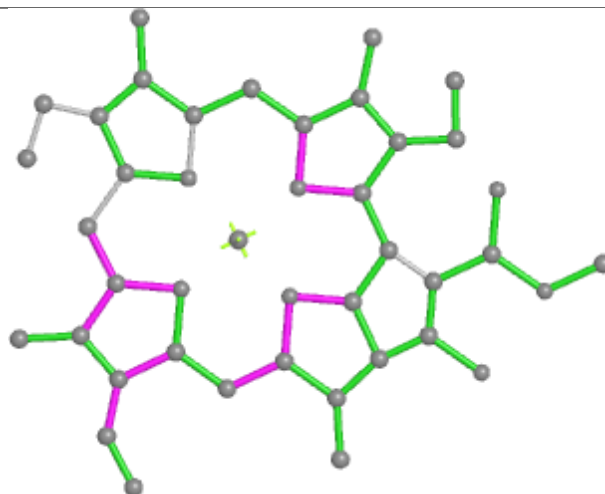


Rings

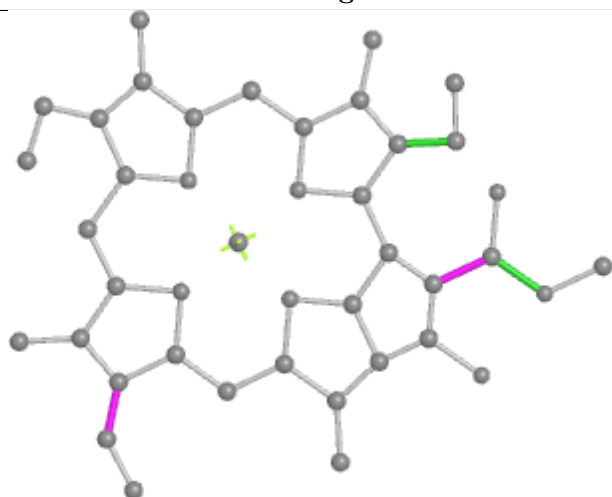
Ligand CLA B 809



Bond lengths



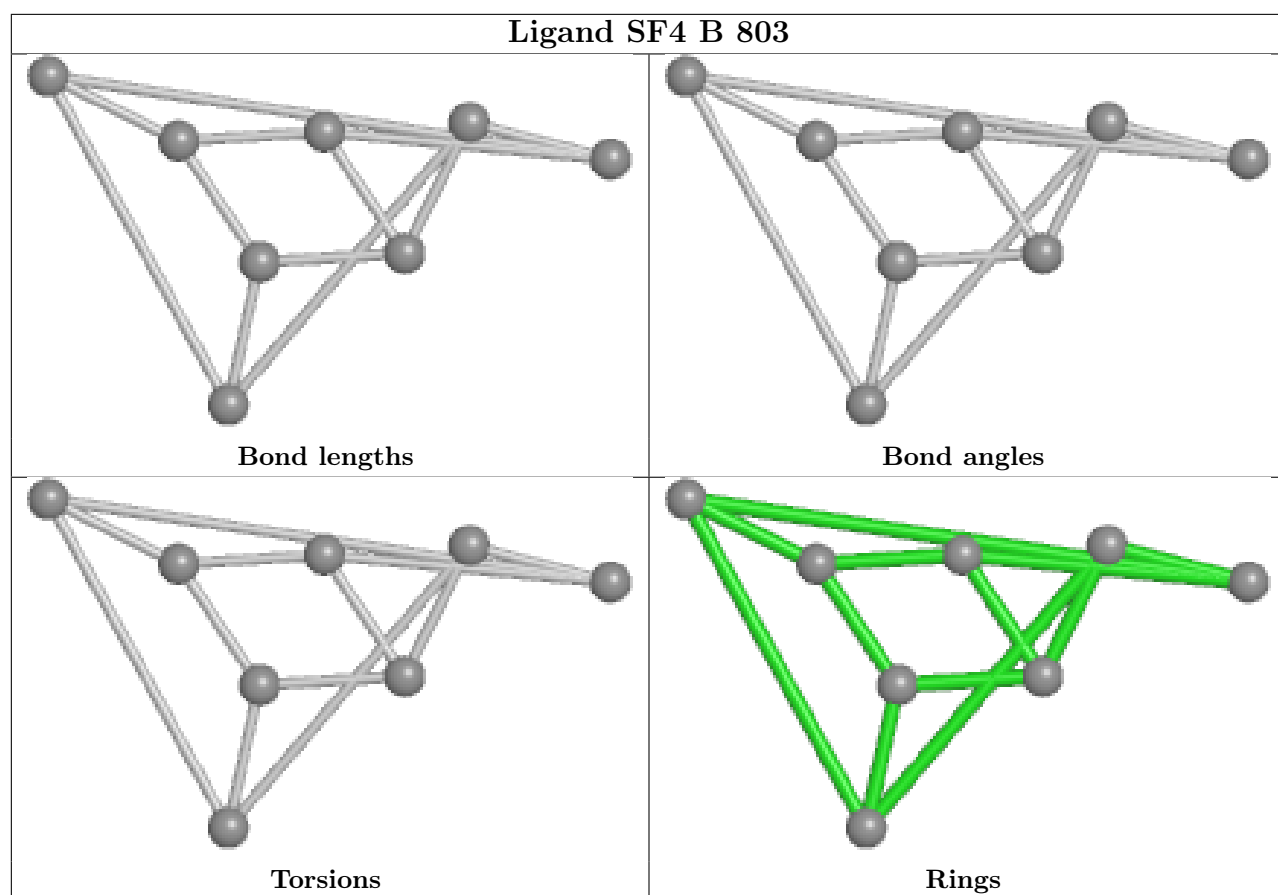
Bond angles



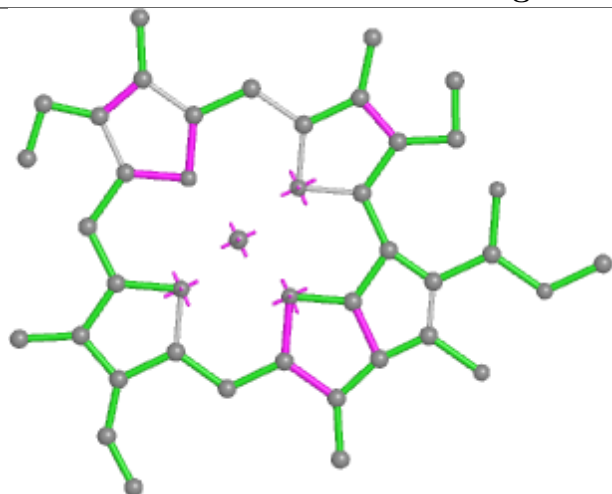
Torsions



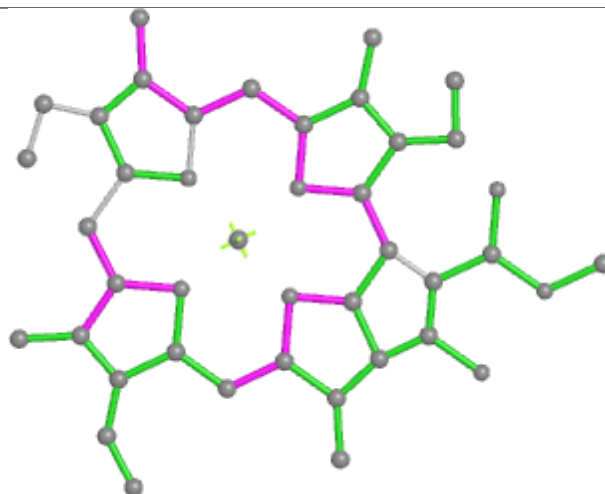
Rings



Ligand CLA A 822



Bond lengths



Bond angles

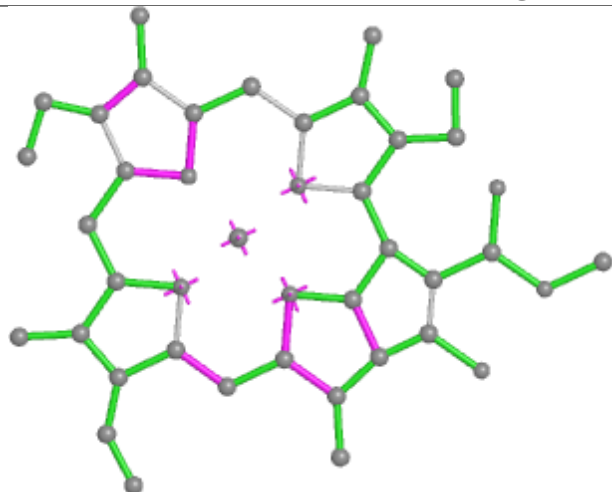


Torsions

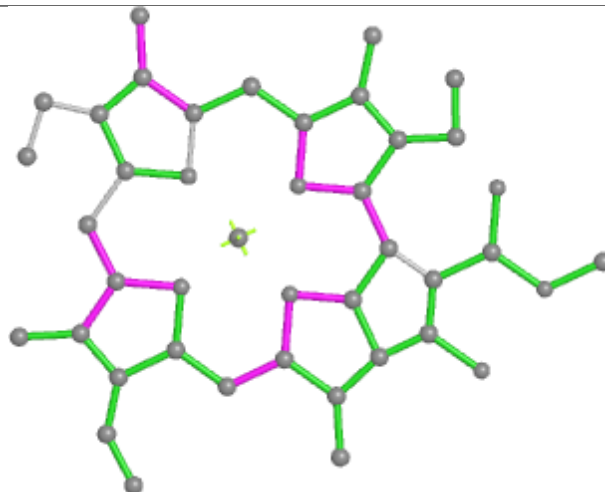


Rings

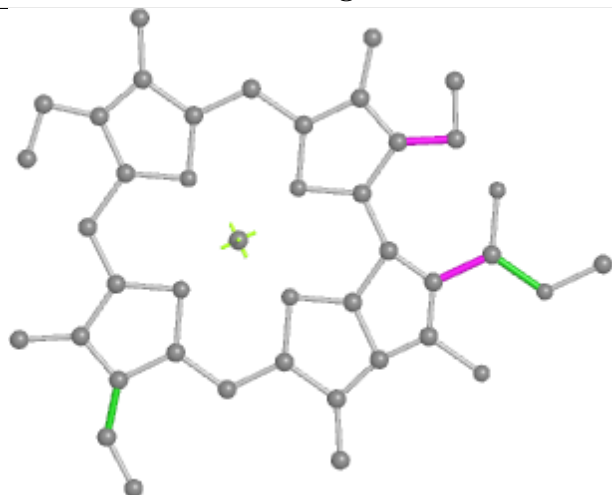
Ligand CLA B 825



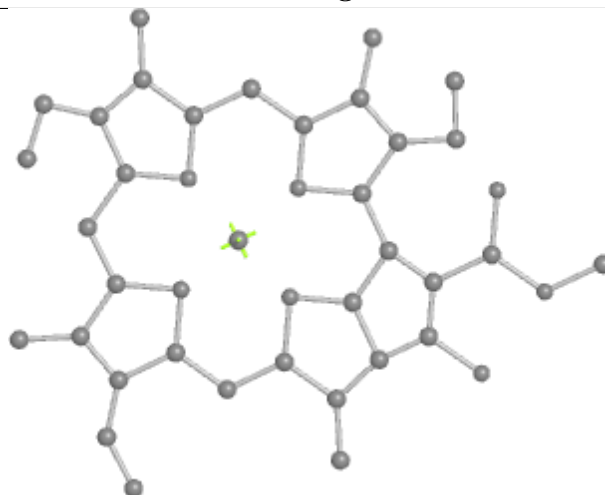
Bond lengths



Bond angles

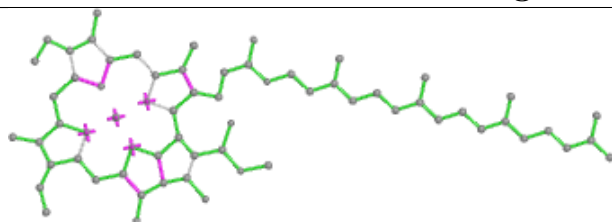


Torsions

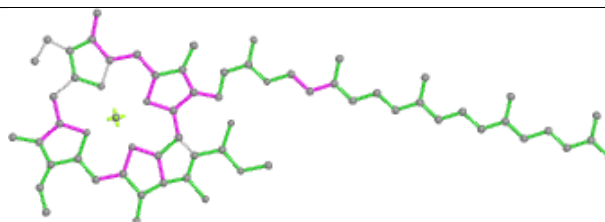


Rings

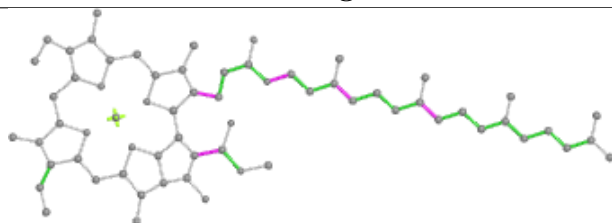
Ligand CLA B 815



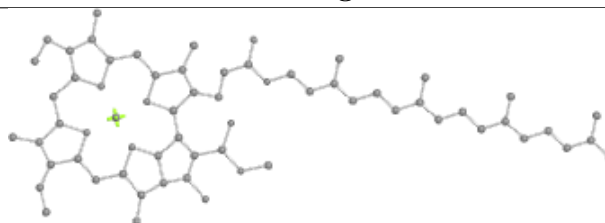
Bond lengths



Bond angles

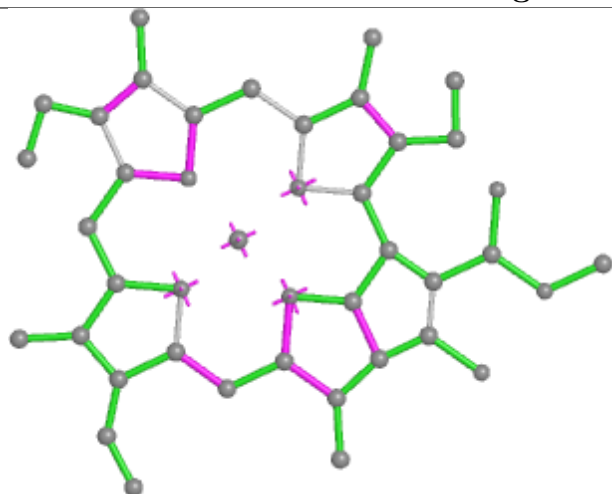


Torsions

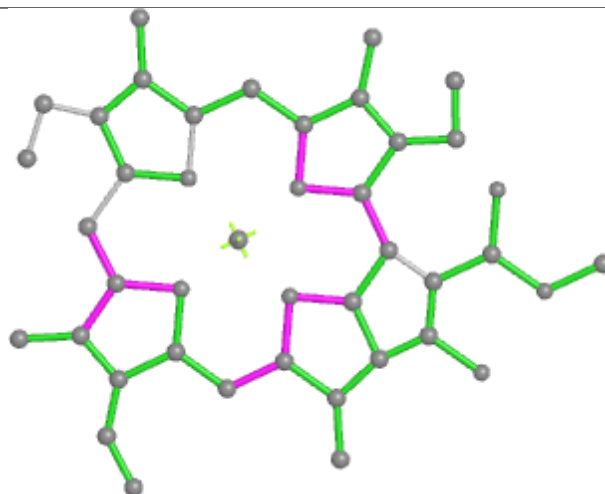


Rings

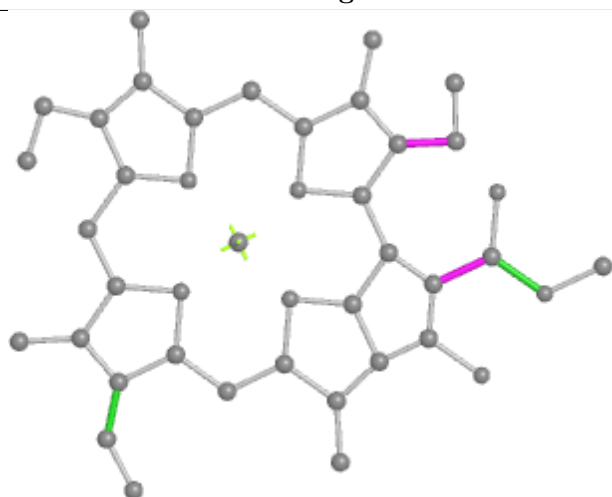
Ligand CLA A 837



Bond lengths



Bond angles

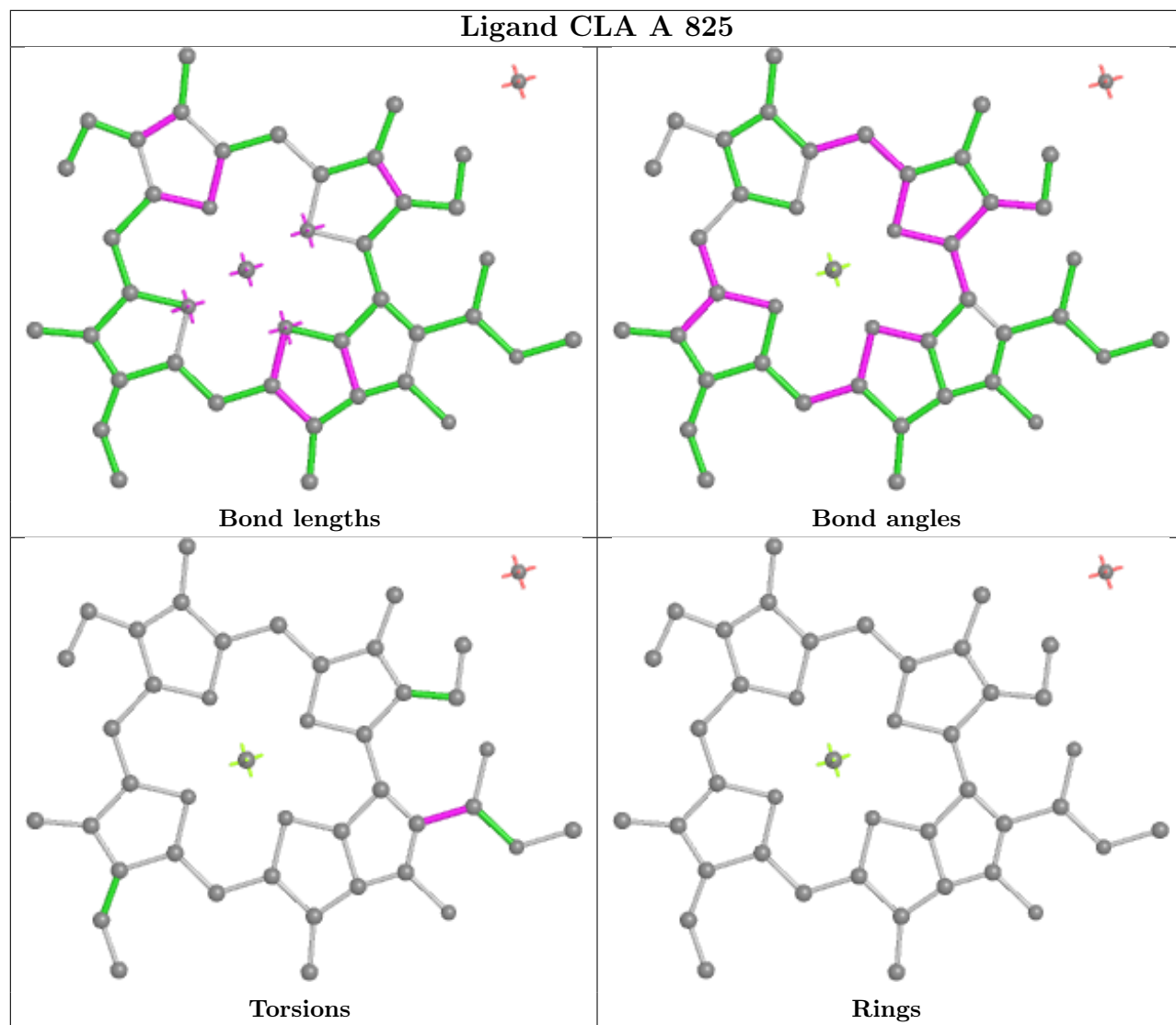


Torsions

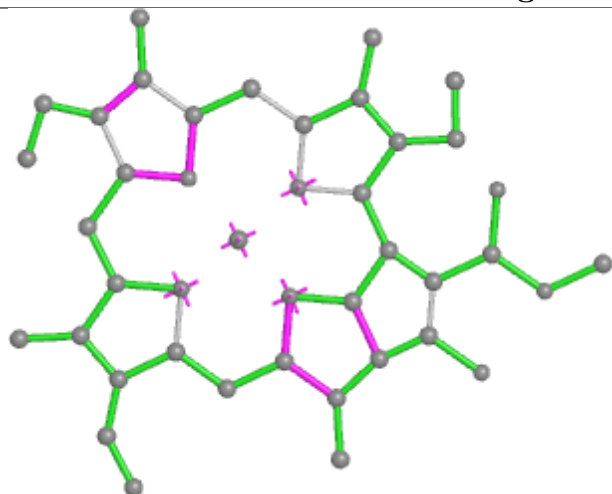


Rings

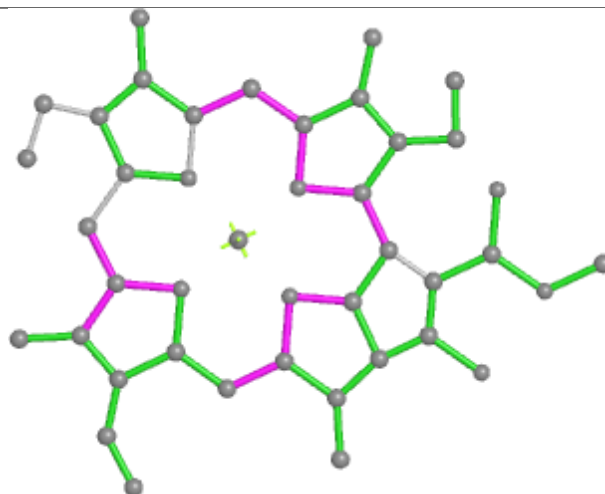
Ligand CLA A 825



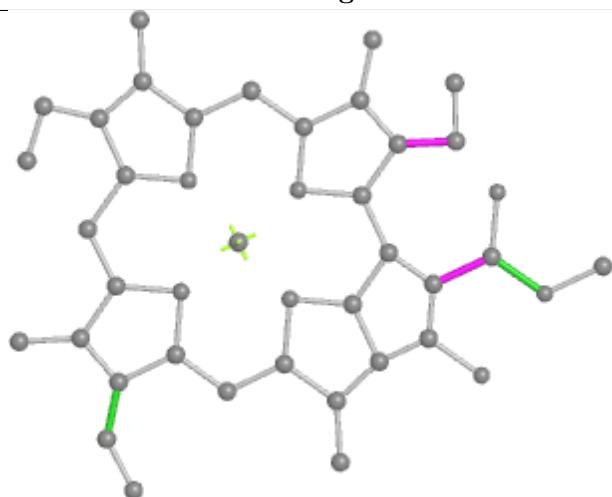
Ligand CLA 1 610



Bond lengths



Bond angles

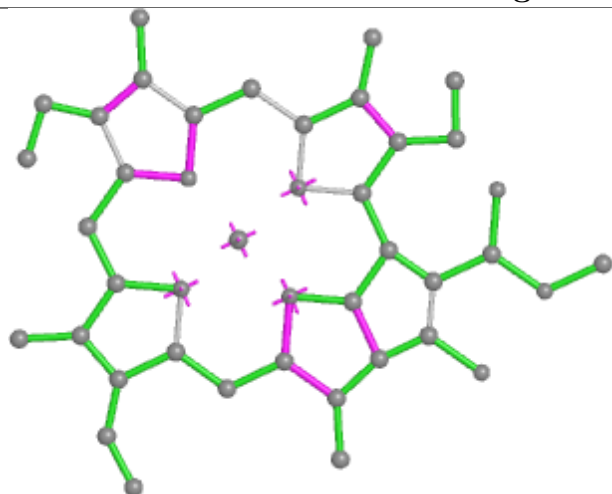


Torsions

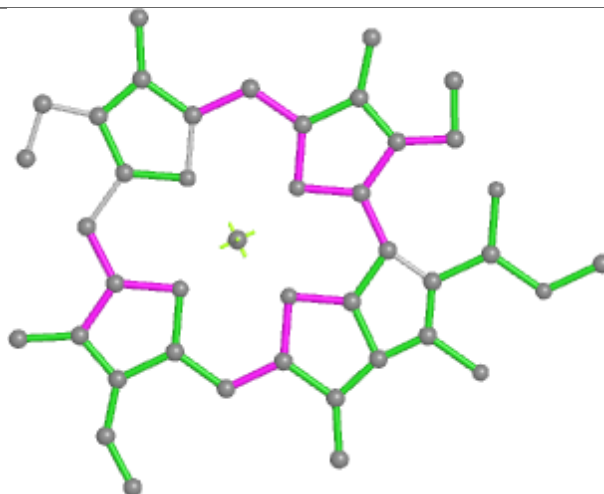


Rings

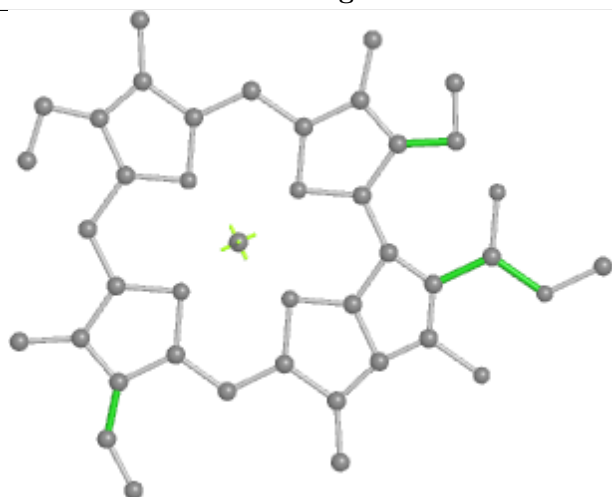
Ligand CLA B 831



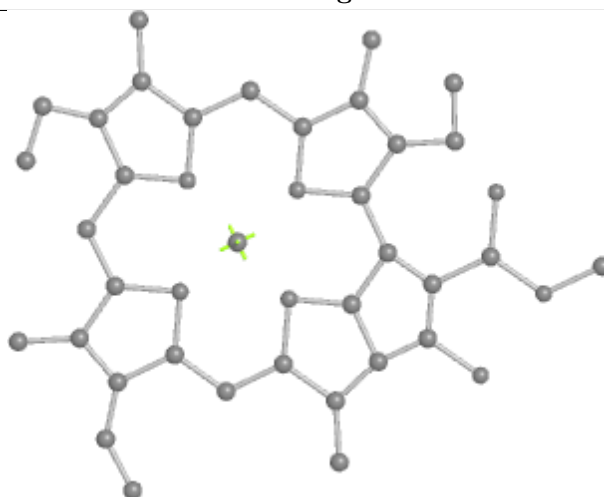
Bond lengths



Bond angles

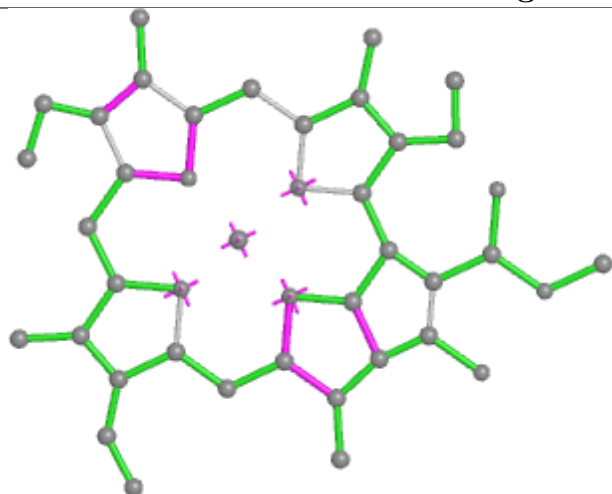


Torsions

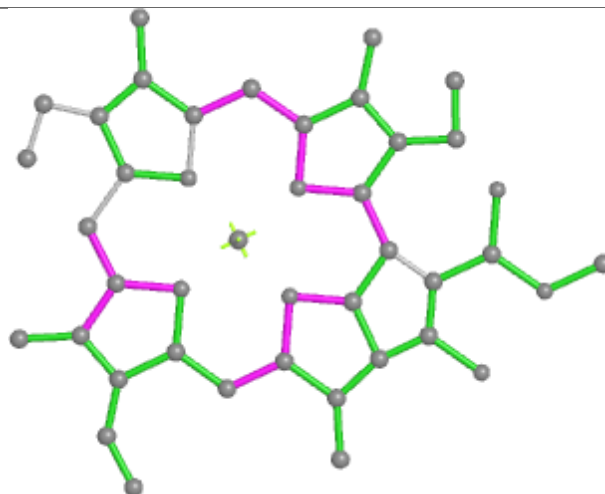


Rings

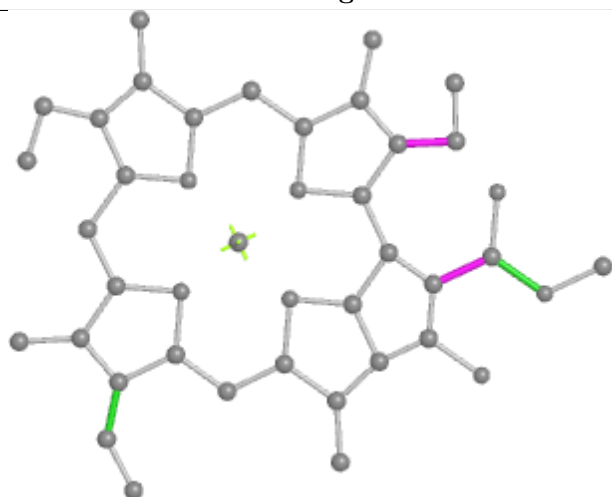
Ligand CLA 5 307



Bond lengths



Bond angles

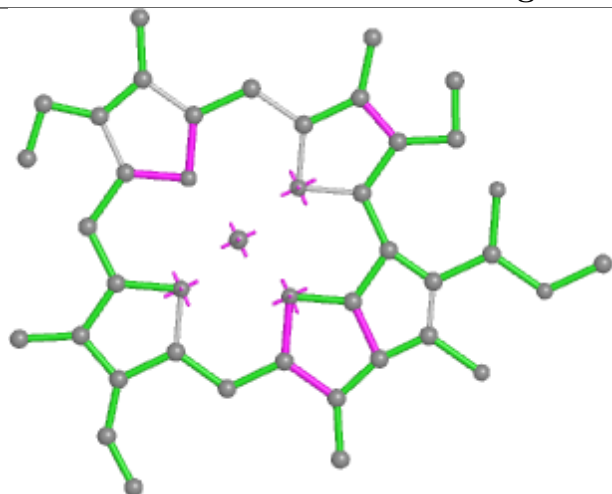


Torsions

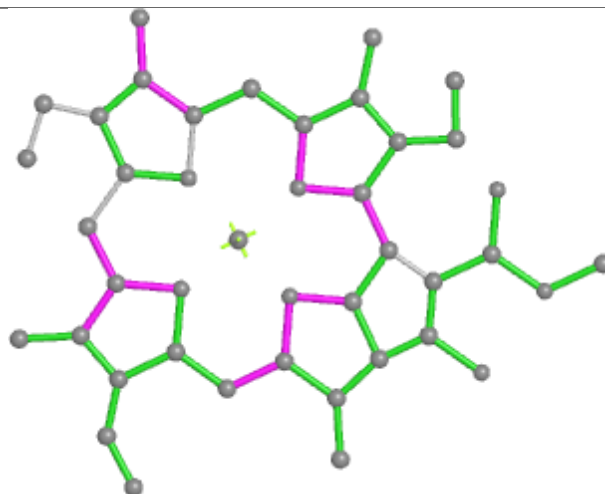


Rings

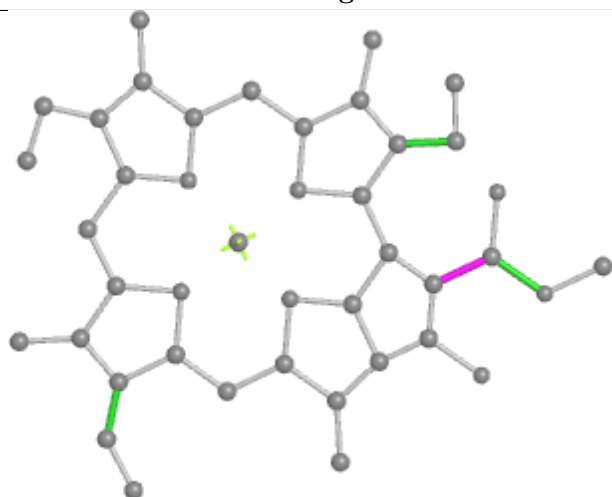
Ligand CLA 3 311



Bond lengths



Bond angles

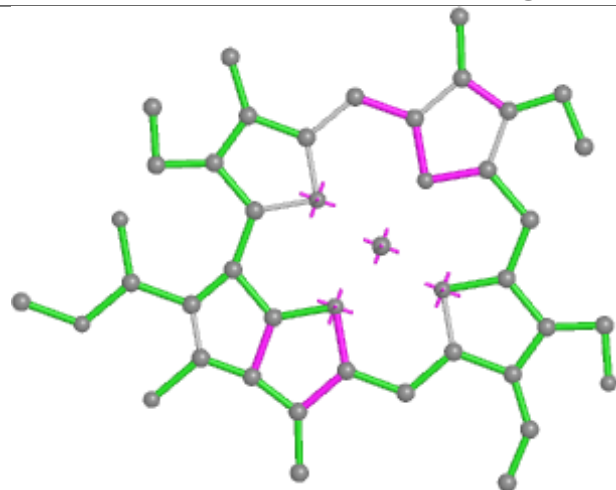


Torsions

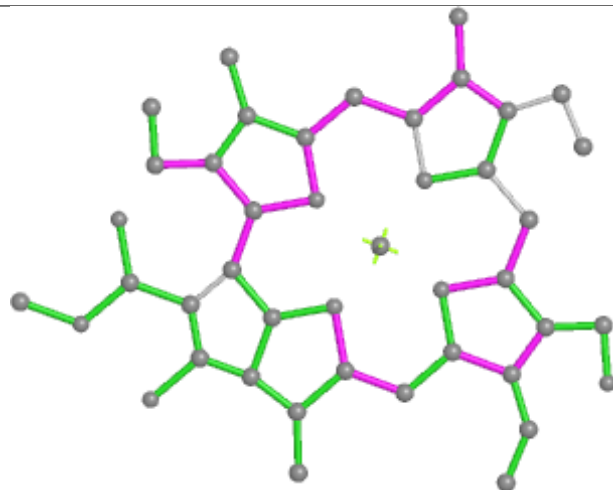


Rings

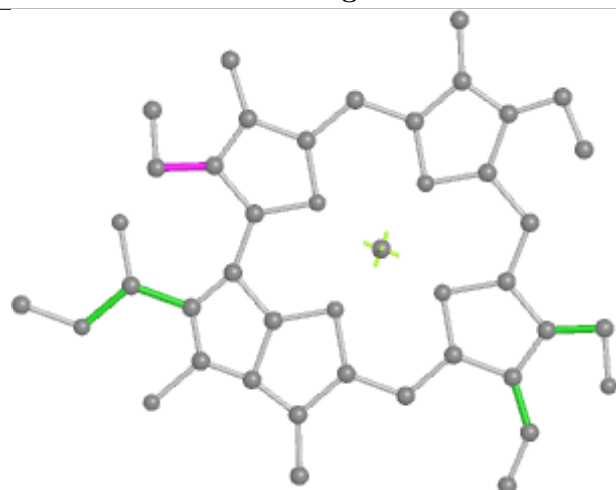
Ligand CHL 6 605



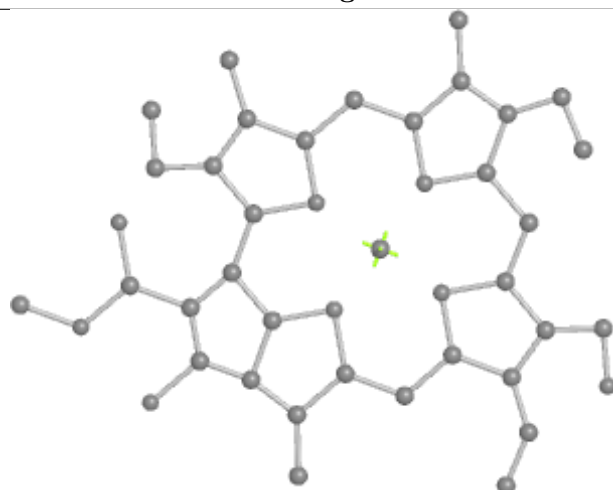
Bond lengths



Bond angles

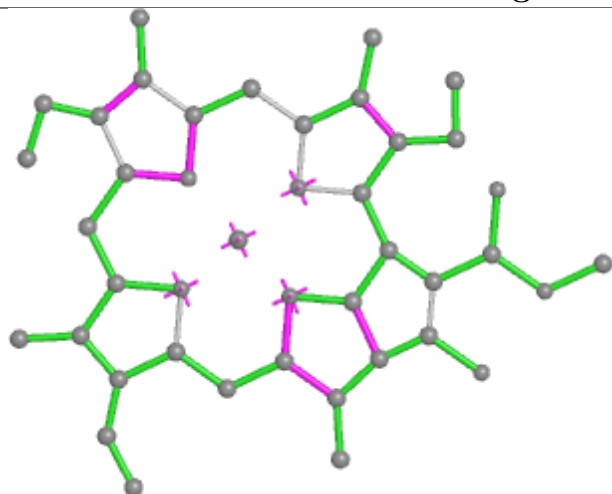


Torsions

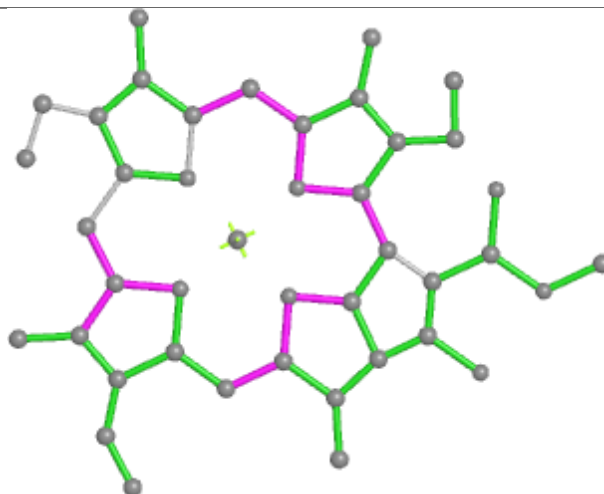


Rings

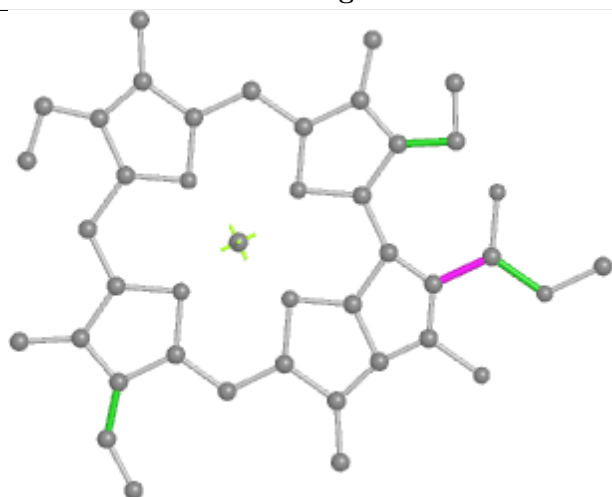
Ligand CLA A 836



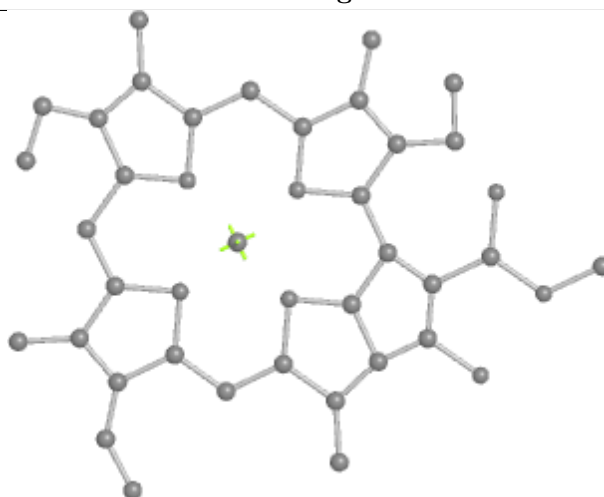
Bond lengths



Bond angles

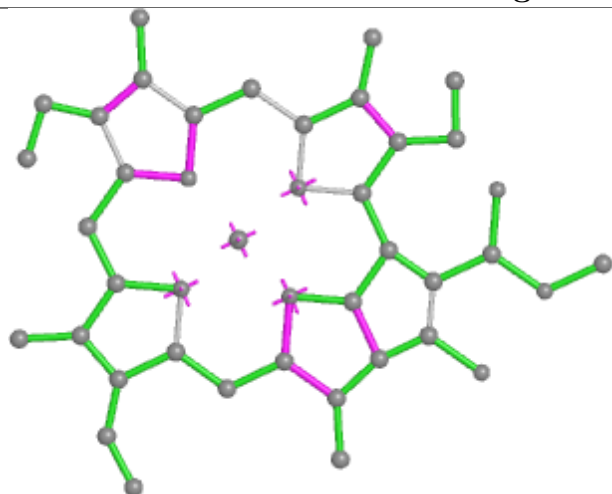


Torsions

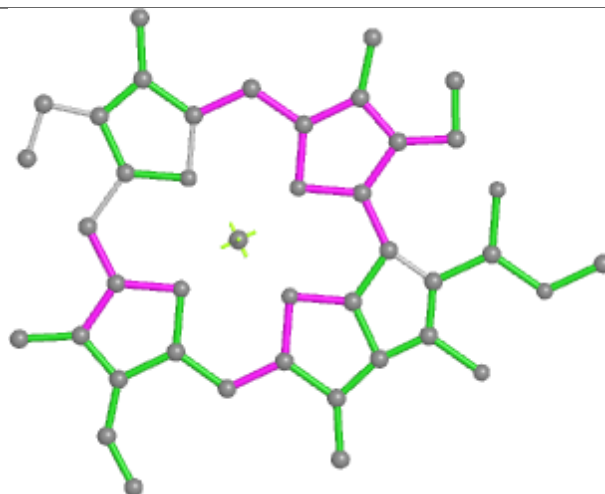


Rings

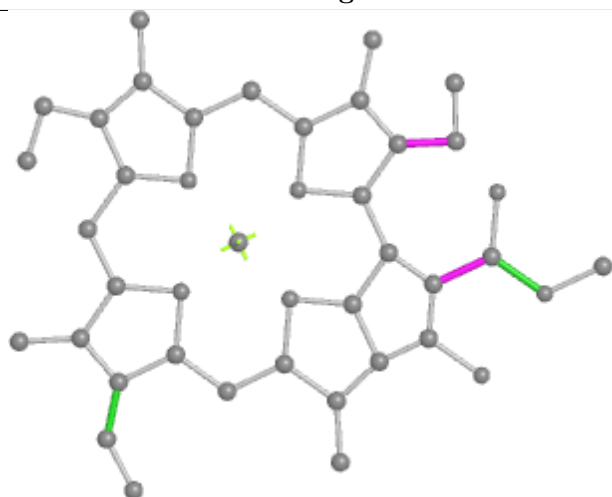
Ligand CLA B 812



Bond lengths



Bond angles

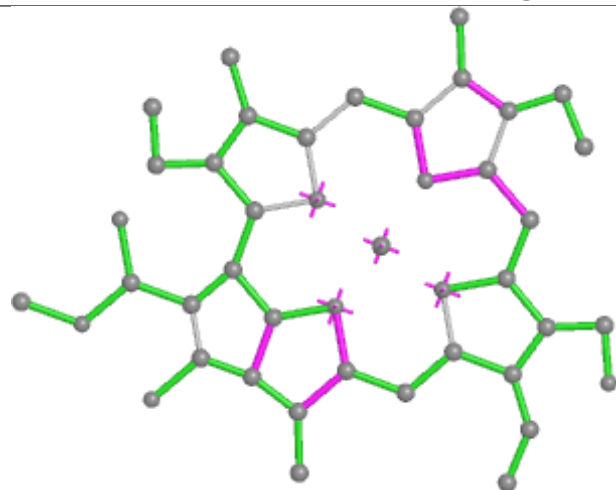


Torsions

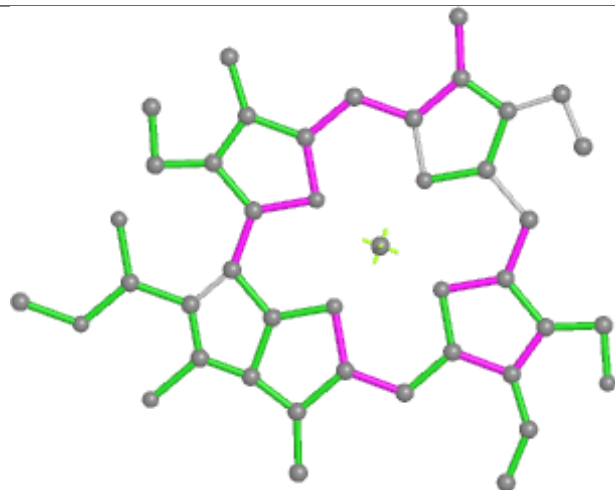


Rings

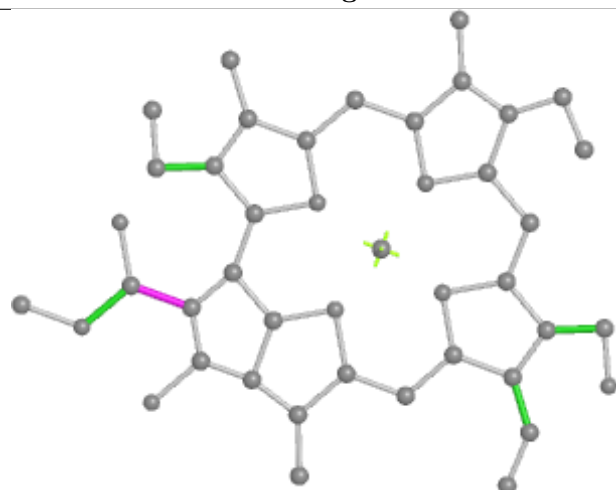
Ligand CHL Z 601



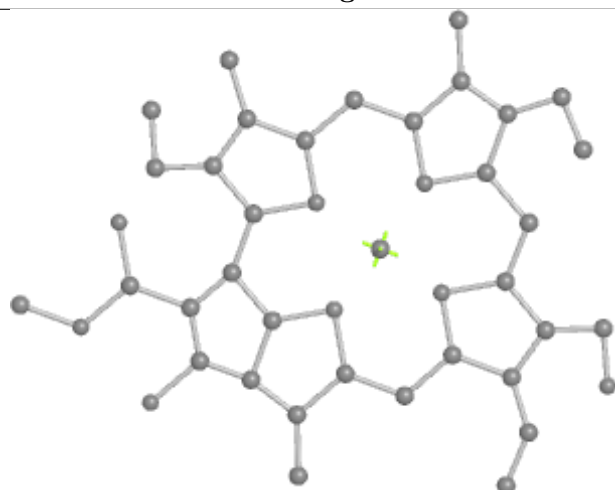
Bond lengths



Bond angles

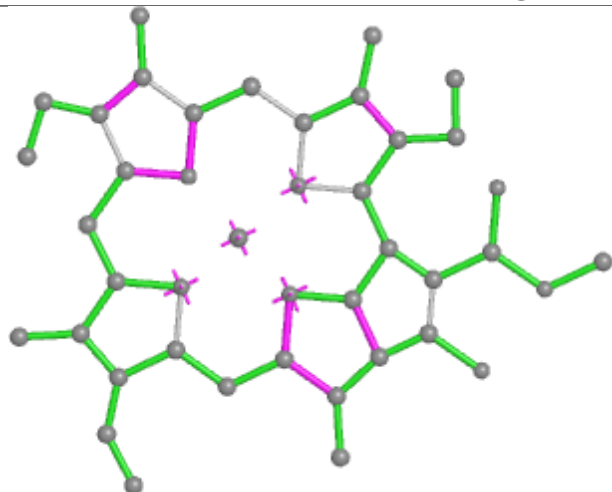


Torsions

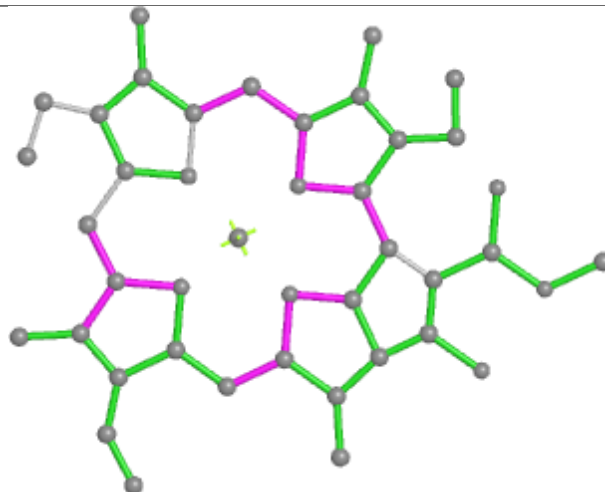


Rings

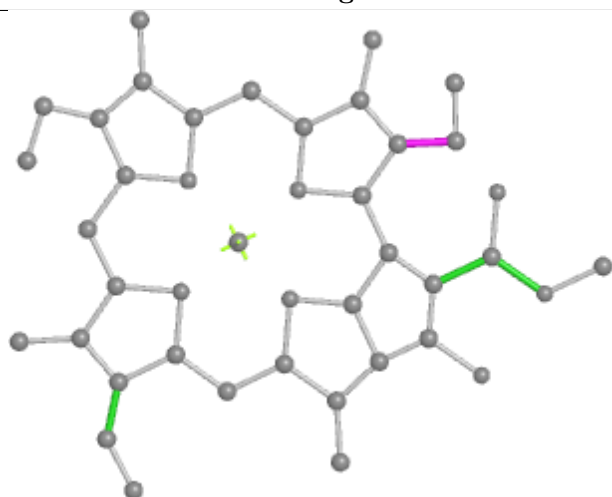
Ligand CLA A 833



Bond lengths



Bond angles

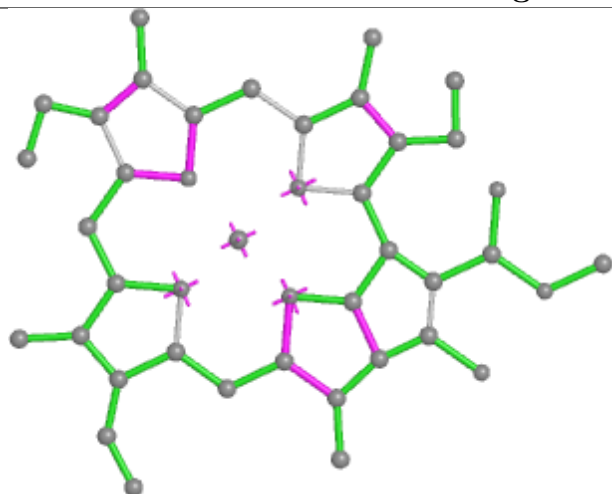


Torsions

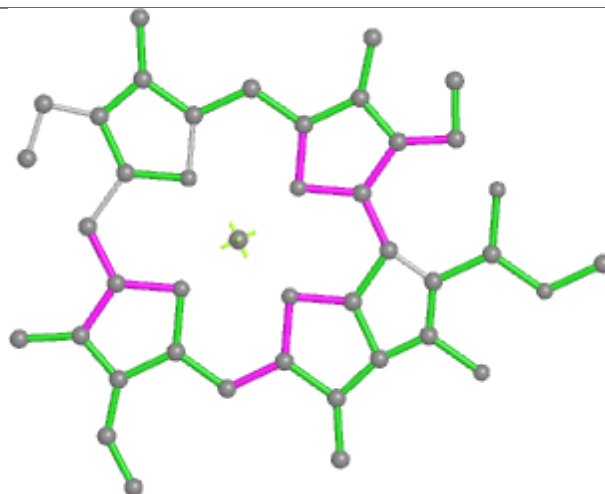


Rings

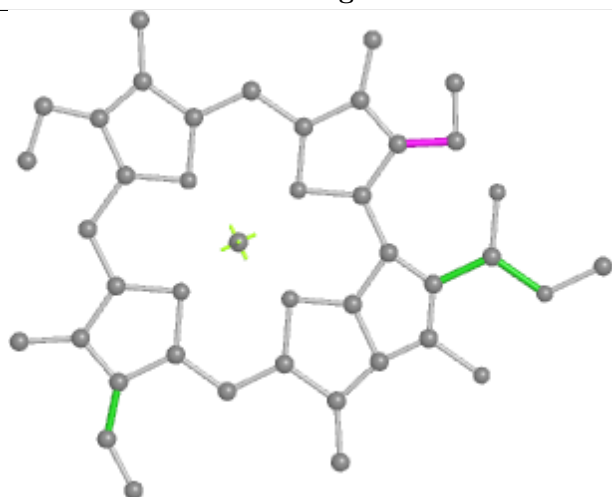
Ligand CLA A 828



Bond lengths



Bond angles

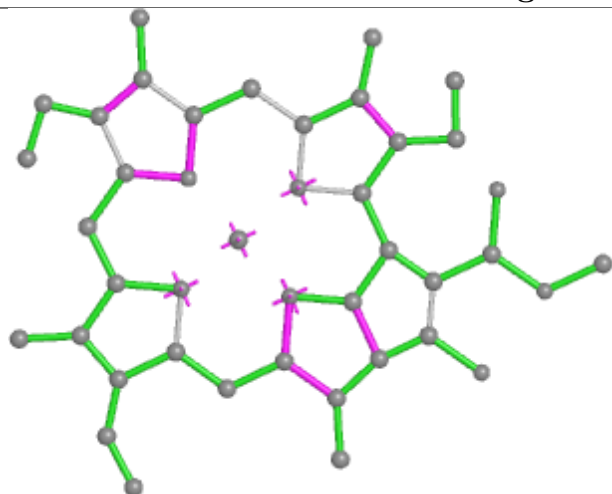


Torsions

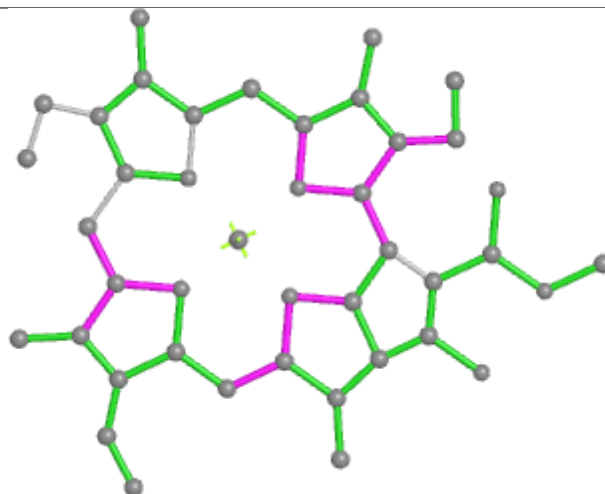


Rings

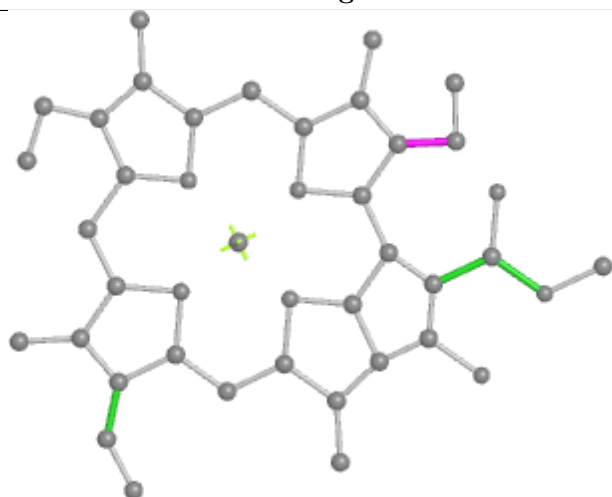
Ligand CLA 5 312



Bond lengths



Bond angles

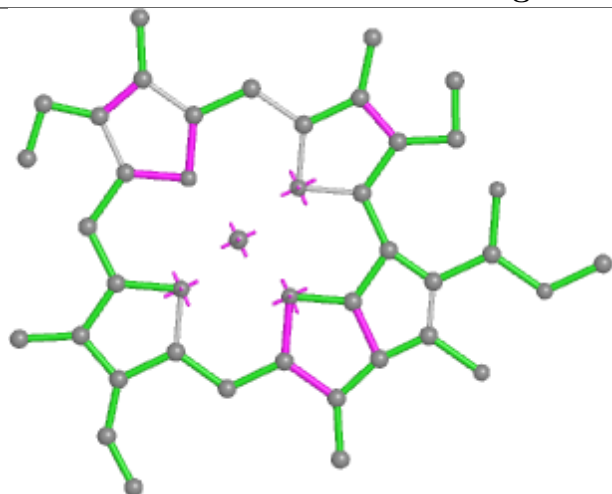


Torsions

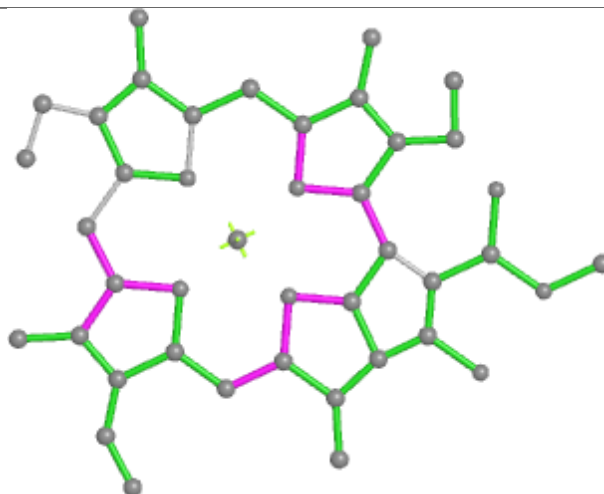


Rings

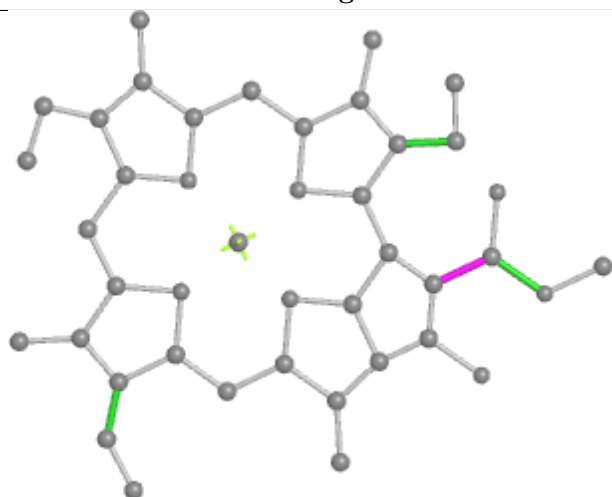
Ligand CLA A 803



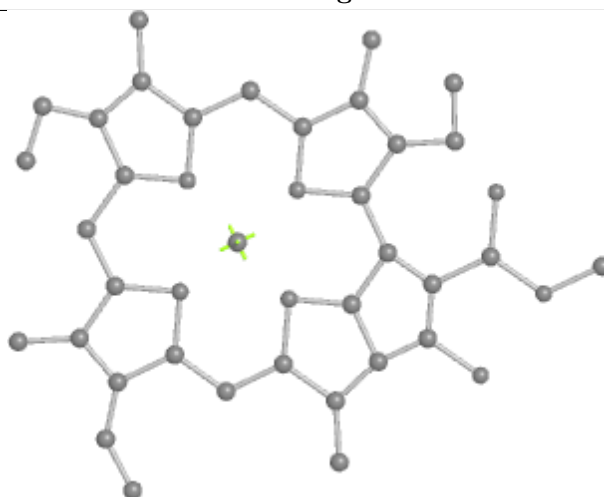
Bond lengths



Bond angles

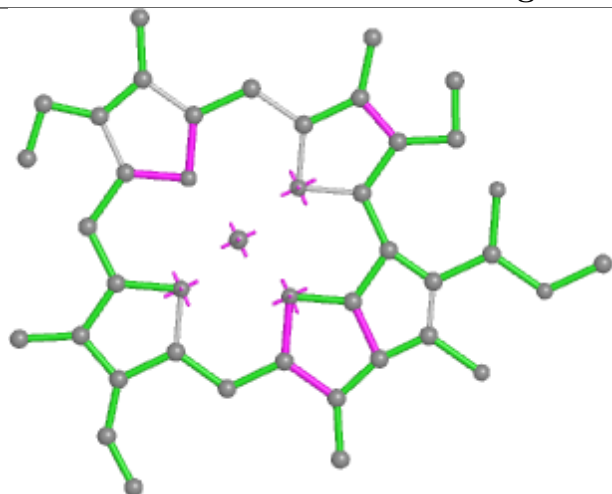


Torsions

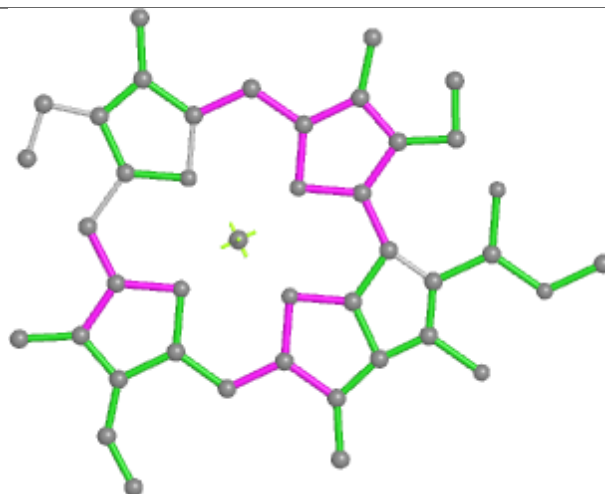


Rings

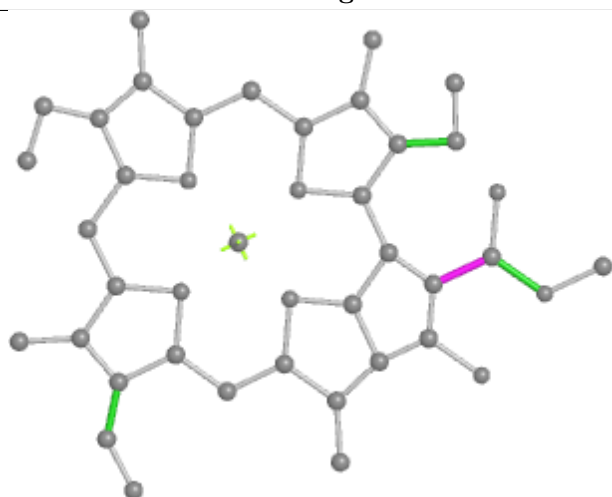
Ligand CLA 7 614



Bond lengths



Bond angles

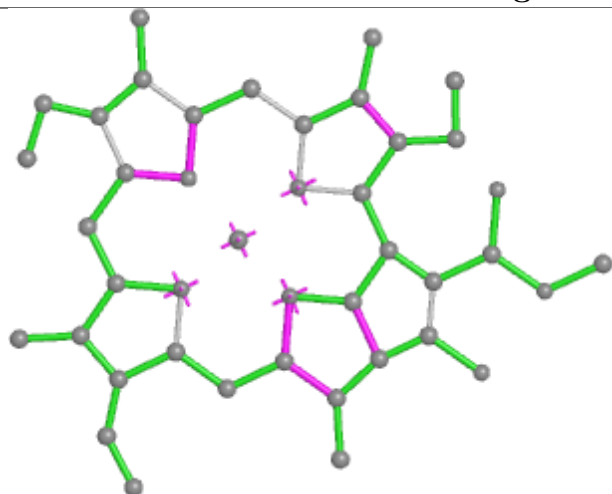


Torsions

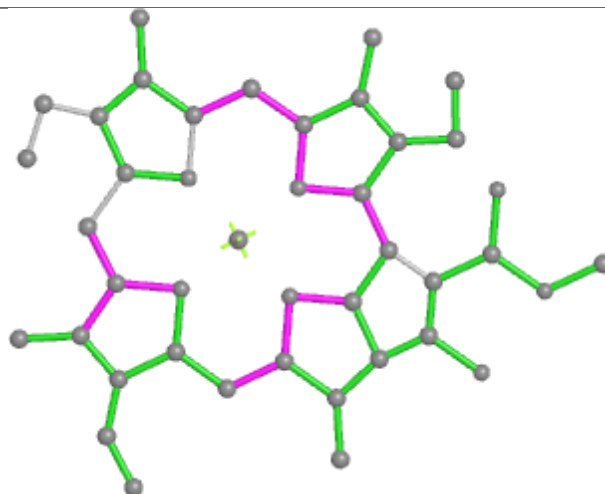


Rings

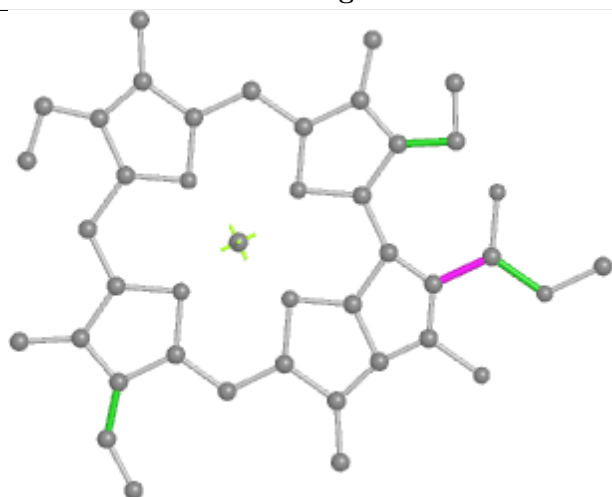
Ligand CLA B 839



Bond lengths



Bond angles

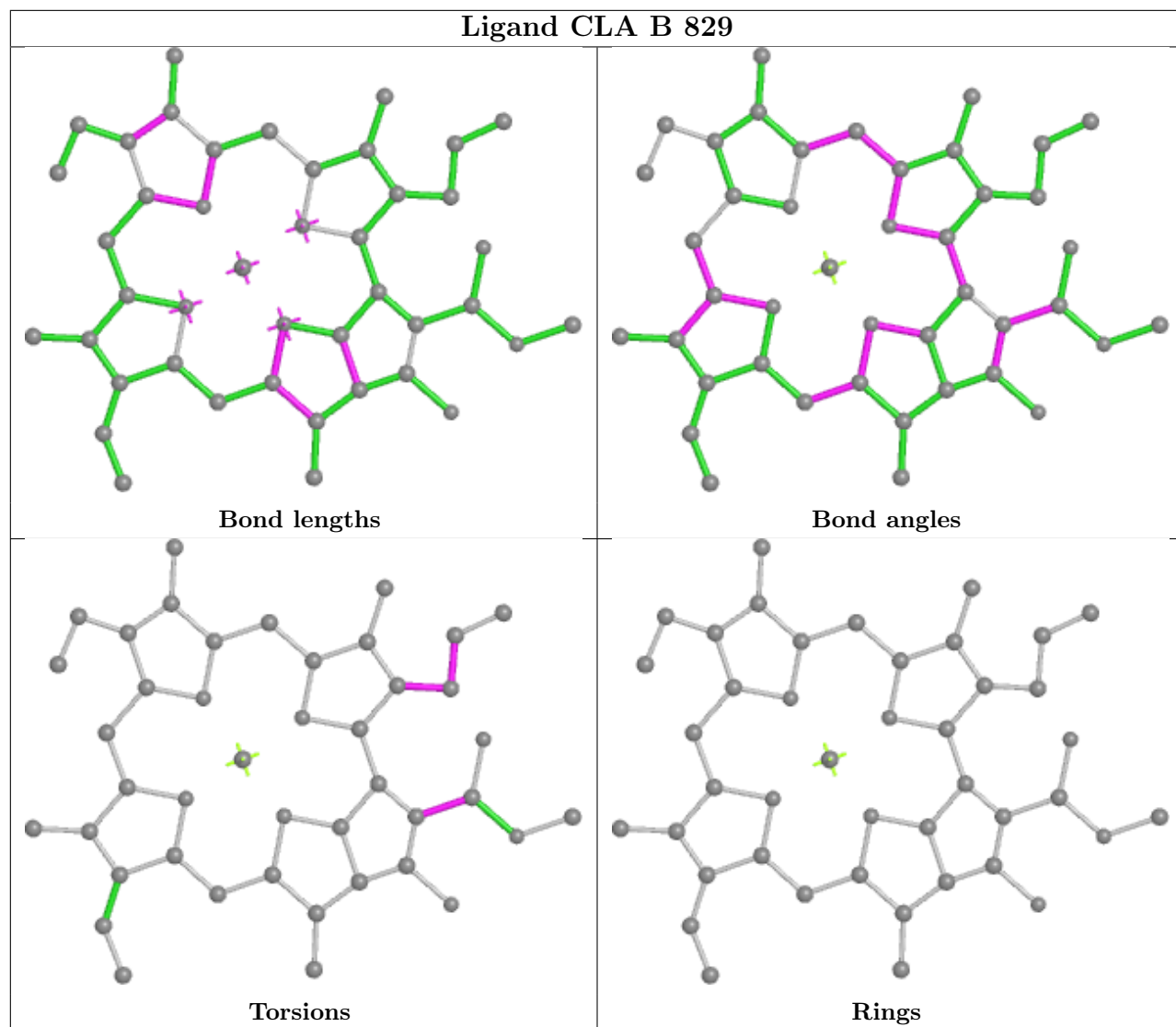


Torsions

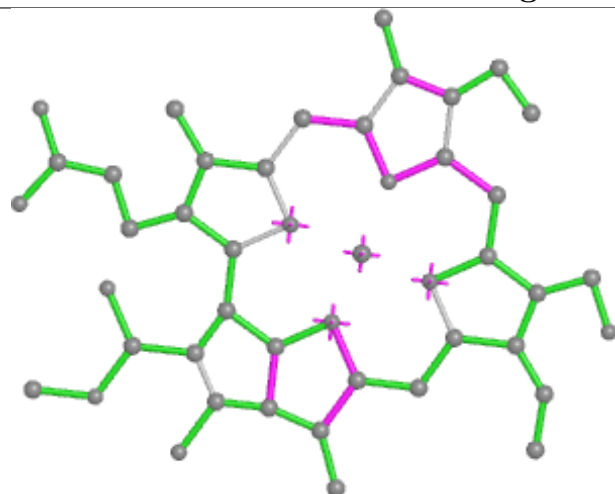


Rings

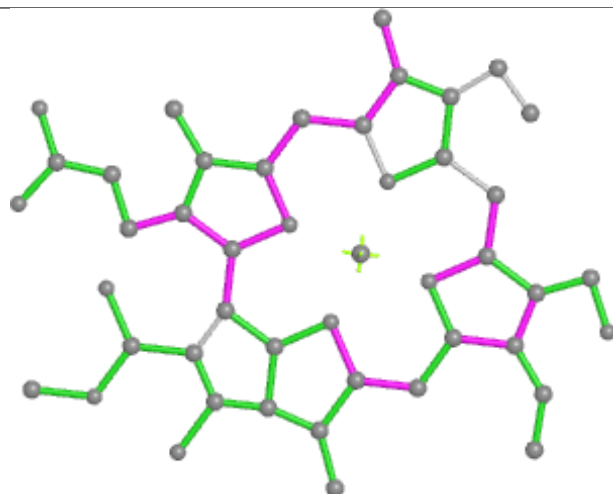
Ligand CLA B 829



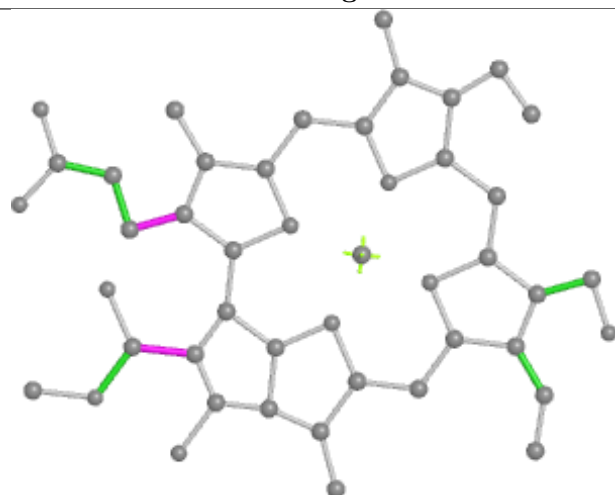
Ligand CHL 5 305



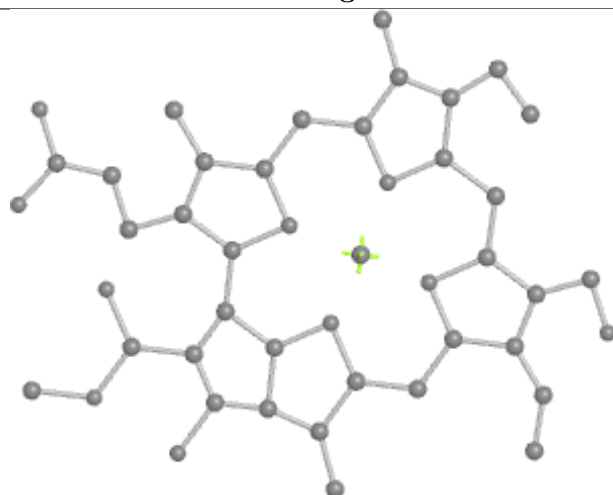
Bond lengths



Bond angles

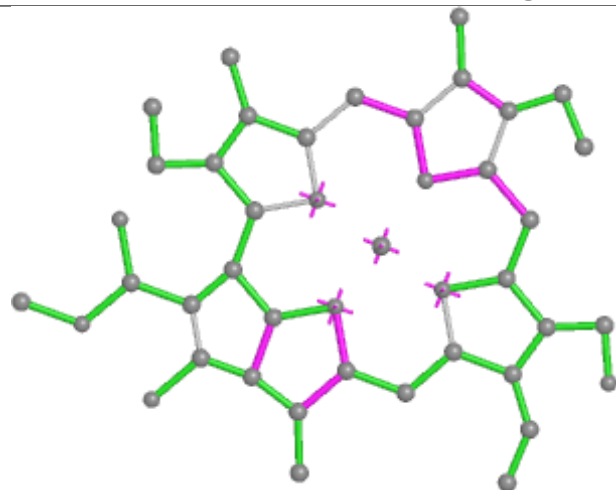


Torsions

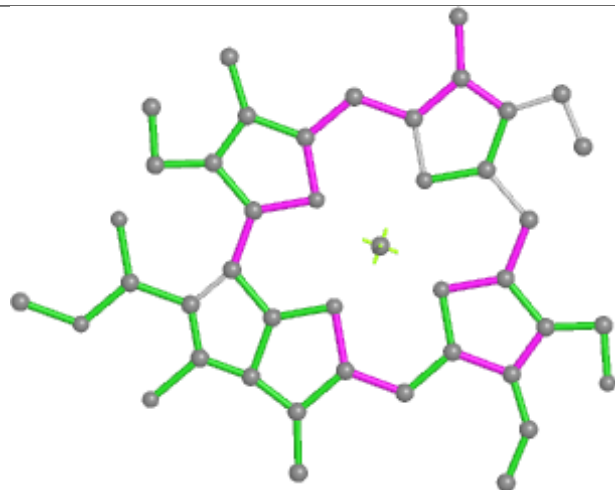


Rings

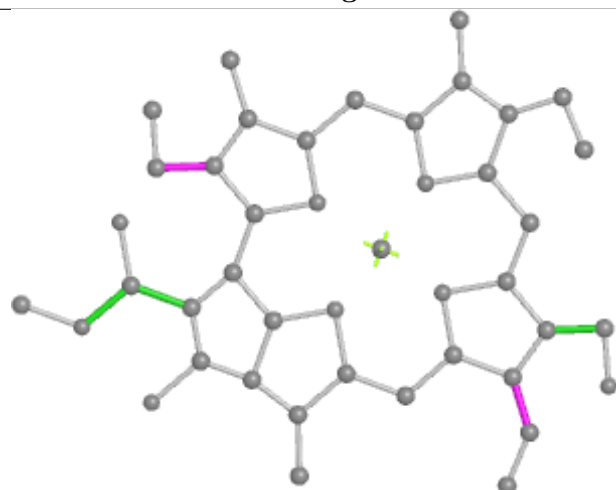
Ligand CHL 6 606



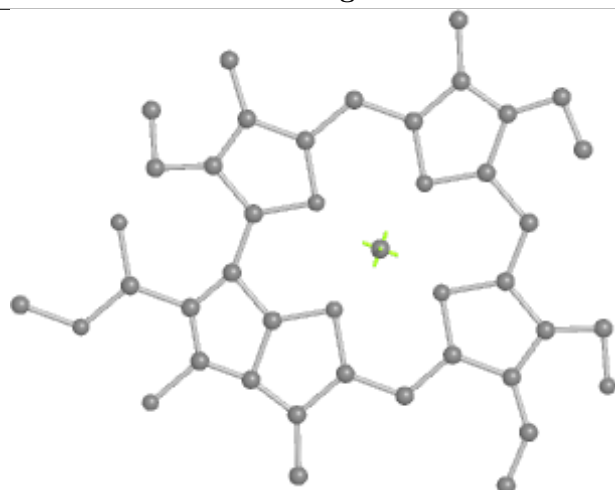
Bond lengths



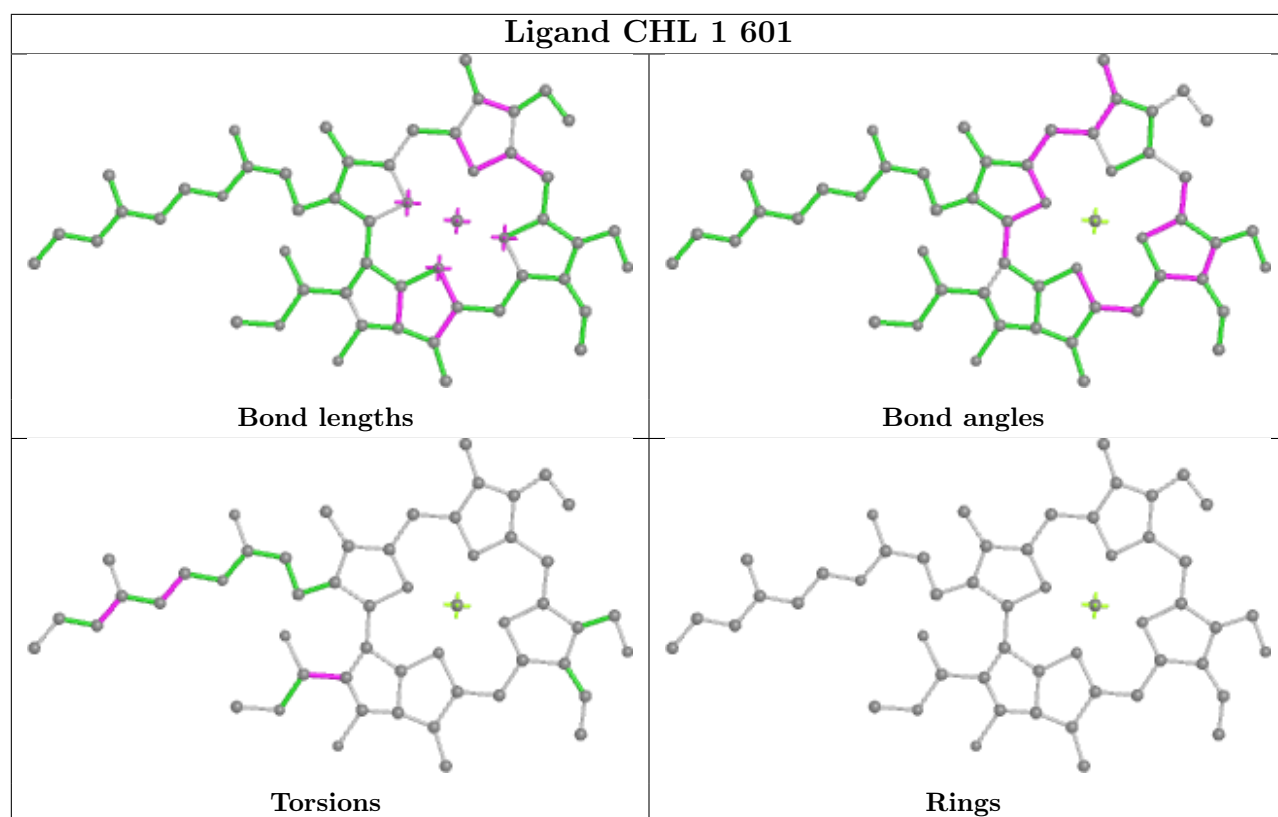
Bond angles



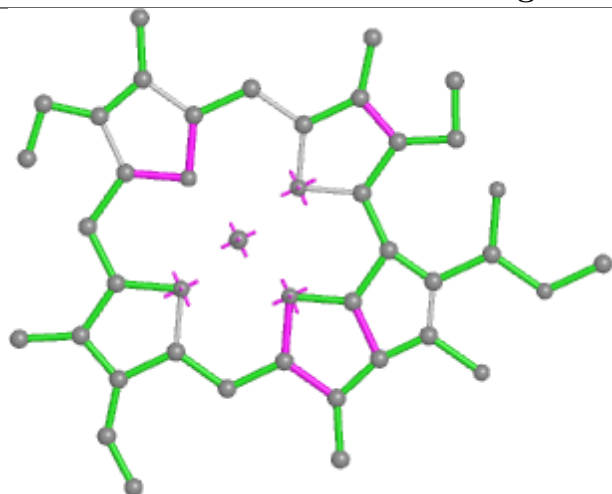
Torsions



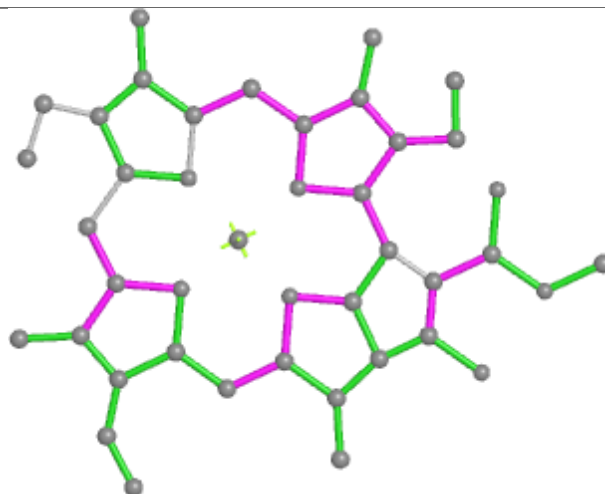
Rings



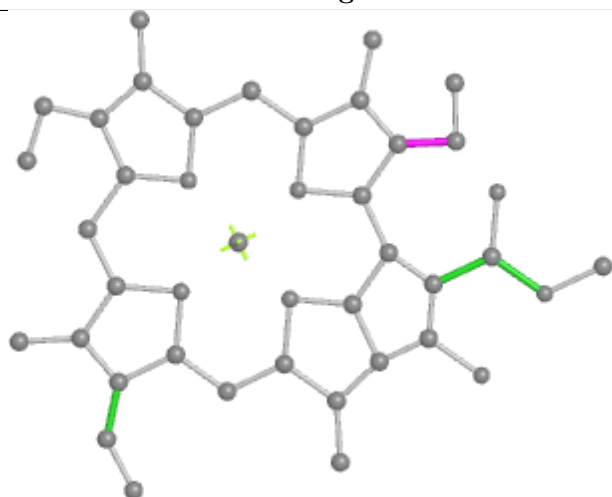
Ligand CLA 3 306



Bond lengths



Bond angles

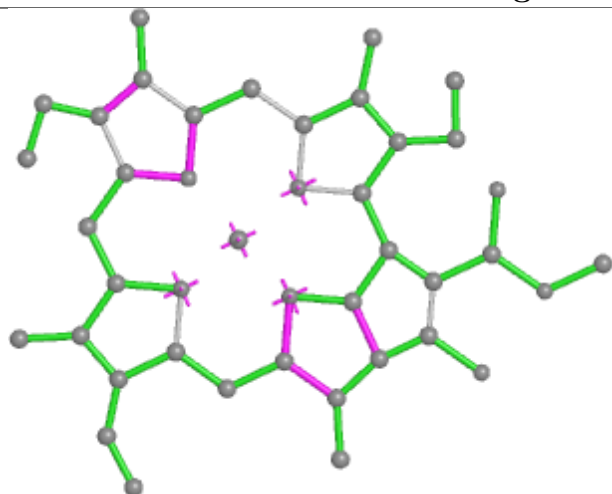


Torsions

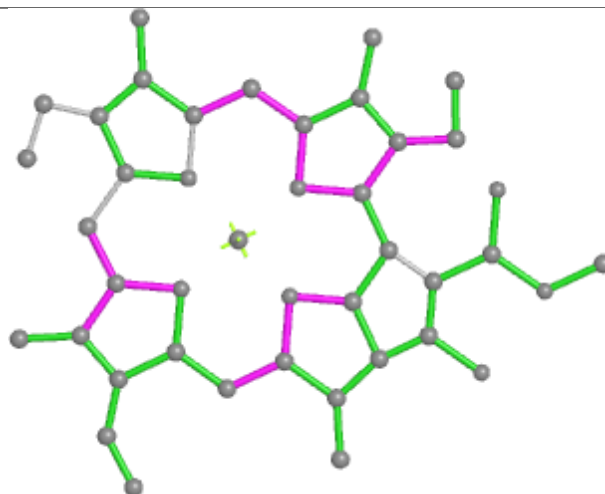


Rings

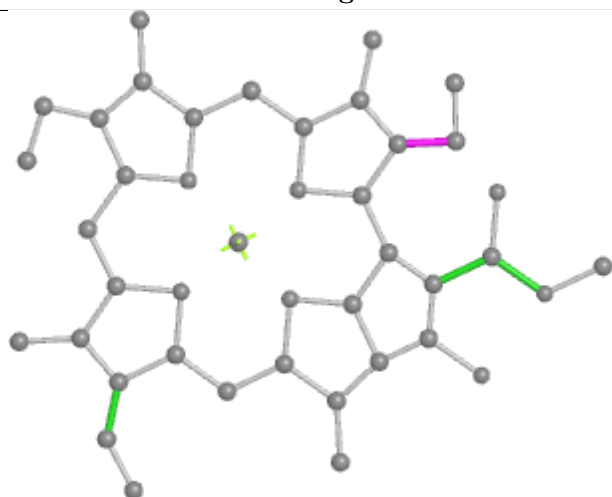
Ligand CLA B 826



Bond lengths



Bond angles

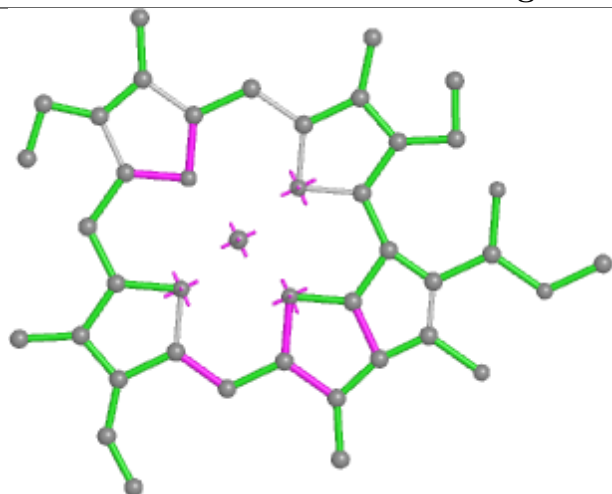


Torsions

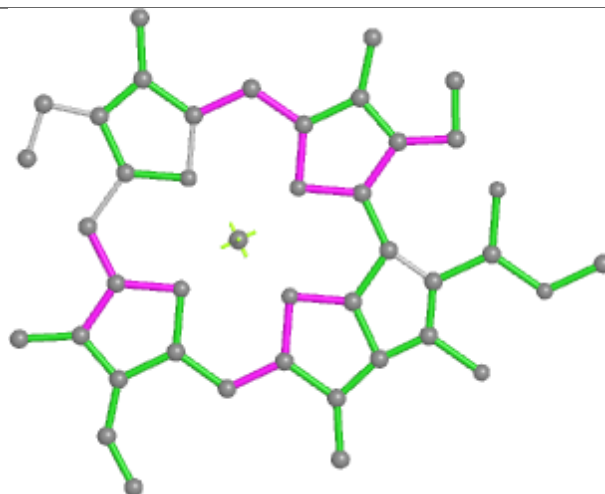


Rings

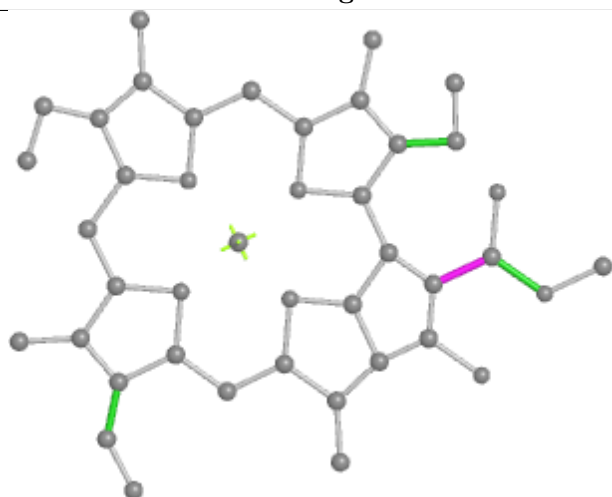
Ligand CLA 5 311



Bond lengths



Bond angles

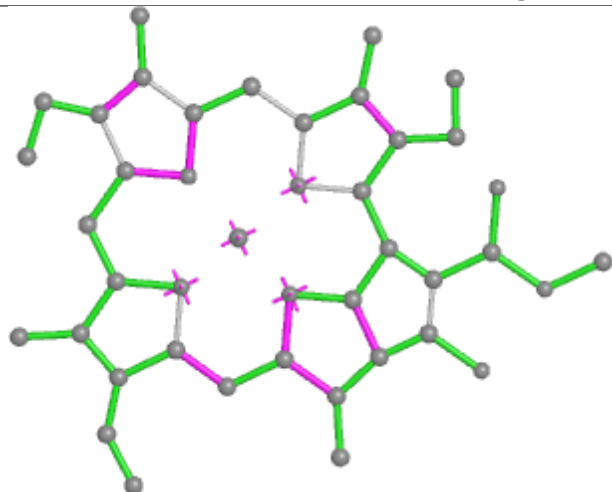


Torsions

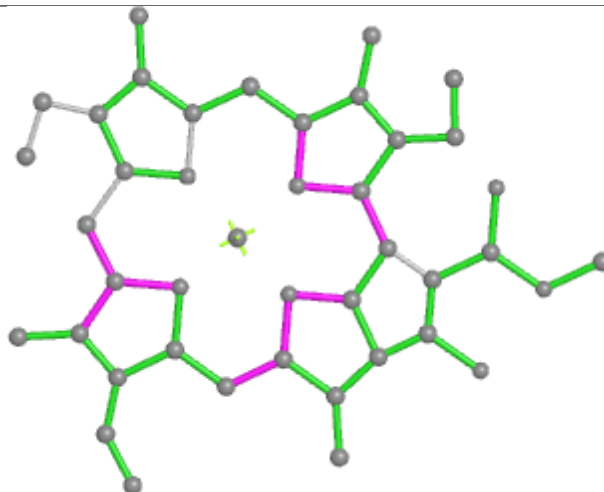


Rings

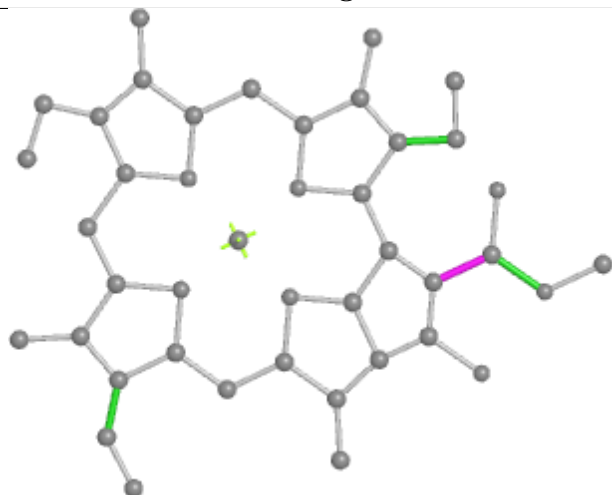
Ligand CLA A 843



Bond lengths



Bond angles

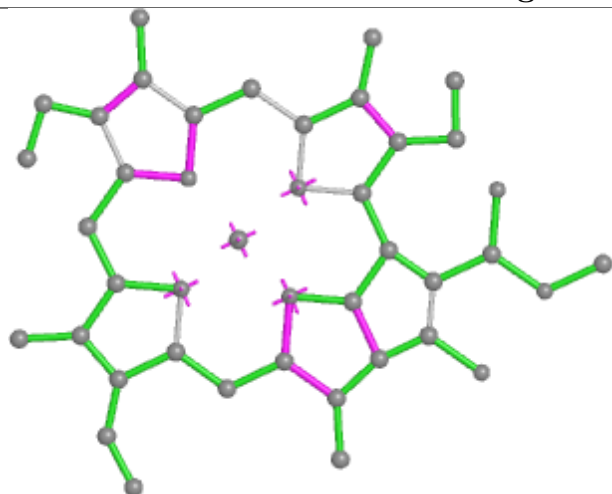


Torsions

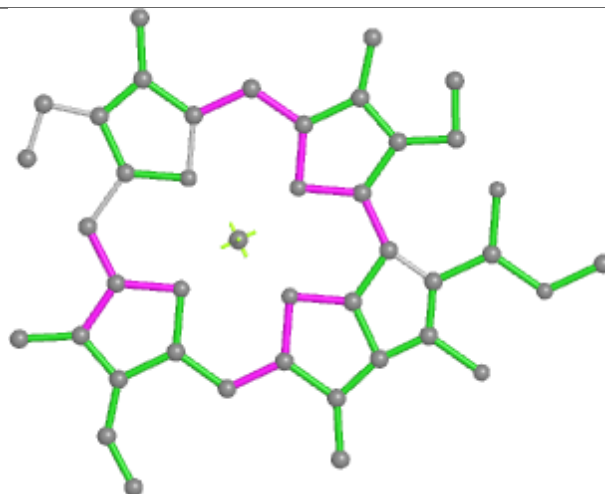


Rings

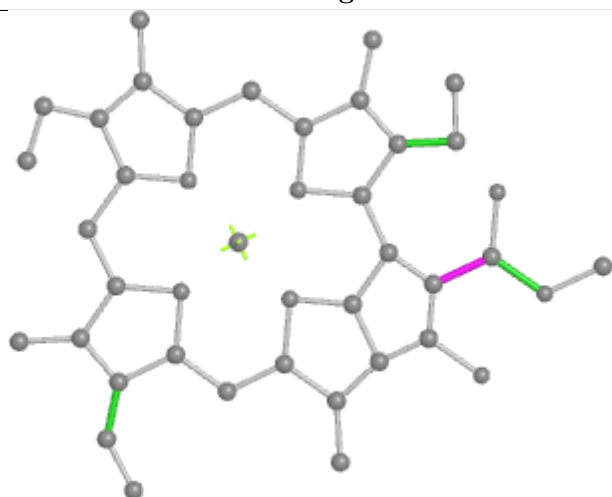
Ligand CLA 4 601



Bond lengths



Bond angles

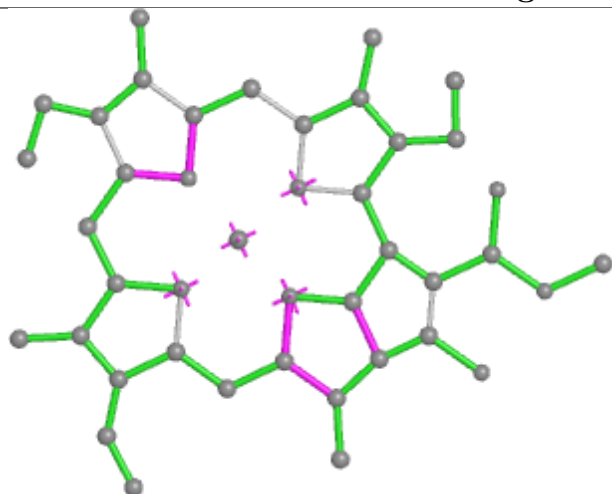


Torsions

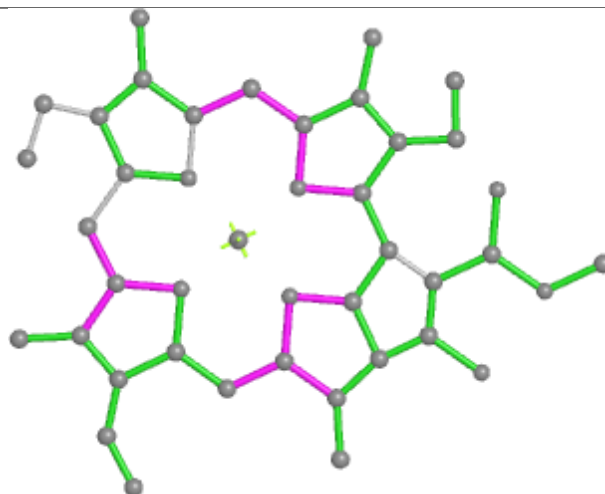


Rings

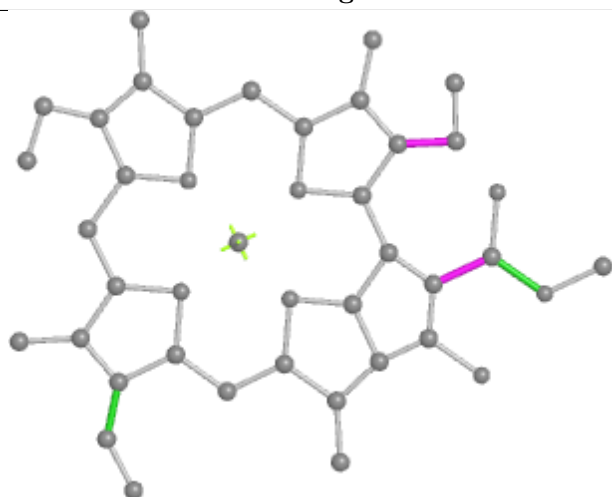
Ligand CLA 5 308



Bond lengths



Bond angles

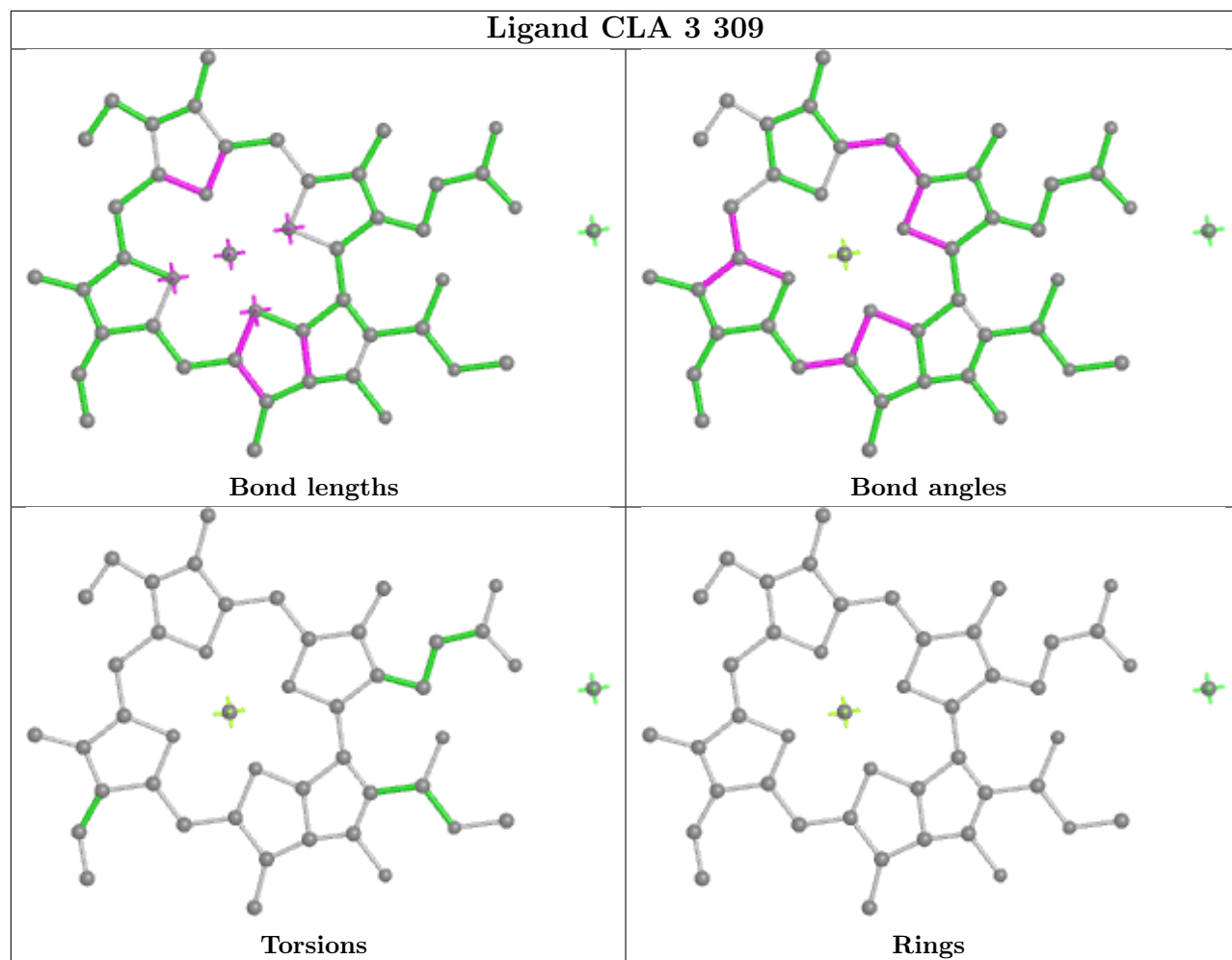


Torsions

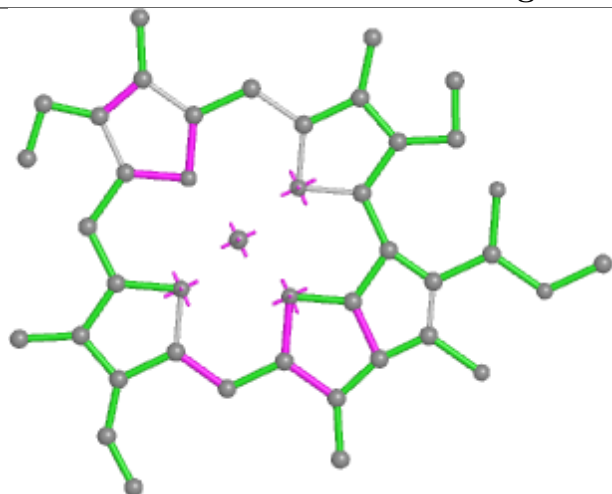


Rings

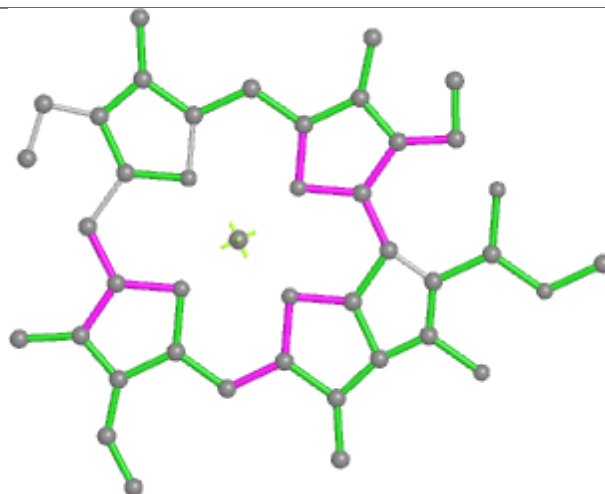
Ligand CLA 3 309



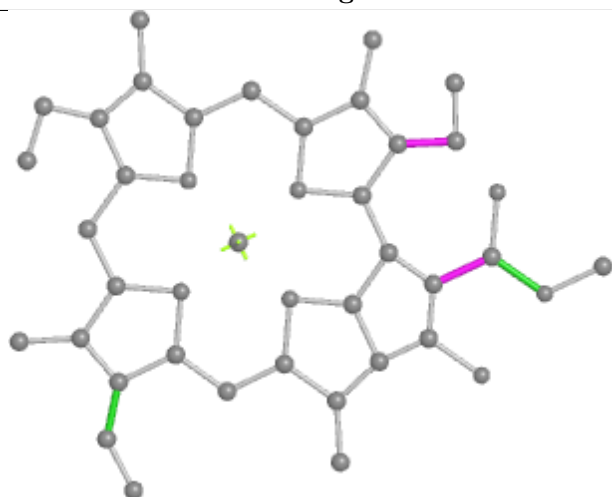
Ligand CLA 3 302



Bond lengths



Bond angles

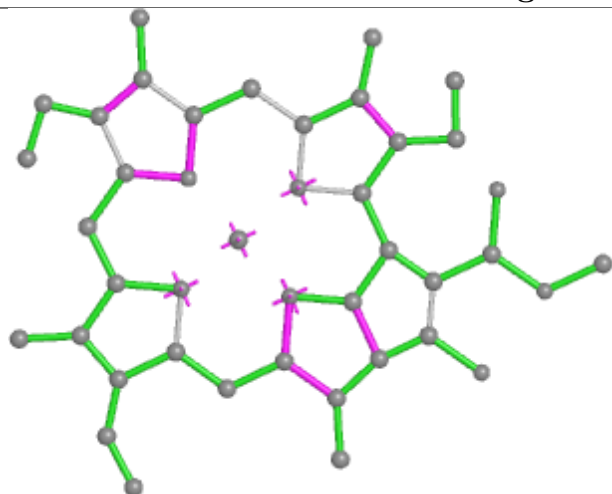


Torsions

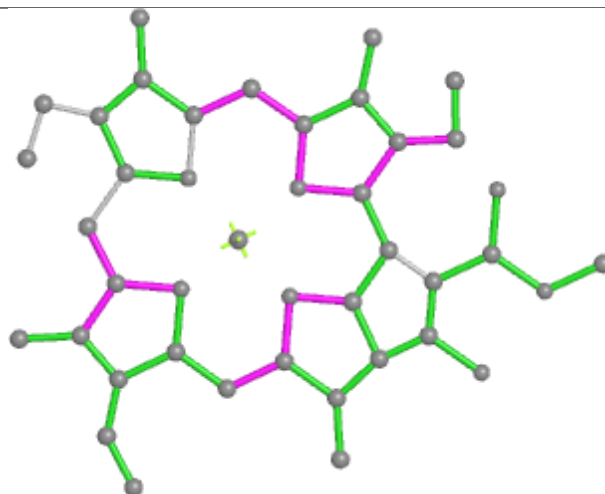


Rings

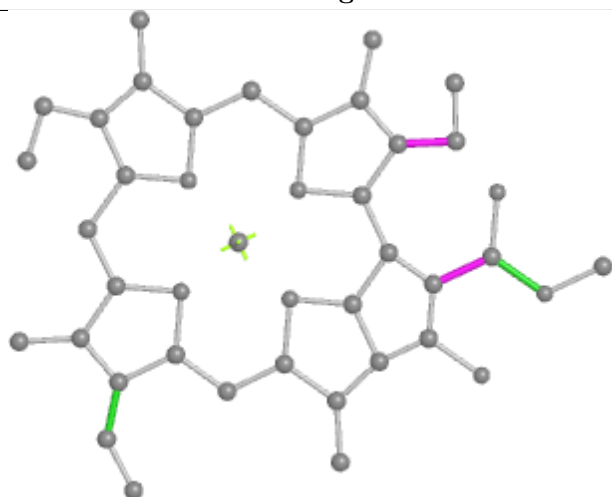
Ligand CLA 5 309



Bond lengths



Bond angles

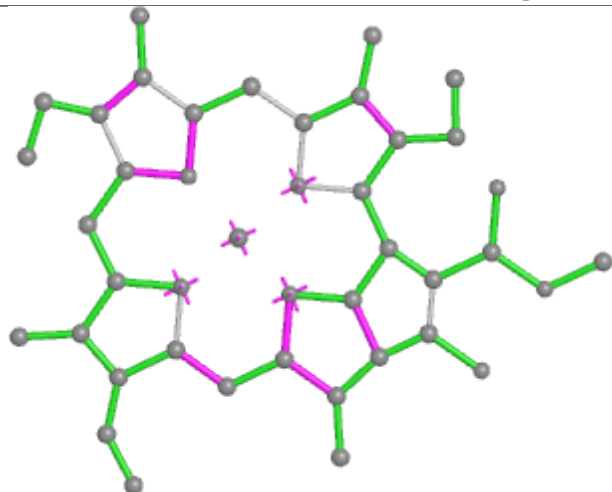


Torsions

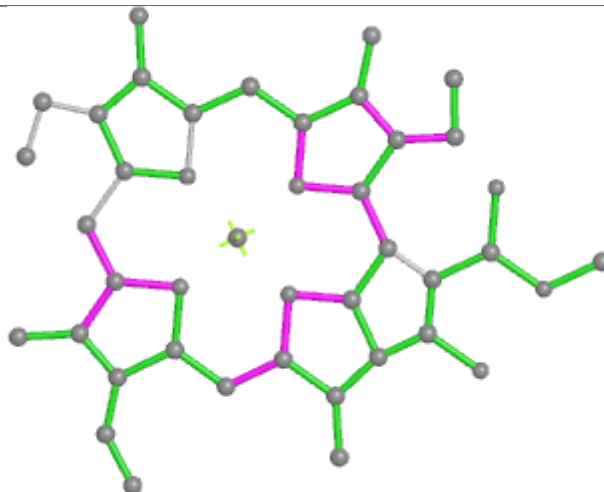


Rings

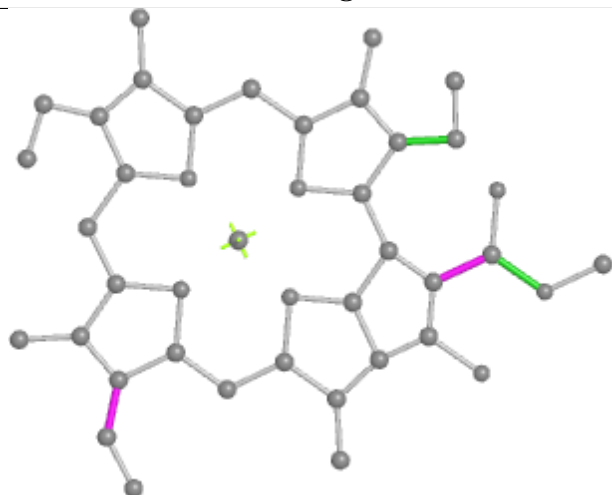
Ligand CLA 8 607



Bond lengths



Bond angles

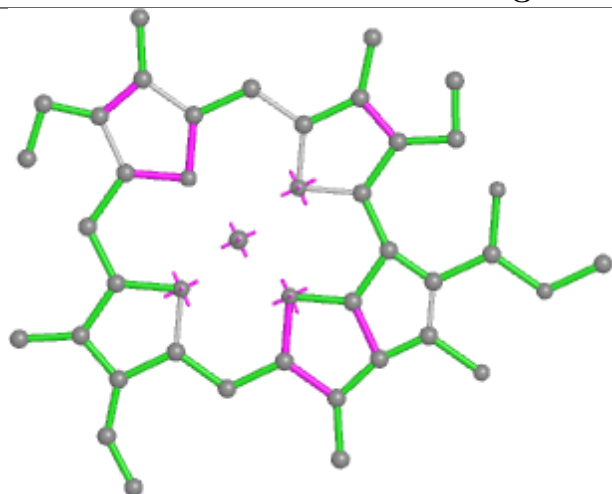


Torsions

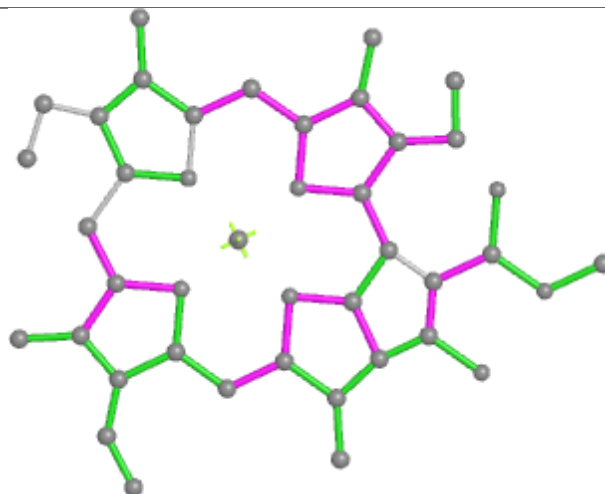


Rings

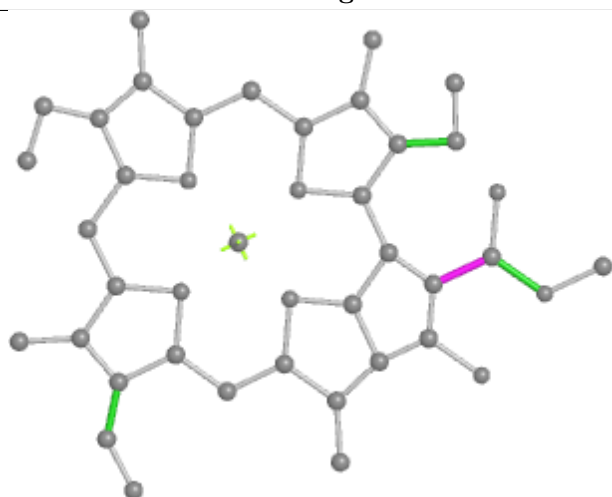
Ligand CLA B 806



Bond lengths



Bond angles

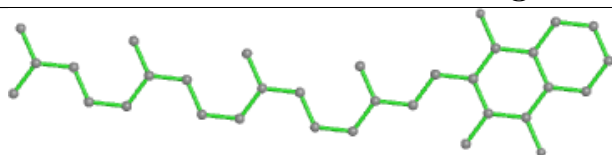


Torsions

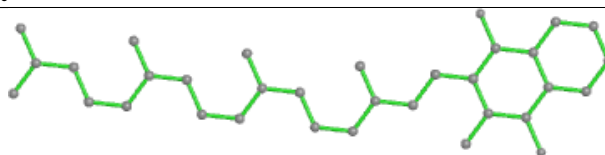


Rings

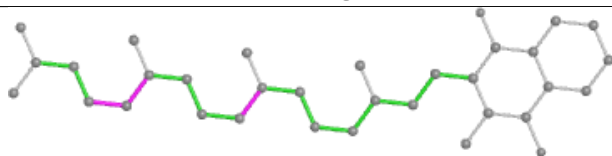
Ligand PQN A 840



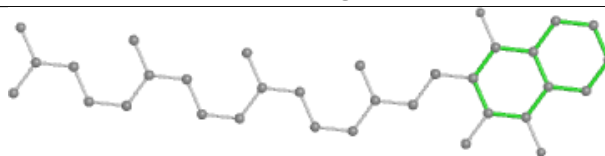
Bond lengths



Bond angles

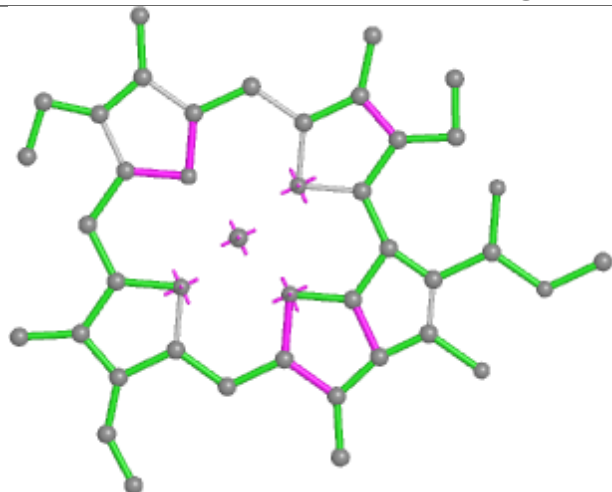


Torsions

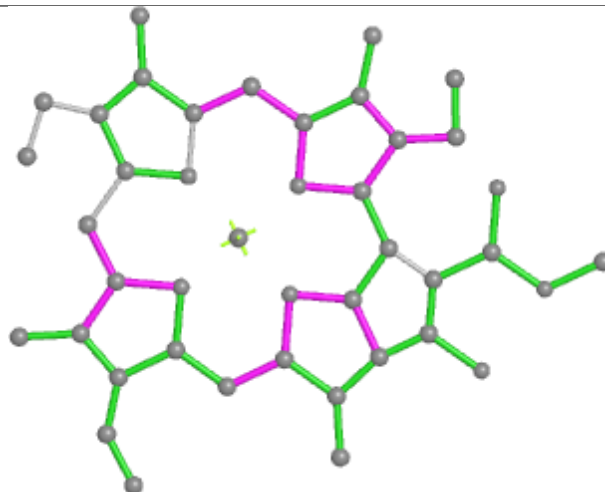


Rings

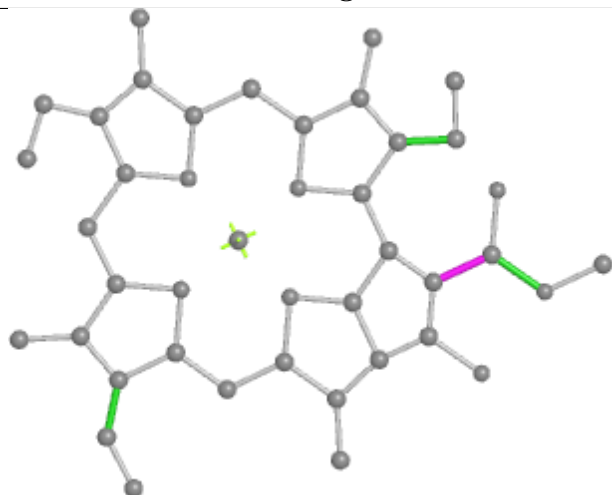
Ligand CLA 7 603



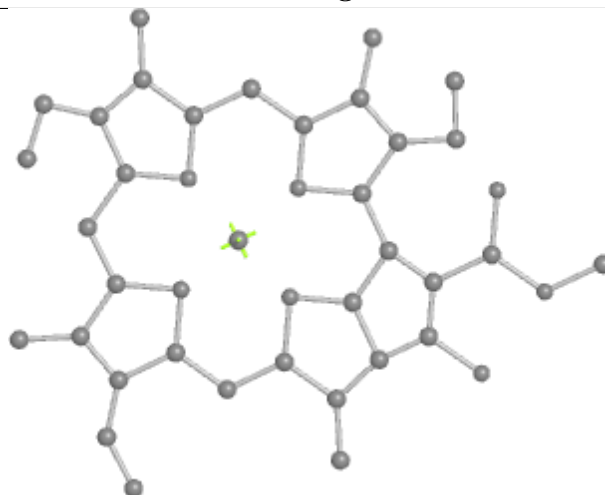
Bond lengths



Bond angles

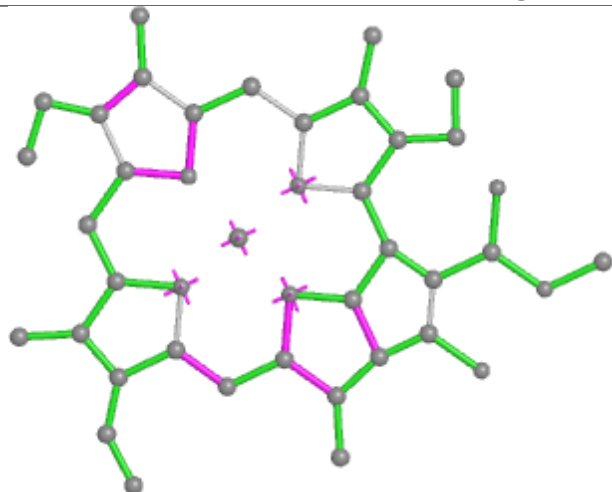


Torsions

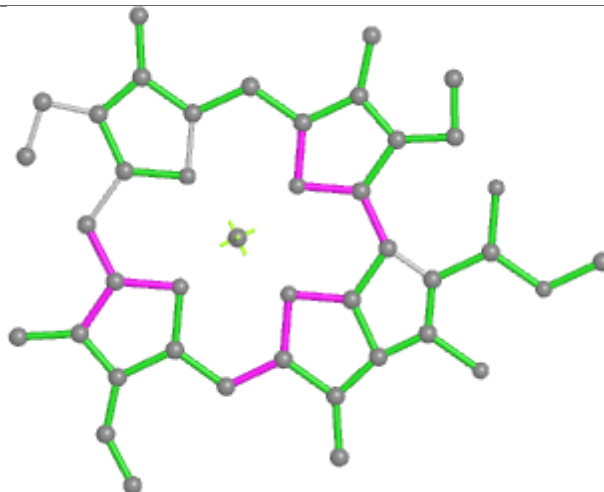


Rings

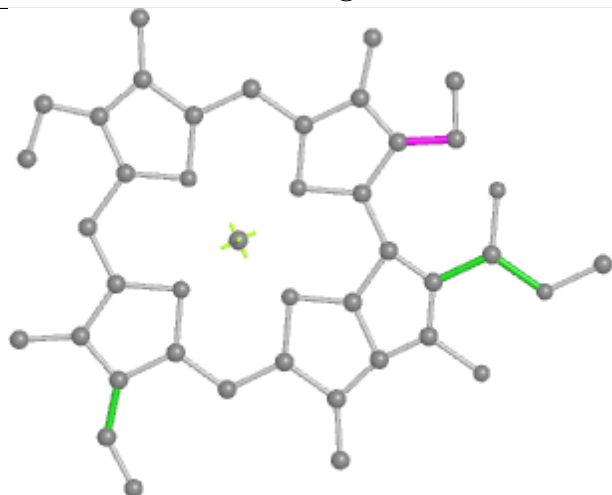
Ligand CLA A 814



Bond lengths



Bond angles

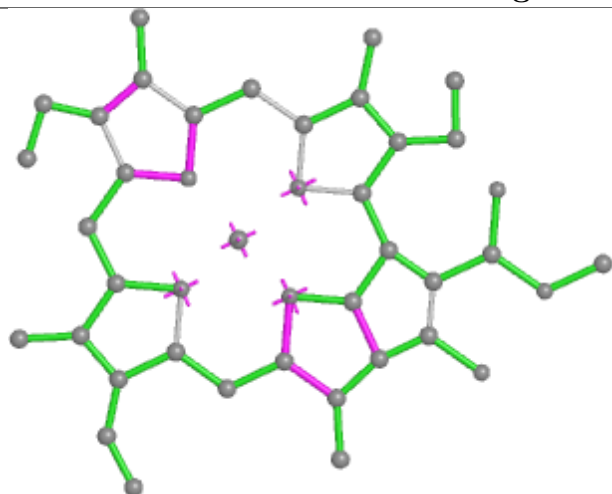


Torsions

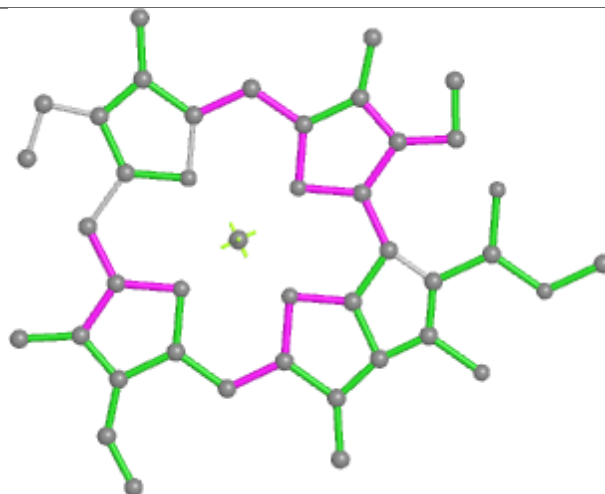


Rings

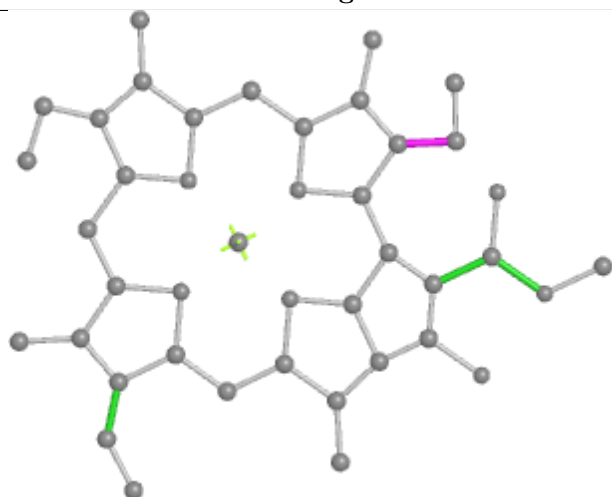
Ligand CLA A 817



Bond lengths



Bond angles

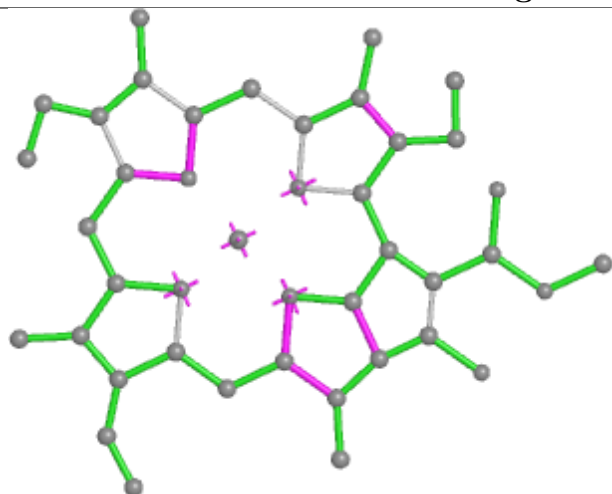


Torsions

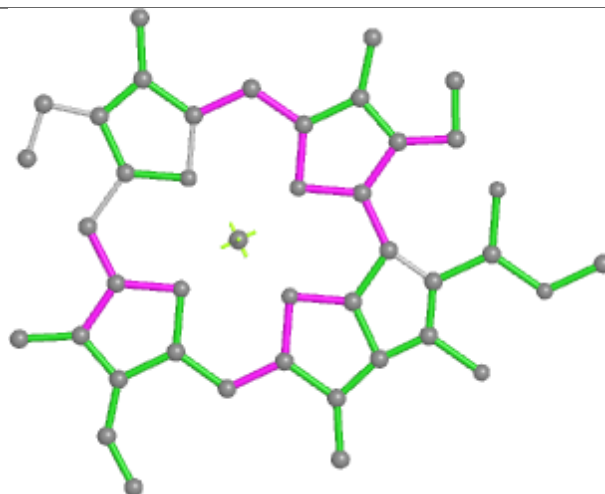


Rings

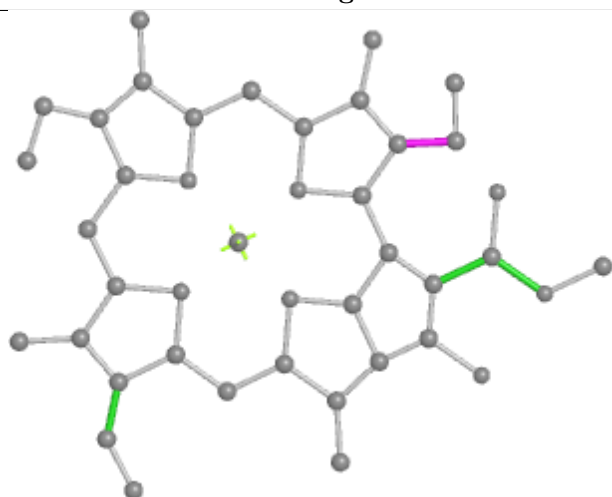
Ligand CLA F 301



Bond lengths



Bond angles

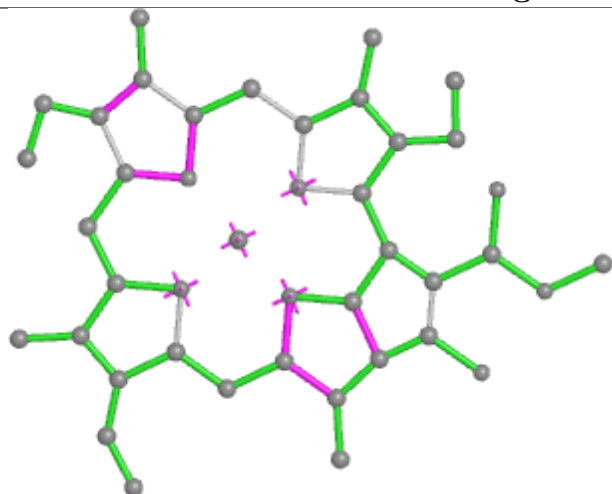


Torsions

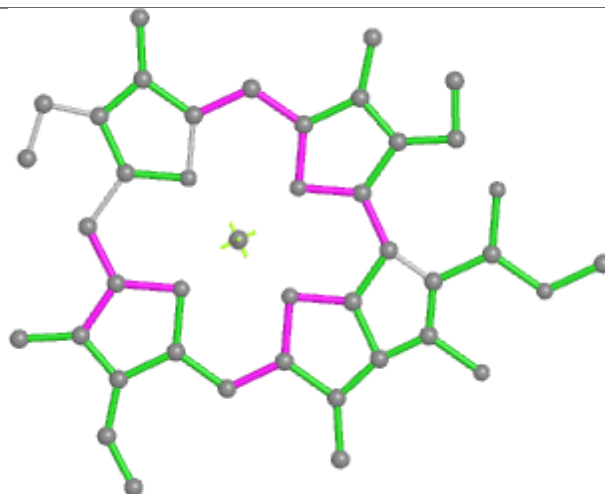


Rings

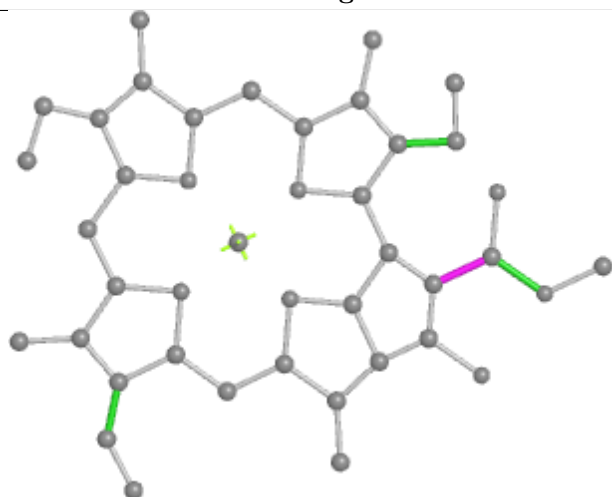
Ligand CLA B 833



Bond lengths



Bond angles

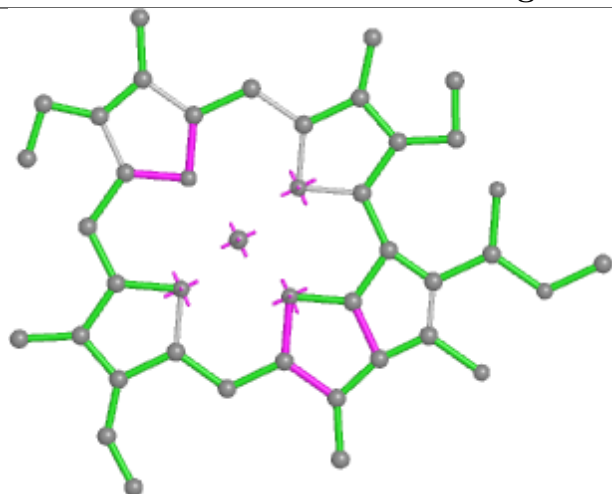


Torsions

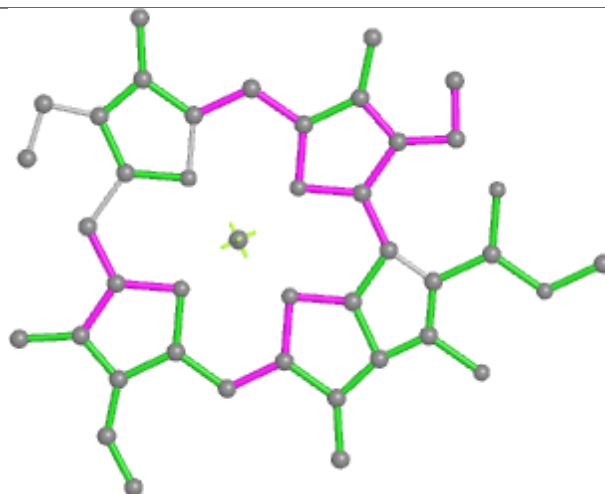


Rings

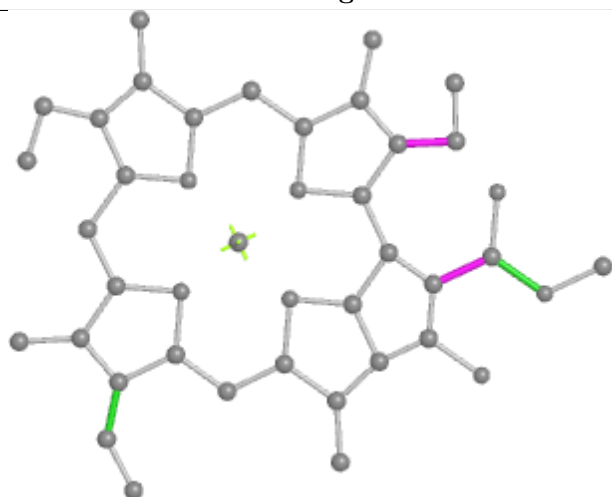
Ligand CLA 1 607



Bond lengths



Bond angles

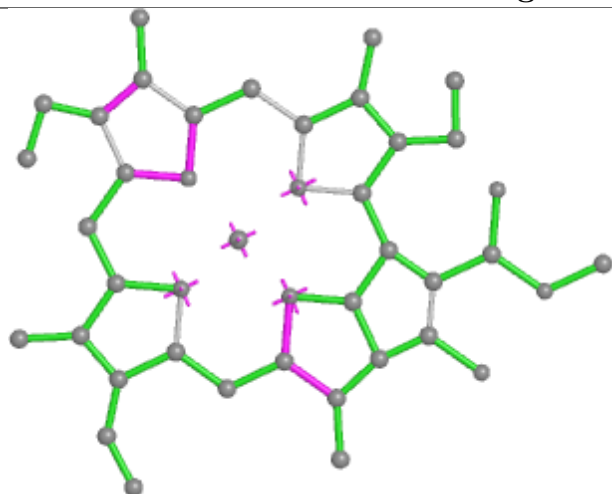


Torsions

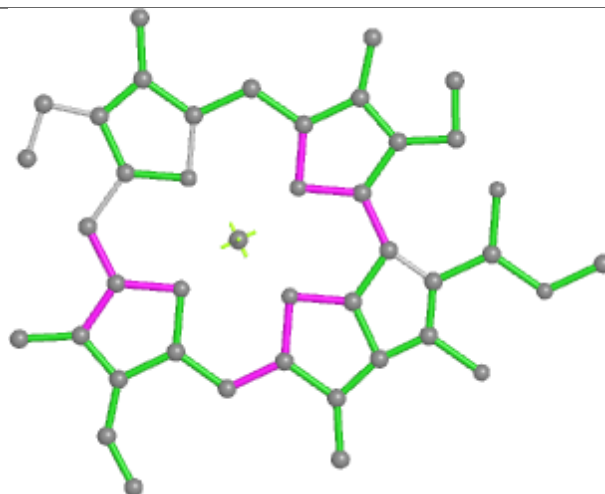


Rings

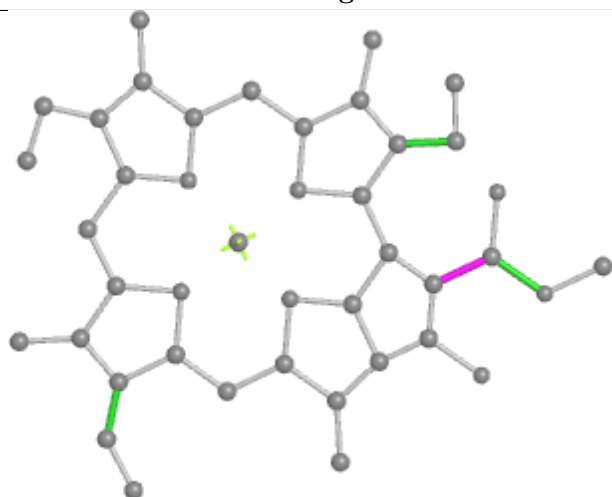
Ligand CLA 1 609



Bond lengths



Bond angles

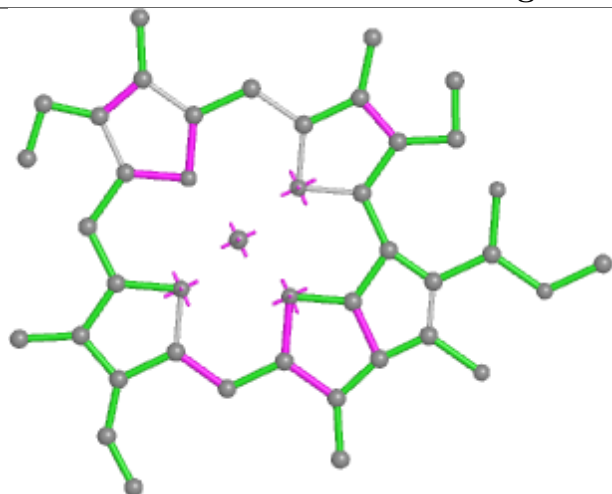


Torsions

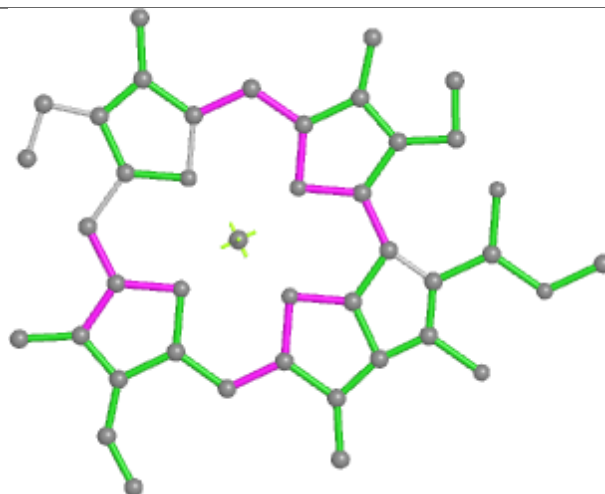


Rings

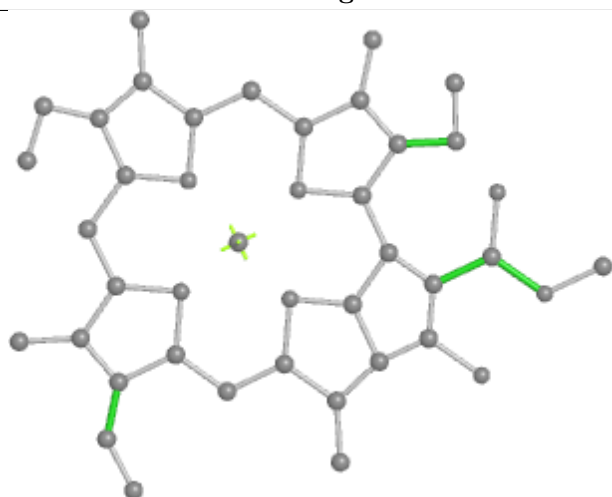
Ligand CLA 5 310



Bond lengths



Bond angles

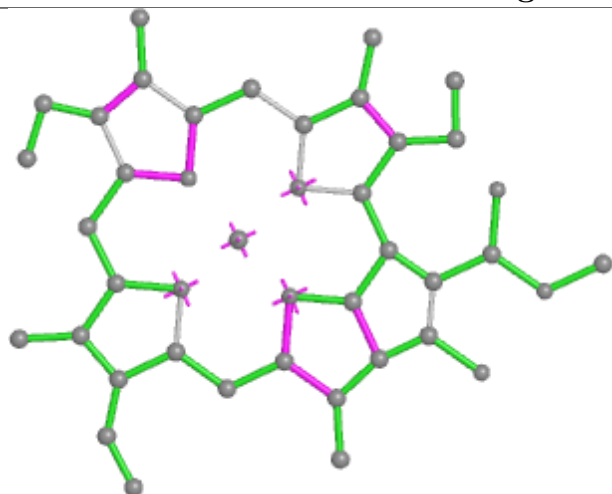


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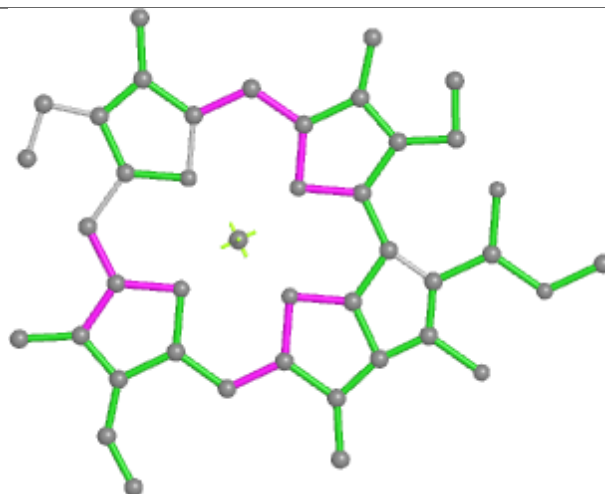


Rings

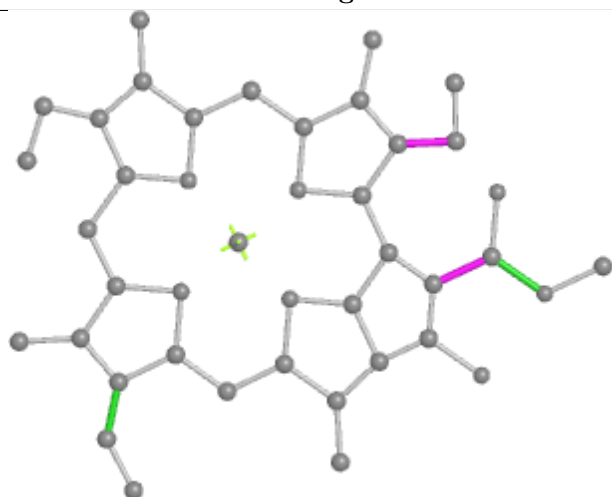
Ligand CLA 8 611



Bond lengths



Bond angles

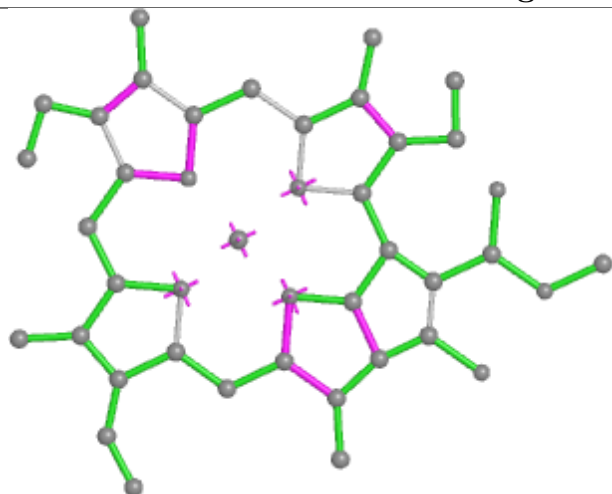


Torsions

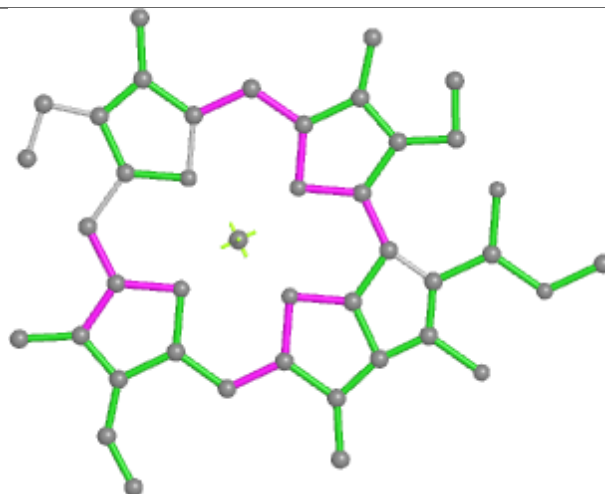


Rings

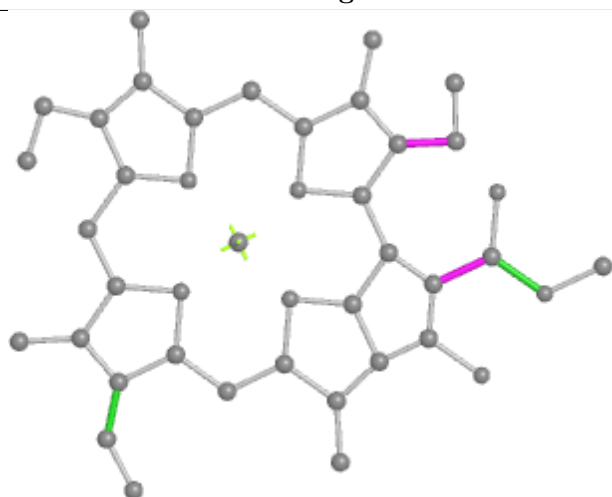
Ligand CLA 8 613



Bond lengths



Bond angles

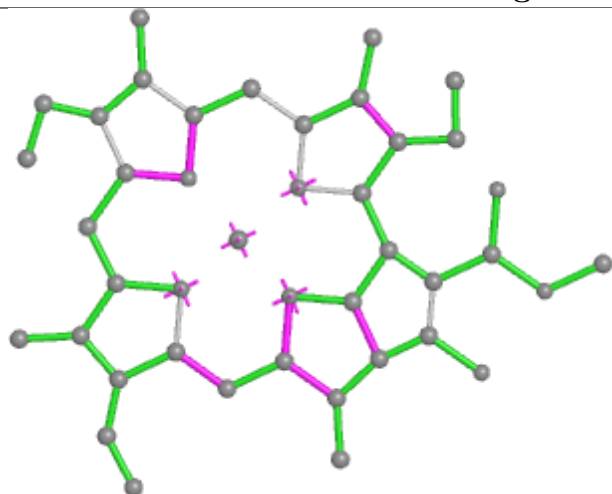


Torsions

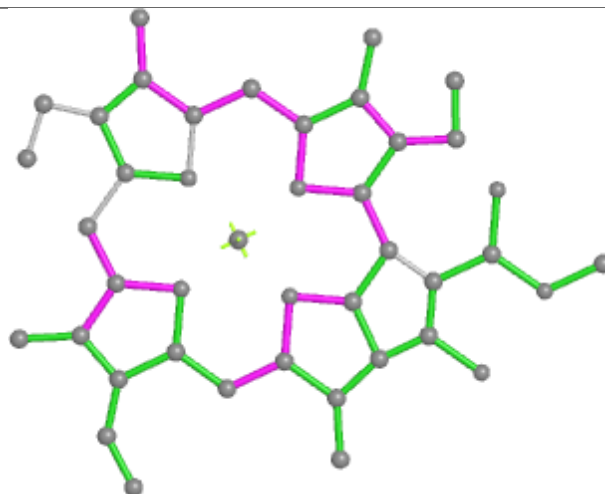


Rings

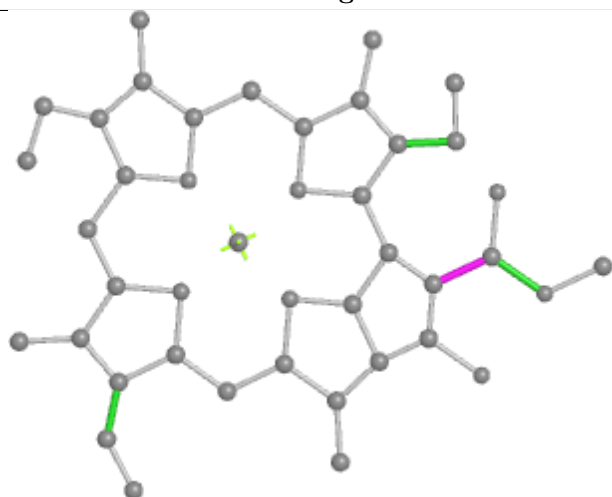
Ligand CLA B 823



Bond lengths



Bond angles

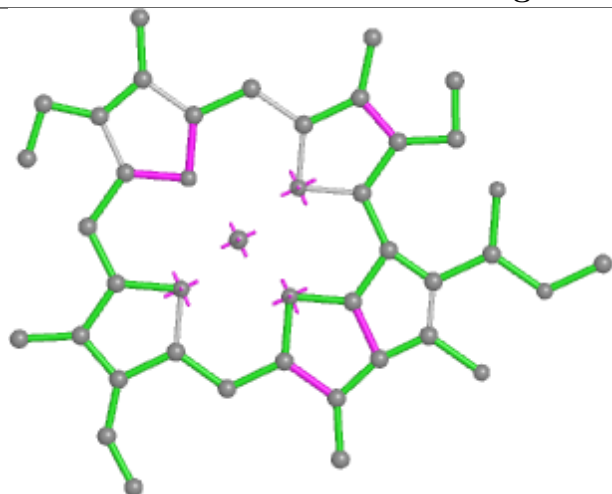


Torsions

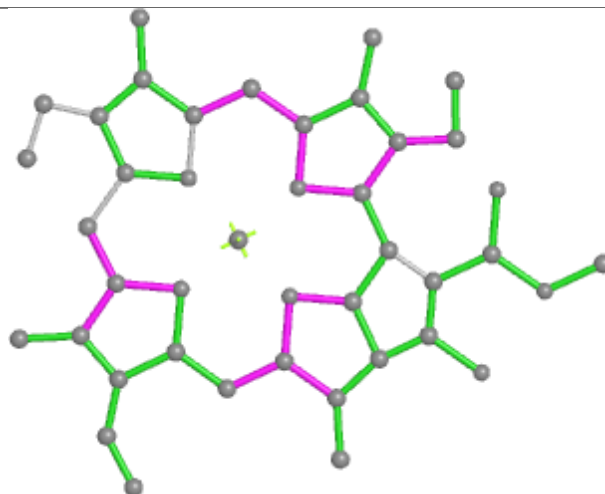


Rings

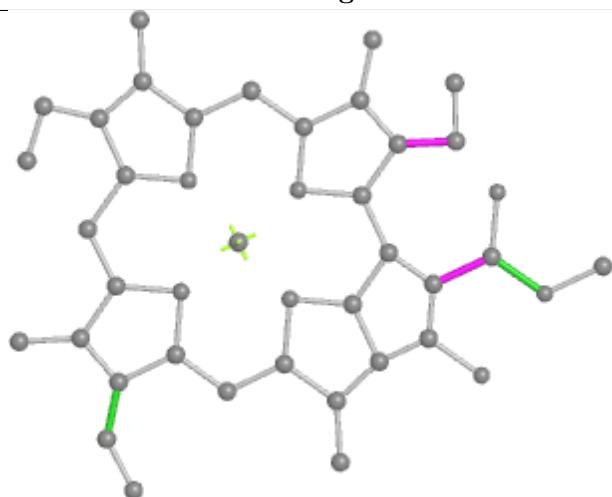
Ligand CLA B 801



Bond lengths



Bond angles

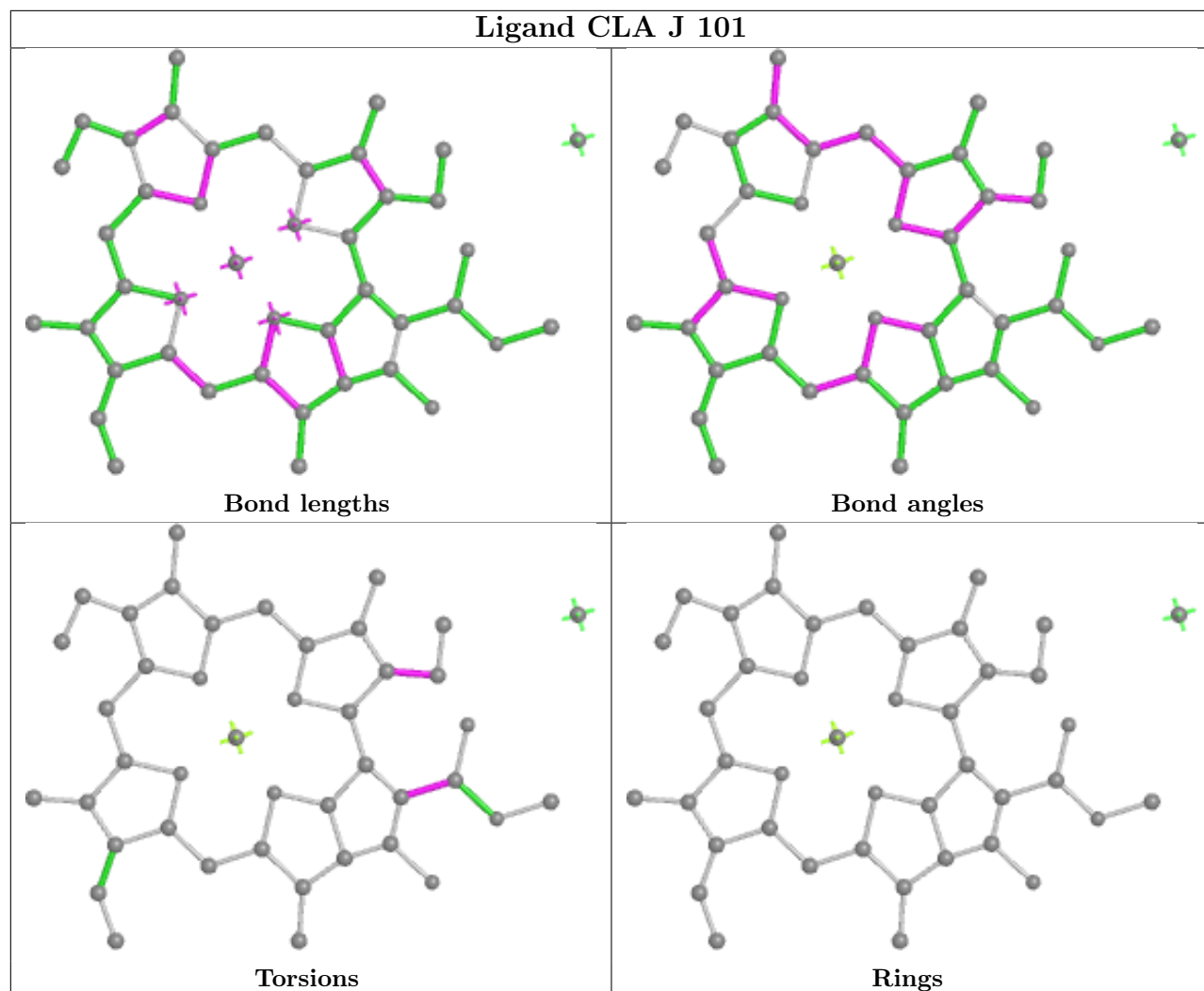


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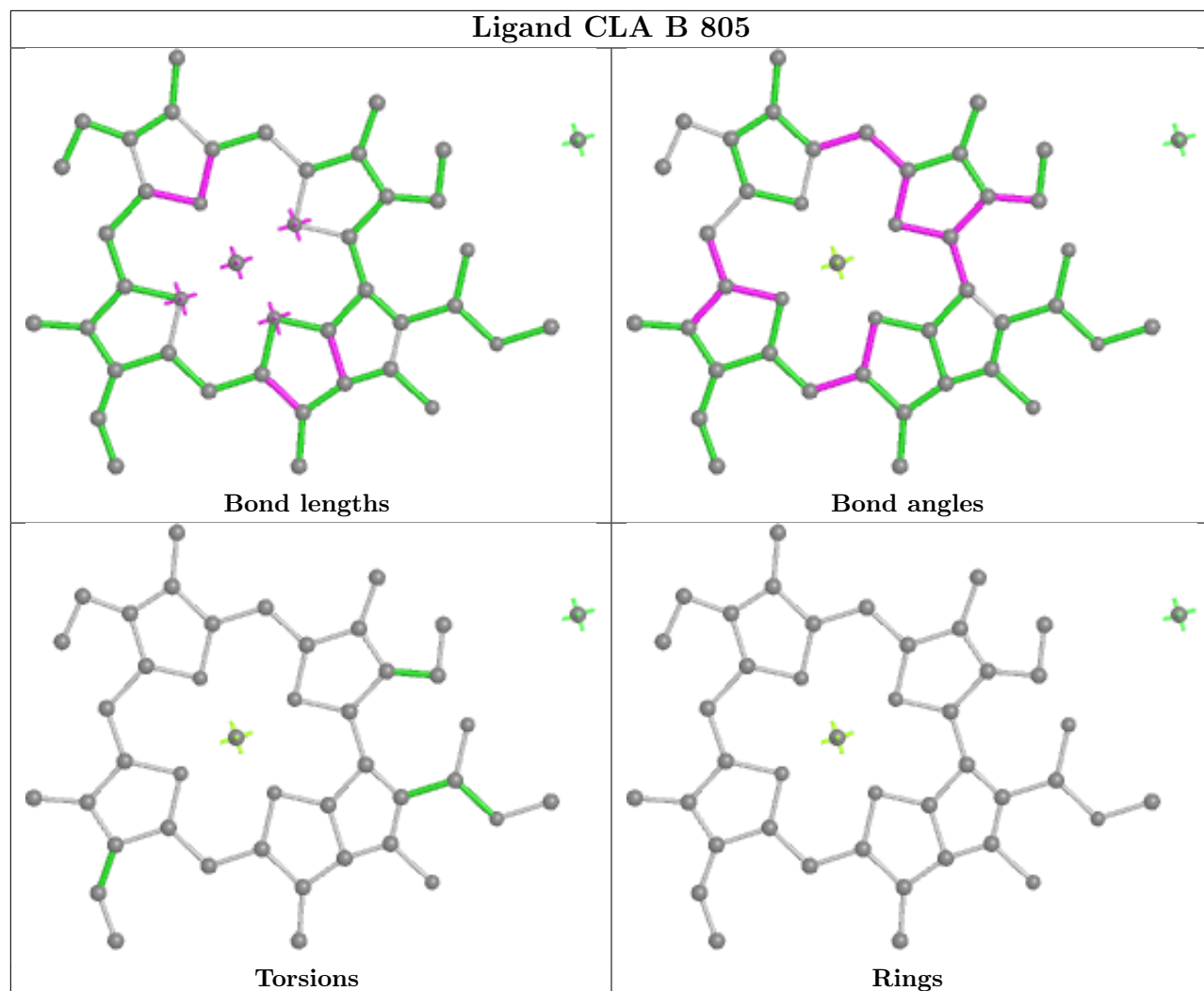


Rings

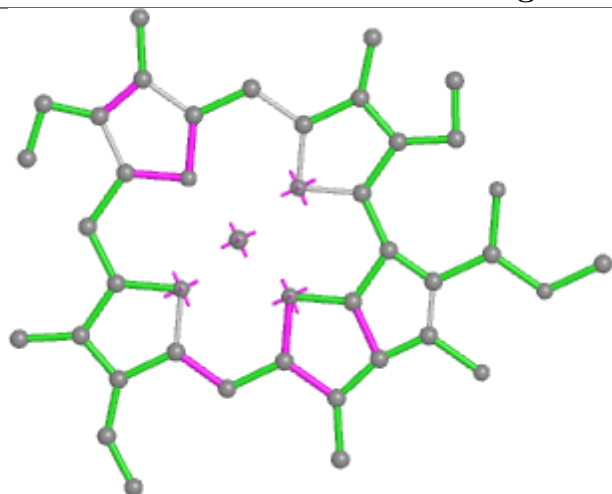
Ligand CLA J 101



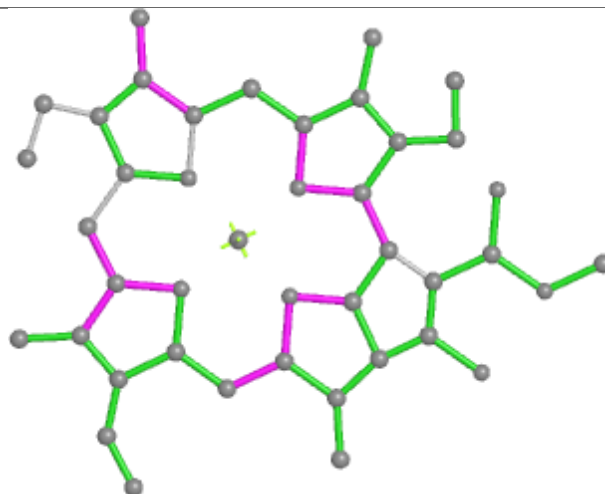
Ligand CLA B 805



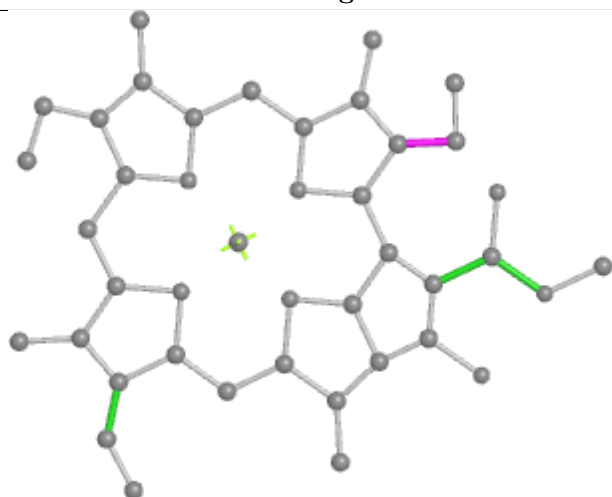
Ligand CLA 5 302



Bond lengths



Bond angles

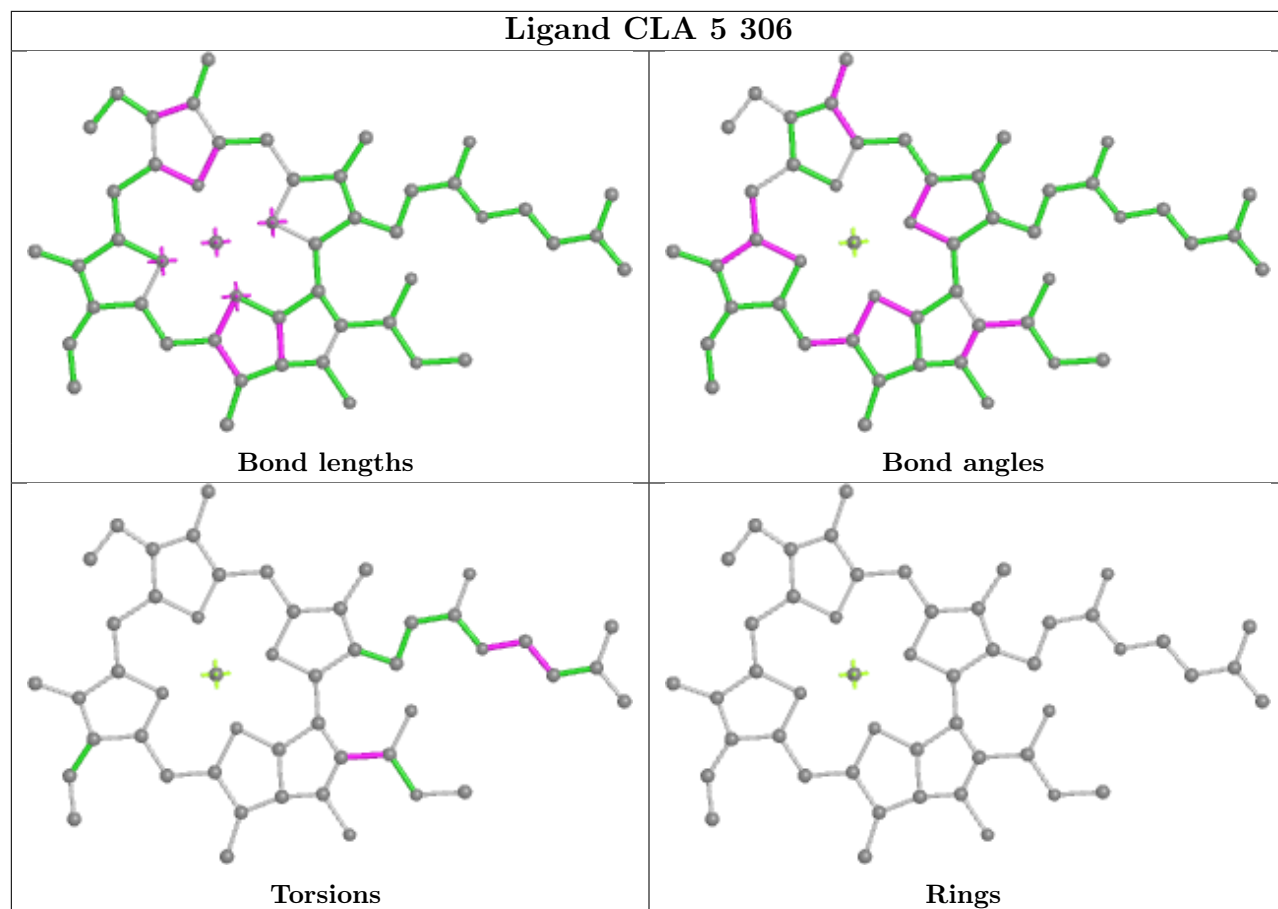


Torsions

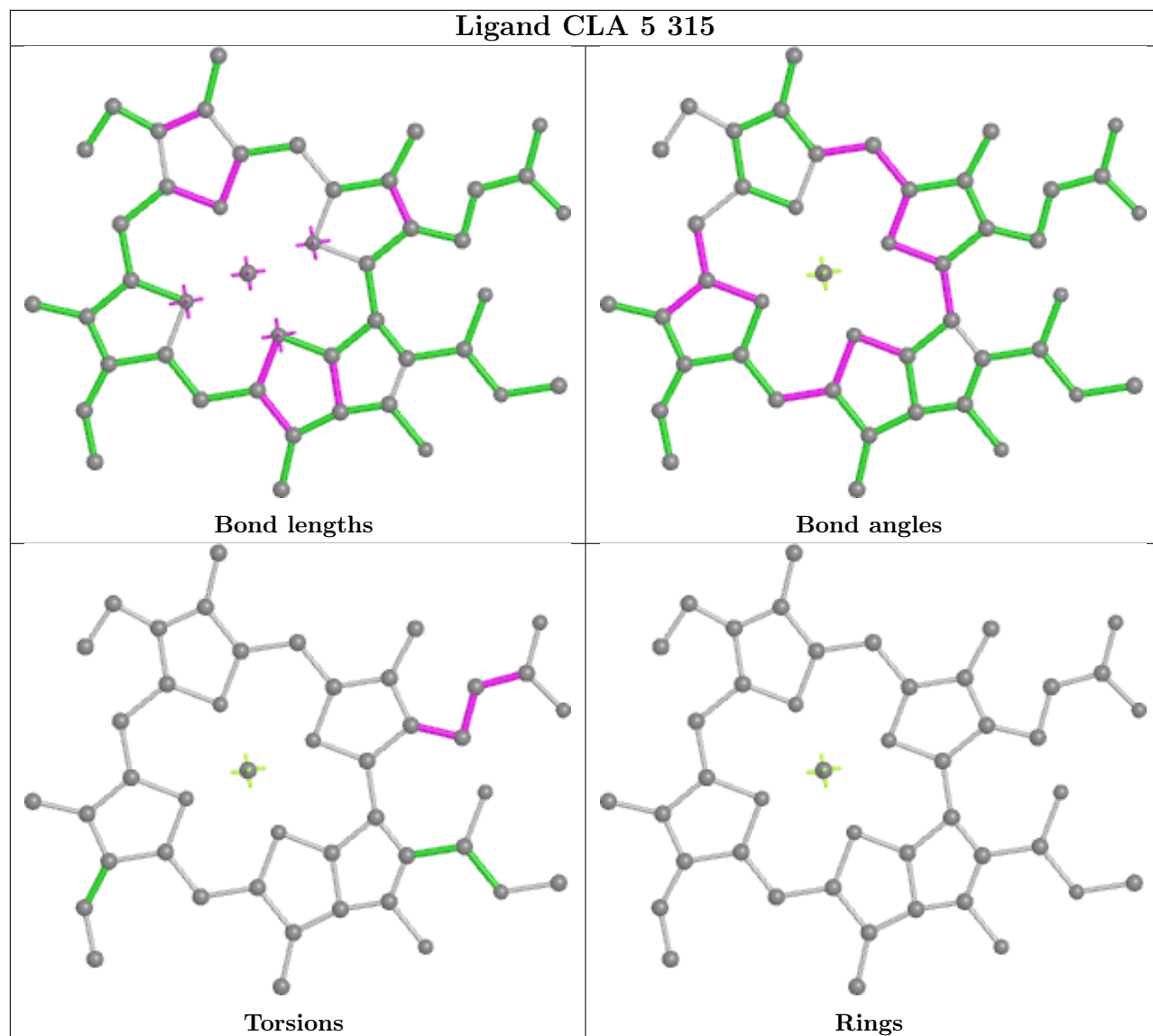


Rings

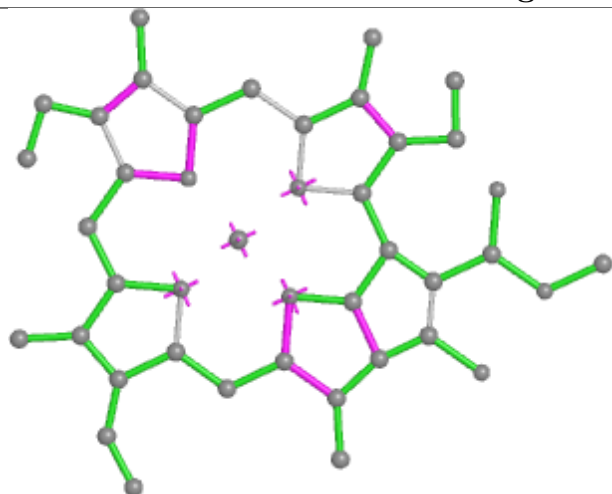
Ligand CLA 5 306



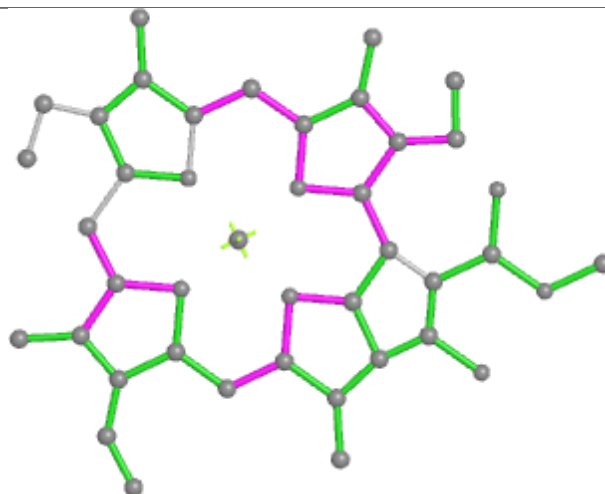
Ligand CLA 5 315



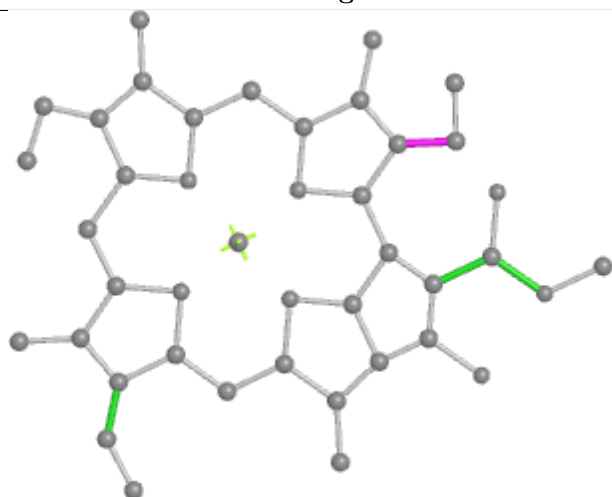
Ligand CLA 3 313



Bond lengths



Bond angles

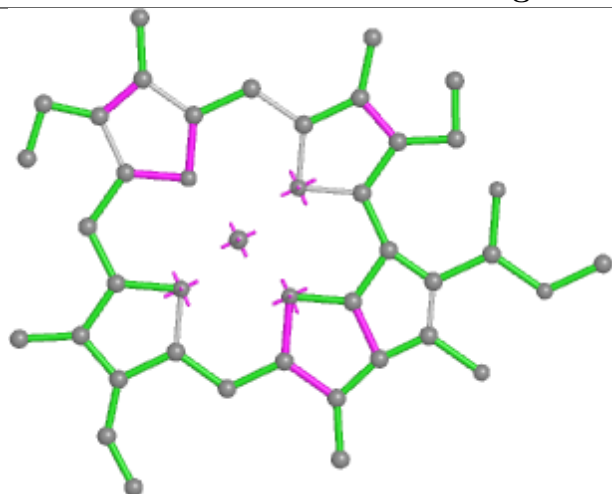


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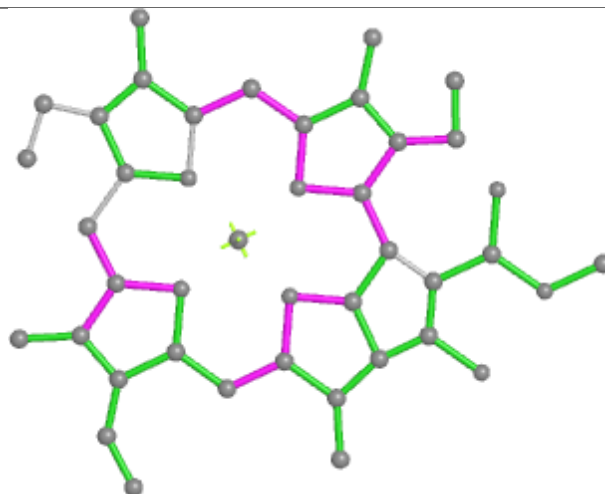


Rings

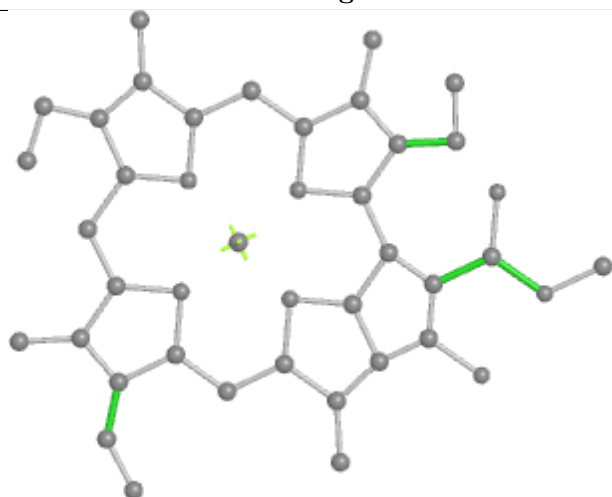
Ligand CLA A 824



Bond lengths



Bond angles

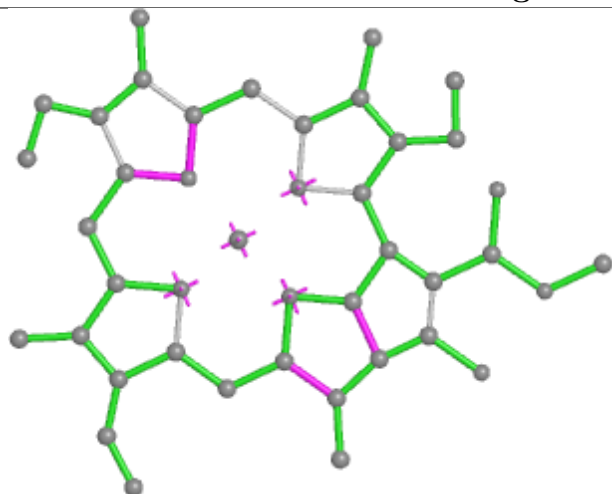


Torsions

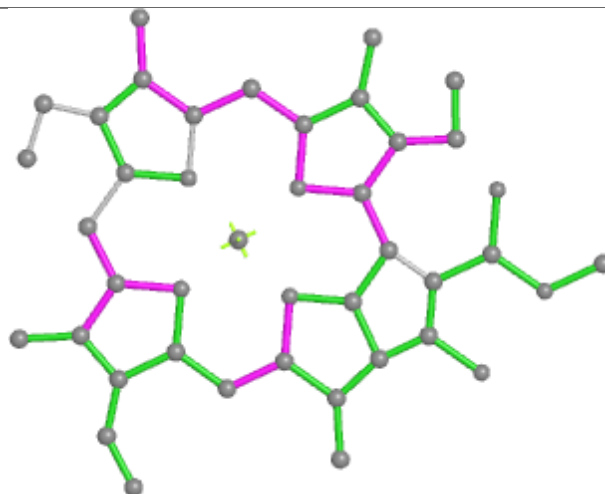


Rings

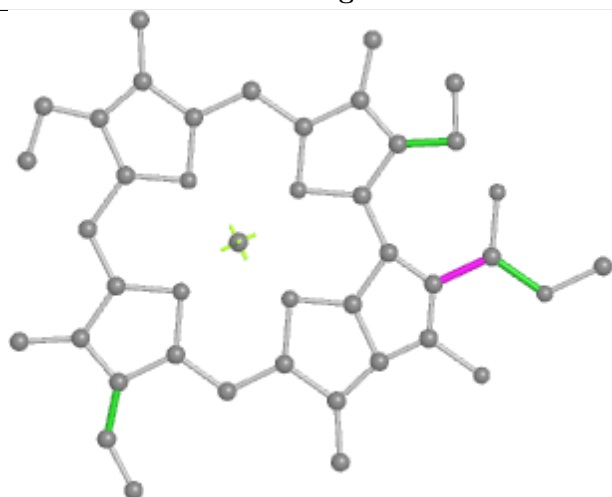
Ligand CLA A 842



Bond lengths



Bond angles

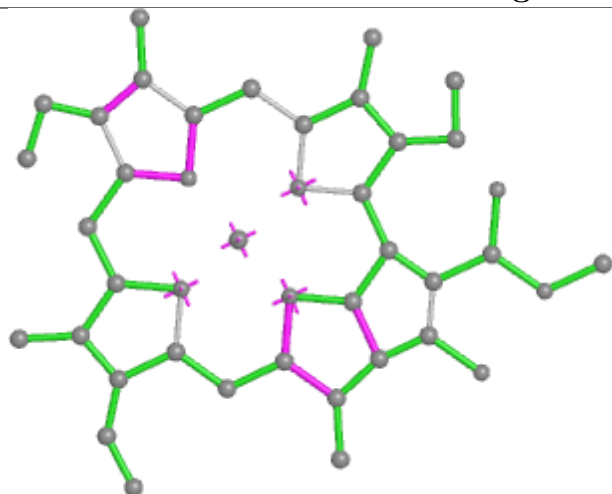


Torsions

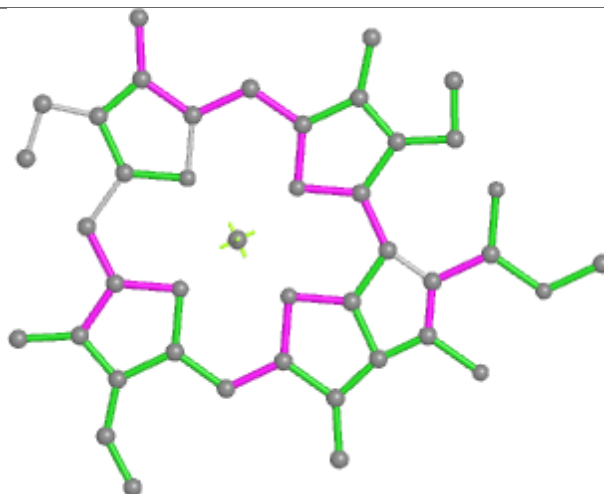


Rings

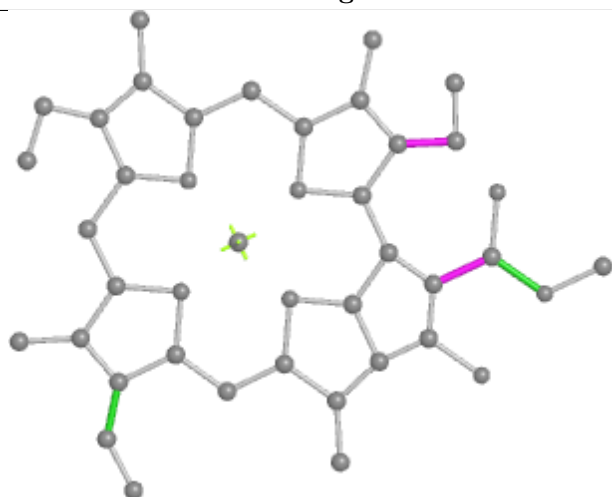
Ligand CLA A 838



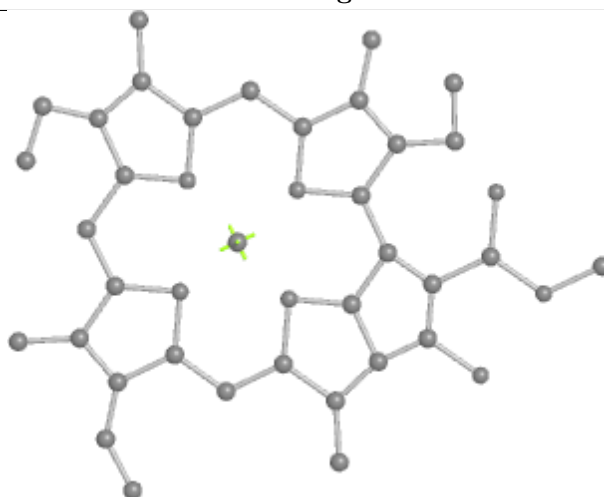
Bond lengths



Bond angles

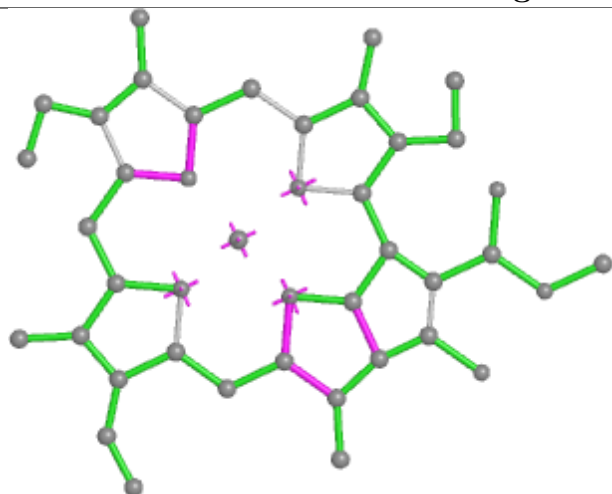


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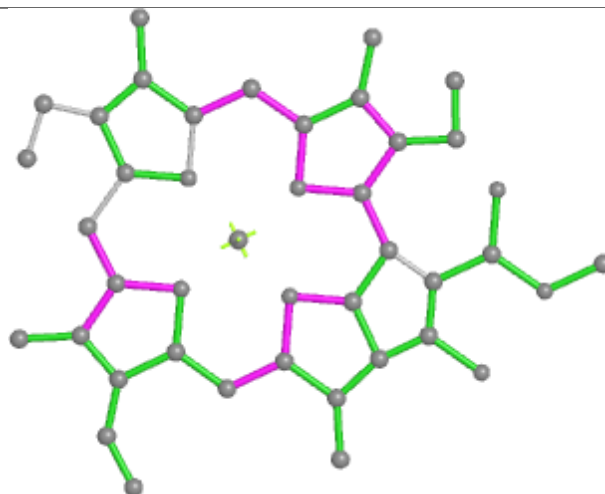


Rings

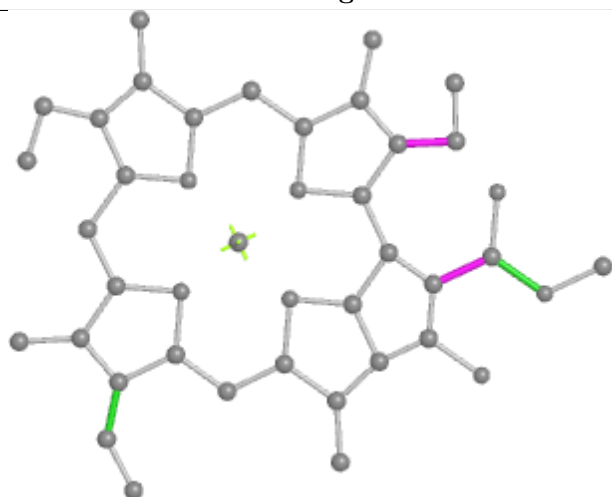
Ligand CLA B 820



Bond lengths



Bond angles

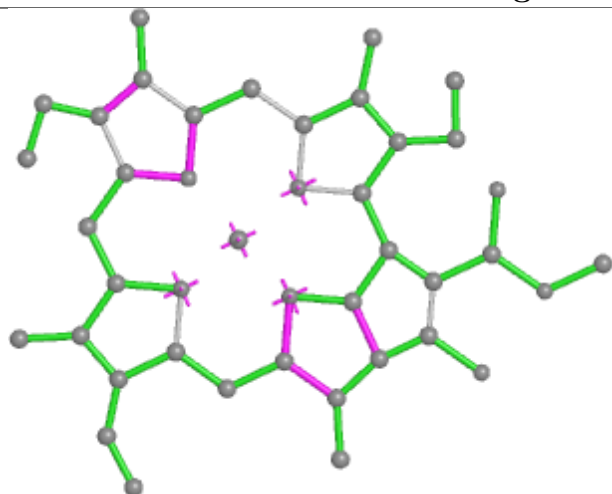


Torsions

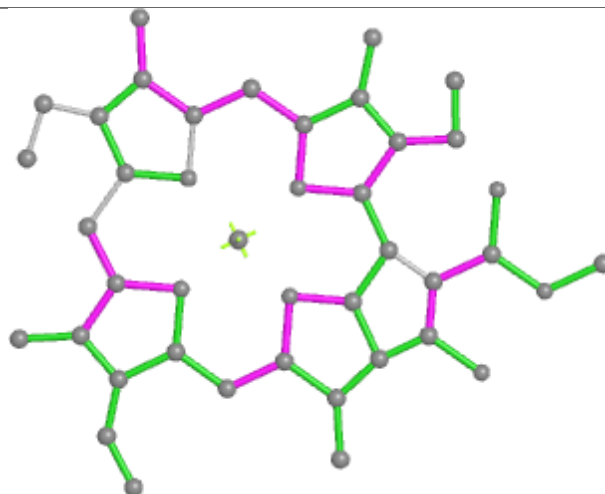


Rings

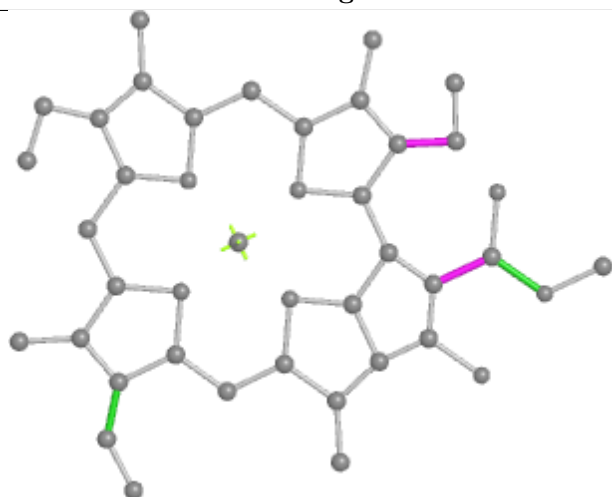
Ligand CLA B 818



Bond lengths



Bond angles

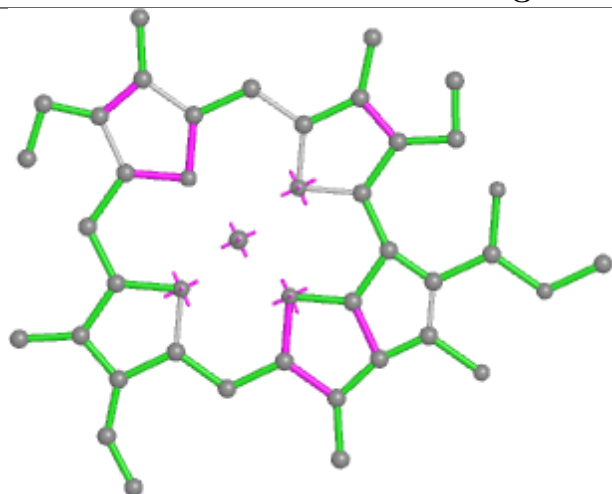


Torsions

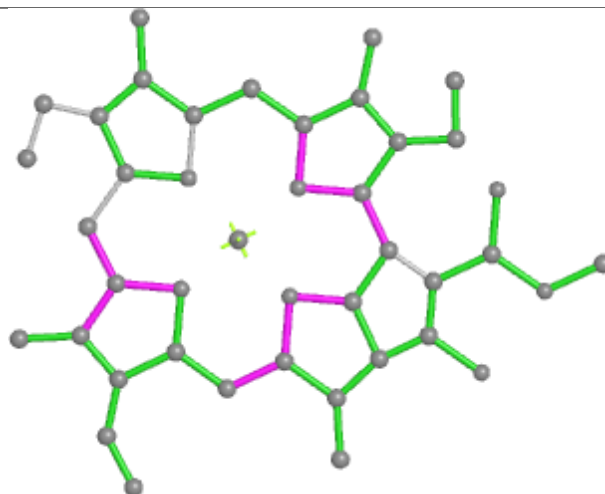


Rings

Ligand CLA B 836



Bond lengths



Bond angles

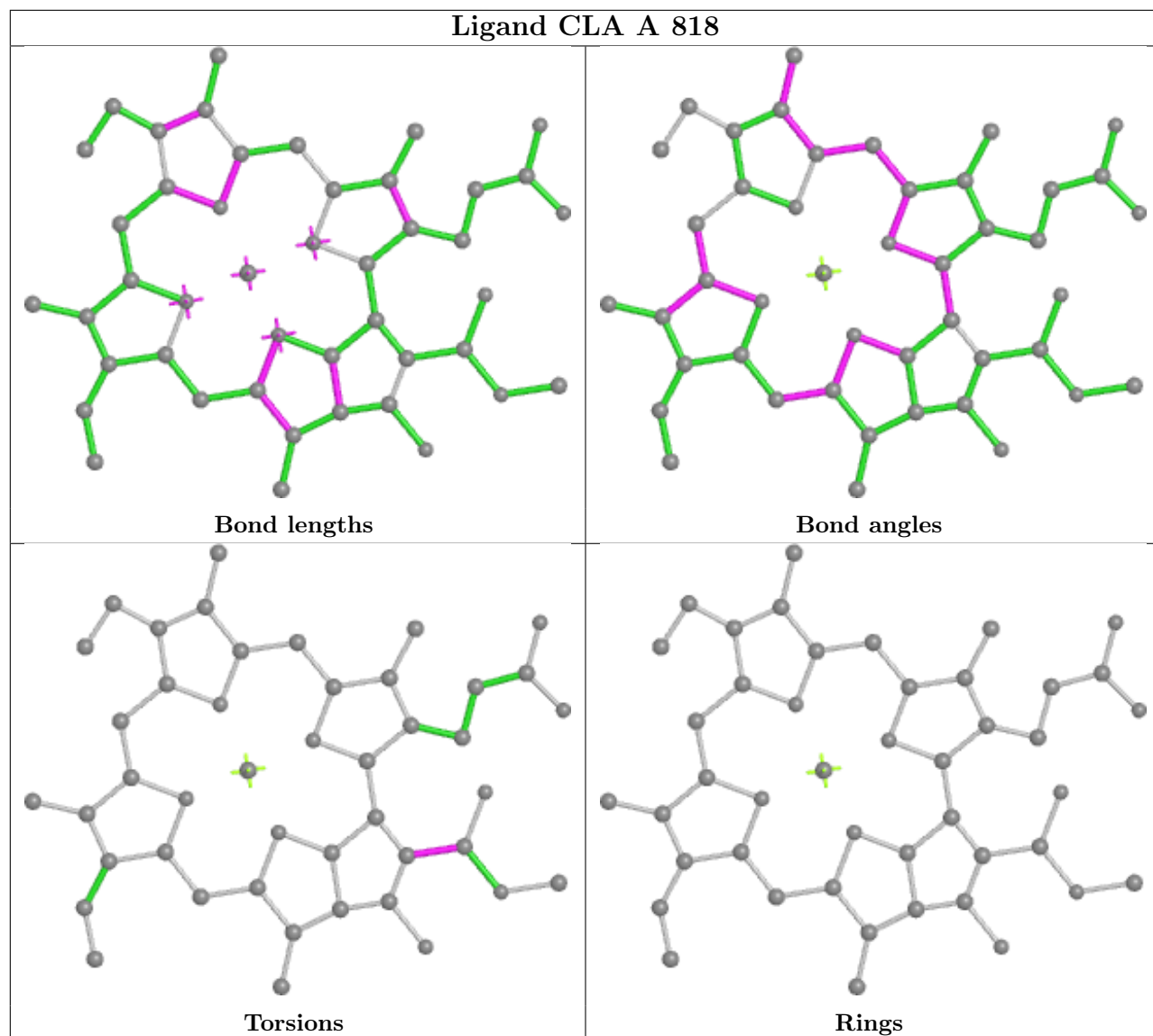


Torsions

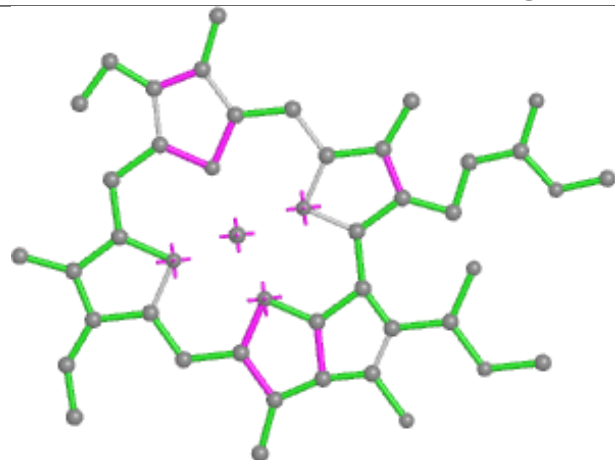


Rings

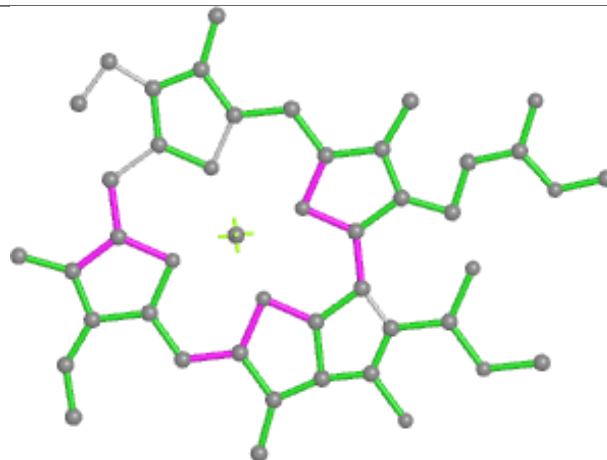
Ligand CLA A 818



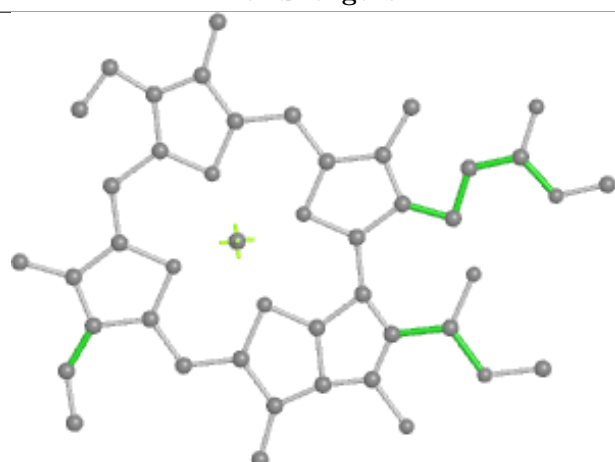
Ligand CLA 8 612



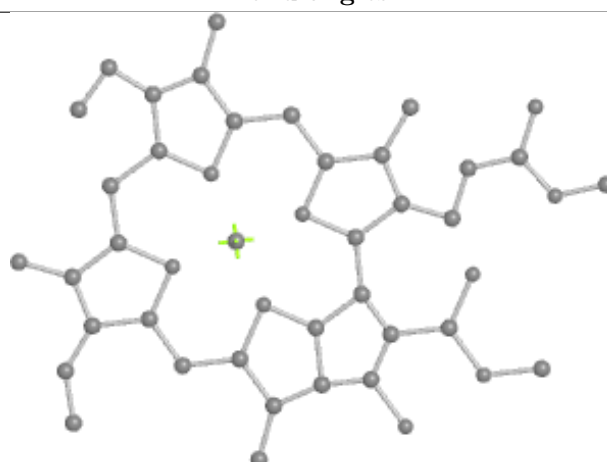
Bond lengths



Bond angles

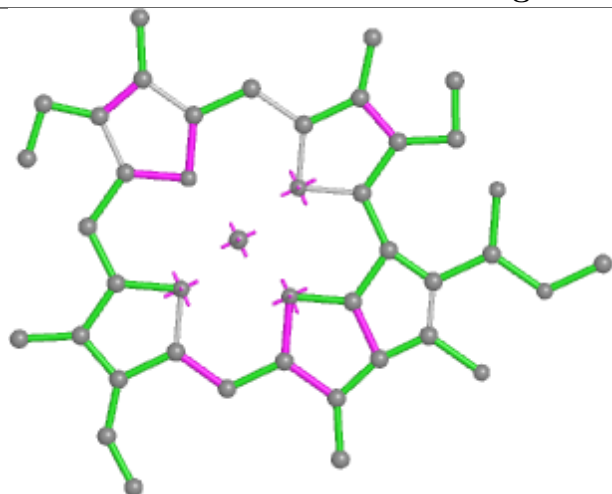


Torsions

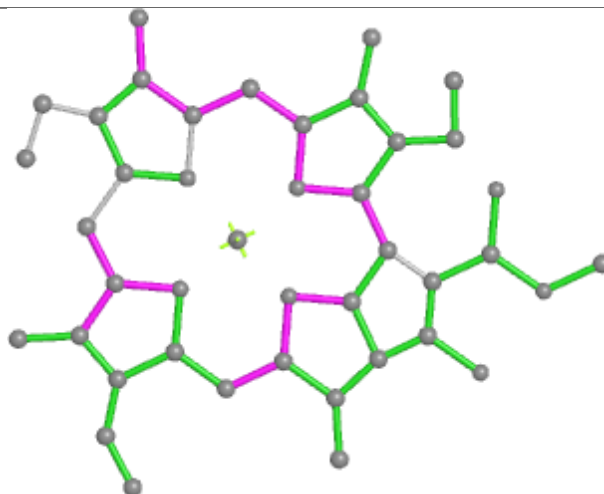


Rings

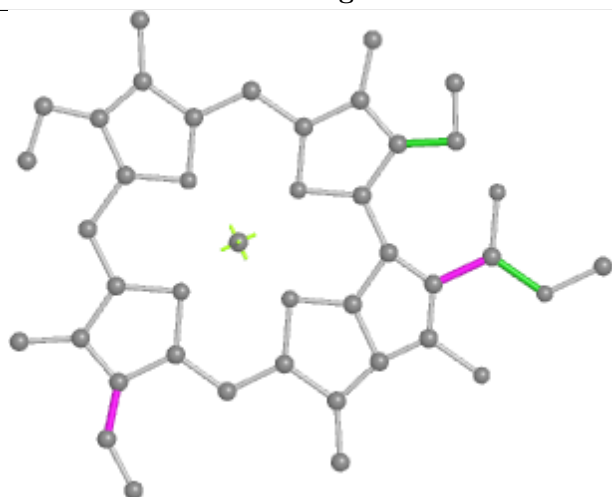
Ligand CLA A 835



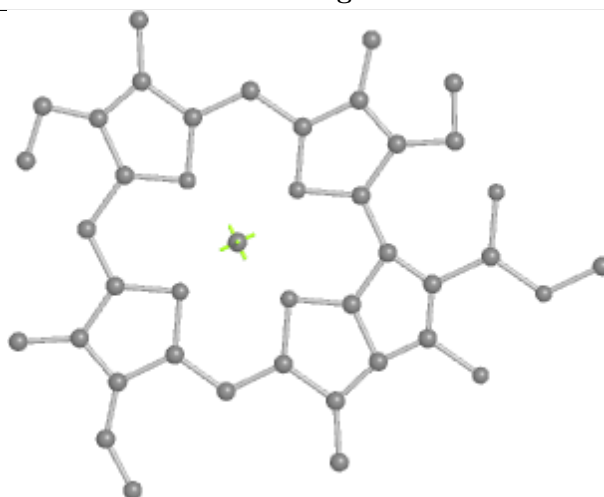
Bond lengths



Bond angles

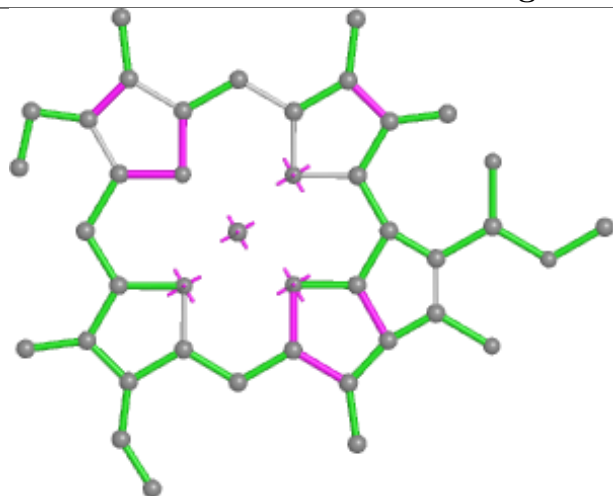


Torsions

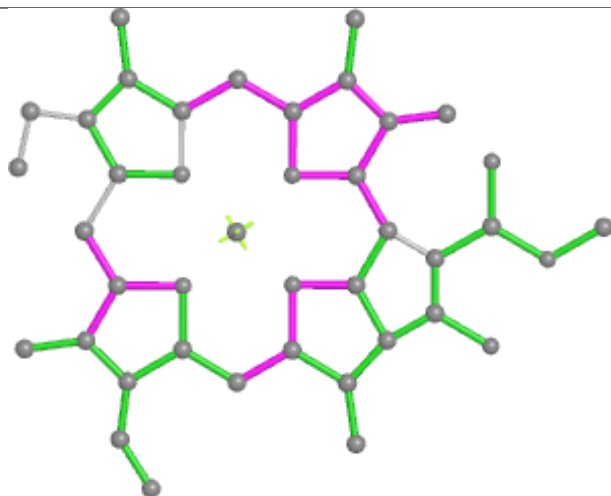


Rings

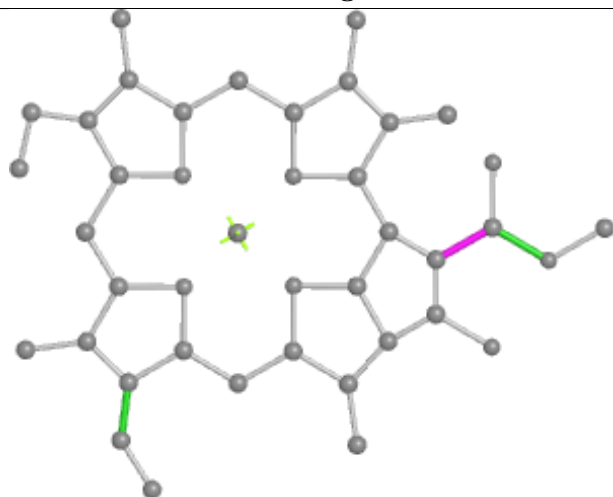
Ligand CLA 7 610



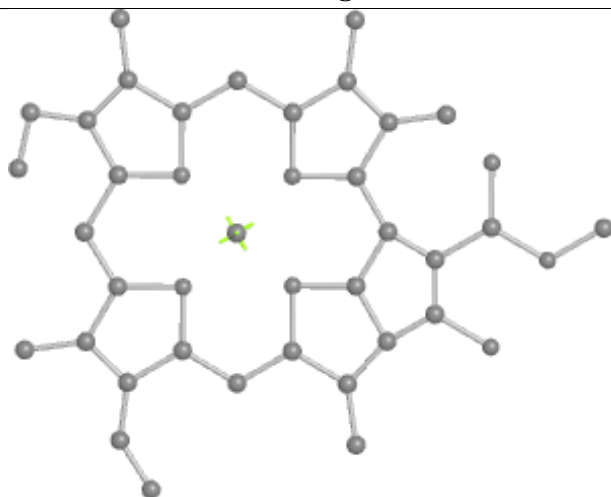
Bond lengths



Bond angles

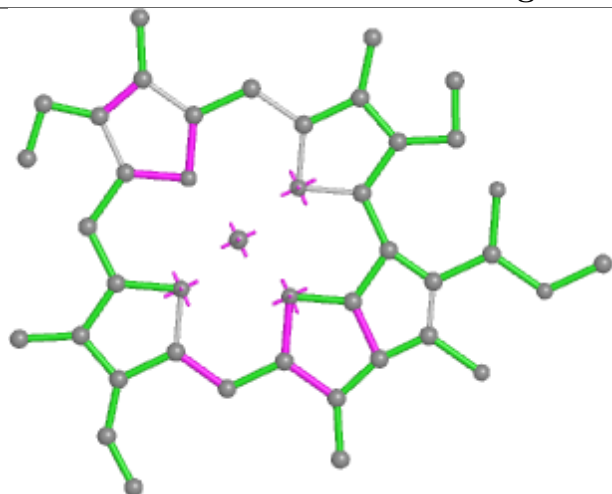


Torsions

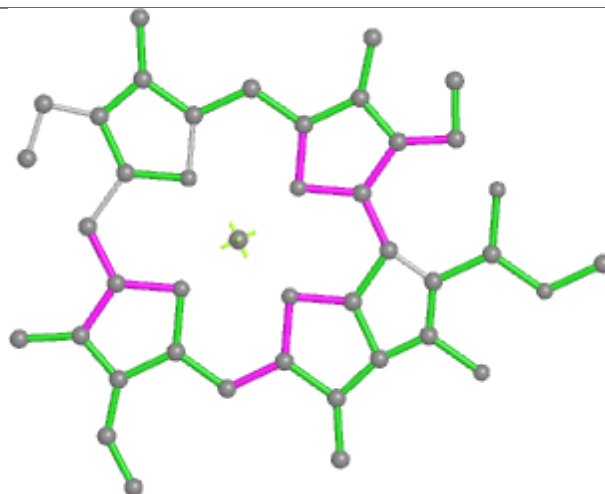


Rings

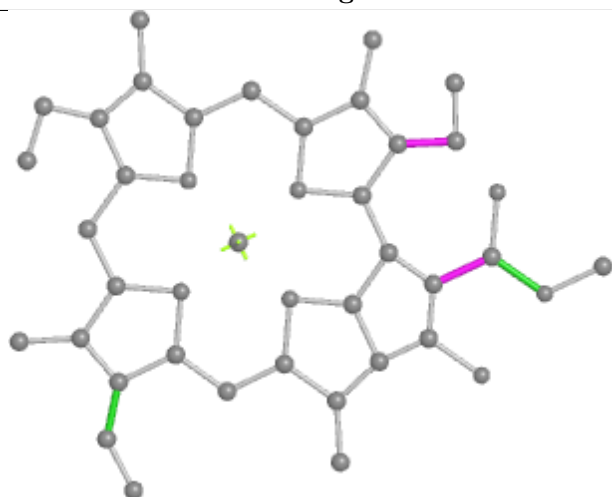
Ligand CLA 7 602



Bond lengths



Bond angles

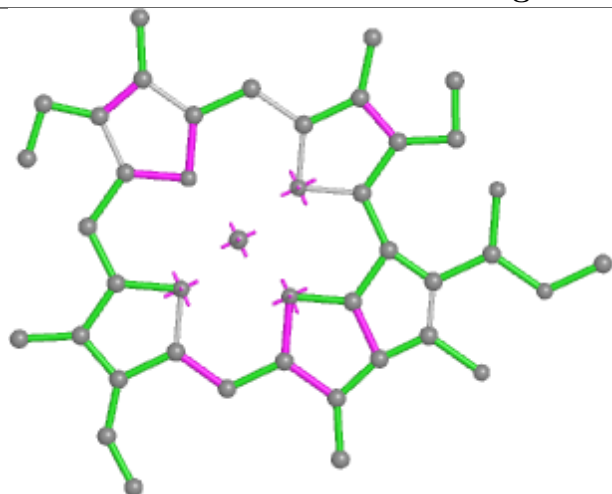


Torsions

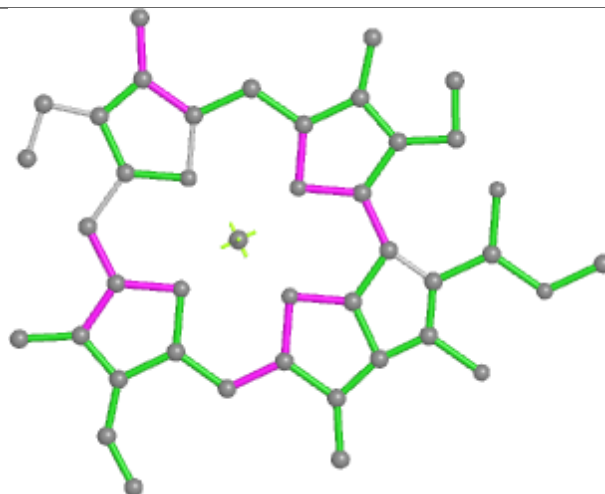


Rings

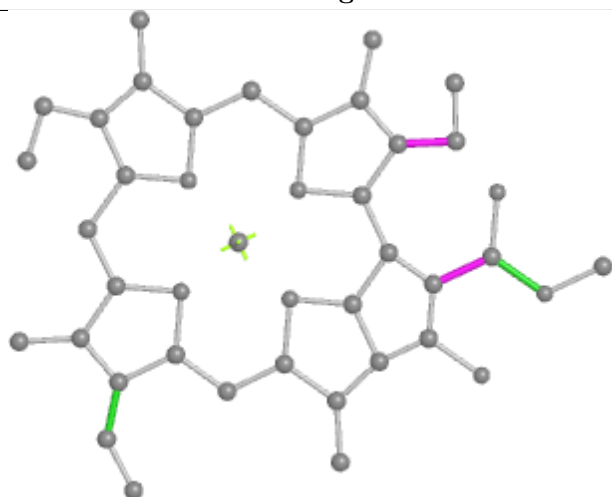
Ligand CLA A 812



Bond lengths



Bond angles

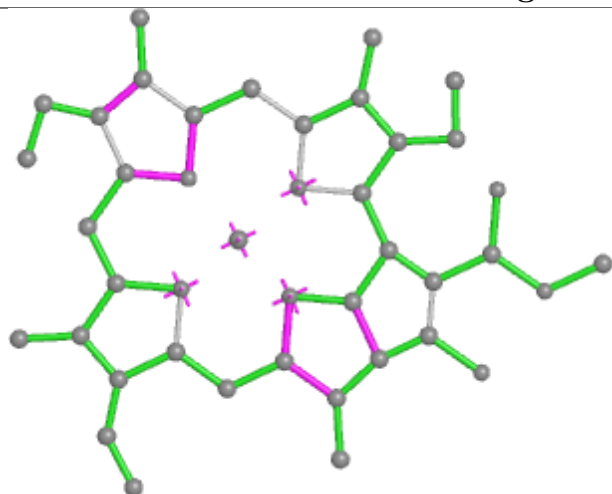


Torsions

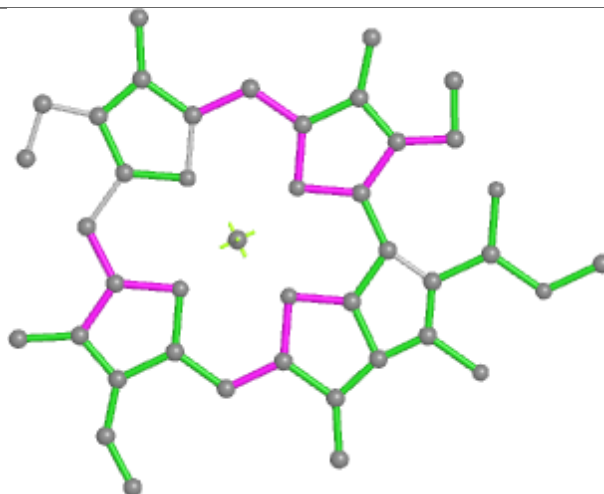


Rings

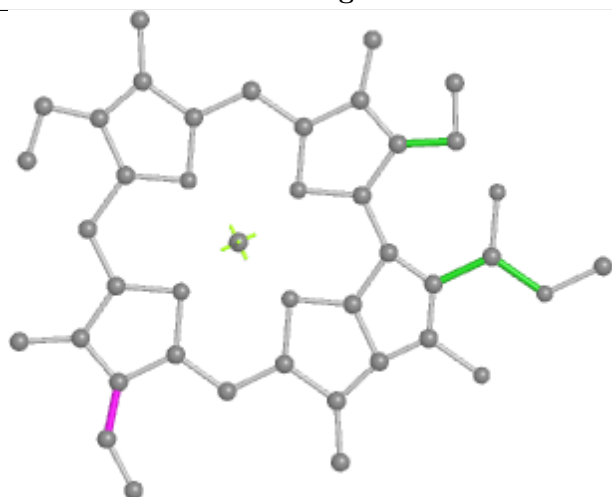
Ligand CLA 3 312



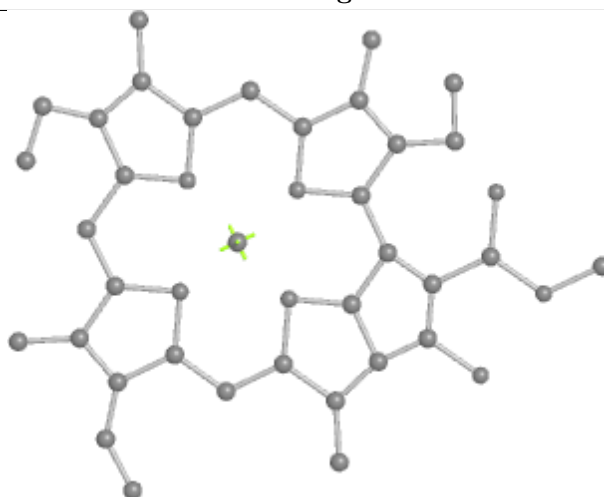
Bond lengths



Bond angles

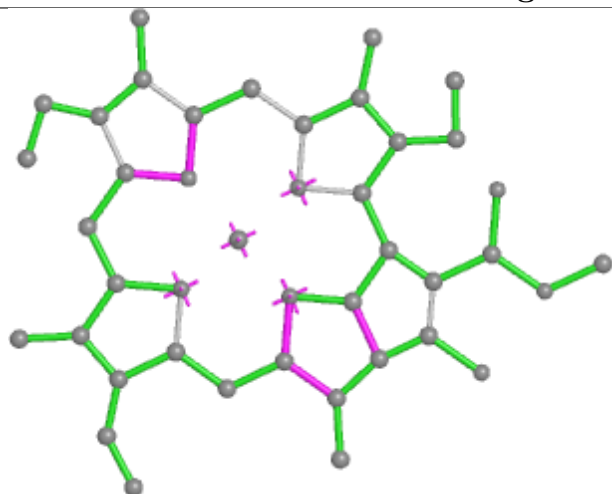


Torsions

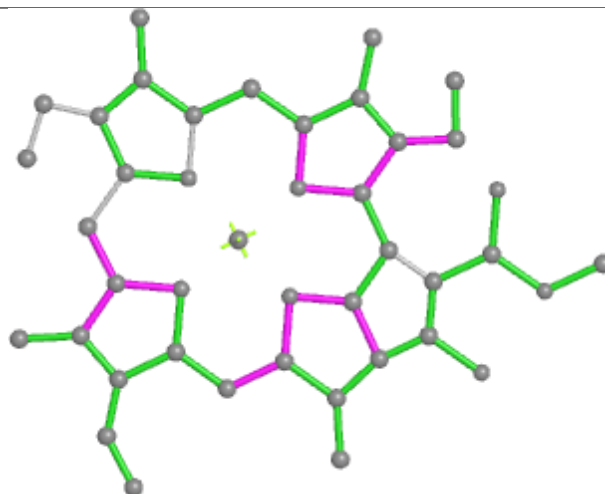


Rings

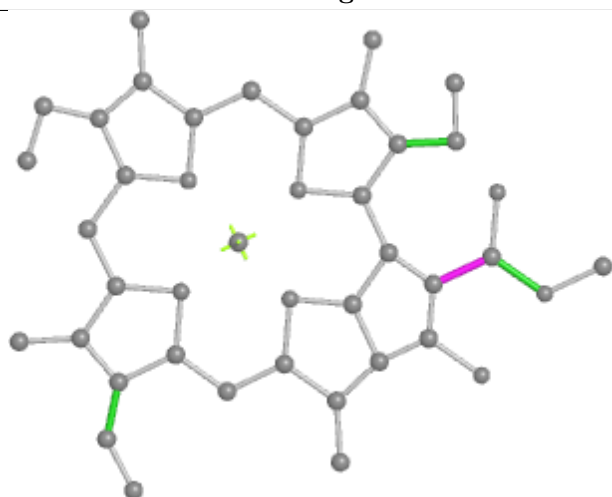
Ligand CLA 7 608



Bond lengths



Bond angles

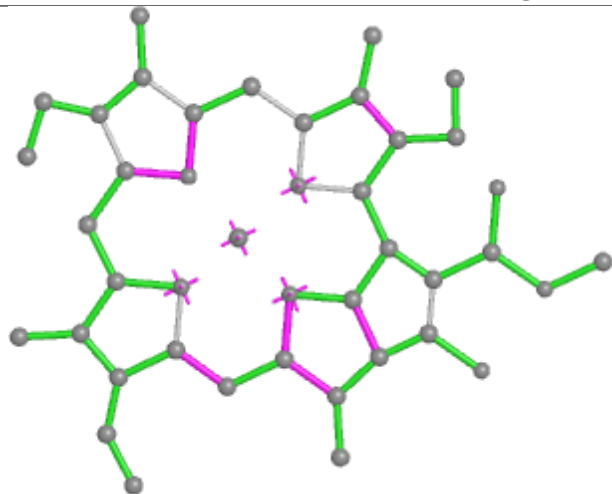


Torsions

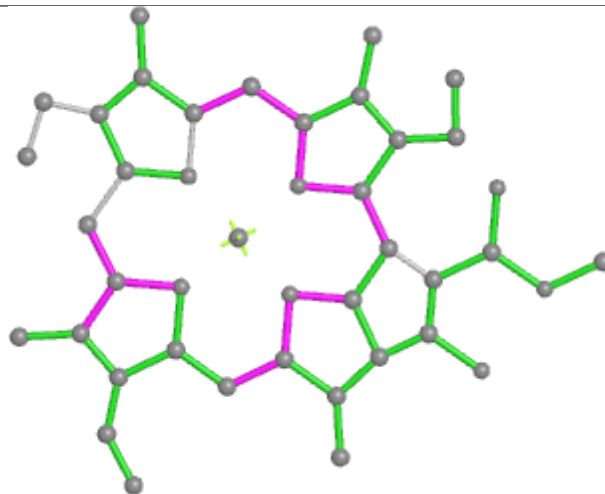


Rings

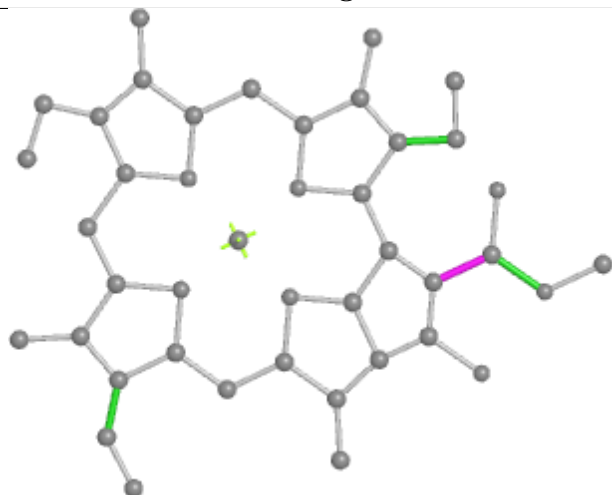
Ligand CLA 8 614



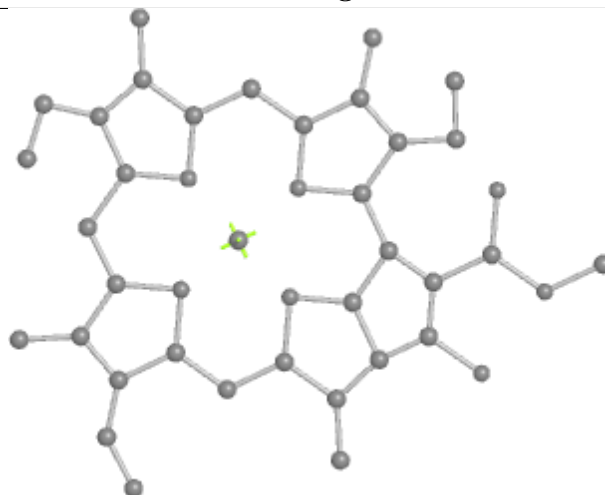
Bond lengths



Bond angles

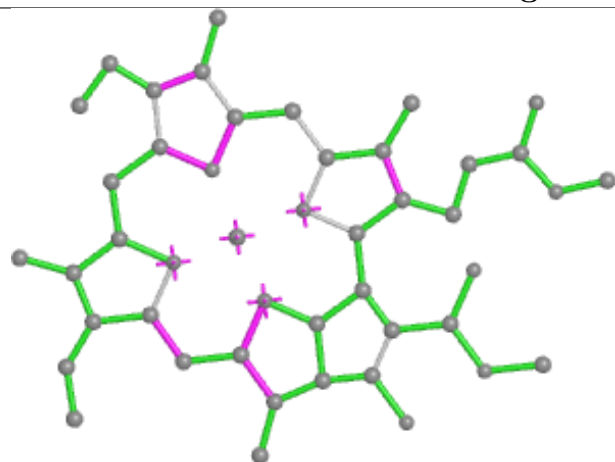


Torsions

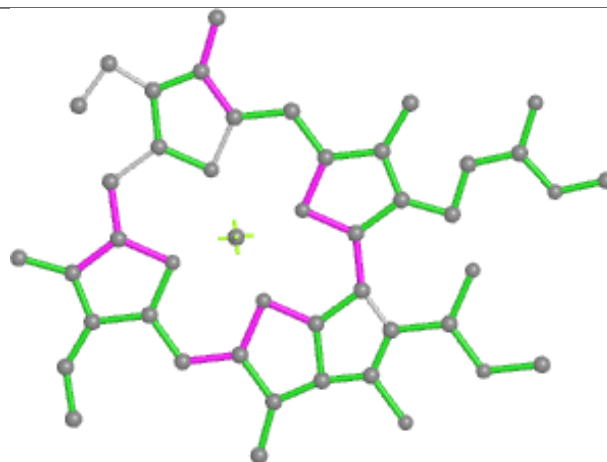


Rings

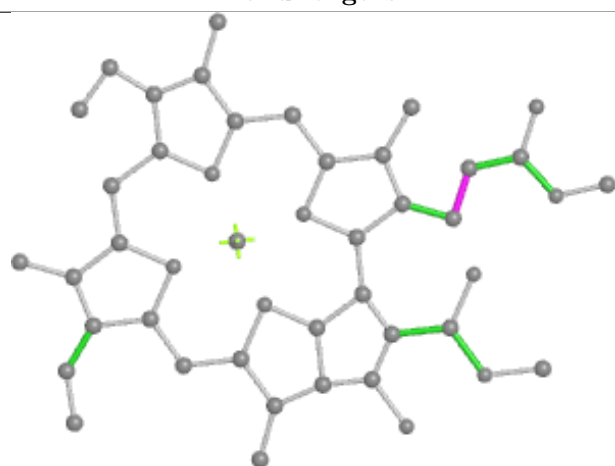
Ligand CLA 6 609



Bond lengths



Bond angles

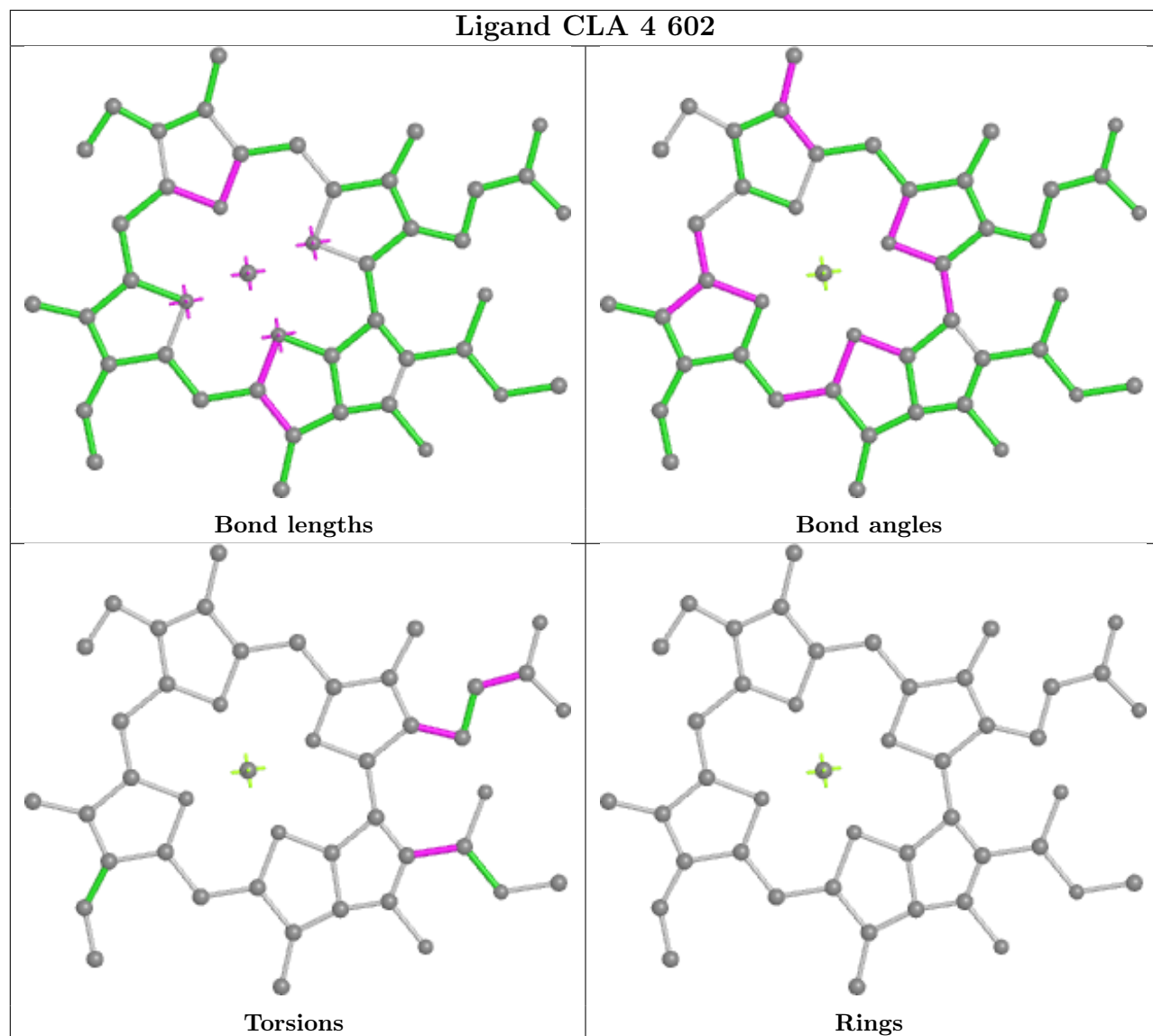


Torsions

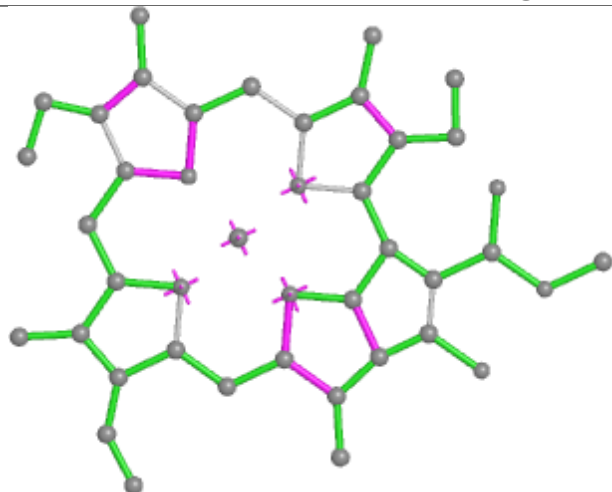


Rings

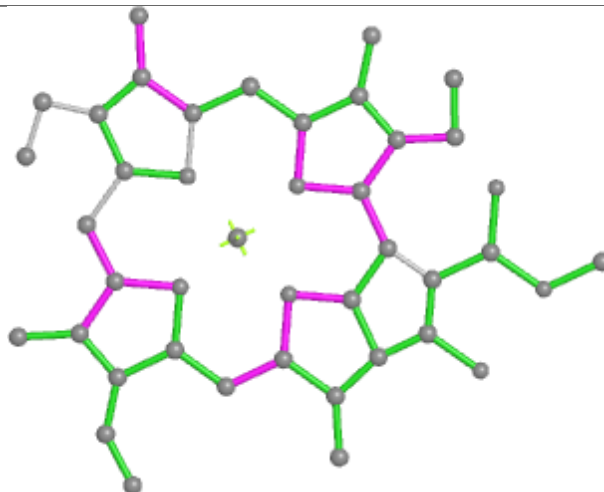
Ligand CLA 4 602



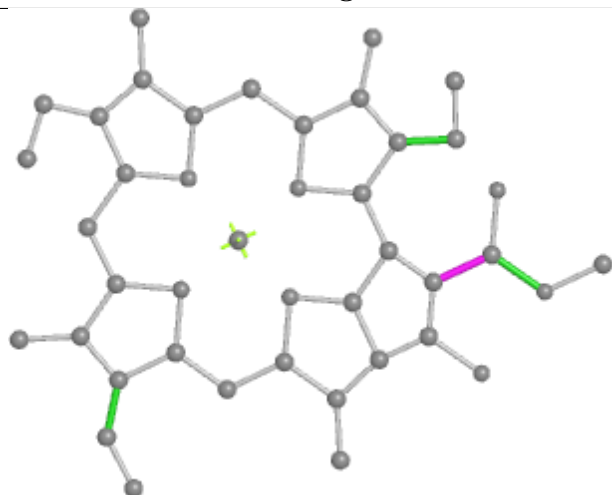
Ligand CLA 6 601



Bond lengths



Bond angles

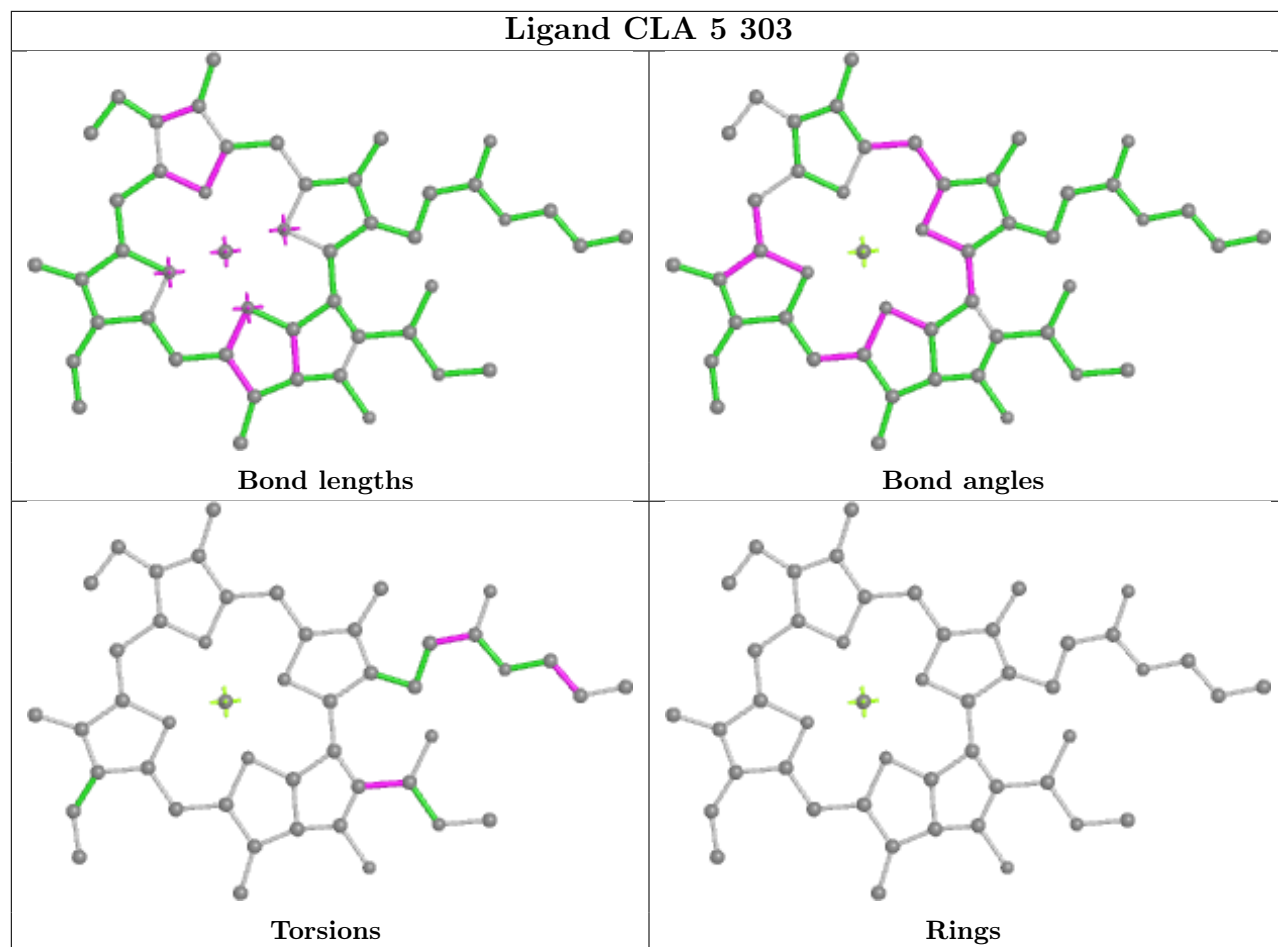


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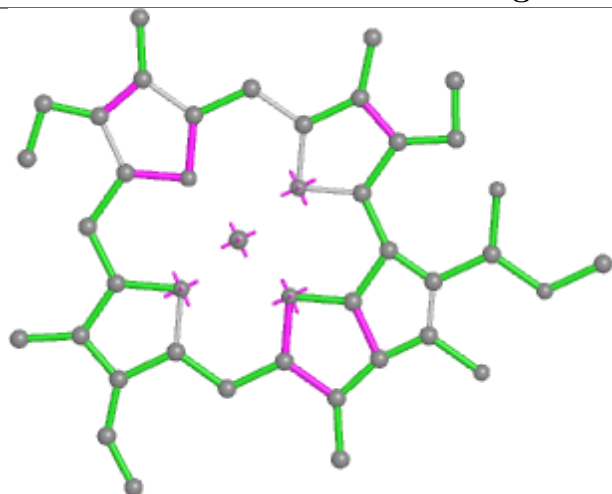


Rings

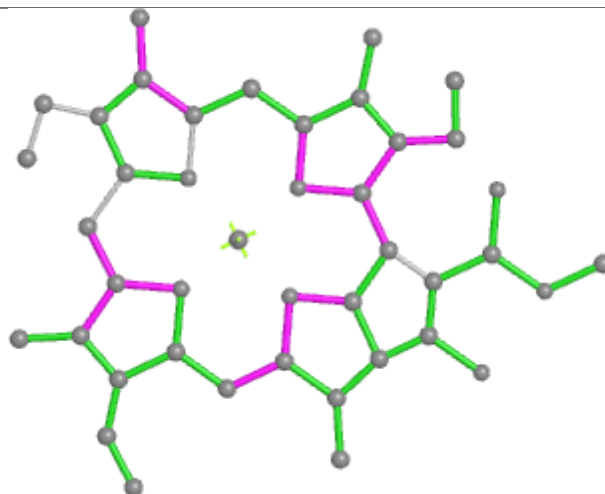
Ligand CLA 5 303



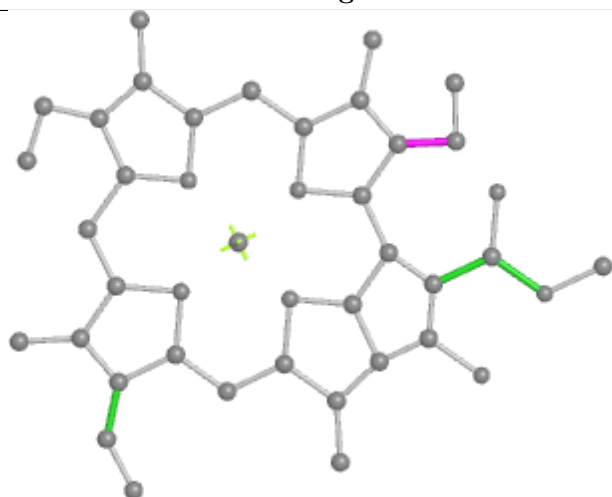
Ligand CLA A 805



Bond lengths



Bond angles

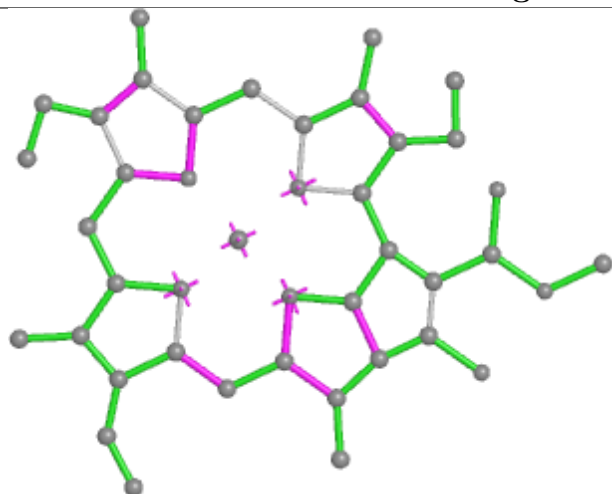


Torsions

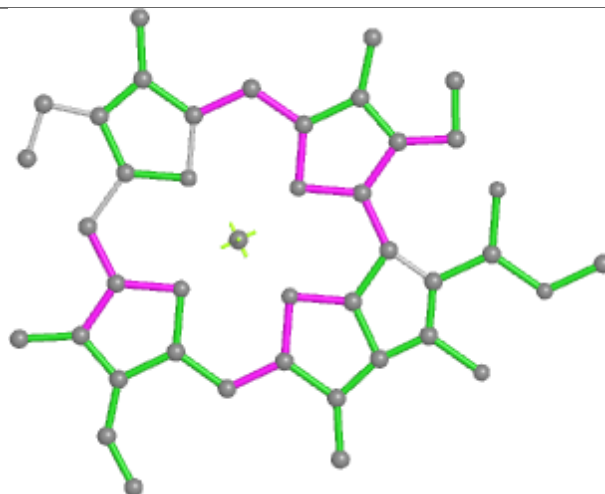


Rings

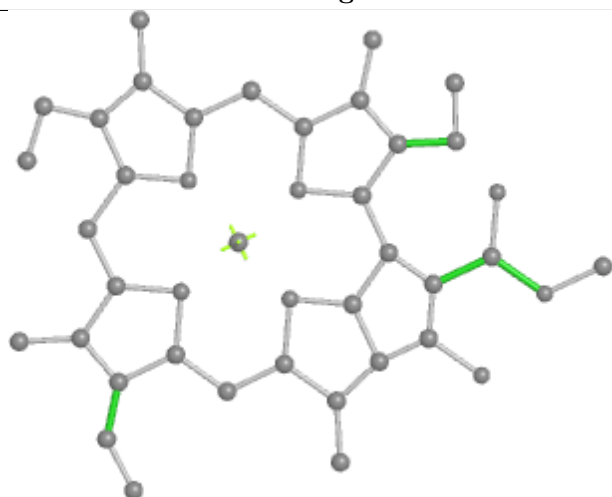
Ligand CLA A 827



Bond lengths



Bond angles

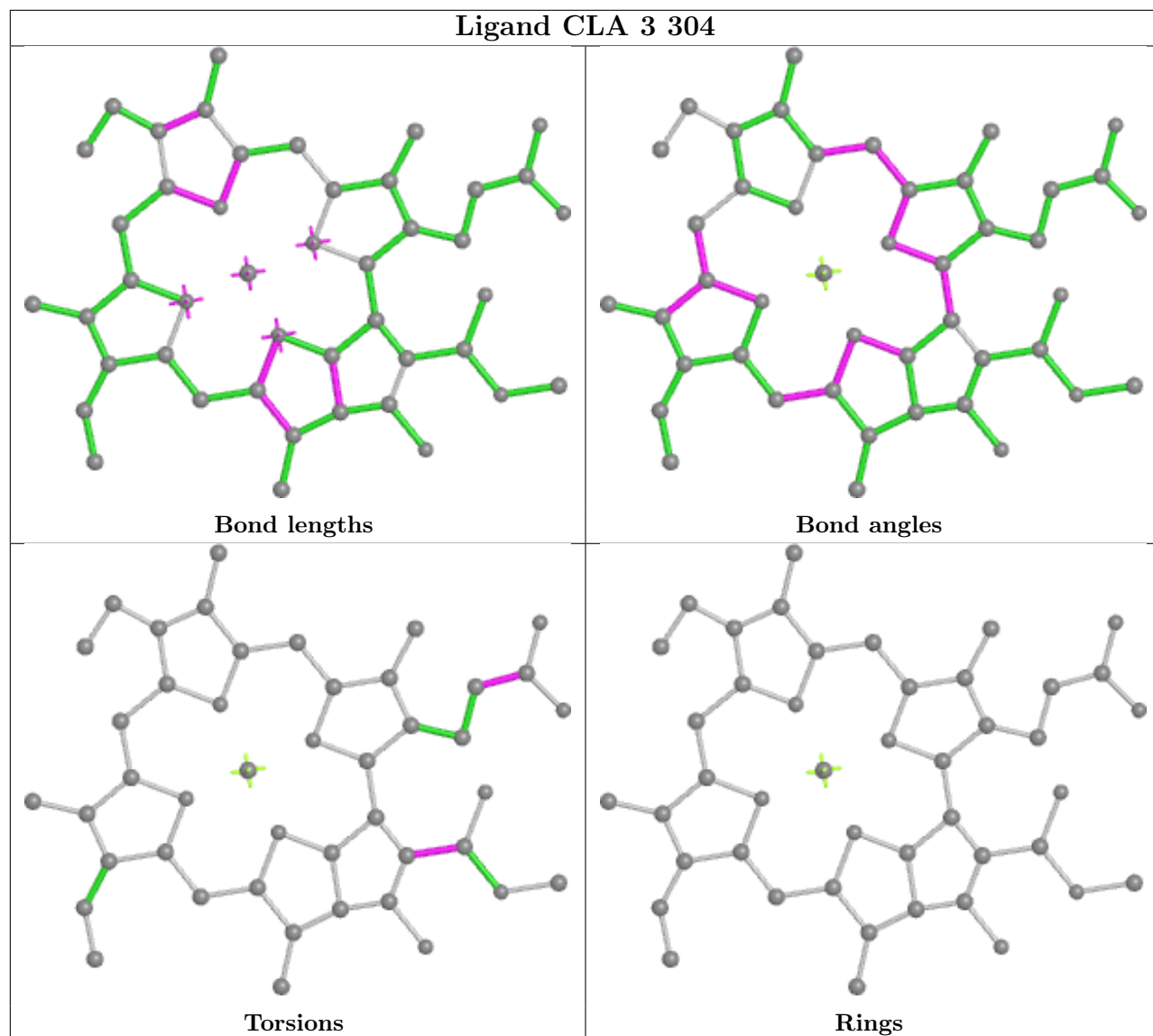


Torsions

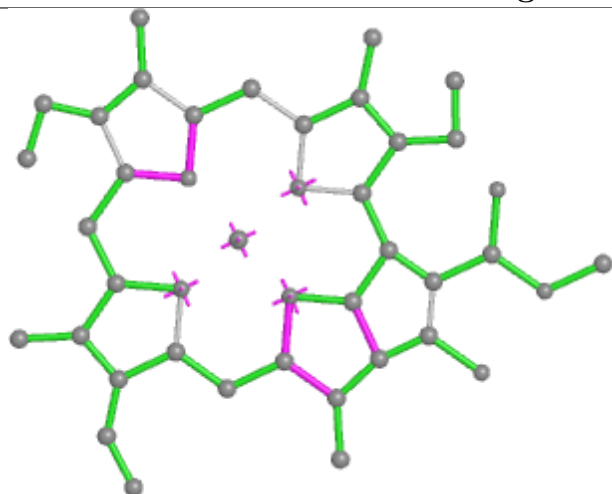


Rings

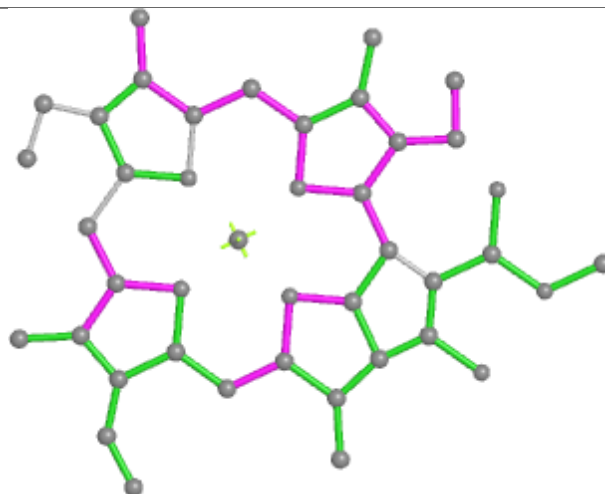
Ligand CLA 3 304



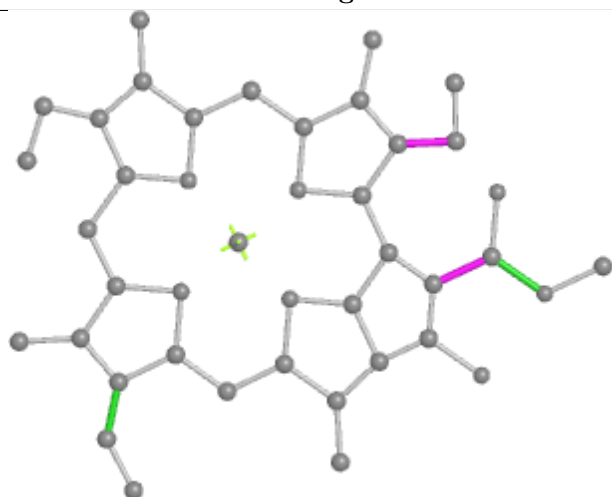
Ligand CLA 4 603



Bond lengths



Bond angles

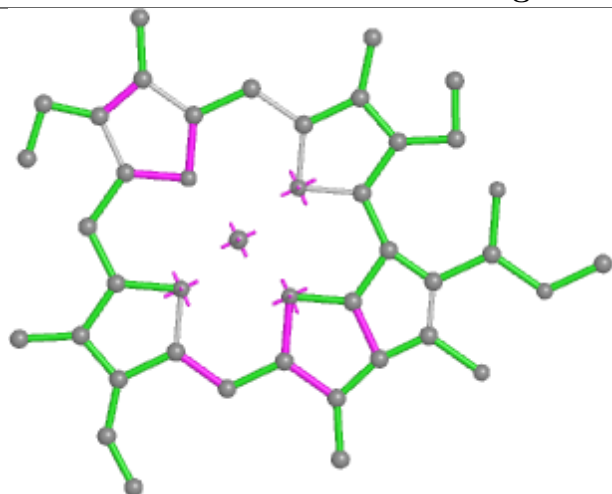


Torsions

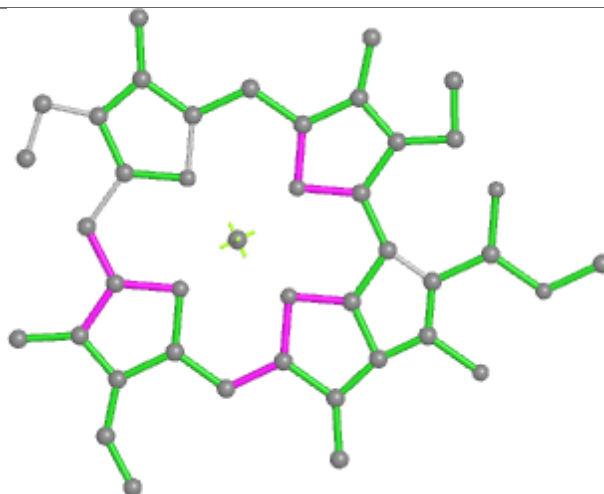


Rings

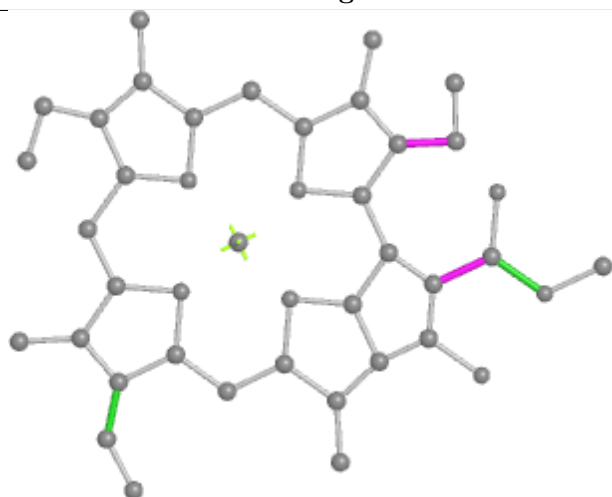
Ligand CLA A 820



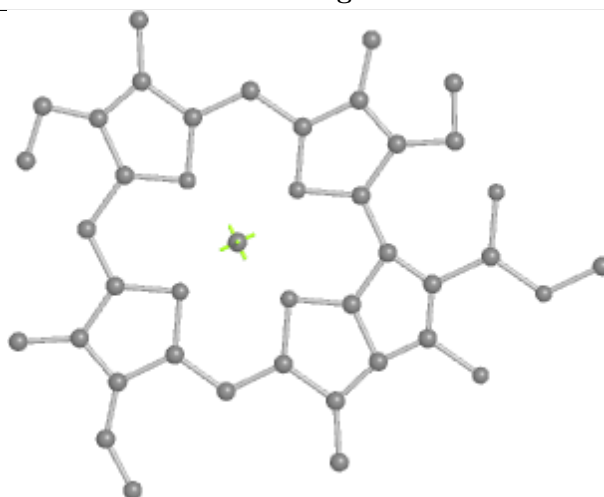
Bond lengths



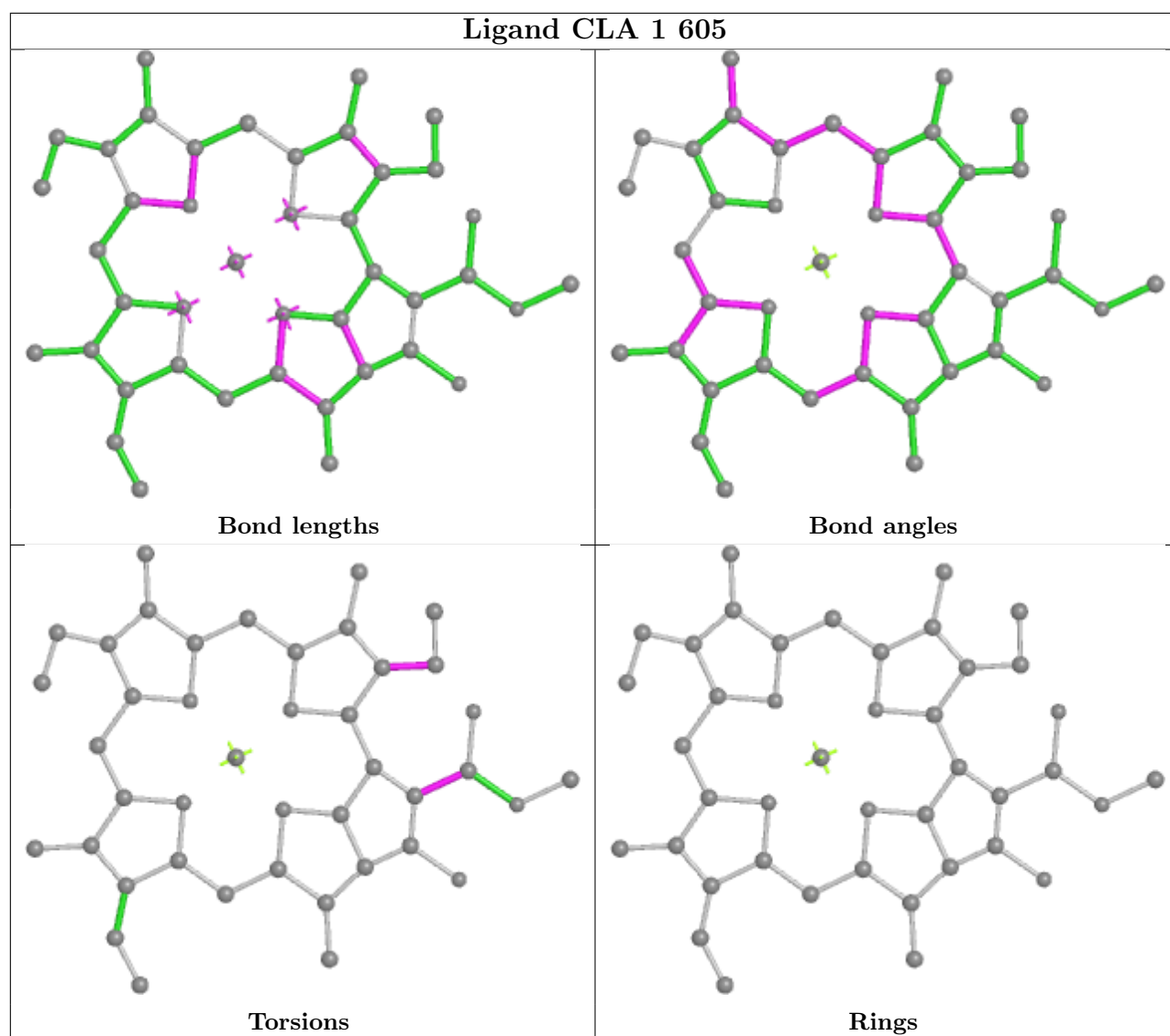
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

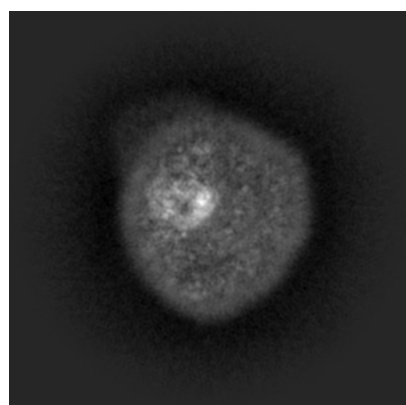
6 Map visualisation [i](#)

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

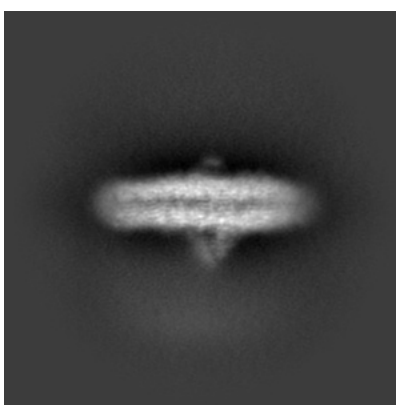
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

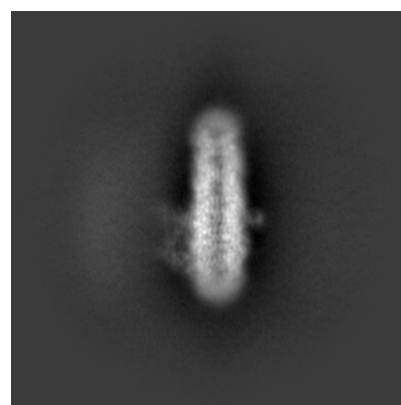
6.1.1 Primary map



X



Y

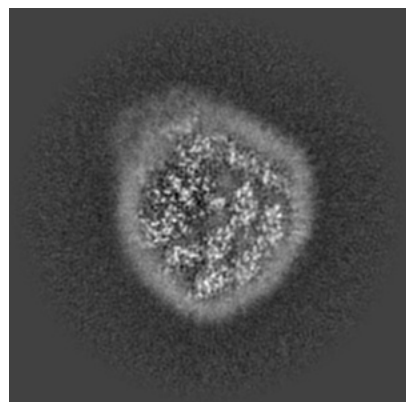


Z

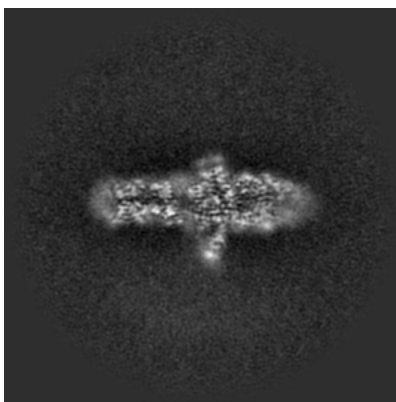
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

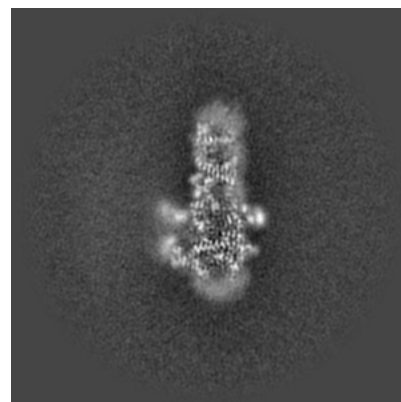
6.2.1 Primary map



X Index: 196



Y Index: 196

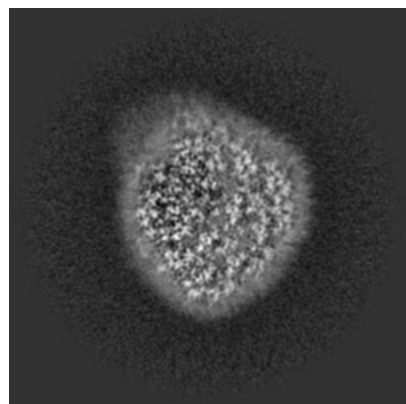


Z Index: 196

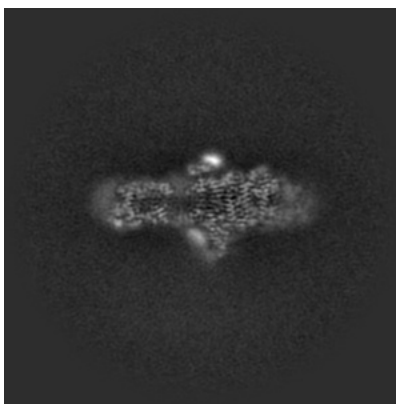
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

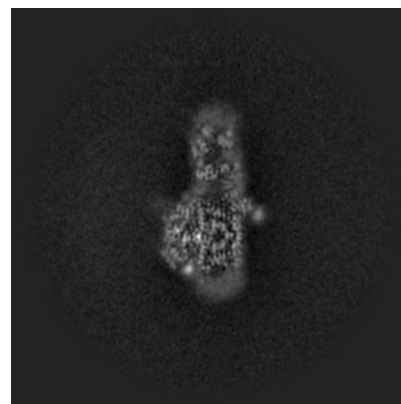
6.3.1 Primary map



X Index: 190



Y Index: 185

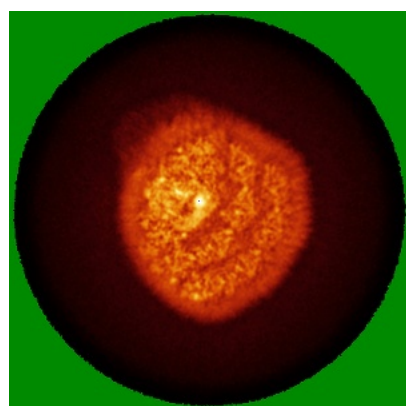


Z Index: 213

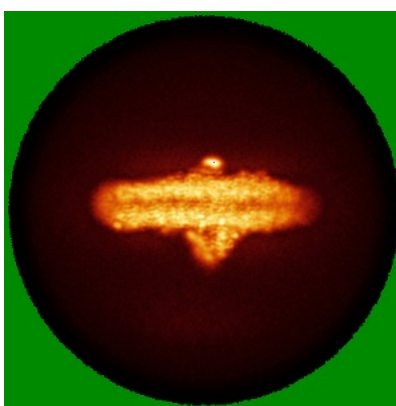
The images above show the largest variance slices of the map in three orthogonal directions.

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

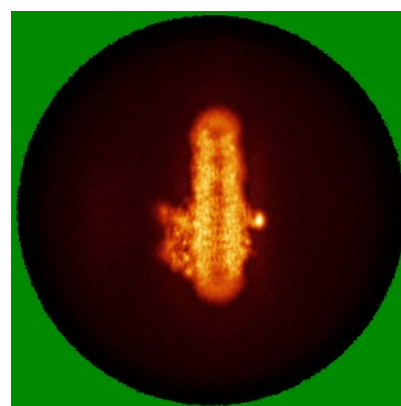
6.4.1 Primary map



X



Y

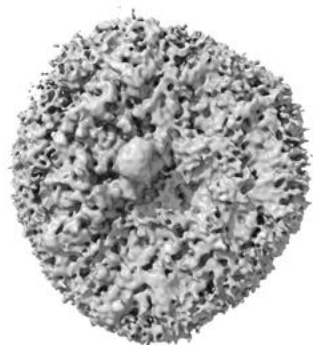


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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.

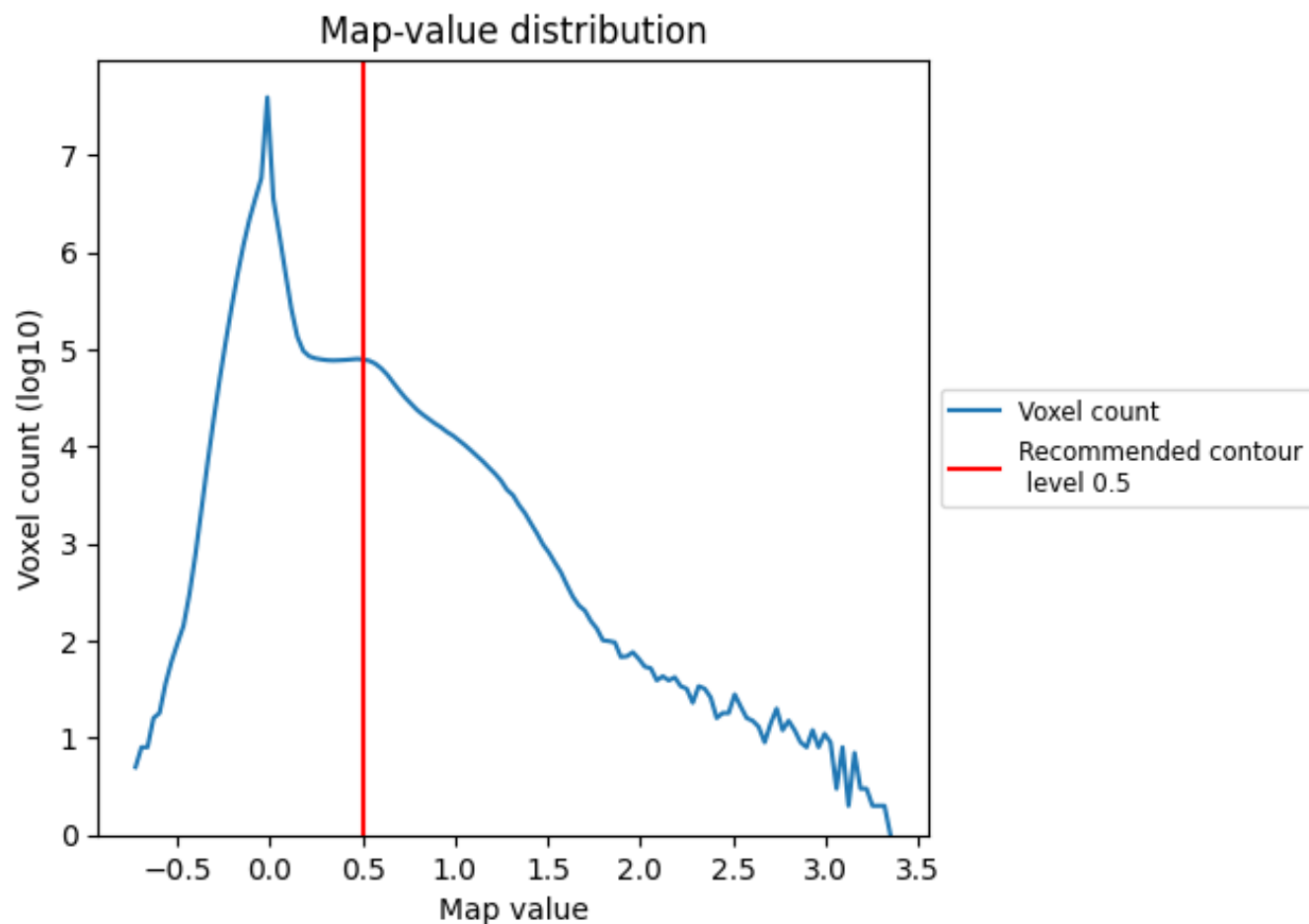
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

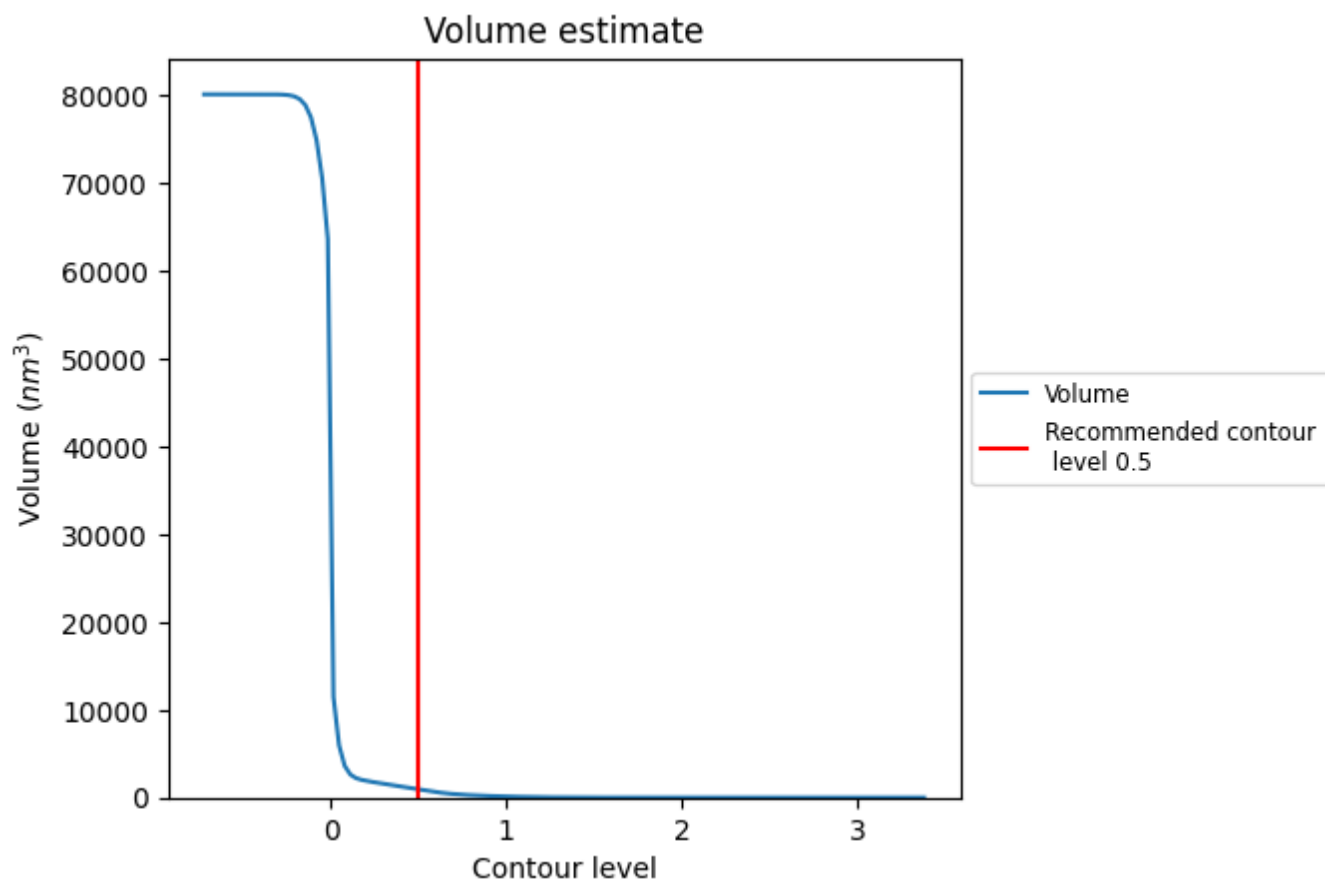
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

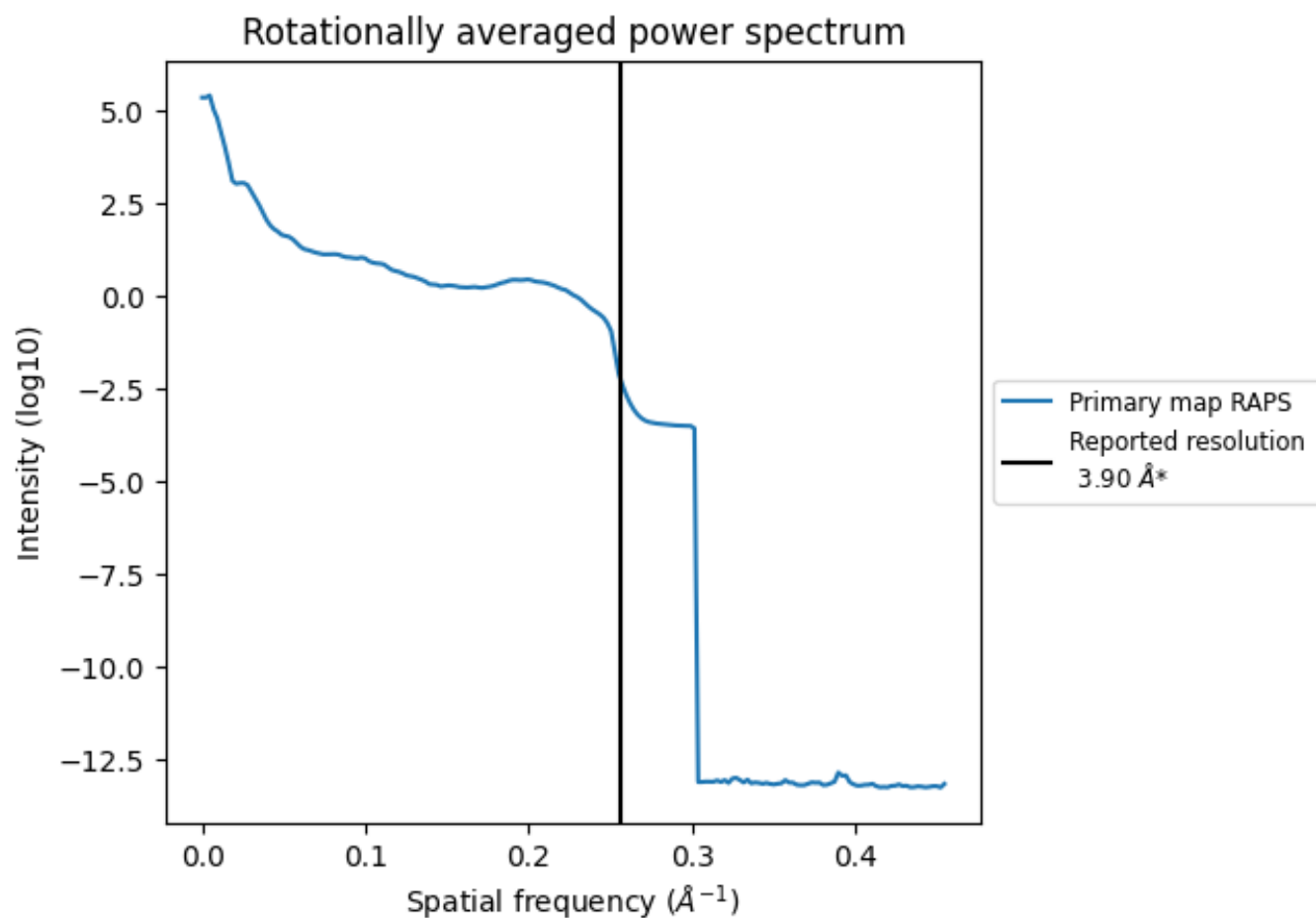
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 932 nm^3 ; 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.

7.3 Rotationally averaged power spectrum ⓘ

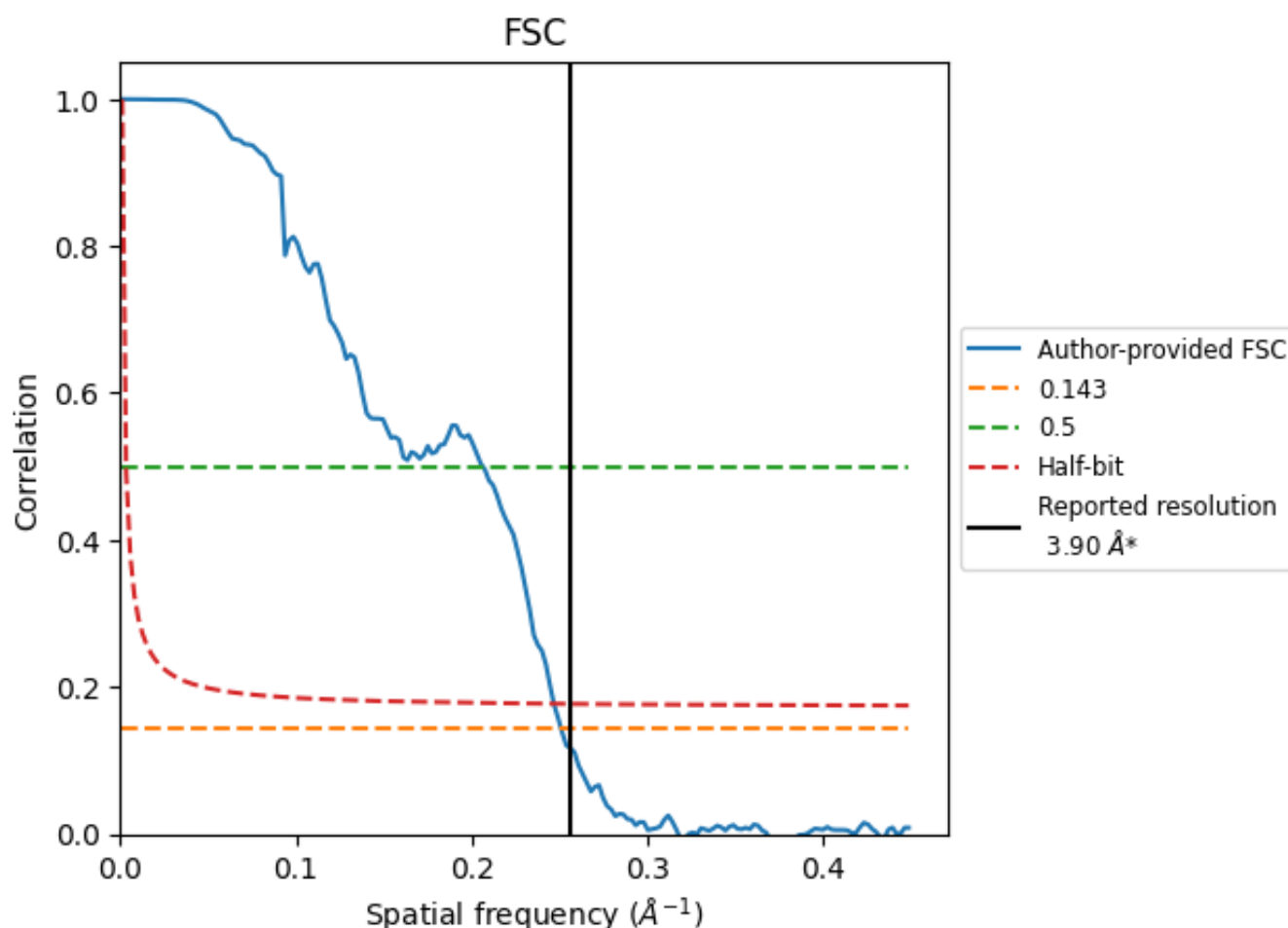


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

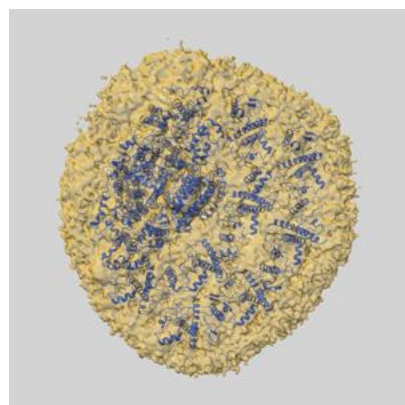
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.98	4.84	4.05
Unmasked-calculated*	-	-	-

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

9 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 [3](#) on page [22](#).

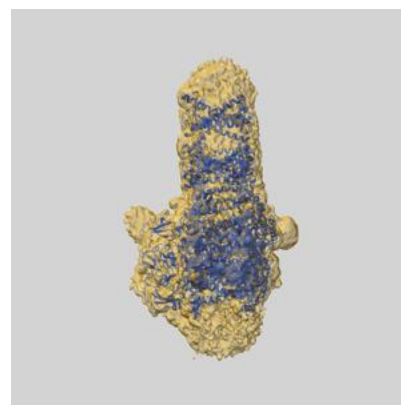
9.1 Map-model overlay [i](#)



X



Y



Z

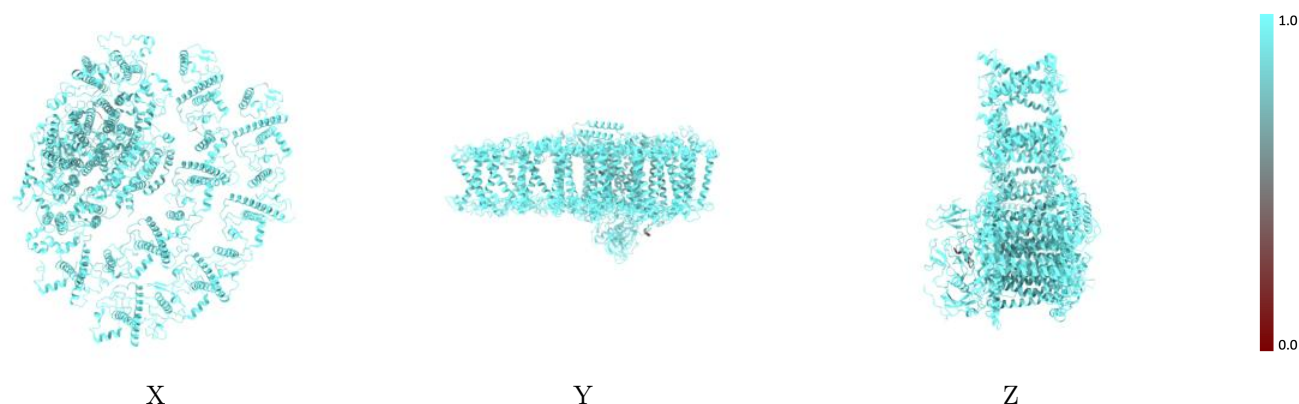
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



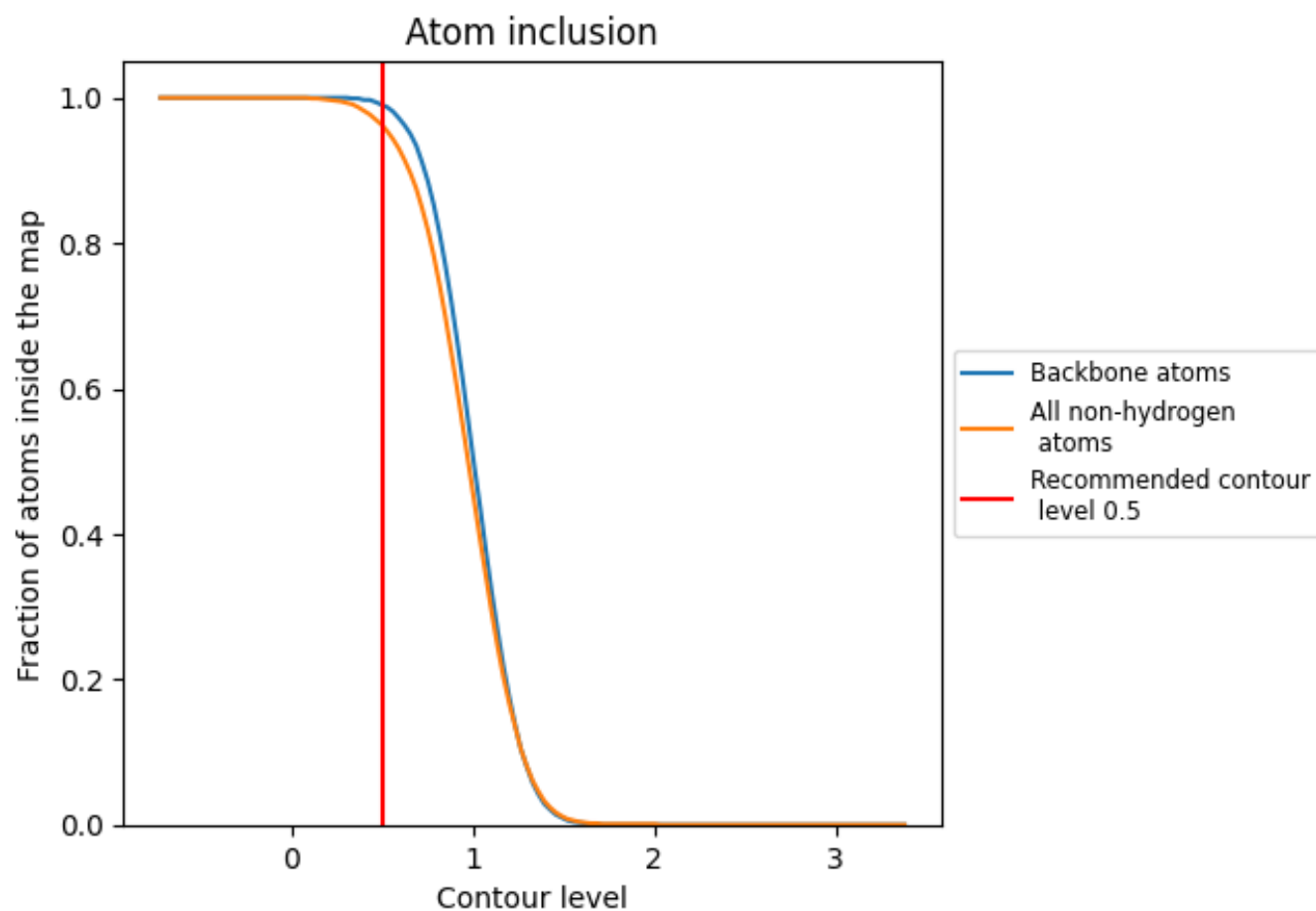
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



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

9.5 Map-model fit summary ⓘ

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

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

